



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:01 PM GMT

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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

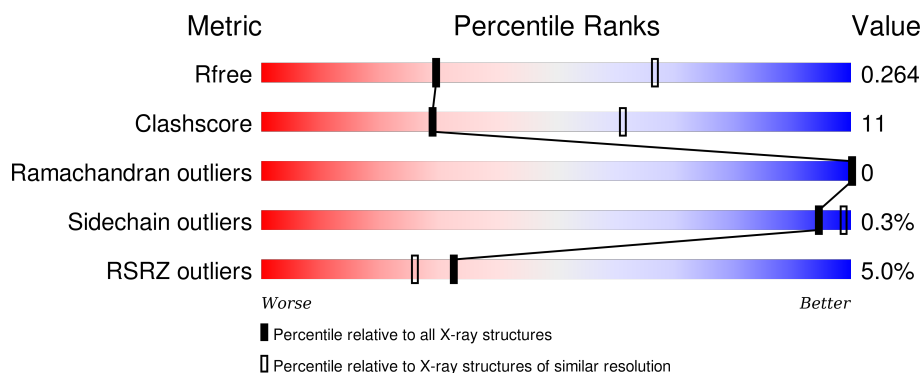
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.89 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))
$R_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	526	
1	B	526	
1	C	526	
1	D	526	
1	E	526	

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Mol	Chain	Length	Quality of chain
1	F	526	 % 69% 18% 12%

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	GOL	B	601	-	-	-	X
2	GOL	C	602	-	-	-	X
2	GOL	C	603	-	-	-	X
2	GOL	D	601	-	-	-	X
2	GOL	F	602	-	-	-	X
3	GAL	A	602	-	-	-	X
3	GAL	A	603	-	-	X	X
3	GAL	B	604	-	-	X	-
3	GAL	C	605	-	-	X	X
3	GAL	E	603	-	-	X	-
3	GAL	F	604	-	-	X	X
4	GAL	F	607	-	-	-	X

## 2 Entry composition

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

There are 216 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	3	Total	C	O	0	0
			34	18	16		
3	B	3	Total	C	O	0	0
			34	18	16		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	3	Total	C	O	0	0
			34	18	16		
3	E	3	Total	C	O	0	0
			34	18	16		
3	F	3	Total	C	O	0	0
			34	18	16		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	2	Total	C	O	0	0
			23	12	11		

- Molecule 5 is water.

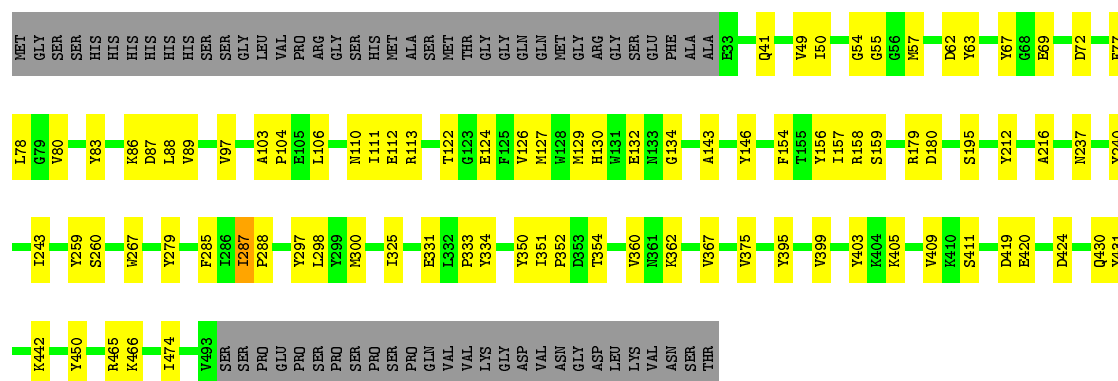
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	O	0	0
			4	4		
5	C	9	Total	O	0	0
			9	9		
5	E	2	Total	O	0	0
			2	2		
5	F	4	Total	O	0	0
			4	4		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

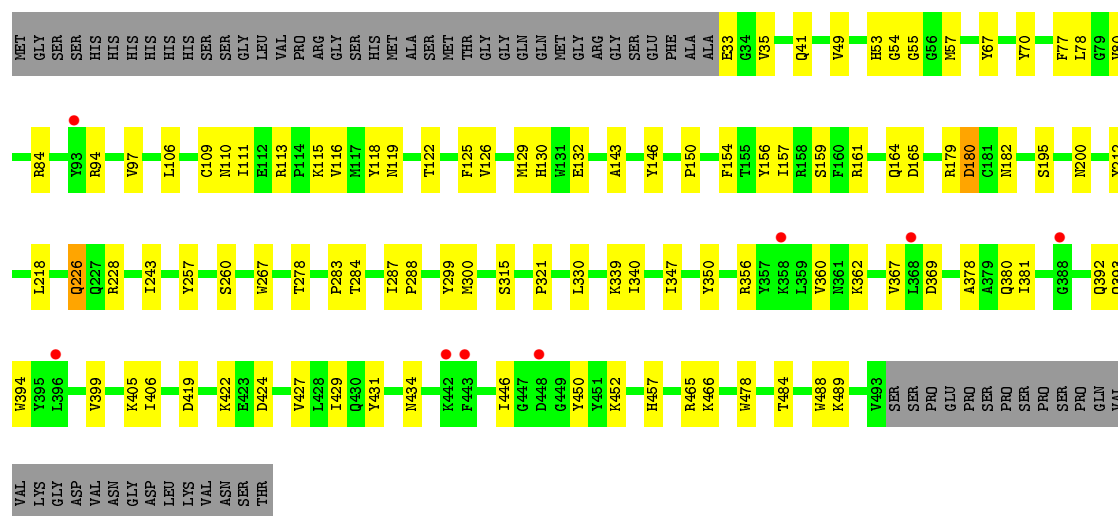
#### • Molecule 1: Ricin B lectin

Chain A: 



