



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:01 PM GMT

PDB ID : 3VSF  
Title : Crystal structure of 1,3Gal43A, an exo-beta-1,3-Galactanase from Clostridium thermocellum  
Authors : Jiang, D.; Fan, J.; Wang, X.; Zhao, Y.; Huang, B.; Zhang, X.C.  
Deposited on : 2012-04-25  
Resolution : 2.76 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

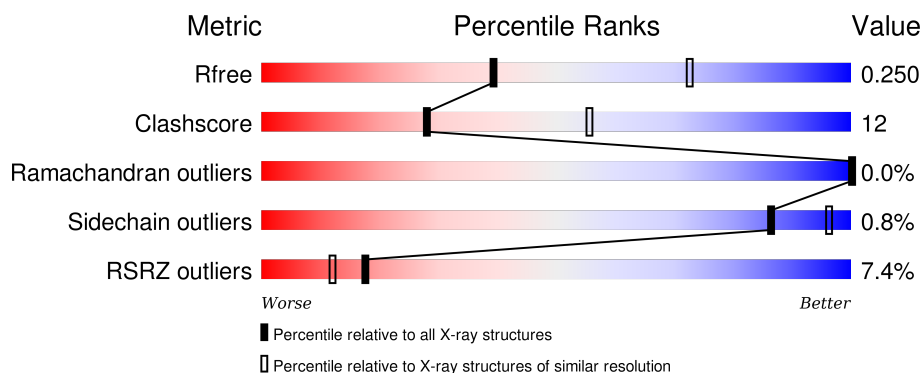
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.76 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	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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>5%</div> <div>67% 20% 12%</div> </div>
1	B	526	<div> <div>9%</div> <div>66% 21% 12%</div> </div>
1	C	526	<div> <div>%</div> <div>76% 15% 8%</div> </div>
1	D	526	<div> <div>21%</div> <div>57% 30% 12%</div> </div>
1	E	526	<div> <div>2%</div> <div>67% 20% 12%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	526	 % 72% 16% 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	A	602	-	-	X	X
2	GOL	B	601	-	-	-	X
2	GOL	C	601	-	-	X	-
2	GOL	C	602	-	-	-	X
2	GOL	C	603	-	-	-	X
2	GOL	E	601	-	-	-	X
2	GOL	F	601	-	-	X	-
2	GOL	F	603	-	-	X	-
2	GOL	F	604	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22233 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

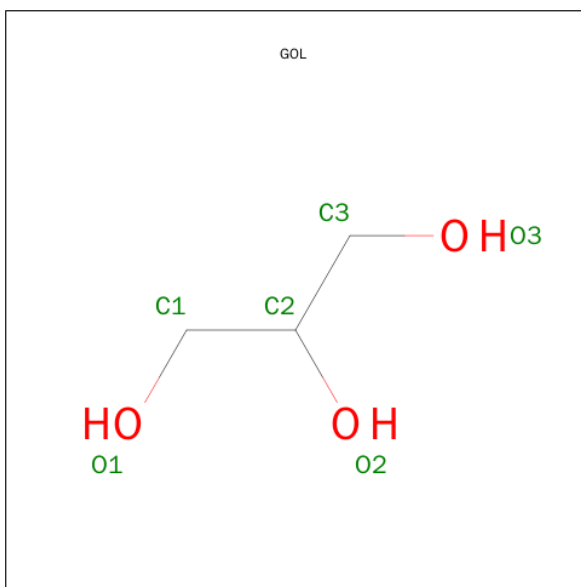
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Chain	Residue	Modelled	Actual	Comment	Reference
F	-30	HIS	-	EXPRESSION TAG	UNP A3DD67
F	-29	HIS	-	EXPRESSION TAG	UNP A3DD67
F	-28	HIS	-	EXPRESSION TAG	UNP A3DD67
F	-27	HIS	-	EXPRESSION TAG	UNP A3DD67
F	-26	HIS	-	EXPRESSION TAG	UNP A3DD67
F	-25	SER	-	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	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		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		

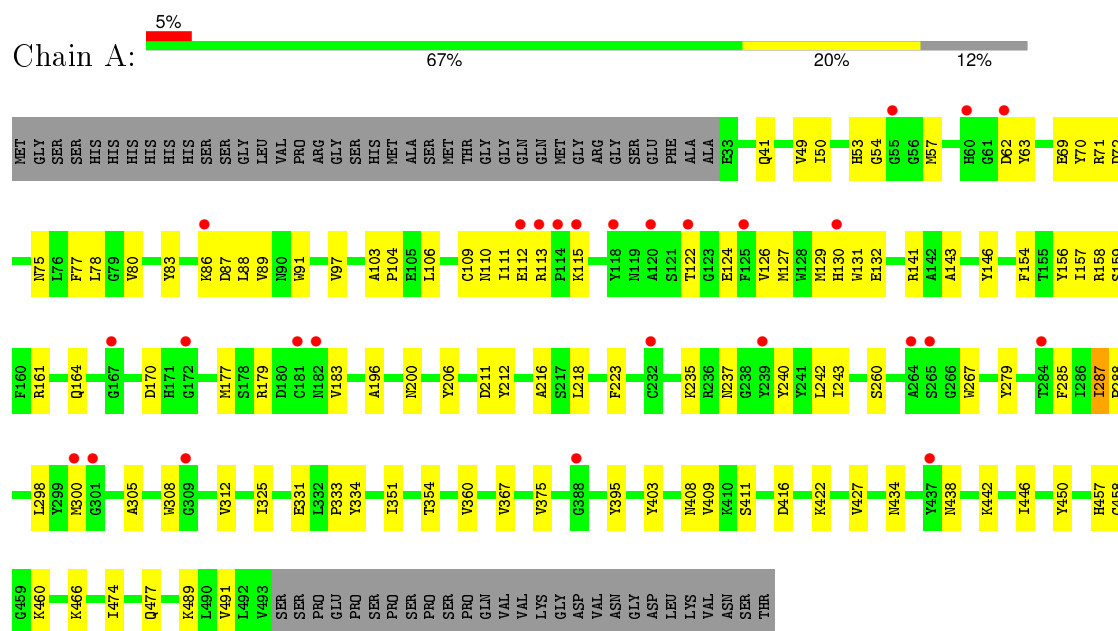
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total 4	O 4	0	0
3	C	12	Total 12	O 12	0	0
3	E	2	Total 2	O 2	0	0
3	F	4	Total 4	O 4	0	0

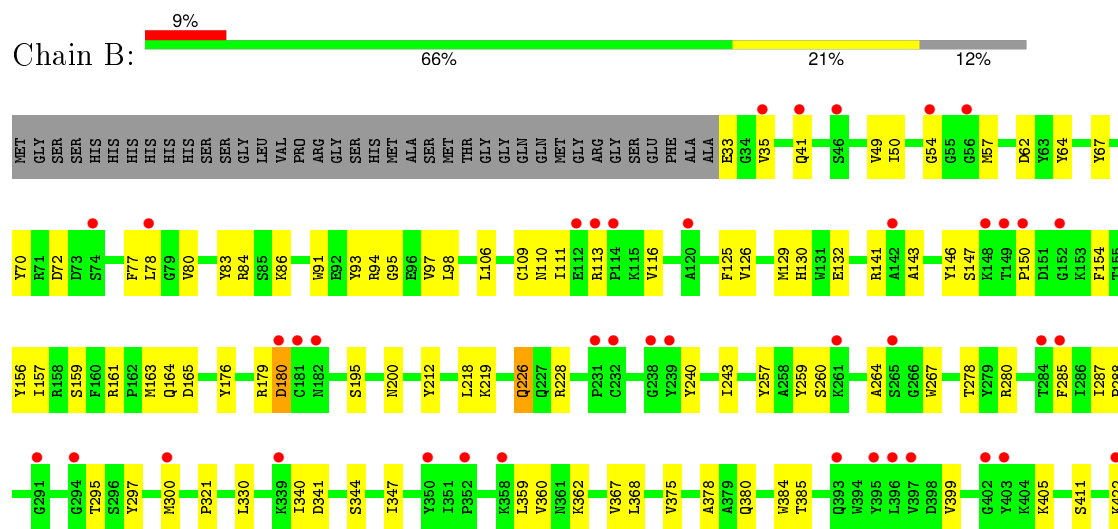
### 3 Residue-property plots

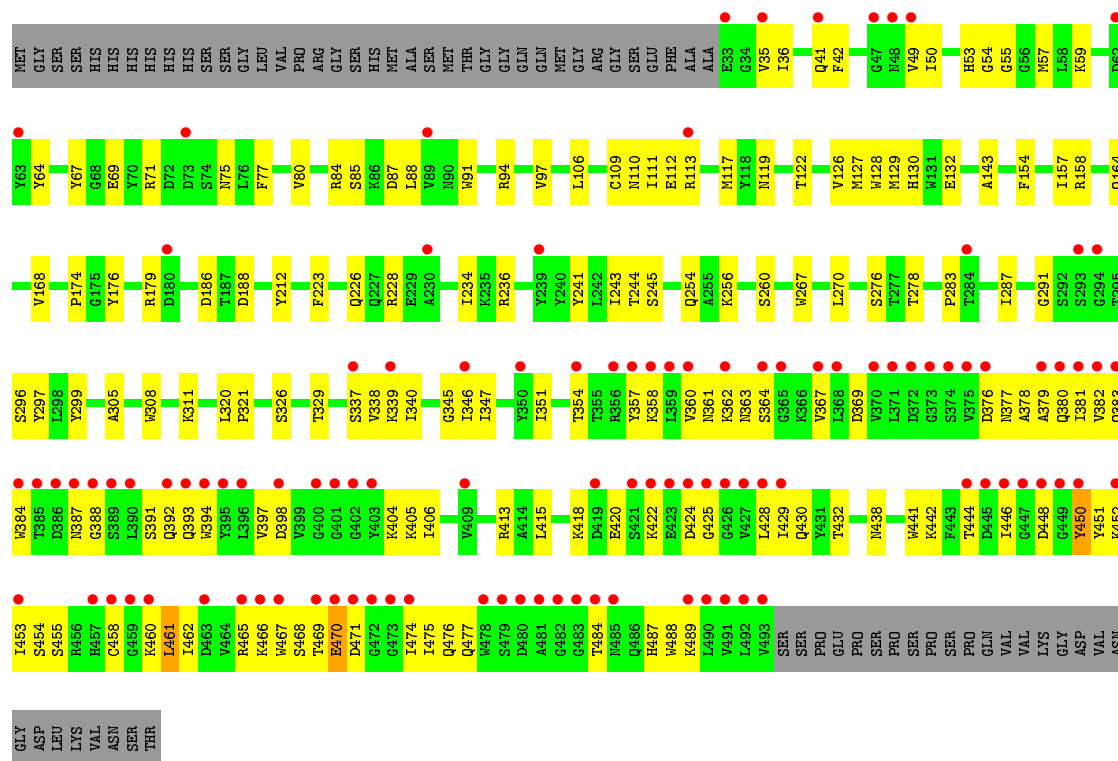
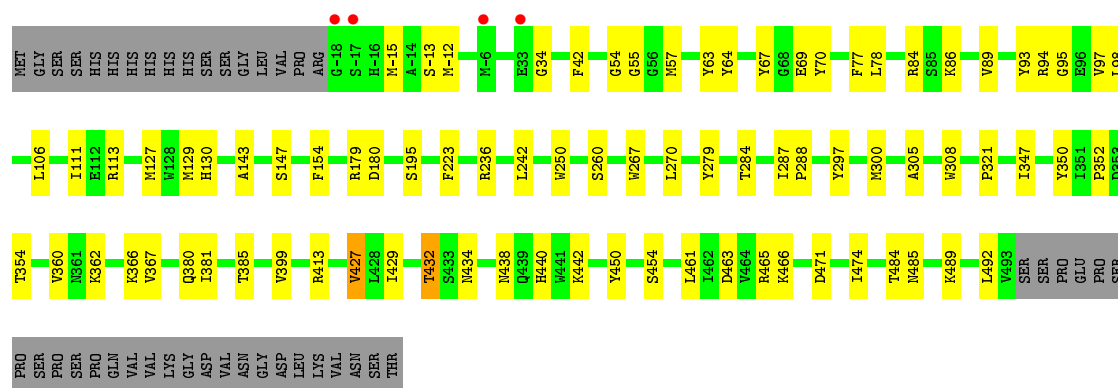
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

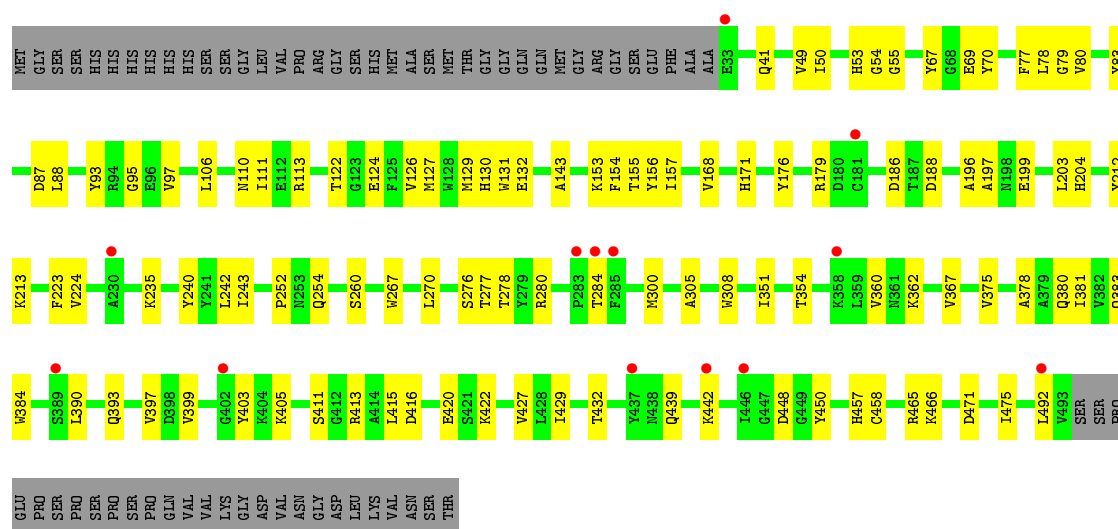
#### • Molecule 1: Ricin B lectin



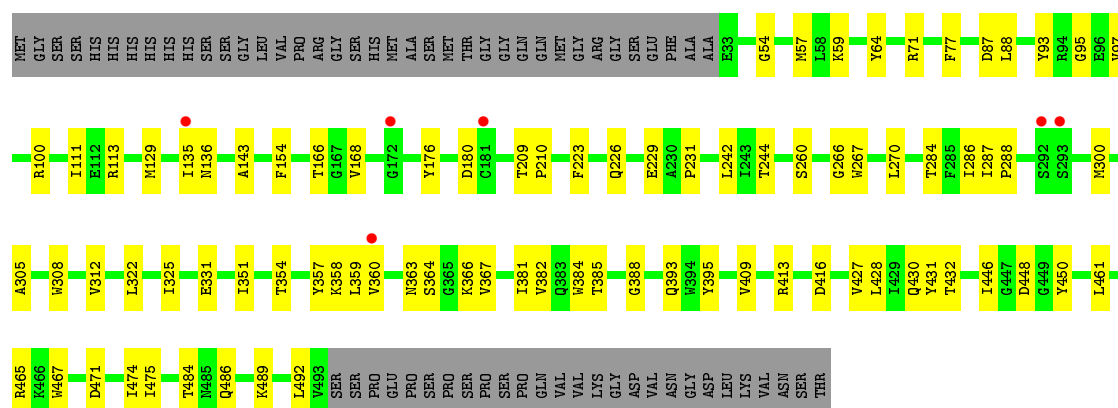
#### • Molecule 1: Ricin B lectin







● Molecule 1: Ricin B lectin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.60Å 122.51Å 405.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.55 – 2.76 37.55 – 2.76	Depositor EDS
% Data completeness (in resolution range)	98.1 (37.55-2.76) 98.1 (37.55-2.76)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.16 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.236 , 0.257 0.226 , 0.250	Depositor DCC
$R_{free}$ test set	2464 reflections (1.81%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.5	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 37.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 136199 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	22233	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.89% 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

