



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:07 AM UTC

PDB ID : 3VSZ / pdb_00003vsz
Title : Crystal structure of Ct1,3Gal43A in complex with galactan
Authors : Jiang, D.; Fan, J.; Wang, X.; Zhao, Y.; Huang, B.; Zhang, X.C.
Deposited on : 2012-05-18
Resolution : 2.89 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

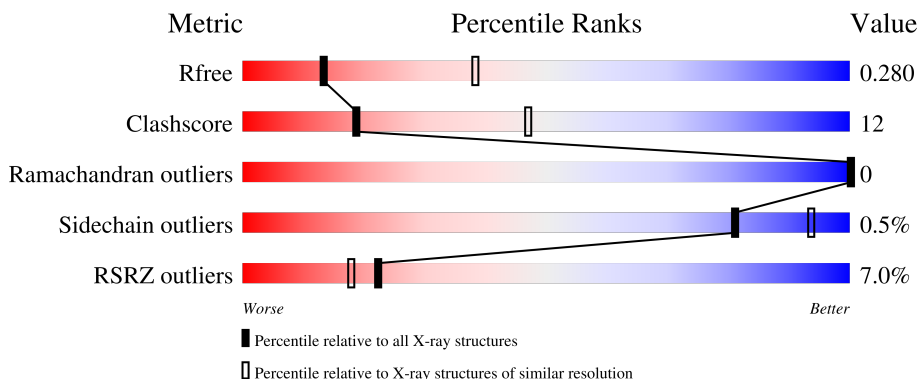
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	526	 4% 70% 17% 12%
1	B	526	 5% 68% 19% 12%
1	C	526	 2% 74% 18% 8%
1	D	526	 22% 61% 26% 12%
1	E	526	 2% 69% 19% 12%

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Mol	Chain	Length	Quality of chain
1	F	526	 3% 70% 18% 12%
2	G	3	 100%
2	H	3	 100%
2	I	3	 100%
2	J	3	 100%
2	K	3	 100%
3	L	2	 100%

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
2	GAL	G	2	-	-	X	-
2	GAL	H	2	-	-	X	-
2	GAL	I	2	-	-	X	-
2	GAL	J	2	-	-	X	-
2	GAL	K	2	-	-	X	-

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 22399 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 Ricin B lectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	461	3664	2323	623	703	15	0	0	0
1	B	461	3664	2323	623	703	15	0	0	0
1	C	482	3807	2406	651	732	18	0	0	0
1	D	461	3664	2323	623	703	15	0	0	0
1	E	461	3664	2323	623	703	15	0	0	0
1	F	461	3664	2323	623	703	15	0	0	0

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MET	-	expression tag	UNP A3DD67
A	-34	GLY	-	expression tag	UNP A3DD67
A	-33	SER	-	expression tag	UNP A3DD67
A	-32	SER	-	expression tag	UNP A3DD67
A	-31	HIS	-	expression tag	UNP A3DD67
A	-30	HIS	-	expression tag	UNP A3DD67
A	-29	HIS	-	expression tag	UNP A3DD67
A	-28	HIS	-	expression tag	UNP A3DD67
A	-27	HIS	-	expression tag	UNP A3DD67
A	-26	HIS	-	expression tag	UNP A3DD67
A	-25	SER	-	expression tag	UNP A3DD67
A	-24	SER	-	expression tag	UNP A3DD67
A	-23	GLY	-	expression tag	UNP A3DD67
A	-22	LEU	-	expression tag	UNP A3DD67
A	-21	VAL	-	expression tag	UNP A3DD67
A	-20	PRO	-	expression tag	UNP A3DD67
A	-19	ARG	-	expression tag	UNP A3DD67

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	expression tag	UNP A3DD67
A	-17	SER	-	expression tag	UNP A3DD67
A	-16	HIS	-	expression tag	UNP A3DD67
A	-15	MET	-	expression tag	UNP A3DD67
A	-14	ALA	-	expression tag	UNP A3DD67
A	-13	SER	-	expression tag	UNP A3DD67
A	-12	MET	-	expression tag	UNP A3DD67
A	-11	THR	-	expression tag	UNP A3DD67
A	-10	GLY	-	expression tag	UNP A3DD67
A	-9	GLY	-	expression tag	UNP A3DD67
A	-8	GLN	-	expression tag	UNP A3DD67
A	-7	GLN	-	expression tag	UNP A3DD67
A	-6	MET	-	expression tag	UNP A3DD67
A	-5	GLY	-	expression tag	UNP A3DD67
A	-4	ARG	-	expression tag	UNP A3DD67
A	-3	GLY	-	expression tag	UNP A3DD67
A	-2	SER	-	expression tag	UNP A3DD67
A	-1	GLU	-	expression tag	UNP A3DD67
A	0	PHE	-	expression tag	UNP A3DD67
B	-35	MET	-	expression tag	UNP A3DD67
B	-34	GLY	-	expression tag	UNP A3DD67
B	-33	SER	-	expression tag	UNP A3DD67
B	-32	SER	-	expression tag	UNP A3DD67
B	-31	HIS	-	expression tag	UNP A3DD67
B	-30	HIS	-	expression tag	UNP A3DD67
B	-29	HIS	-	expression tag	UNP A3DD67
B	-28	HIS	-	expression tag	UNP A3DD67
B	-27	HIS	-	expression tag	UNP A3DD67
B	-26	HIS	-	expression tag	UNP A3DD67
B	-25	SER	-	expression tag	UNP A3DD67
B	-24	SER	-	expression tag	UNP A3DD67
B	-23	GLY	-	expression tag	UNP A3DD67
B	-22	LEU	-	expression tag	UNP A3DD67
B	-21	VAL	-	expression tag	UNP A3DD67
B	-20	PRO	-	expression tag	UNP A3DD67
B	-19	ARG	-	expression tag	UNP A3DD67
B	-18	GLY	-	expression tag	UNP A3DD67
B	-17	SER	-	expression tag	UNP A3DD67
B	-16	HIS	-	expression tag	UNP A3DD67
B	-15	MET	-	expression tag	UNP A3DD67
B	-14	ALA	-	expression tag	UNP A3DD67
B	-13	SER	-	expression tag	UNP A3DD67

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	MET	-	expression tag	UNP A3DD67
B	-11	THR	-	expression tag	UNP A3DD67
B	-10	GLY	-	expression tag	UNP A3DD67
B	-9	GLY	-	expression tag	UNP A3DD67
B	-8	GLN	-	expression tag	UNP A3DD67
B	-7	GLN	-	expression tag	UNP A3DD67
B	-6	MET	-	expression tag	UNP A3DD67
B	-5	GLY	-	expression tag	UNP A3DD67
B	-4	ARG	-	expression tag	UNP A3DD67
B	-3	GLY	-	expression tag	UNP A3DD67
B	-2	SER	-	expression tag	UNP A3DD67
B	-1	GLU	-	expression tag	UNP A3DD67
B	0	PHE	-	expression tag	UNP A3DD67
C	-35	MET	-	expression tag	UNP A3DD67
C	-34	GLY	-	expression tag	UNP A3DD67
C	-33	SER	-	expression tag	UNP A3DD67
C	-32	SER	-	expression tag	UNP A3DD67
C	-31	HIS	-	expression tag	UNP A3DD67
C	-30	HIS	-	expression tag	UNP A3DD67
C	-29	HIS	-	expression tag	UNP A3DD67
C	-28	HIS	-	expression tag	UNP A3DD67
C	-27	HIS	-	expression tag	UNP A3DD67
C	-26	HIS	-	expression tag	UNP A3DD67
C	-25	SER	-	expression tag	UNP A3DD67
C	-24	SER	-	expression tag	UNP A3DD67
C	-23	GLY	-	expression tag	UNP A3DD67
C	-22	LEU	-	expression tag	UNP A3DD67
C	-21	VAL	-	expression tag	UNP A3DD67
C	-20	PRO	-	expression tag	UNP A3DD67
C	-19	ARG	-	expression tag	UNP A3DD67
C	-18	GLY	-	expression tag	UNP A3DD67
C	-17	SER	-	expression tag	UNP A3DD67
C	-16	HIS	-	expression tag	UNP A3DD67
C	-15	MET	-	expression tag	UNP A3DD67
C	-14	ALA	-	expression tag	UNP A3DD67
C	-13	SER	-	expression tag	UNP A3DD67
C	-12	MET	-	expression tag	UNP A3DD67
C	-11	THR	-	expression tag	UNP A3DD67
C	-10	GLY	-	expression tag	UNP A3DD67
C	-9	GLY	-	expression tag	UNP A3DD67
C	-8	GLN	-	expression tag	UNP A3DD67
C	-7	GLN	-	expression tag	UNP A3DD67

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	MET	-	expression tag	UNP A3DD67
C	-5	GLY	-	expression tag	UNP A3DD67
C	-4	ARG	-	expression tag	UNP A3DD67
C	-3	GLY	-	expression tag	UNP A3DD67
C	-2	SER	-	expression tag	UNP A3DD67
C	-1	GLU	-	expression tag	UNP A3DD67
C	0	PHE	-	expression tag	UNP A3DD67
D	-35	MET	-	expression tag	UNP A3DD67
D	-34	GLY	-	expression tag	UNP A3DD67
D	-33	SER	-	expression tag	UNP A3DD67
D	-32	SER	-	expression tag	UNP A3DD67
D	-31	HIS	-	expression tag	UNP A3DD67
D	-30	HIS	-	expression tag	UNP A3DD67
D	-29	HIS	-	expression tag	UNP A3DD67
D	-28	HIS	-	expression tag	UNP A3DD67
D	-27	HIS	-	expression tag	UNP A3DD67
D	-26	HIS	-	expression tag	UNP A3DD67
D	-25	SER	-	expression tag	UNP A3DD67
D	-24	SER	-	expression tag	UNP A3DD67
D	-23	GLY	-	expression tag	UNP A3DD67
D	-22	LEU	-	expression tag	UNP A3DD67
D	-21	VAL	-	expression tag	UNP A3DD67
D	-20	PRO	-	expression tag	UNP A3DD67
D	-19	ARG	-	expression tag	UNP A3DD67
D	-18	GLY	-	expression tag	UNP A3DD67
D	-17	SER	-	expression tag	UNP A3DD67
D	-16	HIS	-	expression tag	UNP A3DD67
D	-15	MET	-	expression tag	UNP A3DD67
D	-14	ALA	-	expression tag	UNP A3DD67
D	-13	SER	-	expression tag	UNP A3DD67
D	-12	MET	-	expression tag	UNP A3DD67
D	-11	THR	-	expression tag	UNP A3DD67
D	-10	GLY	-	expression tag	UNP A3DD67
D	-9	GLY	-	expression tag	UNP A3DD67
D	-8	GLN	-	expression tag	UNP A3DD67
D	-7	GLN	-	expression tag	UNP A3DD67
D	-6	MET	-	expression tag	UNP A3DD67
D	-5	GLY	-	expression tag	UNP A3DD67
D	-4	ARG	-	expression tag	UNP A3DD67
D	-3	GLY	-	expression tag	UNP A3DD67
D	-2	SER	-	expression tag	UNP A3DD67
D	-1	GLU	-	expression tag	UNP A3DD67

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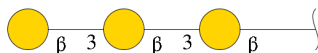
Chain	Residue	Modelled	Actual	Comment	Reference
D	0	PHE	-	expression tag	UNP A3DD67
E	-35	MET	-	expression tag	UNP A3DD67
E	-34	GLY	-	expression tag	UNP A3DD67
E	-33	SER	-	expression tag	UNP A3DD67
E	-32	SER	-	expression tag	UNP A3DD67
E	-31	HIS	-	expression tag	UNP A3DD67
E	-30	HIS	-	expression tag	UNP A3DD67
E	-29	HIS	-	expression tag	UNP A3DD67
E	-28	HIS	-	expression tag	UNP A3DD67
E	-27	HIS	-	expression tag	UNP A3DD67
E	-26	HIS	-	expression tag	UNP A3DD67
E	-25	SER	-	expression tag	UNP A3DD67
E	-24	SER	-	expression tag	UNP A3DD67
E	-23	GLY	-	expression tag	UNP A3DD67
E	-22	LEU	-	expression tag	UNP A3DD67
E	-21	VAL	-	expression tag	UNP A3DD67
E	-20	PRO	-	expression tag	UNP A3DD67
E	-19	ARG	-	expression tag	UNP A3DD67
E	-18	GLY	-	expression tag	UNP A3DD67
E	-17	SER	-	expression tag	UNP A3DD67
E	-16	HIS	-	expression tag	UNP A3DD67
E	-15	MET	-	expression tag	UNP A3DD67
E	-14	ALA	-	expression tag	UNP A3DD67
E	-13	SER	-	expression tag	UNP A3DD67
E	-12	MET	-	expression tag	UNP A3DD67
E	-11	THR	-	expression tag	UNP A3DD67
E	-10	GLY	-	expression tag	UNP A3DD67
E	-9	GLY	-	expression tag	UNP A3DD67
E	-8	GLN	-	expression tag	UNP A3DD67
E	-7	GLN	-	expression tag	UNP A3DD67
E	-6	MET	-	expression tag	UNP A3DD67
E	-5	GLY	-	expression tag	UNP A3DD67
E	-4	ARG	-	expression tag	UNP A3DD67
E	-3	GLY	-	expression tag	UNP A3DD67
E	-2	SER	-	expression tag	UNP A3DD67
E	-1	GLU	-	expression tag	UNP A3DD67
E	0	PHE	-	expression tag	UNP A3DD67
F	-35	MET	-	expression tag	UNP A3DD67
F	-34	GLY	-	expression tag	UNP A3DD67
F	-33	SER	-	expression tag	UNP A3DD67
F	-32	SER	-	expression tag	UNP A3DD67
F	-31	HIS	-	expression tag	UNP A3DD67

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-30	HIS	-	expression tag	UNP A3DD67
F	-29	HIS	-	expression tag	UNP A3DD67
F	-28	HIS	-	expression tag	UNP A3DD67
F	-27	HIS	-	expression tag	UNP A3DD67
F	-26	HIS	-	expression tag	UNP A3DD67
F	-25	SER	-	expression tag	UNP A3DD67
F	-24	SER	-	expression tag	UNP A3DD67
F	-23	GLY	-	expression tag	UNP A3DD67
F	-22	LEU	-	expression tag	UNP A3DD67
F	-21	VAL	-	expression tag	UNP A3DD67
F	-20	PRO	-	expression tag	UNP A3DD67
F	-19	ARG	-	expression tag	UNP A3DD67
F	-18	GLY	-	expression tag	UNP A3DD67
F	-17	SER	-	expression tag	UNP A3DD67
F	-16	HIS	-	expression tag	UNP A3DD67
F	-15	MET	-	expression tag	UNP A3DD67
F	-14	ALA	-	expression tag	UNP A3DD67
F	-13	SER	-	expression tag	UNP A3DD67
F	-12	MET	-	expression tag	UNP A3DD67
F	-11	THR	-	expression tag	UNP A3DD67
F	-10	GLY	-	expression tag	UNP A3DD67
F	-9	GLY	-	expression tag	UNP A3DD67
F	-8	GLN	-	expression tag	UNP A3DD67
F	-7	GLN	-	expression tag	UNP A3DD67
F	-6	MET	-	expression tag	UNP A3DD67
F	-5	GLY	-	expression tag	UNP A3DD67
F	-4	ARG	-	expression tag	UNP A3DD67
F	-3	GLY	-	expression tag	UNP A3DD67
F	-2	SER	-	expression tag	UNP A3DD67
F	-1	GLU	-	expression tag	UNP A3DD67
F	0	PHE	-	expression tag	UNP A3DD67

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-3)-beta-D-galactopyranose-e-(1-3)-beta-D-galactopyranose.



