Full wwPDB X-ray Structure Validation Report (i)

Mar 9, 2024 – 04:06 PM EST

PDB ID	:	3VSZ
Title	:	Crystal structure of Ct1,3Gal43A in complex with galactan
Authors	:	Jiang, D.; Fan, J.; Wang, X.; Zhao, Y.; Huang, B.; Zhang, X.C.
Deposited on	:	2012-05-18
Resolution	:	2.89 Å(reported)

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

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

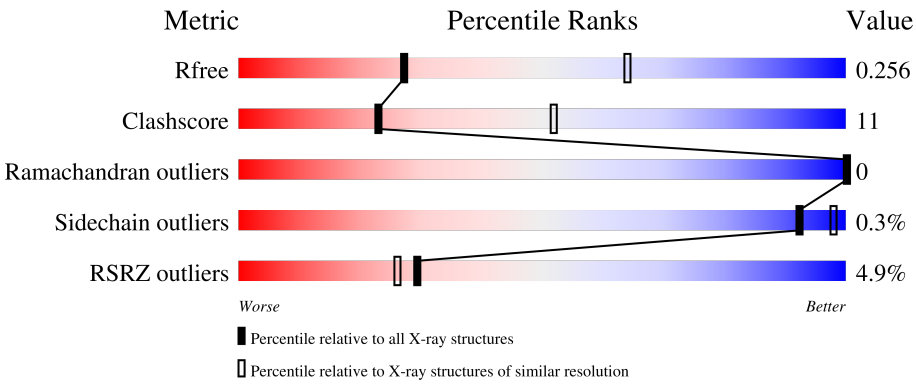
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.89 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	71% 17% 12%
1	B	526	2% 69% 18% 12%
1	C	526	76% 16% 8%
1	D	526	22% 63% 25% 12%
1	E	526	2% 70% 18% 12%

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Mol	Chain	Length	Quality of chain
1	F	526	% 69% 18% 12%
2	G	3	100%
2	H	3	100%
2	I	3	100%
2	J	3	100%
2	K	3	100%
3	L	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GAL	G	2	-	-	X	-
2	GAL	H	2	-	-	X	-
2	GAL	I	2	-	-	X	-
2	GAL	J	2	-	-	X	-
2	GAL	K	2	-	-	X	-
4	GOL	C	603	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 22399 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ricin B lectin.

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

There are 216 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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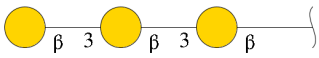
Chain	Residue	Modelled	Actual	Comment	Reference
F	-30	HIS	-	expression tag	UNP A3DD67
F	-29	HIS	-	expression tag	UNP A3DD67
F	-28	HIS	-	expression tag	UNP A3DD67
F	-27	HIS	-	expression tag	UNP A3DD67
F	-26	HIS	-	expression tag	UNP A3DD67
F	-25	SER	-	expression tag	UNP A3DD67
F	-24	SER	-	expression tag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

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



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

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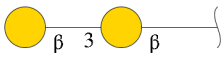
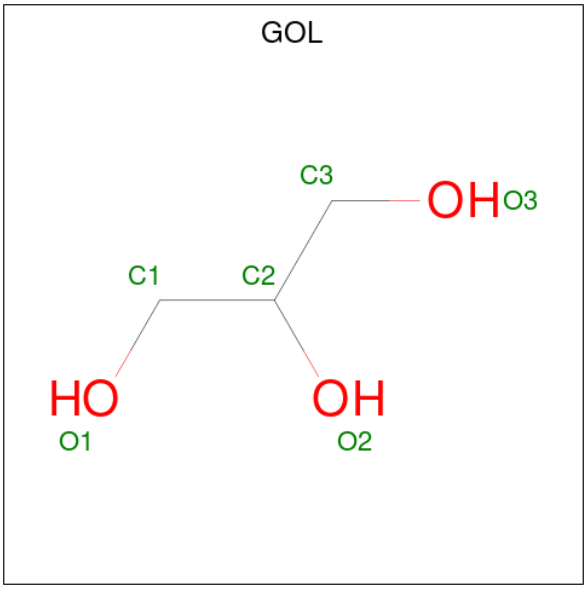
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	H	3	34	18	16	0	0	0
2	I	3	34	18	16	0	0	0
2	J	3	34	18	16	0	0	0
2	K	3	34	18	16	0	0	0

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



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 5 is water.

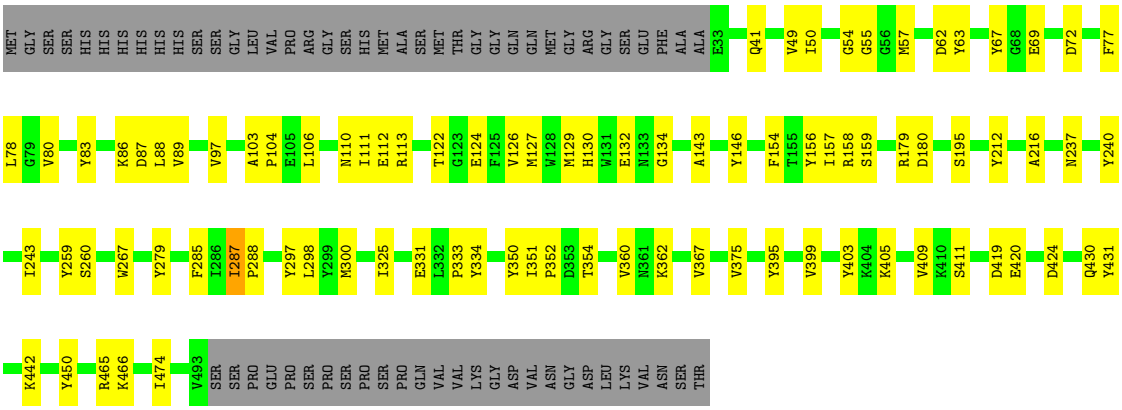
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	4	4	4	0	0
			Total	O		
5	C	9	9	9	0	0
			Total	O		
5	E	2	2	2	0	0
			Total	O		
5	F	4	4	4	0	0

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.

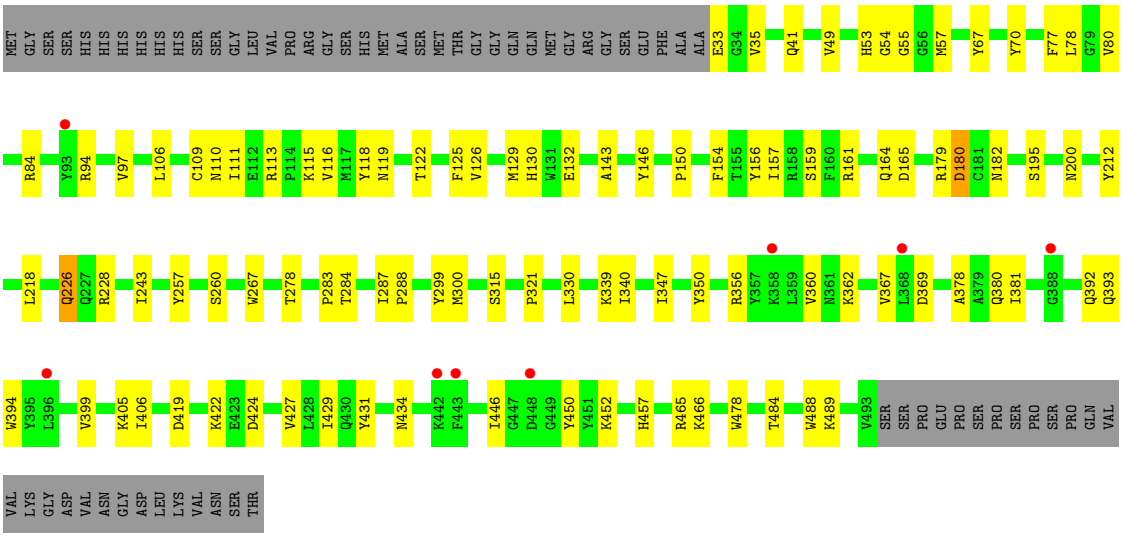
• Molecule 1: Ricin B lectin

Chain A: 71% 17% 12%



• Molecule 1: Ricin B lectin

Chain B: 2% 69% 18% 12%



• Molecule 1: Ricin B lectin

Chain C: 76% 16% 8%

MET GLY SER SER HIS HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG G-18 S-13 M-12 R-4 G34 V35 I36 T40 Q41 F42 I50 G54 G55 G56 M57 L58 K59 Y63 Y64 Y67 G68 E69 F77 Y83 R84 S85 K86 D87 L88 V89 R94

V97 P104 E105 L106 N107 H108 C109 N110 I111 E112 R113 V116 M129 N136 A143 F154 T155 Y156 F223 K235 Y240 Y241 L242 S245 W250 S260 W267 L270 P283 T284 F285 I286 I287 P288 M300 A305 W308 Y317 I340

T354 V360 N361 K362 V367 N377 A378 T385 V399 R413 D419 V427 L428 I429 Q430 Y431 T432 S433 N434 H440 I446 Y450 Y451 K452 R465 D471 I474 W478 T484 N485 K489 L492 V493 SER SER PRO GLU PRO SER PRO SER PRO

SER PRO GLN VAL VAL LYS GLY ASP VAL ASN GLY ASP LEU LYS VAL ASN SER THR

- Molecule 1: Ricin B lectin

Chain D: 22% 63% 25% 12%

MET GLY SER SER HIS HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET ALA SER MET THR GLY GLY GLN GLN MET GLY ARG GLY SER GLU PHE ALA ALA E33 G34 V35 Q41 F42 V49 I50 H51 A52 H53 G54 G55 Y64 Y67 G68 E69 Y70 R71

N75 L76 F77 V80 R84 D87 L88 Y93 R94 V97 L106 N110 I111 E112 R113 M117 Y118 N119 M127 W128 M129 E132 N133 G134 I135 N136 A143 S147 F154 T155 Y156 I157 R158 V168 Y176 D211 R228 I234 K235 R236

Y241 L242 I243 T244 S245 T248 N251 Q254 A255 K256 Y259 S260 A264 W267 L270 S276 T277 T278 P283 T284 G291 S292 S293 S296 Y297 L298 Y299 M300 L320 P321 L330 E331 L332 V338 K339 I340 G345 I346 I347 Y350 I351 T354 T355

R356 Y357 K358 L359 V360 N361 K362 N363 S364 G365 K366 V367 L368 D369 V370 L371 D372 G373 S374 V375 D376 N377 A378 A379 Q380 I381 V382 Q383 W384 N387 G388 S389 Q392 Q393 W394 Y395 L396 V397 D398 V399 G400 G401 G402 Y403 K404 K405 I406 V407 N408 V409 R413 A414 L415 D416 Y417 E420

S421 K422 E423 D424 G425 G426 V427 L428 I429 Q430 Y431 T432 G436 Y437 N438 Q439 H440 W441 K442 F443 T444 D445 I446 G447 D448 C449 Y450 Y451 K452 I453 S454 S455 R456 H457 C458 G459 K460 L461 I462 D463 V464 R465 K466 W467 S468 T469 E470 D471 G472 G473 I474 I475 Q476 Q477 W478 S479 D480 A481 G482

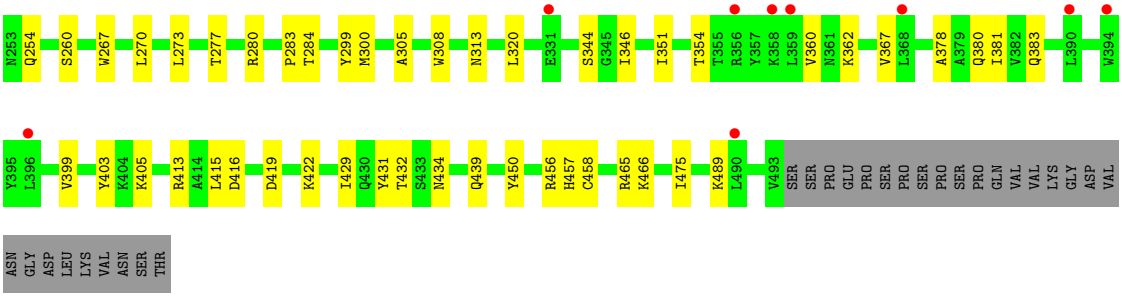
G483 T484 N485 Q486 H487 W488 K489 L490 V491 L492 V493 SER SER PRO GLU PRO SER PRO SER PRO SER PRO GLN VAL VAL LYS GLY ASP VAL ASN GLY ASP LEU LYS VAL ASN SER THR

