



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:01 PM GMT

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](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

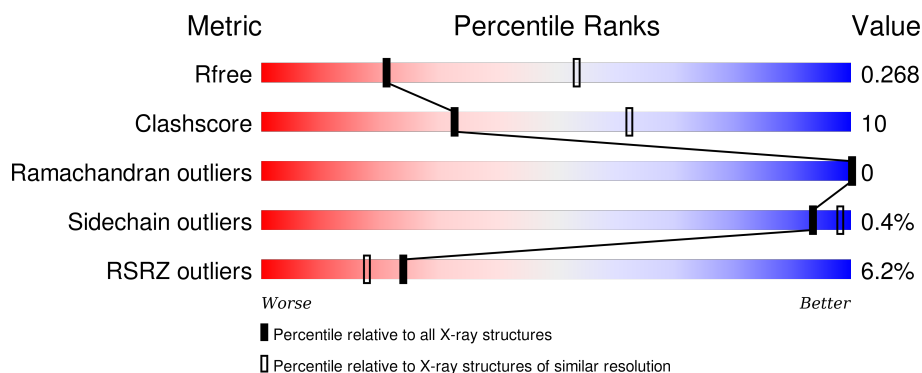
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.91 Å.

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




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1643 (2.94-2.90)
Clashscore	102246	1871 (2.94-2.90)
Ramachandran outliers	100387	1824 (2.94-2.90)
Sidechain outliers	100360	1826 (2.94-2.90)
RSRZ outliers	91569	1650 (2.94-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	<div> <div>2%</div> <div>68% 19% 12%</div> </div>
1	B	526	<div> <div>6%</div> <div>67% 20% 12%</div> </div>
1	C	526	<div> <div>75% 17% 8%</div> </div>
1	D	526	<div> <div>23%</div> <div>59% 28% 12%</div> </div>
1	E	526	<div> <div>2%</div> <div>71% 16% 12%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	526	 70% 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	LAT	F	601	-	-	-	X
3	GOL	F	603	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22283 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ricin B lectin.

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

There are 216 discrepancies between the modelled and reference sequences:

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

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

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

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

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

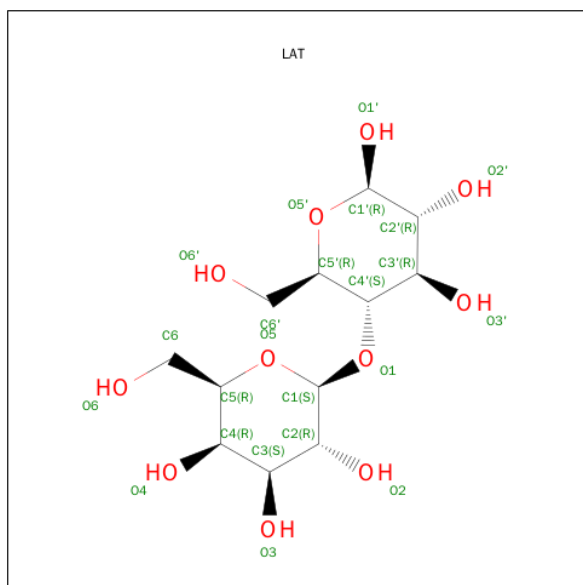
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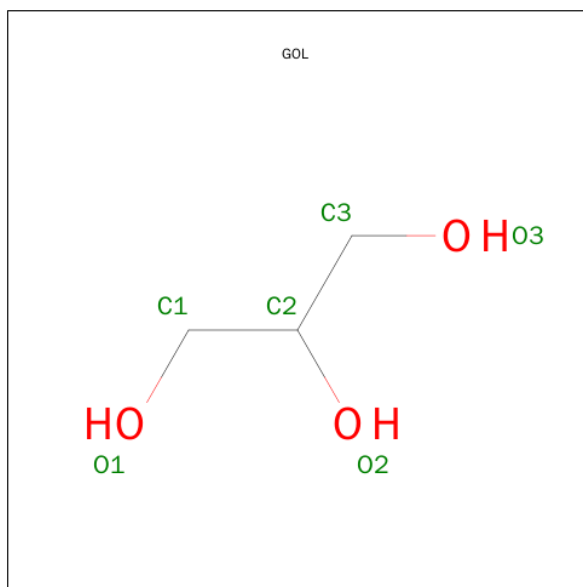
Chain	Residue	Modelled	Actual	Comment	Reference
F	-30	HIS	-	EXPRESSION TAG	UNP A3DD67
F	-29	HIS	-	EXPRESSION TAG	UNP A3DD67
F	-28	HIS	-	EXPRESSION TAG	UNP A3DD67
F	-27	HIS	-	EXPRESSION TAG	UNP A3DD67
F	-26	HIS	-	EXPRESSION TAG	UNP A3DD67
F	-25	SER	-	EXPRESSION TAG	UNP A3DD67
F	-24	SER	-	EXPRESSION TAG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

- Molecule 2 is SUGAR (BETA-LACTOSE) (three-letter code: LAT) (formula: C<sub>12</sub>H<sub>22</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			23	12	11		
2	B	1	Total	C	O	0	0
			23	12	11		
2	C	1	Total	C	O	0	0
			23	12	11		
2	E	1	Total	C	O	0	0
			23	12	11		
2	F	1	Total	C	O	0	0
			23	12	11		
2	F	1	Total	C	O	0	0
			23	12	11		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).