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	0.20	0/3762	0.35	0/5104
1	C	0.21	0/3907	0.35	0/5295
1	D	0.22	0/3762	0.37	0/5104
1	E	0.21	0/3762	0.36	0/5104
1	F	0.21	0/3762	0.36	0/5104
All	All	0.21	0/22717	0.36	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	88	0
1	B	3664	0	3480	87	0
1	C	3807	0	3613	66	0
1	D	3664	0	3480	131	0
1	E	3664	0	3480	72	0
1	F	3664	0	3480	68	0
2	A	12	0	16	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	12	0	16	4	0
2	C	24	0	32	9	0
2	D	6	0	8	0	0
2	E	6	0	8	0	0
2	F	24	0	32	9	0
3	A	4	0	0	1	0
3	C	12	0	0	0	0
3	E	2	0	0	0	0
3	F	4	0	0	0	0
All	All	22233	0	21125	505	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 12.

All (505) 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	1.52	0.89
1:C:485:ASN:HD21	2:C:601:GOL:H11	1.35	0.89
1:D:465:ARG:HG2	1:D:466:LYS:HG2	1.56	0.86
1:D:340:ILE:HG22	1:D:347:ILE:HG22	1.58	0.84
1:D:254:GLN:HG2	1:D:276:SER:HA	1.60	0.83
1:B:84:ARG:HE	1:B:94:ARG:HE	1.26	0.82
1:D:321:PRO:HB3	1:D:347:ILE:HD13	1.60	0.82
1:D:422:LYS:HG3	1:D:458:CYS:HB3	1.62	0.81
1:C:-12:MET:HG3	1:E:155:THR:HG22	1.61	0.81
1:F:57:MET:HE1	1:F:287:ILE:HG21	1.62	0.81
1:F:461:LEU:HD11	1:F:486:GLN:HB3	1.65	0.78
1:A:285:PHE:HE2	1:A:287:ILE:HG23	1.50	0.77
1:E:80:VAL:HG21	1:E:127:MET:HE1	1.66	0.77
1:A:285:PHE:CE2	1:A:287:ILE:HG23	2.20	0.76
1:A:110:ASN:HB2	1:A:132:GLU:HB2	1.69	0.75
1:D:380:GLN:HA	1:D:429:ILE:HG22	1.69	0.74
1:C:57:MET:HE2	1:C:287:ILE:HD13	1.69	0.74
1:B:446:ILE:HD13	1:B:452:LYS:HG3	1.69	0.73
1:B:219:LYS:HE3	1:B:264:ALA:HB2	1.69	0.73
1:D:455:SER:N	1:D:461:LEU:HD11	2.04	0.73
1:C:465:ARG:HH21	1:C:474:ILE:HG21	1.54	0.72
1:E:252:PRO:HB2	1:E:277:THR:HG23	1.72	0.72
1:D:420:GLU:HG2	1:D:438:ASN:ND2	2.05	0.71
1:C:360:VAL:HG22	1:C:367:VAL:HG12	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:TYR:CZ	1:B:78:LEU:HD11	2.24	0.71
1:F:360:VAL:HG22	1:F:367:VAL:HG12	1.73	0.71
1:D:453:ILE:O	1:D:461:LEU:HG	1.92	0.70
1:D:454:SER:HA	1:D:461:LEU:HD21	1.72	0.70
1:A:422:LYS:HD3	1:A:458:CYS:HB3	1.73	0.70
1:E:416:ASP:HB3	1:E:439:GLN:HG2	1.73	0.70
1:D:360:VAL:HG12	1:D:489:LYS:HB2	1.73	0.70
1:D:110:ASN:HB2	1:D:132:GLU:HB2	1.73	0.70
1:E:422:LYS:HD3	1:E:458:CYS:HB3	1.75	0.69
1:B:360:VAL:HG22	1:B:367:VAL:HG12	1.73	0.69
1:D:387:ASN:H	1:D:392:GLN:HE22	1.41	0.68
1:A:260:SER:HB2	1:A:267:TRP:HA	1.76	0.68
1:D:69:GLU:OE1	1:D:112:GLU:HA	1.94	0.67
1:D:450:TYR:CE2	1:D:489:LYS:HE3	2.29	0.67
1:E:70:TYR:O	1:E:78:LEU:HB3	1.94	0.67
1:A:72:ASP:HB3	1:A:78:LEU:HD12	1.76	0.67
1:D:484:THR:HA	1:D:487:HIS:CD2	2.29	0.67
1:B:84:ARG:NE	1:B:94:ARG:HE	1.93	0.67
1:A:157:ILE:HG22	1:A:158:ARG:HG2	1.77	0.66
1:D:450:TYR:CD1	1:D:489:LYS:HG3	2.30	0.66
1:F:113:ARG:HE	2:F:603:GOL:H31	1.61	0.66
1:F:465:ARG:HH21	1:F:474:ILE:HG21	1.61	0.66
1:A:422:LYS:HE2	1:A:457:HIS:CE1	2.31	0.65
1:D:381:ILE:HG12	1:D:429:ILE:HA	1.79	0.65
1:A:77:PHE:CE2	1:A:111:ILE:HD12	2.32	0.65
1:C:260:SER:HB2	1:C:267:TRP:HA	1.79	0.64
1:B:72:ASP:HA	1:B:78:LEU:HD23	1.78	0.64