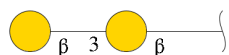
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	G	3	34	18	16	0	0	0

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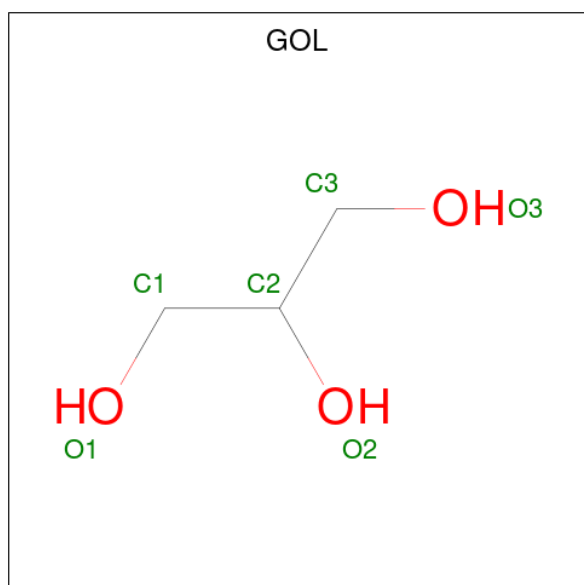
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	H	3	Total	C	O	0	0	0
			34	18	16			
2	I	3	Total	C	O	0	0	0
			34	18	16			
2	J	3	Total	C	O	0	0	0
			34	18	16			
2	K	3	Total	C	O	0	0	0
			34	18	16			

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-3)-beta-D-galactopyranoside.



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

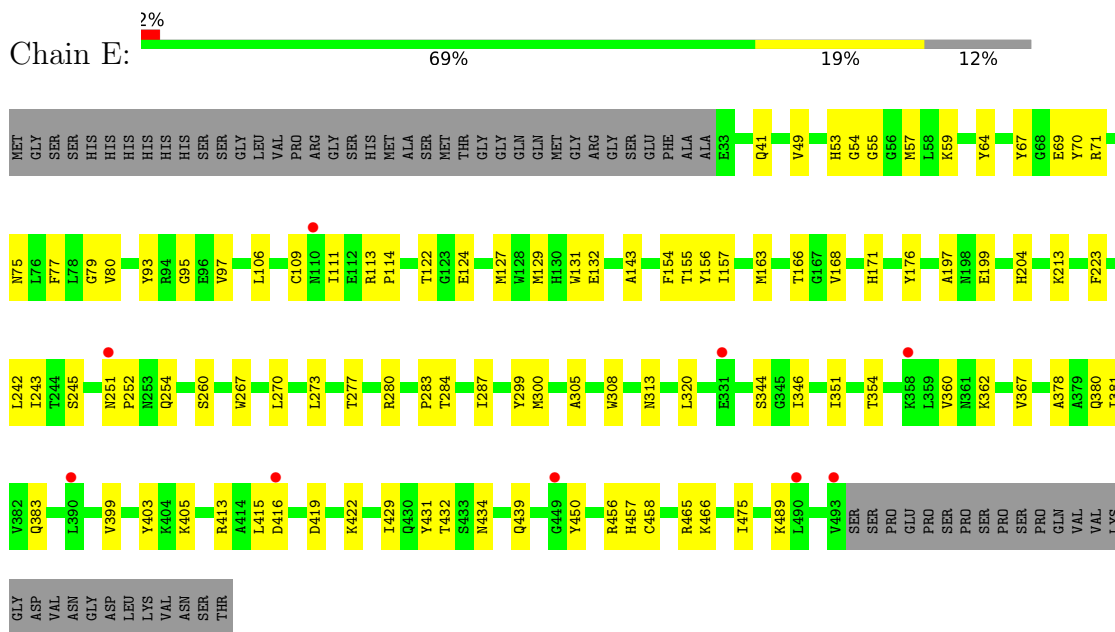
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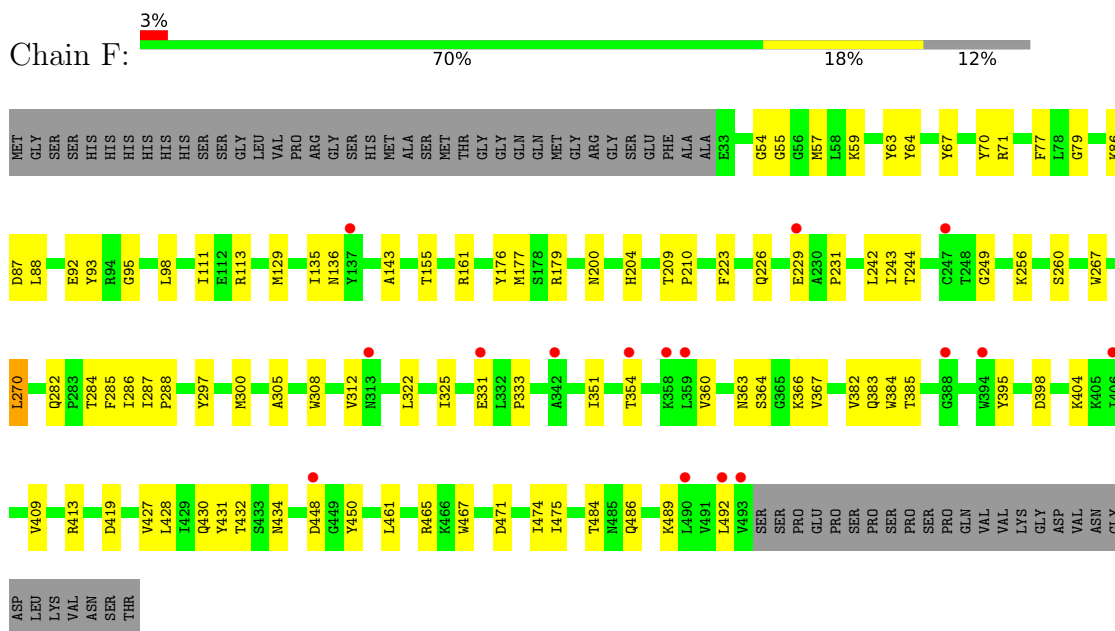
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0
4	F	1	Total C O 6 3 3	0	0
4	F	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

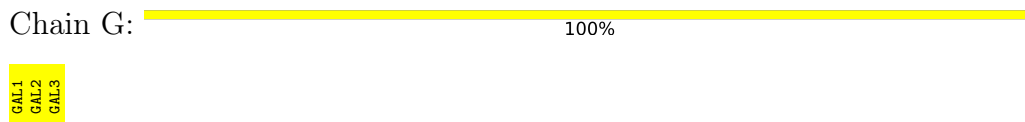
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total O 4 4	0	0
5	C	9	Total O 9 9	0	0
5	E	2	Total O 2 2	0	0
5	F	4	Total O 4 4	0	0



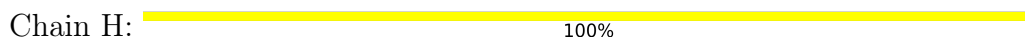
• Molecule 1: Ricin B lectin



• Molecule 2: beta-D-galactopyranose-(1-3)-beta-D-galactopyranose-(1-3)-beta-D-galactopyranose




• Molecule 2: beta-D-galactopyranose-(1-3)-beta-D-galactopyranose-(1-3)-beta-D-galactopyranose



GAL1
GAL2
GAL3


- Molecule 2: beta-D-galactopyranose-(1-3)-beta-D-galactopyranose-(1-3)-beta-D-galactopyranose

Chain I:  100%GAL1
GAL2
GAL3

- Molecule 2: beta-D-galactopyranose-(1-3)-beta-D-galactopyranose-(1-3)-beta-D-galactopyranose

Chain J:  100%GAL1
GAL2
GAL3

- Molecule 2: beta-D-galactopyranose-(1-3)-beta-D-galactopyranose-(1-3)-beta-D-galactopyranose

Chain K:  100%GAL1
GAL2
GAL3

- Molecule 3: beta-D-galactopyranose-(1-3)-beta-D-galactopyranose

Chain L:  100%GAL1
GAL2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.79Å 122.60Å 405.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.88 – 2.89 48.88 – 2.89	Depositor EDS
% Data completeness (in resolution range)	90.5 (48.88-2.89) 94.9 (48.88-2.89)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.91Å)	Xtrriage
Refinement program	PHENIX 1.7_650	Depositor
R, R_{free}	0.239 , 0.262 (Not available) , 0.280	Depositor DCC
R_{free} test set	2040 reflections (1.78%)	wwPDB-VP
Wilson B-factor (Å ²)	60.8	Xtrriage
Anisotropy	0.638	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22399	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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: GAL, GOL

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	0.24	0/3762	0.68	2/5104 (0.0%)
1	B	0.24	0/3762	0.66	0/5104
1	C	0.25	0/3907	0.67	0/5295
1	D	0.26	0/3762	0.70	1/5104 (0.0%)
1	E	0.25	0/3762	0.70	0/5104
1	F	0.25	0/3762	0.69	0/5104
All	All	0.25	0/22717	0.68	3/30815 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	461	LEU	N-CA-C	6.95	119.98	109.41
1	A	351	ILE	CA-C-N	5.41	125.08	119.56
1	A	351	ILE	C-N-CA	5.41	125.08	119.56

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	3664	0	3480	78	0
1	B	3664	0	3480	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3807	0	3613	79	0
1	D	3664	0	3480	116	0
1	E	3664	0	3480	80	0
1	F	3664	0	3480	77	0
2	G	34	0	30	15	0
2	H	34	0	30	17	0
2	I	34	0	30	16	0
2	J	34	0	30	20	0
2	K	34	0	30	13	0
3	L	23	0	21	3	0
4	A	6	0	8	0	0
4	B	12	0	16	0	0
4	C	18	0	24	2	0
4	D	6	0	8	0	0
4	E	6	0	8	0	0
4	F	12	0	16	0	0
5	A	4	0	0	1	0
5	C	9	0	0	0	0
5	E	2	0	0	0	0
5	F	4	0	0	0	0
All	All	22399	0	21264	517	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 12.