- Molecule 1: Ricin B lectin

Chain E: 2% 70% 18% 12%

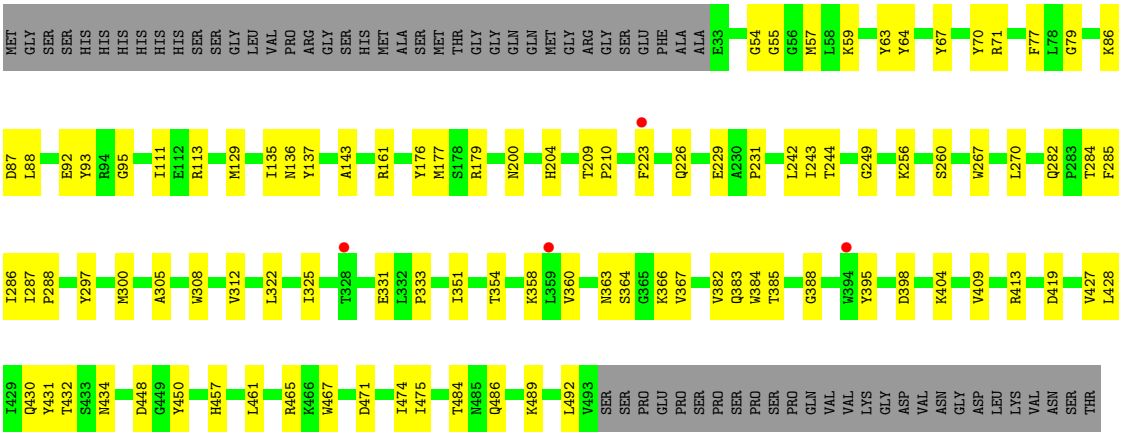
MET GLY SER SER HIS HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET ALA SER MET THR GLY GLY GLN GLN MET GLY ARG GLY SER GLU PHE ALA ALA E33 Q41 V49 H53 G54 G55 K59 Y64 Y67 G68 E69 Y70 R71 N75 L76

F77 L78 G79 V80 Y93 R94 G95 E96 V97 L106 C109 N110 I111 E112 R113 T122 G123 E124 M127 W128 M129 H130 W131 E132 A143 F154 T155 Y156 I157 V168 H171 Y176 A197 N198 E199 H204 K213 F223 L242 I243 T244 S245 N251 P252



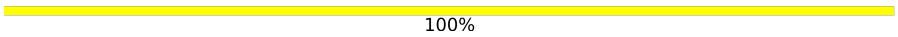
• Molecule 1: Ricin B lectin

Chain F:



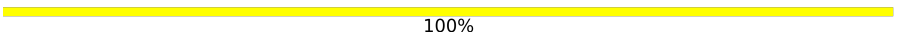
• Molecule 2: beta-D-galactopyranose-(1-3)-beta-D-galactopyranose-(1-3)-beta-D-galactopyranose

Chain G:



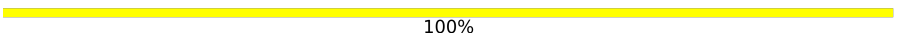
• Molecule 2: beta-D-galactopyranose-(1-3)-beta-D-galactopyranose-(1-3)-beta-D-galactopyranose

Chain H:



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

Chain I:



