



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:06 PM UTC

PDB ID : 3VT0 / pdb_00003vt0
Title : Crystal structure of Ct1,3Gal43A in complex with lactose
Authors : Jiang, D.; Fan, J.; Wang, X.; Zhao, Y.; Huang, B.; Zhang, X.C.
Deposited on : 2012-05-18
Resolution : 2.91 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

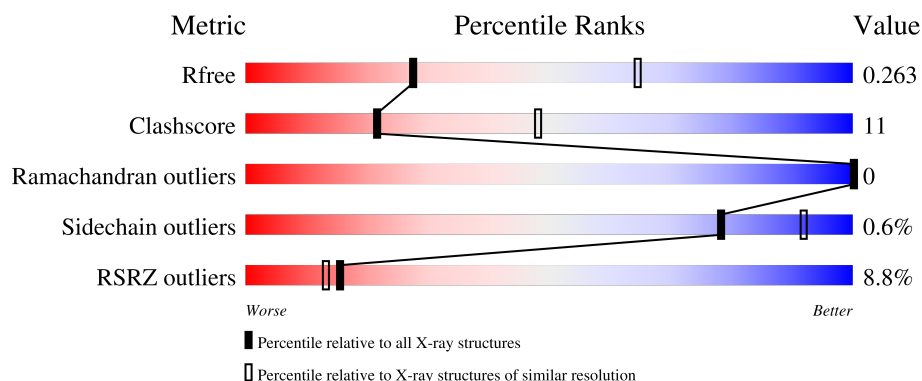
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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.



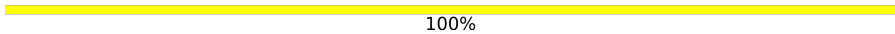
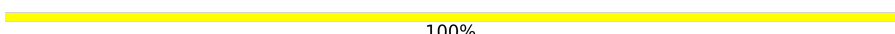
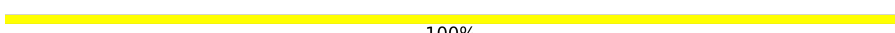
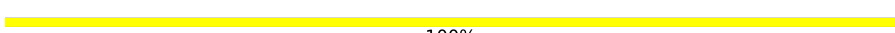
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	5% 67% 21% 12%
1	B	526	10% 67% 20% 12%
1	C	526	2% 74% 18% 8%
1	D	526	23% 58% 29% 12%
1	E	526	3% 71% 17% 12%

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Mol	Chain	Length	Quality of chain
1	F	526	 4% 70% 18% 12%
2	G	2	 100%
2	H	2	 50% 50%
2	I	2	 50% 50%
2	J	2	 100%
2	K	2	 100%
2	L	2	 100%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22283 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
1	A	461	Total	C	N	O	S	0	0	0
			3664	2323	623	703	15			
1	B	461	Total	C	N	O	S	0	0	0
			3664	2323	623	703	15			
1	C	482	Total	C	N	O	S	0	0	0
			3807	2406	651	732	18			
1	D	461	Total	C	N	O	S	0	0	0
			3664	2323	623	703	15			
1	E	461	Total	C	N	O	S	0	0	0
			3664	2323	623	703	15			
1	F	461	Total	C	N	O	S	0	0	0
			3664	2323	623	703	15			

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-(1-4)-beta-D-glucopyranose.



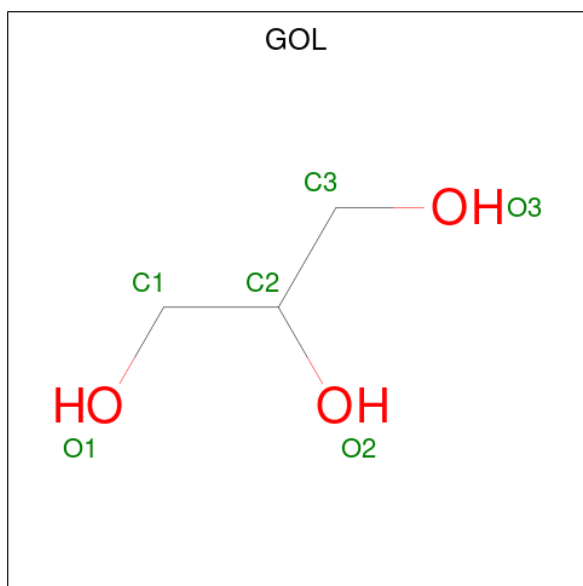
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	G	2	Total	C	O	0	0	0
			23	12	11			

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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

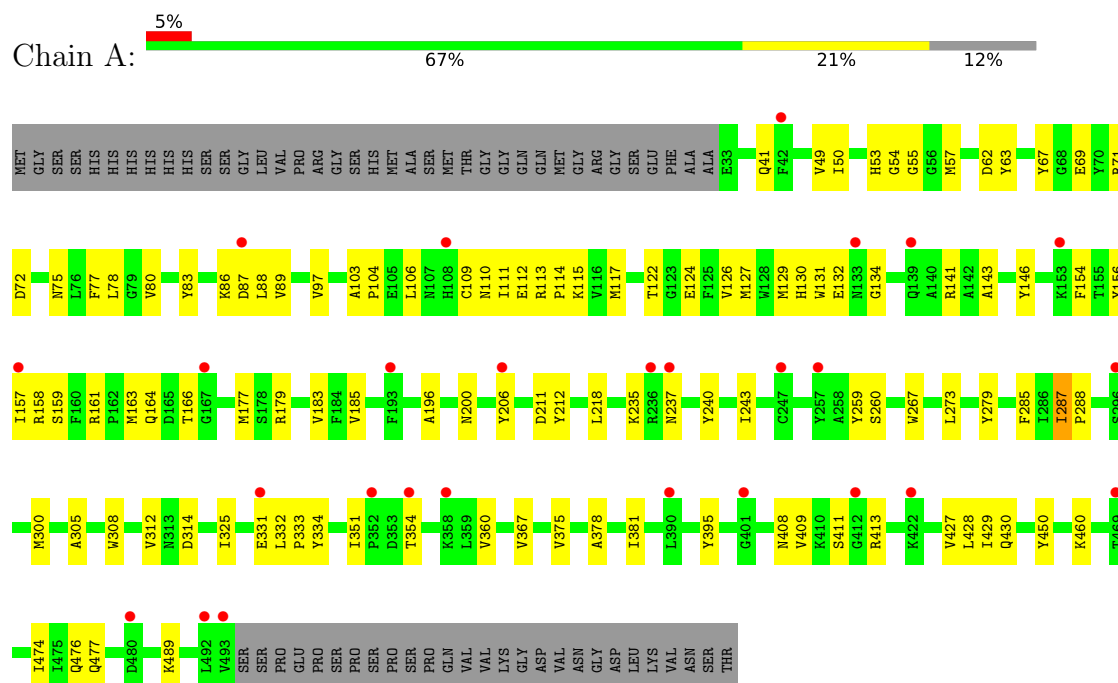


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		

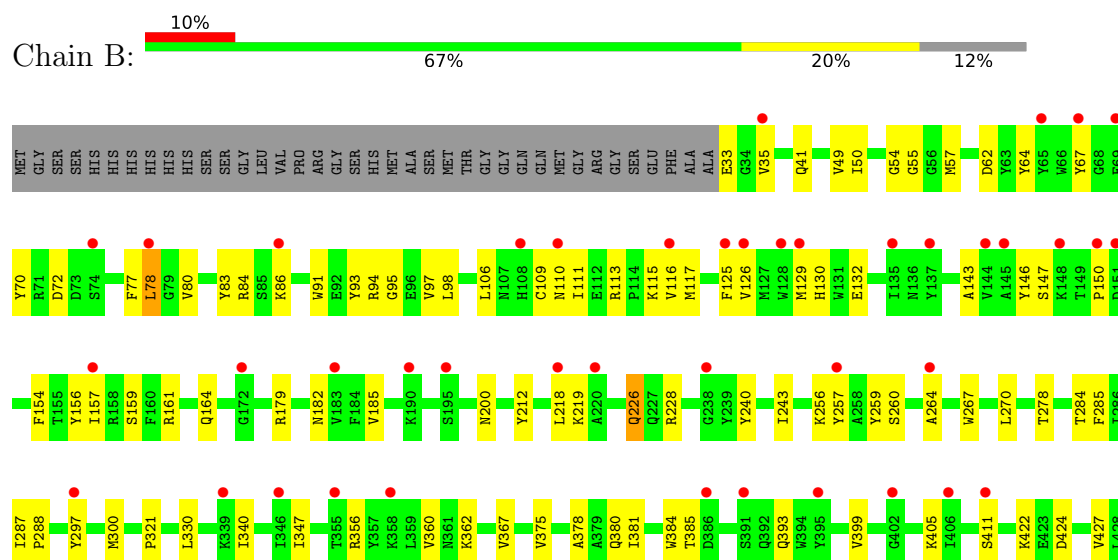
3 Residue-property plots [i](#)

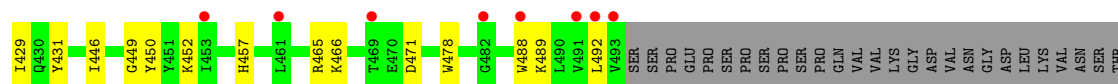
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Ricin B lectin

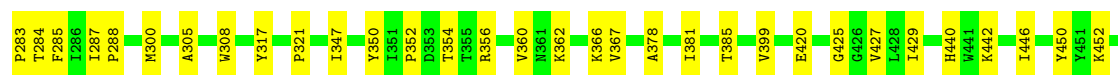
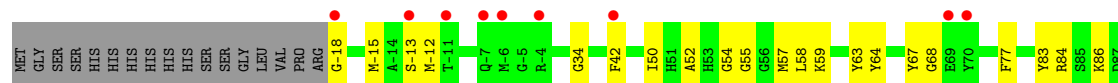
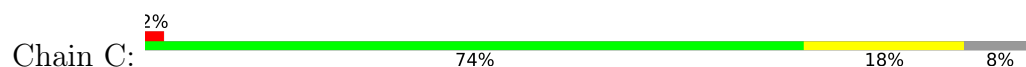


• Molecule 1: Ricin B lectin

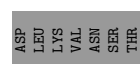
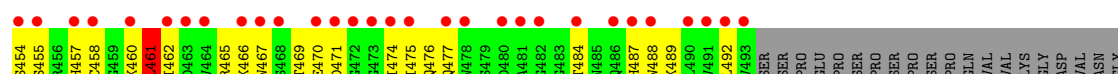
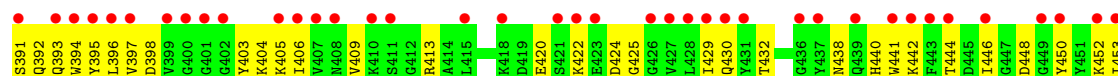
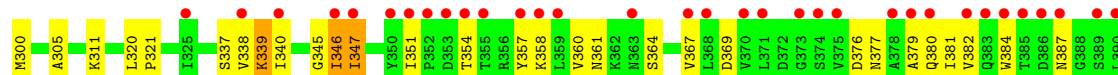
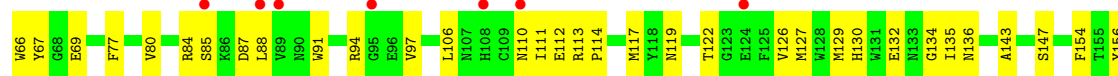
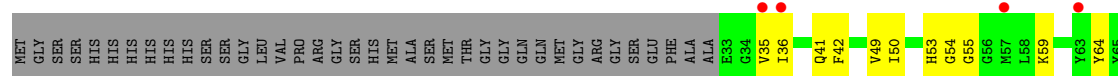