1:D:35:VAL:HG22	1:D:339:LYS:HA	1.77	0.64
1:B:378:ALA:HA	1:B:429:ILE:HD12	1.80	0.64
1:A:360:VAL:HG22	1:A:367:VAL:HG12	1.80	0.64
1:F:113:ARG:HH21	2:F:603:GOL:H31	1.62	0.64
1:D:442:LYS:HB3	1:D:454:SER:OG	1.97	0.64
1:F:223:PHE:HB3	1:F:226:GLN:HG3	1.80	0.64
1:D:450:TYR:HA	1:D:489:LYS:HA	1.81	0.63
1:C:54:GLY:O	1:C:113:ARG:HA	1.98	0.63
1:E:77:PHE:CD1	1:E:111:ILE:HB	2.33	0.63
1:D:347:ILE:O	1:D:347:ILE:HD12	1.98	0.63
1:D:360:VAL:CG1	1:D:489:LYS:HB2	2.28	0.63
1:F:260:SER:HB2	1:F:267:TRP:HA	1.81	0.63
1:D:80:VAL:HG21	1:D:127:MET:HE1	1.81	0.62
1:D:380:GLN:NE2	1:D:474:ILE:HG13	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:366:LYS:HE3	1:F:385:THR:HG22	1.81	0.62
1:D:53:HIS:O	1:D:69:GLU:HG2	2.00	0.62
1:D:106:LEU:HD22	1:D:111:ILE:HD11	1.82	0.62
1:A:287:ILE:HD11	1:A:300:MET:HE3	1.81	0.62
1:E:416:ASP:CB	1:E:439:GLN:HG2	2.30	0.61
1:A:97:VAL:HB	1:A:154:PHE:CD2	2.36	0.61
1:C:434:ASN:HD21	2:C:602:GOL:H12	1.64	0.61
1:E:420:GLU:HB3	1:E:457:HIS:CE1	2.36	0.61
1:D:361:ASN:HB3	1:D:364:SER:OG	1.99	0.61
1:D:467:TRP:HH2	1:D:484:THR:HG1	1.48	0.61
1:B:340:ILE:HG22	1:B:347:ILE:HG23	1.82	0.61
1:C:438:ASN:HD21	2:C:602:GOL:H11	1.66	0.61
1:B:161:ARG:O	1:B:164:GLN:HG3	2.01	0.61
1:C:466:LYS:H	2:C:601:GOL:H31	1.67	0.60
1:D:260:SER:HB2	1:D:267:TRP:HA	1.84	0.60
1:F:450:TYR:CE1	1:F:489:LYS:HB2	2.37	0.60
1:C:98:LEU:HD22	1:C:127:MET:HE1	1.83	0.60
1:D:377:ASN:HD21	1:D:432:THR:HG23	1.67	0.60
1:F:54:GLY:O	1:F:113:ARG:HA	2.02	0.60
1:E:171:HIS:CE1	1:E:199:GLU:HB2	2.36	0.59
1:C:413:ARG:NH1	1:C:432:THR:HG22	2.17	0.59
1:B:179:ARG:HG3	1:B:200:ASN:OD1	2.02	0.59
1:F:71:ARG:HD3	1:F:312:VAL:HG11	1.84	0.59
1:B:163:MET:HE2	1:B:176:TYR:HE2	1.67	0.59
1:B:72:ASP:HB3	1:B:78:LEU:HB3	1.85	0.59
1:C:450:TYR:CE1	1:C:489:LYS:HB2	2.38	0.59
1:E:360:VAL:HG22	1:E:367:VAL:HG12	1.84	0.59
1:E:54:GLY:O	1:E:113:ARG:HA	2.02	0.58
1:B:126:VAL:HG21	1:B:212:TYR:HB2	1.86	0.58
1:B:463:ASP:OD2	2:B:602:GOL:H11	2.02	0.58
1:E:157:ILE:HD11	1:E:213:LYS:HD2	1.86	0.58
1:F:358:LYS:HZ2	1:F:388:GLY:HA2	1.69	0.58
1:C:-13:SER:HA	1:C:492:LEU:HD11	1.86	0.58
1:B:362:LYS:HE2	1:B:450:TYR:CZ	2.38	0.57
1:B:156:TYR:OH	1:B:159:SER:HB3	2.05	0.57
1:E:260:SER:HB2	1:E:267:TRP:HA	1.86	0.57
1:B:41:GLN:HB3	1:B:49:VAL:HG23	1.86	0.57
1:C:362:LYS:HE3	1:C:484:THR:HG22	1.86	0.57
1:C:129:MET:HG2	1:C:143:ALA:HB3	1.85	0.57
1:F:428:LEU:HD12	1:F:475:ILE:HG22	1.87	0.57
1:E:168:VAL:HG11	1:E:176:TYR:CE1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:ILE:HD11	1:E:131:TRP:HD1	1.68	0.57
1:B:449:GLY:O	1:B:489:LYS:HA	2.04	0.57
1:D:444:THR:OG1	1:D:452:LYS:HB2	2.05	0.56
1:B:97:VAL:HB	1:B:154:PHE:CD2	2.40	0.56
1:A:279:TYR:CD2	1:A:334:TYR:HB2	2.40	0.56
1:C:223:PHE:HE2	1:C:242:LEU:HD23	1.69	0.56
1:D:424:ASP:OD2	1:D:460:LYS:HD3	2.05	0.56
1:E:80:VAL:HG21	1:E:127:MET:CE	2.36	0.56
1:A:466:LYS:HG2	1:C:250:TRP:CE2	2.40	0.56
1:D:42:PHE:HB2	1:D:50:ILE:HD11	1.86	0.56
1:E:53:HIS:O	1:E:69:GLU:HG2	2.05	0.56
1:D:380:GLN:HE22	1:D:474:ILE:HG13	1.70	0.56
1:C:279:TYR:HA	2:C:603:GOL:H11	1.89	0.56
1:A:129:MET:HG2	1:A:143:ALA:HB3	1.88	0.55
1:B:129:MET:HG2	1:B:143:ALA:HB3	1.88	0.55