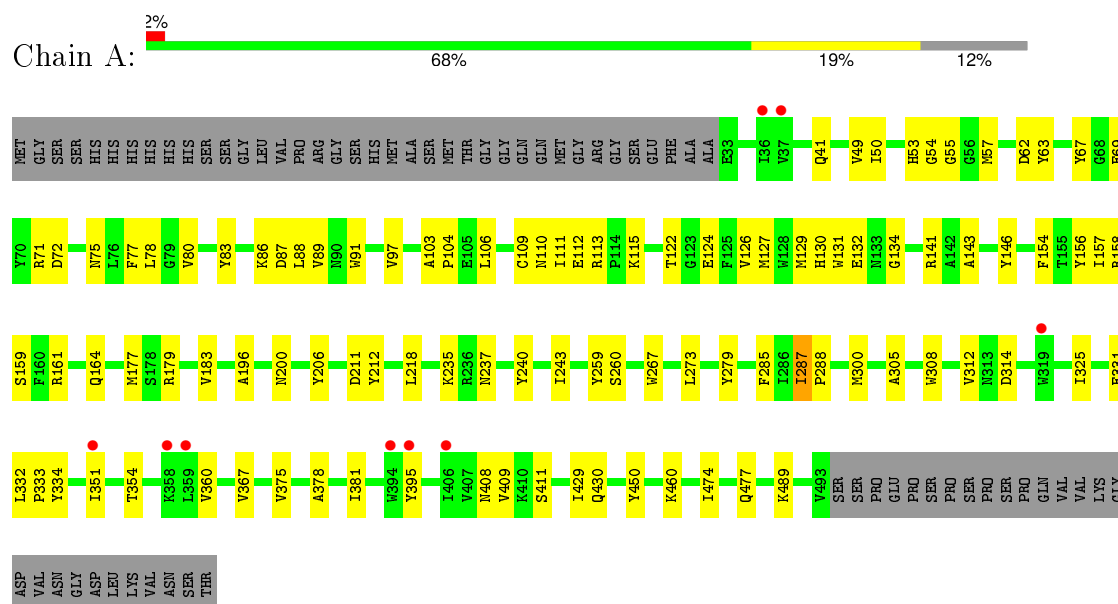


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		

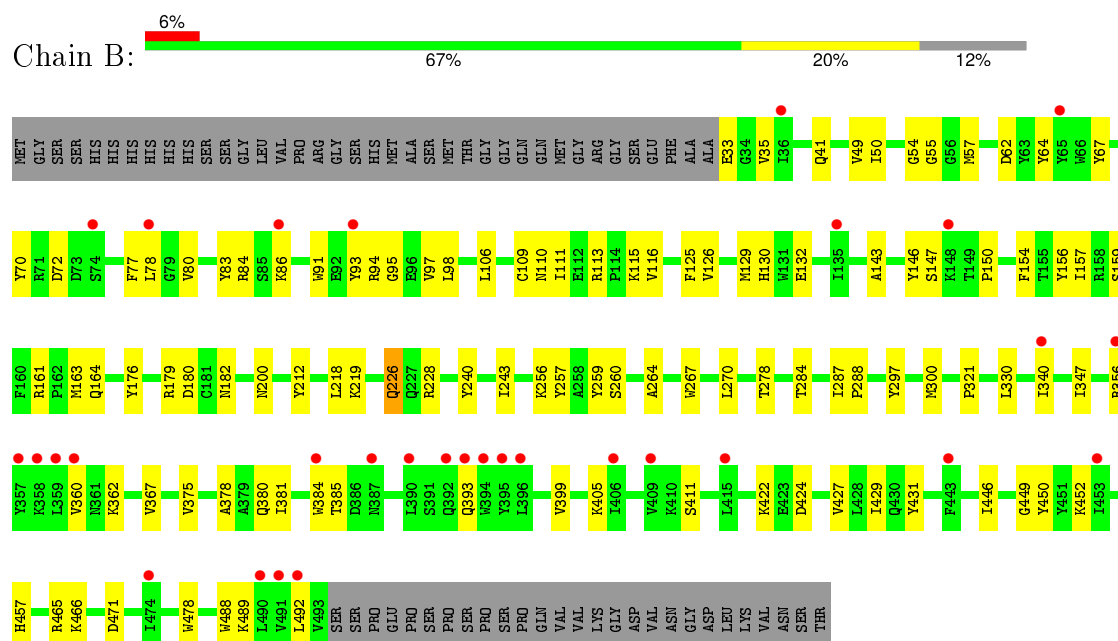
### 3 Residue-property plots

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

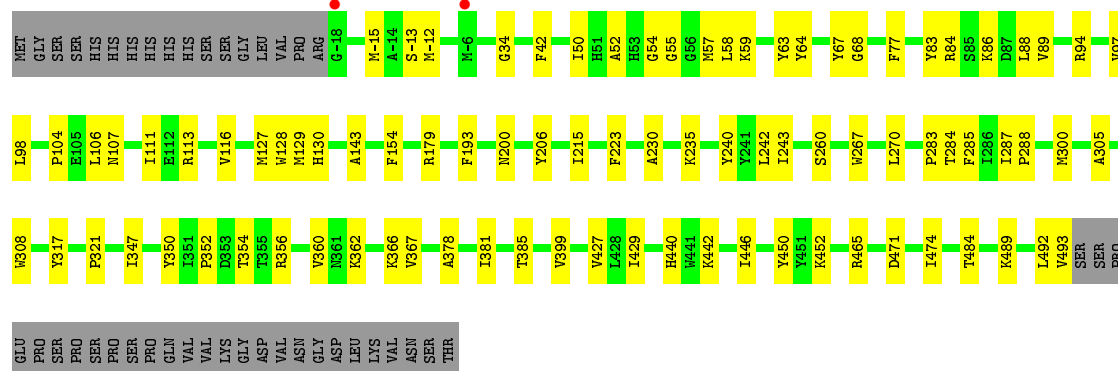


#### • Molecule 1: Ricin B lectin



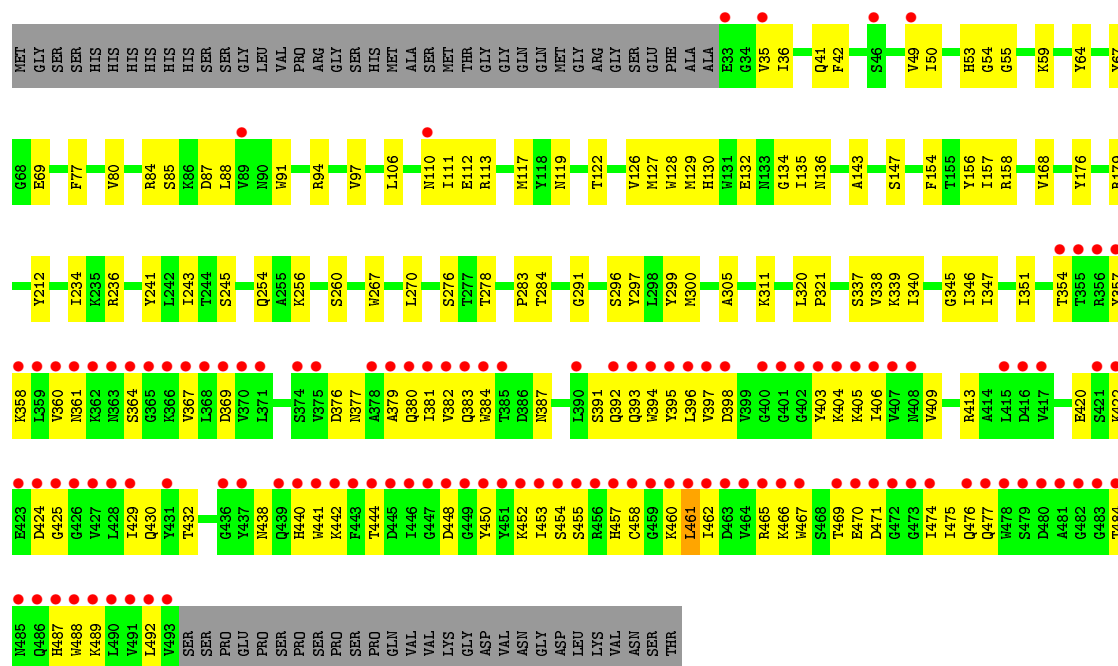
- Molecule 1: Ricin B lectin

Chain C:  75% 17% 8%



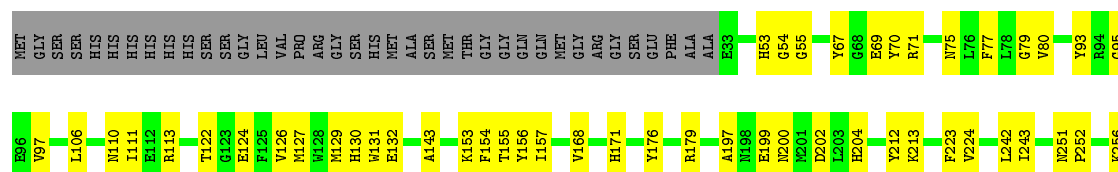
- Molecule 1: Ricin B lectin

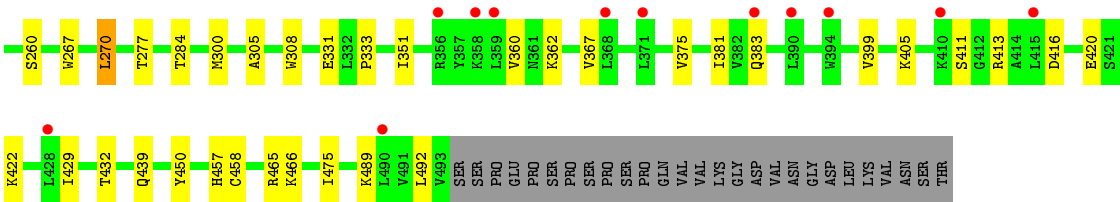
Chain D: 



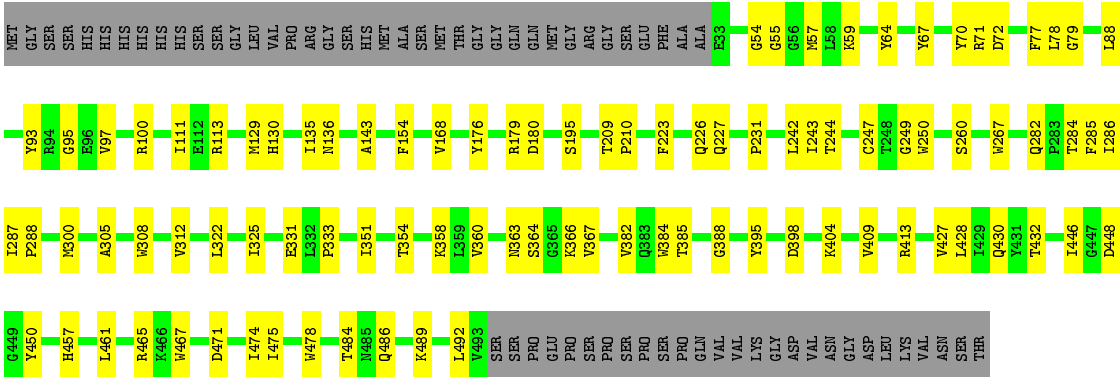
- Molecule 1: Ricin B lectin

Chain E: 





• 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, $\alpha$ , $\beta$ , $\gamma$	107.69Å 122.38Å 404.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.29 – 2.91 49.29 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.29-2.91) 99.6 (49.29-2.91)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.67 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.253 , 0.269 0.252 , 0.268	Depositor DCC
$R_{free}$ test set	2116 reflections (1.84%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.0	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.4	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 117218 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	22283	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: LAT, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.20	0/3762	0.35	0/5104
1	B	0.21	0/3762	0.35	0/5104
1	C	0.21	0/3907	0.35	0/5295
1	D	0.21	0/3762	0.36	0/5104
1	E	0.21	0/3762	0.36	0/5104
1	F	0.21	0/3762	0.35	0/5104
All	All	0.21	0/22717	0.35	0/30815