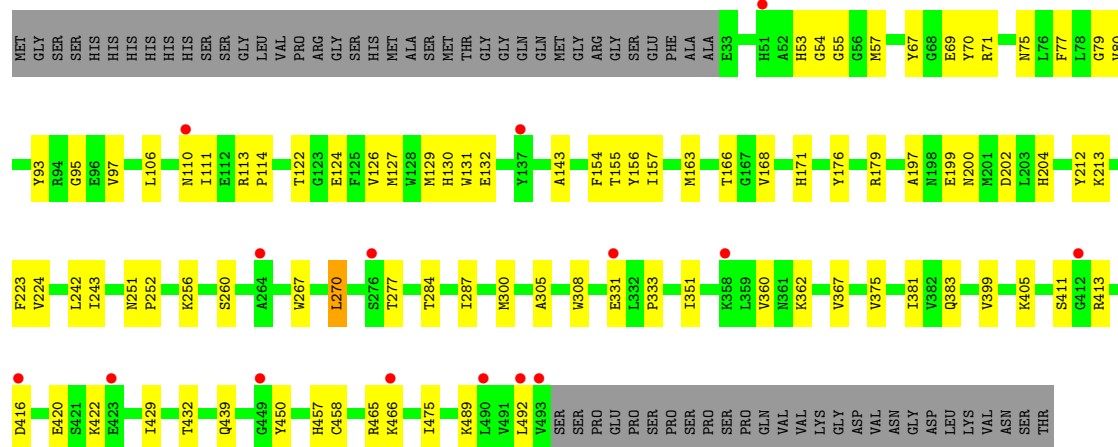
● Molecule 1: Ricin B lectin



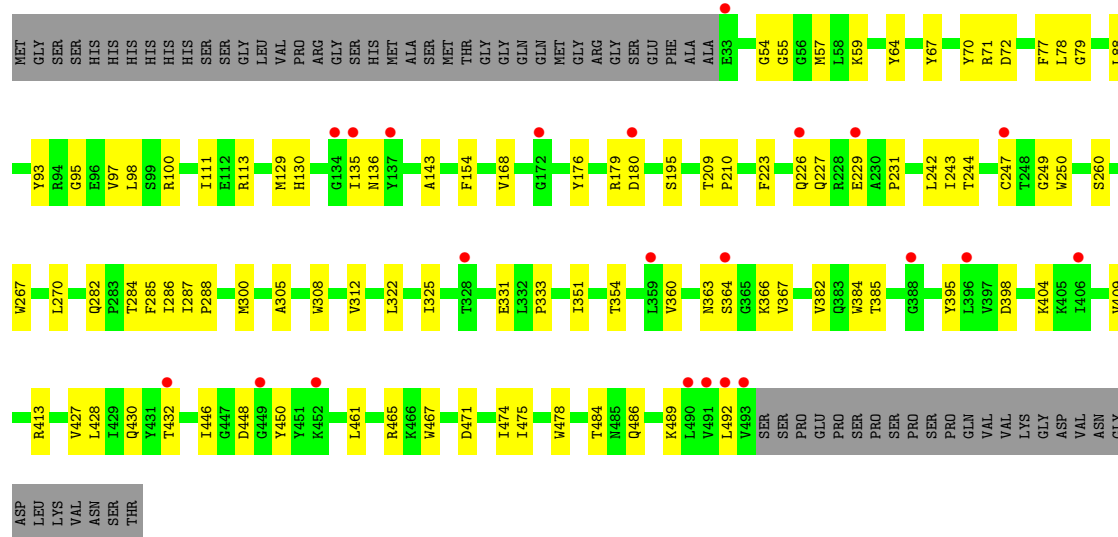
● Molecule 1: Ricin B lectin



● Molecule 1: Ricin B lectin



• Molecule 1: Ricin B lectin



• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose



BGC1
GAL2

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose



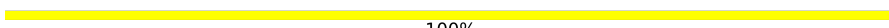
BGC1
GAL2

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain I:  50% 50%

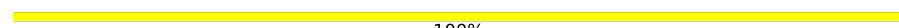
BGC1
GAL2

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain J:  100%

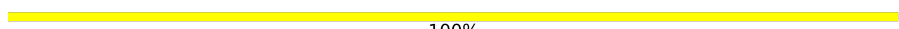
BGC1
GAL2

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain K:  100%

BGC1
GAL2

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain L:  100%

BGC1
GAL2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.69Å 122.38Å 404.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.29 – 2.91 49.29 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.29-2.91) 99.5 (49.29-2.91)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.7_650	Depositor
R, R_{free}	0.253 , 0.269 0.245 , 0.263	Depositor DCC
R_{free} test set	2116 reflections (1.81%)	wwPDB-VP
Wilson B-factor (Å ²)	63.0	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	22283	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, BGC, GAL

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	0.23	0/3762	0.66	0/5104
1	B	0.24	0/3762	0.64	0/5104
1	C	0.24	0/3907	0.65	0/5295
1	D	0.24	0/3762	0.67	1/5104 (0.0%)
1	E	0.23	0/3762	0.66	0/5104
1	F	0.24	0/3762	0.65	0/5104
All	All	0.24	0/22717	0.65	1/30815 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	461	LEU	N-CA-C	6.96	120.00	109.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3664	0	3480	78	0
1	B	3664	0	3480	79	0
1	C	3807	0	3613	62	0
1	D	3664	0	3480	124	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3664	0	3480	58	0
1	F	3664	0	3480	71	0
2	G	23	0	20	0	0
2	H	23	0	20	1	0
2	I	23	0	20	1	0
2	J	23	0	20	0	0
2	K	23	0	21	6	0
2	L	23	0	21	1	0
3	A	6	0	8	0	0
3	C	6	0	8	0	0
3	F	6	0	8	2	0
All	All	22283	0	21159	470	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 11.

