



Full wwPDB X-ray Structure Validation Report i

Mar 9, 2024 – 04:07 PM EST

PDB ID : 3VT0
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 i 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](#) i) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

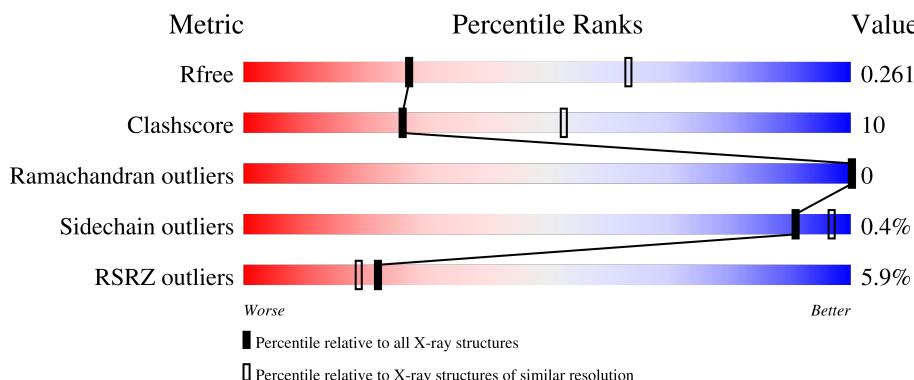
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

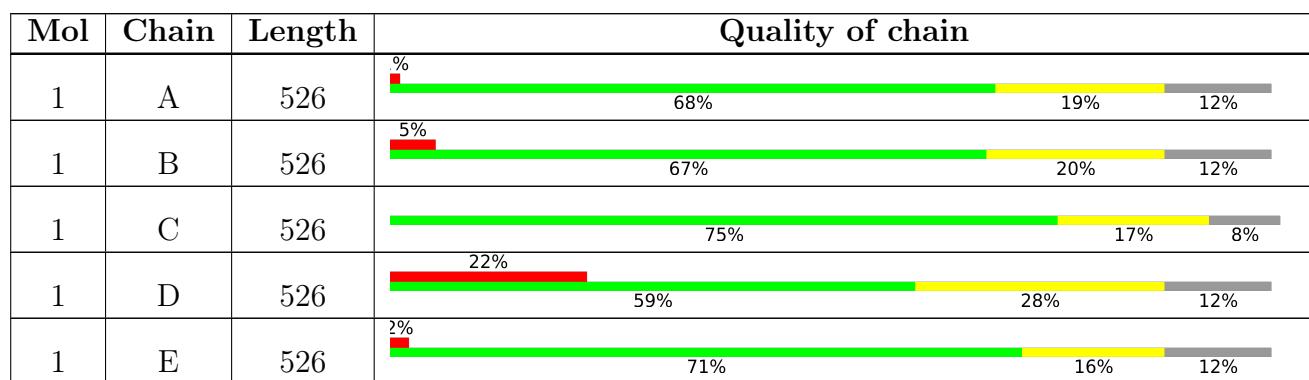
The reported resolution of this entry is 2.91 Å.

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.



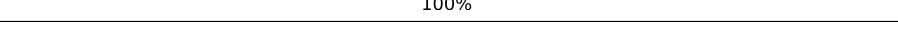
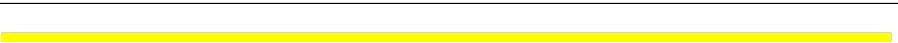
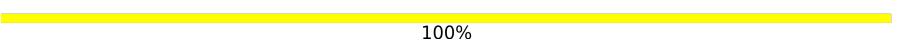
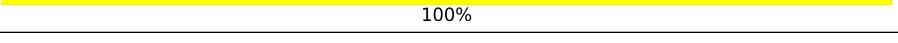
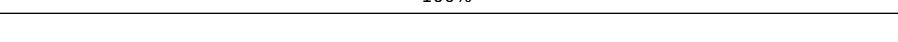
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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 <=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.



Continued on next page...

Continued from previous page...

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

2 Entry composition i

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 3664	N 2323	O 623	S 703	15	0	0
1	B	461	Total	C 3664	N 2323	O 623	S 703	15	0	0
1	C	482	Total	C 3807	N 2406	O 651	S 732	18	0	0
1	D	461	Total	C 3664	N 2323	O 623	S 703	15	0	0
1	E	461	Total	C 3664	N 2323	O 623	S 703	15	0	0
1	F	461	Total	C 3664	N 2323	O 623	S 703	15	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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.



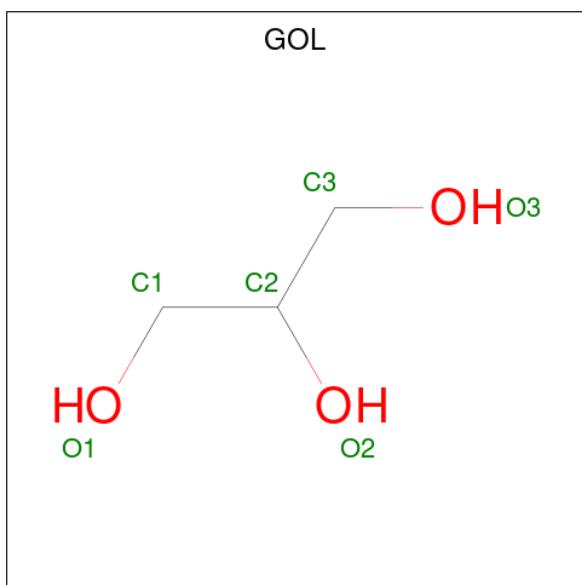
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	G	2	Total C O 23 12 11	0	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).

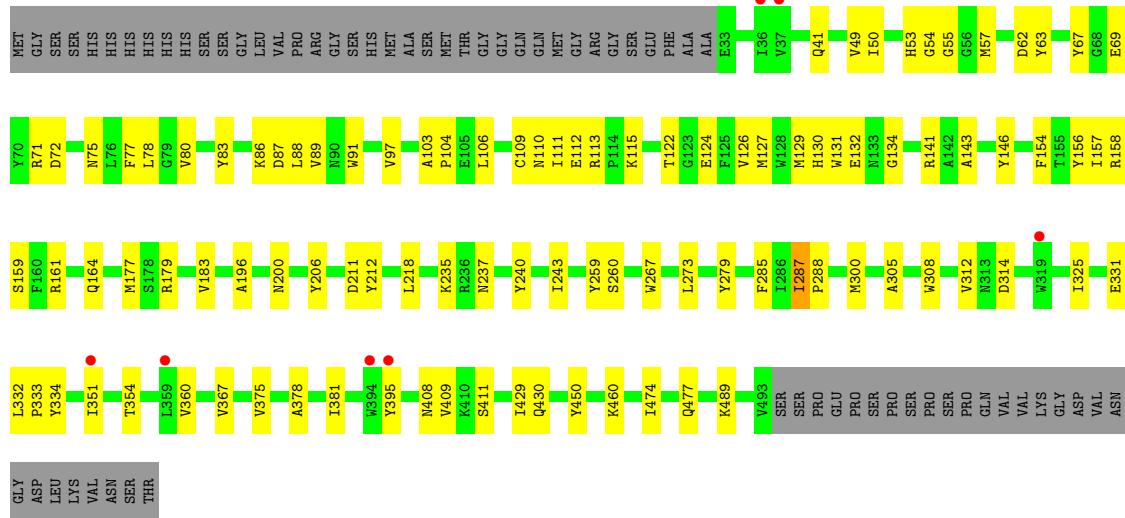


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0

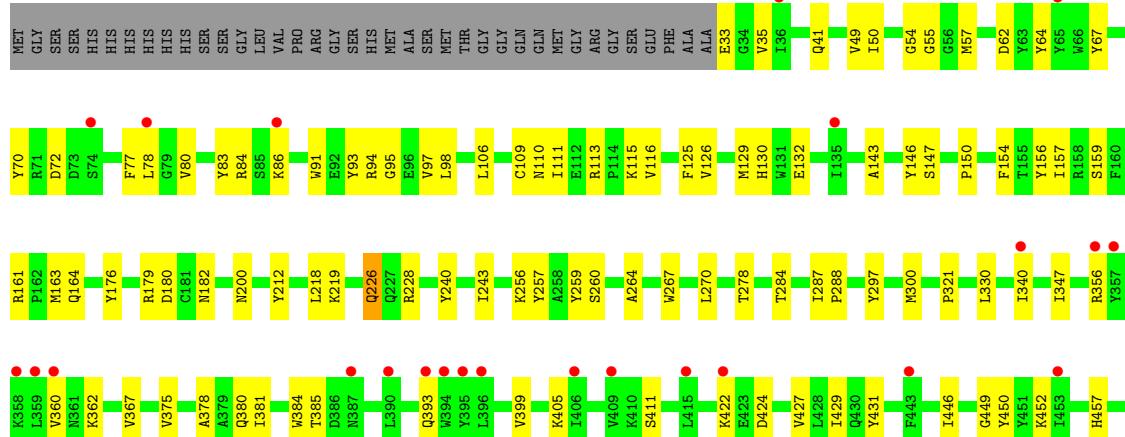
3 Residue-property plots

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

- Molecule 1: Ricin B lectin



- Molecule 1: Ricin B lectin

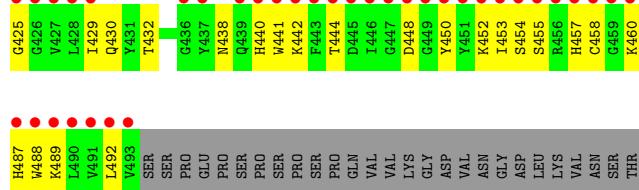
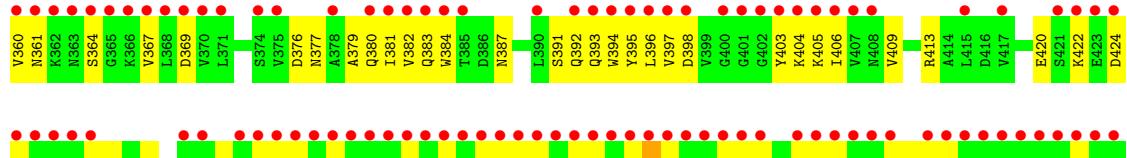
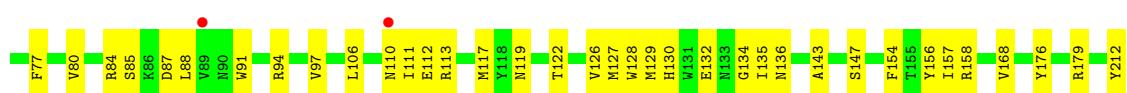
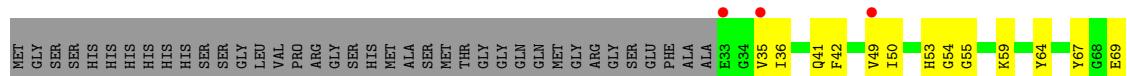