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

Chain J: 100%

GAL1
GAL2
GAL3

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

Chain K: 100%

GAL1
GAL2
GAL3

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

Chain L: 100%

GAL1
GAL2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	107.79Å 122.60Å 405.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.88 – 2.89 48.88 – 2.89	Depositor EDS
% Data completeness (in resolution range)	90.5 (48.88-2.89) 94.9 (48.88-2.89)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.7_650	Depositor
R, R_{free}	0.239 , 0.262 0.234 , 0.256	Depositor DCC
R_{free} test set	2038 reflections (1.78%)	wwPDB-VP
Wilson B-factor (Å^2)	60.8	Xtriage
Anisotropy	0.638	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 41.7	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	0.91	EDS
Total number of atoms	22399	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	0.21	0/3762	0.38	0/5104
1	B	0.20	0/3762	0.38	0/5104
1	C	0.21	0/3907	0.38	0/5295
1	D	0.21	0/3762	0.40	0/5104
1	E	0.21	0/3762	0.38	0/5104
1	F	0.21	0/3762	0.38	0/5104
All	All	0.21	0/22717	0.38	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	77	0
1	B	3664	0	3480	79	0
1	C	3807	0	3613	73	0
1	D	3664	0	3480	108	0
1	E	3664	0	3480	77	0
1	F	3664	0	3480	74	0
2	G	34	0	30	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	34	0	30	17	0
2	I	34	0	30	16	0
2	J	34	0	30	20	0
2	K	34	0	30	13	0
3	L	23	0	21	4	0
4	A	6	0	8	0	0
4	B	12	0	16	0	0
4	C	18	0	24	2	0
4	D	6	0	8	0	0
4	E	6	0	8	0	0
4	F	12	0	16	0	0
5	A	4	0	0	1	0
5	C	9	0	0	0	0
5	E	2	0	0	0	0
5	F	4	0	0	0	0
All	All	22399	0	21264	497	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 (497) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:453:ILE:HG13	1:D:461:LEU:HD11	1.21	1.14
1:D:446:ILE:HD11	1:D:452:LYS:HG3	1.27	1.13
2:J:2:GAL:H3	2:J:3:GAL:O2	1.55	1.03
2:H:2:GAL:H3	2:H:3:GAL:O2	1.59	1.00
1:D:453:ILE:HG13	1:D:461:LEU:CD1	1.94	0.96
1:B:419:ASP:OD1	2:H:2:GAL:O2	1.86	0.92
1:D:453:ILE:CG1	1:D:461:LEU:HD11	1.98	0.91
2:I:2:GAL:H3	2:I:3:GAL:O2	1.70	0.89
1:D:340:ILE:HG22	1:D:347:ILE:HG22	1.57	0.87
1:C:419:ASP:OD1	2:I:1:GAL:O2	1.92	0.87
1:B:419:ASP:HA	2:H:2:GAL:H2	1.60	0.84
1:C:34:GLY:HA2	1:C:89:VAL:HG21	1.59	0.82
1:D:380:GLN:HA	1:D:429:ILE:HG22	1.62	0.82
1:C:57:MET:HE2	1:C:287:ILE:HD13	1.63	0.80
1:F:282:GLN:HE22	3:L:2:GAL:H61	1.47	0.80
1:A:419:ASP:OD1	2:G:2:GAL:O2	1.99	0.80
1:D:465:ARG:HG2	1:D:466:LYS:HG2	1.64	0.79
1:E:419:ASP:HA	2:J:2:GAL:H2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:VAL:HG22	1:C:367:VAL:HG12	1.65	0.79
1:C:419:ASP:OD1	2:I:2:GAL:O2	2.00	0.78
1:A:285:PHE:HE2	1:A:287:ILE:HG23	1.50	0.77
1:D:422:LYS:HG3	1:D:458:CYS:HB3	1.67	0.77
2:J:2:GAL:C3	2:J:3:GAL:O2	2.30	0.77
2:H:2:GAL:C3	2:H:3:GAL:O2	2.33	0.77
1:E:422:LYS:HD3	1:E:458:CYS:HB3	1.65	0.76
1:F:461:LEU:HD11	1:F:486:GLN:HB3	1.67	0.76
1:A:285:PHE:CE2	1:A:287:ILE:HG23	2.21	0.76
1:C:260:SER:HB2	1:C:267:TRP:HA	1.69	0.76
1:C:-12:MET:HG3	1:E:155:THR:HG22	1.67	0.75
1:D:321:PRO:HB3	1:D:347:ILE:HD13	1.67	0.75
1:F:434:ASN:HD21	2:K:2:GAL:H61	1.51	0.74
1:B:84:ARG:HE	1:B:94:ARG:HE	1.34	0.74
1:E:431:TYR:CD2	2:J:2:GAL:H62	2.23	0.74
1:D:254:GLN:HG2	1:D:276:SER:HA	1.69	0.74
1:A:72:ASP:HB3	1:A:78:LEU:HD12	1.70	0.73
1:A:419:ASP:HA	2:G:2:GAL:H2	1.69	0.72
1:E:252:PRO:HB2	1:E:277:THR:HG23	1.72	0.71
1:B:419:ASP:HA	2:H:2:GAL:C2	2.21	0.70
1:D:443:PHE:CE2	1:D:453:ILE:HG22	2.26	0.70
1:F:229:GLU:CD	3:L:2:GAL:H62	2.12	0.70
2:I:2:GAL:C3	2:I:3:GAL:O2	2.40	0.70
1:B:356:ARG:HD3	1:B:393:GLN:NE2	2.08	0.69
1:A:419:ASP:HA	2:G:2:GAL:O3	1.93	0.69
1:B:419:ASP:CA	2:H:2:GAL:H2	2.23	0.69
1:E:111:ILE:HD11	1:E:131:TRP:HD1	1.57	0.69
1:F:360:VAL:HG22	1:F:367:VAL:HG12	1.74	0.69
1:B:360:VAL:HG22	1:B:367:VAL:HG12	1.73	0.68
1:C:223:PHE:HE2	1:C:242:LEU:HD23	1.57	0.68
1:E:54:GLY:O	1:E:113:ARG:HA	1.94	0.68
1:F:260:SER:HB2	1:F:267:TRP:HA	1.76	0.68
1:F:223:PHE:HE2	1:F:242:LEU:HD23	1.59	0.67
1:F:419:ASP:HA	2:K:2:GAL:O3	1.94	0.67
1:E:419:ASP:HA	2:J:2:GAL:C2	2.25	0.66
1:E:434:ASN:HD21	2:J:2:GAL:H61	1.60	0.66
1:A:157:ILE:HG22	1:A:158:ARG:HG2	1.78	0.66
1:C:465:ARG:HH21	1:C:474:ILE:HG21	1.61	0.65
1:D:461:LEU:HD12	1:D:462:ILE:H	1.60	0.65
1:D:377:ASN:HD21	1:D:432:THR:HG23	1.61	0.65
1:E:53:HIS:O	1:E:69:GLU:HG2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:419:ASP:HA	2:I:2:GAL:H2	1.79	0.64
1:F:77:PHE:CD1	1:F:111:ILE:HB	2.32	0.64
1:B:54:GLY:O	1:B:113:ARG:HA	1.98	0.63
1:F:57:MET:HE2	1:F:287:ILE:HD13	1.79	0.63
1:B:419:ASP:H	2:H:2:GAL:H2	1.64	0.62
1:D:420:GLU:HG2	1:D:438:ASN:ND2	2.14	0.62
1:C:84:ARG:HH21	1:C:94:ARG:NH1	1.98	0.62
1:A:420:GLU:OE1	2:G:3:GAL:H62	1.99	0.62
1:E:360:VAL:HG22	1:E:367:VAL:HG12	1.81	0.62
1:E:419:ASP:OD1	2:J:1:GAL:O2	2.17	0.62
1:E:413:ARG:NH1	1:E:432:THR:HG22	2.15	0.62
1:D:110:ASN:OD1	1:D:134:GLY:HA2	2.00	0.62
1:E:419:ASP:OD1	2:J:2:GAL:O2	2.12	0.61
1:E:383:GLN:HB3	1:E:475:ILE:HD11	1.82	0.61
1:B:179:ARG:HG3	1:B:200:ASN:OD1	2.00	0.61
1:C:77:PHE:CD1	1:C:111:ILE:HB	2.36	0.61
1:E:129:MET:HG2	1:E:143:ALA:HB3	1.82	0.61
1:B:106:LEU:HD11	1:B:156:TYR:CD2	2.36	0.61
1:D:395:TYR:CE2	1:D:409:VAL:HG22	2.36	0.61
1:D:387:ASN:H	1:D:392:GLN:HE22	1.47	0.60
1:C:485:ASN:HD21	4:C:601:GOL:H11	1.66	0.60
1:A:331:GLU:HG2	1:A:333:PRO:HD3	1.82	0.60
1:D:360:VAL:HA	1:D:367:VAL:HA	1.82	0.60
1:C:413:ARG:NH1	1:C:432:THR:HG22	2.17	0.60
1:D:380:GLN:HE22	1:D:474:ILE:HG13	1.66	0.60
1:F:71:ARG:HD3	1:F:312:VAL:HG11	1.83	0.60
1:C:55:GLY:HA3	1:C:67:TYR:O	2.02	0.60
1:D:35:VAL:HG22	1:D:339:LYS:HA	1.83	0.59
1:A:419:ASP:HA	2:G:2:GAL:C2	2.31	0.59
1:B:84:ARG:NE	1:B:94:ARG:HE	1.99	0.59
1:B:431:TYR:HE1	2:H:1:GAL:HO4	1.49	0.59
1:E:197:ALA:HB3	1:E:204:HIS:CE1	2.38	0.59
1:F:419:ASP:OD1	2:K:2:GAL:O2	2.17	0.59
1:F:428:LEU:HD12	1:F:475:ILE:HG22	1.84	0.59
1:B:419:ASP:HA	2:H:2:GAL:O3	2.03	0.59
1:B:419:ASP:N	2:H:2:GAL:H2	2.18	0.59
1:D:347:ILE:HD12	1:D:347:ILE:O	2.02	0.59
1:A:287:ILE:HD11	1:A:300:MET:HE3	1.83	0.59
1:C:54:GLY:O	1:C:113:ARG:HA	2.02	0.59
1:B:161:ARG:O	1:B:164:GLN:HG3	2.02	0.59
1:F:54:GLY:O	1:F:113:ARG:HA	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:SER:HB2	1:A:267:TRP:HA	1.84	0.58
1:E:77:PHE:CD1	1:E:111:ILE:HB	2.37	0.58
1:B:70:TYR:CZ	1:B:78:LEU:HD11	2.38	0.58
1:E:419:ASP:CA	2:J:2:GAL:H2	2.33	0.58
1:A:97:VAL:HB	1:A:154:PHE:CD2	2.38	0.58
1:D:415:LEU:HD21	1:D:462:ILE:HD11	1.85	0.58
1:A:419:ASP:OD1	2:G:1:GAL:O2	2.20	0.58
1:C:450:TYR:CE1	1:C:489:LYS:HB2	2.39	0.58
1:D:97:VAL:HB	1:D:154:PHE:CD2	2.39	0.58
1:D:260:SER:HB2	1:D:267:TRP:HA	1.86	0.58
1:D:380:GLN:NE2	1:D:474:ILE:HG13	2.19	0.58
1:B:419:ASP:OD1	2:H:1:GAL:O2	2.21	0.58
1:D:55:GLY:HA3	1:D:67:TYR:O	2.03	0.58
1:A:54:GLY:O	1:A:113:ARG:HA	2.04	0.57
1:D:41:GLN:HB3	1:D:49:VAL:HG13	1.86	0.57
1:D:360:VAL:HG12	1:D:489:LYS:HB2	1.86	0.57
1:E:223:PHE:HE2	1:E:242:LEU:HD23	1.67	0.57
1:B:446:ILE:HD13	1:B:452:LYS:HG3	1.85	0.57
1:D:84:ARG:HG2	1:D:94:ARG:HD3	1.85	0.57
1:D:106:LEU:HD22	1:D:111:ILE:HD11	1.85	0.57
1:E:416:ASP:HB3	1:E:439:GLN:HG2	1.85	0.57
1:F:431:TYR:CE1	2:K:1:GAL:O4	2.57	0.57
1:B:41:GLN:HB3	1:B:49:VAL:HG23	1.86	0.57
1:B:431:TYR:CD2	2:H:2:GAL:H62	2.39	0.57
1:A:360:VAL:HG22	1:A:367:VAL:HG12	1.86	0.56
1:F:231:PRO:HA	1:F:244:THR:HG22	1.87	0.56
1:D:54:GLY:O	1:D:113:ARG:HA	2.04	0.56
1:B:380:GLN:HE22	1:B:427:VAL:HG13	1.71	0.56
1:D:361:ASN:HB3	1:D:364:SER:OG	2.06	0.56
1:F:431:TYR:CD2	2:K:2:GAL:H62	2.40	0.56
1:C:419:ASP:H	2:I:2:GAL:H2	1.70	0.56
1:F:286:ILE:HD13	1:F:322:LEU:HD22	1.86	0.56
1:B:260:SER:HB2	1:B:267:TRP:HA	1.88	0.56
1:C:419:ASP:HA	2:I:2:GAL:C2	2.35	0.56
1:E:277:THR:HG22	1:E:277:THR:O	2.06	0.56
1:F:256:LYS:HD3	1:F:270:LEU:HB3	1.88	0.56
1:E:157:ILE:HD11	1:E:213:LYS:HD2	1.88	0.55
1:F:223:PHE:CE2	1:F:242:LEU:HD23	2.41	0.55
1:D:450:TYR:CE2	1:D:489:LYS:HE3	2.42	0.55
1:B:67:TYR:CE2	1:B:116:VAL:HG21	2.42	0.55
1:D:42:PHE:HB2	1:D:50:ILE:HD11	1.87	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	1.89	0.55
1:F:363:ASN:HB2	1:F:484:THR:OG1	2.07	0.55
1:D:296:SER:HB2	1:D:347:ILE:HD11	1.89	0.55
1:F:434:ASN:HD21	2:K:2:GAL:C6	2.21	0.54
1:D:291:GLY:HA3	1:D:345:GLY:HA3	1.89	0.54
1:A:279:TYR:CE2	1:A:334:TYR:HB2	2.43	0.54
1:B:55:GLY:HA3	1:B:67:TYR:O	2.07	0.54
1:D:360:VAL:CG1	1:D:489:LYS:HB2	2.37	0.54
1:D:462:ILE:HA	1:D:476:GLN:O	2.08	0.54
1:E:260:SER:HB2	1:E:267:TRP:HA	1.90	0.54
1:A:77:PHE:CD1	1:A:111:ILE:HB	2.42	0.54
1:B:110:ASN:HB2	1:B:132:GLU:HB2	1.90	0.54
1:A:103:ALA:HB3	1:A:106:LEU:HG	1.90	0.54
1:B:340:ILE:HG22	1:B:347:ILE:HG23	1.89	0.54
1:D:381:ILE:HG12	1:D:429:ILE:HA	1.89	0.54
1:F:419:ASP:OD1	2:K:1:GAL:O2	2.26	0.54
1:B:284:THR:HG22	1:B:300:MET:O	2.06	0.54
1:A:419:ASP:CA	2:G:2:GAL:H2	2.35	0.54
1:C:63:TYR:CE1	1:C:86:LYS:HE3	2.43	0.54
1:D:256:LYS:HD3	1:D:270:LEU:HB3	1.90	0.54
1:D:443:PHE:CD2	1:D:453:ILE:HG22	2.43	0.54
1:E:431:TYR:CE1	2:J:1:GAL:O4	2.61	0.54
1:B:130:HIS:CE1	1:B:179:ARG:HD3	2.43	0.53
1:C:63:TYR:CE1	1:C:84:ARG:NH1	2.76	0.53
1:C:97:VAL:HB	1:C:154:PHE:CD2	2.42	0.53
1:B:419:ASP:OD1	2:H:2:GAL:C2	2.56	0.53
1:C:362:LYS:HE3	1:C:484:THR:HG22	1.90	0.53
1:D:424:ASP:OD2	1:D:460:LYS:HD3	2.08	0.53
1:B:106:LEU:HD21	1:B:156:TYR:CE2	2.44	0.53
1:B:156:TYR:OH	1:B:159:SER:HB3	2.07	0.53
1:D:441:TRP:HA	1:D:454:SER:O	2.08	0.53
1:A:62:ASP:O	1:A:86:LYS:HG2	2.08	0.53
1:C:-13:SER:HA	1:C:492:LEU:HD11	1.90	0.53
1:D:484:THR:HA	1:D:487:HIS:CD2	2.42	0.53
1:D:453:ILE:HD11	1:D:462:ILE:HB	1.91	0.53
1:F:398:ASP:HA	1:F:404:LYS:HG2	1.91	0.53
1:B:97:VAL:HB	1:B:154:PHE:CD2	2.44	0.53
1:E:284:THR:HG22	1:E:300:MET:O	2.08	0.53
1:A:112:GLU:HB2	5:A:703:HOH:O	2.08	0.53
1:C:129:MET:HG2	1:C:143:ALA:HB3	1.91	0.53
1:D:110:ASN:HB2	1:D:132:GLU:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:305:ALA:HA	1:F:308:TRP:CZ2	2.43	0.53
1:E:168:VAL:HG11	1:E:176:TYR:CE1	2.43	0.52
1:E:419:ASP:H	2:J:2:GAL:H2	1.75	0.52
1:A:63:TYR:CE1	1:A:86:LYS:HE3	2.44	0.52
1:B:434:ASN:HD21	2:H:2:GAL:H61	1.74	0.52
1:C:84:ARG:HE	1:C:94:ARG:CZ	2.22	0.52
1:D:245:SER:HB3	1:D:283:PRO:HD2	1.90	0.52
1:F:135:ILE:HG22	1:F:136:ASN:HD22	1.74	0.52
1:A:279:TYR:CD2	1:A:334:TYR:HB2	2.44	0.52
1:B:78:LEU:C	1:B:78:LEU:HD12	2.29	0.52
1:D:450:TYR:CD1	1:D:489:LYS:HG3	2.44	0.52
1:A:419:ASP:OD1	2:G:2:GAL:C2	2.58	0.52
1:D:384:TRP:CZ3	1:D:471:ASP:HB3	2.44	0.52
1:D:444:THR:OG1	1:D:452:LYS:HB2	2.10	0.52
1:E:97:VAL:HB	1:E:154:PHE:CD2	2.45	0.52
1:C:59:LYS:HD3	1:C:64:TYR:CE1	2.44	0.52
1:B:129:MET:HG2	1:B:143:ALA:HB3	1.91	0.52
1:E:171:HIS:CE1	1:E:199:GLU:HB2	2.45	0.52
1:C:84:ARG:HE	1:C:94:ARG:NE	2.07	0.52
1:E:431:TYR:CE2	2:J:2:GAL:H62	2.45	0.51
2:J:2:GAL:O2	2:J:3:GAL:C2	2.58	0.51
1:E:416:ASP:CB	1:E:439:GLN:HG2	2.40	0.51
1:D:236:ARG:HA	1:D:297:TYR:OH	2.10	0.51
1:C:57:MET:CE	1:C:287:ILE:HG21	2.41	0.51
1:D:80:VAL:HG21	1:D:127:MET:HE1	1.93	0.51
2:I:1:GAL:HO2	2:I:2:GAL:HO2	1.58	0.51
1:B:97:VAL:HB	1:B:154:PHE:HD2	1.75	0.51
1:F:331:GLU:HG2	1:F:333:PRO:HD3	1.93	0.51
1:A:80:VAL:HG11	1:A:127:MET:HE3	1.91	0.51
1:D:157:ILE:HG22	1:D:158:ARG:HG2	1.92	0.51
1:E:434:ASN:ND2	2:J:2:GAL:H61	2.26	0.51
1:F:431:TYR:HE1	2:K:1:GAL:O4	1.93	0.51
1:D:284:THR:HG22	1:D:300:MET:O	2.11	0.50
1:E:80:VAL:HG11	1:E:127:MET:HE3	1.93	0.50
1:E:277:THR:HG22	1:E:280:ARG:H	1.76	0.50
1:C:58:LEU:HD22	1:C:116:VAL:HG12	1.93	0.50
1:D:71:ARG:HG2	1:D:75:ASN:C	2.32	0.50
1:D:453:ILE:CD1	1:D:462:ILE:HD12	2.42	0.50
1:A:69:GLU:HG2	1:A:112:GLU:HA	1.92	0.50
1:E:70:TYR:HB3	1:E:79:GLY:O	2.12	0.50
1:E:465:ARG:HG2	1:E:466:LYS:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:VAL:HG21	1:A:212:TYR:HB2	1.92	0.50
1:B:431:TYR:HE1	2:H:1:GAL:O4	1.95	0.50
1:C:419:ASP:HA	2:I:2:GAL:O3	2.11	0.50
1:F:59:LYS:HD3	1:F:64:TYR:CE1	2.47	0.50
1:D:476:GLN:HG2	1:D:477:GLN:H	1.77	0.50
1:E:122:THR:OG1	1:E:124:GLU:HG2	2.11	0.50