All (470) 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:57:MET:HE2	1:C:287:ILE:HG21	1.52	0.91
1:C:34:GLY:HA2	1:C:89:VAL:HG21	1.53	0.89
1:F:57:MET:HE2	1:F:287:ILE:HG21	1.54	0.89
1:B:84:ARG:HE	1:B:94:ARG:HE	1.22	0.88
1:D:321:PRO:HB3	1:D:347:ILE:HD13	1.58	0.85
1:D:422:LYS:HG3	1:D:458:CYS:HB3	1.58	0.84
1:E:422:LYS:HD3	1:E:458:CYS:HB3	1.59	0.84
1:C:-12:MET:HG3	1:E:155:THR:HG22	1.61	0.83
1:D:465:ARG:HG2	1:D:466:LYS:HG2	1.61	0.82
1:D:254:GLN:HG2	1:D:276:SER:HA	1.61	0.81
1:D:340:ILE:HG22	1:D:347:ILE:HG22	1.61	0.81
1:B:360:VAL:HG22	1:B:367:VAL:HG12	1.68	0.75
1:F:461:LEU:HD11	1:F:486:GLN:HB3	1.68	0.75
1:C:465:ARG:HH21	1:C:474:ILE:HG21	1.53	0.74
1:C:360:VAL:HG22	1:C:367:VAL:HG12	1.69	0.74
1:E:416:ASP:HB3	1:E:439:GLN:HG2	1.69	0.73
1:D:163:MET:HE3	1:D:166:THR:HG21	1.69	0.73
1:F:360:VAL:HG22	1:F:367:VAL:HG12	1.71	0.72
1:C:260:SER:HB2	1:C:267:TRP:HA	1.72	0.72
1:A:285:PHE:CE2	1:A:287:ILE:HG23	2.25	0.71
1:E:80:VAL:HG21	1:E:127:MET:HE1	1.73	0.71
1:A:110:ASN:HB2	1:A:132:GLU:HB2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:PHE:HE2	1:A:287:ILE:HG23	1.57	0.70
1:D:380:GLN:HA	1:D:429:ILE:HG22	1.73	0.70
1:B:219:LYS:HE3	1:B:264:ALA:HB2	1.72	0.70
1:E:54:GLY:O	1:E:113:ARG:HA	1.92	0.70
1:A:72:ASP:HB3	1:A:78:LEU:HD12	1.75	0.69
1:A:360:VAL:HG22	1:A:367:VAL:HG12	1.73	0.69
1:D:110:ASN:HB2	1:D:132:GLU:HB2	1.74	0.69
1:D:387:ASN:H	1:D:392:GLN:HE22	1.40	0.69
1:D:455:SER:N	1:D:461:LEU:HD11	2.08	0.69
1:E:360:VAL:HG22	1:E:367:VAL:HG12	1.76	0.68
1:D:453:ILE:O	1:D:461:LEU:HG	1.94	0.67
1:D:454:SER:HA	1:D:461:LEU:HD21	1.77	0.67
1:B:356:ARG:HD3	1:B:393:GLN:NE2	2.10	0.67
1:D:484:THR:HA	1:D:487:HIS:CD2	2.30	0.66
1:A:287:ILE:HD11	1:A:300:MET:HE3	1.78	0.66
1:A:157:ILE:HG22	1:A:158:ARG:HG2	1.78	0.66
1:D:377:ASN:HD21	1:D:432:THR:HG23	1.61	0.66
1:F:428:LEU:HD12	1:F:475:ILE:HG22	1.78	0.65
1:C:129:MET:HG2	1:C:143:ALA:HB3	1.79	0.65
1:B:179:ARG:HG3	1:B:200:ASN:OD1	1.97	0.65
1:A:260:SER:HB2	1:A:267:TRP:HA	1.78	0.65
1:D:450:TYR:CE2	1:D:489:LYS:HE3	2.32	0.65
1:F:260:SER:HB2	1:F:267:TRP:HA	1.79	0.65
1:C:98:LEU:HD22	1:C:127:MET:HE1	1.78	0.65
1:C:-18:GLY:HA3	1:C:-15:MET:HE2	1.78	0.64
1:D:381:ILE:HG12	1:D:429:ILE:HA	1.79	0.64
1:D:69:GLU:OE1	1:D:112:GLU:HA	1.98	0.64
1:D:420:GLU:HG2	1:D:438:ASN:ND2	2.12	0.64
1:E:77:PHE:CD1	1:E:111:ILE:HB	2.33	0.64
1:C:54:GLY:O	1:C:113:ARG:HA	1.98	0.64
1:A:331:GLU:HG2	1:A:333:PRO:HD3	1.79	0.63
1:E:416:ASP:CB	1:E:439:GLN:HG2	2.29	0.63
1:E:420:GLU:HB3	1:E:457:HIS:CE1	2.34	0.63
1:D:42:PHE:HB2	1:D:50:ILE:HD11	1.80	0.62
1:E:53:HIS:O	1:E:69:GLU:HG2	2.00	0.62
1:F:77:PHE:CD1	1:F:111:ILE:HB	2.34	0.62
1:D:35:VAL:HG22	1:D:339:LYS:HA	1.80	0.62
1:D:53:HIS:O	1:D:69:GLU:HG2	1.99	0.62
1:F:98:LEU:HD23	1:F:129:MET:HE1	1.81	0.61
1:F:54:GLY:O	1:F:113:ARG:HA	1.99	0.61
1:F:250:TRP:CZ3	2:K:2:GAL:H61	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:SER:HB2	1:D:267:TRP:HA	1.83	0.61
1:B:54:GLY:O	1:B:113:ARG:HA	2.01	0.60
1:D:360:VAL:HA	1:D:367:VAL:HA	1.82	0.60
1:A:77:PHE:CE2	1:A:111:ILE:HD12	2.37	0.60
1:E:171:HIS:CE1	1:E:199:GLU:HB2	2.36	0.60
1:A:97:VAL:HB	1:A:154:PHE:CD2	2.37	0.60
1:D:347:ILE:HD12	1:D:347:ILE:O	2.01	0.60
1:E:111:ILE:HD11	1:E:131:TRP:HD1	1.67	0.59
1:E:260:SER:HB2	1:E:267:TRP:HA	1.84	0.59
1:D:380:GLN:NE2	1:D:474:ILE:HG13	2.17	0.59
1:B:84:ARG:NE	1:B:94:ARG:HE	1.95	0.59
1:B:161:ARG:O	1:B:164:GLN:HG3	2.02	0.59
1:C:450:TYR:CE1	1:C:489:LYS:HB2	2.38	0.59
1:E:252:PRO:HB2	1:E:277:THR:HG23	1.85	0.59
1:D:450:TYR:CD1	1:D:489:LYS:HG3	2.37	0.59
1:B:340:ILE:HG22	1:B:347:ILE:HG23	1.83	0.59
1:D:106:LEU:HD22	1:D:111:ILE:HD11	1.84	0.59
1:B:70:TYR:CZ	1:B:78:LEU:HD11	2.38	0.59
1:D:442:LYS:HB3	1:D:454:SER:OG	2.03	0.58
1:D:360:VAL:HG12	1:D:489:LYS:HB2	1.85	0.58
1:E:110:ASN:HB2	1:E:132:GLU:HB2	1.85	0.58
1:F:111:ILE:HG12	1:F:129:MET:HE2	1.85	0.58
1:D:361:ASN:HB3	1:D:364:SER:OG	2.03	0.58
1:E:129:MET:HG2	1:E:143:ALA:HB3	1.86	0.58
1:F:168:VAL:HG11	1:F:176:TYR:CE1	2.39	0.58
1:B:117:MET:HE3	1:B:185:VAL:HG22	1.87	0.57
1:D:360:VAL:CG1	1:D:489:LYS:HB2	2.34	0.57
1:F:285:PHE:HB3	1:F:300:MET:HE3	1.85	0.57
1:C:84:ARG:HH21	1:C:94:ARG:NH1	2.02	0.57
1:B:72:ASP:HB3	1:B:78:LEU:HB3	1.85	0.57
1:B:97:VAL:HB	1:B:154:PHE:CD2	2.40	0.57
1:E:97:VAL:HB	1:E:154:PHE:CD2	2.40	0.56
1:E:422:LYS:HE2	1:E:457:HIS:CD2	2.40	0.56
1:B:106:LEU:HD22	1:B:111:ILE:HD11	1.87	0.56
1:D:454:SER:C	1:D:461:LEU:HD11	2.30	0.56
1:D:97:VAL:HB	1:D:154:PHE:CD2	2.40	0.56
1:D:420:GLU:HB3	1:D:457:HIS:CE1	2.41	0.56
1:B:431:TYR:CE1	2:H:2:GAL:H62	2.40	0.56
1:B:110:ASN:HB2	1:B:132:GLU:HB2	1.88	0.56
1:F:71:ARG:HD3	1:F:312:VAL:HG11	1.87	0.56
1:F:223:PHE:HE2	1:F:242:LEU:HD23	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:223:PHE:HB3	1:F:226:GLN:HG3	1.88	0.55
1:A:103:ALA:HB3	1:A:106:LEU:HG	1.88	0.55
1:A:279:TYR:CD2	1:A:334:TYR:HB2	2.41	0.55
1:D:80:VAL:HG21	1:D:127:MET:HE1	1.89	0.55
1:F:249:GLY:H	2:K:1:BGC:C6	2.20	0.55
1:F:478:TRP:CZ3	3:F:601:GOL:H31	2.42	0.55
1:C:97:VAL:HB	1:C:154:PHE:CD2	2.41	0.55
1:B:41:GLN:HB3	1:B:49:VAL:HG23	1.88	0.55
1:A:54:GLY:O	1:A:113:ARG:HA	2.05	0.55
1:D:380:GLN:HE22	1:D:474:ILE:HG13	1.71	0.55
1:B:129:MET:HG2	1:B:143:ALA:HB3	1.89	0.55
1:F:366:LYS:HE3	1:F:385:THR:HG22	1.89	0.55
1:B:156:TYR:OH	1:B:159:SER:HB3	2.07	0.55
1:D:424:ASP:OD2	1:D:460:LYS:HD3	2.06	0.55
1:A:69:GLU:HG2	1:A:112:GLU:HA	1.88	0.54
1:F:227:GLN:HG2	1:F:247:CYS:SG	2.47	0.54
1:A:117:MET:HE3	1:A:185:VAL:HG22	1.89	0.54
1:D:256:LYS:HD3	1:D:270:LEU:HB3	1.89	0.54
1:C:163:MET:HE3	1:C:166:THR:HG21	1.89	0.54
1:D:441:TRP:HA	1:D:454:SER:O	2.07	0.54
1:B:55:GLY:HA3	1:B:67:TYR:O	2.08	0.54
1:D:453:ILE:HG23	1:D:461:LEU:HD12	1.89	0.54
1:A:63:TYR:CE1	1:A:86:LYS:HE3	2.43	0.54
1:E:163:MET:HE3	1:E:166:THR:HG21	1.89	0.53
1:F:398:ASP:HA	1:F:404:LYS:HG2	1.91	0.53
1:A:114:PRO:HB2	1:A:127:MET:HE3	1.91	0.53
1:B:77:PHE:CE1	1:B:80:VAL:HG23	2.43	0.53
1:B:126:VAL:HG21	1:B:212:TYR:HB2	1.90	0.53
1:E:80:VAL:HG21	1:E:127:MET:CE	2.38	0.53
1:F:250:TRP:CH2	2:K:2:GAL:H61	2.44	0.53
1:F:465:ARG:HH21	1:F:474:ILE:HG21	1.74	0.53
1:B:378:ALA:HA	1:B:429:ILE:HD12	1.91	0.53
1:C:77:PHE:CD1	1:C:111:ILE:HB	2.44	0.53
1:C:63:TYR:CE1	1:C:86:LYS:HE3	2.44	0.53
1:A:325:ILE:HD11	1:A:331:GLU:OE2	2.10	0.52
1:B:57:MET:HE3	1:B:287:ILE:HG21	1.91	0.52
1:D:41:GLN:HB3	1:D:49:VAL:HG13	1.90	0.52
1:B:78:LEU:C	1:B:78:LEU:HD12	2.35	0.52
1:B:446:ILE:HD13	1:B:452:LYS:HG3	1.90	0.52
1:C:84:ARG:HE	1:C:94:ARG:NE	2.06	0.52
1:E:179:ARG:HG3	1:E:200:ASN:OD1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:93:TYR:CZ	1:F:95:GLY:HA2	2.44	0.52
1:A:63:TYR:CZ	1:A:86:LYS:HE3	2.44	0.52
1:B:226:GLN:HB3	1:B:228:ARG:HG2	1.90	0.52
1:D:54:GLY:O	1:D:113:ARG:HA	2.09	0.52
1:E:168:VAL:HG11	1:E:176:TYR:CE1	2.44	0.52
1:D:376:ASP:C	1:D:413:ARG:HH12	2.17	0.52
1:F:450:TYR:CE1	1:F:489:LYS:HB2	2.45	0.52
1:B:97:VAL:HB	1:B:154:PHE:HD2	1.74	0.52
1:B:362:LYS:HE2	1:B:450:TYR:CZ	2.45	0.52
1:D:476:GLN:HG2	1:D:477:GLN:H	1.75	0.52
1:B:260:SER:HB2	1:B:267:TRP:HA	1.92	0.52
1:E:223:PHE:HE2	1:E:242:LEU:HD23	1.74	0.51
1:D:157:ILE:HG22	1:D:158:ARG:HG2	1.91	0.51
1:A:129:MET:HG2	1:A:143:ALA:HB3	1.91	0.51
1:C:-13:SER:HA	1:C:492:LEU:HD11	1.92	0.51
1:B:422:LYS:HE3	1:B:457:HIS:NE2	2.26	0.51
1:C:223:PHE:HE2	1:C:242:LEU:HD23	1.76	0.51
1:A:378:ALA:HA	1:A:429:ILE:HD12	1.93	0.51
1:D:299:TYR:HB3	1:D:320:LEU:O	2.11	0.51
1:A:237:ASN:OD1	1:F:448:ASP:HA	2.10	0.51
1:B:72:ASP:HA	1:B:78:LEU:HD23	1.92	0.51
1:C:179:ARG:HG3	1:C:200:ASN:OD1	2.11	0.51
1:A:106:LEU:HD11	1:A:156:TYR:CD2	2.45	0.50
1:C:55:GLY:HA3	1:C:67:TYR:O	2.12	0.50
1:E:157:ILE:HD11	1:E:213:LYS:HD2	1.93	0.50
1:F:478:TRP:CD2	3:F:601:GOL:H11	2.47	0.50
1:A:126:VAL:HG21	1:A:212:TYR:HB2	1.92	0.50
1:B:288:PRO:HG3	1:B:297:TYR:CE1	2.45	0.50
1:F:249:GLY:H	2:K:1:BGC:H6C2	1.76	0.50
1:D:84:ARG:HG2	1:D:94:ARG:HD3	1.93	0.50
1:E:277:THR:HG22	1:E:277:THR:O	2.12	0.50
1:D:55:GLY:HA3	1:D:67:TYR:O	2.11	0.50
1:D:245:SER:HB3	1:D:283:PRO:HD2	1.93	0.50
1:F:59:LYS:HD3	1:F:64:TYR:CE1	2.47	0.50
1:F:135:ILE:HG22	1:F:136:ASN:HD22	1.76	0.50
1:D:382:VAL:HG21	1:D:384:TRP:HE1	1.77	0.50
1:E:420:GLU:HB3	1:E:457:HIS:HE1	1.77	0.50
1:B:77:PHE:HE1	1:B:80:VAL:HG23	1.76	0.49
1:C:442:LYS:HG3	1:F:100:ARG:NH1	2.27	0.49
1:B:67:TYR:CE2	1:B:116:VAL:HG21	2.47	0.49
1:B:380:GLN:HE22	1:B:427:VAL:HG13	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:GLY:HA3	1:E:67:TYR:O	2.12	0.49
1:E:381:ILE:HG12	1:E:429:ILE:HA	1.93	0.49
1:D:285:PHE:HB3	1:D:300:MET:HE3	1.94	0.49
1:D:381:ILE:HG22	1:D:475:ILE:HG13	1.94	0.49
1:B:218:LEU:O	1:B:218:LEU:HD12	2.12	0.49
1:D:358:LYS:HG2	1:D:392:GLN:O	2.12	0.49
1:F:325:ILE:HD11	1:F:331:GLU:OE1	2.11	0.49
1:D:377:ASN:ND2	1:D:432:THR:HG23	2.28	0.49
1:D:450:TYR:HA	1:D:489:LYS:HA	1.95	0.49
1:D:460:LYS:O	1:D:461:LEU:HD13	2.13	0.49
1:C:106:LEU:HD22	1:C:111:ILE:HD11	1.95	0.49
1:D:236:ARG:HA	1:D:297:TYR:OH	2.13	0.49
1:D:382:VAL:HA	1:D:475:ILE:HG12	1.95	0.49
1:F:135:ILE:HD12	1:F:135:ILE:N	2.28	0.49
1:C:98:LEU:HD22	1:C:127:MET:CE	2.42	0.48
1:C:362:LYS:HE3	1:C:484:THR:HG22	1.94	0.48
1:E:70:TYR:HB3	1:E:79:GLY:O	2.12	0.48
1:D:462:ILE:HA	1:D:476:GLN:O	2.13	0.48
1:F:325:ILE:H	1:F:325:ILE:HD12	1.79	0.48
1:D:77:PHE:CD1	1:D:111:ILE:HB	2.48	0.48
1:D:425:GLY:HA2	1:D:476:GLN:CD	2.39	0.48
1:E:383:GLN:O	1:E:383:GLN:HG3	2.12	0.48
1:A:146:TYR:CD2	1:A:157:ILE:HD11	2.49	0.48
1:F:305:ALA:HA	1:F:308:TRP:CZ2	2.48	0.48
1:A:50:ILE:HG23	1:A:83:TYR:CE1	2.49	0.48
1:B:321:PRO:HB3	1:B:347:ILE:HG22	1.95	0.48
1:E:93:TYR:CZ	1:E:95:GLY:HA2	2.49	0.48
1:A:57:MET:CB	1:A:300:MET:HE1	2.45	0.47
1:B:50:ILE:HG23	1:B:83:TYR:CE1	2.50	0.47
1:F:430:GLN:O	1:F:430:GLN:HG3	2.14	0.47
1:A:395:TYR:CE2	1:A:409:VAL:HG22	2.49	0.47
1:D:126:VAL:HG21	1:D:212:TYR:HB2	1.95	0.47
1:E:126:VAL:HG21	1:E:212:TYR:HB2	1.94	0.47
1:D:398:ASP:HA	1:D:404:LYS:HG2	1.94	0.47
1:F:231:PRO:HA	1:F:244:THR:HG22	1.95	0.47
1:A:161:ARG:O	1:A:164:GLN:HG3	2.14	0.47
1:B:109:CYS:HB2	1:B:132:GLU:O	2.15	0.47
1:C:285:PHE:HE2	1:C:287:ILE:HB	1.80	0.47
1:C:378:ALA:HA	1:C:429:ILE:HD12	1.97	0.47
1:D:454:SER:CA	1:D:461:LEU:HD11	2.45	0.47
1:E:252:PRO:HB2	1:E:277:THR:CG2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:70:TYR:HB3	1:F:79:GLY:O	2.15	0.47
1:B:356:ARG:HD3	1:B:393:GLN:HE22	1.79	0.47
1:D:474:ILE:HD12	1:D:474:ILE:N	2.30	0.47
1:E:284:THR:HG22	1:E:300:MET:O	2.14	0.47
1:E:383:GLN:HB3	1:E:475:ILE:HD11	1.97	0.47
1:D:395:TYR:CE2	1:D:409:VAL:HG22	2.49	0.47
1:F:331:GLU:HG2	1:F:333:PRO:HD3	1.97	0.47
1:C:362:LYS:HB2	1:C:450:TYR:CE1	2.49	0.47
1:D:364:SER:HA	1:D:469:THR:OG1	2.14	0.47
1:D:338:VAL:HG12	1:D:340:ILE:HG23	1.96	0.47
1:D:376:ASP:O	1:D:379:ALA:HB2	2.14	0.46
1:F:285:PHE:HE2	1:F:287:ILE:HB	1.79	0.46
1:F:363:ASN:HB2	1:F:484:THR:OG1	2.15	0.46