All (517) 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:D:453:ILE:HG13	1:D:461:LEU:HD11	1.21	1.14
1:D:446:ILE:HD11	1:D:452:LYS:HG3	1.27	1.13
2:J:2:GAL:H3	2:J:3:GAL:O2	1.55	1.03
2:H:2:GAL:H3	2:H:3:GAL:O2	1.59	1.00
1:D:453:ILE:HG13	1:D:461:LEU:CD1	1.94	0.96
1:C:57:MET:HE2	1:C:287:ILE:HG21	1.50	0.93
1:B:419:ASP:OD1	2:H:2:GAL:O2	1.86	0.92
1:D:453:ILE:CG1	1:D:461:LEU:HD11	1.98	0.91
2:I:2:GAL:H3	2:I:3:GAL:O2	1.70	0.89
1:D:340:ILE:HG22	1:D:347:ILE:HG22	1.57	0.87
1:C:419:ASP:OD1	2:I:1:GAL:O2	1.92	0.87
1:B:419:ASP:HA	2:H:2:GAL:H2	1.60	0.84
1:F:57:MET:HE2	1:F:287:ILE:HG21	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:GLY:HA2	1:C:89:VAL:HG21	1.59	0.82
1:D:380:GLN:HA	1:D:429:ILE:HG22	1.62	0.82
1:F:282:GLN:HE22	3:L:2:GAL:H61	1.47	0.80
1:A:419:ASP:OD1	2:G:2:GAL:O2	1.99	0.80
1:D:465:ARG:HG2	1:D:466:LYS:HG2	1.64	0.79
1:E:419:ASP:HA	2:J:2:GAL:H2	1.64	0.79
1:C:360:VAL:HG22	1:C:367:VAL:HG12	1.65	0.79
1:C:419:ASP:OD1	2:I:2:GAL:O2	2.00	0.78
1:A:285:PHE:HE2	1:A:287:ILE:HG23	1.50	0.77
1:D:422:LYS:HG3	1:D:458:CYS:HB3	1.67	0.77
2:J:2:GAL:C3	2:J:3:GAL:O2	2.30	0.77
2:H:2:GAL:C3	2:H:3:GAL:O2	2.33	0.77
1:E:422:LYS:HD3	1:E:458:CYS:HB3	1.65	0.76
1:F:461:LEU:HD11	1:F:486:GLN:HB3	1.67	0.76
1:A:285:PHE:CE2	1:A:287:ILE:HG23	2.21	0.76
1:C:260:SER:HB2	1:C:267:TRP:HA	1.69	0.76
1:C:-12:MET:HG3	1:E:155:THR:HG22	1.67	0.75
1:D:321:PRO:HB3	1:D:347:ILE:HD13	1.67	0.75
1:F:229:GLU:CD	3:L:2:GAL:H62	2.12	0.75
1:F:434:ASN:HD21	2:K:2:GAL:H61	1.51	0.74
1:B:84:ARG:HE	1:B:94:ARG:HE	1.34	0.74
1:E:431:TYR:CD2	2:J:2:GAL:H62	2.23	0.74
1:D:254:GLN:HG2	1:D:276:SER:HA	1.69	0.74
1:A:72:ASP:HB3	1:A:78:LEU:HD12	1.70	0.73
1:A:419:ASP:HA	2:G:2:GAL:H2	1.69	0.72
1:E:252:PRO:HB2	1:E:277:THR:HG23	1.72	0.71
1:E:80:VAL:HG21	1:E:127:MET:HE1	1.72	0.71
1:B:419:ASP:HA	2:H:2:GAL:C2	2.21	0.70
1:D:443:PHE:CE2	1:D:453:ILE:HG22	2.26	0.70
2:I:2:GAL:C3	2:I:3:GAL:O2	2.40	0.70
1:B:356:ARG:HD3	1:B:393:GLN:NE2	2.08	0.69
1:A:419:ASP:HA	2:G:2:GAL:O3	1.93	0.69
1:B:419:ASP:CA	2:H:2:GAL:H2	2.23	0.69
1:E:111:ILE:HD11	1:E:131:TRP:HD1	1.57	0.69
1:F:360:VAL:HG22	1:F:367:VAL:HG12	1.74	0.69
1:B:360:VAL:HG22	1:B:367:VAL:HG12	1.73	0.68
1:C:223:PHE:HE2	1:C:242:LEU:HD23	1.57	0.68
1:E:54:GLY:O	1:E:113:ARG:HA	1.94	0.68
1:F:260:SER:HB2	1:F:267:TRP:HA	1.76	0.68
1:F:223:PHE:HE2	1:F:242:LEU:HD23	1.59	0.67
1:F:419:ASP:HA	2:K:2:GAL:O3	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:419:ASP:HA	2:J:2:GAL:C2	2.25	0.66
1:E:434:ASN:HD21	2:J:2:GAL:H61	1.60	0.66
1:A:157:ILE:HG22	1:A:158:ARG:HG2	1.78	0.66
1:C:465:ARG:HH21	1:C:474:ILE:HG21	1.61	0.65
1:D:461:LEU:HD12	1:D:462:ILE:H	1.60	0.65
1:D:377:ASN:HD21	1:D:432:THR:HG23	1.61	0.65
1:E:53:HIS:O	1:E:69:GLU:HG2	1.97	0.65
1:C:419:ASP:HA	2:I:2:GAL:H2	1.79	0.64
1:F:77:PHE:CD1	1:F:111:ILE:HB	2.32	0.64
1:B:54:GLY:O	1:B:113:ARG:HA	1.98	0.63
1:B:419:ASP:H	2:H:2:GAL:H2	1.64	0.62
1:D:420:GLU:HG2	1:D:438:ASN:ND2	2.14	0.62
1:C:84:ARG:HH21	1:C:94:ARG:NH1	1.98	0.62
1:A:420:GLU:OE1	2:G:3:GAL:H62	1.99	0.62
1:A:163:MET:HE3	1:A:166:THR:HG21	1.80	0.62
1:E:360:VAL:HG22	1:E:367:VAL:HG12	1.81	0.62
1:E:413:ARG:NH1	1:E:432:THR:HG22	2.15	0.62
1:D:110:ASN:OD1	1:D:134:GLY:HA2	2.00	0.62
1:E:419:ASP:OD1	2:J:2:GAL:O2	2.12	0.61
1:A:114:PRO:HB2	1:A:127:MET:HE3	1.82	0.61
1:E:383:GLN:HB3	1:E:475:ILE:HD11	1.82	0.61
1:B:179:ARG:HG3	1:B:200:ASN:OD1	2.00	0.61
1:C:77:PHE:CD1	1:C:111:ILE:HB	2.36	0.61
1:F:98:LEU:HD23	1:F:129:MET:HE1	1.82	0.61
1:E:129:MET:HG2	1:E:143:ALA:HB3	1.82	0.61
1:B:106:LEU:HD11	1:B:156:TYR:CD2	2.36	0.61
1:D:163:MET:HE3	1:D:166:THR:HG21	1.83	0.61
1:D:395:TYR:CE2	1:D:409:VAL:HG22	2.36	0.61
1:D:387:ASN:H	1:D:392:GLN:HE22	1.47	0.60
1:C:485:ASN:HD21	4:C:601:GOL:H11	1.66	0.60
1:A:331:GLU:HG2	1:A:333:PRO:HD3	1.82	0.60
1:D:360:VAL:HA	1:D:367:VAL:HA	1.82	0.60
1:C:163:MET:HE3	1:C:166:THR:HG21	1.82	0.60
1:C:413:ARG:NH1	1:C:432:THR:HG22	2.17	0.60
1:D:380:GLN:HE22	1:D:474:ILE:HG13	1.66	0.60
1:F:71:ARG:HD3	1:F:312:VAL:HG11	1.83	0.60
1:A:287:ILE:HD11	1:A:300:MET:HE3	1.82	0.60
1:C:55:GLY:HA3	1:C:67:TYR:O	2.02	0.60
1:D:35:VAL:HG22	1:D:339:LYS:HA	1.83	0.59
1:A:419:ASP:HA	2:G:2:GAL:C2	2.31	0.59
1:B:84:ARG:NE	1:B:94:ARG:HE	1.99	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:TYR:HE1	2:H:1:GAL:HO4	1.49	0.59
1:E:197:ALA:HB3	1:E:204:HIS:CE1	2.38	0.59
1:F:419:ASP:OD1	2:K:2:GAL:O2	2.17	0.59
1:F:428:LEU:HD12	1:F:475:ILE:HG22	1.84	0.59
1:B:419:ASP:HA	2:H:2:GAL:O3	2.03	0.59
1:B:419:ASP:N	2:H:2:GAL:H2	2.18	0.59
1:D:347:ILE:HD12	1:D:347:ILE:O	2.02	0.59
1:C:54:GLY:O	1:C:113:ARG:HA	2.02	0.59
1:B:161:ARG:O	1:B:164:GLN:HG3	2.02	0.59
1:F:54:GLY:O	1:F:113:ARG:HA	2.02	0.58
1:A:260:SER:HB2	1:A:267:TRP:HA	1.84	0.58
1:E:77:PHE:CD1	1:E:111:ILE:HB	2.37	0.58
1:B:70:TYR:CZ	1:B:78:LEU:HD11	2.38	0.58
1:E:419:ASP:CA	2:J:2:GAL:H2	2.33	0.58
1:A:97:VAL:HB	1:A:154:PHE:CD2	2.38	0.58
1:B:57:MET:HE3	1:B:287:ILE:HG21	1.85	0.58
1:D:415:LEU:HD21	1:D:462:ILE:HD11	1.85	0.58
1:A:419:ASP:OD1	2:G:1:GAL:O2	2.20	0.58
1:C:450:TYR:CE1	1:C:489:LYS:HB2	2.39	0.58
1:D:97:VAL:HB	1:D:154:PHE:CD2	2.39	0.58
1:D:260:SER:HB2	1:D:267:TRP:HA	1.86	0.58
1:D:380:GLN:NE2	1:D:474:ILE:HG13	2.19	0.58
1:D:55:GLY:HA3	1:D:67:TYR:O	2.03	0.58
1:F:111:ILE:HG12	1:F:129:MET:HE2	1.86	0.58
1:A:54:GLY:O	1:A:113:ARG:HA	2.04	0.57
1:D:41:GLN:HB3	1:D:49:VAL:HG13	1.86	0.57
1:D:360:VAL:HG12	1:D:489:LYS:HB2	1.86	0.57
1:E:223:PHE:HE2	1:E:242:LEU:HD23	1.67	0.57
1:B:78:LEU:C	1:B:78:LEU:HD12	2.29	0.57
1:B:446:ILE:HD13	1:B:452:LYS:HG3	1.85	0.57
1:D:84:ARG:HG2	1:D:94:ARG:HD3	1.85	0.57
1:D:106:LEU:HD22	1:D:111:ILE:HD11	1.85	0.57
1:E:416:ASP:HB3	1:E:439:GLN:HG2	1.85	0.57
1:F:431:TYR:CE1	2:K:1:GAL:O4	2.57	0.57
1:D:117:MET:HE2	1:D:183:VAL:HB	1.85	0.57
1:B:41:GLN:HB3	1:B:49:VAL:HG23	1.86	0.57
1:B:431:TYR:CD2	2:H:2:GAL:H62	2.39	0.57
1:A:360:VAL:HG22	1:A:367:VAL:HG12	1.86	0.56
1:F:231:PRO:HA	1:F:244:THR:HG22	1.87	0.56
1:D:54:GLY:O	1:D:113:ARG:HA	2.04	0.56
1:B:380:GLN:HE22	1:B:427:VAL:HG13	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:361:ASN:HB3	1:D:364:SER:OG	2.06	0.56
1:F:431:TYR:CD2	2:K:2:GAL:H62	2.40	0.56
1:C:419:ASP:H	2:I:2:GAL:H2	1.70	0.56
1:F:286:ILE:HD13	1:F:322:LEU:HD22	1.86	0.56
1:B:260:SER:HB2	1:B:267:TRP:HA	1.88	0.56
1:C:419:ASP:HA	2:I:2:GAL:C2	2.35	0.56
1:E:277:THR:HG22	1:E:277:THR:O	2.06	0.56
1:F:256:LYS:HD3	1:F:270:LEU:HB3	1.88	0.56
1:E:157:ILE:HD11	1:E:213:LYS:HD2	1.88	0.55
1:F:223:PHE:CE2	1:F:242:LEU:HD23	2.41	0.55
1:D:450:TYR:CE2	1:D:489:LYS:HE3	2.42	0.55
1:B:67:TYR:CE2	1:B:116:VAL:HG21	2.42	0.55
1:B:419:ASP:OD1	2:H:1:GAL:O2	2.21	0.55
1:D:42:PHE:HB2	1:D:50:ILE:HD11	1.87	0.55
1:F:223:PHE:HB3	1:F:226:GLN:HG3	1.89	0.55
1:D:71:ARG:HG2	1:D:75:ASN:C	2.32	0.55
1:F:363:ASN:HB2	1:F:484:THR:OG1	2.07	0.55
1:D:296:SER:HB2	1:D:347:ILE:HD11	1.89	0.55
1:F:434:ASN:HD21	2:K:2:GAL:C6	2.21	0.54
1:D:291:GLY:HA3	1:D:345:GLY:HA3	1.89	0.54
1:A:279:TYR:CE2	1:A:334:TYR:HB2	2.43	0.54
1:B:55:GLY:HA3	1:B:67:TYR:O	2.07	0.54
1:D:360:VAL:CG1	1:D:489:LYS:HB2	2.37	0.54
1:D:462:ILE:HA	1:D:476:GLN:O	2.08	0.54
1:E:260:SER:HB2	1:E:267:TRP:HA	1.90	0.54
1:A:77:PHE:CD1	1:A:111:ILE:HB	2.42	0.54
1:B:110:ASN:HB2	1:B:132:GLU:HB2	1.90	0.54
1:A:103:ALA:HB3	1:A:106:LEU:HG	1.90	0.54
1:D:376:ASP:C	1:D:413:ARG:HH12	2.14	0.54
1:E:419:ASP:OD1	2:J:1:GAL:O2	2.17	0.54
1:B:340:ILE:HG22	1:B:347:ILE:HG23	1.89	0.54
1:D:381:ILE:HG12	1:D:429:ILE:HA	1.89	0.54
1:E:114:PRO:HB2	1:E:127:MET:HE3	1.90	0.54
1:F:419:ASP:OD1	2:K:1:GAL:O2	2.26	0.54
1:B:284:THR:HG22	1:B:300:MET:O	2.06	0.54
1:A:419:ASP:CA	2:G:2:GAL:H2	2.35	0.54
1:C:63:TYR:CE1	1:C:86:LYS:HE3	2.43	0.54
1:D:256:LYS:HD3	1:D:270:LEU:HB3	1.90	0.54
1:D:443:PHE:CD2	1:D:453:ILE:HG22	2.43	0.54
1:E:431:TYR:CE1	2:J:1:GAL:O4	2.61	0.54