1:D:377:ASN:HD21	1:D:432:THR:H	1.59	0.49
1:A:325:ILE:HD11	1:A:331:GLU:OE2	2.12	0.49
1:C:235:LYS:HD2	1:C:240:TYR:CE2	2.47	0.49
1:D:376:ASP:C	1:D:413:ARG:HH12	2.14	0.49
2:G:1:GAL:O2	2:G:2:GAL:O2	2.30	0.49
1:B:57:MET:HE2	1:B:287:ILE:HG21	1.94	0.49
1:B:321:PRO:HB3	1:B:347:ILE:HG22	1.94	0.49
1:C:399:VAL:HG21	1:C:440:HIS:NE2	2.27	0.49
2:J:2:GAL:O2	2:J:3:GAL:H2	2.13	0.49
1:E:252:PRO:HB2	1:E:277:THR:CG2	2.42	0.49
1:F:363:ASN:ND2	1:F:467:TRP:HE3	2.10	0.49
2:K:3:GAL:HO4	2:K:3:GAL:HO6	1.60	0.49
1:A:122:THR:OG1	1:A:124:GLU:HG2	2.13	0.48
1:B:106:LEU:HD22	1:B:111:ILE:HD11	1.94	0.48
1:B:218:LEU:O	1:B:218:LEU:HD12	2.13	0.48
1:B:356:ARG:HD3	1:B:393:GLN:HE22	1.78	0.48
1:F:135:ILE:HD12	1:F:135:ILE:N	2.28	0.48
1:F:430:GLN:O	1:F:430:GLN:HG3	2.13	0.48
1:F:431:TYR:CE1	2:K:1:GAL:H4	2.48	0.48
1:C:362:LYS:HB2	1:C:450:TYR:CE1	2.47	0.48
1:D:117:MET:HE3	1:D:128:TRP:CD1	2.48	0.48
1:F:465:ARG:HH21	1:F:474:ILE:HG21	1.78	0.48
1:B:125:PHE:CZ	1:B:150:PRO:HG3	2.49	0.48
1:B:434:ASN:ND2	2:H:2:GAL:H61	2.28	0.48
1:C:419:ASP:CA	2:I:2:GAL:H2	2.44	0.48
1:D:443:PHE:HE2	1:D:453:ILE:HG22	1.73	0.48
1:F:129:MET:CG	1:F:143:ALA:HB3	2.43	0.48
1:F:284:THR:HG22	1:F:300:MET:O	2.14	0.48
1:A:129:MET:HG2	1:A:143:ALA:HB3	1.95	0.48
1:A:146:TYR:CD2	1:A:157:ILE:HD11	2.48	0.48
1:D:35:VAL:HG21	1:D:350:TYR:CD1	2.48	0.48
1:B:115:LYS:HG3	1:B:182:ASN:HA	1.96	0.48
1:B:369:ASP:HB2	1:B:392:GLN:HG2	1.96	0.48
1:C:77:PHE:CZ	1:C:111:ILE:HD12	2.48	0.48
1:D:147:SER:HB2	1:D:154:PHE:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:360:VAL:O	1:D:488:TRP:HA	2.13	0.48
1:F:431:TYR:CE1	2:K:1:GAL:C4	2.97	0.48
1:A:424:ASP:O	1:C:136:ASN:HB2	2.14	0.48
1:D:474:ILE:HD12	1:D:474:ILE:N	2.29	0.48
1:C:64:TYR:CG	1:C:88:LEU:HD21	2.49	0.47
1:D:448:ASP:O	1:D:489:LYS:HE2	2.14	0.47
1:B:378:ALA:HA	1:B:429:ILE:HD12	1.96	0.47
1:C:42:PHE:CE2	1:C:317:TYR:HB2	2.49	0.47
1:E:80:VAL:HG21	1:E:127:MET:CE	2.43	0.47
1:E:41:GLN:HB3	1:E:49:VAL:HG13	1.96	0.47
1:A:431:TYR:CE1	2:G:1:GAL:H4	2.49	0.47
1:B:283:PRO:HB3	1:B:299:TYR:HE1	1.78	0.47
1:F:434:ASN:ND2	2:K:2:GAL:H61	2.26	0.47
1:D:168:VAL:HG21	1:D:176:TYR:CE1	2.50	0.47
1:A:110:ASN:OD1	1:A:134:GLY:HA2	2.15	0.47
1:B:53:HIS:CD2	1:B:315:SER:HB2	2.49	0.47
1:D:119:ASN:HD21	1:D:211:ASP:HA	1.79	0.47
1:E:383:GLN:O	1:E:383:GLN:HG3	2.14	0.47
1:F:249:GLY:HA2	3:L:1:GAL:O4	2.15	0.47
1:F:325:ILE:H	1:F:325:ILE:HD12	1.80	0.47
1:D:299:TYR:HB3	1:D:320:LEU:O	2.15	0.47
1:E:245:SER:HB3	1:E:283:PRO:HD2	1.97	0.47
1:F:366:LYS:HE3	1:F:385:THR:HG22	1.97	0.47
1:B:146:TYR:CD2	1:B:157:ILE:HD11	2.50	0.47
1:A:419:ASP:H	2:G:2:GAL:H2	1.80	0.47
1:F:129:MET:HG2	1:F:143:ALA:HB3	1.96	0.47
1:F:209:THR:HB	1:F:210:PRO:HD2	1.98	0.47
2:J:2:GAL:O2	2:J:3:GAL:O2	2.30	0.47
1:B:450:TYR:CE1	1:B:489:LYS:HB2	2.50	0.46
1:C:69:GLU:HG3	1:C:111:ILE:O	2.15	0.46
1:C:431:TYR:CE2	2:I:2:GAL:H61	2.50	0.46
1:E:419:ASP:N	2:J:2:GAL:H2	2.30	0.46
1:C:104:PRO:HA	1:C:107:ASN:OD1	2.16	0.46
1:C:64:TYR:O	1:C:84:ARG:HA	2.15	0.46
1:D:106:LEU:HD11	1:D:156:TYR:CD2	2.50	0.46
1:D:453:ILE:O	1:D:461:LEU:HD13	2.14	0.46
1:D:461:LEU:O	1:D:477:GLN:HA	2.15	0.46
1:C:413:ARG:HH12	1:C:432:THR:HG22	1.80	0.46
1:D:453:ILE:HD11	1:D:462:ILE:HD12	1.98	0.46
1:E:109:CYS:HB2	1:E:132:GLU:O	2.15	0.46
1:E:254:GLN:NE2	1:E:273:LEU:H	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:422:LYS:HE2	1:E:457:HIS:CD2	2.51	0.46
1:F:70:TYR:HB3	1:F:79:GLY:O	2.16	0.46
1:F:325:ILE:HD11	1:F:331:GLU:OE1	2.16	0.46
1:D:379:ALA:HB3	1:D:430:GLN:HG2	1.97	0.46
1:E:71:ARG:HB2	1:E:313:ASN:HD21	1.81	0.46
1:A:110:ASN:HB2	1:A:132:GLU:HB2	1.98	0.46
1:F:395:TYR:CE2	1:F:409:VAL:HG22	2.51	0.46
1:A:237:ASN:OD1	1:F:448:ASP:HA	2.16	0.45
1:A:351:ILE:HD12	1:A:351:ILE:N	2.31	0.45
1:C:419:ASP:N	2:I:2:GAL:H2	2.31	0.45
1:F:413:ARG:NH1	1:F:432:THR:HG22	2.31	0.45
1:C:223:PHE:CE2	1:C:242:LEU:HD23	2.43	0.45
1:C:270:LEU:HD12	1:C:270:LEU:N	2.31	0.45
1:E:351:ILE:N	1:E:351:ILE:HD12	2.30	0.45
1:A:375:VAL:HG12	1:A:411:SER:HB3	1.97	0.45
1:D:248:THR:O	1:D:251:ASN:HB2	2.16	0.45
1:F:382:VAL:HA	1:F:475:ILE:HG12	1.98	0.45
1:C:284:THR:HG22	1:C:300:MET:O	2.17	0.45
1:A:156:TYR:OH	1:A:159:SER:HB3	2.17	0.45
1:C:-13:SER:HA	1:C:492:LEU:CD1	2.47	0.45
1:D:77:PHE:CD1	1:D:111:ILE:HB	2.51	0.45
1:B:381:ILE:HG12	1:B:429:ILE:HA	1.99	0.45
1:C:385:THR:HG23	1:C:471:ASP:OD1	2.16	0.45
1:D:450:TYR:HB3	1:D:487:HIS:HB3	1.98	0.45
1:A:63:TYR:CZ	1:A:86:LYS:HE3	2.52	0.45
1:F:419:ASP:HA	2:K:2:GAL:H2	1.99	0.45
2:G:1:GAL:HO2	2:G:2:GAL:HO2	1.61	0.45
1:E:106:LEU:HD11	1:E:156:TYR:CD2	2.50	0.45
1:E:431:TYR:HE1	2:J:1:GAL:O4	2.00	0.45
1:B:146:TYR:HD2	1:B:157:ILE:HD11	1.81	0.45
1:C:106:LEU:HD22	1:C:111:ILE:HD11	1.99	0.45
1:C:492:LEU:HD12	1:C:492:LEU:N	2.32	0.45
1:F:285:PHE:HE2	1:F:287:ILE:HB	1.81	0.45
1:D:35:VAL:CG2	1:D:339:LYS:HE3	2.47	0.45
1:D:80:VAL:HG11	1:D:127:MET:HE3	1.99	0.45
1:D:278:THR:HG22	1:D:278:THR:O	2.17	0.45
1:E:197:ALA:HB3	1:E:204:HIS:ND1	2.32	0.45
1:E:305:ALA:HA	1:E:308:TRP:CZ2	2.52	0.45
1:F:351:ILE:HD12	1:F:351:ILE:N	2.32	0.45
1:A:97:VAL:HB	1:A:154:PHE:HD2	1.78	0.44
1:A:243:ILE:N	1:A:243:ILE:HD12	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:381:ILE:HG13	1:E:415:LEU:CD1	2.47	0.44
1:F:55:GLY:HA3	1:F:67:TYR:O	2.17	0.44
1:F:450:TYR:CE1	1:F:489:LYS:HB2	2.51	0.44
1:A:55:GLY:HA3	1:A:67:TYR:O	2.17	0.44
1:B:339:LYS:HB2	1:B:350:TYR:HB2	2.00	0.44
1:E:111:ILE:HD11	1:E:131:TRP:CD1	2.45	0.44
1:B:118:TYR:HD2	1:B:125:PHE:CE1	2.35	0.44
1:D:243:ILE:N	1:D:243:ILE:HD12	2.32	0.44
1:F:93:TYR:CZ	1:F:95:GLY:HA2	2.52	0.44
1:A:474:ILE:HD12	1:A:474:ILE:N	2.33	0.44
1:B:33:GLU:HG2	1:B:35:VAL:HG12	1.98	0.44
1:D:354:THR:HG22	1:D:354:THR:O	2.18	0.44
1:D:366:LYS:HE3	1:D:383:GLN:OE1	2.18	0.44
1:E:362:LYS:HD3	1:E:450:TYR:CZ	2.53	0.44
1:F:161:ARG:HH22	1:F:177:MET:HG2	1.83	0.44
1:A:50:ILE:HG23	1:A:83:TYR:CE1	2.53	0.44
1:A:466:LYS:HB3	1:C:250:TRP:CD1	2.53	0.44
1:D:53:HIS:O	1:D:69:GLU:HG2	2.17	0.44
1:D:338:VAL:HG12	1:D:340:ILE:HG23	1.98	0.44
1:E:399:VAL:HG11	1:E:405:LYS:HG3	1.99	0.44
1:F:287:ILE:HA	1:F:288:PRO:HD3	1.86	0.44
1:A:399:VAL:HG11	1:A:405:LYS:HG3	2.00	0.44
1:E:380:GLN:HE21	1:E:381:ILE:N	2.15	0.44
1:B:287:ILE:HA	1:B:288:PRO:HD3	1.88	0.44
1:C:354:THR:HG22	1:C:354:THR:O	2.17	0.44
1:D:77:PHE:CZ	1:D:111:ILE:HD12	2.53	0.44
1:F:288:PRO:HG3	1:F:297:TYR:CE1	2.53	0.44
2:I:2:GAL:O2	2:I:3:GAL:O2	2.30	0.44
1:A:41:GLN:HB3	1:A:49:VAL:HG23	1.99	0.43
1:A:130:HIS:CD2	1:A:179:ARG:HA	2.54	0.43
1:A:216:ALA:O	1:B:165:ASP:HA	2.18	0.43
1:A:403:TYR:CD1	1:A:442:LYS:HB2	2.53	0.43
1:B:57:MET:CE	1:B:287:ILE:HG21	2.47	0.43
1:B:422:LYS:HE3	1:B:457:HIS:NE2	2.33	0.43
1:C:106:LEU:HD11	1:C:156:TYR:CD2	2.53	0.43
1:D:461:LEU:CD1	1:D:462:ILE:H	2.30	0.43
1:E:55:GLY:HA3	1:E:67:TYR:O	2.18	0.43
1:E:93:TYR:CZ	1:E:95:GLY:HA2	2.53	0.43
1:E:413:ARG:HH11	1:E:432:THR:HG22	1.83	0.43
1:C:434:ASN:HD21	2:I:2:GAL:C6	2.32	0.43
1:D:228:ARG:HB3	1:D:244:THR:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:ASP:N	2:G:2:GAL:H2	2.33	0.43
1:B:362:LYS:HG3	1:B:484:THR:HB	1.99	0.43
1:D:119:ASN:ND2	1:D:211:ASP:HA	2.33	0.43
1:A:106:LEU:HD11	1:A:156:TYR:CD2	2.53	0.43
1:B:362:LYS:HE2	1:B:450:TYR:CZ	2.53	0.43
1:E:299:TYR:HB3	1:E:320:LEU:O	2.17	0.43
1:C:305:ALA:HA	1:C:308:TRP:CZ2	2.53	0.43
1:D:35:VAL:HG23	1:D:339:LYS:HE3	2.00	0.43
1:D:35:VAL:HG21	1:D:350:TYR:CG	2.54	0.43
1:E:380:GLN:HE21	1:E:381:ILE:H	1.67	0.43
1:F:87:ASP:O	1:F:88:LEU:HB2	2.19	0.43
1:A:288:PRO:HG3	1:A:297:TYR:CE1	2.54	0.43
1:A:362:LYS:HD3	1:A:450:TYR:CZ	2.53	0.43
1:D:87:ASP:O	1:D:88:LEU:HB2	2.19	0.43
1:D:394:TRP:CE3	1:D:406:ILE:HG22	2.54	0.43
1:A:77:PHE:CZ	1:A:80:VAL:HG23	2.54	0.42
1:C:57:MET:HE1	1:C:287:ILE:HG21	2.00	0.42
1:D:376:ASP:O	1:D:379:ALA:HB2	2.19	0.42
1:D:377:ASN:ND2	1:D:432:THR:HG23	2.29	0.42
1:D:382:VAL:HA	1:D:475:ILE:HG12	2.01	0.42
1:E:59:LYS:HD3	1:E:64:TYR:CE1	2.54	0.42
1:D:135:ILE:HG13	1:D:136:ASN:ND2	2.35	0.42
1:E:344:SER:HB3	1:E:346:ILE:HD13	2.00	0.42
2:H:2:GAL:O2	2:H:3:GAL:O2	2.33	0.42
1:A:87:ASP:O	1:A:88:LEU:HB2	2.19	0.42
1:A:287:ILE:HD12	1:A:298:LEU:HB3	2.00	0.42
1:C:377:ASN:OD1	1:C:431:TYR:HA	2.20	0.42
1:E:129:MET:CG	1:E:143:ALA:HB3	2.50	0.42
1:A:240:TYR:O	1:A:259:TYR:HA	2.18	0.42
1:B:450:TYR:HA	1:B:488:TRP:O	2.19	0.42
1:C:285:PHE:HE2	1:C:287:ILE:HB	1.84	0.42
1:C:431:TYR:CD2	2:I:2:GAL:C6	3.02	0.42
1:E:277:THR:HG22	1:E:280:ARG:HA	2.02	0.42
1:E:450:TYR:CE1	1:E:489:LYS:HB2	2.55	0.42
1:F:325:ILE:HD12	1:F:325:ILE:N	2.33	0.42
1:F:364:SER:OG	1:F:366:LYS:HG2	2.19	0.42
1:F:383:GLN:HB3	1:F:475:ILE:HD11	2.02	0.42
1:A:103:ALA:HB1	1:A:104:PRO:HD2	2.00	0.42
1:A:395:TYR:CE2	1:A:409:VAL:HG22	2.55	0.42
1:B:399:VAL:HG11	1:B:405:LYS:HG3	2.02	0.42
1:E:251:ASN:HA	1:E:252:PRO:HD3	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:243:ILE:N	1:F:243:ILE:HD12	2.34	0.42
1:F:358:LYS:HZ2	1:F:388:GLY:HA2	1.83	0.42
1:B:109:CYS:HB2	1:B:132:GLU:O	2.20	0.42
1:D:395:TYR:CZ	1:D:409:VAL:HG22	2.55	0.42
1:F:354:THR:HG22	1:F:354:THR:O	2.20	0.42
1:A:354:THR:HG22	1:A:354:THR:O	2.20	0.42
1:B:130:HIS:CE1	1:B:179:ARG:HA	2.54	0.42
1:B:465:ARG:HG2	1:B:466:LYS:HG2	2.02	0.42
1:A:474:ILE:HD12	1:A:474:ILE:H	1.84	0.41
1:C:287:ILE:HA	1:C:288:PRO:HD3	1.87	0.41
1:C:431:TYR:CD2	2:I:2:GAL:H62	2.55	0.41
1:D:361:ASN:HB2	1:D:488:TRP:CZ3	2.54	0.41
1:D:351:ILE:N	1:D:351:ILE:HD12	2.35	0.41
1:B:243:ILE:HD12	1:B:243:ILE:N	2.36	0.41
1:E:431:TYR:CE1	2:J:1:GAL:H4	2.55	0.41
1:E:431:TYR:CE1	2:J:1:GAL:C4	3.04	0.41
1:F:63:TYR:CE1	1:F:86:LYS:HE3	2.55	0.41
1:A:57:MET:CB	1:A:300:MET:HE1	2.51	0.41
1:C:378:ALA:HA	1:C:429:ILE:HD12	2.02	0.41
1:C:478:TRP:CE3	4:C:601:GOL:H32	2.55	0.41
1:D:129:MET:CG	1:D:143:ALA:HB3	2.51	0.41
1:E:243:ILE:HD12	1:E:243:ILE:N	2.35	0.41
1:F:176:TYR:CD1	1:F:204:HIS:HE1	2.38	0.41
1:A:87:ASP:OD1	1:A:89:VAL:HB	2.20	0.41
1:B:226:GLN:HB3	1:B:228:ARG:HG2	2.01	0.41
1:C:77:PHE:HB2	1:C:111:ILE:H	1.85	0.41
1:C:446:ILE:HG21	1:C:452:LYS:HG3	2.02	0.41
1:D:320:LEU:HB2	1:D:332:LEU:HD11	2.01	0.41
1:B:424:ASP:HB3	1:B:478:TRP:CE3	2.56	0.41
1:B:257:TYR:CE2	1:B:330:LEU:HD13	2.55	0.41
1:C:50:ILE:HG23	1:C:83:TYR:CE1	2.56	0.41
1:F:179:ARG:HD2	1:F:200:ASN:OD1	2.21	0.41
1:D:64:TYR:CG	1:D:88:LEU:HD21	2.56	0.41
1:A:130:HIS:NE2	1:A:179:ARG:HA	2.36	0.41
1:A:465:ARG:HH21	1:A:474:ILE:HG21	1.86	0.41
1:B:180:ASP:O	1:B:195:SER:HA	2.20	0.41
1:B:278:THR:HG22	1:B:278:THR:O	2.21	0.41
1:C:223:PHE:CD1	1:C:270:LEU:HD11	2.56	0.41
1:C:245:SER:HB3	1:C:283:PRO:HD2	2.03	0.41
1:D:293:SER:OG	1:D:346:ILE:HD13	2.21	0.41
1:E:71:ARG:NH1	1:E:75:ASN:HD21	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:354:THR:HG22	1:E:354:THR:O	2.21	0.41
1:A:287:ILE:CD1	1:A:298:LEU:HB3	2.52	0.40
1:B:57:MET:HE2	1:B:57:MET:HB3	2.01	0.40
1:B:394:TRP:CE3	1:B:406:ILE:HG22	2.56	0.40
1:E:80:VAL:HG21	1:E:127:MET:HE3	2.03	0.40
1:B:77:PHE:CE1	1:B:80:VAL:HG23	2.56	0.40
1:B:119:ASN:HB3	1:B:122:THR:OG1	2.20	0.40
1:B:126:VAL:HG21	1:B:212:TYR:HB2	2.02	0.40
1:C:106:LEU:HA	1:C:109:CYS:SG	2.61	0.40
1:D:52:ALA:CA	1:D:68:GLY:HA3	2.51	0.40
1:D:77:PHE:CE1	1:D:111:ILE:HD12	2.57	0.40
1:A:405:LYS:HE2	1:A:405:LYS:HB3	1.86	0.40
1:A:419:ASP:HA	2:G:2:GAL:C3	2.51	0.40
1:A:430:GLN:O	1:A:430:GLN:HG3	2.20	0.40
1:A:431:TYR:HE1	2:G:1:GAL:H4	1.87	0.40
1:C:40:THR:HB	1:F:92:GLU:OE2	2.21	0.40
1:D:381:ILE:HG22	1:D:475:ILE:HG13	2.03	0.40
1:F:492:LEU:N	1:F:492:LEU:HD12	2.36	0.40
1:A:57:MET:HB3	1:A:300:MET:HE1	2.04	0.40
1:A:180:ASP:O	1:A:195:SER:HA	2.20	0.40
1:A:350:TYR:O	1:A:352:PRO:HD3	2.21	0.40
1:C:36:ILE:HD13	1:C:340:ILE:HD12	2.03	0.40
1:D:234:ILE:HD11	1:D:241:TYR:HB2	2.03	0.40
1:F:367:VAL:HG22	1:F:384:TRP:O	2.21	0.40
1:E:378:ALA:HA	1:E:429:ILE:HD12	2.03	0.40
1:E:403:TYR:CZ	1:E:456:ARG:HG3	2.56	0.40
1:F:137:TYR:OH	3:L:1:GAL:O2	2.32	0.40
1:F:385:THR:HG23	1:F:471:ASP:OD1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