- Molecule 1: Ricin B lectin

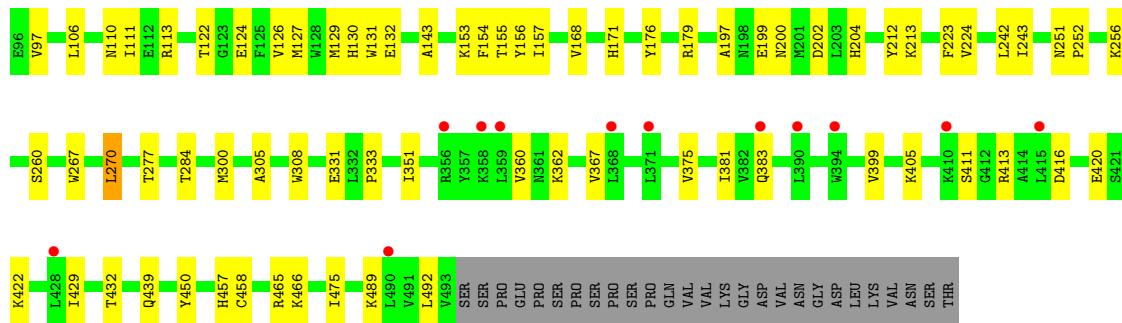


- Molecule 1: Ricin B lectin



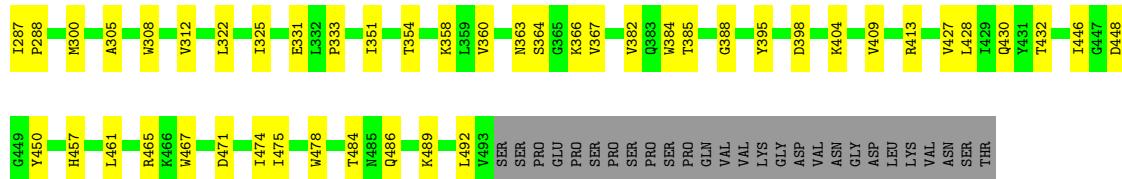
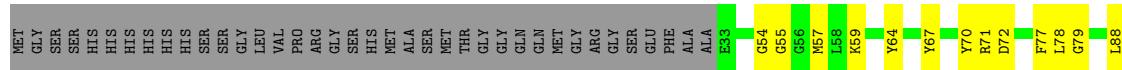
- Molecule 1: Ricin B lectin





- Molecule 1: Ricin B lectin

Chain F: 70% 18% 12%



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

Chain G: 100%



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

Chain H: 50%



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

Chain I: 100%



- 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 i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.69 Å 122.38 Å 404.66 Å 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) 99.6 (49.29-2.91)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	2.67 (at 2.91 Å)	Xtriage
Refinement program	PHENIX 1.7_650	Depositor
R , R_{free}	0.253 , 0.269 0.244 , 0.261	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)	0.33 , 44.4	EDS
L-test for twinning ²	$< L > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	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 $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

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

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	0.20	0/3762	0.35	0/5104
1	B	0.21	0/3762	0.35	0/5104
1	C	0.21	0/3907	0.35	0/5295
1	D	0.21	0/3762	0.36	0/5104
1	E	0.21	0/3762	0.36	0/5104
1	F	0.21	0/3762	0.35	0/5104
All	All	0.21	0/22717	0.35	0/30815

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts i

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3664	0	3480	72	0
1	B	3664	0	3480	78	0
1	C	3807	0	3613	60	0
1	D	3664	0	3480	119	0
1	E	3664	0	3480	57	0
1	F	3664	0	3480	69	0
2	G	23	0	20	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	23	0	20	1	0
2	I	23	0	20	0	0
2	J	23	0	20	0	0
2	K	23	0	21	5	0
2	L	23	0	21	0	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	451	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 10.

All (451) 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:34:GLY:HA2	1:C:89:VAL:HG21	1.53	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:C:57:MET:HE2	1:C:287:ILE:HD13	1.70	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:A:110:ASN:HB2	1:A:132:GLU:HB2	1.73	0.70
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:57:MET:HE2	1:F:287:ILE:HD13	1.78	0.66
1:D:484:THR:HA	1:D:487:HIS:CD2	2.30	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:C:98:LEU:HD22	1:C:127:MET:HE1	1.78	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: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:A:287:ILE:HD11	1:A:300:MET:HE3	1.82	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:360:VAL:CG1	1:D:489:LYS:HB2	2.34	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: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
1:F:223:PHE:HB3	1:F:226:GLN:HG3	1.88	0.55
1:A:80:VAL:HG11	1:A:127:MET:HE3	1.89	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:F:249:GLY:H	2:K:1:BGC:C6	2.20	0.55
1:F:478:TRP:CZ3	3:F:603: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:80:VAL:HG21	1:D:127:MET:HE1	1.89	0.54
1:D:256:LYS:HD3	1:D:270:LEU:HB3	1.89	0.54
1:E:80:VAL:HG21	1:E:127:MET:CE	2.38	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:F:398:ASP:HA	1:F:404:LYS:HG2	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: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: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
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: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:D:454:SER:C	1:D:461:LEU:HD11	2.30	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:LYS:HE3	1:B:457:HIS:NE2	2.26	0.51
1:C:57:MET:HE1	1:C:287:ILE:HG21	1.93	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:E:80:VAL:HG21	1:E:127:MET:HE3	1.93	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:603: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
1:E:80:VAL:HG11	1:E:127:MET:HE3	1.94	0.49
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: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:C:-15:MET:HE3	1:E:153:LYS:HE2	1.94	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:382:VAL:HA	1:D:475:ILE:HG12	1.95	0.49
1:E:383:GLN:O	1:E:383:GLN:HG3	2.12	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: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: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:D:376:ASP:C	1:D:413:ARG:HH12	2.17	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
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:A:57:MET:CB	1:A:300:MET:HE1	2.45	0.47
1:B:78:LEU:C	1:B:78:LEU:HD12	2.35	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:F:358:LYS:HZ2	1:F:388:GLY:HA2	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:80:VAL:HG11	1:D:127:MET:HE3	1.96	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: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:C:57:MET:CE	1:C:287:ILE:HG21	2.46	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:97:VAL:HB	1:A:154:PHE:HD2	1.81	0.45
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:TYR:CZ	1:B:95:GLY:HA2	2.52	0.45
1:D:117:MET:HE3	1:D:128:TRP:CD1	2.51	0.45
1:D:234:ILE:HD11	1:D:241:TYR:HB2	1.98	0.45
1:F:57:MET:CE	1:F:287:ILE:HG21	2.47	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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:425:GLY:HA2	1:D:476:GLN:CD	2.39	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: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:F:57:MET:HE1	1:F:287:ILE:HG21	2.00	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: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: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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:351:ILE:N	1:D:351:ILE:HD12	2.34	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:364:SER:OG	1:F:366:LYS:HG2	2.19	0.43
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:A:57:MET:HE2	1:A:91:TRP:CH2	2.54	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: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:D:467:TRP:HH2	1:D:484:THR:HG1	1.68	0.42
1:E:197:ALA:HB3	1:E:204:HIS:CE1	2.55	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
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:B:163:MET:HE2	1:B:176:TYR:HE2	1.85	0.41
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: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:F:111:ILE:HG21	1:F:129:MET:HE2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:ASP:CA	1:B:78:LEU:HD23	2.50	0.41
1:A:57:MET:HB3	1:A:300:MET:HE1	2.02	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:D:117:MET:HE3	1:D:128:TRP:HD1	1.85	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:408:ASN:HB3	1:A:411:SER:O	2.21	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:234:ILE:CD1	1:D:241:TYR:HB2	2.51	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [\(i\)](#)

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%)	388 (100%)	1 (0%)	92 98
1	B	389/442 (88%)	387 (100%)	2 (0%)	88 96
1	C	402/442 (91%)	401 (100%)	1 (0%)	93 98
1	D	389/442 (88%)	386 (99%)	3 (1%)	81 93
1	E	389/442 (88%)	388 (100%)	1 (0%)	92 98
1	F	389/442 (88%)	387 (100%)	2 (0%)	88 96
All	All	2347/2652 (88%)	2337 (100%)	10 (0%)	91 97

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	287	ILE
1	B	180	ASP
1	B	226	GLN
1	C	427	VAL
1	D	383	GLN
1	D	461	LEU
1	D	470	GLU
1	E	270	LEU
1	F	427	VAL
1	F	457	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	393	GLN
1	B	487	HIS
1	D	377	ASN
1	D	380	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	392	GLN
1	D	430	GLN
1	D	457	HIS
1	E	171	HIS
1	E	457	HIS
1	F	313	ASN