1:B:130:HIS:CE1	1:B:179:ARG:HD3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:TYR:CE1	1:C:84:ARG:NH1	2.76	0.53
1:C:97:VAL:HB	1:C:154:PHE:CD2	2.42	0.53
1:B:419:ASP:OD1	2:H:2:GAL:C2	2.56	0.53
1:C:362:LYS:HE3	1:C:484:THR:HG22	1.90	0.53
1:D:424:ASP:OD2	1:D:460:LYS:HD3	2.08	0.53
1:B:106:LEU:HD21	1:B:156:TYR:CE2	2.44	0.53
1:B:156:TYR:OH	1:B:159:SER:HB3	2.07	0.53
1:D:441:TRP:HA	1:D:454:SER:O	2.08	0.53
1:A:62:ASP:O	1:A:86:LYS:HG2	2.08	0.53
1:C:-13:SER:HA	1:C:492:LEU:HD11	1.90	0.53
1:D:484:THR:HA	1:D:487:HIS:CD2	2.42	0.53
1:D:453:ILE:HD11	1:D:462:ILE:HB	1.91	0.53
1:F:398:ASP:HA	1:F:404:LYS:HG2	1.91	0.53
1:B:97:VAL:HB	1:B:154:PHE:CD2	2.44	0.53
1:E:284:THR:HG22	1:E:300:MET:O	2.08	0.53
1:A:112:GLU:HB2	5:A:701:HOH:O	2.08	0.53
1:C:129:MET:HG2	1:C:143:ALA:HB3	1.91	0.53
1:D:110:ASN:HB2	1:D:132:GLU:HB2	1.91	0.53
1:F:305:ALA:HA	1:F:308:TRP:CZ2	2.43	0.53
1:E:168:VAL:HG11	1:E:176:TYR:CE1	2.43	0.52
1:E:419:ASP:H	2:J:2:GAL:H2	1.75	0.52
1:A:63:TYR:CE1	1:A:86:LYS:HE3	2.44	0.52
1:B:434:ASN:HD21	2:H:2:GAL:H61	1.74	0.52
1:C:84:ARG:HE	1:C:94:ARG:CZ	2.22	0.52
1:D:245:SER:HB3	1:D:283:PRO:HD2	1.90	0.52
1:F:135:ILE:HG22	1:F:136:ASN:HD22	1.74	0.52
1:A:279:TYR:CD2	1:A:334:TYR:HB2	2.44	0.52
1:C:-6:MET:HE2	1:F:155:THR:HG21	1.90	0.52
1:D:450:TYR:CD1	1:D:489:LYS:HG3	2.44	0.52
1:A:419:ASP:OD1	2:G:2:GAL:C2	2.58	0.52
1:D:384:TRP:CZ3	1:D:471:ASP:HB3	2.44	0.52
1:D:444:THR:OG1	1:D:452:LYS:HB2	2.10	0.52
1:E:97:VAL:HB	1:E:154:PHE:CD2	2.45	0.52
1:C:59:LYS:HD3	1:C:64:TYR:CE1	2.44	0.52
1:B:129:MET:HG2	1:B:143:ALA:HB3	1.91	0.52
1:E:171:HIS:CE1	1:E:199:GLU:HB2	2.45	0.52
1:A:117:MET:HE3	1:A:185:VAL:HG22	1.92	0.52
1:C:84:ARG:HE	1:C:94:ARG:NE	2.07	0.52
1:E:431:TYR:CE2	2:J:2:GAL:H62	2.45	0.51
2:J:2:GAL:O2	2:J:3:GAL:C2	2.58	0.51
1:E:416:ASP:CB	1:E:439:GLN:HG2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:ARG:HA	1:D:297:TYR:OH	2.10	0.51
1:B:97:VAL:HB	1:B:154:PHE:HD2	1.75	0.51
1:F:331:GLU:HG2	1:F:333:PRO:HD3	1.93	0.51
1:D:157:ILE:HG22	1:D:158:ARG:HG2	1.92	0.51
1:E:434:ASN:ND2	2:J:2:GAL:H61	2.26	0.51
1:F:431:TYR:HE1	2:K:1:GAL:O4	1.93	0.51
1:D:284:THR:HG22	1:D:300:MET:O	2.11	0.50
1:E:277:THR:HG22	1:E:280:ARG:H	1.76	0.50
1:C:58:LEU:HD22	1:C:116:VAL:HG12	1.93	0.50
1:D:453:ILE:CD1	1:D:462:ILE:HD12	2.42	0.50
1:A:69:GLU:HG2	1:A:112:GLU:HA	1.92	0.50
1:E:70:TYR:HB3	1:E:79:GLY:O	2.12	0.50
1:E:465:ARG:HG2	1:E:466:LYS:HG2	1.93	0.50
1:A:126:VAL:HG21	1:A:212:TYR:HB2	1.92	0.50
1:B:431:TYR:HE1	2:H:1:GAL:O4	1.95	0.50
1:C:419:ASP:HA	2:I:2:GAL:O3	2.11	0.50
1:F:59:LYS:HD3	1:F:64:TYR:CE1	2.47	0.50
1:D:476:GLN:HG2	1:D:477:GLN:H	1.77	0.50
1:E:122:THR:OG1	1:E:124:GLU:HG2	2.11	0.50
1:D:377:ASN:HD21	1:D:432:THR:H	1.59	0.49
1:D:80:VAL:HG21	1:D:127:MET:HE1	1.94	0.49
2:I:1:GAL:HO2	2:I:2:GAL:HO2	1.60	0.49
1:A:325:ILE:HD11	1:A:331:GLU:OE2	2.12	0.49
1:C:235:LYS:HD2	1:C:240:TYR:CE2	2.47	0.49
2:G:1:GAL:O2	2:G:2:GAL:O2	2.30	0.49
1:B:321:PRO:HB3	1:B:347:ILE:HG22	1.94	0.49
1:C:399:VAL:HG21	1:C:440:HIS:NE2	2.27	0.49
2:J:2:GAL:O2	2:J:3:GAL:H2	2.13	0.49
1:E:252:PRO:HB2	1:E:277:THR:CG2	2.42	0.49
1:F:363:ASN:ND2	1:F:467:TRP:HE3	2.10	0.49
1:D:285:PHE:HB3	1:D:300:MET:HE3	1.95	0.49
1:A:122:THR:OG1	1:A:124:GLU:HG2	2.13	0.48
1:B:106:LEU:HD22	1:B:111:ILE:HD11	1.94	0.48
1:B:218:LEU:O	1:B:218:LEU:HD12	2.13	0.48
1:B:356:ARG:HD3	1:B:393:GLN:HE22	1.78	0.48
1:F:135:ILE:HD12	1:F:135:ILE:N	2.28	0.48
1:F:430:GLN:O	1:F:430:GLN:HG3	2.13	0.48
1:F:431:TYR:CE1	2:K:1:GAL:H4	2.48	0.48
1:C:362:LYS:HB2	1:C:450:TYR:CE1	2.47	0.48
1:F:465:ARG:HH21	1:F:474:ILE:HG21	1.78	0.48
1:B:125:PHE:CZ	1:B:150:PRO:HG3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:ASN:ND2	2:H:2:GAL:H61	2.28	0.48
1:C:419:ASP:CA	2:I:2:GAL:H2	2.44	0.48
1:D:443:PHE:HE2	1:D:453:ILE:HG22	1.73	0.48
1:F:129:MET:CG	1:F:143:ALA:HB3	2.43	0.48
1:F:284:THR:HG22	1:F:300:MET:O	2.14	0.48
1:A:129:MET:HG2	1:A:143:ALA:HB3	1.95	0.48
1:A:146:TYR:CD2	1:A:157:ILE:HD11	2.48	0.48
1:D:35:VAL:HG21	1:D:350:TYR:CD1	2.48	0.48
1:B:115:LYS:HG3	1:B:182:ASN:HA	1.96	0.48
1:B:369:ASP:HB2	1:B:392:GLN:HG2	1.96	0.48
1:C:77:PHE:CZ	1:C:111:ILE:HD12	2.48	0.48
1:D:147:SER:HB2	1:D:154:PHE:HA	1.95	0.48
1:D:360:VAL:O	1:D:488:TRP:HA	2.13	0.48
1:F:431:TYR:CE1	2:K:1:GAL:C4	2.97	0.48
1:A:424:ASP:O	1:C:136:ASN:HB2	2.14	0.48
1:D:474:ILE:HD12	1:D:474:ILE:N	2.29	0.48
1:E:163:MET:HE3	1:E:166:THR:HG21	1.96	0.48
1:C:64:TYR:CG	1:C:88:LEU:HD21	2.49	0.47
1:D:448:ASP:O	1:D:489:LYS:HE2	2.14	0.47
1:B:378:ALA:HA	1:B:429:ILE:HD12	1.96	0.47
1:C:42:PHE:CE2	1:C:317:TYR:HB2	2.49	0.47
1:E:41:GLN:HB3	1:E:49:VAL:HG13	1.96	0.47
1:F:57:MET:HB2	1:F:300:MET:HE1	1.95	0.47
2:K:3:GAL:HO4	2:K:3:GAL:HO6	1.62	0.47
1:A:431:TYR:CE1	2:G:1:GAL:H4	2.49	0.47
1:B:283:PRO:HB3	1:B:299:TYR:HE1	1.78	0.47
1:F:434:ASN:ND2	2:K:2:GAL:H61	2.26	0.47
1:D:168:VAL:HG21	1:D:176:TYR:CE1	2.50	0.47
1:A:110:ASN:OD1	1:A:134:GLY:HA2	2.15	0.47
1:B:53:HIS:CD2	1:B:315:SER:HB2	2.49	0.47
1:D:119:ASN:HD21	1:D:211:ASP:HA	1.79	0.47
1:F:249:GLY:HA2	3:L:1:GAL:O4	2.15	0.47
1:F:325:ILE:H	1:F:325:ILE:HD12	1.80	0.47
1:D:299:TYR:HB3	1:D:320:LEU:O	2.15	0.47
1:E:245:SER:HB3	1:E:283:PRO:HD2	1.97	0.47
1:F:366:LYS:HE3	1:F:385:THR:HG22	1.97	0.47
1:B:146:TYR:CD2	1:B:157:ILE:HD11	2.50	0.47
1:A:419:ASP:H	2:G:2:GAL:H2	1.80	0.47
1:C:-18:GLY:HA3	1:C:-15:MET:HE2	1.97	0.47
1:F:129:MET:HG2	1:F:143:ALA:HB3	1.96	0.47
1:F:209:THR:HB	1:F:210:PRO:HD2	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2:GAL:O2	2:J:3:GAL:O2	2.30	0.47
1:B:450:TYR:CE1	1:B:489:LYS:HB2	2.50	0.46
1:C:69:GLU:HG3	1:C:111:ILE:O	2.15	0.46
1:C:431:TYR:CE2	2:I:2:GAL:H61	2.50	0.46
1:E:419:ASP:N	2:J:2:GAL:H2	2.30	0.46
1:F:285:PHE:HB3	1:F:300:MET:HE3	1.96	0.46
1:E:80:VAL:HG21	1:E:127:MET:CE	2.43	0.46
1:C:104:PRO:HA	1:C:107:ASN:OD1	2.16	0.46
1:E:383:GLN:O	1:E:383:GLN:HG3	2.14	0.46
1:C:64:TYR:O	1:C:84:ARG:HA	2.15	0.46
1:D:106:LEU:HD11	1:D:156:TYR:CD2	2.50	0.46
1:D:453:ILE:O	1:D:461:LEU:HD13	2.14	0.46
1:D:461:LEU:O	1:D:477:GLN:HA	2.15	0.46
1:C:413:ARG:HH12	1:C:432:THR:HG22	1.80	0.46
1:D:453:ILE:HD11	1:D:462:ILE:HD12	1.98	0.46
1:E:109:CYS:HB2	1:E:132:GLU:O	2.15	0.46
1:E:254:GLN:NE2	1:E:273:LEU:H	2.14	0.46
1:E:422:LYS:HE2	1:E:457:HIS:CD2	2.51	0.46
1:F:70:TYR:HB3	1:F:79:GLY:O	2.16	0.46
1:F:325:ILE:HD11	1:F:331:GLU:OE1	2.16	0.46
1:B:117:MET:HE3	1:B:185:VAL:HG22	1.98	0.46
1:D:379:ALA:HB3	1:D:430:GLN:HG2	1.97	0.46
1:E:71:ARG:HB2	1:E:313:ASN:HD21	1.81	0.46
1:A:110:ASN:HB2	1:A:132:GLU:HB2	1.98	0.46
1:F:395:TYR:CE2	1:F:409:VAL:HG22	2.51	0.46
1:A:237:ASN:OD1	1:F:448:ASP:HA	2.16	0.45
1:A:351:ILE:HD12	1:A:351:ILE:N	2.31	0.45
1:C:419:ASP:N	2:I:2:GAL:H2	2.31	0.45
1:F:413:ARG:NH1	1:F:432:THR:HG22	2.31	0.45
1:C:223:PHE:CE2	1:C:242:LEU:HD23	2.43	0.45
1:C:270:LEU:HD12	1:C:270:LEU:N	2.31	0.45
1:E:351:ILE:N	1:E:351:ILE:HD12	2.30	0.45
1:A:375:VAL:HG12	1:A:411:SER:HB3	1.97	0.45
1:D:248:THR:O	1:D:251:ASN:HB2	2.16	0.45
1:E:57:MET:HE3	1:E:287:ILE:HG21	1.98	0.45
1:F:382:VAL:HA	1:F:475:ILE:HG12	1.98	0.45
1:C:284:THR:HG22	1:C:300:MET:O	2.17	0.45
1:A:156:TYR:OH	1:A:159:SER:HB3	2.17	0.45
1:C:-13:SER:HA	1:C:492:LEU:CD1	2.47	0.45
1:D:77:PHE:CD1	1:D:111:ILE:HB	2.51	0.45
1:B:381:ILE:HG12	1:B:429:ILE:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:385:THR:HG23	1:C:471:ASP:OD1	2.16	0.45
1:D:450:TYR:HB3	1:D:487:HIS:HB3	1.98	0.45
1:A:63:TYR:CZ	1:A:86:LYS:HE3	2.52	0.45
1:F:419:ASP:HA	2:K:2:GAL:H2	1.99	0.45
2:G:1:GAL:HO2	2:G:2:GAL:HO2	1.61	0.45
1:D:114:PRO:HB2	1:D:127:MET:HE3	1.98	0.45
1:E:106:LEU:HD11	1:E:156:TYR:CD2	2.50	0.45
1:E:431:TYR:HE1	2:J:1:GAL:O4	2.00	0.45
1:B:146:TYR:HD2	1:B:157:ILE:HD11	1.81	0.45
1:C:106:LEU:HD22	1:C:111:ILE:HD11	1.99	0.45
1:C:492:LEU:HD12	1:C:492:LEU:N	2.32	0.45
1:F:285:PHE:HE2	1:F:287:ILE:HB	1.81	0.45
1:D:35:VAL:CG2	1:D:339:LYS:HE3	2.47	0.45
1:D:278:THR:HG22	1:D:278:THR:O	2.17	0.45