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

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	389/442 (88%)	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%)	388 (100%)	1 (0%)	92	98
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%)	2339 (100%)	8 (0%)	92	98

All (8) 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	E	270	LEU
1	F	427	VAL

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Mol	Chain	Res	Type
1	F	457	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	B	130	HIS
1	B	487	HIS
1	C	53	HIS
1	D	380	GLN
1	D	392	GLN
1	E	171	HIS
1	E	457	HIS
1	F	282	GLN
1	F	313	ASN
1	F	477	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

17 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GAL	G	1	2	12,12,12	0.55	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	G	2	2	11,11,12	0.66	0	15,15,17	0.64	0
2	GAL	G	3	2	11,11,12	0.68	0	15,15,17	0.64	0
2	GAL	H	1	2	12,12,12	0.55	0	17,17,17	0.53	0
2	GAL	H	2	2	11,11,12	0.66	0	15,15,17	0.64	0
2	GAL	H	3	2	11,11,12	0.68	0	15,15,17	0.63	0
2	GAL	I	1	2	12,12,12	0.55	0	17,17,17	0.53	0
2	GAL	I	2	2	11,11,12	0.67	0	15,15,17	0.63	0
2	GAL	I	3	2	11,11,12	0.67	0	15,15,17	0.64	0
2	GAL	J	1	2	12,12,12	0.56	0	17,17,17	0.53	0
2	GAL	J	2	2	11,11,12	0.67	0	15,15,17	0.63	0
2	GAL	J	3	2	11,11,12	0.67	0	15,15,17	0.64	0
2	GAL	K	1	2	12,12,12	0.54	0	17,17,17	0.52	0
2	GAL	K	2	2	11,11,12	0.67	0	15,15,17	0.64	0
2	GAL	K	3	2	11,11,12	0.68	0	15,15,17	0.64	0
3	GAL	L	1	3	12,12,12	0.56	0	17,17,17	0.53	0
3	GAL	L	2	3	11,11,12	0.67	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	GAL	G	1	2	-	2/2/22/22	0/1/1/1
2	GAL	G	2	2	-	2/2/19/22	0/1/1/1
2	GAL	G	3	2	-	0/2/19/22	0/1/1/1
2	GAL	H	1	2	-	2/2/22/22	0/1/1/1
2	GAL	H	2	2	-	1/2/19/22	0/1/1/1
2	GAL	H	3	2	-	2/2/19/22	0/1/1/1
2	GAL	I	1	2	-	2/2/22/22	0/1/1/1
2	GAL	I	2	2	-	2/2/19/22	0/1/1/1
2	GAL	I	3	2	-	0/2/19/22	0/1/1/1
2	GAL	J	1	2	-	2/2/22/22	0/1/1/1
2	GAL	J	2	2	-	0/2/19/22	0/1/1/1
2	GAL	J	3	2	-	2/2/19/22	0/1/1/1
2	GAL	K	1	2	-	2/2/22/22	0/1/1/1
2	GAL	K	2	2	-	0/2/19/22	0/1/1/1
2	GAL	K	3	2	-	0/2/19/22	0/1/1/1
3	GAL	L	1	3	-	2/2/22/22	0/1/1/1
3	GAL	L	2	3	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (23) torsion outliers are listed below:

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

There are no ring outliers.