1:A:235:LYS:HD2	1:A:240:TYR:CE2	2.50	0.46
1:C:321:PRO:HB3	1:C:347:ILE:HG22	1.95	0.46
1:E:71:ARG:HH11	1:E:75:ASN:ND2	2.13	0.46
1:A:62:ASP:O	1:A:86:LYS:HG2	2.16	0.46
1:C:235:LYS:HD2	1:C:240:TYR:CE2	2.51	0.46
1:D:291:GLY:HA3	1:D:345:GLY:HA3	1.96	0.46
1:D:384:TRP:CZ3	1:D:471:ASP:HB3	2.50	0.46
1:D:444:THR:OG1	1:D:452:LYS:HB2	2.16	0.46
1:E:305:ALA:HA	1:E:308:TRP:CZ2	2.51	0.46
1:B:147:SER:HB2	1:B:154:PHE:HA	1.97	0.46
1:D:296:SER:HB2	1:D:347:ILE:HD11	1.97	0.46
1:A:57:MET:HE3	1:A:300:MET:HE1	1.98	0.46
1:F:55:GLY:HA3	1:F:67:TYR:O	2.16	0.46
1:D:35:VAL:HG11	1:D:337:SER:HB3	1.98	0.46
1:D:129:MET:CG	1:D:143:ALA:HB3	2.46	0.46
1:D:448:ASP:O	1:D:489:LYS:HE2	2.15	0.46
1:F:282:GLN:HE22	2:K:2:GAL:H3	1.81	0.46
1:B:83:TYR:HB3	1:B:91:TRP:HB3	1.98	0.46
1:F:286:ILE:HD13	1:F:322:LEU:HD22	1.97	0.46
1:A:375:VAL:HG12	1:A:411:SER:HB3	1.97	0.45
1:C:58:LEU:HD22	1:C:116:VAL:HG12	1.97	0.45
1:A:41:GLN:HB3	1:A:49:VAL:HG23	1.98	0.45
1:A:122:THR:OG1	1:A:124:GLU:HG2	2.16	0.45
1:A:129:MET:CG	1:A:143:ALA:HB3	2.46	0.45
1:B:130:HIS:CE1	1:B:179:ARG:HD3	2.51	0.45
1:E:362:LYS:HD3	1:E:450:TYR:CZ	2.51	0.45
1:A:57:MET:HB2	1:A:300:MET:HE1	1.97	0.45
1:A:97:VAL:HB	1:A:154:PHE:HD2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:ILE:HD12	1:A:351:ILE:N	2.32	0.45
1:D:147:SER:HB2	1:D:154:PHE:HA	1.98	0.45
1:D:357:TYR:O	1:D:393:GLN:HA	2.17	0.45
1:D:377:ASN:HD21	1:D:432:THR:H	1.65	0.45
1:F:223:PHE:CE2	1:F:242:LEU:HD23	2.51	0.45
1:A:87:ASP:OD1	1:A:89:VAL:HB	2.17	0.45
1:C:77:PHE:CZ	1:C:111:ILE:HD12	2.51	0.45
1:C:366:LYS:HE3	1:C:385:THR:HG22	1.99	0.45
1:D:243:ILE:N	1:D:243:ILE:HD12	2.31	0.45
1:D:360:VAL:O	1:D:488:TRP:HA	2.16	0.45
2:L:1:BGC:O3	2:L:2:GAL:O5	2.34	0.45
1:B:93:TYR:CZ	1:B:95:GLY:HA2	2.52	0.45
1:D:234:ILE:HD11	1:D:241:TYR:HB2	1.98	0.45
1:F:284:THR:HG22	1:F:300:MET:O	2.17	0.45
1:A:55:GLY:HA3	1:A:67:TYR:O	2.16	0.45
1:C:59:LYS:HD3	1:C:64:TYR:CE1	2.52	0.45
1:C:350:TYR:O	1:C:352:PRO:HD3	2.17	0.45
1:D:114:PRO:HB2	1:D:127:MET:HE3	1.98	0.45
1:F:287:ILE:HA	1:F:288:PRO:HD3	1.86	0.45
1:A:474:ILE:HD12	1:A:474:ILE:N	2.32	0.45
1:C:64:TYR:O	1:C:84:ARG:HA	2.17	0.45
1:C:287:ILE:HA	1:C:288:PRO:HD3	1.85	0.45
1:E:351:ILE:N	1:E:351:ILE:HD12	2.31	0.45
1:A:206:TYR:CE1	1:A:218:LEU:HD23	2.53	0.44
1:B:465:ARG:HG2	1:B:466:LYS:HG2	1.99	0.44
1:C:381:ILE:HG12	1:C:429:ILE:HA	1.98	0.44
1:F:395:TYR:CE2	1:F:409:VAL:HG22	2.53	0.44
1:F:351:ILE:HD12	1:F:351:ILE:N	2.32	0.44
1:C:399:VAL:HG21	1:C:440:HIS:NE2	2.33	0.44
1:D:42:PHE:HB2	1:D:50:ILE:CD1	2.47	0.44
1:D:284:THR:HG22	1:D:300:MET:O	2.17	0.44
1:D:454:SER:HA	1:D:461:LEU:CD2	2.45	0.44
1:D:87:ASP:O	1:D:88:LEU:HB2	2.18	0.44
1:A:243:ILE:N	1:A:243:ILE:HD12	2.33	0.44
1:A:381:ILE:HG12	1:A:429:ILE:HA	1.98	0.44
1:D:467:TRP:HH2	1:D:484:THR:OG1	2.00	0.44
1:E:202:ASP:OD1	1:E:224:VAL:HG23	2.16	0.44
1:E:465:ARG:HG2	1:E:466:LYS:HG2	1.99	0.44
1:A:156:TYR:OH	1:A:159:SER:HB3	2.18	0.44
1:C:50:ILE:HG23	1:C:83:TYR:CE1	2.52	0.44
1:B:106:LEU:HD11	1:B:156:TYR:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:385:THR:HG23	1:C:471:ASP:OD1	2.17	0.44
1:E:106:LEU:HD11	1:E:156:TYR:CD2	2.52	0.44
1:C:270:LEU:HD12	1:C:270:LEU:N	2.32	0.44
1:D:85:SER:HB3	1:D:91:TRP:HA	1.98	0.44
1:F:325:ILE:HD12	1:F:325:ILE:N	2.32	0.44
1:A:474:ILE:HD12	1:A:474:ILE:H	1.82	0.44
1:F:64:TYR:CG	1:F:88:LEU:HD21	2.53	0.44
1:D:461:LEU:HD13	1:D:461:LEU:HA	1.55	0.43
1:A:279:TYR:CE2	1:A:334:TYR:HB2	2.53	0.43
1:B:146:TYR:CD2	1:B:157:ILE:HD11	2.53	0.43
1:B:287:ILE:HA	1:B:288:PRO:HD3	1.90	0.43
1:B:381:ILE:HG12	1:B:429:ILE:HA	2.00	0.43
1:D:106:LEU:HD11	1:D:156:TYR:CD2	2.53	0.43
1:D:168:VAL:HG21	1:D:176:TYR:CE1	2.52	0.43
1:D:387:ASN:H	1:D:392:GLN:NE2	2.12	0.43
1:E:492:LEU:HD12	1:E:492:LEU:N	2.33	0.43
1:B:399:VAL:HG11	1:B:405:LYS:HG3	2.01	0.43
1:C:57:MET:HE3	1:C:64:TYR:CD1	2.54	0.43
1:C:354:THR:HG22	1:C:354:THR:O	2.17	0.43
1:D:110:ASN:OD1	1:D:134:GLY:HA2	2.19	0.43
1:D:453:ILE:C	1:D:461:LEU:HG	2.44	0.43
1:A:103:ALA:HB1	1:A:104:PRO:HD2	1.99	0.43
1:A:131:TRP:CE3	1:A:141:ARG:HD2	2.52	0.43
1:B:385:THR:HG23	1:B:471:ASP:OD1	2.18	0.43
1:B:424:ASP:HB3	1:B:478:TRP:CE3	2.53	0.43
1:B:450:TYR:HA	1:B:488:TRP:O	2.18	0.43
1:C:284:THR:HG22	1:C:300:MET:O	2.18	0.43
1:D:135:ILE:HG13	1:D:136:ASN:ND2	2.34	0.43
1:F:363:ASN:ND2	1:F:467:TRP:HE3	2.16	0.43
1:B:240:TYR:O	1:B:259:TYR:HA	2.18	0.43
1:C:305:ALA:HA	1:C:308:TRP:CZ2	2.53	0.43
1:F:57:MET:HB2	1:F:300:MET:HE1	2.01	0.43
1:F:209:THR:HB	1:F:210:PRO:HD2	2.01	0.43
1:F:492:LEU:N	1:F:492:LEU:HD12	2.33	0.43
1:C:243:ILE:N	1:C:243:ILE:HD12	2.34	0.43
1:C:425:GLY:HA2	1:C:476:GLN:CD	2.44	0.43
1:E:375:VAL:HG12	1:E:411:SER:HB3	2.01	0.43
1:A:110:ASN:OD1	1:A:134:GLY:HA2	2.18	0.43
1:A:305:ALA:HA	1:A:308:TRP:CZ2	2.53	0.43
1:D:357:TYR:CE2	1:D:492:LEU:HG	2.54	0.43
1:D:381:ILE:HD11	1:D:430:GLN:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:TYR:CE2	1:B:330:LEU:HD13	2.53	0.43
1:C:63:TYR:CE1	1:C:84:ARG:NH1	2.87	0.43
1:D:117:MET:HE2	1:D:183:VAL:HB	2.00	0.43
1:D:305:ALA:HB3	1:D:311:LYS:O	2.18	0.43
1:E:256:LYS:HD2	1:E:270:LEU:HD23	2.00	0.43
1:A:115:LYS:HB3	1:A:183:VAL:HG22	2.01	0.43
1:C:52:ALA:HB1	1:C:68:GLY:HA3	2.00	0.43
1:D:278:THR:HG22	1:D:278:THR:O	2.18	0.43
1:E:130:HIS:CE1	1:E:179:ARG:HA	2.54	0.43
1:F:384:TRP:CE3	1:F:471:ASP:HB3	2.53	0.43
1:B:33:GLU:HG2	1:B:35:VAL:HG12	1.99	0.43
1:B:126:VAL:HG11	1:B:212:TYR:O	2.18	0.43
1:C:130:HIS:CE1	1:C:179:ARG:HD3	2.54	0.43
1:D:351:ILE:N	1:D:351:ILE:HD12	2.34	0.43
1:D:460:LYS:C	1:D:461:LEU:HD22	2.43	0.43
1:E:122:THR:OG1	1:E:124:GLU:HG2	2.18	0.43
1:E:399:VAL:HG11	1:E:405:LYS:HG3	2.01	0.43
1:F:229:GLU:CD	2:K:2:GAL:O2	2.62	0.43
1:F:364:SER:OG	1:F:366:LYS:HG2	2.19	0.43
1:D:234:ILE:C	1:D:234:ILE:HD12	2.44	0.42
1:F:243:ILE:N	1:F:243:ILE:HD12	2.33	0.42
1:A:161:ARG:HH22	1:A:177:MET:HG2	1.83	0.42
1:B:285:PHE:HB3	1:B:300:MET:HE3	2.00	0.42
1:A:87:ASP:O	1:A:88:LEU:HB2	2.18	0.42
1:A:460:LYS:HB2	1:A:477:GLN:HG2	2.01	0.42
1:B:450:TYR:CE1	1:B:489:LYS:HB2	2.54	0.42
1:E:130:HIS:CE1	1:E:179:ARG:HD3	2.54	0.42
1:B:64:TYR:O	1:B:84:ARG:HA	2.20	0.42
1:B:125:PHE:CZ	1:B:150:PRO:HG3	2.54	0.42
1:C:420:GLU:CD	2:I:1:BGC:H6C1	2.45	0.42
1:D:59:LYS:HD3	1:D:64:TYR:CD1	2.54	0.42
1:D:454:SER:HA	1:D:461:LEU:HD11	2.00	0.42
1:E:57:MET:HE3	1:E:287:ILE:HG21	2.01	0.42
1:E:197:ALA:HB3	1:E:204:HIS:CE1	2.55	0.42
1:F:57:MET:HE3	1:F:64:TYR:CD1	2.54	0.42
1:B:243:ILE:HD12	1:B:243:ILE:N	2.35	0.42
1:F:97:VAL:HB	1:F:154:PHE:CD2	2.55	0.42
1:B:321:PRO:HB3	1:B:347:ILE:CG2	2.49	0.42
1:E:331:GLU:HG2	1:E:333:PRO:HD3	2.02	0.42
1:E:450:TYR:CE1	1:E:489:LYS:HB2	2.55	0.42
1:D:397:VAL:HB	1:D:405:LYS:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:PRO:HB2	1:E:127:MET:HE3	2.02	0.42
1:E:413:ARG:NH1	1:E:432:THR:HG22	2.35	0.42
1:D:64:TYR:CG	1:D:88:LEU:HD21	2.55	0.42
1:D:394:TRP:CE3	1:D:406:ILE:HG22	2.55	0.42
1:A:240:TYR:O	1:A:259:TYR:HA	2.19	0.42
1:A:287:ILE:HA	1:A:288:PRO:HD3	1.89	0.42
1:D:354:THR:HG22	1:D:354:THR:O	2.20	0.42
1:D:36:ILE:HD12	1:D:42:PHE:CZ	2.55	0.41
1:F:70:TYR:O	1:F:78:LEU:HB2	2.19	0.41
1:F:130:HIS:CD2	1:F:179:ARG:HA	2.54	0.41
1:F:180:ASP:O	1:F:195:SER:HA	2.19	0.41
1:A:450:TYR:CE2	1:A:489:LYS:HE3	2.55	0.41
1:D:454:SER:HA	1:D:461:LEU:CG	2.50	0.41
1:E:243:ILE:HD12	1:E:243:ILE:N	2.35	0.41
1:F:382:VAL:HA	1:F:475:ILE:HG12	2.02	0.41
1:A:80:VAL:HG21	1:A:127:MET:HE1	2.02	0.41
1:A:411:SER:C	1:A:413:ARG:H	2.28	0.41
1:C:129:MET:CG	1:C:143:ALA:HB3	2.47	0.41
1:C:356:ARG:HB2	1:C:493:VAL:HG21	2.01	0.41
1:B:72:ASP:CA	1:B:78:LEU:HD23	2.50	0.41
1:A:354:THR:HG22	1:A:354:THR:O	2.20	0.41
1:B:384:TRP:CZ3	1:B:471:ASP:HB3	2.54	0.41
1:B:466:LYS:HE2	1:B:466:LYS:HA	2.01	0.41
1:E:251:ASN:HA	1:E:252:PRO:HD3	1.94	0.41
1:F:385:THR:HG23	1:F:471:ASP:OD1	2.20	0.41
1:A:430:GLN:O	1:A:430:GLN:HG3	2.19	0.41
1:B:284:THR:HG22	1:B:300:MET:O	2.20	0.41
1:F:354:THR:HG22	1:F:354:THR:O	2.21	0.41
1:A:161:ARG:NH2	1:A:177:MET:HG2	2.36	0.41
1:B:62:ASP:O	1:B:86:LYS:HG2	2.21	0.41
1:C:104:PRO:HA	1:C:107:ASN:OD1	2.20	0.41
1:D:357:TYR:HE1	1:D:396:LEU:HD12	1.86	0.41
1:E:71:ARG:HH11	1:E:75:ASN:HD21	1.67	0.41
1:A:53:HIS:HD2	1:A:312:VAL:HG12	1.85	0.41
1:A:71:ARG:NH1	1:A:312:VAL:HG11	2.36	0.41
1:C:206:TYR:HB3	1:C:215:ILE:HG23	2.03	0.41
1:C:230:ALA:HB1	1:C:283:PRO:O	2.20	0.41
1:A:71:ARG:HB3	1:A:75:ASN:HA	2.01	0.41
1:A:80:VAL:HG11	1:A:127:MET:HE1	2.03	0.41
1:A:163:MET:HE3	1:A:166:THR:HG21	2.02	0.41
1:A:408:ASN:HB3	1:A:411:SER:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:LEU:HD13	1:A:476:GLN:C	2.46	0.41
1:B:80:VAL:HB	1:B:98:LEU:HB3	2.03	0.41
1:C:42:PHE:CE2	1:C:317:TYR:HB2	2.56	0.41
1:C:84:ARG:HE	1:C:94:ARG:CZ	2.34	0.41
1:C:128:TRP:HB3	1:C:193:PHE:CE1	2.56	0.41
1:D:66:TRP:CD1	1:D:66:TRP:C	2.99	0.41
1:D:234:ILE:CD1	1:D:241:TYR:HB2	2.51	0.41
1:D:467:TRP:HH2	1:D:484:THR:HG1	1.69	0.41
1:F:72:ASP:HB3	1:F:78:LEU:HD11	2.02	0.41
1:F:129:MET:CG	1:F:143:ALA:HB3	2.51	0.41
1:F:461:LEU:CD1	1:F:486:GLN:HB3	2.43	0.41
1:A:109:CYS:HB2	1:A:132:GLU:O	2.21	0.41
1:B:384:TRP:CE3	1:B:471:ASP:HB3	2.55	0.41
1:B:492:LEU:HD12	1:B:492:LEU:N	2.36	0.41
1:D:369:ASP:OD1	1:D:391:SER:HB2	2.21	0.41
1:B:111:ILE:HA	1:B:130:HIS:O	2.21	0.40
1:D:296:SER:OG	1:D:347:ILE:HG13	2.21	0.40
1:F:446:ILE:HG12	1:F:450:TYR:O	2.21	0.40
1:B:70:TYR:OH	1:B:78:LEU:HD11	2.22	0.40
1:A:273:LEU:HD11	1:A:332:LEU:HB2	2.02	0.40
1:B:256:LYS:HD3	1:B:270:LEU:HB3	2.04	0.40
1:B:278:THR:HG22	1:B:278:THR:O	2.22	0.40
1:B:375:VAL:HG12	1:B:411:SER:HB3	2.03	0.40
1:C:446:ILE:HG21	1:C:452:LYS:HG3	2.04	0.40
1:D:345:GLY:O	1:D:346:ILE:HD12	2.22	0.40
1:D:403:TYR:HB3	1:D:440:HIS:HB3	2.03	0.40
1:F:413:ARG:NH1	1:F:432:THR:HG22	2.36	0.40
1:A:41:GLN:HE22	1:A:314:ASP:HA	1.86	0.40
1:A:130:HIS:NE2	1:A:179:ARG:HA	2.37	0.40
1:A:196:ALA:HB1	1:A:200:ASN:HA	2.03	0.40
1:B:449:GLY:O	1:B:489:LYS:HA	2.22	0.40
1:A:211:ASP:O	1:A:212:TYR:HB2	2.20	0.40
1:B:115:LYS:HG3	1:B:182:ASN:HA	2.03	0.40
1:C:64:TYR:CG	1:C:88:LEU:HD21	2.56	0.40
1:D:35:VAL:CG2	1:D:339:LYS:HE3	2.51	0.40
1:D:119:ASN:HB3	1:D:122:THR:OG1	2.22	0.40
1:D:129:MET:HG2	1:D:143:ALA:HB3	2.03	0.40
1:D:130:HIS:CE1	1:D:179:ARG:HA	2.57	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	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%)	460 (96%)	20 (4%)	0	100	100
1	D	459/526 (87%)	429 (94%)	30 (6%)	0	100	100
1	E	459/526 (87%)	439 (96%)	20 (4%)	0	100	100
1	F	459/526 (87%)	440 (96%)	19 (4%)	0	100	100
All	All	2775/3156 (88%)	2638 (95%)	137 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	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%)	383 (98%)	6 (2%)	57	82
1	E	389/442 (88%)	388 (100%)	1 (0%)	86	95
1	F	389/442 (88%)	387 (100%)	2 (0%)	81	93
All	All	2347/2652 (88%)	2333 (99%)	14 (1%)	78	92