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [\(i\)](#)

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	1.60	3 (25%)	17,17,17	0.95	0
2	GAL	G	2	2	11,11,12	2.21	5 (45%)	15,15,17	0.91	1 (6%)
2	BGC	H	1	2	12,12,12	1.62	3 (25%)	17,17,17	1.11	0
2	GAL	H	2	2	11,11,12	2.20	5 (45%)	15,15,17	0.82	0
2	BGC	I	1	2	12,12,12	1.60	2 (16%)	17,17,17	1.00	0
2	GAL	I	2	2	11,11,12	2.16	5 (45%)	15,15,17	1.14	1 (6%)
2	BGC	J	1	2	12,12,12	1.59	3 (25%)	17,17,17	1.34	2 (11%)
2	GAL	J	2	2	11,11,12	2.17	5 (45%)	15,15,17	1.12	2 (13%)
2	BGC	K	1	2	12,12,12	0.45	0	17,17,17	0.53	0
2	GAL	K	2	2	11,11,12	0.27	0	15,15,17	0.64	0
2	BGC	L	1	2	12,12,12	0.45	0	17,17,17	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GAL	L	2	2	11,11,12	0.26	0	15,15,17	0.64	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
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 (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	2	GAL	C2-C3	-4.01	1.46	1.52
2	J	2	GAL	C4-C3	-3.96	1.42	1.52
2	G	2	GAL	C4-C3	-3.96	1.42	1.52
2	G	2	GAL	C2-C3	-3.94	1.46	1.52
2	H	2	GAL	C4-C3	-3.89	1.42	1.52
2	I	2	GAL	C2-C3	-3.87	1.46	1.52
2	J	2	GAL	C2-C3	-3.83	1.46	1.52
2	I	2	GAL	C4-C3	-3.82	1.42	1.52
2	I	1	BGC	O5-C1	3.65	1.52	1.42
2	G	1	BGC	O5-C1	3.64	1.52	1.42
2	H	1	BGC	O5-C1	3.62	1.51	1.42
2	J	1	BGC	O5-C1	3.59	1.51	1.42
2	G	2	GAL	O5-C1	-2.72	1.39	1.43
2	H	2	GAL	O5-C1	-2.70	1.39	1.43
2	I	2	GAL	O5-C1	-2.61	1.39	1.43
2	J	2	GAL	O5-C1	-2.39	1.39	1.43
2	J	1	BGC	C3-C2	-2.32	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	BGC	C3-C2	-2.31	1.46	1.52
2	J	2	GAL	O5-C5	2.27	1.48	1.43
2	H	1	BGC	C1-C2	-2.26	1.46	1.52
2	I	1	BGC	C3-C2	-2.26	1.46	1.52
2	G	1	BGC	C3-C2	-2.24	1.46	1.52
2	J	1	BGC	C1-C2	-2.16	1.47	1.52
2	I	2	GAL	O3-C3	2.10	1.47	1.43
2	H	2	GAL	O3-C3	2.09	1.47	1.43
2	G	1	BGC	C1-C2	-2.08	1.47	1.52
2	J	2	GAL	O3-C3	2.07	1.47	1.43
2	I	2	GAL	O5-C5	2.06	1.47	1.43
2	G	2	GAL	O5-C5	2.06	1.47	1.43
2	G	2	GAL	O3-C3	2.05	1.47	1.43
2	H	2	GAL	O5-C5	2.02	1.47	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1	BGC	C4-C3-C2	2.88	115.86	110.82
2	I	2	GAL	C1-C2-C3	2.86	113.19	109.67
2	J	2	GAL	C1-C2-C3	2.46	112.69	109.67
2	J	1	BGC	C3-C4-C5	2.39	114.50	110.24
2	G	2	GAL	C1-C2-C3	2.34	112.55	109.67
2	J	2	GAL	O6-C6-C5	2.03	118.25	111.29

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	G	1	BGC	C4-C5-C6-O6
2	L	2	GAL	C4-C5-C6-O6
2	J	1	BGC	O5-C5-C6-O6
2	L	2	GAL	O5-C5-C6-O6
2	K	1	BGC	C4-C5-C6-O6
2	J	2	GAL	C4-C5-C6-O6
2	I	1	BGC	C4-C5-C6-O6
2	K	1	BGC	O5-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

Continued on next page...

Continued from previous page...

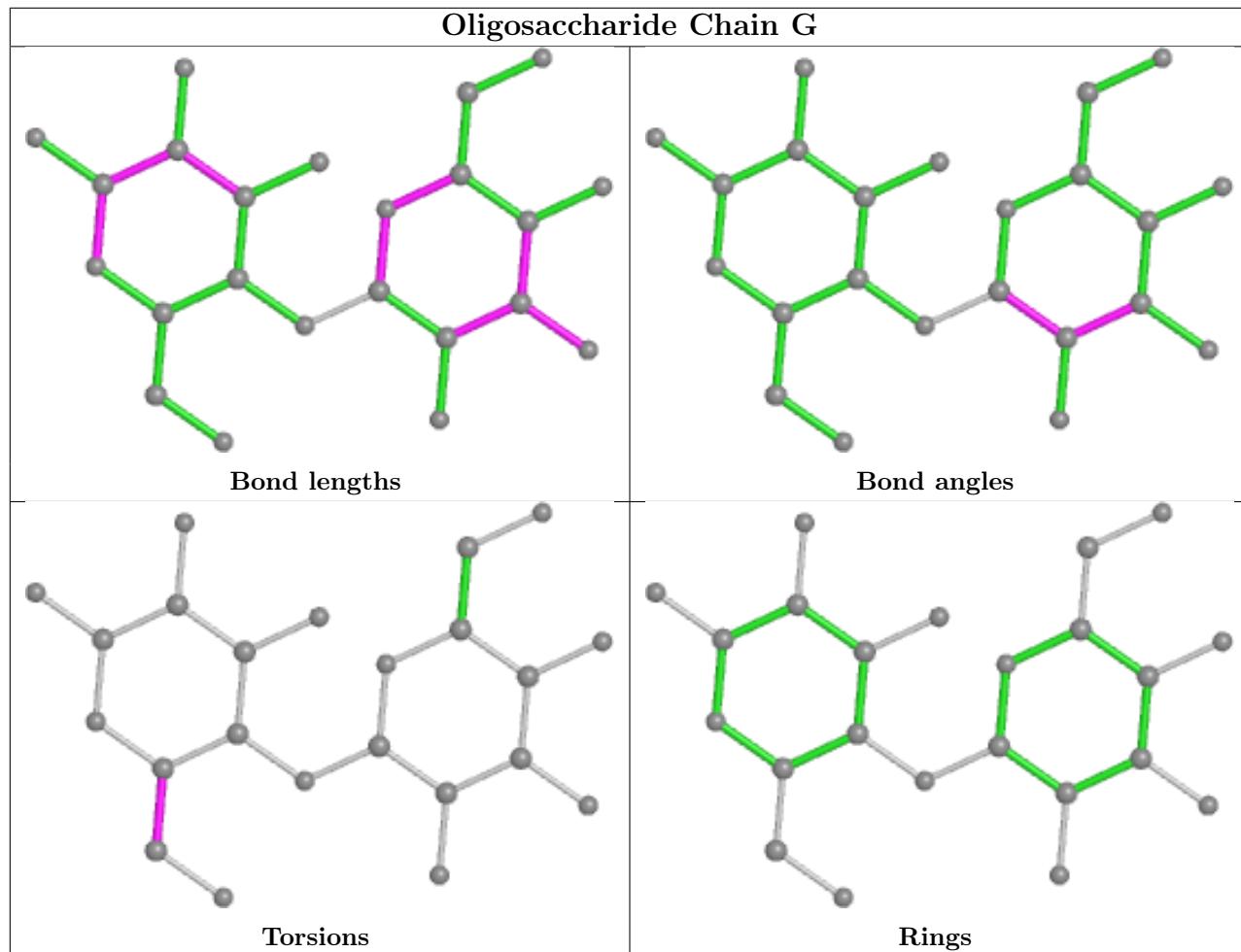
Mol	Chain	Res	Type	Atoms
2	L	1	BGC	C4-C5-C6-O6