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3664	0	3480	72	0
1	B	3664	0	3480	78	0
1	C	3807	0	3613	60	0
1	D	3664	0	3480	119	0
1	E	3664	0	3480	57	0
1	F	3664	0	3480	69	0
2	A	23	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	23	0	21	1	0
2	C	23	0	21	0	0
2	E	23	0	21	0	0
2	F	46	0	44	5	0
3	A	6	0	8	0	0
3	C	6	0	8	0	0
3	F	6	0	8	2	0
All	All	22283	0	21165	451	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (451) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:GLY:HA2	1:C:89:VAL:HG21	1.53	0.89
1:B:84:ARG:HE	1:B:94:ARG:HE	1.22	0.88
1:D:321:PRO:HB3	1:D:347:ILE:HD13	1.58	0.85
1:D:422:LYS:HG3	1:D:458:CYS:HB3	1.58	0.84
1:E:422:LYS:HD3	1:E:458:CYS:HB3	1.59	0.84
1:C:-12:MET:HG3	1:E:155:THR:HG22	1.61	0.83
1:D:465:ARG:HG2	1:D:466:LYS:HG2	1.61	0.82
1:D:254:GLN:HG2	1:D:276:SER:HA	1.61	0.81
1:D:340:ILE:HG22	1:D:347:ILE:HG22	1.61	0.81
1:B:360:VAL:HG22	1:B:367:VAL:HG12	1.68	0.75
1:F:461:LEU:HD11	1:F:486:GLN:HB3	1.68	0.75
1:C:465:ARG:HH21	1:C:474:ILE:HG21	1.53	0.74
1:C:360:VAL:HG22	1:C:367:VAL:HG12	1.69	0.74
1:E:416:ASP:HB3	1:E:439:GLN:HG2	1.69	0.73
1:C:57:MET:HE2	1:C:287:ILE:HD13	1.70	0.73
1:F:360:VAL:HG22	1:F:367:VAL:HG12	1.71	0.72
1:C:260:SER:HB2	1:C:267:TRP:HA	1.72	0.72
1:A:285:PHE:CE2	1:A:287:ILE:HG23	2.25	0.71
1:A:110:ASN:HB2	1:A:132:GLU:HB2	1.73	0.70
1:A:285:PHE:HE2	1:A:287:ILE:HG23	1.57	0.70
1:D:380:GLN:HA	1:D:429:ILE:HG22	1.73	0.70
1:B:219:LYS:HE3	1:B:264:ALA:HB2	1.72	0.70
1:E:54:GLY:O	1:E:113:ARG:HA	1.92	0.70
1:A:360:VAL:HG22	1:A:367:VAL:HG12	1.73	0.69
1:D:110:ASN:HB2	1:D:132:GLU:HB2	1.74	0.69
1:D:455:SER:N	1:D:461:LEU:HD11	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ASP:HB3	1:A:78:LEU:HD12	1.75	0.69
1:D:387:ASN:H	1:D:392:GLN:HE22	1.40	0.69
1:E:360:VAL:HG22	1:E:367:VAL:HG12	1.76	0.68
1:D:453:ILE:O	1:D:461:LEU:HG	1.94	0.67
1:D:454:SER:HA	1:D:461:LEU:HD21	1.77	0.67
1:B:356:ARG:HD3	1:B:393:GLN:NE2	2.10	0.67
1:F:57:MET:HE2	1:F:287:ILE:HD13	1.78	0.66
1:D:484:THR:HA	1:D:487:HIS:CD2	2.30	0.66
1:D:377:ASN:HD21	1:D:432:THR:HG23	1.61	0.66
1:A:157:ILE:HG22	1:A:158:ARG:HG2	1.78	0.66
1:F:428:LEU:HD12	1:F:475:ILE:HG22	1.78	0.65
1:C:129:MET:HG2	1:C:143:ALA:HB3	1.79	0.65
1:B:179:ARG:HG3	1:B:200:ASN:OD1	1.97	0.65
1:C:98:LEU:HD22	1:C:127:MET:HE1	1.78	0.65
1:A:260:SER:HB2	1:A:267:TRP:HA	1.78	0.65
1:D:450:TYR:CE2	1:D:489:LYS:HE3	2.32	0.65
1:F:260:SER:HB2	1:F:267:TRP:HA	1.79	0.65
1:D:381:ILE:HG12	1:D:429:ILE:HA	1.79	0.64
1:D:69:GLU:OE1	1:D:112:GLU:HA	1.98	0.64
1:D:420:GLU:HG2	1:D:438:ASN:ND2	2.12	0.64
1:E:77:PHE:CD1	1:E:111:ILE:HB	2.33	0.64
1:C:54:GLY:O	1:C:113:ARG:HA	1.98	0.64
1:A:331:GLU:HG2	1:A:333:PRO:HD3	1.79	0.63
1:E:416:ASP:CB	1:E:439:GLN:HG2	2.29	0.63
1:E:420:GLU:HB3	1:E:457:HIS:CE1	2.34	0.63
1:D:42:PHE:HB2	1:D:50:ILE:HD11	1.80	0.62
1:E:53:HIS:O	1:E:69:GLU:HG2	2.00	0.62
1:F:77:PHE:CD1	1:F:111:ILE:HB	2.34	0.62
1:D:53:HIS:O	1:D:69:GLU:HG2	1.99	0.62
1:D:35:VAL:HG22	1:D:339:LYS:HA	1.80	0.62
1:A:287:ILE:HD11	1:A:300:MET:HE3	1.82	0.61
1:F:54:GLY:O	1:F:113:ARG:HA	1.99	0.61
1:F:250:TRP:CZ3	2:F:601:LAT:H61	2.36	0.61
1:D:260:SER:HB2	1:D:267:TRP:HA	1.83	0.61
1:D:360:VAL:HA	1:D:367:VAL:HA	1.82	0.60
1:B:54:GLY:O	1:B:113:ARG:HA	2.01	0.60
1:A:77:PHE:CE2	1:A:111:ILE:HD12	2.37	0.60
1:E:171:HIS:CE1	1:E:199:GLU:HB2	2.36	0.60
1:D:347:ILE:O	1:D:347:ILE:HD12	2.01	0.60
1:A:97:VAL:HB	1:A:154:PHE:CD2	2.37	0.60
1:E:111:ILE:HD11	1:E:131:TRP:HD1	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:260:SER:HB2	1:E:267:TRP:HA	1.84	0.59
1:D:380:GLN:NE2	1:D:474:ILE:HG13	2.17	0.59
1:B:84:ARG:NE	1:B:94:ARG:HE	1.95	0.59
1:B:161:ARG:O	1:B:164:GLN:HG3	2.02	0.59
1:C:450:TYR:CE1	1:C:489:LYS:HB2	2.38	0.59
1:E:252:PRO:HB2	1:E:277:THR:HG23	1.85	0.59
1:D:450:TYR:CD1	1:D:489:LYS:HG3	2.37	0.59
1:B:340:ILE:HG22	1:B:347:ILE:HG23	1.83	0.59
1:D:106:LEU:HD22	1:D:111:ILE:HD11	1.84	0.59
1:B:70:TYR:CZ	1:B:78:LEU:HD11	2.38	0.59
1:D:442:LYS:HB3	1:D:454:SER:OG	2.03	0.58
1:D:360:VAL:HG12	1:D:489:LYS:HB2	1.85	0.58
1:E:110:ASN:HB2	1:E:132:GLU:HB2	1.85	0.58
1:D:361:ASN:HB3	1:D:364:SER:OG	2.03	0.58
1:E:129:MET:HG2	1:E:143:ALA:HB3	1.86	0.58
1:F:168:VAL:HG11	1:F:176:TYR:CE1	2.39	0.58
1:D:360:VAL:CG1	1:D:489:LYS:HB2	2.34	0.57
1:C:84:ARG:HH21	1:C:94:ARG:NH1	2.02	0.57
1:B:72:ASP:HB3	1:B:78:LEU:HB3	1.85	0.57
1:B:97:VAL:HB	1:B:154:PHE:CD2	2.40	0.57
1:E:422:LYS:HE2	1:E:457:HIS:CD2	2.40	0.56
1:E:97:VAL:HB	1:E:154:PHE:CD2	2.40	0.56
1:B:106:LEU:HD22	1:B:111:ILE:HD11	1.87	0.56
1:D:97:VAL:HB	1:D:154:PHE:CD2	2.40	0.56
1:D:420:GLU:HB3	1:D:457:HIS:CE1	2.41	0.56
1:B:431:TYR:CE1	2:B:601:LAT:H62	2.40	0.56
1:F:71:ARG:HD3	1:F:312:VAL:HG11	1.87	0.56
1:B:110:ASN:HB2	1:B:132:GLU:HB2	1.88	0.56
1:F:223:PHE:HB3	1:F:226:GLN:HG3	1.88	0.55
1:F:223:PHE:HE2	1:F:242:LEU:HD23	1.70	0.55
1:F:249:GLY:H	2:F:601:LAT:C6'	2.20	0.55
1:F:478:TRP:CZ3	3:F:603:GOL:H31	2.42	0.55
1:A:279:TYR:CD2	1:A:334:TYR:HB2	2.41	0.55
1:A:103:ALA:HB3	1:A:106:LEU:HG	1.88	0.55
1:C:97:VAL:HB	1:C:154:PHE:CD2	2.41	0.55
1:B:41:GLN:HB3	1:B:49:VAL:HG23	1.88	0.55
1:D:380:GLN:HE22	1:D:474:ILE:HG13	1.71	0.55
1:A:54:GLY:O	1:A:113:ARG:HA	2.05	0.55
1:B:129:MET:HG2	1:B:143:ALA:HB3	1.89	0.55
1:F:366:LYS:HE3	1:F:385:THR:HG22	1.89	0.55