All (14) 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	446	ILE
1	D	461	LEU
1	D	470	GLU
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 (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	101	ASN
1	A	476	GLN
1	A	487	HIS
1	B	48	ASN
1	B	75	ASN
1	B	130	HIS
1	C	-8	GLN
1	C	60	HIS
1	C	75	ASN
1	D	254	GLN
1	D	392	GLN
1	D	430	GLN
1	D	457	HIS
1	D	477	GLN
1	D	487	HIS
1	E	171	HIS
1	E	457	HIS
1	F	60	HIS
1	F	107	ASN
1	F	171	HIS
1	F	457	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 ⓘ

12 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	BGC	G	1	2	12,12,12	1.62	3 (25%)	17,17,17	0.95	0
2	GAL	G	2	2	11,11,12	2.16	4 (36%)	15,15,17	0.81	0
2	BGC	H	1	2	12,12,12	1.64	3 (25%)	17,17,17	1.10	0
2	GAL	H	2	2	11,11,12	2.14	4 (36%)	15,15,17	0.74	0
2	BGC	I	1	2	12,12,12	1.62	3 (25%)	17,17,17	0.99	0
2	GAL	I	2	2	11,11,12	2.11	5 (45%)	15,15,17	1.01	1 (6%)
2	BGC	J	1	2	12,12,12	1.61	3 (25%)	17,17,17	1.33	2 (11%)
2	GAL	J	2	2	11,11,12	2.12	4 (36%)	15,15,17	1.00	2 (13%)
2	BGC	K	1	2	12,12,12	0.46	0	17,17,17	0.52	0
2	GAL	K	2	2	11,11,12	0.27	0	15,15,17	0.52	0
2	BGC	L	1	2	12,12,12	0.45	0	17,17,17	0.52	0
2	GAL	L	2	2	11,11,12	0.25	0	15,15,17	0.53	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	BGC	G	1	2	-	2/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	G	2	2	-	0/2/19/22	0/1/1/1
2	BGC	H	1	2	-	1/2/22/22	0/1/1/1
2	GAL	H	2	2	-	0/2/19/22	0/1/1/1
2	BGC	I	1	2	-	2/2/22/22	0/1/1/1
2	GAL	I	2	2	-	0/2/19/22	0/1/1/1
2	BGC	J	1	2	-	2/2/22/22	0/1/1/1
2	GAL	J	2	2	-	2/2/19/22	0/1/1/1
2	BGC	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	BGC	L	1	2	-	1/2/22/22	0/1/1/1
2	GAL	L	2	2	-	2/2/19/22	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	2	GAL	C4-C3	-3.89	1.42	1.52
2	G	2	GAL	C4-C3	-3.89	1.42	1.52
2	H	2	GAL	C2-C3	-3.83	1.46	1.52
2	H	2	GAL	C4-C3	-3.82	1.42	1.52
2	G	2	GAL	C2-C3	-3.77	1.46	1.52
2	I	2	GAL	C4-C3	-3.75	1.42	1.52
2	I	1	BGC	O5-C1	3.74	1.52	1.42
2	G	1	BGC	O5-C1	3.73	1.52	1.42
2	H	1	BGC	O5-C1	3.71	1.51	1.42
2	I	2	GAL	C2-C3	-3.70	1.46	1.52
2	J	1	BGC	O5-C1	3.68	1.51	1.42
2	J	2	GAL	C2-C3	-3.67	1.46	1.52
2	G	2	GAL	O5-C1	-2.58	1.39	1.43
2	H	2	GAL	O5-C1	-2.56	1.39	1.43
2	I	2	GAL	O5-C1	-2.47	1.39	1.43
2	J	2	GAL	O5-C5	2.37	1.48	1.43
2	H	1	BGC	C1-C2	-2.36	1.46	1.52
2	J	1	BGC	C3-C2	-2.28	1.46	1.52
2	H	1	BGC	C3-C2	-2.27	1.46	1.52
2	J	2	GAL	O5-C1	-2.26	1.39	1.43
2	J	1	BGC	C1-C2	-2.25	1.47	1.52
2	I	1	BGC	C3-C2	-2.22	1.46	1.52
2	G	1	BGC	C3-C2	-2.20	1.46	1.52
2	G	1	BGC	C1-C2	-2.17	1.47	1.52
2	I	2	GAL	O5-C5	2.15	1.47	1.43
2	G	2	GAL	O5-C5	2.15	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	2	GAL	O5-C5	2.11	1.47	1.43
2	I	1	BGC	C1-C2	-2.08	1.47	1.52
2	I	2	GAL	O3-C3	2.00	1.47	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1	BGC	C4-C3-C2	2.86	115.86	110.83
2	I	2	GAL	C1-C2-C3	2.43	113.19	109.64
2	J	1	BGC	C3-C4-C5	2.35	114.50	110.23
2	J	2	GAL	C1-C2-C3	2.09	112.69	109.64
2	J	2	GAL	O6-C6-C5	2.03	118.25	111.33

There are no chirality outliers.

All (14) torsion outliers are listed below:

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

There are no ring outliers.

6 monomers are involved in 9 short contacts:

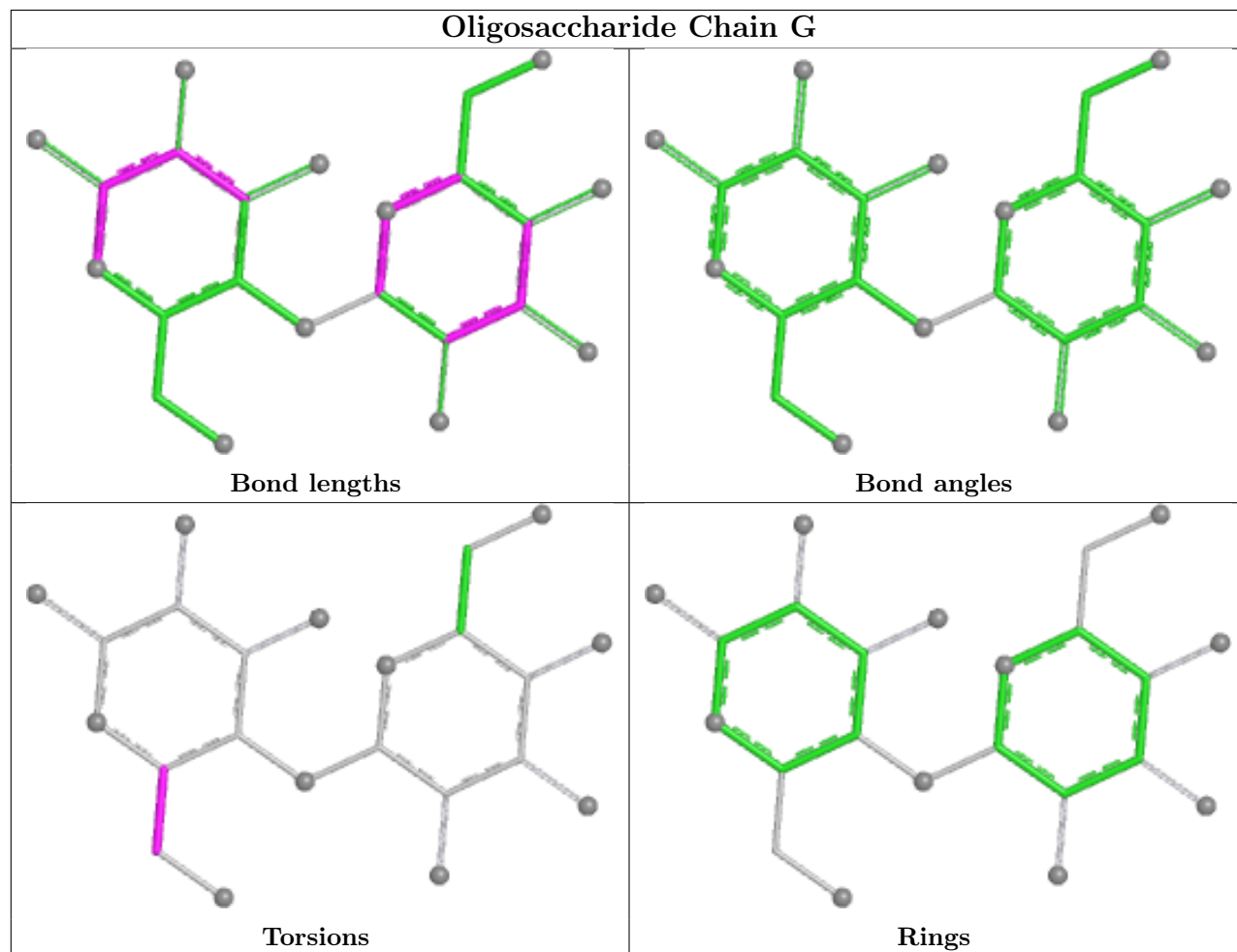
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	1	BGC	1	0
2	L	2	GAL	1	0
2	K	1	BGC	2	0
2	I	1	BGC	1	0
2	H	2	GAL	1	0