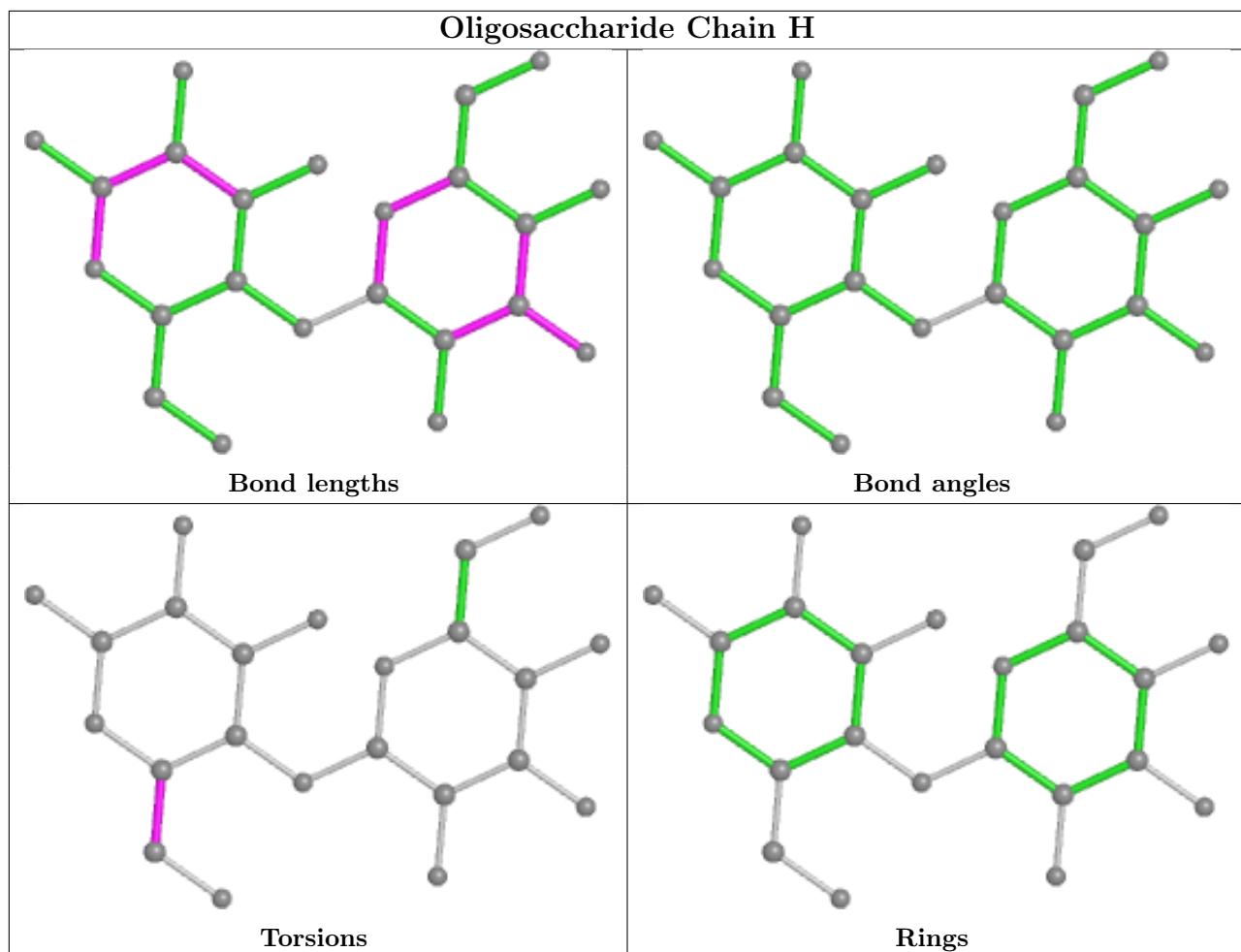
There are no ring outliers.

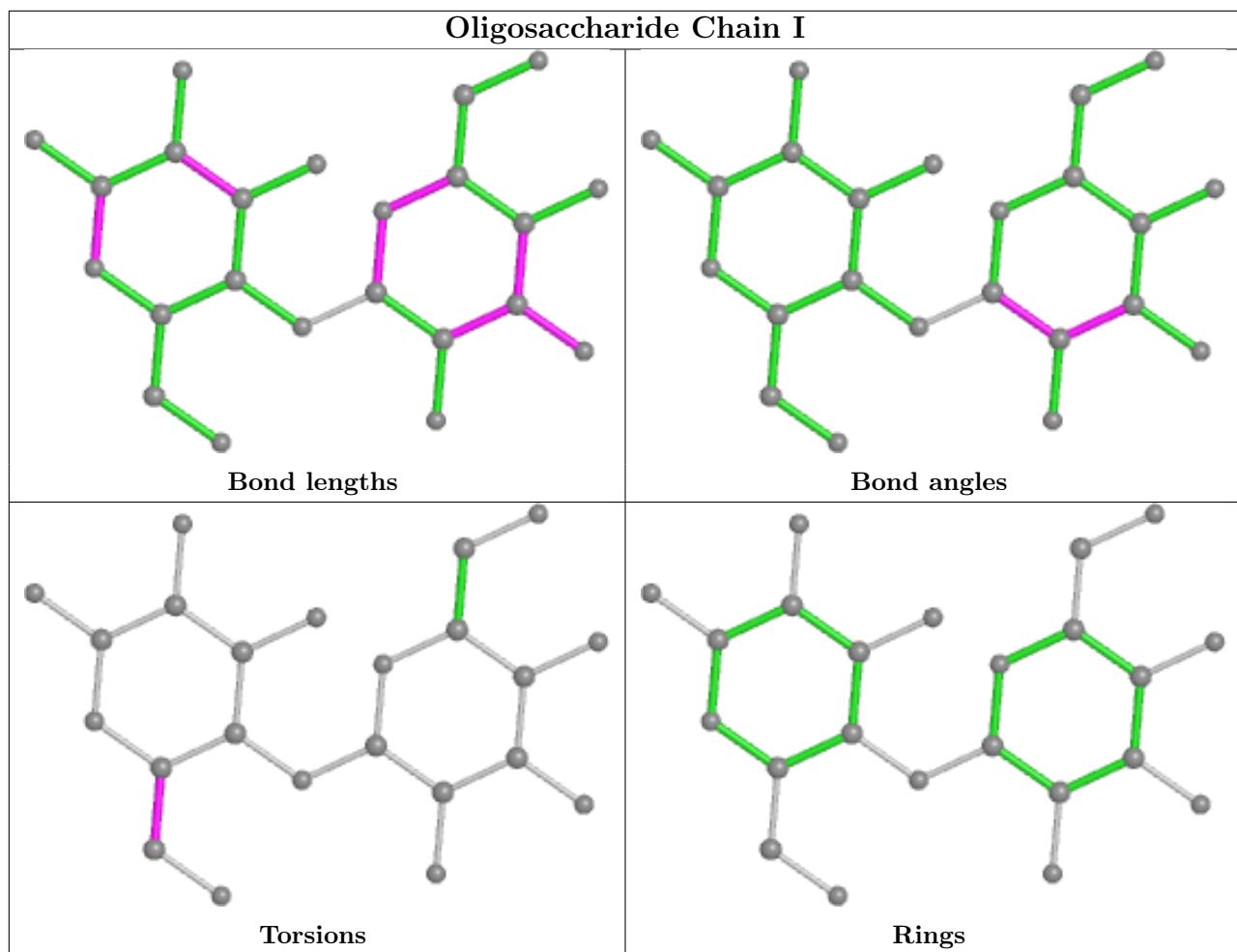
3 monomers are involved in 6 short contacts:

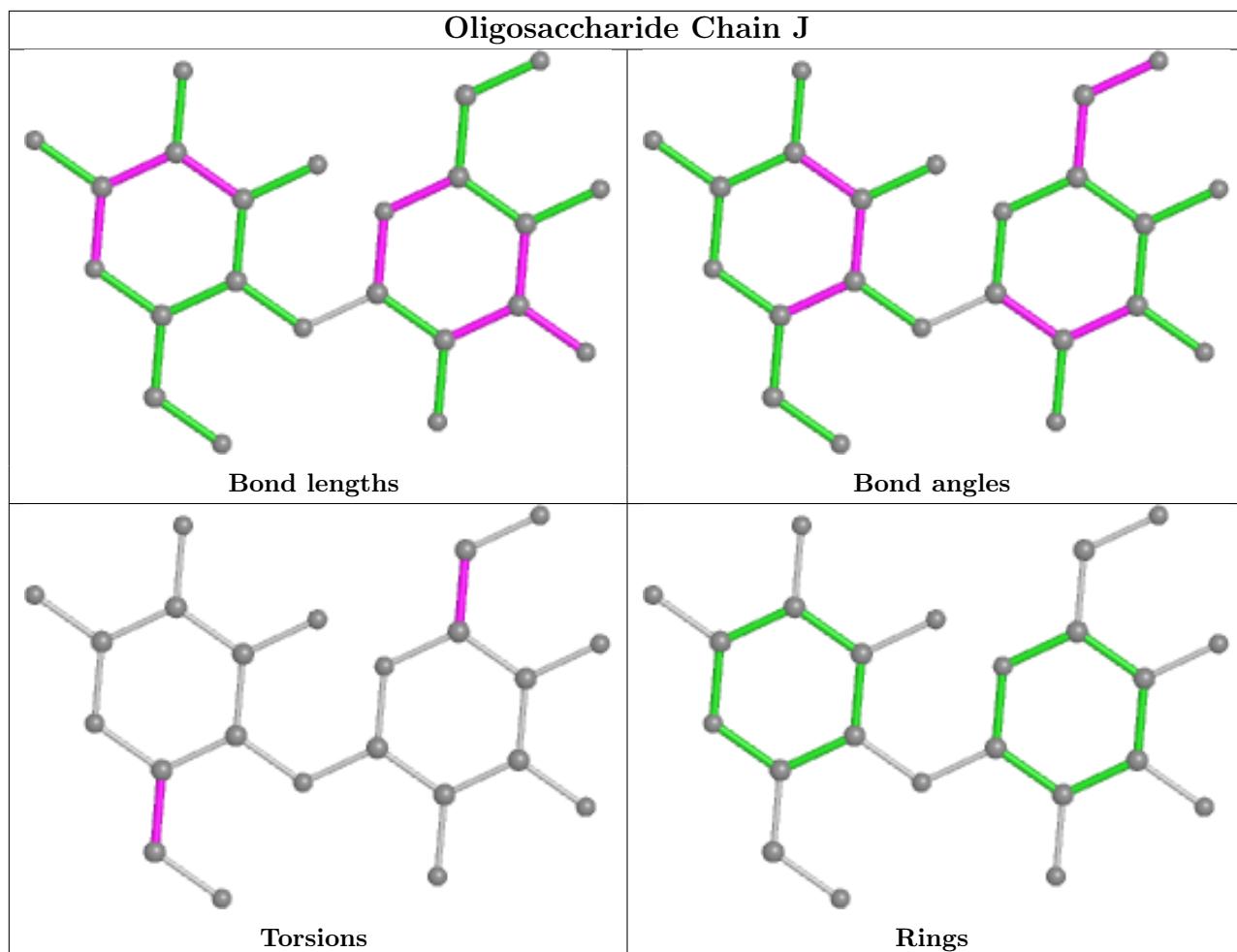
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	2	GAL	3	0
2	K	1	BGC	2	0
2	H	2	GAL	1	0