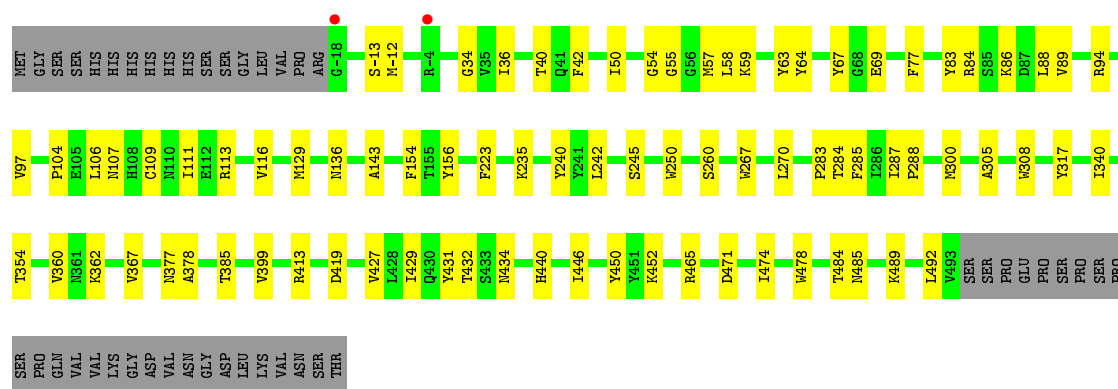
#### • Molecule 1: Ricin B lectin

Chain B: 

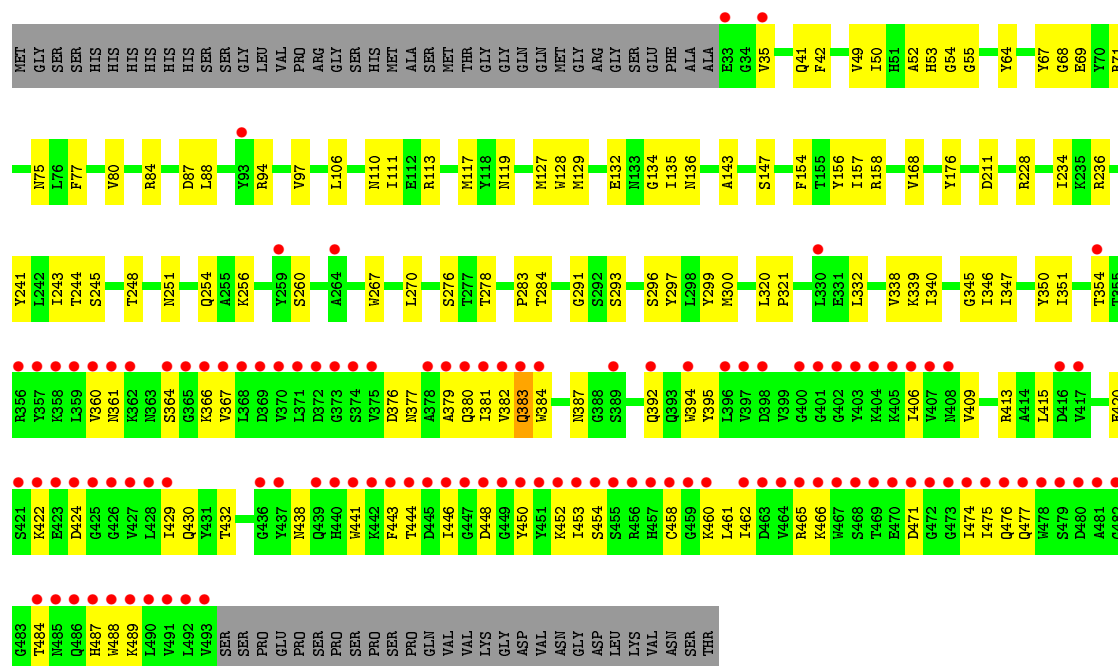


#### • Molecule 1: Ricin B lectin

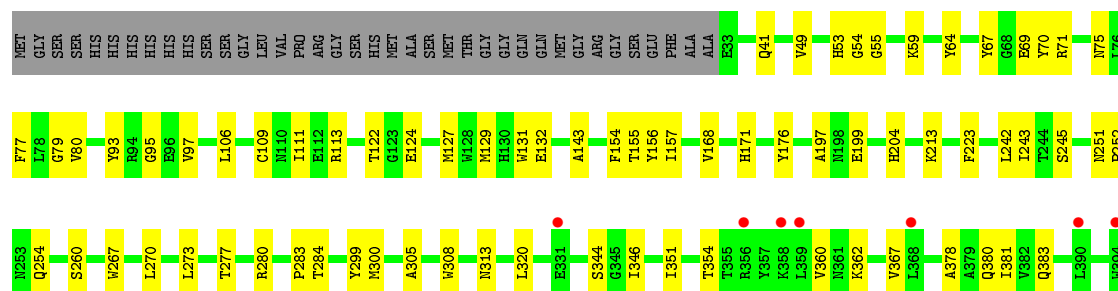
Chain C: 