17 monomers are involved in 85 short contacts:

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

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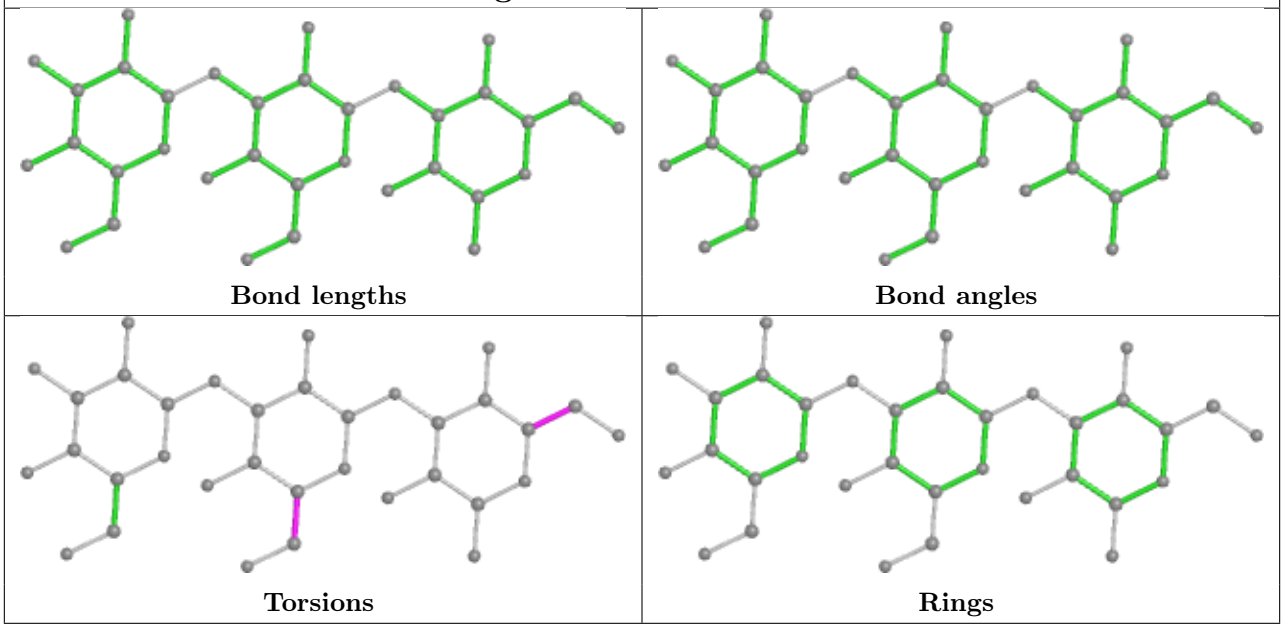
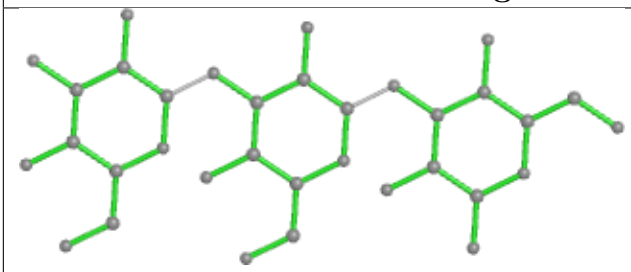
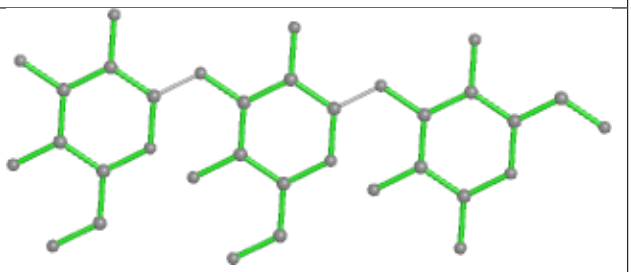
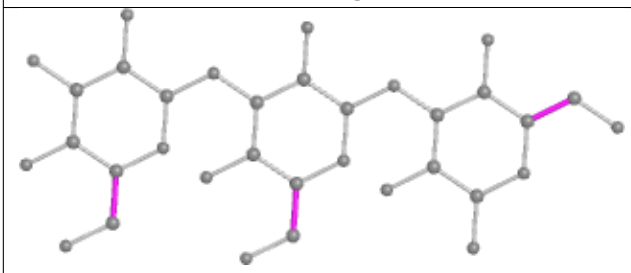
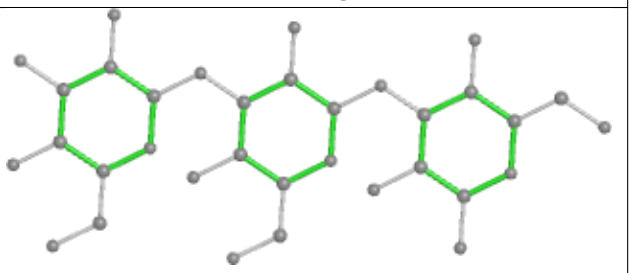
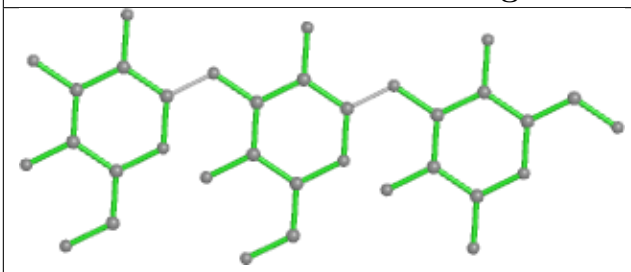
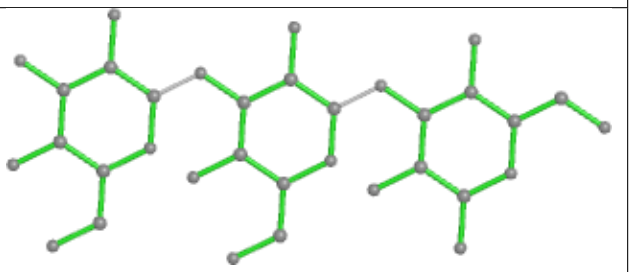
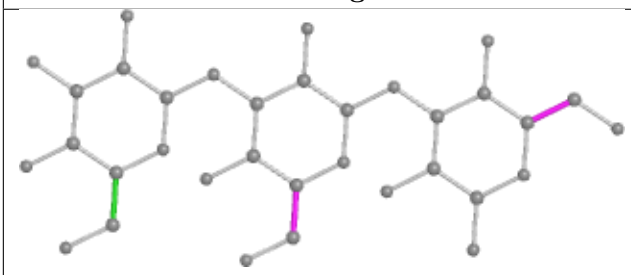
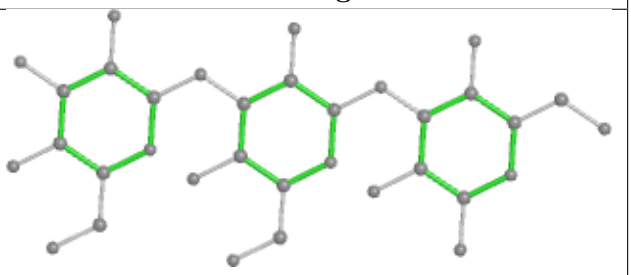
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	2	GAL	14	0
2	J	2	GAL	15	0
2	J	3	GAL	5	0
2	I	1	GAL	2	0
2	K	3	GAL	1	0
3	L	1	GAL	2	0
2	J	1	GAL	5	0
2	H	1	GAL	3	0

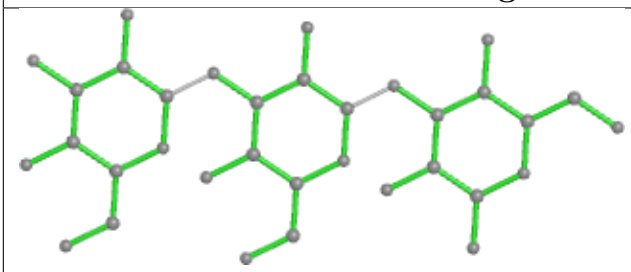
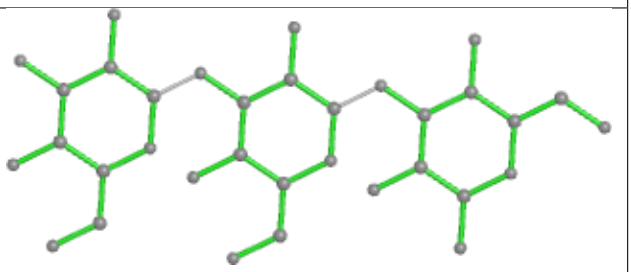
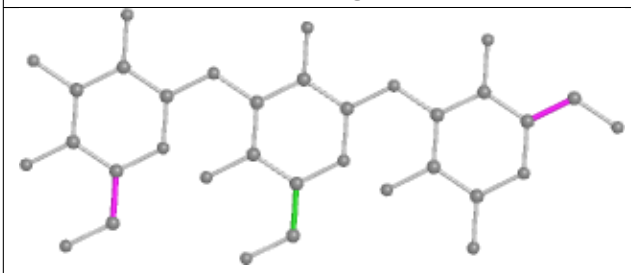
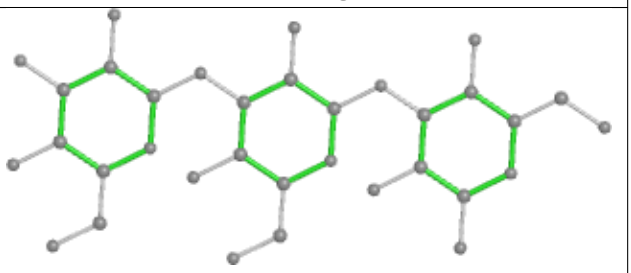
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

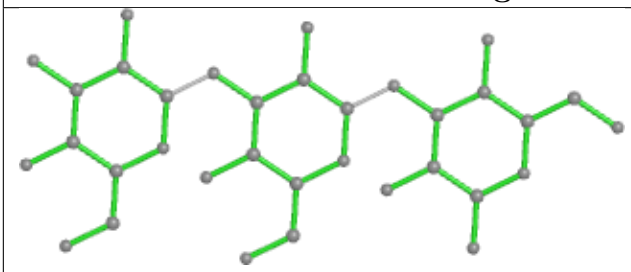
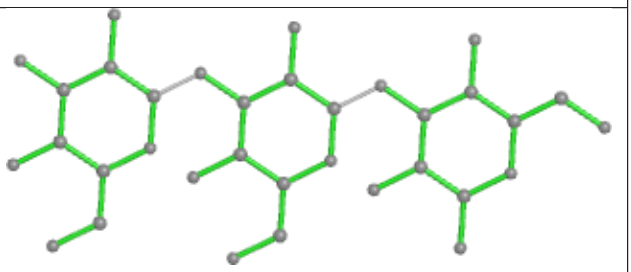
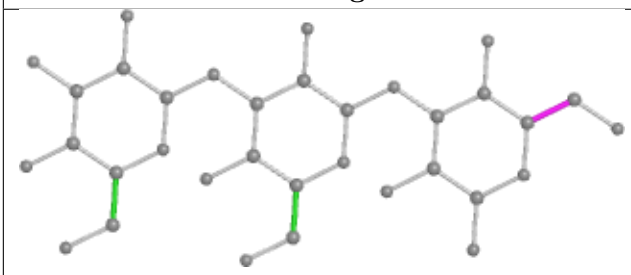
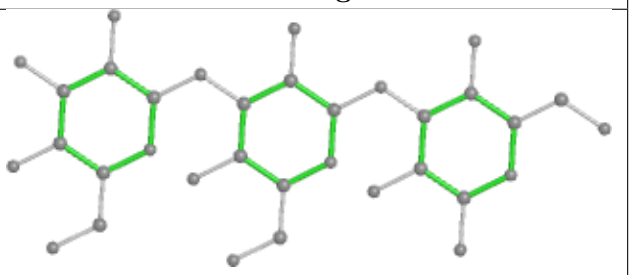
Oligosaccharide Chain G