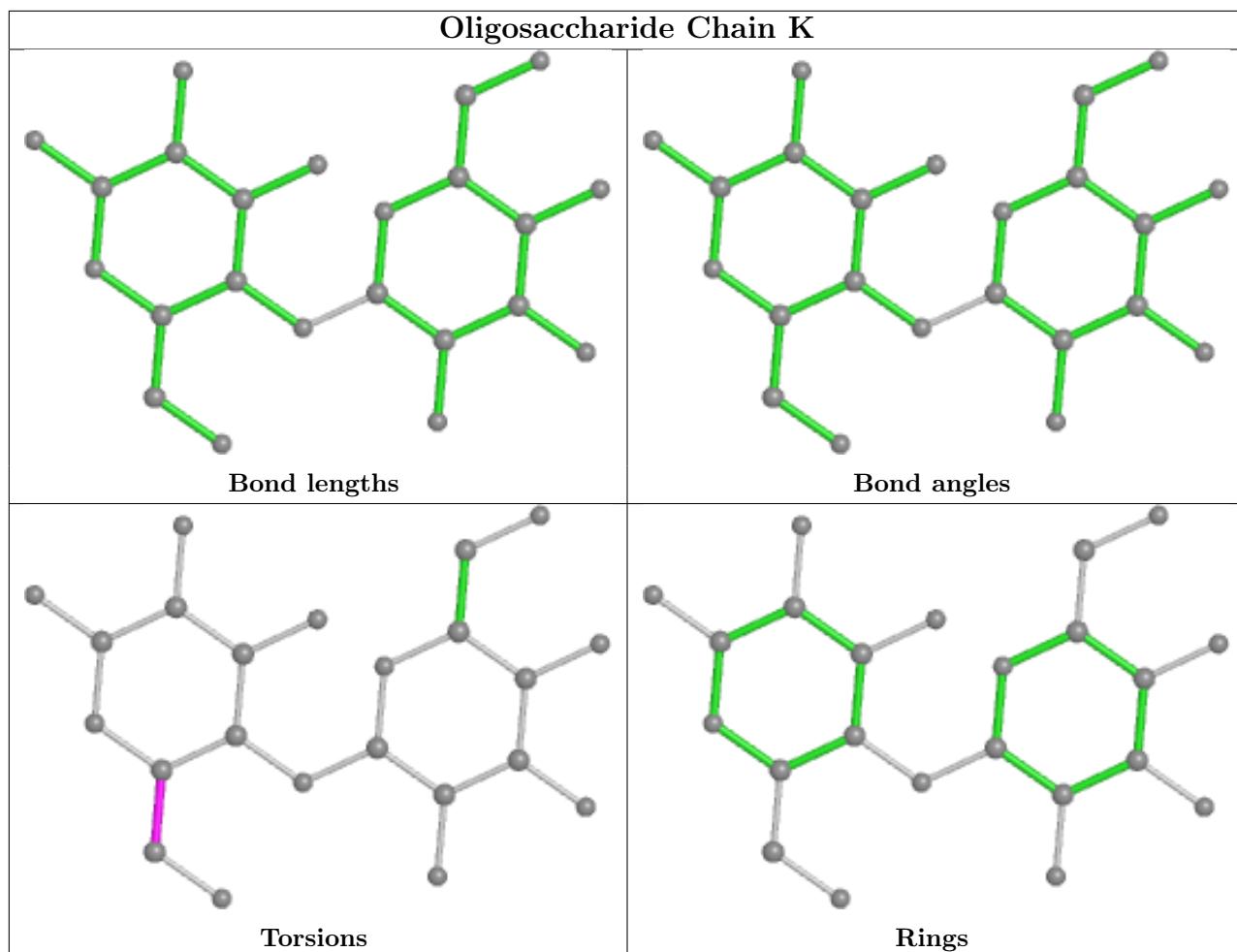
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

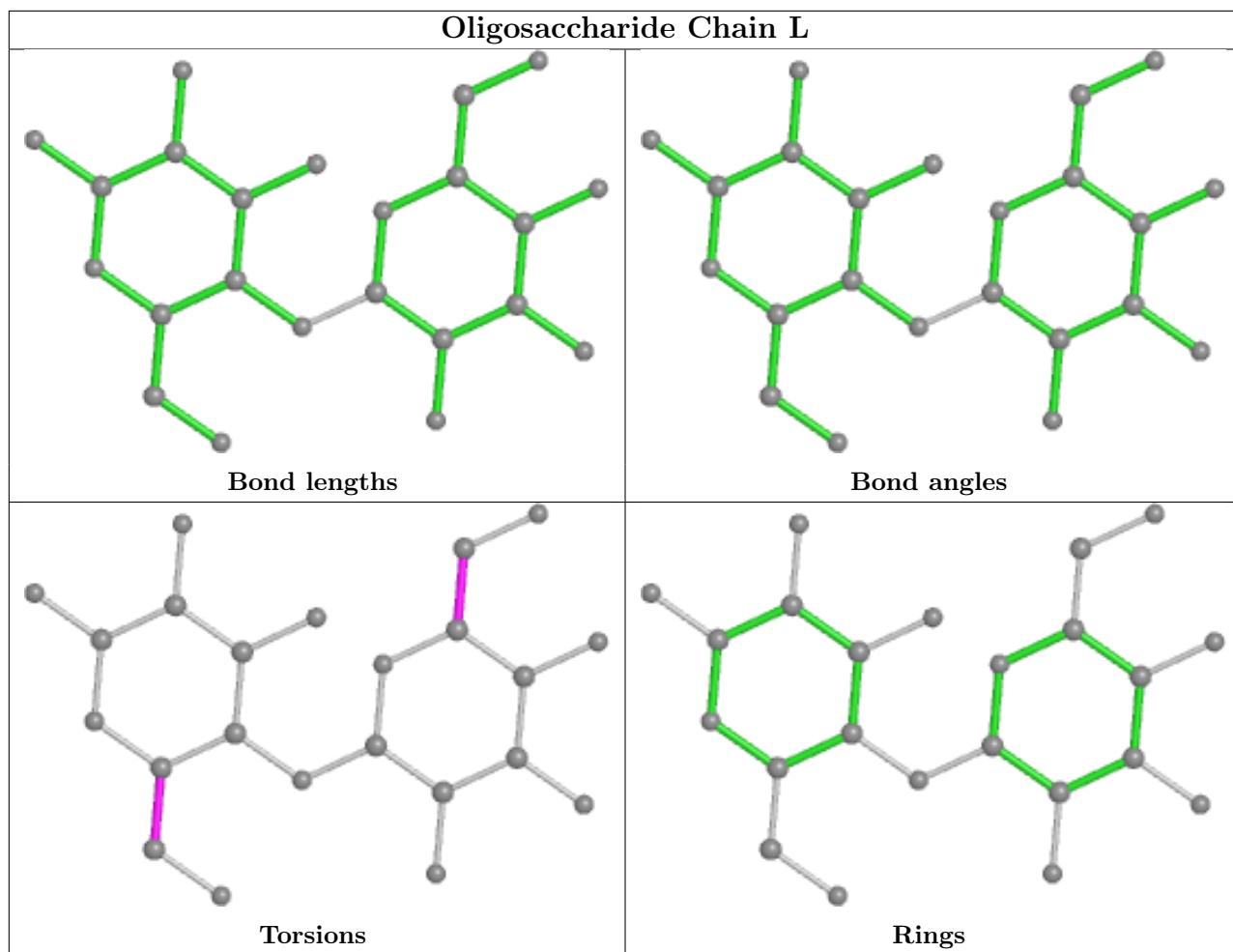












5.6 Ligand geometry (i)

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	602	-	5,5,5	0.36	0	5,5,5	0.26	0
3	GOL	C	602	-	5,5,5	0.35	0	5,5,5	0.23	0
3	GOL	F	603	-	5,5,5	0.38	0	5,5,5	0.25	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	602	-	-	2/4/4/4	-
3	GOL	C	602	-	-	2/4/4/4	-
3	GOL	F	603	-	-	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	A	602	GOL	O1-C1-C2-C3
3	C	602	GOL	O1-C1-C2-C3
3	F	603	GOL	O1-C1-C2-C3
3	C	602	GOL	O1-C1-C2-O2
3	A	602	GOL	O1-C1-C2-O2
3	F	603	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	603	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 i

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	461/526 (87%)	0.37	7 (1%) 73 73	57, 82, 97, 108	0
1	B	461/526 (87%)	0.59	28 (6%) 21 18	68, 91, 110, 114	0
1	C	482/526 (91%)	0.18	2 (0%) 92 92	48, 59, 74, 102	0
1	D	461/526 (87%)	1.30	116 (25%) 0 0	55, 86, 148, 153	0
1	E	461/526 (87%)	0.35	12 (2%) 56 53	54, 69, 85, 97	0
1	F	461/526 (87%)	0.27	0 100 100	47, 65, 83, 101	0
All	All	2787/3156 (88%)	0.51	165 (5%) 22 19	47, 74, 114, 153	0