• Molecule 1: Ricin B lectin



• Molecule 1: Ricin B lectin





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.79Å 122.60Å 405.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.88 – 2.89 48.88 – 2.89	Depositor EDS
% Data completeness (in resolution range)	90.5 (48.88-2.89) 94.9 (48.88-2.89)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.239 , 0.262 0.243 , 0.264	Depositor DCC
$R_{free}$ test set	2040 reflections (1.81%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.8	Xtriage
Anisotropy	0.638	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 41.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 114509 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	22399	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	12	0	16	0	0
2	C	18	0	24	2	0
2	D	6	0	8	0	0
2	E	6	0	8	0	0
2	F	12	0	16	0	0
3	A	34	0	30	15	0
3	B	34	0	30	17	0
3	C	34	0	30	16	0
3	E	34	0	30	20	0
3	F	34	0	30	13	0
4	F	23	0	21	4	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
3:E:603:GAL:H3	3:E:604:GAL:O2	1.55	1.03
3:B:604:GAL:H3	3:B:605: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	3:B:604:GAL:O2	1.86	0.92
1:D:453:ILE:CG1	1:D:461:LEU:HD11	1.98	0.91
3:C:605:GAL:H3	3:C:606: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	3:C:604:GAL:O2	1.92	0.87
1:B:419:ASP:HA	3:B:604: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	4:F:607:GAL:H61	1.47	0.80
1:A:419:ASP:OD1	3:A:603: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	3:E:603: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	3:C:605:GAL:O2	2.00	0.78
1:A:285:PHE:HE2	1:A:287:ILE:HG23	1.50	0.77
3:E:603:GAL:C3	3:E:604:GAL:O2	2.30	0.77
1:D:422:LYS:HG3	1:D:458:CYS:HB3	1.67	0.77
3:B:604:GAL:C3	3:B:605: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	3:F:604:GAL:H61	1.51	0.74
1:E:431:TYR:CD2	3:E:603:GAL:H62	2.23	0.74
1:B:84:ARG:HE	1:B:94:ARG:HE	1.34	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	3:A:603: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	3:B:604: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	4:F:607:GAL:H62	2.12	0.70
3:C:605:GAL:C3	3:C:606:GAL:O2	2.40	0.70
1:B:356:ARG:HD3	1:B:393:GLN:NE2	2.08	0.69
1:B:419:ASP:CA	3:B:604:GAL:H2	2.23	0.69
1:A:419:ASP:HA	3:A:603:GAL:O3	1.93	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:E:54:GLY:O	1:E:113:ARG:HA	1.94	0.68
1:C:223:PHE:HE2	1:C:242:LEU:HD23	1.57	0.68
1:F:260:SER:HB2	1:F:267:TRP:HA	1.76	0.68
1:F:419:ASP:HA	3:F:604:GAL:O3	1.94	0.67
1:F:223:PHE:HE2	1:F:242:LEU:HD23	1.59	0.67
1:E:419:ASP:HA	3:E:603:GAL:C2	2.25	0.66
1:E:434:ASN:HD21	3:E:603:GAL:H61	1.60	0.66
1:A:157:ILE:HG22	1:A:158:ARG:HG2	1.78	0.66
1:D:461:LEU:HD12	1:D:462:ILE:H	1.60	0.65
1:C:465:ARG:HH21	1:C:474:ILE:HG21	1.61	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	3:C:605: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	3:B:604: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	3:A:604:GAL:H62	1.99	0.62
1:E:419:ASP:OD1	3:E:602:GAL:O2	2.17	0.62
1:E:360:VAL:HG22	1:E:367:VAL:HG12	1.81	0.62
1:E:413:ARG:NH1	1:E:432:THR:HG22	2.15	0.62
1:D:110:ASN:OD1	1:D:134:GLY:HA2	2.00	0.62
1:E:419:ASP:OD1	3:E:603: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	2: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:B:431:TYR:HE1	3:B:603:GAL:HO4	1.49	0.59
1:A:419:ASP:HA	3:A:603:GAL:C2	2.31	0.59
1:B:84:ARG:NE	1:B:94:ARG:HE	1.99	0.59
1:F:419:ASP:OD1	3:F:604:GAL:O2	2.17	0.59
1:E:197:ALA:HB3	1:E:204:HIS:CE1	2.38	0.59
1:F:428:LEU:HD12	1:F:475:ILE:HG22	1.84	0.59
1:B:419:ASP:N	3:B:604:GAL:H2	2.18	0.59
1:B:419:ASP:HA	3:B:604:GAL:O3	2.03	0.59
1:D:347:ILE:O	1:D:347:ILE:HD12	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:E:77:PHE:CD1	1:E:111:ILE:HB	2.37	0.58
1:A:260:SER:HB2	1:A:267:TRP:HA	1.84	0.58
1:E:419:ASP:CA	3:E:603:GAL:H2	2.33	0.58
1:B:70:TYR:CZ	1:B:78:LEU:HD11	2.38	0.58
1:D:415:LEU:HD21	1:D:462:ILE:HD11	1.85	0.58
1:A:97:VAL:HB	1:A:154:PHE:CD2	2.38	0.58
1:A:419:ASP:OD1	3:A:602:GAL:O2	2.20	0.58
1:D:380:GLN:NE2	1:D:474:ILE:HG13	2.19	0.58
1:D:97:VAL:HB	1:D:154:PHE:CD2	2.39	0.58
1:C:450:TYR:CE1	1:C:489:LYS:HB2	2.39	0.58
1:D:260:SER:HB2	1:D:267:TRP:HA	1.86	0.58
1:B:419:ASP:OD1	3:B:603: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:F:431:TYR:CE1	3:F:603:GAL:O4	2.57	0.57
1:D:106:LEU:HD22	1:D:111:ILE:HD11	1.85	0.57
1:D:84:ARG:HG2	1:D:94:ARG:HD3	1.85	0.57
1:E:416:ASP:HB3	1:E:439:GLN:HG2	1.85	0.57
1:B:431:TYR:CD2	3:B:604:GAL:H62	2.39	0.57
1:B:41:GLN:HB3	1:B:49:VAL:HG23	1.86	0.57
1:F:231:PRO:HA	1:F:244:THR:HG22	1.87	0.56