1:D:424:ASP:OD2	1:D:460:LYS:HD3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:TYR:OH	1:B:159:SER:HB3	2.07	0.55
1:A:69:GLU:HG2	1:A:112:GLU:HA	1.88	0.54
1:F:227:GLN:HG2	1:F:247:CYS:SG	2.47	0.54
1:D:80:VAL:HG21	1:D:127:MET:HE1	1.89	0.54
1:E:80:VAL:HG21	1:E:127:MET:CE	2.38	0.54
1:D:256:LYS:HD3	1:D:270:LEU:HB3	1.89	0.54
1:D:441:TRP:HA	1:D:454:SER:O	2.07	0.54
1:D:453:ILE:HG23	1:D:461:LEU:HD12	1.89	0.54
1:B:55:GLY:HA3	1:B:67:TYR:O	2.08	0.54
1:A:63:TYR:CE1	1:A:86:LYS:HE3	2.43	0.54
1:F:398:ASP:HA	1:F:404:LYS:HG2	1.91	0.53
1:F:250:TRP:CH2	2:F:601:LAT:H61	2.44	0.53
1:B:77:PHE:CE1	1:B:80:VAL:HG23	2.43	0.53
1:B:126:VAL:HG21	1:B:212:TYR:HB2	1.90	0.53
1:A:80:VAL:HG11	1:A:127:MET:HE3	1.91	0.53
1:F:465:ARG:HH21	1:F:474:ILE:HG21	1.74	0.53
1:B:378:ALA:HA	1:B:429:ILE:HD12	1.91	0.53
1:C:77:PHE:CD1	1:C:111:ILE:HB	2.44	0.53
1:C:63:TYR:CE1	1:C:86:LYS:HE3	2.44	0.53
1:A:325:ILE:HD11	1:A:331:GLU:OE2	2.10	0.52
1:B:57:MET:HE3	1:B:287:ILE:HG21	1.91	0.52
1:D:41:GLN:HB3	1:D:49:VAL:HG13	1.90	0.52
1:C:84:ARG:HE	1:C:94:ARG:NE	2.06	0.52
1:B:446:ILE:HD13	1:B:452:LYS:HG3	1.90	0.52
1:E:179:ARG:HG3	1:E:200:ASN:OD1	2.10	0.52
1:F:93:TYR:CZ	1:F:95:GLY:HA2	2.44	0.52
1:A:63:TYR:CZ	1:A:86:LYS:HE3	2.44	0.52
1:D:54:GLY:O	1:D:113:ARG:HA	2.09	0.52
1:E:168:VAL:HG11	1:E:176:TYR:CE1	2.44	0.52
1:B:226:GLN:HB3	1:B:228:ARG:HG2	1.90	0.52
1:F:450:TYR:CE1	1:F:489:LYS:HB2	2.45	0.52
1:B:97:VAL:HB	1:B:154:PHE:HD2	1.74	0.52
1:B:362:LYS:HE2	1:B:450:TYR:CZ	2.45	0.52
1:D:476:GLN:HG2	1:D:477:GLN:H	1.75	0.52
1:D:454:SER:C	1:D:461:LEU:HD11	2.30	0.52
1:B:260:SER:HB2	1:B:267:TRP:HA	1.92	0.52
1:E:223:PHE:HE2	1:E:242:LEU:HD23	1.74	0.51
1:D:157:ILE:HG22	1:D:158:ARG:HG2	1.91	0.51
1:A:129:MET:HG2	1:A:143:ALA:HB3	1.91	0.51
1:C:-13:SER:HA	1:C:492:LEU:HD11	1.92	0.51
1:C:57:MET:HE1	1:C:287:ILE:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:LYS:HE3	1:B:457:HIS:NE2	2.26	0.51
1:C:223:PHE:HE2	1:C:242:LEU:HD23	1.76	0.51
1:D:299:TYR:HB3	1:D:320:LEU:O	2.11	0.51
1:A:378:ALA:HA	1:A:429:ILE:HD12	1.93	0.51
1:E:80:VAL:HG21	1:E:127:MET:HE3	1.93	0.51
1:A:237:ASN:OD1	1:F:448:ASP:HA	2.10	0.51
1:B:72:ASP:HA	1:B:78:LEU:HD23	1.92	0.51
1:C:179:ARG:HG3	1:C:200:ASN:OD1	2.11	0.51
1:A:106:LEU:HD11	1:A:156:TYR:CD2	2.45	0.50
1:E:157:ILE:HD11	1:E:213:LYS:HD2	1.93	0.50
1:C:55:GLY:HA3	1:C:67:TYR:O	2.12	0.50
1:F:478:TRP:CD2	3:F:603:GOL:H11	2.47	0.50
1:A:126:VAL:HG21	1:A:212:TYR:HB2	1.92	0.50
1:F:249:GLY:H	2:F:601:LAT:H6'2	1.76	0.50
1:B:288:PRO:HG3	1:B:297:TYR:CE1	2.45	0.50
1:E:277:THR:HG22	1:E:277:THR:O	2.12	0.50
1:D:84:ARG:HG2	1:D:94:ARG:HD3	1.93	0.50
1:F:59:LYS:HD3	1:F:64:TYR:CE1	2.47	0.50
1:F:135:ILE:HG22	1:F:136:ASN:HD22	1.76	0.50
1:D:245:SER:HB3	1:D:283:PRO:HD2	1.93	0.50
1:D:55:GLY:HA3	1:D:67:TYR:O	2.11	0.50
1:E:420:GLU:HB3	1:E:457:HIS:HE1	1.77	0.50
1:D:382:VAL:HG21	1:D:384:TRP:HE1	1.77	0.50
1:B:77:PHE:HE1	1:B:80:VAL:HG23	1.76	0.49
1:C:442:LYS:HG3	1:F:100:ARG:NH1	2.27	0.49
1:E:80:VAL:HG11	1:E:127:MET:HE3	1.94	0.49
1:B:67:TYR:CE2	1:B:116:VAL:HG21	2.47	0.49
1:B:380:GLN:HE22	1:B:427:VAL:HG13	1.77	0.49
1:E:381:ILE:HG12	1:E:429:ILE:HA	1.93	0.49
1:E:55:GLY:HA3	1:E:67:TYR:O	2.12	0.49
1:D:381:ILE:HG22	1:D:475:ILE:HG13	1.94	0.49
1:D:358:LYS:HG2	1:D:392:GLN:O	2.12	0.49
1:C:-15:MET:HE3	1:E:153:LYS:HE2	1.94	0.49
1:B:218:LEU:O	1:B:218:LEU:HD12	2.12	0.49
1:F:325:ILE:HD11	1:F:331:GLU:OE1	2.11	0.49
1:D:460:LYS:O	1:D:461:LEU:HD13	2.13	0.49
1:D:377:ASN:ND2	1:D:432:THR:HG23	2.28	0.49
1:D:450:TYR:HA	1:D:489:LYS:HA	1.95	0.49
1:D:382:VAL:HA	1:D:475:ILE:HG12	1.95	0.49
1:C:106:LEU:HD22	1:C:111:ILE:HD11	1.95	0.49
1:D:236:ARG:HA	1:D:297:TYR:OH	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:135:ILE:HD12	1:F:135:ILE:N	2.28	0.49
1:E:383:GLN:HG3	1:E:383:GLN:O	2.12	0.49
1:C:98:LEU:HD22	1:C:127:MET:CE	2.42	0.48
1:C:362:LYS:HE3	1:C:484:THR:HG22	1.94	0.48
1:E:70:TYR:HB3	1:E:79:GLY:O	2.12	0.48
1:D:462:ILE:HA	1:D:476:GLN:O	2.13	0.48
1:F:325:ILE:HD12	1:F:325:ILE:H	1.79	0.48
1:D:77:PHE:CD1	1:D:111:ILE:HB	2.48	0.48
1:A:146:TYR:CD2	1:A:157:ILE:HD11	2.49	0.48
1:F:305:ALA:HA	1:F:308:TRP:CZ2	2.48	0.48
1:B:321:PRO:HB3	1:B:347:ILE:HG22	1.95	0.48
1:A:50:ILE:HG23	1:A:83:TYR:CE1	2.49	0.48
1:E:93:TYR:CZ	1:E:95:GLY:HA2	2.49	0.48
1:F:430:GLN:O	1:F:430:GLN:HG3	2.14	0.47
1:B:50:ILE:HG23	1:B:83:TYR:CE1	2.50	0.47
1:D:126:VAL:HG21	1:D:212:TYR:HB2	1.95	0.47
1:E:126:VAL:HG21	1:E:212:TYR:HB2	1.94	0.47
1:A:395:TYR:CE2	1:A:409:VAL:HG22	2.49	0.47
1:D:376:ASP:C	1:D:413:ARG:HH12	2.17	0.47
1:F:231:PRO:HA	1:F:244:THR:HG22	1.95	0.47
1:D:398:ASP:HA	1:D:404:LYS:HG2	1.94	0.47
1:C:285:PHE:HE2	1:C:287:ILE:HB	1.80	0.47
1:D:454:SER:CA	1:D:461:LEU:HD11	2.45	0.47
1:E:252:PRO:HB2	1:E:277:THR:CG2	2.44	0.47
1:B:109:CYS:HB2	1:B:132:GLU:O	2.15	0.47
1:A:161:ARG:O	1:A:164:GLN:HG3	2.14	0.47
1:C:378:ALA:HA	1:C:429:ILE:HD12	1.97	0.47
1:F:70:TYR:HB3	1:F:79:GLY:O	2.15	0.47
1:D:474:ILE:N	1:D:474:ILE:HD12	2.30	0.47
1:B:356:ARG:HD3	1:B:393:GLN:HE22	1.79	0.47
1:E:383:GLN:HB3	1:E:475:ILE:HD11	1.97	0.47
1:E:284:THR:HG22	1:E:300:MET:O	2.14	0.47
1:A:57:MET:CB	1:A:300:MET:HE1	2.45	0.47
1:B:78:LEU:C	1:B:78:LEU:HD12	2.35	0.47
1:D:395:TYR:CE2	1:D:409:VAL:HG22	2.49	0.47
1:F:331:GLU:HG2	1:F:333:PRO:HD3	1.97	0.47
1:C:362:LYS:HB2	1:C:450:TYR:CE1	2.49	0.47