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	359	LEU	9.2
1	D	380	GLN	8.7
1	D	368	LEU	8.2
1	D	491	VAL	8.0
1	D	490	LEU	7.8
1	D	450	TYR	7.3
1	D	374	SER	7.2
1	D	443	PHE	7.1
1	D	484	THR	6.8
1	D	371	LEU	6.3
1	D	394	TRP	6.2
1	D	367	VAL	6.1
1	D	382	VAL	6.1
1	D	357	TYR	5.9
1	D	354	THR	5.7
1	D	478	TRP	5.7
1	D	444	THR	5.5
1	D	452	LYS	5.4
1	D	423	GLU	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	448	ASP	5.3
1	D	442	LYS	5.3
1	D	401	GLY	5.3
1	D	474	ILE	5.1
1	D	466	LYS	4.9
1	D	445	ASP	4.9
1	D	471	ASP	4.9
1	D	467	TRP	4.8
1	D	360	VAL	4.8
1	D	489	LYS	4.8
1	D	453	ILE	4.8
1	D	441	TRP	4.8
1	D	407	VAL	4.7
1	D	451	TYR	4.7
1	D	425	GLY	4.6
1	D	481	ALA	4.6
1	D	487	HIS	4.6
1	D	428	LEU	4.5
1	D	462	ILE	4.5
1	D	426	GLY	4.5
1	D	492	LEU	4.5
1	D	458	CYS	4.5
1	D	449	GLY	4.5
1	D	427	VAL	4.5
1	D	479	SER	4.4
1	D	402	GLY	4.4
1	D	459	GLY	4.4
1	D	383	GLN	4.3
1	D	356	ARG	4.3
1	D	364	SER	4.3
1	D	424	ASP	4.2
1	D	396	LEU	4.2
1	D	358	LYS	4.2
1	D	446	ILE	4.1
1	D	381	ILE	4.1
1	B	358	LYS	4.0
1	D	437	TYR	4.0
1	D	488	TRP	4.0
1	D	392	GLN	3.9
1	D	460	LYS	3.9
1	D	370	VAL	3.9
1	D	363	ASN	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	469	THR	3.8
1	D	405	LYS	3.8
1	D	384	TRP	3.8
1	D	456	ARG	3.8
1	D	365	GLY	3.7
1	D	472	GLY	3.7
1	B	491	VAL	3.6
1	D	470	GLU	3.6
1	D	447	GLY	3.6
1	D	480	ASP	3.6
1	D	35	VAL	3.5
1	D	362	LYS	3.5
1	D	422	LYS	3.5
1	B	490	LEU	3.4
1	D	454	SER	3.4
1	D	417	VAL	3.4
1	D	440	HIS	3.4
1	D	406	ILE	3.4
1	D	486	GLN	3.3
1	D	421	SER	3.2
1	B	396	LEU	3.2
1	D	463	ASP	3.2
1	D	439	GLN	3.2
1	D	390	LEU	3.2
1	D	395	TYR	3.1
1	D	89	VAL	3.1
1	D	110	ASN	3.1
1	D	465	ARG	3.1
1	E	359	LEU	3.1
1	D	408	ASN	3.0
1	D	400	GLY	2.9
1	D	477	GLN	2.9
1	D	403	TYR	2.9
1	B	340	ILE	2.9
1	D	366	LYS	2.9
1	B	65	TYR	2.9
1	B	356	ARG	2.9
1	D	33	GLU	2.9
1	B	360	VAL	2.8
1	D	398	ASP	2.8
1	D	473	GLY	2.8
1	D	355	THR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	397	VAL	2.7
1	E	394	TRP	2.7
1	D	361	ASN	2.7
1	B	406	ILE	2.7
1	D	378	ALA	2.6
1	A	395	TYR	2.6
1	B	135	ILE	2.6
1	B	394	TRP	2.6
1	E	490	LEU	2.6
1	D	393	GLN	2.6
1	B	393	GLN	2.6
1	B	387	ASN	2.6
1	B	415	LEU	2.6
1	D	415	LEU	2.5
1	D	482	GLY	2.5
1	D	493	VAL	2.5
1	C	-18	GLY	2.5
1	B	74	SER	2.5
1	E	383	GLN	2.5
1	B	86	LYS	2.4
1	D	404	LYS	2.4
1	A	359	LEU	2.4
1	D	429	ILE	2.4
1	E	390	LEU	2.4
1	E	428	LEU	2.4
1	C	-6	MET	2.4
1	A	351	ILE	2.4
1	D	436	GLY	2.4
1	B	359	LEU	2.4
1	B	395	TYR	2.4
1	B	390	LEU	2.4
1	E	356	ARG	2.3
1	B	78	LEU	2.3
1	B	492	LEU	2.3
1	D	461	LEU	2.3
1	A	394	TRP	2.3
1	B	443	PHE	2.3
1	D	483	GLY	2.3
1	D	476	GLN	2.3
1	E	415	LEU	2.3
1	D	485	ASN	2.3
1	A	36	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	464	VAL	2.2
1	A	37	VAL	2.2
1	B	453	ILE	2.2
1	D	457	HIS	2.2
1	E	368	LEU	2.2
1	D	375	VAL	2.2
1	E	358	LYS	2.2
1	D	455	SER	2.2
1	D	385	THR	2.1
1	B	409	VAL	2.1
1	D	49	VAL	2.1
1	B	36	ILE	2.0
1	B	357	TYR	2.0
1	B	474	ILE	2.0
1	B	422	LYS	2.0
1	E	410	LYS	2.0
1	E	371	LEU	2.0
1	D	351	ILE	2.0
1	D	369	ASP	2.0
1	A	319	TRP	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.

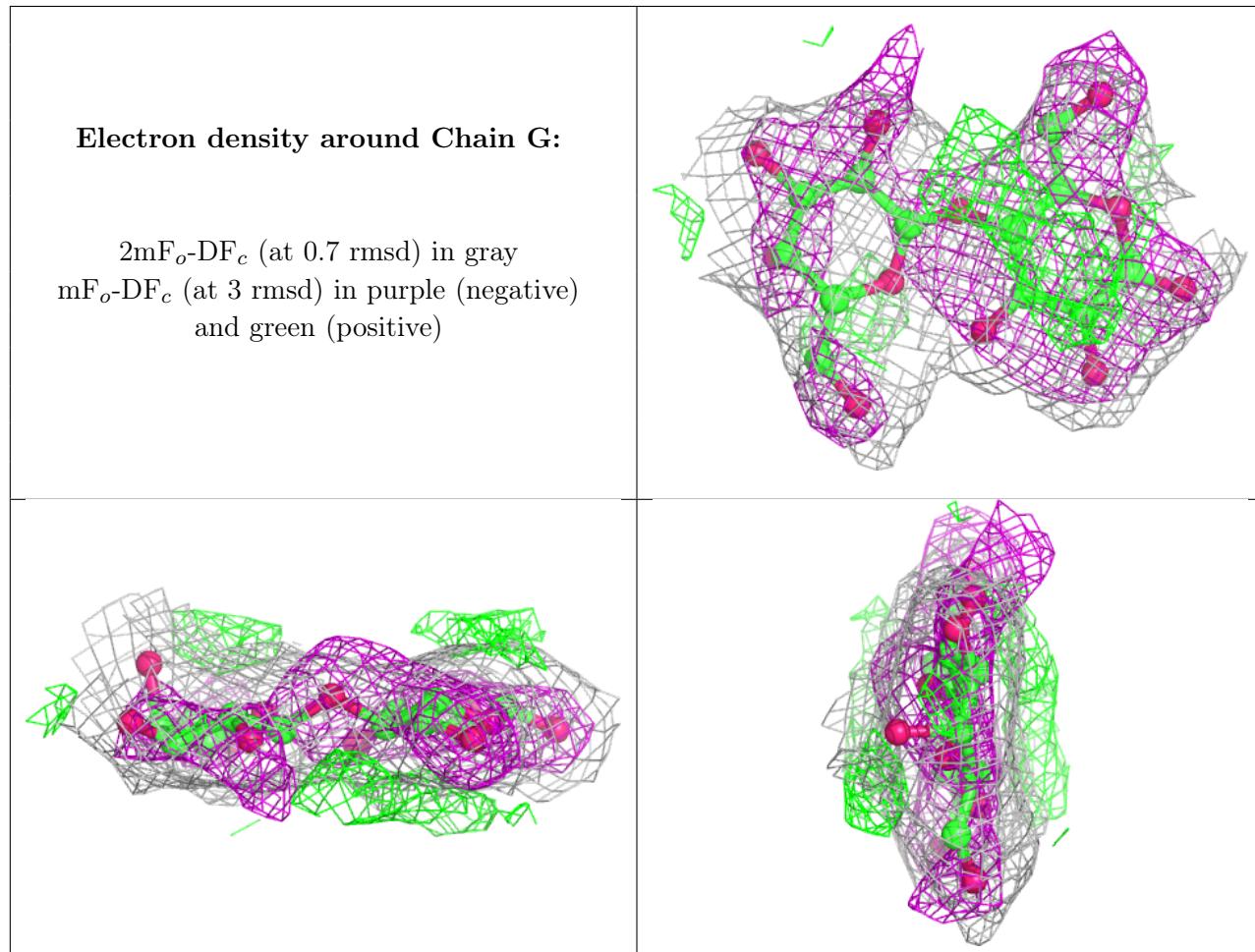
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BGC	K	1	12/12	0.75	0.30	19,19,19,19	0
2	GAL	K	2	11/12	0.87	0.37	19,19,19,19	0
2	BGC	H	1	12/12	0.88	0.23	19,19,19,19	0
2	BGC	G	1	12/12	0.91	0.22	19,19,19,19	0
2	BGC	L	1	12/12	0.91	0.18	19,19,19,19	0
2	GAL	I	2	11/12	0.92	0.12	19,19,19,19	0
2	BGC	I	1	12/12	0.92	0.19	19,19,19,19	0
2	BGC	J	1	12/12	0.93	0.21	19,19,19,19	0