1:A:360:VAL:HG22	1:A:367:VAL:HG12	1.86	0.56
1:D:54:GLY:O	1:D:113:ARG:HA	2.04	0.56
1:D:361:ASN:HB3	1:D:364:SER:OG	2.06	0.56
1:B:380:GLN:HE22	1:B:427:VAL:HG13	1.71	0.56
1:F:431:TYR:CD2	3:F:604:GAL:H62	2.40	0.56
1:C:419:ASP:H	3:C:605: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	3:C:605: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:F:223:PHE:CE2	1:F:242:LEU:HD23	2.41	0.55
1:E:157:ILE:HD11	1:E:213:LYS:HD2	1.88	0.55
1:D:450:TYR:CE2	1:D:489:LYS:HE3	2.42	0.55
1:F:223:PHE:HB3	1:F:226:GLN:HG3	1.89	0.55
1:B:67:TYR:CE2	1:B:116:VAL:HG21	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:PHE:HB2	1:D:50:ILE:HD11	1.87	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	3:F:604:GAL:C6	2.21	0.54
1:D:291:GLY:HA3	1:D:345:GLY:HA3	1.89	0.54
1:D:462:ILE:HA	1:D:476:GLN:O	2.08	0.54
1:D:360:VAL:CG1	1:D:489:LYS:HB2	2.37	0.54
1:B:55:GLY:HA3	1:B:67:TYR:O	2.07	0.54
1:E:260:SER:HB2	1:E:267:TRP:HA	1.90	0.54
1:A:279:TYR:CE2	1:A:334:TYR:HB2	2.43	0.54
1:A:77:PHE:CD1	1:A:111:ILE:HB	2.42	0.54
1:B:110:ASN:HB2	1:B:132:GLU:HB2	1.90	0.54
1:A:103:ALA:HB3	1:A:106:LEU:HG	1.90	0.54
1:D:381:ILE:HG12	1:D:429:ILE:HA	1.89	0.54
1:B:340:ILE:HG22	1:B:347:ILE:HG23	1.89	0.54
1:F:419:ASP:OD1	3:F:603:GAL:O2	2.26	0.54
1:B:284:THR:HG22	1:B:300:MET:O	2.06	0.54
1:D:443:PHE:CD2	1:D:453:ILE:HG22	2.43	0.54
1:E:431:TYR:CE1	3:E:602:GAL:O4	2.61	0.54
1:A:419:ASP:CA	3:A:603: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:C:63:TYR:CE1	1:C:84:ARG:NH1	2.76	0.53
1:B:130:HIS:CE1	1:B:179:ARG:HD3	2.43	0.53
1:C:97:VAL:HB	1:C:154:PHE:CD2	2.42	0.53
1:B:419:ASP:OD1	3:B:604: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:D:484:THR:HA	1:D:487:HIS:CD2	2.42	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: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:E:284:THR:HG22	1:E:300:MET:O	2.08	0.53
1:B:97:VAL:HB	1:B:154:PHE:CD2	2.44	0.53
1:C:129:MET:HG2	1:C:143:ALA:HB3	1.91	0.53
1:A:112:GLU:HB2	5:A:703:HOH:O	2.08	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:419:ASP:H	3:E:603:GAL:H2	1.75	0.52
1:E:168:VAL:HG11	1:E:176:TYR:CE1	2.43	0.52
1:B:434:ASN:HD21	3:B:604:GAL:H61	1.74	0.52
1:C:84:ARG:HE	1:C:94:ARG:CZ	2.22	0.52
1:A:63:TYR:CE1	1:A:86:LYS:HE3	2.44	0.52
1:F:135:ILE:HG22	1:F:136:ASN:HD22	1.74	0.52
1:D:245:SER:HB3	1:D:283:PRO:HD2	1.90	0.52
1:D:450:TYR:CD1	1:D:489:LYS:HG3	2.44	0.52
1:B:78:LEU:HD12	1:B:78:LEU:C	2.29	0.52
1:A:279:TYR:CD2	1:A:334:TYR:HB2	2.44	0.52
1:D:444:THR:OG1	1:D:452:LYS:HB2	2.10	0.52
1:A:419:ASP:OD1	3:A:603:GAL:C2	2.58	0.52
1:E:97:VAL:HB	1:E:154:PHE:CD2	2.45	0.52
1:D:384:TRP:CZ3	1:D:471:ASP:HB3	2.44	0.52
1:C:59:LYS:HD3	1:C:64:TYR:CE1	2.44	0.52
1:E:171:HIS:CE1	1:E:199:GLU:HB2	2.45	0.52
1:B:129:MET:HG2	1:B:143:ALA:HB3	1.91	0.52
1:C:84:ARG:HE	1:C:94:ARG:NE	2.07	0.52
1:E:431:TYR:CE2	3:E:603:GAL:H62	2.45	0.51
3:E:603:GAL:O2	3:E:604: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
3:C:604:GAL:HO2	3:C:605: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:E:434:ASN:ND2	3:E:603:GAL:H61	2.26	0.51
1:F:431:TYR:HE1	3:F:603:GAL:O4	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:80:VAL:HG11	1:E:127:MET:HE3	1.93	0.50
1:D:284:THR:HG22	1:D:300:MET:O	2.11	0.50
1:E:277:THR:HG22	1:E:280:ARG:H	1.76	0.50
1:C:58:LEU:HD22	1:C:116:VAL:HG12	1.93	0.50
1:D:453:ILE:CD1	1:D:462:ILE:HD12	2.42	0.50
1:D:71:ARG:HG2	1:D:75:ASN:C	2.32	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:B:431:TYR:HE1	3:B:603:GAL:O4	1.95	0.50
1:C:419:ASP:HA	3:C:605:GAL:O3	2.11	0.50
1:A:126:VAL:HG21	1:A:212:TYR:HB2	1.92	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
3:A:602:GAL:O2	3:A:603:GAL:O2	2.30	0.49
1:D:376:ASP:C	1:D:413:ARG:HH12	2.14	0.49
1:B:57:MET:HE2	1:B:287:ILE:HG21	1.94	0.49
3:E:603:GAL:O2	3:E:604:GAL:H2	2.13	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
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
3:F:605:GAL:HO6	3:F:605:GAL:HO4	1.60	0.49
1:F:431:TYR:CE1	3:F:603:GAL:H4	2.48	0.48
1:B:356:ARG:HD3	1:B:393:GLN:HE22	1.78	0.48
1:B:106:LEU:HD22	1:B:111:ILE:HD11	1.94	0.48
1:F:135:ILE:HD12	1:F:135:ILE:N	2.28	0.48
1:A:122:THR:OG1	1:A:124:GLU:HG2	2.13	0.48
1:B:218:LEU:O	1:B:218:LEU:HD12	2.13	0.48
1:F:430:GLN:O	1:F:430:GLN:HG3	2.13	0.48
1:C:362:LYS:HB2	1:C:450:TYR:CE1	2.47	0.48
3:A:602:GAL:HO2	3:A:603:GAL:HO2	1.57	0.48
1:F:465:ARG:HH21	1:F:474:ILE:HG21	1.78	0.48
1:D:117:MET:HE3	1:D:128:TRP:CD1	2.48	0.48
1:D:443:PHE:HE2	1:D:453:ILE:HG22	1.73	0.48
1:B:434:ASN:ND2	3:B:604:GAL:H61	2.28	0.48
1:C:419:ASP:CA	3:C:605:GAL:H2	2.44	0.48