1:F:77:PHE:CD1	1:F:111:ILE:HB	2.41	0.55
1:F:363:ASN:HB2	1:F:484:THR:OG1	2.07	0.55
1:A:63:TYR:CZ	1:A:86:LYS:HE3	2.41	0.55
1:F:231:PRO:HA	1:F:244:THR:HG22	1.88	0.55
1:F:416:ASP:OD2	2:F:601:GOL:H11	2.07	0.55
1:C:385:THR:HG23	1:C:471:ASP:OD1	2.07	0.55
1:D:382:VAL:HG21	1:D:384:TRP:HE1	1.72	0.55
1:D:157:ILE:HG22	1:D:158:ARG:HG2	1.88	0.54
1:C:55:GLY:HA3	1:C:67:TYR:O	2.07	0.54
1:D:462:ILE:HA	1:D:476:GLN:O	2.08	0.54
1:D:448:ASP:O	1:D:489:LYS:HE2	2.07	0.54
1:A:237:ASN:OD1	1:F:448:ASP:HA	2.07	0.54
1:D:256:LYS:HD3	1:D:270:LEU:HB3	1.90	0.54
1:C:84:ARG:HH21	1:C:94:ARG:NH1	2.06	0.54
1:C:106:LEU:HD22	1:C:111:ILE:HD11	1.89	0.54
1:B:226:GLN:HB3	1:B:228:ARG:HG2	1.90	0.54
1:D:360:VAL:HA	1:D:367:VAL:HA	1.89	0.53
1:D:398:ASP:OD1	1:D:404:LYS:HG2	2.08	0.53
1:F:180:ASP:OD2	1:F:229:GLU:HG2	2.08	0.53
1:F:325:ILE:HD11	1:F:331:GLU:OE1	2.08	0.53
1:E:97:VAL:HB	1:E:154:PHE:CD2	2.42	0.53
1:D:441:TRP:HA	1:D:454:SER:O	2.07	0.53
1:A:331:GLU:HG2	1:A:333:PRO:HD3	1.89	0.53
1:A:106:LEU:HD11	1:A:156:TYR:CD2	2.43	0.53
1:E:277:THR:HG22	1:E:277:THR:O	2.08	0.53
1:A:325:ILE:HD11	1:A:331:GLU:OE2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:VAL:HG11	1:D:127:MET:HE3	1.90	0.53
1:B:130:HIS:CE1	1:B:179:ARG:HD3	2.43	0.53
1:A:63:TYR:CE1	1:A:86:LYS:HE3	2.44	0.53
1:B:422:LYS:HE3	1:B:457:HIS:NE2	2.24	0.53
1:E:383:GLN:HG3	1:E:383:GLN:O	2.09	0.52
1:C:97:VAL:HB	1:C:154:PHE:CD2	2.44	0.52
1:E:110:ASN:HB2	1:E:132:GLU:HB2	1.91	0.52
1:A:80:VAL:HG11	1:A:127:MET:HE3	1.92	0.52
1:B:106:LEU:HD22	1:B:111:ILE:HD11	1.92	0.52
1:C:63:TYR:CE1	1:C:86:LYS:HE3	2.44	0.52
1:A:122:THR:OG1	1:A:124:GLU:HG2	2.10	0.52
1:D:454:SER:HA	1:D:461:LEU:CD2	2.39	0.52
1:C:57:MET:HE1	1:C:287:ILE:HG21	1.92	0.52
1:D:460:LYS:O	1:D:461:LEU:HD13	2.10	0.52
1:B:466:LYS:N	2:B:602:GOL:O2	2.42	0.52
1:D:41:GLN:HB3	1:D:49:VAL:HG13	1.91	0.52
1:F:168:VAL:HG11	1:F:176:TYR:CE1	2.45	0.52
1:A:69:GLU:HG2	1:A:112:GLU:HA	1.91	0.52
1:C:434:ASN:ND2	2:C:602:GOL:H12	2.24	0.52
1:B:67:TYR:CE2	1:B:116:VAL:HG21	2.45	0.52
1:F:223:PHE:HE2	1:F:242:LEU:HD23	1.74	0.51
1:F:416:ASP:CG	2:F:601:GOL:H11	2.30	0.51
1:C:57:MET:CE	1:C:287:ILE:HG21	2.40	0.51
1:E:422:LYS:CD	1:E:458:CYS:HB3	2.41	0.51
1:B:54:GLY:O	1:B:113:ARG:HA	2.10	0.51
1:B:72:ASP:CA	1:B:78:LEU:HD23	2.40	0.51
1:D:467:TRP:HH2	1:D:484:THR:OG1	1.92	0.51
1:E:223:PHE:HE2	1:E:242:LEU:HD23	1.74	0.51
1:D:299:TYR:HB3	1:D:320:LEU:O	2.11	0.51
1:D:454:SER:C	1:D:461:LEU:HD11	2.30	0.51
1:B:97:VAL:HB	1:B:154:PHE:HD2	1.75	0.51
1:D:54:GLY:O	1:D:113:ARG:HA	2.11	0.51
1:A:57:MET:CB	1:A:300:MET:HE1	2.40	0.51
1:C:77:PHE:CD1	1:C:111:ILE:HB	2.46	0.51
1:D:468:SER:OG	1:D:470:GLU:HG2	2.10	0.51
1:B:110:ASN:HB2	1:B:132:GLU:HB2	1.92	0.51
1:D:358:LYS:HG2	1:D:392:GLN:O	2.11	0.50
1:B:218:LEU:O	1:B:218:LEU:HD12	2.10	0.50
1:E:277:THR:HG22	1:E:280:ARG:H	1.75	0.50
1:E:383:GLN:HB3	1:E:475:ILE:HD11	1.94	0.50
1:C:466:LYS:H	2:C:601:GOL:C3	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:338:VAL:HG12	1:D:340:ILE:HG23	1.93	0.50
1:D:126:VAL:HG21	1:D:212:TYR:HB2	1.93	0.50
1:F:431:TYR:CD2	2:F:601:GOL:H12	2.47	0.50