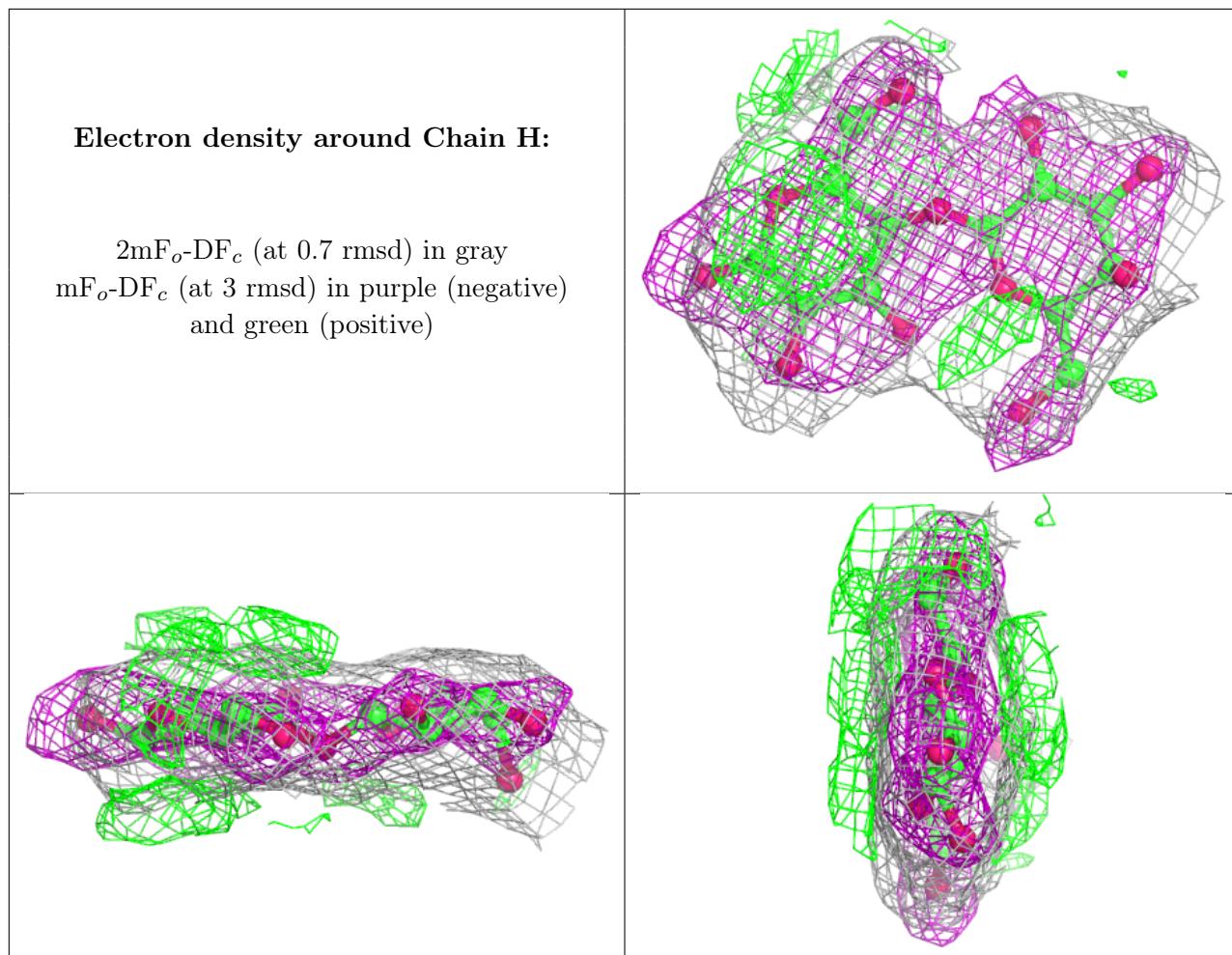
Continued on next page...

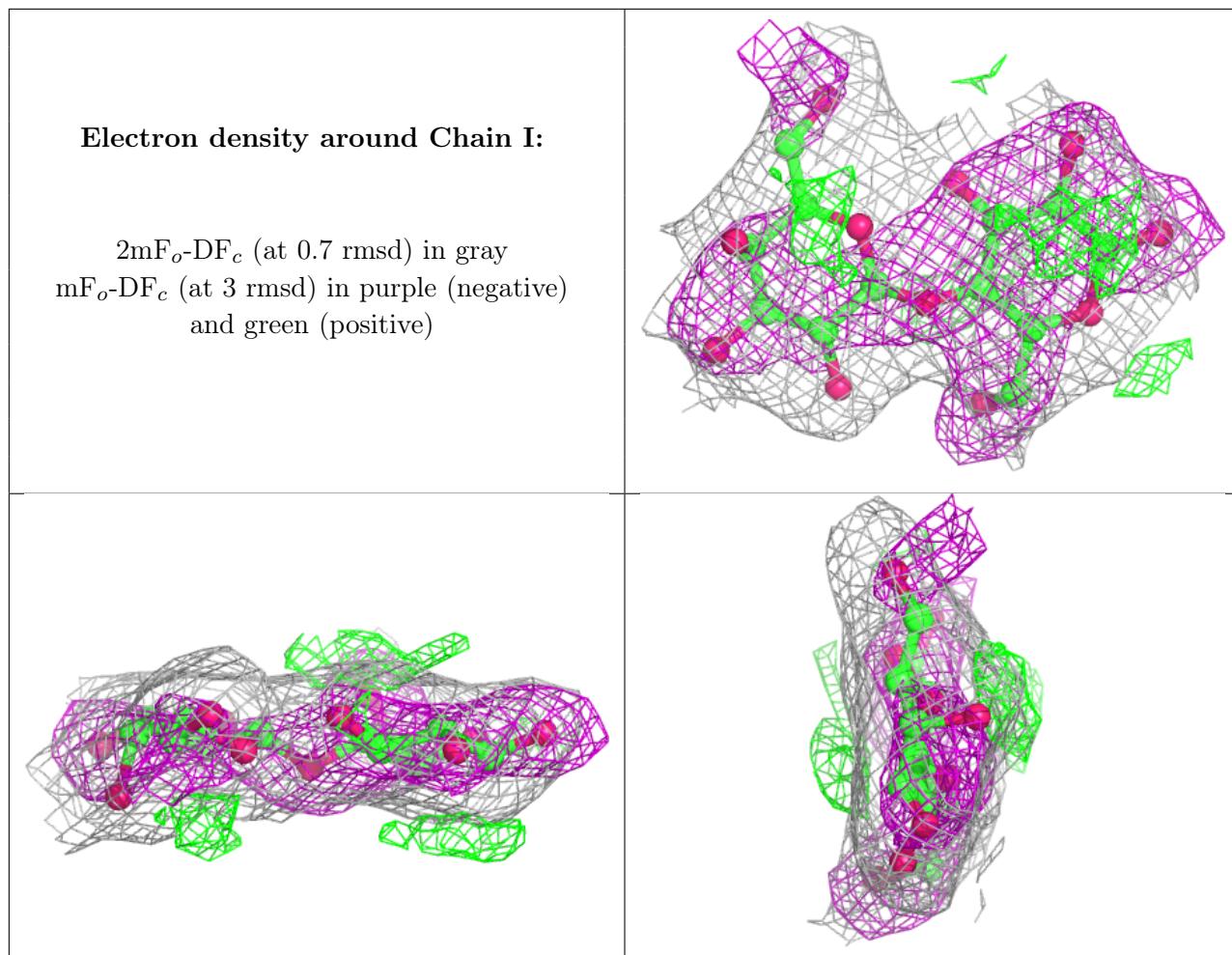
Continued from previous page...

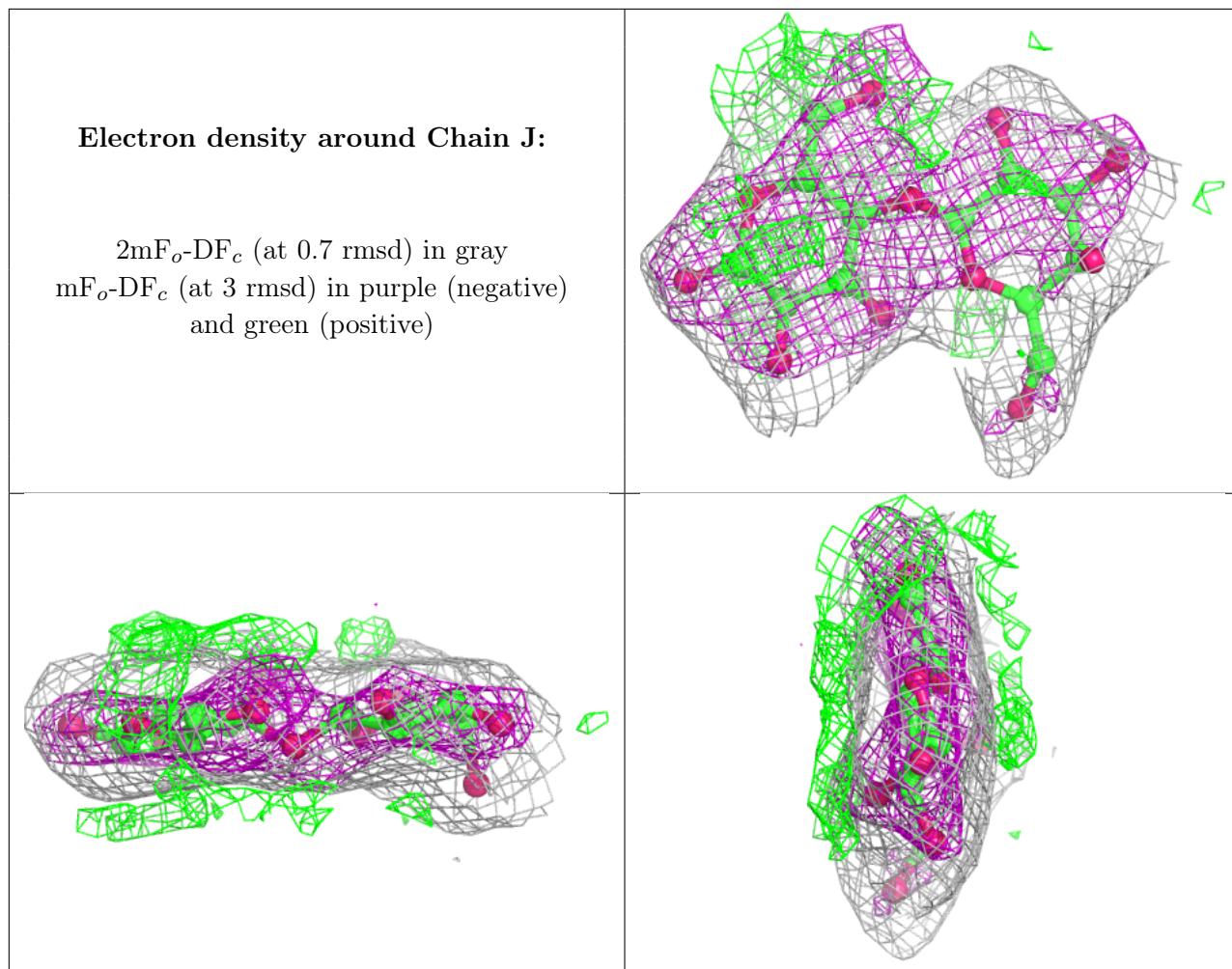
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GAL	G	2	11/12	0.93	0.17	19,19,19,19	0
2	GAL	L	2	11/12	0.93	0.14	19,19,19,19	0
2	GAL	H	2	11/12	0.95	0.20	19,19,19,19	0
2	GAL	J	2	11/12	0.96	0.20	19,19,19,19	0