1:F:284:THR:HG22	1:F:300:MET:O	2.14	0.48
1:F:129:MET:CG	1:F:143:ALA:HB3	2.43	0.48
1:B:125:PHE:CZ	1:B:150:PRO:HG3	2.49	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:A:129:MET:HG2	1:A:143:ALA:HB3	1.95	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:F:431:TYR:CE1	3:F:603:GAL:C4	2.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:PHE:CZ	1:C:111:ILE:HD12	2.48	0.48
1:D:360:VAL:O	1:D:488:TRP:HA	2.13	0.48
1:D:147:SER:HB2	1:D:154:PHE:HA	1.95	0.48
1:D:474:ILE:HD12	1:D:474:ILE:N	2.29	0.48
1:A:424:ASP:O	1:C:136:ASN:HB2	2.14	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:E:80:VAL:HG21	1:E:127:MET:CE	2.43	0.47
1:C:42:PHE:CE2	1:C:317:TYR:HB2	2.49	0.47
1:B:378:ALA:HA	1:B:429:ILE:HD12	1.96	0.47
1:E:41:GLN:HB3	1:E:49:VAL:HG13	1.96	0.47
1:A:431:TYR:CE1	3:A:602: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	3:F:604:GAL:H61	2.26	0.47
1:D:168:VAL:HG21	1:D:176:TYR:CE1	2.50	0.47
1:E:383:GLN:O	1:E:383:GLN:HG3	2.14	0.47
1:F:325:ILE:HD12	1:F:325:ILE:H	1.80	0.47
1:A:110:ASN:OD1	1:A:134:GLY:HA2	2.15	0.47
1:D:119:ASN:HD21	1:D:211:ASP:HA	1.79	0.47
1:F:249:GLY:HA2	4:F:606:GAL:O4	2.15	0.47
1:B:53:HIS:CD2	1:B:315:SER:HB2	2.49	0.47
1:F:366:LYS:HE3	1:F:385:THR:HG22	1.97	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:B:146:TYR:CD2	1:B:157:ILE:HD11	2.50	0.47
3:E:603:GAL:O2	3:E:604:GAL:O2	2.30	0.47
1:A:419:ASP:H	3:A:603: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
1:E:419:ASP:N	3:E:603:GAL:H2	2.30	0.46
1:C:431:TYR:CE2	3:C:605:GAL:H61	2.50	0.46
1:C:69:GLU:HG3	1:C:111:ILE:O	2.15	0.46
1:B:450:TYR:CE1	1:B:489:LYS:HB2	2.50	0.46
1:C:104:PRO:HA	1:C:107:ASN:OD1	2.16	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: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: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:422:LYS:HE2	1:E:457:HIS:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:325:ILE:HD11	1:F:331:GLU:OE1	2.16	0.46
1:E:109:CYS:HB2	1:E:132:GLU:O	2.15	0.46
1:F:70:TYR:HB3	1:F:79:GLY:O	2.16	0.46
1:E:254:GLN:NE2	1:E:273:LEU:H	2.14	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:C:419:ASP:N	3:C:605:GAL:H2	2.31	0.45
1:A:351:ILE:N	1:A:351:ILE:HD12	2.31	0.45
1:A:237:ASN:OD1	1:F:448:ASP:HA	2.16	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:N	1:C:270:LEU:HD12	2.31	0.45
1:E:351:ILE:N	1:E:351:ILE:HD12	2.30	0.45
1:F:382:VAL:HA	1:F:475:ILE:HG12	1.98	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:C:284:THR:HG22	1:C:300:MET:O	2.17	0.45
1:D:77:PHE:CD1	1:D:111:ILE:HB	2.51	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:450:TYR:HB3	1:D:487:HIS:HB3	1.98	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:F:419:ASP:HA	3:F:604:GAL:H2	1.99	0.45
1:A:63:TYR:CZ	1:A:86:LYS:HE3	2.52	0.45
1:E:431:TYR:HE1	3:E:602:GAL:O4	2.00	0.45
1:E:106:LEU:HD11	1:E:156:TYR:CD2	2.50	0.45
1:F:285:PHE:HE2	1:F:287:ILE:HB	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:B:146:TYR:HD2	1:B:157:ILE:HD11	1.81	0.45
1:D:35:VAL:CG2	1:D:339:LYS:HE3	2.47	0.45
1:E:197:ALA:HB3	1:E:204:HIS:ND1	2.32	0.45
1:D:80:VAL:HG11	1:D:127:MET:HE3	1.99	0.45
1:E:305:ALA:HA	1:E:308:TRP:CZ2	2.52	0.45
1:D:278:THR:HG22	1:D:278:THR:O	2.17	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:450:TYR:CE1	1:F:489:LYS:HB2	2.51	0.44
1:F:55:GLY:HA3	1:F:67:TYR:O	2.17	0.44
1:E:111:ILE:HD11	1:E:131:TRP:CD1	2.45	0.44
1:B:339:LYS:HB2	1:B:350:TYR:HB2	2.00	0.44
1:A:55:GLY:HA3	1:A:67:TYR:O	2.17	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:E:362:LYS:HD3	1:E:450:TYR:CZ	2.53	0.44
1:A:474:ILE:N	1:A:474:ILE:HD12	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:F:161:ARG:HH22	1:F:177:MET:HG2	1.83	0.44
1:D:338:VAL:HG12	1:D:340:ILE:HG23	1.98	0.44
1:F:287:ILE:HA	1:F:288:PRO:HD3	1.86	0.44
1:A:466:LYS:HB3	1:C:250:TRP:CD1	2.53	0.44
1:E:399:VAL:HG11	1:E:405:LYS:HG3	1.99	0.44
1:A:50:ILE:HG23	1:A:83:TYR:CE1	2.53	0.44
1:D:53:HIS:O	1:D:69:GLU:HG2	2.17	0.44
1:E:380:GLN:HE21	1:E:381:ILE:N	2.15	0.44
1:A:399:VAL:HG11	1:A:405:LYS:HG3	2.00	0.44
3:C:605:GAL:O2	3:C:606:GAL:O2	2.30	0.44
1:F:288:PRO:HG3	1:F:297:TYR:CE1	2.53	0.44
1:D:77:PHE:CZ	1:D:111:ILE:HD12	2.53	0.44
1:B:287:ILE:HA	1:B:288:PRO:HD3	1.88	0.44
1:C:354:THR:O	1:C:354:THR:HG22	2.17	0.44
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:A:403:TYR:CD1	1:A:442:LYS:HB2	2.53	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:41:GLN:HB3	1:A:49:VAL:HG23	1.99	0.43
1:D:461:LEU:CD1	1:D:462:ILE:H	2.30	0.43
1:C:106:LEU:HD11	1:C:156:TYR:CD2	2.53	0.43
1:E:55:GLY:HA3	1:E:67:TYR:O	2.18	0.43