1:D:364:SER:HA	1:D:469:THR:OG1	2.14	0.47
1:D:338:VAL:HG12	1:D:340:ILE:HG23	1.96	0.47
1:F:358:LYS:HZ2	1:F:388:GLY:HA2	1.79	0.47
1:F:285:PHE:HE2	1:F:287:ILE:HB	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:376:ASP:O	1:D:379:ALA:HB2	2.14	0.46
1:F:363:ASN:HB2	1:F:484:THR:OG1	2.15	0.46
1:D:80:VAL:HG11	1:D:127:MET:HE3	1.96	0.46
1:C:321:PRO:HB3	1:C:347:ILE:HG22	1.95	0.46
1:E:71:ARG:HH11	1:E:75:ASN:ND2	2.13	0.46
1:A:235:LYS:HD2	1:A:240:TYR:CE2	2.50	0.46
1:D:384:TRP:CZ3	1:D:471:ASP:HB3	2.50	0.46
1:A:62:ASP:O	1:A:86:LYS:HG2	2.16	0.46
1:C:235:LYS:HD2	1:C:240:TYR:CE2	2.51	0.46
1:D:291:GLY:HA3	1:D:345:GLY:HA3	1.96	0.46
1:D:444:THR:OG1	1:D:452:LYS:HB2	2.16	0.46
1:E:305:ALA:HA	1:E:308:TRP:CZ2	2.51	0.46
1:D:296:SER:HB2	1:D:347:ILE:HD11	1.97	0.46
1:B:147:SER:HB2	1:B:154:PHE:HA	1.97	0.46
1:F:55:GLY:HA3	1:F:67:TYR:O	2.16	0.46
1:D:448:ASP:O	1:D:489:LYS:HE2	2.15	0.46
1:D:35:VAL:HG11	1:D:337:SER:HB3	1.98	0.46
1:D:129:MET:CG	1:D:143:ALA:HB3	2.46	0.46
1:C:57:MET:CE	1:C:287:ILE:HG21	2.46	0.46
1:F:282:GLN:HE22	2:F:601:LAT:H3	1.81	0.46
1:B:83:TYR:HB3	1:B:91:TRP:HB3	1.98	0.46
1:F:286:ILE:HD13	1:F:322:LEU:HD22	1.97	0.46
1:C:58:LEU:HD22	1:C:116:VAL:HG12	1.97	0.45
1:A:375:VAL:HG12	1:A:411:SER:HB3	1.97	0.45
1:B:130:HIS:CE1	1:B:179:ARG:HD3	2.51	0.45
1:A:129:MET:CG	1:A:143:ALA:HB3	2.46	0.45
1:A:122:THR:OG1	1:A:124:GLU:HG2	2.16	0.45
1:A:41:GLN:HB3	1:A:49:VAL:HG23	1.98	0.45
1:E:362:LYS:HD3	1:E:450:TYR:CZ	2.51	0.45
1:D:377:ASN:HD21	1:D:432:THR:H	1.65	0.45
1:A:97:VAL:HB	1:A:154:PHE:HD2	1.81	0.45
1:D:147:SER:HB2	1:D:154:PHE:HA	1.98	0.45
1:F:223:PHE:CE2	1:F:242:LEU:HD23	2.51	0.45
1:A:351:ILE:N	1:A:351:ILE:HD12	2.32	0.45
1:D:357:TYR:O	1:D:393:GLN:HA	2.17	0.45
1:C:77:PHE:CZ	1:C:111:ILE:HD12	2.51	0.45
1:A:87:ASP:OD1	1:A:89:VAL:HB	2.17	0.45
1:D:360:VAL:O	1:D:488:TRP:HA	2.16	0.45
1:D:243:ILE:N	1:D:243:ILE:HD12	2.31	0.45
1:C:366:LYS:HE3	1:C:385:THR:HG22	1.99	0.45
1:F:57:MET:CE	1:F:287:ILE:HG21	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:MET:HE3	1:D:128:TRP:CD1	2.51	0.45
1:D:234:ILE:HD11	1:D:241:TYR:HB2	1.98	0.45
1:F:284:THR:HG22	1:F:300:MET:O	2.17	0.45
1:B:93:TYR:CZ	1:B:95:GLY:HA2	2.52	0.45
1:F:287:ILE:HA	1:F:288:PRO:HD3	1.86	0.45
1:C:59:LYS:HD3	1:C:64:TYR:CE1	2.52	0.45
1:C:350:TYR:O	1:C:352:PRO:HD3	2.17	0.45
1:A:55:GLY:HA3	1:A:67:TYR:O	2.16	0.45
1:C:287:ILE:HA	1:C:288:PRO:HD3	1.85	0.45
1:C:64:TYR:O	1:C:84:ARG:HA	2.17	0.45
1:E:351:ILE:N	1:E:351:ILE:HD12	2.31	0.45
1:A:474:ILE:N	1:A:474:ILE:HD12	2.32	0.45
1:C:381:ILE:HG12	1:C:429:ILE:HA	1.98	0.44
1:A:206:TYR:CE1	1:A:218:LEU:HD23	2.53	0.44
1:F:395:TYR:CE2	1:F:409:VAL:HG22	2.53	0.44
1:B:465:ARG:HG2	1:B:466:LYS:HG2	1.99	0.44
1:F:351:ILE:HD12	1:F:351:ILE:N	2.32	0.44
1:D:454:SER:HA	1:D:461:LEU:CD2	2.45	0.44
1:D:42:PHE:HB2	1:D:50:ILE:CD1	2.47	0.44
1:D:284:THR:HG22	1:D:300:MET:O	2.17	0.44
1:C:399:VAL:HG21	1:C:440:HIS:NE2	2.33	0.44
1:D:87:ASP:O	1:D:88:LEU:HB2	2.18	0.44
1:D:467:TRP:HH2	1:D:484:THR:OG1	2.00	0.44
1:A:381:ILE:HG12	1:A:429:ILE:HA	1.98	0.44
1:E:202:ASP:OD1	1:E:224:VAL:HG23	2.16	0.44
1:A:243:ILE:N	1:A:243:ILE:HD12	2.33	0.44
1:E:465:ARG:HG2	1:E:466:LYS:HG2	1.99	0.44
1:A:156:TYR:OH	1:A:159:SER:HB3	2.18	0.44
1:C:50:ILE:HG23	1:C:83:TYR:CE1	2.52	0.44
1:B:106:LEU:HD11	1:B:156:TYR:CD2	2.53	0.44
1:C:385:THR:HG23	1:C:471:ASP:OD1	2.17	0.44
1:E:106:LEU:HD11	1:E:156:TYR:CD2	2.52	0.44
1:F:325:ILE:HD12	1:F:325:ILE:N	2.32	0.44
1:D:85:SER:HB3	1:D:91:TRP:HA	1.98	0.44
1:C:270:LEU:N	1:C:270:LEU:HD12	2.32	0.44
1:F:64:TYR:CG	1:F:88:LEU:HD21	2.53	0.44
1:A:474:ILE:H	1:A:474:ILE:HD12	1.82	0.44
1:D:461:LEU:HA	1:D:461:LEU:HD13	1.55	0.43
1:D:387:ASN:H	1:D:392:GLN:NE2	2.12	0.43
1:D:106:LEU:HD11	1:D:156:TYR:CD2	2.53	0.43
1:A:279:TYR:CE2	1:A:334:TYR:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:ILE:HG12	1:B:429:ILE:HA	2.00	0.43
1:B:287:ILE:HA	1:B:288:PRO:HD3	1.90	0.43
1:D:425:GLY:HA2	1:D:476:GLN:CD	2.39	0.43
1:B:146:TYR:CD2	1:B:157:ILE:HD11	2.53	0.43
1:D:168:VAL:HG21	1:D:176:TYR:CE1	2.52	0.43
1:E:492:LEU:HD12	1:E:492:LEU:N	2.33	0.43
1:D:110:ASN:OD1	1:D:134:GLY:HA2	2.19	0.43
1:F:57:MET:HE1	1:F:287:ILE:HG21	2.00	0.43
1:B:399:VAL:HG11	1:B:405:LYS:HG3	2.01	0.43
1:C:354:THR:O	1:C:354:THR:HG22	2.17	0.43
1:A:103:ALA:HB1	1:A:104:PRO:HD2	1.99	0.43
1:B:450:TYR:HA	1:B:488:TRP:O	2.18	0.43
1:F:363:ASN:ND2	1:F:467:TRP:HE3	2.16	0.43
1:D:135:ILE:HG13	1:D:136:ASN:ND2	2.34	0.43
1:B:385:THR:HG23	1:B:471:ASP:OD1	2.18	0.43
1:B:424:ASP:HB3	1:B:478:TRP:CE3	2.53	0.43
1:A:131:TRP:CE3	1:A:141:ARG:HD2	2.52	0.43
1:C:284:THR:HG22	1:C:300:MET:O	2.18	0.43
1:B:240:TYR:O	1:B:259:TYR:HA	2.18	0.43
1:F:209:THR:HB	1:F:210:PRO:HD2	2.01	0.43
1:F:492:LEU:N	1:F:492:LEU:HD12	2.33	0.43
1:C:305:ALA:HA	1:C:308:TRP:CZ2	2.53	0.43
1:E:375:VAL:HG12	1:E:411:SER:HB3	2.01	0.43
1:C:243:ILE:N	1:C:243:ILE:HD12	2.34	0.43
1:A:110:ASN:OD1	1:A:134:GLY:HA2	2.18	0.43
1:D:381:ILE:HD11	1:D:430:GLN:HB3	2.01	0.43
1:D:357:TYR:CE2	1:D:492:LEU:HG	2.54	0.43
1:A:305:ALA:HA	1:A:308:TRP:CZ2	2.53	0.43
1:C:63:TYR:CE1	1:C:84:ARG:NH1	2.87	0.43
1:B:257:TYR:CE2	1:B:330:LEU:HD13	2.53	0.43
1:D:305:ALA:HB3	1:D:311:LYS:O	2.18	0.43
1:E:256:LYS:HD2	1:E:270:LEU:HD23	2.00	0.43
1:F:384:TRP:CE3	1:F:471:ASP:HB3	2.53	0.43