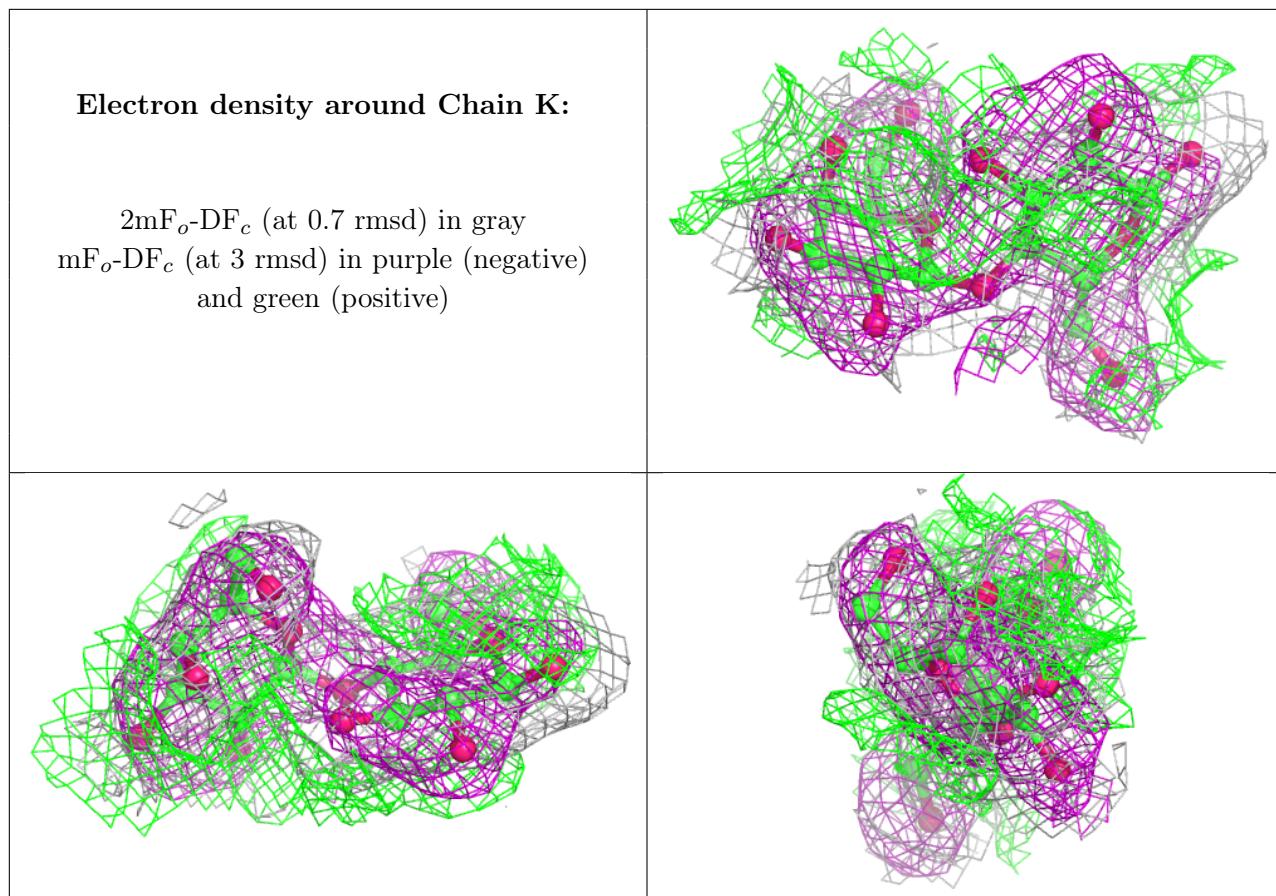
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

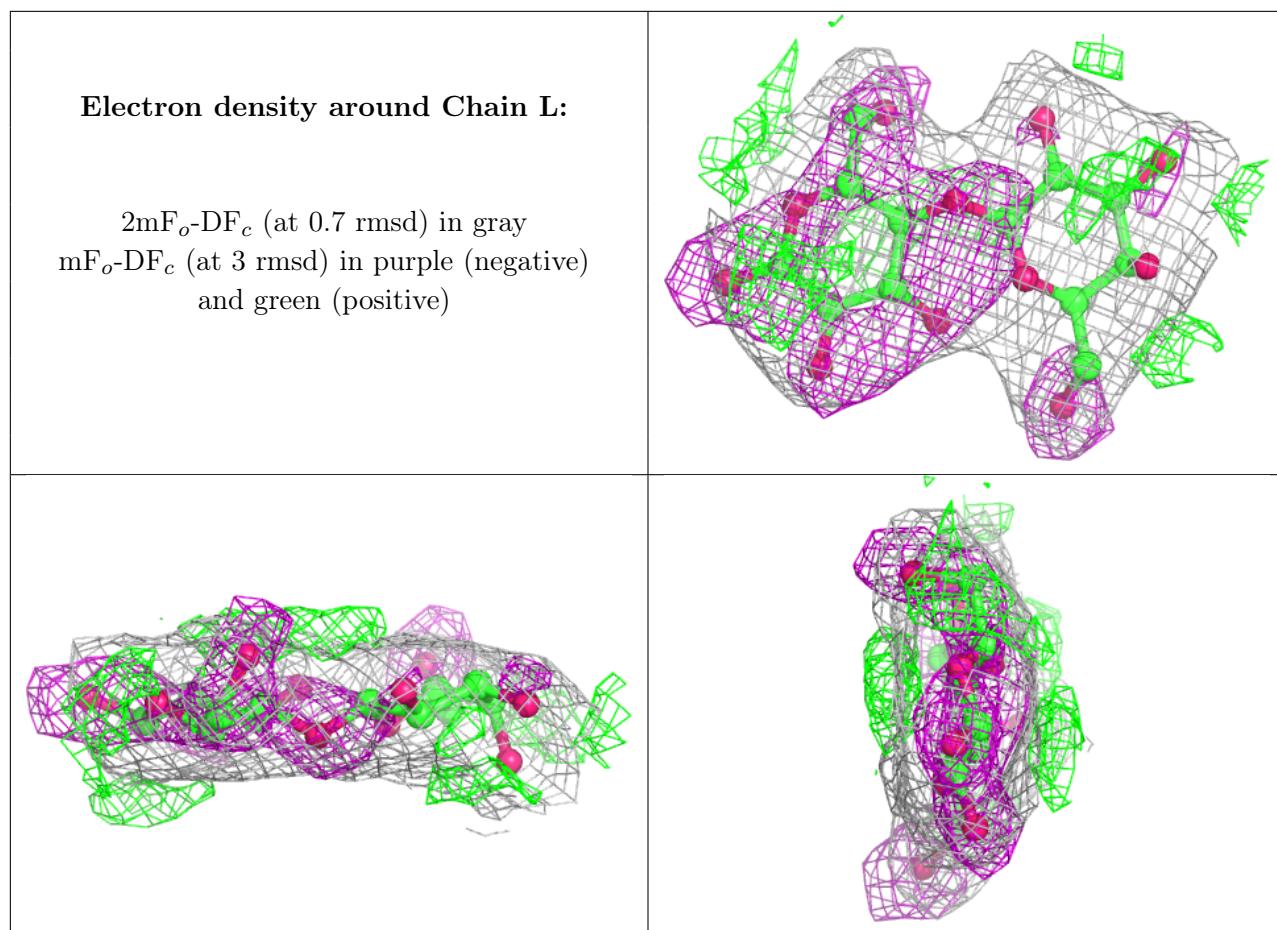












6.4 Ligands [\(i\)](#)

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	603	6/6	0.94	0.28	19,19,19,19	0
3	GOL	C	602	6/6	0.95	0.25	19,19,19,19	0
3	GOL	A	602	6/6	0.96	0.15	19,19,19,19	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.