1:E:413:ARG:HH11	1:E:432:THR:HG22	1.83	0.43
1:E:93:TYR:CZ	1:E:95:GLY:HA2	2.53	0.43
1:C:434:ASN:HD21	3:C:605: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	3:A:603: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:D:35:VAL:HG23	1:D:339:LYS:HE3	2.00	0.43
1:C:305:ALA:HA	1:C:308:TRP:CZ2	2.53	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:D:87:ASP:O	1:D:88:LEU:HB2	2.19	0.43
1:A:362:LYS:HD3	1:A:450:TYR:CZ	2.53	0.43
1:A:288:PRO:HG3	1:A:297:TYR:CE1	2.54	0.43
1:D:394:TRP:CE3	1:D:406:ILE:HG22	2.54	0.43
1:C:57:MET:HE1	1:C:287:ILE:HG21	2.00	0.42
1:A:77:PHE:CZ	1:A:80:VAL:HG23	2.54	0.42
1:D:376:ASP:O	1:D:379:ALA:HB2	2.19	0.42
1:D:382:VAL:HA	1:D:475:ILE:HG12	2.01	0.42
1:D:377:ASN:ND2	1:D:432:THR:HG23	2.29	0.42
1:E:59:LYS:HD3	1:E:64:TYR:CE1	2.54	0.42
3:B:604:GAL:O2	3:B:605:GAL:O2	2.33	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
1:C:377:ASN:OD1	1:C:431:TYR:HA	2.20	0.42
1:A:287:ILE:HD12	1:A:298:LEU:HB3	2.00	0.42
1:E:129:MET:CG	1:E:143:ALA:HB3	2.50	0.42
1:A:87:ASP:O	1:A:88:LEU:HB2	2.19	0.42
1:C:431:TYR:CD2	3:C:605:GAL:C6	3.02	0.42
1:C:285:PHE:HE2	1:C:287:ILE:HB	1.84	0.42
1:E:277:THR:HG22	1:E:280:ARG:HA	2.02	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:B:450:TYR:HA	1:B:488:TRP:O	2.19	0.42
1:E:450:TYR:CE1	1:E:489:LYS:HB2	2.55	0.42
1:A:240:TYR:O	1:A:259:TYR:HA	2.18	0.42
1:F:383:GLN:HB3	1:F:475:ILE:HD11	2.02	0.42
1:E:251:ASN:HA	1:E:252:PRO:HD3	1.93	0.42
1:A:103:ALA:HB1	1:A:104:PRO:HD2	2.00	0.42
1:F:358:LYS:HZ2	1:F:388:GLY:HA2	1.83	0.42
1:B:399:VAL:HG11	1:B:405:LYS:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:243:ILE:HD12	1:F:243:ILE:N	2.34	0.42
1:A:395:TYR:CE2	1:A:409:VAL:HG22	2.55	0.42
1:D:395:TYR:CZ	1:D:409:VAL:HG22	2.55	0.42
1:B:109:CYS:HB2	1:B:132:GLU:O	2.20	0.42
1:F:354:THR:O	1:F:354:THR:HG22	2.20	0.42
1:A:354:THR:O	1:A:354:THR:HG22	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:C:431:TYR:CD2	3:C:605:GAL:H62	2.55	0.41
1:C:287:ILE:HA	1:C:288:PRO:HD3	1.87	0.41
1:D:361:ASN:HB2	1:D:488:TRP:CZ3	2.54	0.41
1:A:474:ILE:H	1:A:474:ILE:HD12	1.84	0.41
1:D:351:ILE:HD12	1:D:351:ILE:N	2.35	0.41
1:E:431:TYR:CE1	3:E:602:GAL:C4	3.04	0.41
1:E:431:TYR:CE1	3:E:602:GAL:H4	2.55	0.41
1:F:63:TYR:CE1	1:F:86:LYS:HE3	2.55	0.41
1:B:243:ILE:HD12	1:B:243:ILE:N	2.36	0.41
1:A:57:MET:CB	1:A:300:MET:HE1	2.51	0.41
1:C:478:TRP:CE3	2:C:601:GOL:H32	2.55	0.41
1:D:129:MET:CG	1:D:143:ALA:HB3	2.51	0.41
1:C:378:ALA:HA	1:C:429:ILE:HD12	2.02	0.41
1:F:176:TYR:CD1	1:F:204:HIS:HE1	2.38	0.41
1:E:243:ILE:N	1:E:243:ILE:HD12	2.35	0.41
1:C:77:PHE:HB2	1:C:111:ILE:H	1.85	0.41
1:D:320:LEU:HB2	1:D:332:LEU:HD11	2.01	0.41
1:A:87:ASP:OD1	1:A:89:VAL:HB	2.20	0.41
1:C:446:ILE:HG21	1:C:452:LYS:HG3	2.02	0.41
1:B:226:GLN:HB3	1:B:228:ARG:HG2	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:F:179:ARG:HD2	1:F:200:ASN:OD1	2.21	0.41
1:C:50:ILE:HG23	1:C:83:TYR:CE1	2.56	0.41
1:D:64:TYR:CG	1:D:88:LEU:HD21	2.56	0.41
1:C:223:PHE:CD1	1:C:270:LEU:HD11	2.56	0.41
1:E:71:ARG:NH1	1:E:75:ASN:HD21	2.19	0.41
1:A:465:ARG:HH21	1:A:474:ILE:HG21	1.86	0.41
1:A:130:HIS:NE2	1:A:179:ARG:HA	2.36	0.41
1:B:180:ASP:O	1:B:195:SER:HA	2.20	0.41
1:D:293:SER:OG	1:D:346:ILE:HD13	2.21	0.41
1:B:278:THR:O	1:B:278:THR:HG22	2.21	0.41
1:C:245:SER:HB3	1:C:283:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:354:THR:O	1:E:354:THR:HG22	2.21	0.41
1:A:287:ILE:CD1	1:A:298:LEU:HB3	2.52	0.40
1:E:80:VAL:HG21	1:E:127:MET:HE3	2.03	0.40
1:B:57:MET:HB3	1:B:57:MET:HE2	2.01	0.40
1:B:394:TRP:CE3	1:B:406:ILE:HG22	2.56	0.40
1:C:106:LEU:HA	1:C:109:CYS:SG	2.61	0.40
1:D:77:PHE:CE1	1:D:111:ILE:HD12	2.57	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:B:77:PHE:CE1	1:B:80:VAL:HG23	2.56	0.40
1:D:52:ALA:CA	1:D:68:GLY:HA3	2.51	0.40
1:D:381:ILE:HG22	1:D:475:ILE:HG13	2.03	0.40
1:A:419:ASP:HA	3:A:603:GAL:C3	2.51	0.40
1:A:431:TYR:HE1	3:A:602:GAL:H4	1.87	0.40
1:A:405:LYS:HB3	1:A:405:LYS:HE2	1.86	0.40
1:A:430:GLN:O	1:A:430:GLN:HG3	2.20	0.40
1:F:492:LEU:N	1:F:492:LEU:HD12	2.36	0.40
1:C:40:THR:HB	1:F:92:GLU:OE2	2.21	0.40
1:A:57:MET:HB3	1:A:300:MET:HE1	2.04	0.40
1:F:367:VAL:HG22	1:F:384:TRP:O	2.21	0.40
1:A:350:TYR:O	1:A:352:PRO:HD3	2.21	0.40
1:A:180:ASP:O	1:A:195:SER:HA	2.20	0.40
1:D:234:ILE:HD11	1:D:241:TYR:HB2	2.03	0.40
1:C:36:ILE:HD13	1:C:340:ILE:HD12	2.03	0.40
1:F:137:TYR:OH	4:F:606:GAL:O2	2.32	0.40
1:F:385:THR:HG23	1:F:471:ASP:OD1	2.21	0.40
1:E:403:TYR:CZ	1:E:456:ARG:HG3	2.56	0.40
1:E:378:ALA:HA	1:E:429:ILE:HD12	2.03	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 ⓘ