1:C:321:PRO:HB3	1:C:347:ILE:HG22	1.93	0.50
1:C:-15:MET:HE3	1:E:153:LYS:HE2	1.92	0.50
1:A:438:ASN:HD21	2:A:602:GOL:H11	1.75	0.50
1:A:103:ALA:HB3	1:A:106:LEU:HG	1.94	0.49
1:D:453:ILE:HG23	1:D:461:LEU:HD12	1.95	0.49
1:F:135:ILE:HD12	1:F:135:ILE:N	2.27	0.49
1:D:364:SER:HA	1:D:469:THR:OG1	2.12	0.49
1:A:161:ARG:NH2	1:A:177:MET:HG2	2.27	0.49
1:F:93:TYR:CZ	1:F:95:GLY:HA2	2.47	0.49
1:D:384:TRP:CZ3	1:D:471:ASP:HB3	2.47	0.49
1:D:450:TYR:HA	1:D:489:LYS:CA	2.42	0.49
1:E:420:GLU:HB3	1:E:457:HIS:HE1	1.77	0.49
1:C:84:ARG:HE	1:C:94:ARG:NE	2.10	0.49
1:C:98:LEU:HD22	1:C:127:MET:CE	2.42	0.49
1:D:476:GLN:HG2	1:D:477:GLN:H	1.77	0.49
1:D:376:ASP:O	1:D:379:ALA:HB2	2.12	0.49
1:F:57:MET:HE2	1:F:287:ILE:HD13	1.95	0.49
1:D:369:ASP:OD1	1:D:391:SER:HB2	2.13	0.49
1:D:87:ASP:O	1:D:88:LEU:HB2	2.13	0.49
1:A:54:GLY:O	1:A:113:ARG:HA	2.12	0.49
1:B:62:ASP:O	1:B:86:LYS:HG2	2.13	0.49
1:F:59:LYS:HD3	1:F:64:TYR:CE1	2.48	0.48
1:D:97:VAL:HB	1:D:154:PHE:CD2	2.47	0.48
1:B:385:THR:HG23	1:B:471:ASP:OD1	2.13	0.48
1:A:71:ARG:HB3	1:A:75:ASN:HA	1.95	0.48
1:B:465:ARG:HG2	1:B:466:LYS:HG2	1.95	0.48
1:A:62:ASP:O	1:A:86:LYS:HG2	2.14	0.48
1:E:465:ARG:HG2	1:E:466:LYS:HG2	1.96	0.48
1:C:284:THR:HG22	1:C:300:MET:O	2.12	0.48
1:D:377:ASN:HD21	1:D:432:THR:H	1.61	0.48
1:D:117:MET:HE3	1:D:128:TRP:CD1	2.47	0.48
1:B:288:PRO:HG3	1:B:297:TYR:CE1	2.48	0.48
1:A:375:VAL:HG12	1:A:411:SER:HB3	1.94	0.48
1:D:55:GLY:HA3	1:D:67:TYR:O	2.13	0.48
1:B:83:TYR:HB3	1:B:91:TRP:HB3	1.96	0.48
1:E:70:TYR:HB3	1:E:79:GLY:O	2.14	0.47
1:D:296:SER:HB2	1:D:347:ILE:HD11	1.95	0.47
1:B:93:TYR:CZ	1:B:95:GLY:HA2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:LEU:HD12	1:B:368:LEU:HD22	1.95	0.47
1:C:413:ARG:HH12	1:C:432:THR:HG22	1.79	0.47
1:B:50:ILE:HG23	1:B:83:TYR:CE1	2.49	0.47
1:E:305:ALA:HA	1:E:308:TRP:CZ2	2.50	0.47
1:D:278:THR:O	1:D:278:THR:HG22	2.13	0.47
1:E:129:MET:HG2	1:E:143:ALA:HB3	1.97	0.47
1:F:364:SER:OG	1:F:366:LYS:HG2	2.14	0.47
1:D:381:ILE:HG22	1:D:475:ILE:HG13	1.96	0.47
1:A:422:LYS:HE2	1:A:457:HIS:ND1	2.29	0.47
1:F:446:ILE:HG12	1:F:450:TYR:O	2.15	0.47
1:E:492:LEU:HD12	1:E:492:LEU:H	1.79	0.47
1:D:454:SER:HA	1:D:461:LEU:CG	2.45	0.47
1:D:35:VAL:HG11	1:D:337:SER:HB3	1.96	0.47
1:C:366:LYS:HE3	1:C:385:THR:HG22	1.97	0.47
1:A:416:ASP:OD2	2:A:602:GOL:H11	2.14	0.47
1:B:77:PHE:CE1	1:B:80:VAL:HG23	2.49	0.47
1:D:357:TYR:O	1:D:393:GLN:HA	2.15	0.47
1:B:399:VAL:HG11	1:B:405:LYS:HG3	1.97	0.47
1:C:399:VAL:HG21	1:C:440:HIS:NE2	2.29	0.47
1:A:126:VAL:HG21	1:A:212:TYR:HB2	1.95	0.47
1:D:377:ASN:ND2	1:D:432:THR:HG23	2.28	0.47
1:F:305:ALA:HA	1:F:308:TRP:CZ2	2.49	0.47
1:D:450:TYR:N	1:D:489:LYS:HG2	2.30	0.47
1:A:161:ARG:O	1:A:164:GLN:HG3	2.14	0.47
1:B:240:TYR:O	1:B:259:TYR:HA	2.15	0.47
1:E:254:GLN:OE1	1:E:276:SER:HA	2.15	0.47
1:B:80:VAL:HB	1:B:98:LEU:HB3	1.96	0.46
1:E:284:THR:HG22	1:E:300:MET:O	2.14	0.46
1:D:461:LEU:HA	1:D:461:LEU:HD13	1.54	0.46
1:D:305:ALA:HB3	1:D:311:LYS:O	2.15	0.46
1:A:131:TRP:CE3	1:A:141:ARG:HD2	2.49	0.46
1:D:394:TRP:CE3	1:D:406:ILE:HG22	2.50	0.46
1:C:465:ARG:NH2	1:C:474:ILE:HG21	2.26	0.46
1:D:376:ASP:C	1:D:413:ARG:HH12	2.18	0.46
1:D:453:ILE:C	1:D:461:LEU:HG	2.36	0.46