1:E:197:ALA:HB3	1:E:204:HIS:ND1	2.32	0.45
1:E:305:ALA:HA	1:E:308:TRP:CZ2	2.52	0.45
1:F:351:ILE:HD12	1:F:351:ILE:N	2.32	0.45
1:A:97:VAL:HB	1:A:154:PHE:HD2	1.78	0.44
1:A:243:ILE:N	1:A:243:ILE:HD12	2.33	0.44
1:C:71:ARG:HG2	1:C:75:ASN:C	2.43	0.44
1:E:381:ILE:HG13	1:E:415:LEU:CD1	2.47	0.44
1:F:55:GLY:HA3	1:F:67:TYR:O	2.17	0.44
1:F:450:TYR:CE1	1:F:489:LYS:HB2	2.51	0.44
1:A:55:GLY:HA3	1:A:67:TYR:O	2.17	0.44
1:B:339:LYS:HB2	1:B:350:TYR:HB2	2.00	0.44
1:E:111:ILE:HD11	1:E:131:TRP:CD1	2.45	0.44
1:B:118:TYR:HD2	1:B:125:PHE:CE1	2.35	0.44
1:D:243:ILE:N	1:D:243:ILE:HD12	2.32	0.44
1:F:93:TYR:CZ	1:F:95:GLY:HA2	2.52	0.44
1:A:474:ILE:HD12	1:A:474:ILE:N	2.33	0.44
1:B:33:GLU:HG2	1:B:35:VAL:HG12	1.98	0.44
1:D:354:THR:HG22	1:D:354:THR:O	2.18	0.44
1:D:366:LYS:HE3	1:D:383:GLN:OE1	2.18	0.44
1:E:362:LYS:HD3	1:E:450:TYR:CZ	2.53	0.44
1:F:161:ARG:HH22	1:F:177:MET:HG2	1.83	0.44
1:A:50:ILE:HG23	1:A:83:TYR:CE1	2.53	0.44
1:A:466:LYS:HB3	1:C:250:TRP:CD1	2.53	0.44
1:D:53:HIS:O	1:D:69:GLU:HG2	2.17	0.44
1:D:338:VAL:HG12	1:D:340:ILE:HG23	1.98	0.44
1:E:399:VAL:HG11	1:E:405:LYS:HG3	1.99	0.44
1:F:287:ILE:HA	1:F:288:PRO:HD3	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:VAL:HG11	1:A:405:LYS:HG3	2.00	0.44
1:E:380:GLN:HE21	1:E:381:ILE:N	2.15	0.44
1:B:287:ILE:HA	1:B:288:PRO:HD3	1.88	0.44
1:C:354:THR:HG22	1:C:354:THR:O	2.17	0.44
1:D:77:PHE:CZ	1:D:111:ILE:HD12	2.53	0.44
1:F:288:PRO:HG3	1:F:297:TYR:CE1	2.53	0.44
2:I:2:GAL:O2	2:I:3:GAL:O2	2.30	0.44
1:A:41:GLN:HB3	1:A:49:VAL:HG23	1.99	0.43
1:A:130:HIS:CD2	1:A:179:ARG:HA	2.54	0.43
1:A:216:ALA:O	1:B:165:ASP:HA	2.18	0.43
1:A:403:TYR:CD1	1:A:442:LYS:HB2	2.53	0.43
1:B:422:LYS:HE3	1:B:457:HIS:NE2	2.33	0.43
1:C:106:LEU:HD11	1:C:156:TYR:CD2	2.53	0.43
1:D:461:LEU:CD1	1:D:462:ILE:H	2.30	0.43
1:E:55:GLY:HA3	1:E:67:TYR:O	2.18	0.43
1:C:201:MET:HE3	1:C:225:GLY:HA2	2.00	0.43
1:E:93:TYR:CZ	1:E:95:GLY:HA2	2.53	0.43
1:E:413:ARG:HH11	1:E:432:THR:HG22	1.83	0.43
1:C:434:ASN:HD21	2:I:2:GAL:C6	2.32	0.43
1:D:228:ARG:HB3	1:D:244:THR:HB	2.00	0.43
1:A:419:ASP:N	2:G:2:GAL:H2	2.33	0.43
1:B:57:MET:CE	1:B:287:ILE:HG21	2.47	0.43
1:B:362:LYS:HG3	1:B:484:THR:HB	1.99	0.43
1:D:66:TRP:CD1	1:D:66:TRP:C	2.96	0.43
1:D:119:ASN:ND2	1:D:211:ASP:HA	2.33	0.43
1:A:106:LEU:HD11	1:A:156:TYR:CD2	2.53	0.43
1:B:362:LYS:HE2	1:B:450:TYR:CZ	2.53	0.43
1:E:299:TYR:HB3	1:E:320:LEU:O	2.17	0.43
1:C:305:ALA:HA	1:C:308:TRP:CZ2	2.53	0.43
1:D:35:VAL:HG23	1:D:339:LYS:HE3	2.00	0.43
1:D:35:VAL:HG21	1:D:350:TYR:CG	2.54	0.43
1:E:380:GLN:HE21	1:E:381:ILE:H	1.67	0.43
1:F:87:ASP:O	1:F:88:LEU:HB2	2.19	0.43
1:A:288:PRO:HG3	1:A:297:TYR:CE1	2.54	0.43
1:A:362:LYS:HD3	1:A:450:TYR:CZ	2.53	0.43
1:D:87:ASP:O	1:D:88:LEU:HB2	2.19	0.43
1:D:394:TRP:CE3	1:D:406:ILE:HG22	2.54	0.43
1:A:77:PHE:CZ	1:A:80:VAL:HG23	2.54	0.42
1:D:376:ASP:O	1:D:379:ALA:HB2	2.19	0.42
1:D:377:ASN:ND2	1:D:432:THR:HG23	2.29	0.42
1:D:382:VAL:HA	1:D:475:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:59:LYS:HD3	1:E:64:TYR:CE1	2.54	0.42
1:E:114:PRO:CB	1:E:127:MET:HE3	2.49	0.42
1:D:135:ILE:HG13	1:D:136:ASN:ND2	2.35	0.42
1:E:344:SER:HB3	1:E:346:ILE:HD13	2.00	0.42
2:H:2:GAL:O2	2:H:3:GAL:O2	2.33	0.42
1:A:287:ILE:HD12	1:A:298:LEU:HB3	2.00	0.42
1:C:377:ASN:OD1	1:C:431:TYR:HA	2.20	0.42
1:E:129:MET:CG	1:E:143:ALA:HB3	2.50	0.42
1:A:57:MET:CB	1:A:300:MET:HE1	2.49	0.42
1:A:87:ASP:O	1:A:88:LEU:HB2	2.19	0.42
1:A:240:TYR:O	1:A:259:TYR:HA	2.18	0.42
1:B:450:TYR:HA	1:B:488:TRP:O	2.19	0.42
1:C:285:PHE:HE2	1:C:287:ILE:HB	1.84	0.42
1:C:431:TYR:CD2	2:I:2:GAL:C6	3.02	0.42
1:E:277:THR:HG22	1:E:280:ARG:HA	2.02	0.42
1:E:450:TYR:CE1	1:E:489:LYS:HB2	2.55	0.42
1:F:325:ILE:HD12	1:F:325:ILE:N	2.33	0.42
1:F:364:SER:OG	1:F:366:LYS:HG2	2.19	0.42
1:F:383:GLN:HB3	1:F:475:ILE:HD11	2.02	0.42
1:A:103:ALA:HB1	1:A:104:PRO:HD2	2.00	0.42
1:A:395:TYR:CE2	1:A:409:VAL:HG22	2.55	0.42
1:B:399:VAL:HG11	1:B:405:LYS:HG3	2.02	0.42
1:E:251:ASN:HA	1:E:252:PRO:HD3	1.93	0.42
1:F:243:ILE:N	1:F:243:ILE:HD12	2.34	0.42
1:B:109:CYS:HB2	1:B:132:GLU:O	2.20	0.42
1:D:395:TYR:CZ	1:D:409:VAL:HG22	2.55	0.42
1:F:354:THR:HG22	1:F:354:THR:O	2.20	0.42
1:A:354:THR:HG22	1:A:354:THR:O	2.20	0.42
1:B:130:HIS:CE1	1:B:179:ARG:HA	2.54	0.42
1:B:465:ARG:HG2	1:B:466:LYS:HG2	2.02	0.42
1:D:453:ILE:C	1:D:461:LEU:HD13	2.44	0.42
1:A:474:ILE:HD12	1:A:474:ILE:H	1.84	0.41
1:C:287:ILE:HA	1:C:288:PRO:HD3	1.87	0.41
1:C:431:TYR:CD2	2:I:2:GAL:H62	2.55	0.41
1:D:361:ASN:HB2	1:D:488:TRP:CZ3	2.54	0.41
1:D:170:ASP:CG	1:D:177:MET:HG3	2.44	0.41
1:D:351:ILE:N	1:D:351:ILE:HD12	2.35	0.41
1:B:243:ILE:HD12	1:B:243:ILE:N	2.36	0.41
1:E:431:TYR:CE1	2:J:1:GAL:H4	2.55	0.41
1:E:431:TYR:CE1	2:J:1:GAL:C4	3.04	0.41
1:F:63:TYR:CE1	1:F:86:LYS:HE3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:ALA:HA	1:C:429:ILE:HD12	2.02	0.41
1:C:478:TRP:CE3	4:C:601:GOL:H32	2.55	0.41
1:D:129:MET:CG	1:D:143:ALA:HB3	2.51	0.41
1:E:243:ILE:HD12	1:E:243:ILE:N	2.35	0.41
1:F:176:TYR:CD1	1:F:204:HIS:HE1	2.38	0.41
1:A:87:ASP:OD1	1:A:89:VAL:HB	2.20	0.41
1:B:226:GLN:HB3	1:B:228:ARG:HG2	2.01	0.41
1:C:77:PHE:HB2	1:C:111:ILE:H	1.85	0.41
1:C:446:ILE:HG21	1:C:452:LYS:HG3	2.02	0.41
1:D:320:LEU:HB2	1:D:332:LEU:HD11	2.01	0.41
1:B:424:ASP:HB3	1:B:478:TRP:CE3	2.56	0.41
1:B:257:TYR:CE2	1:B:330:LEU:HD13	2.55	0.41
1:C:50:ILE:HG23	1:C:83:TYR:CE1	2.56	0.41
1:C:57:MET:HE2	1:C:287:ILE:HD13	2.02	0.41
1:F:179:ARG:HD2	1:F:200:ASN:OD1	2.21	0.41
1:D:64:TYR:CG	1:D:88:LEU:HD21	2.56	0.41
1:A:130:HIS:NE2	1:A:179:ARG:HA	2.36	0.41
1:A:465:ARG:HH21	1:A:474:ILE:HG21	1.86	0.41
1:B:180:ASP:O	1:B:195:SER:HA	2.20	0.41
1:B:278:THR:HG22	1:B:278:THR:O	2.21	0.41
1:C:223:PHE:CD1	1:C:270:LEU:HD11	2.56	0.41
1:C:245:SER:HB3	1:C:283:PRO:HD2	2.03	0.41
1:D:57:MET:HE2	1:D:57:MET:HB3	1.86	0.41
1:D:234:ILE:C	1:D:234:ILE:HD12	2.46	0.41
1:D:293:SER:OG	1:D:346:ILE:HD13	2.21	0.41
1:E:71:ARG:NH1	1:E:75:ASN:HD21	2.19	0.41
1:C:425:GLY:HA2	1:C:476:GLN:CD	2.46	0.41
1:E:354:THR:HG22	1:E:354:THR:O	2.21	0.41
1:A:287:ILE:CD1	1:A:298:LEU:HB3	2.52	0.40
1:B:394:TRP:CE3	1:B:406:ILE:HG22	2.56	0.40
1:B:77:PHE:CE1	1:B:80:VAL:HG23	2.56	0.40
1:B:119:ASN:HB3	1:B:122:THR:OG1	2.20	0.40
1:B:126:VAL:HG21	1:B:212:TYR:HB2	2.02	0.40
1:C:57:MET:CE	1:C:287:ILE:HD13	2.51	0.40
1:C:106:LEU:HA	1:C:109:CYS:SG	2.61	0.40
1:D:52:ALA:CA	1:D:68:GLY:HA3	2.51	0.40
1:D:77:PHE:CE1	1:D:111:ILE:HD12	2.57	0.40
1:A:405:LYS:HE2	1:A:405:LYS:HB3	1.86	0.40
1:A:419:ASP:HA	2:G:2:GAL:C3	2.51	0.40
1:A:430:GLN:O	1:A:430:GLN:HG3	2.20	0.40
1:A:431:TYR:HE1	2:G:1:GAL:H4	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:THR:HB	1:F:92:GLU:OE2	2.21	0.40
1:D:381:ILE:HG22	1:D:475:ILE:HG13	2.03	0.40
1:F:492:LEU:N	1:F:492:LEU:HD12	2.36	0.40
1:A:180:ASP:O	1:A:195:SER:HA	2.20	0.40
1:A:350:TYR:O	1:A:352:PRO:HD3	2.21	0.40
1:C:36:ILE:HD13	1:C:340:ILE:HD12	2.03	0.40
1:D:234:ILE:HD11	1:D:241:TYR:HB2	2.03	0.40
1:F:367:VAL:HG22	1:F:384:TRP:O	2.21	0.40
1:D:117:MET:HE3	1:D:128:TRP:CD1	2.57	0.40
1:E:378:ALA:HA	1:E:429:ILE:HD12	2.03	0.40
1:E:403:TYR:CZ	1:E:456:ARG:HG3	2.56	0.40
1:F:385:THR:HG23	1:F:471:ASP:OD1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	459/526 (87%)	436 (95%)	23 (5%)	0	100	100
1	B	459/526 (87%)	434 (95%)	25 (5%)	0	100	100
1	C	480/526 (91%)	461 (96%)	19 (4%)	0	100	100
1	D	459/526 (87%)	429 (94%)	30 (6%)	0	100	100
1	E	459/526 (87%)	440 (96%)	19 (4%)	0	100	100
1	F	459/526 (87%)	441 (96%)	18 (4%)	0	100	100
All	All	2775/3156 (88%)	2641 (95%)	134 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	389/442 (88%)	387 (100%)	2 (0%)	81	93
1	B	389/442 (88%)	387 (100%)	2 (0%)	81	93
1	C	402/442 (91%)	401 (100%)	1 (0%)	87	96
1	D	389/442 (88%)	385 (99%)	4 (1%)	68	89
1	E	389/442 (88%)	388 (100%)	1 (0%)	86	96
1	F	389/442 (88%)	387 (100%)	2 (0%)	81	93
All	All	2347/2652 (88%)	2335 (100%)	12 (0%)	81	93