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%)	94	99
1	B	389/442 (88%)	387 (100%)	2 (0%)	92	98
1	C	402/442 (91%)	401 (100%)	1 (0%)	95	99
1	D	389/442 (88%)	388 (100%)	1 (0%)	94	99
1	E	389/442 (88%)	388 (100%)	1 (0%)	94	99
1	F	389/442 (88%)	387 (100%)	2 (0%)	92	98
All	All	2347/2652 (88%)	2339 (100%)	8 (0%)	94	99

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

Some 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 ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

17 carbohydrates 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	GAL	A	602	3	12,12,12	0.56	0	17,17,17	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GAL	A	603	3	11,11,12	0.63	0	14,15,17	0.60	0
3	GAL	A	604	3	11,11,12	0.64	0	14,15,17	0.60	0
3	GAL	B	603	3	12,12,12	0.55	0	17,17,17	0.51	0
3	GAL	B	604	3	11,11,12	0.63	0	14,15,17	0.60	0
3	GAL	B	605	3	11,11,12	0.64	0	14,15,17	0.60	0
3	GAL	C	604	3	12,12,12	0.56	0	17,17,17	0.51	0
3	GAL	C	605	3	11,11,12	0.64	0	14,15,17	0.59	0
3	GAL	C	606	3	11,11,12	0.64	0	14,15,17	0.60	0
3	GAL	E	602	3	12,12,12	0.57	0	17,17,17	0.51	0
3	GAL	E	603	3	11,11,12	0.64	0	14,15,17	0.59	0
3	GAL	E	604	3	11,11,12	0.64	0	14,15,17	0.60	0
3	GAL	F	603	3	12,12,12	0.55	0	17,17,17	0.51	0
3	GAL	F	604	3	11,11,12	0.63	0	14,15,17	0.60	0
3	GAL	F	605	3	11,11,12	0.65	0	14,15,17	0.60	0
4	GAL	F	606	4	12,12,12	0.57	0	17,17,17	0.51	0
4	GAL	F	607	4	11,11,12	0.64	0	14,15,17	0.60	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	GAL	A	602	3	-	0/2/22/22	0/1/1/1
3	GAL	A	603	3	-	0/2/19/22	0/1/1/1
3	GAL	A	604	3	-	0/2/19/22	0/1/1/1
3	GAL	B	603	3	-	0/2/22/22	0/1/1/1
3	GAL	B	604	3	-	0/2/19/22	0/1/1/1
3	GAL	B	605	3	-	0/2/19/22	0/1/1/1
3	GAL	C	604	3	-	0/2/22/22	0/1/1/1
3	GAL	C	605	3	-	0/2/19/22	0/1/1/1
3	GAL	C	606	3	-	0/2/19/22	0/1/1/1
3	GAL	E	602	3	-	0/2/22/22	0/1/1/1
3	GAL	E	603	3	-	0/2/19/22	0/1/1/1
3	GAL	E	604	3	-	0/2/19/22	0/1/1/1
3	GAL	F	603	3	-	0/2/22/22	0/1/1/1
3	GAL	F	604	3	-	0/2/19/22	0/1/1/1
3	GAL	F	605	3	-	0/2/19/22	0/1/1/1
4	GAL	F	606	4	-	0/2/22/22	0/1/1/1
4	GAL	F	607	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.



There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 85 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	GAL	5	0
3	A	603	GAL	11	0
3	A	604	GAL	1	0
3	B	603	GAL	3	0
3	B	604	GAL	14	0
3	B	605	GAL	3	0
3	C	604	GAL	2	0
3	C	605	GAL	15	0
3	C	606	GAL	3	0
3	E	602	GAL	5	0
3	E	603	GAL	15	0
3	E	604	GAL	5	0
3	F	603	GAL	5	0
3	F	604	GAL	7	0
3	F	605	GAL	1	0
4	F	606	GAL	2	0
4	F	607	GAL	2	0

## 5.6 Ligand geometry

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	$\# Z  > 2$
2	GOL	A	601	-	5,5,5	0.36	0	5,5,5	0.22	0
2	GOL	B	601	-	5,5,5	0.34	0	5,5,5	0.24	0
2	GOL	B	602	-	5,5,5	0.35	0	5,5,5	0.23	0
2	GOL	C	601	-	5,5,5	0.34	0	5,5,5	0.26	0
2	GOL	C	602	-	5,5,5	0.35	0	5,5,5	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	C	603	-	5,5,5	0.33	0	5,5,5	0.25	0
2	GOL	D	601	-	5,5,5	0.34	0	5,5,5	0.24	0
2	GOL	E	601	-	5,5,5	0.35	0	5,5,5	0.23	0
2	GOL	F	601	-	5,5,5	0.36	0	5,5,5	0.23	0
2	GOL	F	602	-	5,5,5	0.33	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
2	GOL	A	601	-	-	0/4/4/4	0/0/0/0
2	GOL	B	601	-	-	0/4/4/4	0/0/0/0
2	GOL	B	602	-	-	0/4/4/4	0/0/0/0
2	GOL	C	601	-	-	0/4/4/4	0/0/0/0
2	GOL	C	602	-	-	0/4/4/4	0/0/0/0
2	GOL	C	603	-	-	0/4/4/4	0/0/0/0
2	GOL	D	601	-	-	0/4/4/4	0/0/0/0
2	GOL	E	601	-	-	0/4/4/4	0/0/0/0
2	GOL	F	601	-	-	0/4/4/4	0/0/0/0
2	GOL	F	602	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	GOL	2	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	461/526 (87%)	0.23	0 100 100	47, 73, 93, 110	0
1	B	461/526 (87%)	0.37	8 (1%) 73 70	58, 83, 105, 114	0
1	C	482/526 (91%)	0.08	2 (0%) 93 92	40, 55, 72, 109	0
1	D	461/526 (87%)	1.18	114 (24%) 1 0	47, 85, 150, 156	0
1	E	461/526 (87%)	0.28	9 (1%) 68 64	43, 65, 83, 95	0
1	F	461/526 (87%)	0.28	5 (1%) 82 80	40, 61, 80, 102	0
All	All	2787/3156 (88%)	0.40	138 (4%) 32 26	40, 68, 114, 156	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	359	LEU	8.3
1	D	490	LEU	7.6
1	D	443	PHE	7.5
1	D	380	GLN	7.2
1	D	484	THR	6.4
1	D	367	VAL	6.3
1	D	474	ILE	6.1
1	D	368	LEU	6.1
1	D	450	TYR	6.0
1	D	382	VAL	6.0
1	D	402	GLY	6.0
1	D	374	SER	5.9
1	D	383	GLN	5.8
1	D	394	TRP	5.8
1	D	357	TYR	5.7
1	D	491	VAL	5.6
1	D	448	ASP	5.6
1	D	462	ILE	5.6
1	D	426	GLY	5.5