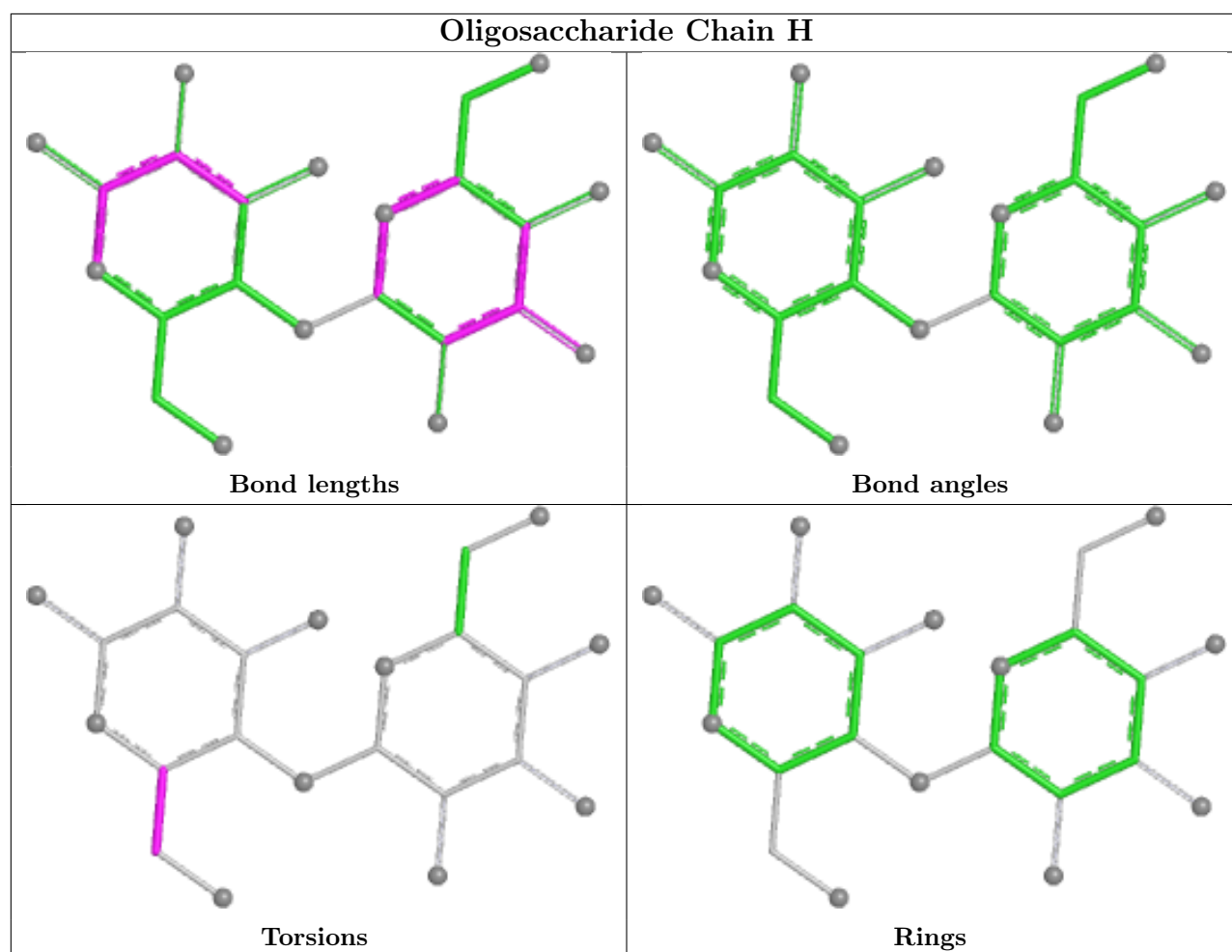
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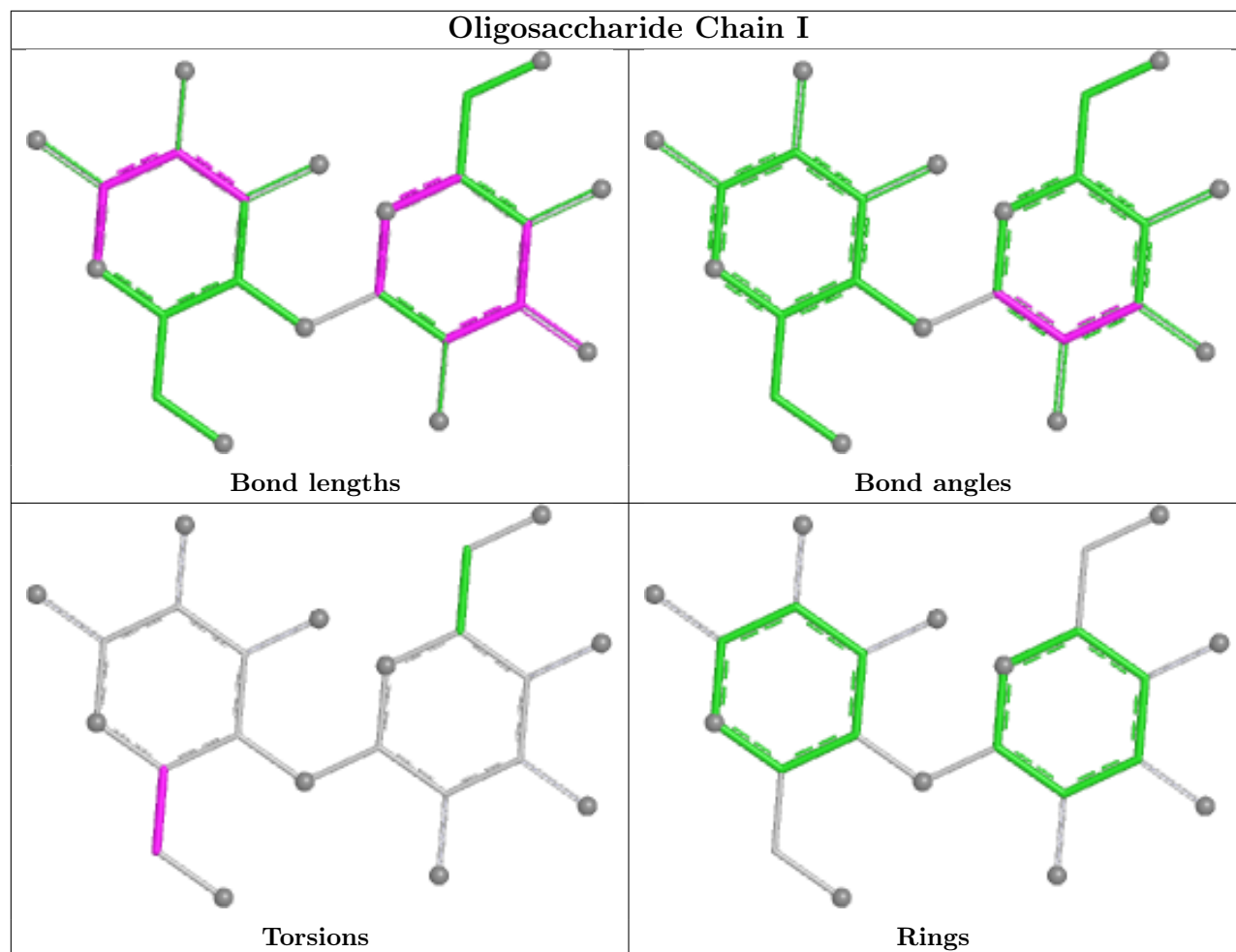
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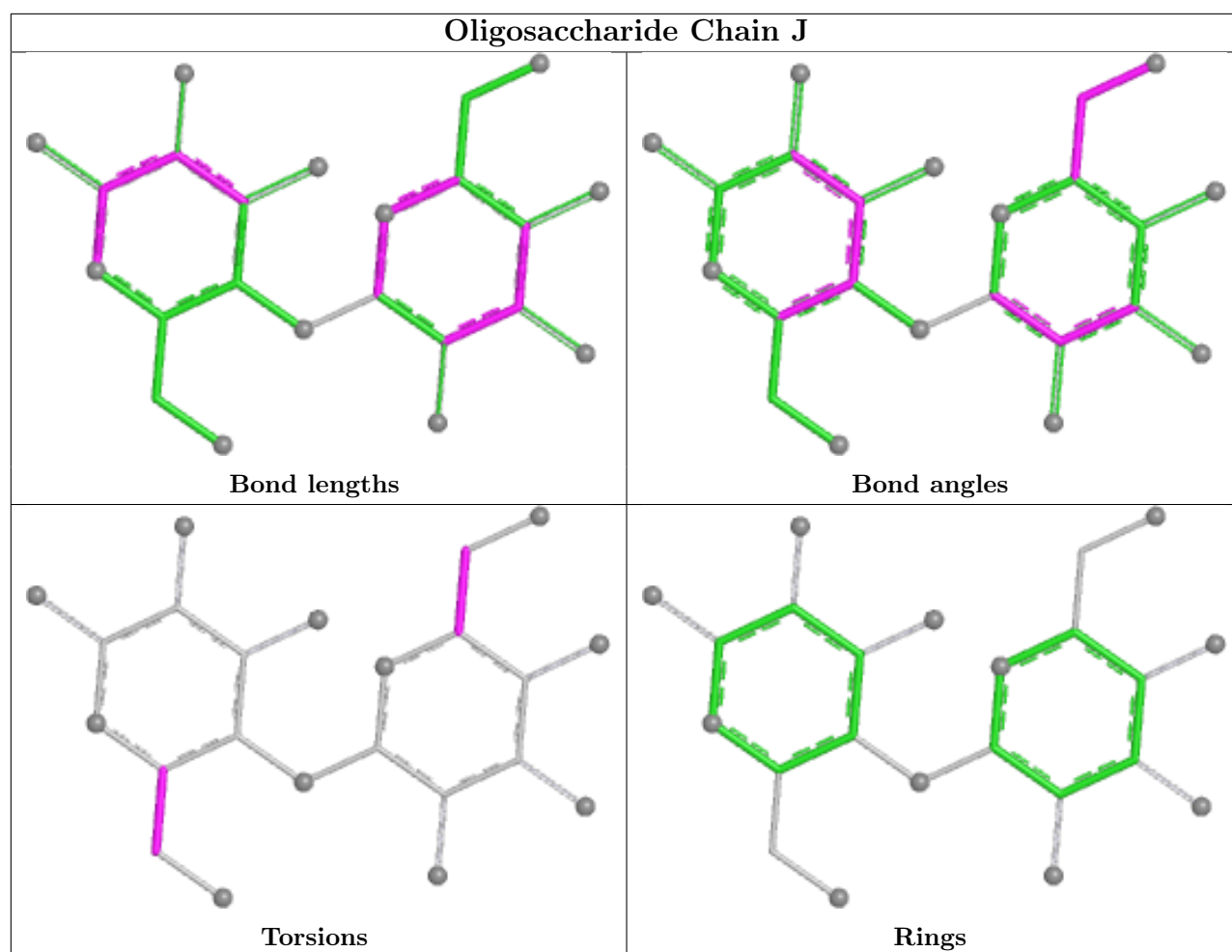
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	2	GAL	4	0

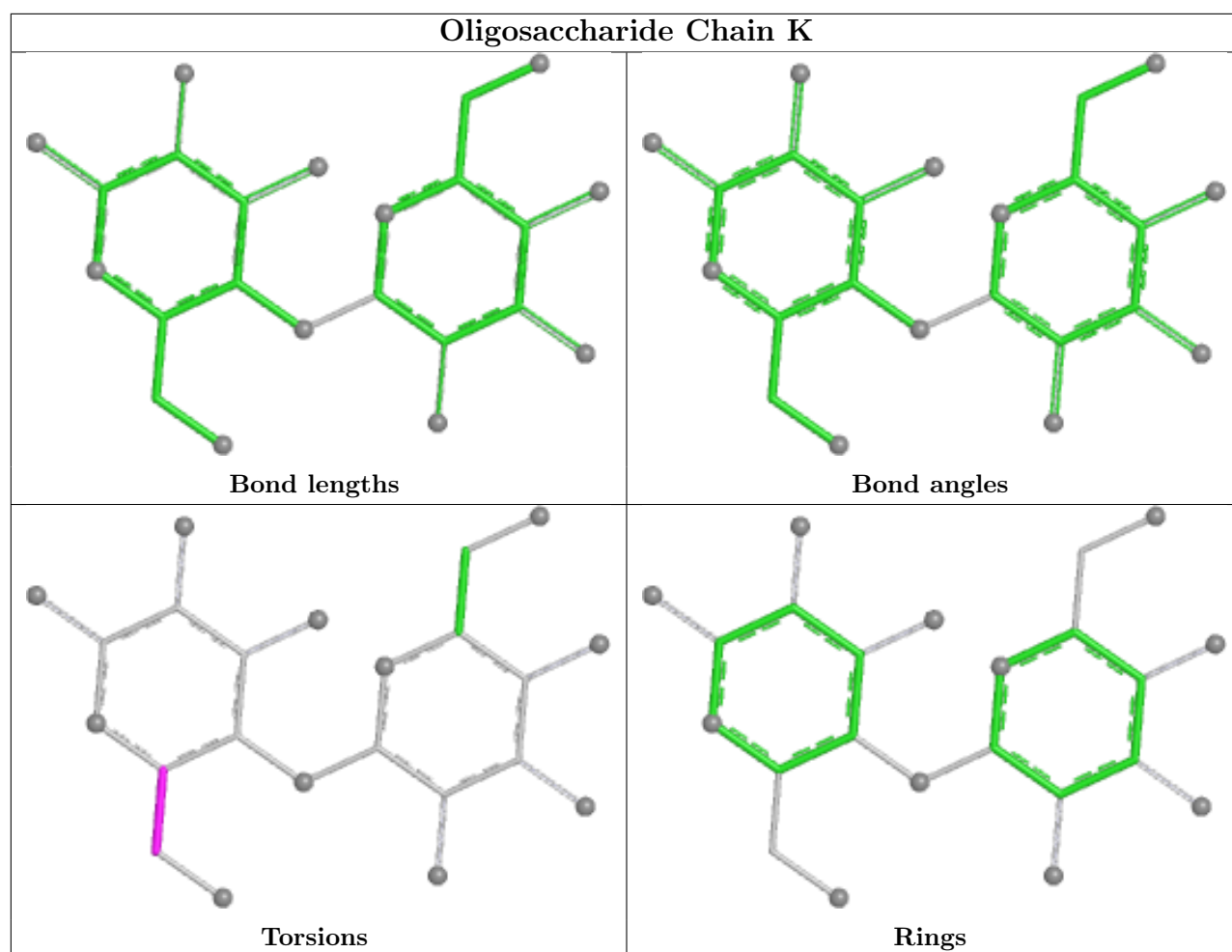
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