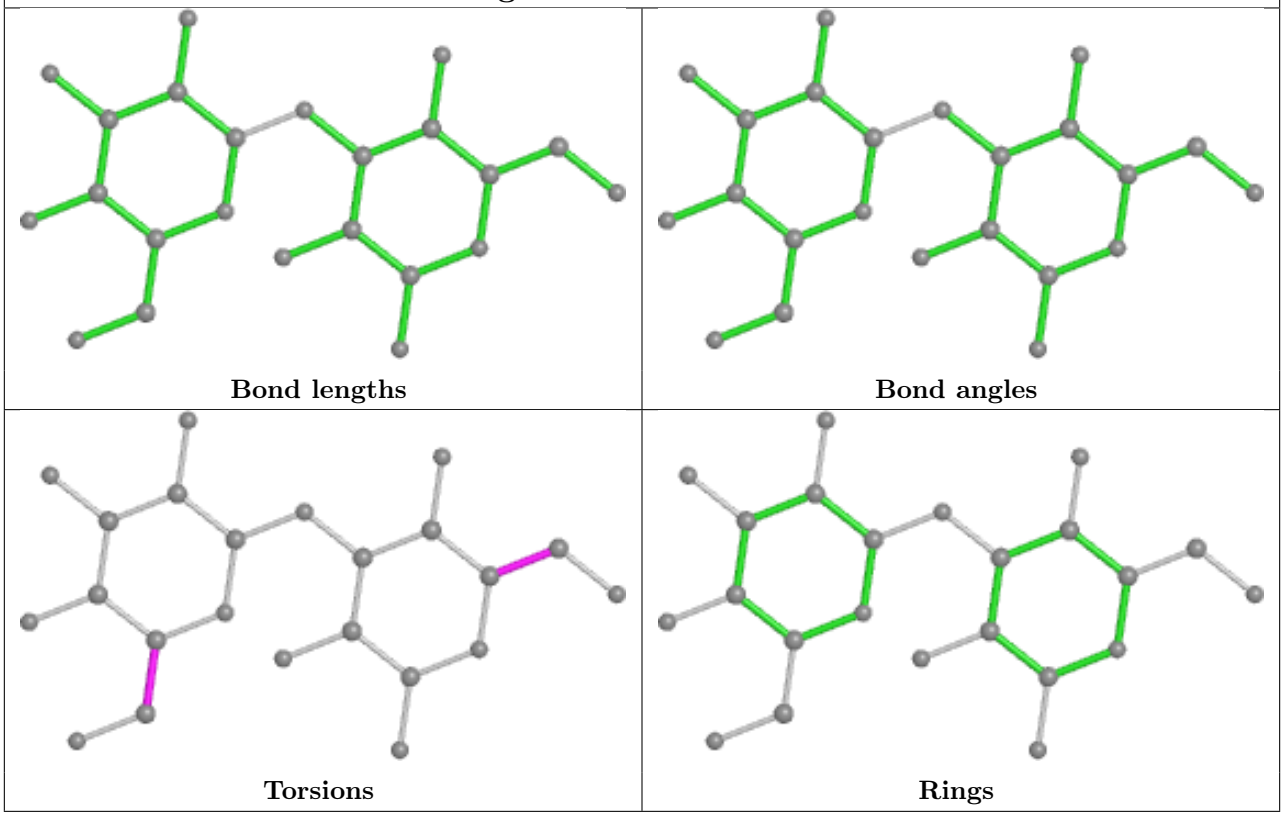
Oligosaccharide Chain H	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain I	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain J	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain K	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain L



5.6 Ligand geometry (i)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GOL	C	601	-	5,5,5	0.36	0	5,5,5	0.31	0
4	GOL	D	601	-	5,5,5	0.36	0	5,5,5	0.28	0
4	GOL	C	602	-	5,5,5	0.37	0	5,5,5	0.26	0
4	GOL	F	602	-	5,5,5	0.36	0	5,5,5	0.29	0
4	GOL	A	601	-	5,5,5	0.37	0	5,5,5	0.26	0
4	GOL	C	603	-	5,5,5	0.36	0	5,5,5	0.30	0
4	GOL	F	601	-	5,5,5	0.38	0	5,5,5	0.27	0
4	GOL	B	601	-	5,5,5	0.36	0	5,5,5	0.28	0
4	GOL	B	602	-	5,5,5	0.37	0	5,5,5	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GOL	E	601	-	5,5,5	0.37	0	5,5,5	0.28	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	C	601	-	-	2/4/4/4	-
4	GOL	D	601	-	-	2/4/4/4	-
4	GOL	C	602	-	-	2/4/4/4	-
4	GOL	F	602	-	-	2/4/4/4	-
4	GOL	A	601	-	-	2/4/4/4	-
4	GOL	C	603	-	-	4/4/4/4	-
4	GOL	F	601	-	-	2/4/4/4	-
4	GOL	B	601	-	-	2/4/4/4	-
4	GOL	B	602	-	-	2/4/4/4	-
4	GOL	E	601	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
4	C	603	GOL	O1-C1-C2-O2
4	A	601	GOL	O1-C1-C2-O2
4	C	601	GOL	O1-C1-C2-O2
4	D	601	GOL	O1-C1-C2-O2
4	E	601	GOL	O1-C1-C2-O2
4	F	601	GOL	O1-C1-C2-O2
4	C	603	GOL	C1-C2-C3-O3
4	C	603	GOL	O2-C2-C3-O3
4	F	602	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
4	C	601	GOL	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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%)	0.22	0	100	100	47, 73, 93, 110	0
1	B	461/526 (87%)	0.35	8 (1%)	70	69	58, 83, 105, 114	0
1	C	482/526 (91%)	0.07	2 (0%)	92	93	40, 55, 72, 109	0
1	D	461/526 (87%)	1.15	114 (24%)	0	0	47, 85, 150, 156	0
1	E	461/526 (87%)	0.27	9 (1%)	65	63	43, 65, 83, 95	0
1	F	461/526 (87%)	0.26	4 (0%)	84	84	40, 61, 80, 102	0
All	All	2787/3156 (88%)	0.38	137 (4%)	29	26	40, 68, 114, 156	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	359	LEU	8.2
1	D	490	LEU	7.5
1	D	443	PHE	7.3
1	D	380	GLN	7.1
1	D	484	THR	6.3
1	D	367	VAL	6.2
1	D	474	ILE	6.0
1	D	368	LEU	6.0
1	D	382	VAL	5.9
1	D	402	GLY	5.9
1	D	450	TYR	5.8
1	D	374	SER	5.7
1	D	383	GLN	5.6
1	D	491	VAL	5.6
1	D	394	TRP	5.6
1	D	357	TYR	5.5
1	D	448	ASP	5.5
1	D	462	ILE	5.5
1	D	426	GLY	5.4

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Mol	Chain	Res	Type	RSRZ
1	D	381	ILE	5.2
1	D	451	TYR	5.2
1	D	445	ASP	5.2
1	D	477	GLN	5.1
1	D	427	VAL	5.1
1	D	452	LYS	5.0
1	D	471	ASP	4.9
1	D	442	LYS	4.9
1	D	371	LEU	4.9
1	D	486	GLN	4.8
1	D	384	TRP	4.7
1	D	449	GLY	4.7
1	D	480	ASP	4.6
1	D	444	THR	4.5
1	D	458	CYS	4.5
1	D	453	ILE	4.5
1	D	423	GLU	4.4
1	D	478	TRP	4.4
1	D	446	ILE	4.4
1	D	472	GLY	4.3
1	D	424	ASP	4.2
1	D	466	LYS	4.2
1	D	479	SER	4.2
1	D	408	ASN	4.2
1	D	378	ALA	4.1
1	D	401	GLY	4.1
1	D	447	GLY	4.1
1	D	481	ALA	4.1
1	D	400	GLY	4.0
1	D	379	ALA	3.9
1	D	396	LEU	3.9
1	D	407	VAL	3.9
1	D	463	ASP	3.8
1	D	360	VAL	3.8
1	D	397	VAL	3.7
1	D	456	ARG	3.6
1	D	459	GLY	3.6
1	D	460	LYS	3.6
1	C	-18	GLY	3.6
1	D	476	GLN	3.5
1	D	470	GLU	3.5
1	D	440	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	465	ARG	3.4
1	D	475	ILE	3.4
1	D	425	GLY	3.4
1	D	457	HIS	3.4
1	D	437	TYR	3.4
1	D	264	ALA	3.3
1	D	405	LYS	3.3
1	D	467	TRP	3.2
1	D	428	LEU	3.1
1	D	489	LYS	3.1
1	D	392	GLN	3.1
1	D	422	LYS	3.0
1	D	375	VAL	3.0
1	D	364	SER	3.0
1	E	358	LYS	2.9
1	D	354	THR	2.9
1	E	359	LEU	2.9
1	D	370	VAL	2.9
1	F	223	PHE	2.9
1	D	35	VAL	2.8
1	D	356	ARG	2.8
1	D	366	LYS	2.8
1	B	448	ASP	2.7
1	E	390	LEU	2.7
1	D	403	TYR	2.7
1	D	421	SER	2.6
1	D	469	THR	2.6
1	B	443	PHE	2.6
1	D	487	HIS	2.6
1	D	372	ASP	2.6
1	D	389	SER	2.6
1	D	468	SER	2.6
1	D	441	TRP	2.6
1	D	417	VAL	2.5
1	D	406	ILE	2.5
1	D	482	GLY	2.5
1	D	473	GLY	2.5
1	E	368	LEU	2.5
1	D	436	GLY	2.4
1	D	398	ASP	2.4
1	D	492	LEU	2.4
1	D	365	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	358	LYS	2.4
1	B	396	LEU	2.4
1	E	490	LEU	2.4
1	D	464	VAL	2.4
1	D	362	LYS	2.3
1	C	-4	ARG	2.3
1	D	485	ASN	2.3
1	B	388	GLY	2.3
1	D	404	LYS	2.3
1	F	359	LEU	2.3
1	F	394	TRP	2.3
1	D	259	TYR	2.3
1	E	331	GLU	2.3
1	B	368	LEU	2.2
1	E	356	ARG	2.2
1	D	416	ASP	2.2
1	D	358	LYS	2.2
1	D	488	TRP	2.2
1	D	33	GLU	2.2
1	D	454	SER	2.2
1	B	442	LYS	2.2
1	E	394	TRP	2.2
1	E	396	LEU	2.2
1	D	369	ASP	2.1
1	D	361	ASN	2.1
1	D	493	VAL	2.1
1	D	429	ILE	2.1
1	B	93	TYR	2.1
1	D	439	GLN	2.1
1	D	93	TYR	2.1
1	D	455	SER	2.0
1	D	373	GLY	2.0
1	F	328	THR	2.0
1	D	330	LEU	2.0

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

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

6.3 Carbohydrates (i)

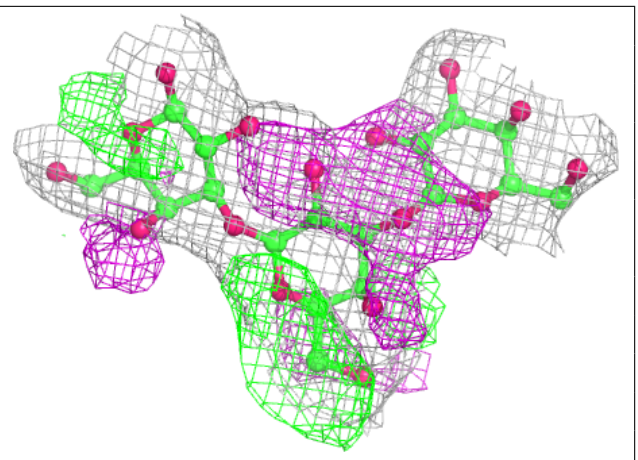
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