1:E:390:LEU:HA	1:E:393:GLN:OE1	2.15	0.46
1:A:87:ASP:O	1:A:88:LEU:HB2	2.14	0.46
1:A:87:ASP:OD1	1:A:89:VAL:HB	2.15	0.46
1:E:362:LYS:HD3	1:E:450:TYR:CZ	2.50	0.46
1:C:485:ASN:HD21	2:C:601:GOL:C1	2.18	0.46
1:C:463:ASP:OD1	2:C:601:GOL:H12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:VAL:HB	1:A:154:PHE:HD2	1.81	0.46
1:C:305:ALA:HA	1:C:308:TRP:CZ2	2.50	0.46
1:A:408:ASN:HB3	1:A:411:SER:O	2.16	0.46
1:D:425:GLY:HA2	1:D:476:GLN:CD	2.35	0.46
1:A:466:LYS:HB3	1:C:250:TRP:CD1	2.52	0.45
1:F:382:VAL:HA	1:F:475:ILE:HG12	1.96	0.45
1:A:434:ASN:HD21	2:A:602:GOL:H12	1.81	0.45
1:A:161:ARG:HH22	1:A:177:MET:HG2	1.82	0.45
1:B:260:SER:HB2	1:B:267:TRP:HA	1.98	0.45
1:B:380:GLN:HE22	1:B:427:VAL:HG13	1.82	0.45
1:A:111:ILE:HD13	1:A:129:MET:SD	2.56	0.45
1:C:454:SER:HB3	1:C:461:LEU:HD23	1.99	0.45
1:D:450:TYR:CG	1:D:489:LYS:HG3	2.51	0.45
1:E:381:ILE:HG12	1:E:429:ILE:HA	1.97	0.45
1:C:442:LYS:HG3	1:F:100:ARG:NH1	2.31	0.45
1:D:291:GLY:HA3	1:D:345:GLY:HA3	1.98	0.45
1:F:57:MET:CE	1:F:287:ILE:HG21	2.40	0.45
1:B:130:HIS:CE1	1:B:179:ARG:HA	2.51	0.45
1:A:434:ASN:HD21	2:A:602:GOL:C1	2.29	0.45
1:E:492:LEU:HD12	1:E:492:LEU:N	2.32	0.45
1:C:350:TYR:O	1:C:352:PRO:HD3	2.17	0.45
1:B:141:ARG:HB3	1:B:161:ARG:HG3	1.98	0.45
1:B:33:GLU:HG2	1:B:35:VAL:HG12	1.98	0.45
1:F:430:GLN:O	1:F:430:GLN:HG3	2.17	0.45
1:F:351:ILE:HD12	1:F:351:ILE:N	2.31	0.45
1:A:354:THR:O	1:A:354:THR:HG22	2.16	0.45
1:D:243:ILE:N	1:D:243:ILE:HD12	2.32	0.45
1:D:59:LYS:HD3	1:D:64:TYR:CD1	2.51	0.45
1:E:378:ALA:HA	1:E:429:ILE:HD12	1.98	0.45
1:D:129:MET:HG2	1:D:143:ALA:HB3	1.98	0.45
1:A:146:TYR:CD2	1:A:157:ILE:HD11	2.52	0.45
1:A:489:LYS:HG2	1:A:491:VAL:HG23	1.98	0.45
1:F:465:ARG:NH2	1:F:474:ILE:HG21	2.29	0.45
1:F:325:ILE:HD12	1:F:325:ILE:N	2.32	0.45
1:D:71:ARG:HG2	1:D:75:ASN:C	2.38	0.45
1:A:50:ILE:HG23	1:A:83:TYR:CE1	2.52	0.45
1:E:106:LEU:HD11	1:E:156:TYR:CD2	2.51	0.45
1:B:106:LEU:HD11	1:B:156:TYR:CD2	2.52	0.45
1:D:36:ILE:HD12	1:D:42:PHE:CZ	2.51	0.45
1:B:109:CYS:HB2	1:B:132:GLU:O	2.18	0.45
1:B:125:PHE:CZ	1:B:150:PRO:HG3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:LYS:HA	1:B:466:LYS:HE2	1.98	0.44
1:B:384:TRP:CZ3	1:B:471:ASP:HB3	2.51	0.44
1:B:341:ASP:HB3	1:B:344:SER:HB2	1.99	0.44
1:E:354:THR:O	1:E:354:THR:HG22	2.17	0.44
1:D:236:ARG:HA	1:D:297:TYR:OH	2.17	0.44
1:D:397:VAL:HB	1:D:405:LYS:HG3	1.97	0.44
1:C:270:LEU:N	1:C:270:LEU:HD12	2.33	0.44
1:D:381:ILE:HD11	1:D:430:GLN:HB3	2.00	0.44
1:B:78:LEU:C	1:B:78:LEU:HD12	2.38	0.44
1:D:363:ASN:HB2	1:D:467:TRP:HZ3	1.80	0.44
1:B:375:VAL:HG12	1:B:411:SER:HB3	1.98	0.44
1:A:235:LYS:HD2	1:A:240:TYR:CE2	2.52	0.44
1:F:166:THR:OG1	1:F:168:VAL:HG23	2.18	0.44
1:B:257:TYR:CE2	1:B:330:LEU:HD13	2.52	0.44
1:A:57:MET:HE2	1:A:91:TRP:CH2	2.52	0.44
1:D:360:VAL:O	1:D:488:TRP:HA	2.17	0.44
1:D:345:GLY:O	1:D:346:ILE:HD12	2.18	0.44
1:E:93:TYR:CZ	1:E:95:GLY:HA2	2.53	0.44
1:D:382:VAL:HA	1:D:475:ILE:HG12	1.98	0.44
1:B:483:GLY:O	1:B:487:HIS:CD2	2.70	0.44
1:A:196:ALA:HB1	1:A:200:ASN:HA	1.99	0.44
1:A:103:ALA:HB1	1:A:104:PRO:HD2	1.98	0.44
1:E:55:GLY:HA3	1:E:67:TYR:O	2.17	0.44