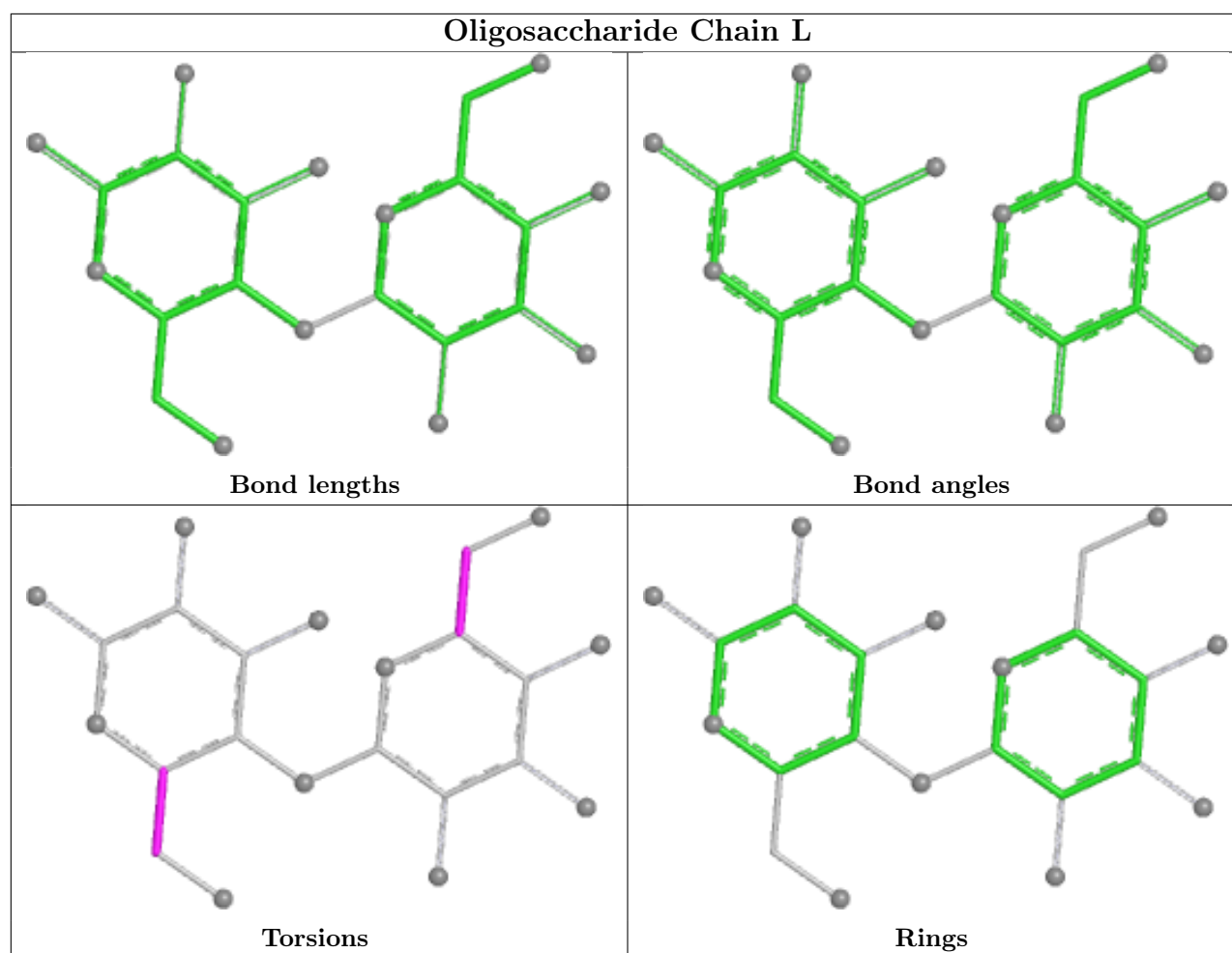












5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
3	GOL	A	601	-	5,5,5	0.37	0	5,5,5	0.30	0
3	GOL	C	601	-	5,5,5	0.35	0	5,5,5	0.26	0
3	GOL	F	601	-	5,5,5	0.39	0	5,5,5	0.29	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	GOL	A	601	-	-	2/4/4/4	-
3	GOL	C	601	-	-	2/4/4/4	-
3	GOL	F	601	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	601	GOL	O1-C1-C2-C3
3	A	601	GOL	O1-C1-C2-C3
3	F	601	GOL	O1-C1-C2-C3
3	C	601	GOL	O1-C1-C2-O2
3	A	601	GOL	O1-C1-C2-O2
3	F	601	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	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%)	0.95	27 (5%) 28 22	57, 82, 97, 108	0
1	B	461/526 (87%)	1.11	50 (10%) 11 9	68, 91, 110, 114	0
1	C	482/526 (91%)	0.39	10 (2%) 63 54	48, 59, 74, 102	0
1	D	461/526 (87%)	1.48	122 (26%) 1 1	55, 86, 148, 153	0
1	E	461/526 (87%)	0.59	15 (3%) 49 39	54, 69, 85, 97	0
1	F	461/526 (87%)	0.59	22 (4%) 35 28	47, 65, 83, 101	0
All	All	2787/3156 (88%)	0.85	246 (8%) 15 13	47, 74, 114, 153	0

All (246) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	390	LEU	6.5
1	D	375	VAL	6.0
1	D	427	VAL	6.0
1	D	493	VAL	5.9
1	D	380	GLN	5.6
1	D	492	LEU	5.5
1	D	453	ILE	5.4
1	D	384	TRP	5.2
1	D	110	ASN	5.1
1	D	443	PHE	5.0
1	F	493	VAL	4.8
1	D	472	GLY	4.8
1	A	493	VAL	4.7
1	B	493	VAL	4.5
1	C	-6	MET	4.3
1	D	464	VAL	4.3
1	D	473	GLY	4.3
1	C	69	GLU	4.3
1	D	374	SER	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	482	GLY	4.1
1	D	478	TRP	4.0
1	D	396	LEU	4.0
1	D	491	VAL	4.0
1	E	110	ASN	3.9
1	D	475	ILE	3.9
1	D	368	LEU	3.8
1	D	383	GLN	3.7
1	D	455	SER	3.7
1	D	415	LEU	3.7
1	D	474	ILE	3.7
1	A	492	LEU	3.7
1	D	452	LYS	3.7
1	D	486	GLN	3.6
1	C	-4	ARG	3.6
1	D	444	THR	3.6
1	D	490	LEU	3.6
1	D	442	LYS	3.5
1	D	373	GLY	3.4
1	E	358	LYS	3.4
1	B	469	THR	3.4
1	D	450	TYR	3.4
1	D	389	SER	3.4
1	D	347	ILE	3.4
1	D	484	THR	3.4
1	D	371	LEU	3.3
1	C	42	PHE	3.3
1	B	492	LEU	3.3
1	D	457	HIS	3.3
1	D	422	LYS	3.2
1	D	441	TRP	3.2
1	D	410	LYS	3.2
1	D	393	GLN	3.1
1	F	388	GLY	3.1
1	D	401	GLY	3.1
1	D	462	ILE	3.1
1	A	133	ASN	3.1
1	D	357	TYR	3.0
1	C	-18	GLY	3.0
1	D	352	PRO	3.0
1	D	353	ASP	2.9
1	D	354	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	426	GLY	2.9
1	D	439	GLN	2.9
1	D	382	VAL	2.9
1	F	492	LEU	2.9
1	D	391	SER	2.9
1	D	370	VAL	2.9
1	D	407	VAL	2.9
1	B	135	ILE	2.9
1	D	358	LYS	2.9
1	D	481	ALA	2.9
1	D	400	GLY	2.8
1	B	150	PRO	2.8
1	A	331	GLU	2.8
1	E	493	VAL	2.8
1	F	449	GLY	2.8
1	C	-13	SER	2.8
1	D	295	THR	2.8
1	D	421	SER	2.8
1	D	395	TYR	2.8
1	B	157	ILE	2.8
1	A	237	ASN	2.8
1	D	57	MET	2.8
1	D	431	TYR	2.8
1	C	110	ASN	2.8
1	B	358	LYS	2.8
1	D	477	GLN	2.7
1	D	355	THR	2.7
1	D	95	GLY	2.7
1	E	412	GLY	2.7
1	F	247	CYS	2.7
1	A	206	TYR	2.7
1	A	139	GLN	2.7
1	D	402	GLY	2.7
1	B	220	ALA	2.7
1	D	63	TYR	2.7
1	A	193	PHE	2.6
1	C	70	TYR	2.6
1	D	436	GLY	2.6
1	B	453	ILE	2.6
1	B	65	TYR	2.6
1	D	408	ASN	2.6
1	D	480	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	378	ALA	2.6
1	A	469	THR	2.6
1	E	492	LEU	2.6
1	F	328	THR	2.6
1	D	351	ILE	2.6
1	A	352	PRO	2.6
1	B	137	TYR	2.6
1	A	157	ILE	2.6
1	B	116	VAL	2.6
1	B	148	LYS	2.5
1	D	367	VAL	2.5
1	D	363	ASN	2.5
1	D	463	ASP	2.5
1	D	471	ASP	2.5
1	F	180	ASP	2.5
1	D	468	SER	2.5
1	E	276	SER	2.5
1	D	394	TRP	2.5
1	E	466	LYS	2.5
1	D	454	SER	2.5
1	B	78	LEU	2.5
1	B	126	VAL	2.5
1	B	144	VAL	2.5
1	D	399	VAL	2.5
1	D	470	GLU	2.5
1	E	264	ALA	2.5
1	A	247	CYS	2.5
1	B	74	SER	2.5
1	B	406	ILE	2.5
1	D	85	SER	2.5
1	D	429	ILE	2.5
1	D	446	ILE	2.5
1	F	364	SER	2.5
1	A	236	ARG	2.5
1	B	110	ASN	2.5
1	D	428	LEU	2.4
1	B	395	TYR	2.4
1	D	385	THR	2.4
1	D	406	ILE	2.4
1	D	397	VAL	2.4
1	A	108	HIS	2.4
1	D	387	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	412	GLY	2.4
1	B	339	LYS	2.4
1	F	33	GLU	2.4
1	B	488	TRP	2.4
1	D	346	ILE	2.4
1	B	151	ASP	2.4
1	F	452	LYS	2.4
1	E	331	GLU	2.4
1	A	296	SER	2.4
1	D	488	TRP	2.4
1	E	137	TYR	2.4
1	F	359	LEU	2.4
1	D	288	PRO	2.4
1	D	338	VAL	2.3
1	D	405	LYS	2.3
1	B	238	GLY	2.3
1	B	402	GLY	2.3
1	B	67	TYR	2.3
1	D	350	TYR	2.3
1	A	422	LYS	2.3
1	F	134	GLY	2.3
1	B	69	GLU	2.3
1	D	264	ALA	2.3
1	D	386	ASP	2.3
1	B	128	TRP	2.3
1	F	137	TYR	2.3
1	F	172	GLY	2.3
1	B	129	MET	2.3
1	D	124	GLU	2.3
1	E	490	LEU	2.3
1	B	346	ILE	2.3
1	D	325	ILE	2.3
1	D	276	SER	2.3
1	D	35	VAL	2.3
1	A	153	LYS	2.2
1	D	418	LYS	2.2
1	D	36	ILE	2.2
1	D	437	TYR	2.2
1	B	482	GLY	2.2
1	B	190	LYS	2.2
1	C	-11	THR	2.2
1	F	432	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	218	LEU	2.2
1	D	359	LEU	2.2
1	F	396	LEU	2.2
1	A	87	ASP	2.2
1	B	257	TYR	2.2
1	E	423	GLU	2.2
1	F	229	GLU	2.2
1	F	135	ILE	2.2
1	A	354	THR	2.2
1	D	467	TRP	2.2
1	B	86	LYS	2.2
1	B	195	SER	2.2
1	F	490	LEU	2.2
1	C	-7	GLN	2.1
1	B	108	HIS	2.1
1	A	390	LEU	2.1
1	B	145	ALA	2.1
1	B	391	SER	2.1
1	D	379	ALA	2.1
1	D	430	GLN	2.1
1	B	491	VAL	2.1
1	E	449	GLY	2.1
1	D	411	SER	2.1
1	D	458	CYS	2.1
1	B	183	VAL	2.1
1	D	89	VAL	2.1
1	F	491	VAL	2.1
1	A	167	GLY	2.1
1	B	355	THR	2.1
1	B	386	ASP	2.1
1	B	461	LEU	2.1
1	D	239	TYR	2.1
1	B	411	SER	2.1
1	A	358	LYS	2.1
1	D	487	HIS	2.1
1	E	51	HIS	2.1
1	F	406	ILE	2.1
1	D	423	GLU	2.1
1	D	241	TYR	2.1
1	D	296	SER	2.0
1	D	466	LYS	2.0
1	D	108	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	226	GLN	2.0
1	D	88	LEU	2.0
1	D	251	ASN	2.0
1	A	401	GLY	2.0
1	B	125	PHE	2.0
1	B	172	GLY	2.0
1	D	449	GLY	2.0
1	D	340	ILE	2.0
1	B	264	ALA	2.0
1	A	257	TYR	2.0
1	B	297	TYR	2.0
1	B	35	VAL	2.0
1	D	236	ARG	2.0
1	A	42	PHE	2.0
1	A	480	ASP	2.0
1	E	416	ASP	2.0
1	D	460	LYS	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($\text{\AA}^2$)	Q<0.9
2	GAL	K	2	11/12	0.65	0.18	19,19,19,19	0
2	BGC	K	1	12/12	0.71	0.16	19,19,19,19	0
2	BGC	H	1	12/12	0.73	0.13	19,19,19,19	0
2	BGC	G	1	12/12	0.81	0.13	19,19,19,19	0
2	BGC	J	1	12/12	0.82	0.12	19,19,19,19	0
2	BGC	I	1	12/12	0.83	0.13	19,19,19,19	0
2	GAL	H	2	11/12	0.86	0.11	19,19,19,19	0
2	BGC	L	1	12/12	0.86	0.12	19,19,19,19	0
2	GAL	J	2	11/12	0.87	0.11	19,19,19,19	0
2	GAL	G	2	11/12	0.87	0.10	19,19,19,19	0
2	GAL	I	2	11/12	0.88	0.10	19,19,19,19	0