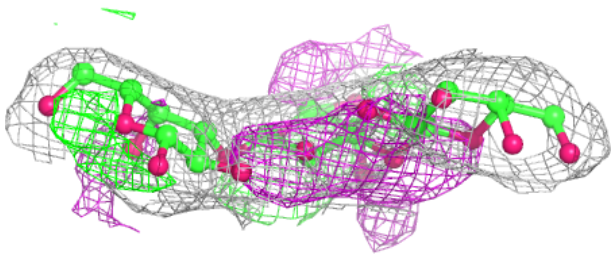
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GAL	G	2	11/12	0.68	0.33	44,49,58,64	0
2	GAL	K	2	11/12	0.73	0.28	45,50,55,61	0
2	GAL	I	2	11/12	0.75	0.32	44,47,54,68	0
2	GAL	G	3	11/12	0.77	0.24	45,55,60,62	0
2	GAL	H	2	11/12	0.77	0.24	48,54,61,62	0
2	GAL	K	1	12/12	0.78	0.27	50,54,62,66	0
2	GAL	J	2	11/12	0.78	0.22	49,56,58,58	0
2	GAL	J	1	12/12	0.81	0.22	51,54,60,62	0
3	GAL	L	2	11/12	0.81	0.34	20,20,20,20	0
2	GAL	G	1	12/12	0.82	0.23	46,50,57,58	0
2	GAL	K	3	11/12	0.83	0.25	48,55,59,62	0
2	GAL	I	3	11/12	0.83	0.22	43,55,61,61	0
3	GAL	L	1	12/12	0.84	0.48	20,20,20,20	0
2	GAL	I	1	12/12	0.84	0.19	43,50,56,59	0
2	GAL	J	3	11/12	0.85	0.19	48,56,64,64	0
2	GAL	H	1	12/12	0.85	0.25	53,56,61,63	0
2	GAL	H	3	11/12	0.86	0.21	50,56,60,63	0

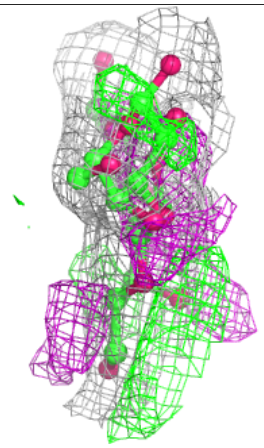
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

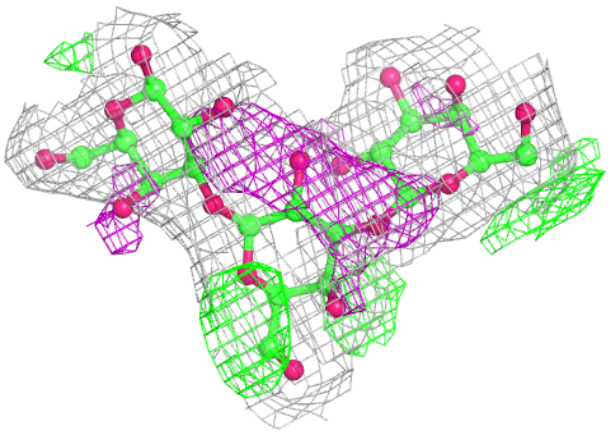


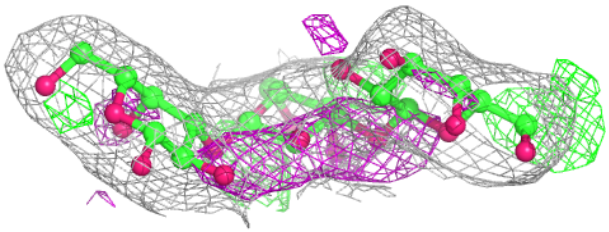


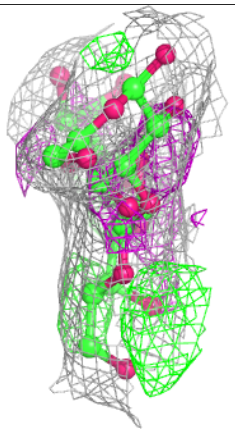


Electron density around Chain H:

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

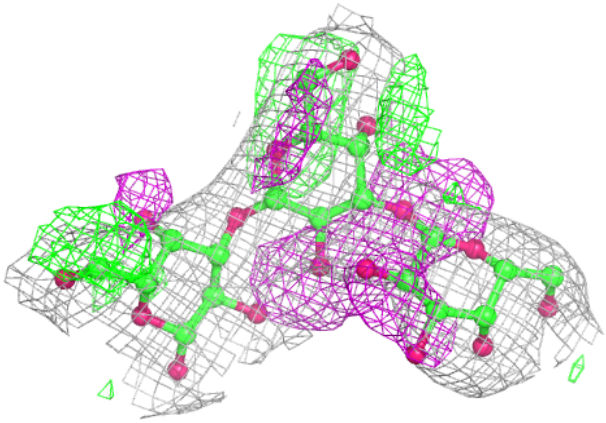


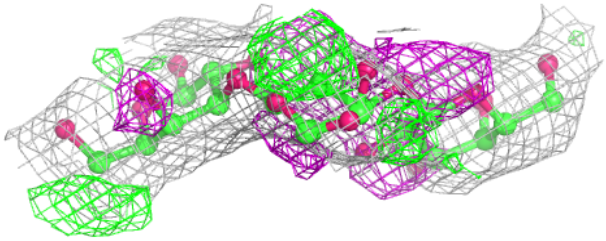


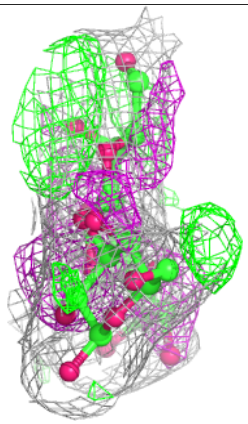


Electron density around Chain I:

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

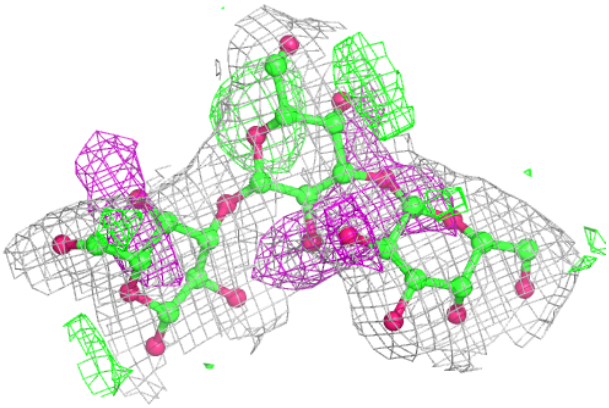


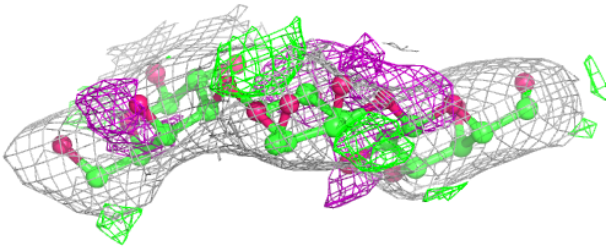


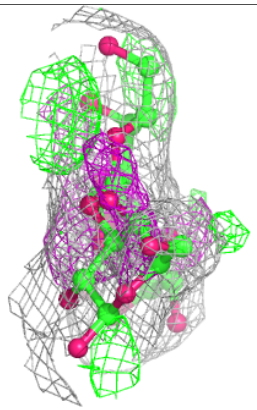


Electron density around Chain J:

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

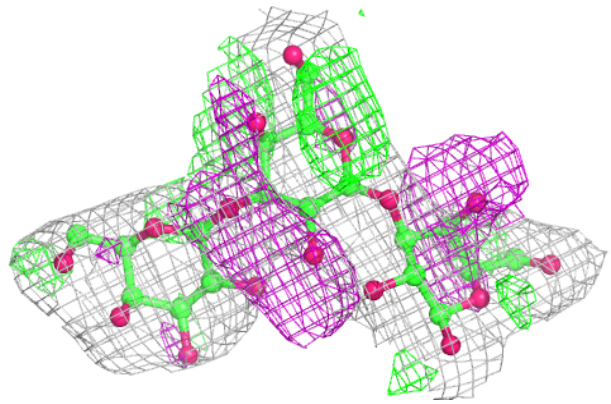


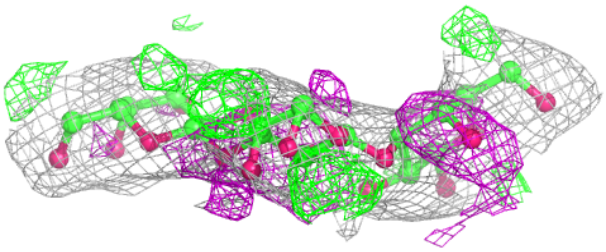


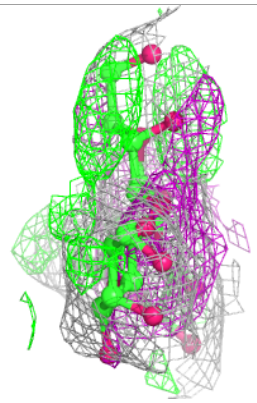


Electron density around Chain K:

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

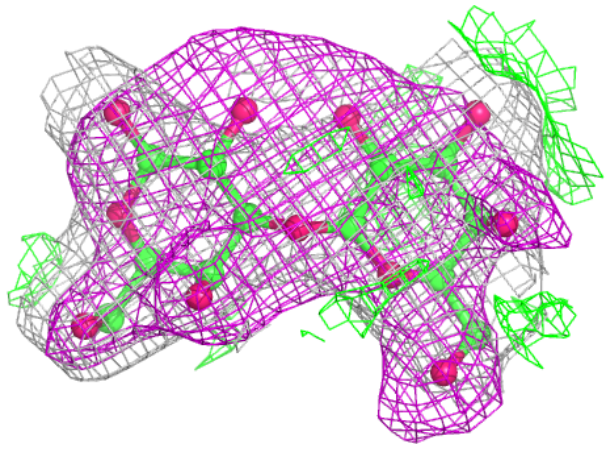


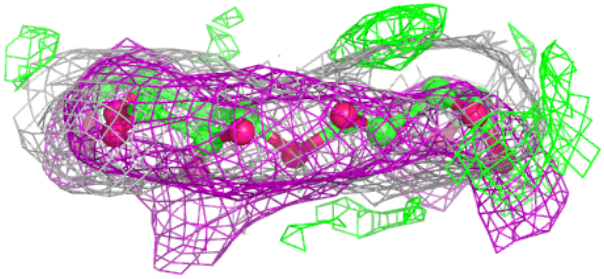


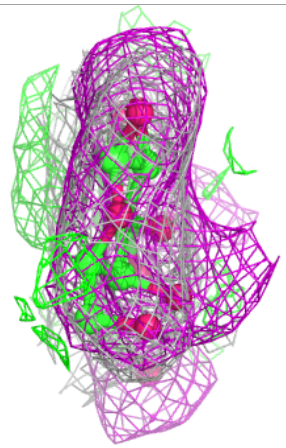


Electron density around Chain L:

$2mF_o$-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
4	GOL	C	603	6/6	0.74	0.53	56,73,83,86	0
4	GOL	C	602	6/6	0.82	0.32	53,65,77,77	0
4	GOL	D	601	6/6	0.85	0.47	83,87,91,93	0
4	GOL	B	602	6/6	0.92	0.18	66,71,75,76	0
4	GOL	F	601	6/6	0.92	0.23	68,71,72,72	0
4	GOL	E	601	6/6	0.93	0.27	66,69,70,71	0
4	GOL	F	602	6/6	0.93	0.47	78,81,87,89	0
4	GOL	B	601	6/6	0.94	0.33	66,81,87,91	0
4	GOL	A	601	6/6	0.94	0.22	54,54,56,56	0
4	GOL	C	601	6/6	0.94	0.21	55,58,62,65	0

6.5 Other polymers (i)

There are no such residues in this entry.