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	287	ILE
1	A	427	VAL
1	B	78	LEU
1	B	226	GLN
1	C	427	VAL
1	D	339	LYS
1	D	346	ILE
1	D	347	ILE
1	D	453	ILE
1	E	270	LEU
1	F	270	LEU
1	F	427	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	51	HIS
1	A	60	HIS
1	A	107	ASN
1	A	313	ASN

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Mol	Chain	Res	Type
1	A	487	HIS
1	B	48	ASN
1	B	53	HIS
1	B	75	ASN
1	B	130	HIS
1	B	361	ASN
1	B	487	HIS
1	C	53	HIS
1	C	75	ASN
1	D	60	HIS
1	D	380	GLN
1	D	392	GLN
1	D	477	GLN
1	E	110	ASN
1	E	171	HIS
1	F	101	ASN
1	F	107	ASN
1	F	171	HIS
1	F	282	GLN
1	F	457	HIS
1	F	477	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 [i](#)

17 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
2	GAL	G	1	2	12,12,12	0.54	0	17,17,17	0.52	0
2	GAL	G	2	2	11,11,12	0.65	0	15,15,17	0.52	0
2	GAL	G	3	2	11,11,12	0.66	0	15,15,17	0.52	0
2	GAL	H	1	2	12,12,12	0.53	0	17,17,17	0.52	0
2	GAL	H	2	2	11,11,12	0.65	0	15,15,17	0.52	0
2	GAL	H	3	2	11,11,12	0.66	0	15,15,17	0.52	0
2	GAL	I	1	2	12,12,12	0.54	0	17,17,17	0.52	0
2	GAL	I	2	2	11,11,12	0.65	0	15,15,17	0.52	0
2	GAL	I	3	2	11,11,12	0.65	0	15,15,17	0.53	0
2	GAL	J	1	2	12,12,12	0.55	0	17,17,17	0.52	0
2	GAL	J	2	2	11,11,12	0.65	0	15,15,17	0.52	0
2	GAL	J	3	2	11,11,12	0.66	0	15,15,17	0.52	0
2	GAL	K	1	2	12,12,12	0.53	0	17,17,17	0.52	0
2	GAL	K	2	2	11,11,12	0.65	0	15,15,17	0.52	0
2	GAL	K	3	2	11,11,12	0.67	0	15,15,17	0.53	0
3	GAL	L	1	3	12,12,12	0.55	0	17,17,17	0.52	0
3	GAL	L	2	3	11,11,12	0.65	0	15,15,17	0.52	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
2	GAL	G	1	2	-	2/2/22/22	0/1/1/1
2	GAL	G	2	2	-	2/2/19/22	0/1/1/1
2	GAL	G	3	2	-	0/2/19/22	0/1/1/1
2	GAL	H	1	2	-	2/2/22/22	0/1/1/1
2	GAL	H	2	2	-	1/2/19/22	0/1/1/1
2	GAL	H	3	2	-	2/2/19/22	0/1/1/1
2	GAL	I	1	2	-	2/2/22/22	0/1/1/1
2	GAL	I	2	2	-	2/2/19/22	0/1/1/1
2	GAL	I	3	2	-	0/2/19/22	0/1/1/1
2	GAL	J	1	2	-	2/2/22/22	0/1/1/1
2	GAL	J	2	2	-	0/2/19/22	0/1/1/1
2	GAL	J	3	2	-	2/2/19/22	0/1/1/1
2	GAL	K	1	2	-	2/2/22/22	0/1/1/1
2	GAL	K	2	2	-	0/2/19/22	0/1/1/1
2	GAL	K	3	2	-	0/2/19/22	0/1/1/1
3	GAL	L	1	3	-	2/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GAL	L	2	3	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (23) torsion outliers are listed below:

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

There are no ring outliers.

17 monomers are involved in 84 short contacts:

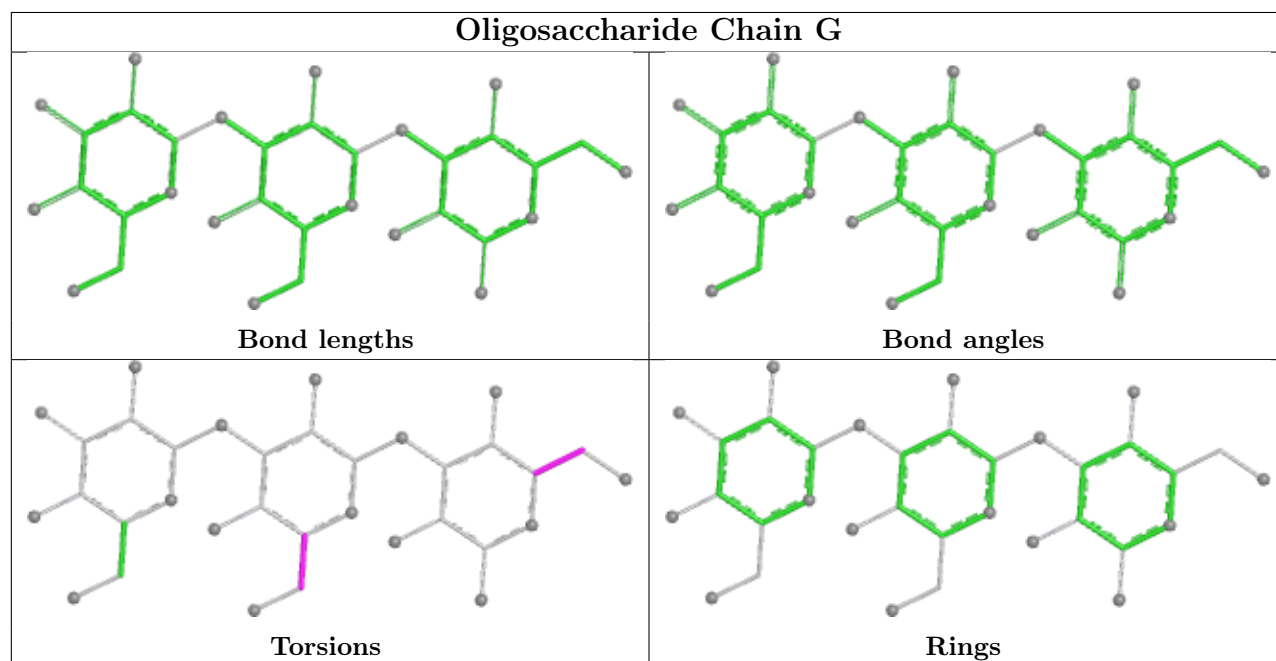
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	2	GAL	15	0
2	G	1	GAL	5	0
2	J	1	GAL	5	0
2	K	3	GAL	1	0

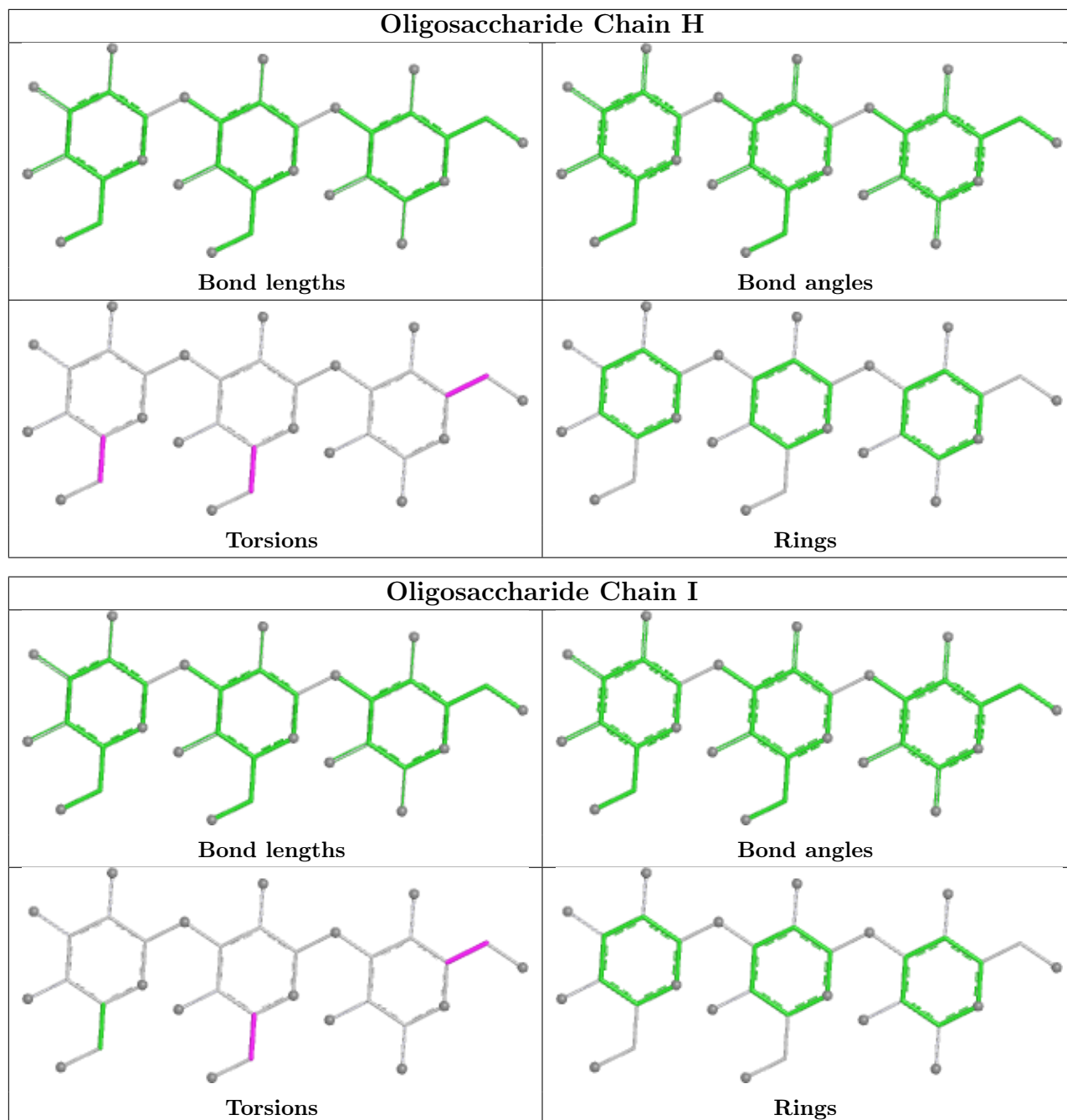
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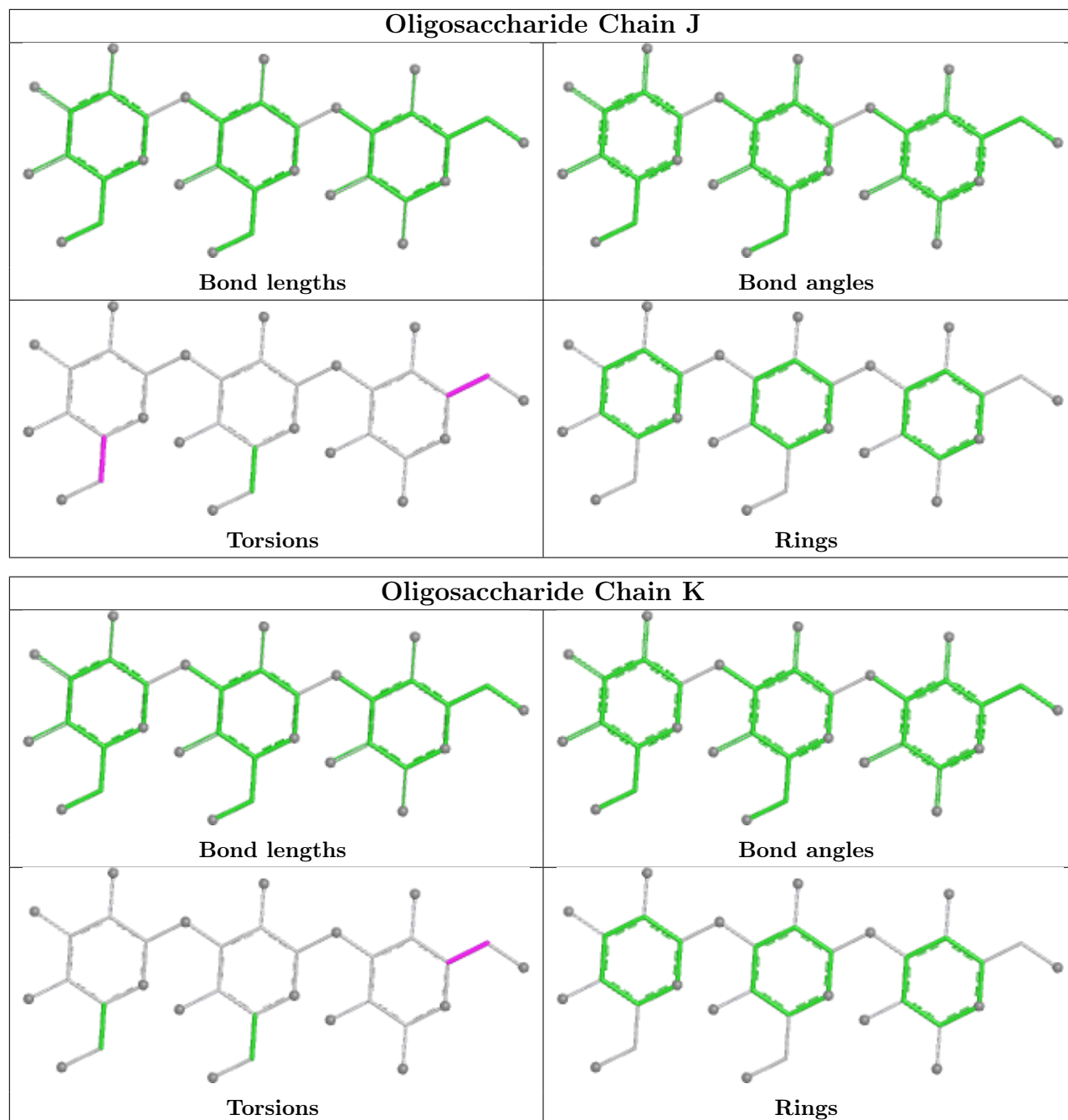
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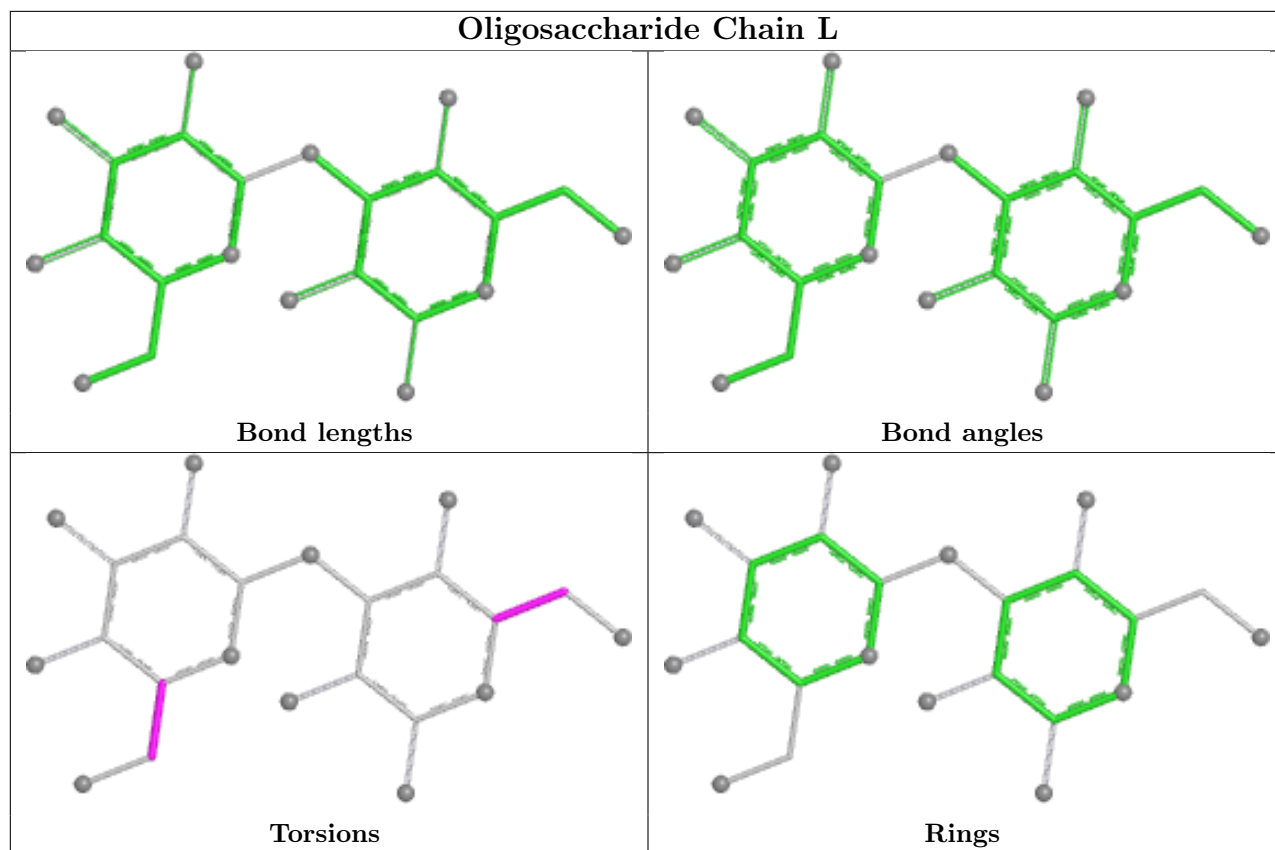
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	1	GAL	5	0
3	L	1	GAL	1	0
2	H	2	GAL	14	0
2	I	1	GAL	2	0
2	G	2	GAL	11	0
2	H	1	GAL	3	0
2	J	2	GAL	15	0
2	J	3	GAL	5	0
3	L	2	GAL	2	0
2	G	3	GAL	1	0
2	I	3	GAL	3	0
2	H	3	GAL	3	0
2	K	2	GAL	7	0