1:E:130:HIS:CE1	1:E:179:ARG:HA	2.54	0.43
1:A:115:LYS:HB3	1:A:183:VAL:HG22	2.01	0.43
1:D:278:THR:O	1:D:278:THR:HG22	2.18	0.43
1:C:52:ALA:HB1	1:C:68:GLY:HA3	2.00	0.43
1:F:364:SER:OG	1:F:366:LYS:HG2	2.19	0.43
1:B:126:VAL:HG11	1:B:212:TYR:O	2.18	0.43
1:C:130:HIS:CE1	1:C:179:ARG:HD3	2.54	0.43
1:E:122:THR:OG1	1:E:124:GLU:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:399:VAL:HG11	1:E:405:LYS:HG3	2.01	0.43
1:B:33:GLU:HG2	1:B:35:VAL:HG12	1.99	0.43
1:D:351:ILE:HD12	1:D:351:ILE:N	2.34	0.43
1:F:243:ILE:HD12	1:F:243:ILE:N	2.33	0.42
1:A:161:ARG:HH22	1:A:177:MET:HG2	1.83	0.42
1:A:57:MET:HE2	1:A:91:TRP:CH2	2.54	0.42
1:E:130:HIS:CE1	1:E:179:ARG:HD3	2.54	0.42
1:B:450:TYR:CE1	1:B:489:LYS:HB2	2.54	0.42
1:A:87:ASP:O	1:A:88:LEU:HB2	2.18	0.42
1:A:460:LYS:HB2	1:A:477:GLN:HG2	2.01	0.42
1:B:64:TYR:O	1:B:84:ARG:HA	2.20	0.42
1:B:125:PHE:CZ	1:B:150:PRO:HG3	2.54	0.42
1:D:454:SER:HA	1:D:461:LEU:HD11	2.00	0.42
1:D:467:TRP:HH2	1:D:484:THR:HG1	1.68	0.42
1:D:59:LYS:HD3	1:D:64:TYR:CD1	2.54	0.42
1:E:197:ALA:HB3	1:E:204:HIS:CE1	2.55	0.42
1:B:243:ILE:N	1:B:243:ILE:HD12	2.35	0.42
1:F:97:VAL:HB	1:F:154:PHE:CD2	2.55	0.42
1:B:321:PRO:HB3	1:B:347:ILE:CG2	2.49	0.42
1:E:450:TYR:CE1	1:E:489:LYS:HB2	2.55	0.42
1:E:331:GLU:HG2	1:E:333:PRO:HD3	2.02	0.42
1:D:397:VAL:HB	1:D:405:LYS:HG3	2.00	0.42
1:E:413:ARG:NH1	1:E:432:THR:HG22	2.35	0.42
1:D:64:TYR:CG	1:D:88:LEU:HD21	2.55	0.42
1:D:394:TRP:CE3	1:D:406:ILE:HG22	2.55	0.42
1:A:287:ILE:HA	1:A:288:PRO:HD3	1.89	0.42
1:A:240:TYR:O	1:A:259:TYR:HA	2.19	0.42
1:D:354:THR:HG22	1:D:354:THR:O	2.20	0.42
1:D:36:ILE:HD12	1:D:42:PHE:CZ	2.55	0.41
1:F:70:TYR:O	1:F:78:LEU:HB2	2.19	0.41
1:F:180:ASP:O	1:F:195:SER:HA	2.19	0.41
1:B:163:MET:HE2	1:B:176:TYR:HE2	1.85	0.41
1:F:130:HIS:CD2	1:F:179:ARG:HA	2.54	0.41
1:D:454:SER:HA	1:D:461:LEU:CG	2.50	0.41
1:F:382:VAL:HA	1:F:475:ILE:HG12	2.02	0.41
1:A:450:TYR:CE2	1:A:489:LYS:HE3	2.55	0.41
1:E:243:ILE:N	1:E:243:ILE:HD12	2.35	0.41
1:C:129:MET:CG	1:C:143:ALA:HB3	2.47	0.41
1:F:111:ILE:HG21	1:F:129:MET:HE2	2.03	0.41
1:C:356:ARG:HB2	1:C:493:VAL:HG21	2.01	0.41
1:B:72:ASP:CA	1:B:78:LEU:HD23	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:MET:HB3	1:A:300:MET:HE1	2.02	0.41
1:E:251:ASN:HA	1:E:252:PRO:HD3	1.94	0.41
1:F:385:THR:HG23	1:F:471:ASP:OD1	2.20	0.41
1:B:466:LYS:HA	1:B:466:LYS:HE2	2.01	0.41
1:B:384:TRP:CZ3	1:B:471:ASP:HB3	2.54	0.41
1:A:354:THR:O	1:A:354:THR:HG22	2.20	0.41
1:D:117:MET:HE3	1:D:128:TRP:HD1	1.85	0.41
1:B:284:THR:HG22	1:B:300:MET:O	2.20	0.41
1:F:354:THR:O	1:F:354:THR:HG22	2.21	0.41
1:A:430:GLN:O	1:A:430:GLN:HG3	2.19	0.41
1:A:161:ARG:NH2	1:A:177:MET:HG2	2.36	0.41
1:E:71:ARG:HH11	1:E:75:ASN:HD21	1.67	0.41
1:D:357:TYR:HE1	1:D:396:LEU:HD12	1.86	0.41
1:B:62:ASP:O	1:B:86:LYS:HG2	2.21	0.41
1:C:104:PRO:HA	1:C:107:ASN:OD1	2.20	0.41
1:C:230:ALA:HB1	1:C:283:PRO:O	2.20	0.41
1:A:53:HIS:HD2	1:A:312:VAL:HG12	1.85	0.41
1:A:71:ARG:NH1	1:A:312:VAL:HG11	2.36	0.41
1:C:206:TYR:HB3	1:C:215:ILE:HG23	2.03	0.41
1:F:461:LEU:CD1	1:F:486:GLN:HB3	2.43	0.41
1:F:129:MET:CG	1:F:143:ALA:HB3	2.51	0.41
1:C:84:ARG:HE	1:C:94:ARG:CZ	2.34	0.41
1:B:80:VAL:HB	1:B:98:LEU:HB3	2.03	0.41
1:F:72:ASP:HB3	1:F:78:LEU:HD11	2.02	0.41
1:A:408:ASN:HB3	1:A:411:SER:O	2.21	0.41
1:D:234:ILE:CD1	1:D:241:TYR:HB2	2.51	0.41
1:A:71:ARG:HB3	1:A:75:ASN:HA	2.01	0.41
1:C:128:TRP:HB3	1:C:193:PHE:CE1	2.56	0.41
1:C:42:PHE:CE2	1:C:317:TYR:HB2	2.56	0.41
1:A:109:CYS:HB2	1:A:132:GLU:O	2.21	0.41
1:B:384:TRP:CE3	1:B:471:ASP:HB3	2.55	0.41
1:D:369:ASP:OD1	1:D:391:SER:HB2	2.21	0.41
1:B:492:LEU:HD12	1:B:492:LEU:N	2.36	0.41
1:D:296:SER:OG	1:D:347:ILE:HG13	2.21	0.40
1:B:111:ILE:HA	1:B:130:HIS:O	2.21	0.40
1:F:446:ILE:HG12	1:F:450:TYR:O	2.21	0.40
1:B:70:TYR:OH	1:B:78:LEU:HD11	2.22	0.40
1:D:345:GLY:O	1:D:346:ILE:HD12	2.22	0.40
1:B:256:LYS:HD3	1:B:270:LEU:HB3	2.04	0.40
1:A:273:LEU:HD11	1:A:332:LEU:HB2	2.02	0.40
1:C:446:ILE:HG21	1:C:452:LYS:HG3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:VAL:HG12	1:B:411:SER:HB3	2.03	0.40
1:D:403:TYR:HB3	1:D:440:HIS:HB3	2.03	0.40
1:B:278:THR:O	1:B:278:THR:HG22	2.22	0.40
1:F:413:ARG:NH1	1:F:432:THR:HG22	2.36	0.40
1:B:449:GLY:O	1:B:489:LYS:HA	2.22	0.40
1:A:41:GLN:HE22	1:A:314:ASP:HA	1.86	0.40
1:A:196:ALA:HB1	1:A:200:ASN:HA	2.03	0.40
1:A:130:HIS:NE2	1:A:179:ARG:HA	2.37	0.40
1:D:35:VAL:CG2	1:D:339:LYS:HE3	2.51	0.40
1:C:64:TYR:CG	1:C:88:LEU:HD21	2.56	0.40
1:A:211:ASP:O	1:A:212:TYR:HB2	2.20	0.40
1:D:129:MET:HG2	1:D:143:ALA:HB3	2.03	0.40
1:D:119:ASN:HB3	1:D:122:THR:OG1	2.22	0.40
1:B:115:LYS:HG3	1:B:182:ASN:HA	2.03	0.40
1:D:130:HIS:CE1	1:D:179:ARG:HA	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	459/526 (87%)	436 (95%)	23 (5%)	0	100	100
1	B	459/526 (87%)	434 (95%)	25 (5%)	0	100	100
1	C	480/526 (91%)	460 (96%)	20 (4%)	0	100	100
1	D	459/526 (87%)	429 (94%)	30 (6%)	0	100	100
1	E	459/526 (87%)	439 (96%)	20 (4%)	0	100	100
1	F	459/526 (87%)	440 (96%)	19 (4%)	0	100	100
All	All	2775/3156 (88%)	2638 (95%)	137 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	389/442 (88%)	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%)	386 (99%)	3 (1%)	86	96
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%)	2337 (100%)	10 (0%)	93	98