1:B:483:GLY:O	1:B:487:HIS:HD2	2.01	0.44
1:D:77:PHE:CD1	1:D:111:ILE:HB	2.53	0.44
1:E:197:ALA:HB3	1:E:204:HIS:CE1	2.53	0.44
1:F:357:TYR:O	1:F:393:GLN:HA	2.18	0.44
1:F:284:THR:HG22	1:F:300:MET:O	2.18	0.44
1:D:387:ASN:H	1:D:392:GLN:NE2	2.11	0.43
1:B:147:SER:HB2	1:B:154:PHE:HA	1.99	0.43
1:F:286:ILE:HD13	1:F:322:LEU:HD22	2.00	0.43
1:E:384:TRP:CZ3	1:E:471:ASP:HB3	2.53	0.43
1:F:287:ILE:HA	1:F:288:PRO:HD3	1.87	0.43
1:F:111:ILE:HG21	1:F:129:MET:HE2	2.00	0.43
1:C:64:TYR:O	1:C:84:ARG:HA	2.18	0.43
1:D:119:ASN:HB3	1:D:122:THR:OG1	2.18	0.43
1:A:109:CYS:HB2	1:A:132:GLU:O	2.19	0.43
1:F:363:ASN:ND2	1:F:467:TRP:HE3	2.17	0.43
1:F:325:ILE:HD12	1:F:325:ILE:H	1.83	0.43
1:E:380:GLN:HE22	1:E:427:VAL:CG2	2.32	0.43
1:C:130:HIS:CE1	1:C:179:ARG:HD3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:LYS:HB2	1:A:477:GLN:HG2	2.01	0.43
1:D:234:ILE:HD11	1:D:241:TYR:HB2	1.99	0.43
1:F:492:LEU:HD12	1:F:492:LEU:H	1.83	0.43
1:A:285:PHE:HE2	1:A:287:ILE:CG2	2.28	0.43
1:C:63:TYR:CE1	1:C:84:ARG:NH1	2.87	0.43
1:F:135:ILE:HG22	1:F:136:ASN:HD22	1.83	0.43
1:F:461:LEU:CD1	1:F:486:GLN:HB3	2.42	0.43
1:A:57:MET:HB3	1:A:300:MET:HE1	1.99	0.43
1:D:474:ILE:N	1:D:474:ILE:HD12	2.33	0.43
1:A:112:GLU:HB2	3:A:703:HOH:O	2.17	0.43
1:A:446:ILE:HG12	1:A:450:TYR:O	2.19	0.43
1:D:129:MET:CG	1:D:143:ALA:HB3	2.48	0.43
1:F:492:LEU:N	1:F:492:LEU:HD12	2.34	0.43
1:D:84:ARG:HG2	1:D:94:ARG:HD3	2.00	0.43
1:C:381:ILE:HG12	1:C:429:ILE:HA	2.00	0.43
1:E:252:PRO:HB2	1:E:277:THR:CG2	2.46	0.43
1:D:362:LYS:HB3	1:D:484:THR:O	2.19	0.43
1:C:362:LYS:HB2	1:C:450:TYR:CE1	2.53	0.43
1:B:146:TYR:CD2	1:B:157:ILE:HD11	2.53	0.43
1:E:375:VAL:HG12	1:E:411:SER:HB3	2.01	0.43
1:B:106:LEU:HD21	1:B:156:TYR:CE2	2.54	0.43
1:E:397:VAL:HB	1:E:405:LYS:HB2	2.01	0.43
1:A:351:ILE:N	1:A:351:ILE:HD12	2.34	0.43
1:B:422:LYS:HG2	1:B:458:CYS:HB3	2.00	0.42
1:E:41:GLN:HB3	1:E:49:VAL:HG13	2.00	0.42
1:E:235:LYS:HD2	1:E:240:TYR:CE2	2.54	0.42
1:D:351:ILE:HD12	1:D:351:ILE:N	2.35	0.42
1:D:451:TYR:H	1:D:488:TRP:H	1.67	0.42
1:B:359:LEU:HD12	1:B:368:LEU:CD2	2.49	0.42
1:A:156:TYR:OH	1:A:159:SER:HB3	2.20	0.42
1:B:285:PHE:HD2	1:B:300:MET:HE3	1.84	0.42
1:E:130:HIS:CE1	1:E:179:ARG:HA	2.54	0.42
1:A:474:ILE:N	1:A:474:ILE:HD12	2.34	0.42
1:F:266:GLY:N	2:F:604:GOL:O3	2.52	0.42
1:C:77:PHE:CZ	1:C:111:ILE:HD12	2.55	0.42
1:E:413:ARG:NH1	1:E:432:THR:HG22	2.35	0.42
1:F:354:THR:O	1:F:354:THR:HG22	2.20	0.42
1:F:97:VAL:HB	1:F:154:PHE:CD2	2.54	0.42
1:F:223:PHE:CE2	1:F:242:LEU:HD23	2.54	0.42
1:A:438:ASN:HD21	2:A:602:GOL:C1	2.33	0.42
1:F:413:ARG:NH1	1:F:432:THR:HG22	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:VAL:HG21	1:E:212:TYR:HB2	2.00	0.42
1:C:492:LEU:N	1:C:492:LEU:HD12	2.35	0.42
1:C:130:HIS:CE1	1:C:179:ARG:HA	2.55	0.42
1:A:115:LYS:HB3	1:A:183:VAL:HG22	2.01	0.42
1:A:287:ILE:HD12	1:A:298:LEU:HB3	2.01	0.42
1:D:377:ASN:O	1:D:378:ALA:HB3	2.19	0.42
1:C:223:PHE:CE2	1:C:242:LEU:HD23	2.53	0.42
1:F:135:ILE:HD12	1:F:135:ILE:H	1.84	0.42
1:A:450:TYR:CE2	1:A:489:LYS:HE3	2.54	0.42
1:D:85:SER:HB3	1:D:91:TRP:HA	2.00	0.42
1:E:87:ASP:O	1:E:88:LEU:HB2	2.19	0.42
1:D:354:THR:HG22	1:D:354:THR:O	2.20	0.42