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









5.6 Ligand geometry [i](#)

10 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	GOL	A	601	-	5,5,5	0.38	0	5,5,5	0.30	0
4	GOL	B	602	-	5,5,5	0.38	0	5,5,5	0.30	0
4	GOL	C	603	-	5,5,5	0.37	0	5,5,5	0.34	0
4	GOL	D	601	-	5,5,5	0.37	0	5,5,5	0.31	0
4	GOL	F	602	-	5,5,5	0.36	0	5,5,5	0.32	0
4	GOL	C	602	-	5,5,5	0.37	0	5,5,5	0.30	0
4	GOL	C	601	-	5,5,5	0.37	0	5,5,5	0.35	0
4	GOL	F	601	-	5,5,5	0.38	0	5,5,5	0.31	0
4	GOL	B	601	-	5,5,5	0.37	0	5,5,5	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	E	601	-	5,5,5	0.37	0	5,5,5	0.32	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	GOL	A	601	-	-	2/4/4/4	-
4	GOL	B	602	-	-	2/4/4/4	-
4	GOL	C	603	-	-	4/4/4/4	-
4	GOL	D	601	-	-	2/4/4/4	-
4	GOL	F	602	-	-	2/4/4/4	-
4	GOL	C	602	-	-	2/4/4/4	-
4	GOL	C	601	-	-	2/4/4/4	-
4	GOL	F	601	-	-	2/4/4/4	-
4	GOL	B	601	-	-	2/4/4/4	-
4	GOL	E	601	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	GOL	O1-C1-C2-C3
4	B	601	GOL	O1-C1-C2-C3
4	B	602	GOL	O1-C1-C2-O2
4	B	602	GOL	O1-C1-C2-C3
4	C	601	GOL	O1-C1-C2-C3
4	C	602	GOL	O1-C1-C2-C3
4	C	603	GOL	O1-C1-C2-C3
4	E	601	GOL	O1-C1-C2-C3
4	D	601	GOL	O1-C1-C2-C3
4	F	601	GOL	O1-C1-C2-C3
4	F	602	GOL	O1-C1-C2-C3
4	B	601	GOL	O1-C1-C2-O2
4	C	602	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	C	603	GOL	O1-C1-C2-O2
4	A	601	GOL	O1-C1-C2-O2
4	C	601	GOL	O1-C1-C2-O2
4	D	601	GOL	O1-C1-C2-O2
4	E	601	GOL	O1-C1-C2-O2
4	F	601	GOL	O1-C1-C2-O2
4	C	603	GOL	O2-C2-C3-O3
4	F	602	GOL	O1-C1-C2-O2
4	C	603	GOL	C1-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	601	GOL	2	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

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	461/526 (87%)	0.71	19 (4%) 41 33	47, 73, 93, 110	0
1	B	461/526 (87%)	0.88	25 (5%) 31 24	58, 83, 105, 114	0
1	C	482/526 (91%)	0.28	11 (2%) 61 52	40, 55, 72, 109	0
1	D	461/526 (87%)	1.29	114 (24%) 2 1	47, 85, 150, 156	0
1	E	461/526 (87%)	0.43	9 (1%) 65 56	43, 65, 83, 95	0
1	F	461/526 (87%)	0.49	16 (3%) 47 38	40, 61, 80, 102	0
All	All	2787/3156 (88%)	0.68	194 (6%) 22 18	40, 68, 114, 156	0

All (194) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	427	VAL	5.2
1	D	493	VAL	5.1
1	D	396	LEU	4.8
1	D	384	TRP	4.7
1	D	375	VAL	4.7
1	D	380	GLN	4.6
1	D	390	LEU	4.6
1	B	493	VAL	4.5
1	D	378	ALA	4.4
1	D	443	PHE	4.0
1	D	492	LEU	4.0
1	F	493	VAL	3.7
1	D	371	LEU	3.7
1	C	-6	MET	3.6
1	C	69	GLU	3.5
1	D	373	GLY	3.5
1	D	457	HIS	3.5
1	A	247	CYS	3.4
1	C	-4	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	453	ILE	3.4
1	D	464	VAL	3.4
1	D	393	GLN	3.3
1	D	35	VAL	3.3
1	D	110	ASN	3.3
1	D	358	LYS	3.2
1	B	358	LYS	3.1
1	A	95	GLY	3.1
1	D	466	LYS	3.1
1	D	397	VAL	3.1
1	E	449	GLY	3.1
1	D	490	LEU	3.1
1	A	133	ASN	3.1
1	C	110	ASN	3.1
1	A	164	GLN	3.1
1	D	410	LYS	3.1
1	F	388	GLY	3.0
1	D	374	SER	3.0
1	D	484	THR	3.0
1	D	450	TYR	3.0
1	D	347	ILE	3.0
1	D	415	LEU	3.0
1	D	408	ASN	3.0
1	F	247	CYS	3.0
1	D	444	THR	3.0
1	D	455	SER	2.9
1	C	42	PHE	2.9
1	B	69	GLU	2.9
1	E	358	LYS	2.9
1	D	446	ILE	2.9
1	D	276	SER	2.8
1	B	469	THR	2.8
1	D	491	VAL	2.8
1	A	493	VAL	2.8
1	D	486	GLN	2.8
1	D	462	ILE	2.8
1	F	492	LEU	2.8
1	D	402	GLY	2.8
1	D	472	GLY	2.8
1	D	382	VAL	2.7
1	E	493	VAL	2.7
1	D	474	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	353	ASP	2.7
1	D	354	THR	2.7
1	D	454	SER	2.7
1	D	441	TRP	2.7
1	A	64	TYR	2.7
1	D	452	LYS	2.7
1	D	416	ASP	2.7
1	D	236	ARG	2.7
1	D	407	VAL	2.7
1	D	478	TRP	2.7
1	D	395	TYR	2.7
1	A	139	GLN	2.7
1	D	394	TRP	2.6
1	B	150	PRO	2.6
1	D	370	VAL	2.6
1	E	331	GLU	2.6
1	D	430	GLN	2.6
1	F	331	GLU	2.6
1	D	352	PRO	2.5
1	D	88	LEU	2.5
1	D	481	ALA	2.5
1	D	411	SER	2.5
1	F	359	LEU	2.5
1	D	383	GLN	2.5
1	D	434	ASN	2.5
1	B	448	ASP	2.5
1	D	405	LYS	2.5
1	D	422	LYS	2.5
1	B	148	LYS	2.5
1	D	463	ASP	2.4
1	D	381	ILE	2.4
1	D	400	GLY	2.4
1	B	220	ALA	2.4
1	F	448	ASP	2.4
1	D	365	GLY	2.4
1	D	239	TYR	2.4
1	D	451	TYR	2.4
1	D	428	LEU	2.4
1	A	229	GLU	2.4
1	D	468	SER	2.4
1	D	379	ALA	2.4
1	D	95	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	274	GLY	2.4
1	D	399	VAL	2.4
1	D	324	PHE	2.4
1	D	437	TYR	2.4
1	C	108	HIS	2.4
1	A	80	VAL	2.3
1	D	338	VAL	2.3
1	B	128	TRP	2.3
1	B	67	TYR	2.3
1	F	354	THR	2.3
1	B	339	LYS	2.3
1	D	442	LYS	2.3
1	D	389	SER	2.3
1	A	108	HIS	2.3
1	B	491	VAL	2.3
1	D	480	ASP	2.3
1	D	164	GLN	2.3
1	E	390	LEU	2.3
1	D	85	SER	2.3
1	D	421	SER	2.3
1	F	137	TYR	2.3
1	A	172	GLY	2.3
1	D	401	GLY	2.3
1	A	331	GLU	2.3
1	B	78	LEU	2.3
1	D	448	ASP	2.3
1	B	108	HIS	2.3
1	B	411	SER	2.3
1	D	465	ARG	2.3
1	D	469	THR	2.3
1	B	33	GLU	2.2
1	E	251	ASN	2.2
1	F	394	TRP	2.2
1	A	81	SER	2.2
1	D	75	ASN	2.2
1	D	237	ASN	2.2
1	E	110	ASN	2.2
1	D	475	ILE	2.2
1	D	386	ASP	2.2
1	D	367	VAL	2.2
1	C	70	TYR	2.2
1	A	93	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	175	GLY	2.2
1	D	431	TYR	2.2
1	B	153	LYS	2.2
1	B	492	LEU	2.2
1	D	359	LEU	2.2
1	D	368	LEU	2.2
1	F	313	ASN	2.2
1	A	416	ASP	2.2
1	D	97	VAL	2.2
1	D	295	THR	2.2
1	D	436	GLY	2.2
1	C	137	TYR	2.2
1	B	331	GLU	2.2
1	D	264	ALA	2.2
1	C	-18	GLY	2.1
1	B	65	TYR	2.1
1	D	403	TYR	2.1
1	D	414	ALA	2.1
1	D	36	ILE	2.1
1	D	50	ILE	2.1
1	D	429	ILE	2.1
1	E	416	ASP	2.1
1	D	482	GLY	2.1
1	F	490	LEU	2.1
1	A	96	GLU	2.1
1	A	157	ILE	2.1
1	C	33	GLU	2.1
1	C	135	ILE	2.1
1	D	346	ILE	2.1
1	D	477	GLN	2.1
1	D	385	THR	2.1
1	F	342	ALA	2.1
1	A	69	GLU	2.1
1	F	406	ILE	2.1
1	A	490	LEU	2.1
1	E	490	LEU	2.1
1	F	229	GLU	2.1
1	B	299	TYR	2.1
1	D	57	MET	2.0
1	D	417	VAL	2.0
1	D	435	GLY	2.0
1	D	325	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	445	ASP	2.0
1	B	412	GLY	2.0
1	D	225	GLY	2.0
1	B	36	ILE	2.0
1	D	351	ILE	2.0
1	F	358	LYS	2.0
1	B	35	VAL	2.0

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](#)

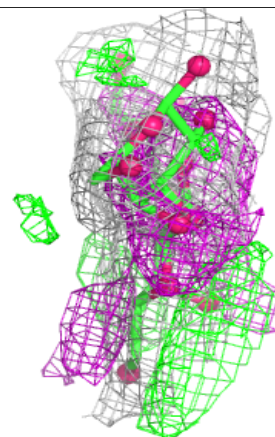
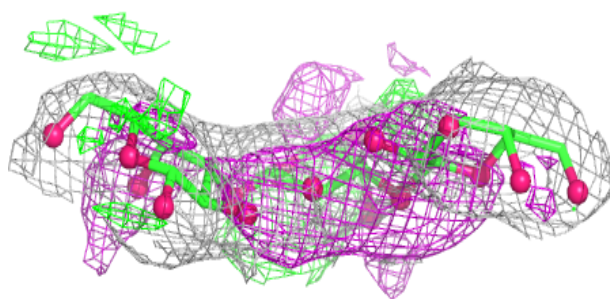
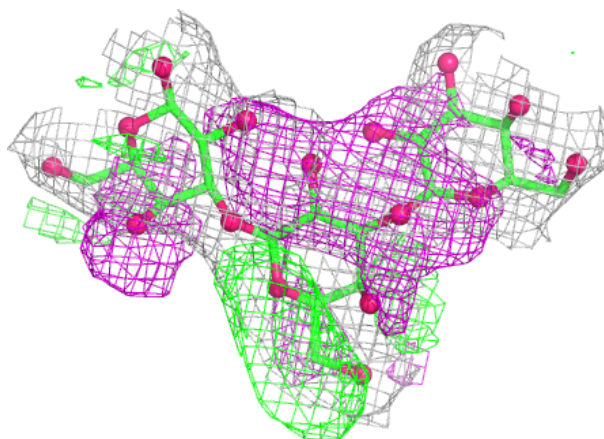
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GAL	G	2	11/12	0.46	0.24	44,49,58,64	0
2	GAL	K	2	11/12	0.53	0.21	45,50,55,61	0
2	GAL	H	3	11/12	0.55	0.16	50,56,60,63	0
2	GAL	I	2	11/12	0.56	0.21	44,47,54,68	0
2	GAL	H	2	11/12	0.56	0.19	48,54,61,62	0
2	GAL	J	2	11/12	0.63	0.17	49,56,58,58	0
2	GAL	K	3	11/12	0.64	0.15	48,55,59,62	0
2	GAL	K	1	12/12	0.66	0.17	50,54,62,66	0
2	GAL	J	3	11/12	0.68	0.14	48,56,64,64	0
2	GAL	I	3	11/12	0.69	0.16	43,55,61,61	0
3	GAL	L	2	11/12	0.69	0.16	20,20,20,20	0
2	GAL	J	1	12/12	0.71	0.15	51,54,60,62	0
2	GAL	G	3	11/12	0.72	0.14	45,55,60,62	0
3	GAL	L	1	12/12	0.72	0.16	20,20,20,20	0
2	GAL	G	1	12/12	0.72	0.16	46,50,57,58	0
2	GAL	I	1	12/12	0.74	0.15	43,50,56,59	0
2	GAL	H	1	12/12	0.75	0.14	53,56,61,63	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.