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

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

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

Mol	Chain	Res	Type
1	B	393	GLN
1	B	487	HIS
1	D	377	ASN
1	D	380	GLN
1	D	392	GLN
1	D	430	GLN
1	D	457	HIS

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Mol	Chain	Res	Type
1	E	171	HIS
1	E	457	HIS
1	F	313	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

9 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	LAT	A	601	-	24,24,24	1.76	6 (25%)	35,35,35	0.98	1 (2%)
3	GOL	A	602	-	5,5,5	0.34	0	5,5,5	0.21	0
2	LAT	B	601	-	24,24,24	1.77	6 (25%)	35,35,35	1.01	2 (5%)
2	LAT	C	601	-	24,24,24	1.74	6 (25%)	35,35,35	1.06	1 (2%)
3	GOL	C	602	-	5,5,5	0.32	0	5,5,5	0.18	0
2	LAT	E	601	-	24,24,24	1.75	6 (25%)	35,35,35	1.19	3 (8%)
2	LAT	F	601	-	24,24,24	0.38	0	35,35,35	0.68	1 (2%)
2	LAT	F	602	-	24,24,24	0.38	0	35,35,35	0.68	1 (2%)
3	GOL	F	603	-	5,5,5	0.36	0	5,5,5	0.17	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	LAT	A	601	-	-	0/8/48/48	0/2/2/2
3	GOL	A	602	-	-	0/4/4/4	0/0/0/0
2	LAT	B	601	-	-	0/8/48/48	0/2/2/2
2	LAT	C	601	-	-	0/8/48/48	0/2/2/2
3	GOL	C	602	-	-	0/4/4/4	0/0/0/0
2	LAT	E	601	-	-	0/8/48/48	0/2/2/2
2	LAT	F	601	-	-	0/8/48/48	0/2/2/2
2	LAT	F	602	-	-	0/8/48/48	0/2/2/2
3	GOL	F	603	-	-	0/4/4/4	0/0/0/0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	LAT	C4-C3	-3.87	1.42	1.52
2	A	601	LAT	C4-C3	-3.87	1.42	1.52
2	B	601	LAT	C4-C3	-3.80	1.42	1.52
2	C	601	LAT	C4-C3	-3.73	1.42	1.52
2	B	601	LAT	C1'-C2'	-3.17	1.46	1.52
2	E	601	LAT	C1'-C2'	-3.04	1.47	1.52
2	A	601	LAT	C1'-C2'	-2.94	1.47	1.52
2	C	601	LAT	C1'-C2'	-2.83	1.47	1.52
2	E	601	LAT	C3'-C2'	-2.28	1.46	1.52
2	B	601	LAT	C3'-C2'	-2.27	1.46	1.52
2	C	601	LAT	C3'-C2'	-2.22	1.46	1.52
2	B	601	LAT	C3-C2	-2.20	1.46	1.52
2	A	601	LAT	C3'-C2'	-2.20	1.46	1.52
2	A	601	LAT	C3-C2	-2.17	1.46	1.52
2	C	601	LAT	C3-C2	-2.13	1.46	1.52
2	E	601	LAT	C3-C2	-2.10	1.46	1.52
2	A	601	LAT	O3-C3	2.02	1.47	1.43
2	E	601	LAT	O3-C3	2.04	1.47	1.43
2	B	601	LAT	O3-C3	2.06	1.47	1.43
2	C	601	LAT	O3-C3	2.07	1.47	1.43
2	E	601	LAT	O5'-C1'	4.67	1.51	1.43
2	B	601	LAT	O5'-C1'	4.70	1.51	1.43
2	A	601	LAT	O5'-C1'	4.72	1.52	1.43
2	C	601	LAT	O5'-C1'	4.74	1.52	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	601	LAT	C1-O1-C4'	-2.38	111.78	118.01
2	F	601	LAT	C1-O1-C4'	-2.38	111.78	118.01
2	F	602	LAT	C1-O1-C4'	-2.36	111.83	118.01
2	B	601	LAT	C1-O1-C4'	-2.32	111.94	118.01
2	A	601	LAT	C1-O1-C4'	-2.18	112.32	118.01
2	C	601	LAT	C1-O1-C4'	-2.04	112.67	118.01
2	E	601	LAT	O6-C6-C5	2.09	118.25	111.33
2	B	601	LAT	C2'-C3'-C4'	2.11	114.23	109.60
2	E	601	LAT	C2'-C3'-C4'	2.85	115.86	109.60