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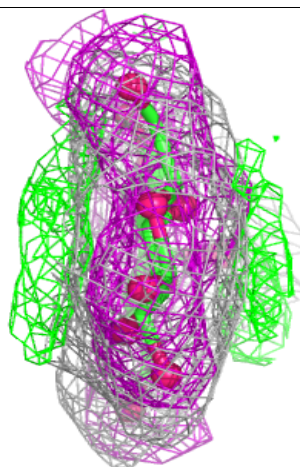
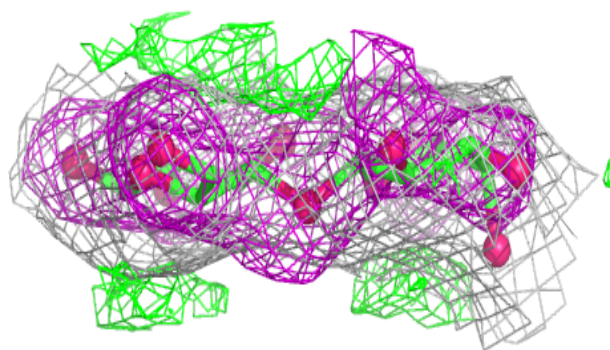
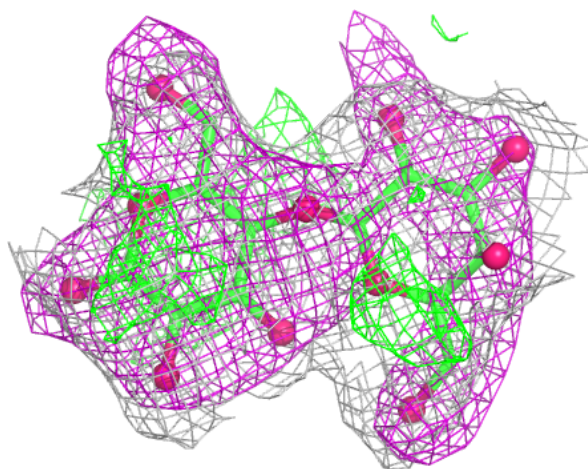
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GAL	L	2	11/12	0.88	0.11	19,19,19,19	0

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.

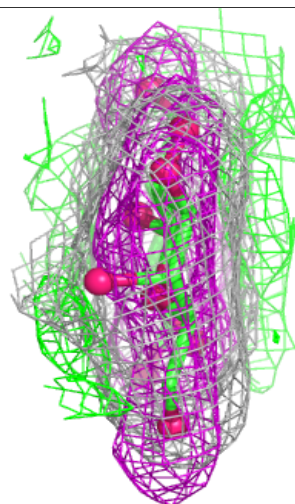
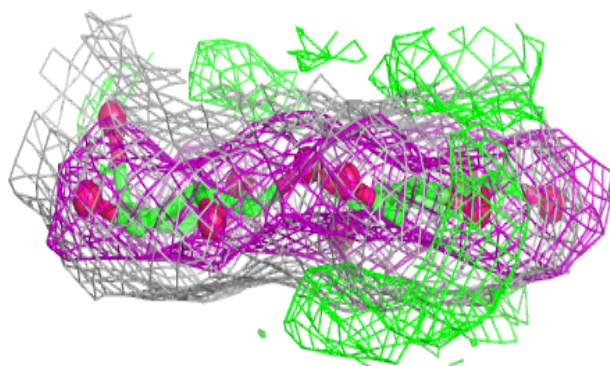
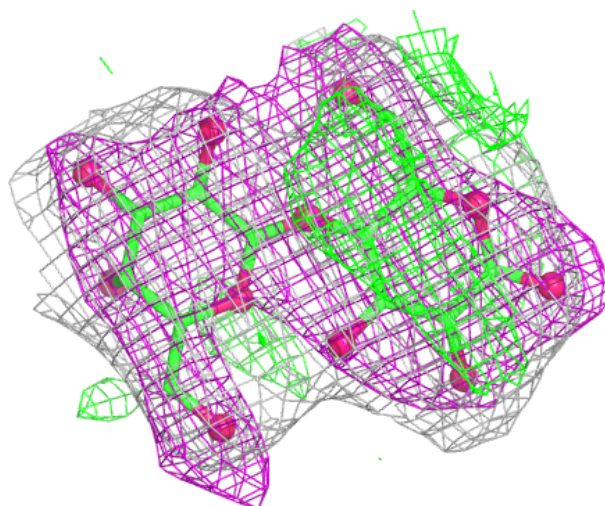
Electron density around Chain G:

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



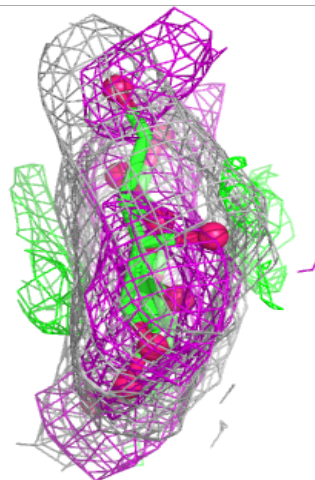
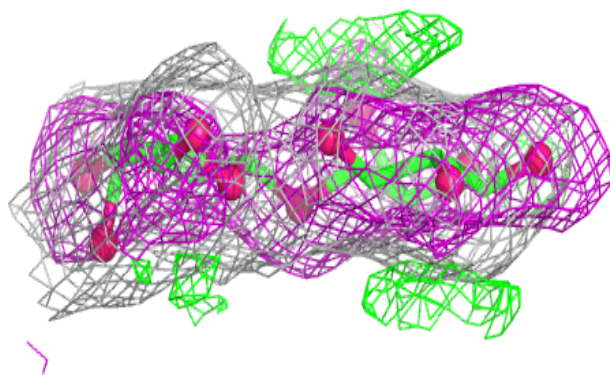
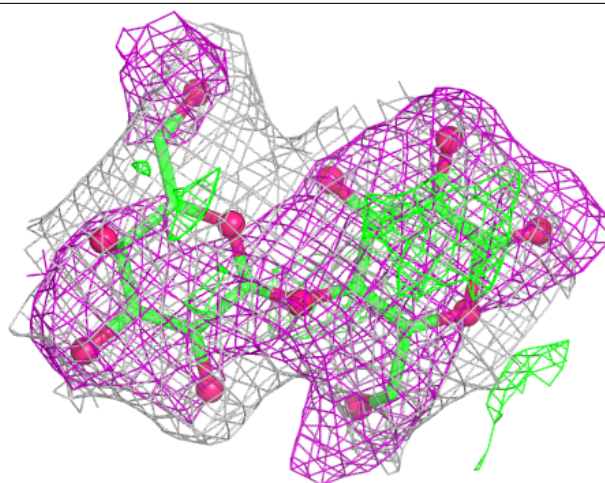
Electron density around Chain H:

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



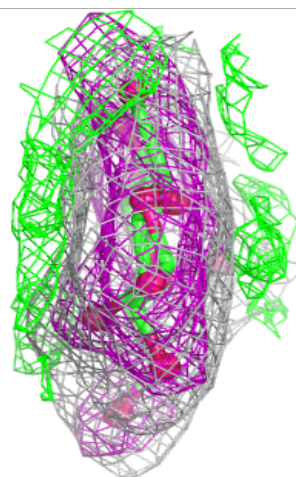
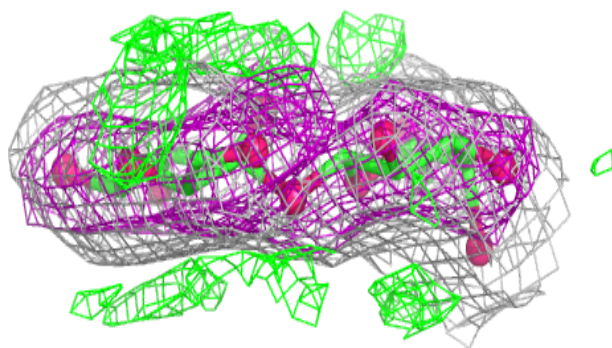
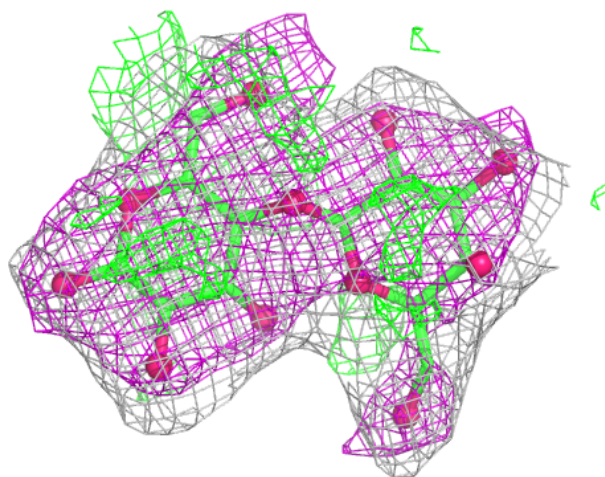
Electron density around Chain I:

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



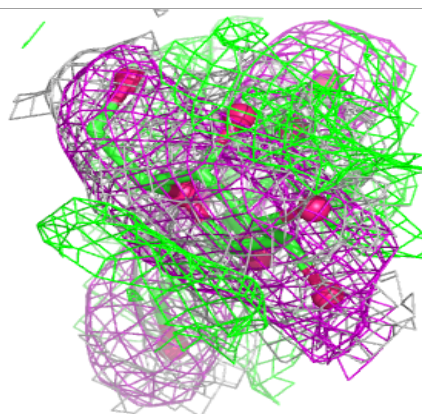
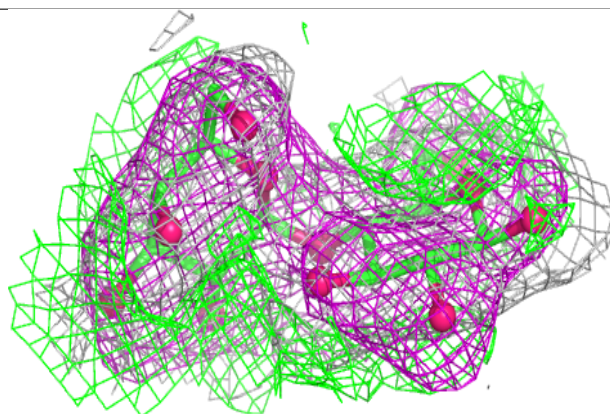
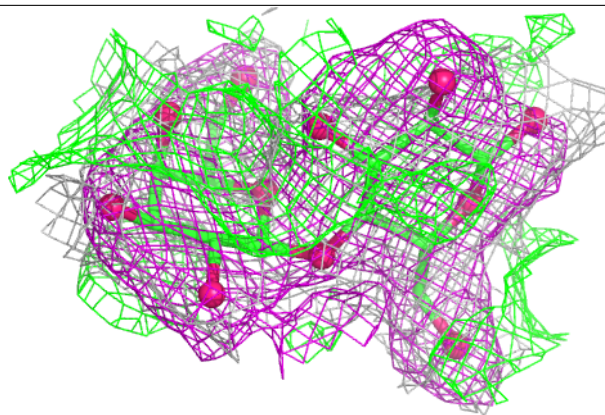
Electron density around Chain J:

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

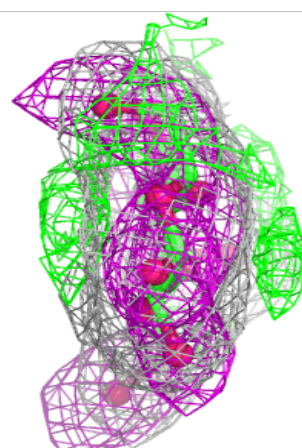
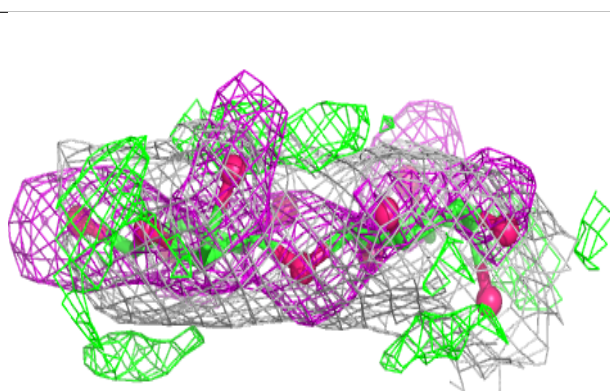
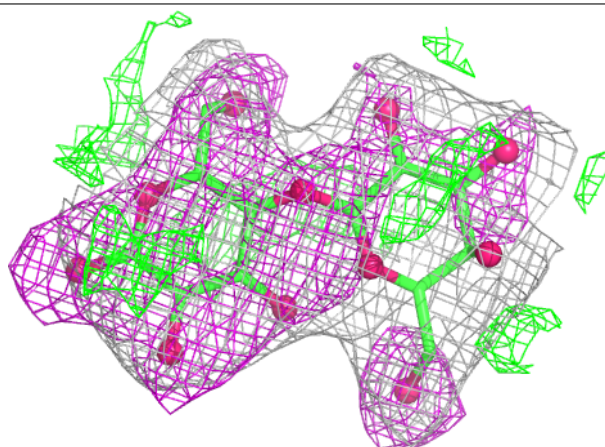


Electron density around Chain K:

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

**Electron density around Chain L:**

$2mF_o-DF_c$ (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
3	GOL	F	601	6/6	0.89	0.28	19,19,19,19	0
3	GOL	C	601	6/6	0.94	0.18	19,19,19,19	0
3	GOL	A	601	6/6	0.96	0.18	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.