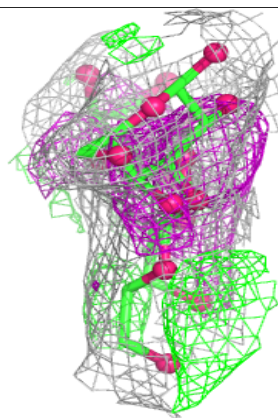
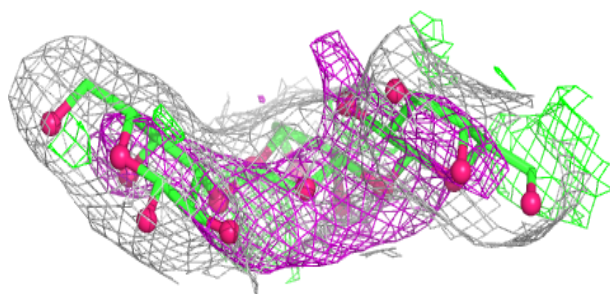
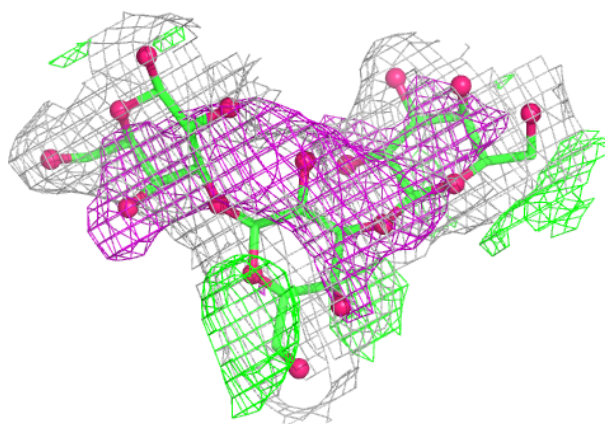
Electron density around Chain G:

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

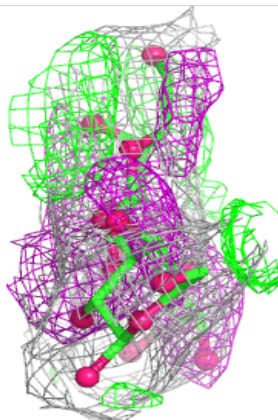
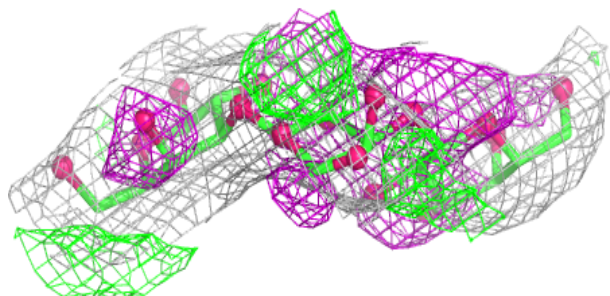
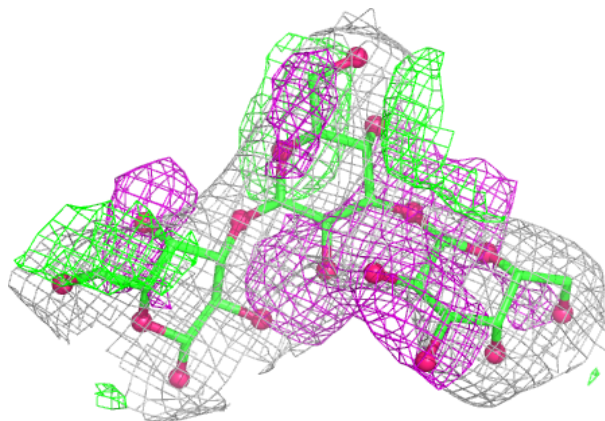


Electron density around Chain H:

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

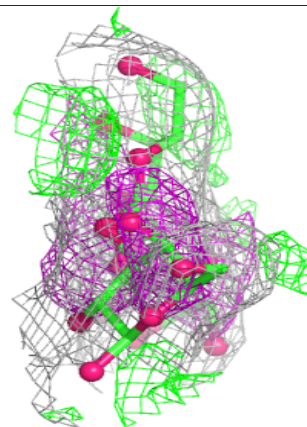
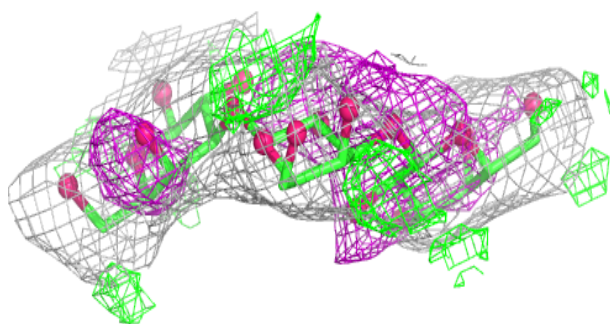
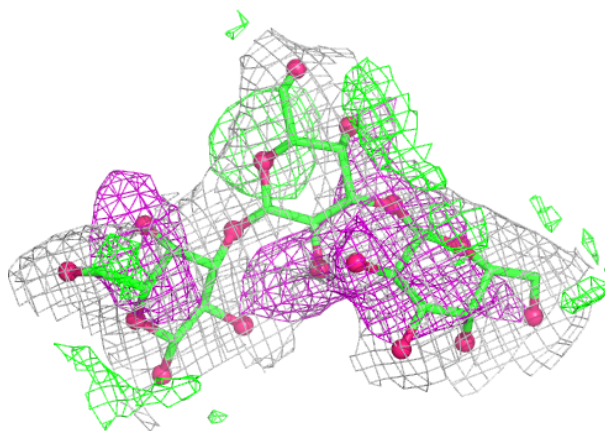
**Electron density around Chain I:**

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

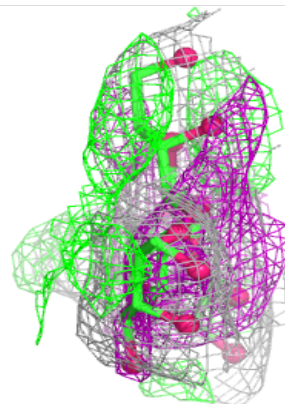
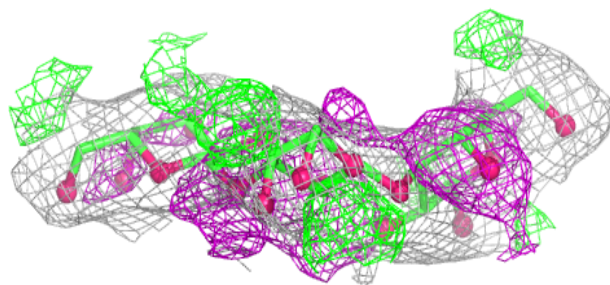
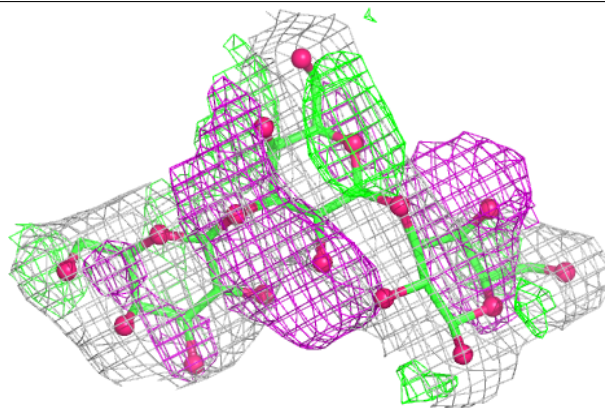


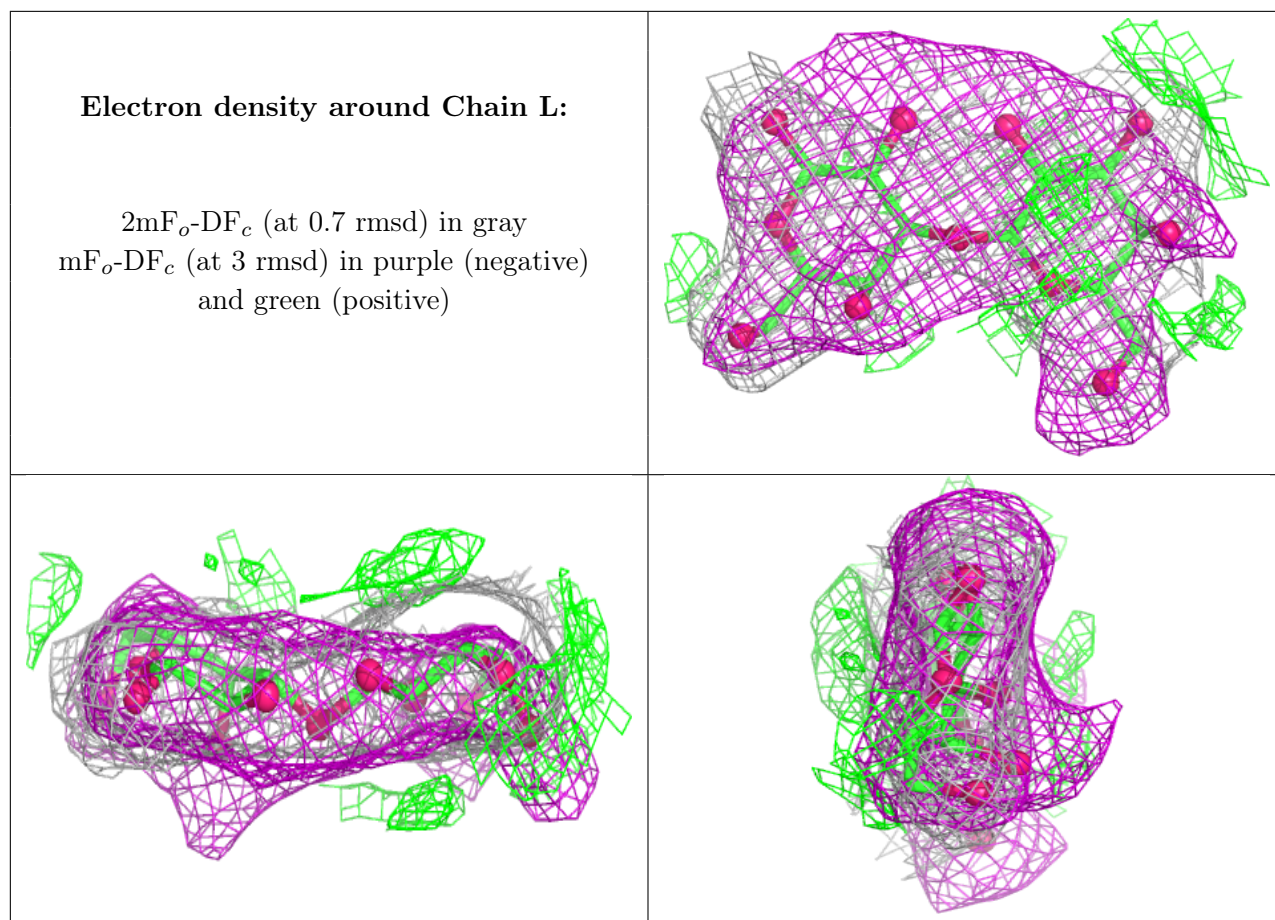
Electron density around Chain J:

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

**Electron density around Chain 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	GOL	C	602	6/6	0.82	0.21	53,65,77,77	0
4	GOL	F	602	6/6	0.83	0.16	78,81,87,89	0
4	GOL	C	603	6/6	0.84	0.33	56,73,83,86	0
4	GOL	F	601	6/6	0.87	0.19	68,71,72,72	0
4	GOL	A	601	6/6	0.87	0.22	54,54,56,56	0
4	GOL	D	601	6/6	0.88	0.19	83,87,91,93	0
4	GOL	C	601	6/6	0.90	0.16	55,58,62,65	0
4	GOL	B	601	6/6	0.91	0.15	66,81,87,91	0
4	GOL	B	602	6/6	0.92	0.17	66,71,75,76	0
4	GOL	E	601	6/6	0.93	0.13	66,69,70,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.