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	LAT	1	0
2	F	601	LAT	5	0
3	F	603	GOL	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 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%)	0.39	9 (1%) 68 64	57, 82, 97, 108	0
1	B	461/526 (87%)	0.62	31 (6%) 21 15	68, 91, 110, 114	0
1	C	482/526 (91%)	0.20	2 (0%) 93 92	48, 59, 74, 102	0
1	D	461/526 (87%)	1.33	119 (25%) 1 0	55, 86, 148, 153	0
1	E	461/526 (87%)	0.37	12 (2%) 59 54	54, 69, 85, 97	0
1	F	461/526 (87%)	0.28	0 100 100	47, 65, 83, 101	0
All	All	2787/3156 (88%)	0.53	173 (6%) 24 18	47, 74, 114, 153	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	359	LEU	9.3
1	D	380	GLN	9.0
1	D	491	VAL	8.3
1	D	368	LEU	8.2
1	D	490	LEU	8.1
1	D	450	TYR	7.5
1	D	374	SER	7.4
1	D	443	PHE	7.3
1	D	484	THR	6.9
1	D	371	LEU	6.4
1	D	394	TRP	6.2
1	D	382	VAL	6.2
1	D	367	VAL	6.1
1	D	357	TYR	6.0
1	D	478	TRP	5.8
1	D	354	THR	5.7
1	D	452	LYS	5.7
1	D	444	THR	5.7
1	D	448	ASP	5.5

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Mol	Chain	Res	Type	RSRZ
1	D	423	GLU	5.4
1	D	474	ILE	5.3
1	D	471	ASP	5.3
1	D	442	LYS	5.3
1	D	441	TRP	5.0
1	D	466	LYS	5.0
1	D	489	LYS	5.0
1	D	401	GLY	5.0
1	D	445	ASP	5.0
1	D	453	ILE	4.9
1	D	451	TYR	4.9
1	D	360	VAL	4.8
1	D	467	TRP	4.8
1	D	428	LEU	4.7
1	D	487	HIS	4.6
1	D	458	CYS	4.6
1	D	462	ILE	4.6
1	D	492	LEU	4.6
1	D	407	VAL	4.6
1	D	449	GLY	4.6
1	D	383	GLN	4.5
1	D	425	GLY	4.5
1	D	481	ALA	4.5
1	D	459	GLY	4.4
1	D	479	SER	4.4
1	D	426	GLY	4.4
1	D	364	SER	4.4
1	D	427	VAL	4.3
1	D	358	LYS	4.3
1	D	396	LEU	4.3
1	D	424	ASP	4.3
1	D	402	GLY	4.2
1	B	358	LYS	4.2
1	D	381	ILE	4.2
1	D	446	ILE	4.1
1	D	488	TRP	4.1
1	D	460	LYS	4.1
1	D	437	TYR	4.1
1	D	469	THR	4.1
1	D	392	GLN	4.0
1	D	472	GLY	4.0
1	D	370	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	363	ASN	4.0
1	D	356	ARG	4.0
1	D	384	TRP	4.0
1	D	470	GLU	3.9
1	D	405	LYS	3.9
1	D	454	SER	3.7
1	B	491	VAL	3.7
1	D	35	VAL	3.7
1	D	365	GLY	3.6
1	D	480	ASP	3.6
1	D	447	GLY	3.6
1	D	456	ARG	3.6
1	D	440	HIS	3.6
1	B	490	LEU	3.5
1	D	439	GLN	3.5
1	D	362	LYS	3.5
1	D	422	LYS	3.5
1	D	486	GLN	3.4
1	D	406	ILE	3.3
1	B	396	LEU	3.3
1	D	417	VAL	3.3
1	D	110	ASN	3.3
1	D	463	ASP	3.2
1	D	390	LEU	3.2
1	D	89	VAL	3.2
1	E	359	LEU	3.1
1	D	421	SER	3.1
1	D	395	TYR	3.0
1	B	65	TYR	3.0
1	D	408	ASN	3.0
1	D	473	GLY	3.0
1	D	465	ARG	2.9
1	D	477	GLN	2.9
1	D	33	GLU	2.9
1	D	366	LYS	2.9
1	D	403	TYR	2.9
1	D	398	ASP	2.9
1	D	355	THR	2.8
1	B	340	ILE	2.8
1	E	394	TRP	2.8
1	D	400	GLY	2.8
1	B	360	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	393	GLN	2.7
1	A	395	TYR	2.7
1	B	394	TRP	2.7
1	B	393	GLN	2.7
1	B	406	ILE	2.7
1	D	397	VAL	2.7
1	D	493	VAL	2.7
1	B	356	ARG	2.7
1	B	387	ASN	2.7
1	E	490	LEU	2.6
1	B	135	ILE	2.6
1	D	361	ASN	2.6
1	C	-18	GLY	2.6
1	D	378	ALA	2.6
1	D	415	LEU	2.6
1	D	436	GLY	2.6
1	B	74	SER	2.6
1	B	415	LEU	2.6
1	B	86	LYS	2.5
1	E	383	GLN	2.5
1	B	492	LEU	2.5
1	B	395	TYR	2.5
1	D	404	LYS	2.5
1	D	429	ILE	2.5
1	D	482	GLY	2.5
1	A	359	LEU	2.5
1	A	394	TRP	2.4
1	D	461	LEU	2.4
1	B	78	LEU	2.4
1	A	351	ILE	2.4
1	B	390	LEU	2.4
1	C	-6	MET	2.4
1	E	428	LEU	2.4
1	D	455	SER	2.4
1	B	443	PHE	2.3
1	E	415	LEU	2.3
1	D	476	GLN	2.3
1	D	485	ASN	2.3
1	E	390	LEU	2.3
1	A	36	ILE	2.3
1	E	358	LYS	2.3
1	A	37	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	457	HIS	2.3
1	B	359	LEU	2.3
1	D	483	GLY	2.3
1	E	356	ARG	2.2
1	B	453	ILE	2.2
1	D	464	VAL	2.2
1	B	384	TRP	2.2
1	D	375	VAL	2.2
1	E	368	LEU	2.1
1	B	357	TYR	2.1
1	E	371	LEU	2.1
1	D	416	ASP	2.1
1	E	410	LYS	2.1
1	B	36	ILE	2.1
1	D	46	SER	2.1
1	A	319	TRP	2.1
1	B	148	LYS	2.1
1	B	474	ILE	2.1
1	B	409	VAL	2.1
1	D	379	ALA	2.1
1	B	392	GLN	2.1
1	D	385	THR	2.0
1	D	431	TYR	2.0
1	D	369	ASP	2.0
1	A	406	ILE	2.0
1	D	49	VAL	2.0
1	A	358	LYS	2.0
1	B	93	TYR	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](#)

There are no carbohydrates in this entry.

## 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. 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	LAT	F	601	23/23	0.79	0.34	2.74	19,19,19,19	0
3	GOL	F	603	6/6	0.94	0.28	2.23	19,19,19,19	0
3	GOL	C	602	6/6	0.95	0.25	1.75	19,19,19,19	0
2	LAT	B	601	23/23	0.90	0.22	0.25	19,19,19,19	0
2	LAT	A	601	23/23	0.90	0.19	0.06	19,19,19,19	0
2	LAT	E	601	23/23	0.94	0.21	-0.29	19,19,19,19	0
2	LAT	F	602	23/23	0.91	0.17	-0.62	19,19,19,19	0
2	LAT	C	601	23/23	0.91	0.16	-1.37	19,19,19,19	0
3	GOL	A	602	6/6	0.97	0.15	-2.53	19,19,19,19	0

## 6.5 Other polymers

There are no such residues in this entry.