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Mol	Chain	Res	Type	RSRZ
1	D	445	ASP	5.3
1	D	451	TYR	5.3
1	D	381	ILE	5.3
1	D	477	GLN	5.2
1	D	427	VAL	5.1
1	D	452	LYS	5.1
1	D	471	ASP	5.1
1	D	442	LYS	5.0
1	D	371	LEU	5.0
1	D	486	GLN	4.9
1	D	384	TRP	4.8
1	D	458	CYS	4.7
1	D	480	ASP	4.7
1	D	449	GLY	4.7
1	D	444	THR	4.7
1	D	453	ILE	4.5
1	D	478	TRP	4.5
1	D	423	GLU	4.5
1	D	446	ILE	4.5
1	D	424	ASP	4.4
1	D	408	ASN	4.3
1	D	472	GLY	4.3
1	D	479	SER	4.3
1	D	466	LYS	4.3
1	D	401	GLY	4.2
1	D	447	GLY	4.2
1	D	378	ALA	4.1
1	D	400	GLY	4.1
1	D	481	ALA	4.0
1	D	463	ASP	4.0
1	D	396	LEU	3.9
1	D	379	ALA	3.9
1	D	407	VAL	3.9
1	D	360	VAL	3.8
1	D	397	VAL	3.7
1	D	460	LYS	3.7
1	D	459	GLY	3.6
1	D	476	GLN	3.6
1	D	470	GLU	3.6
1	C	-18	GLY	3.6
1	D	440	HIS	3.5
1	D	456	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	475	ILE	3.5
1	D	425	GLY	3.5
1	D	457	HIS	3.4
1	D	437	TYR	3.4
1	D	467	TRP	3.4
1	D	405	LYS	3.3
1	D	465	ARG	3.3
1	D	264	ALA	3.2
1	D	428	LEU	3.2
1	D	392	GLN	3.2
1	D	489	LYS	3.1
1	D	422	LYS	3.1
1	D	364	SER	3.0
1	D	375	VAL	3.0
1	E	358	LYS	3.0
1	D	354	THR	3.0
1	E	359	LEU	2.9
1	F	223	PHE	2.9
1	D	370	VAL	2.9
1	D	35	VAL	2.9
1	B	448	ASP	2.8
1	D	366	LYS	2.8
1	D	403	TYR	2.8
1	D	372	ASP	2.7
1	E	390	LEU	2.7
1	D	421	SER	2.7
1	D	469	THR	2.7
1	D	356	ARG	2.7
1	D	468	SER	2.7
1	D	441	TRP	2.6
1	D	487	HIS	2.6
1	D	389	SER	2.6
1	B	443	PHE	2.6
1	D	482	GLY	2.6
1	D	406	ILE	2.6
1	D	473	GLY	2.5
1	D	398	ASP	2.5
1	D	417	VAL	2.5
1	D	365	GLY	2.5
1	E	368	LEU	2.5
1	D	436	GLY	2.5
1	D	492	LEU	2.4

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

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

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

## 6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	GAL	A	603	11/12	0.68	0.33	3.82	44,49,58,64	0
3	GAL	C	605	11/12	0.75	0.31	3.74	44,47,54,68	0
3	GAL	F	604	11/12	0.73	0.28	2.97	45,50,55,61	0
3	GAL	A	602	12/12	0.82	0.23	2.89	46,50,57,58	0
4	GAL	F	607	11/12	0.81	0.34	2.13	20,20,20,20	0
3	GAL	F	603	12/12	0.78	0.27	1.87	50,54,62,66	0
3	GAL	B	604	11/12	0.77	0.24	1.61	48,54,61,62	0
3	GAL	B	603	12/12	0.84	0.24	0.98	53,56,61,63	0
3	GAL	E	603	11/12	0.78	0.22	0.17	49,56,58,58	0
3	GAL	E	602	12/12	0.81	0.22	-0.08	51,54,60,62	0
3	GAL	B	605	11/12	0.86	0.21	-	50,56,60,63	0
3	GAL	E	604	11/12	0.85	0.18	-	48,56,64,64	0
4	GAL	F	606	12/12	0.84	0.47	-	20,20,20,20	0
3	GAL	C	604	12/12	0.85	0.19	-	43,50,56,59	0
3	GAL	C	606	11/12	0.83	0.22	-	43,55,61,61	0
3	GAL	A	604	11/12	0.76	0.24	-	45,55,60,62	0
3	GAL	F	605	11/12	0.83	0.25	-	48,55,59,62	0

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	GOL	C	603	6/6	0.74	0.53	12.14	56,73,83,86	0
2	GOL	D	601	6/6	0.85	0.47	6.96	83,87,91,93	0
2	GOL	C	602	6/6	0.81	0.32	5.49	53,65,77,77	0
2	GOL	B	601	6/6	0.94	0.33	2.76	66,81,87,91	0
2	GOL	F	602	6/6	0.92	0.47	2.16	78,81,87,89	0
2	GOL	F	601	6/6	0.92	0.23	1.57	68,71,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	C	601	6/6	0.94	0.20	0.77	55,58,62,65	0
2	GOL	A	601	6/6	0.94	0.22	0.40	54,54,56,56	0
2	GOL	E	601	6/6	0.93	0.27	0.24	66,69,70,71	0
2	GOL	B	602	6/6	0.92	0.18	-1.37	66,71,75,76	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.