1:B:278:THR:O	1:B:278:THR:HG22	2.20	0.42
1:E:243:ILE:HD12	1:E:243:ILE:N	2.34	0.42
1:D:126:VAL:HG11	1:D:212:TYR:O	2.20	0.42
1:B:287:ILE:HA	1:B:288:PRO:HD3	1.91	0.42
1:A:211:ASP:O	1:A:212:TYR:HB2	2.19	0.42
1:D:186:ASP:HB3	1:D:188:ASP:OD1	2.19	0.42
1:D:454:SER:CA	1:D:461:LEU:HD11	2.50	0.42
1:B:280:ARG:NH2	2:B:601:GOL:H11	2.35	0.42
1:B:180:ASP:O	1:B:195:SER:HA	2.20	0.42
1:E:186:ASP:HB3	1:E:188:ASP:OD1	2.19	0.42
1:D:42:PHE:CD1	1:D:42:PHE:N	2.85	0.41
1:D:117:MET:HE3	1:D:128:TRP:HD1	1.83	0.41
1:E:381:ILE:HG13	1:E:415:LEU:CD1	2.50	0.41
1:A:41:GLN:HB3	1:A:49:VAL:HG23	2.02	0.41
1:F:209:THR:HB	1:F:210:PRO:HD2	2.03	0.41
1:D:228:ARG:HB3	1:D:244:THR:HB	2.01	0.41
1:E:127:MET:HG2	1:E:129:MET:HE2	2.02	0.41
1:B:446:ILE:HD11	1:B:487:HIS:ND1	2.35	0.41
1:D:358:LYS:NZ	1:D:388:GLY:HA2	2.35	0.41
1:F:113:ARG:NE	2:F:603:GOL:H31	2.31	0.41
1:B:129:MET:CG	1:B:143:ALA:HB3	2.49	0.41
1:E:122:THR:OG1	1:E:124:GLU:HG2	2.19	0.41
1:D:245:SER:HB3	1:D:283:PRO:HD2	2.01	0.41
1:E:77:PHE:HB2	1:E:111:ILE:H	1.84	0.41
1:C:-13:SER:HA	1:C:492:LEU:CD1	2.49	0.41
1:F:416:ASP:OD1	2:F:601:GOL:H11	2.19	0.41
1:D:305:ALA:HA	1:D:308:TRP:CZ2	2.55	0.41
1:F:87:ASP:O	1:F:88:LEU:HB2	2.20	0.41
1:C:180:ASP:O	1:C:195:SER:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:TYR:CE2	1:C:78:LEU:HD23	2.56	0.41
1:A:287:ILE:HA	1:A:288:PRO:HD3	1.90	0.41
1:A:70:TYR:OH	1:A:78:LEU:HD22	2.21	0.41
1:A:130:HIS:NE2	1:A:179:ARG:HA	2.36	0.41
1:D:35:VAL:HG23	1:D:339:LYS:HE3	2.02	0.41
1:B:321:PRO:HB3	1:B:347:ILE:CG2	2.50	0.41
1:B:464:VAL:O	2:B:602:GOL:O2	2.37	0.41
1:B:362:LYS:HB2	1:B:450:TYR:CE1	2.55	0.41
1:D:164:GLN:OE1	1:D:174:PRO:HB2	2.20	0.41
1:F:381:ILE:HG22	1:F:475:ILE:HG13	2.02	0.41
1:A:71:ARG:HG2	1:A:75:ASN:OD1	2.21	0.41
1:A:474:ILE:H	1:A:474:ILE:HD12	1.84	0.41
1:A:216:ALA:O	1:B:165:ASP:HA	2.20	0.41
1:D:326:SER:HB3	1:D:329:THR:HB	2.03	0.41
1:E:50:ILE:HG23	1:E:83:TYR:CZ	2.56	0.41
1:A:243:ILE:N	1:A:243:ILE:HD12	2.36	0.41
1:C:287:ILE:HA	1:C:288:PRO:HD3	1.86	0.41
1:F:384:TRP:CE3	1:F:471:ASP:HB3	2.55	0.41
1:F:385:THR:HG23	1:F:471:ASP:OD1	2.20	0.41
1:F:129:MET:CG	1:F:143:ALA:HB3	2.50	0.41
1:C:147:SER:HB2	1:C:154:PHE:HA	2.02	0.41
1:C:380:GLN:HE22	1:C:427:VAL:HG22	1.86	0.41
1:A:206:TYR:CE1	1:A:218:LEU:HD23	2.56	0.41
1:A:53:HIS:HD2	1:A:312:VAL:HG12	1.84	0.41
1:D:130:HIS:CE1	1:D:179:ARG:HA	2.55	0.41
1:E:277:THR:HG22	1:E:280:ARG:HA	2.03	0.41
1:C:93:TYR:CZ	1:C:95:GLY:HA2	2.56	0.41
1:D:168:VAL:HG21	1:D:176:TYR:CE1	2.56	0.41
1:D:57:MET:HE2	1:D:287:ILE:HD13	2.02	0.41
1:D:451:TYR:HB2	1:D:488:TRP:O	2.21	0.41
1:F:113:ARG:NH2	2:F:603:GOL:H31	2.31	0.41
1:A:111:ILE:HA	1:A:130:HIS:O	2.20	0.41
1:B:156:TYR:HH	1:B:159:SER:HB3	1.84	0.41
1:A:279:TYR:CE2	1:A:334:TYR:HB2	2.56	0.41
1:A:170:ASP:OD1	1:A:177:MET:HG3	2.20	0.41
1:E:399:VAL:HG11	1:E:405:LYS:HG3	2.03	0.41
1:A:403:TYR:CD1	1:A:442:LYS:HB2	2.56	0.41
1:B:437:TYR:CD1	1:B:456:ARG:HD3	2.55	0.41
1:E:403:TYR:CE1	1:E:442:LYS:HB2	2.56	0.41
1:E:196:ALA:HA	1:E:203:LEU:HD23	2.02	0.41
1:B:64:TYR:O	1:B:84:ARG:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:PRO:HB3	1:B:347:ILE:HG22	2.03	0.41
1:D:223:PHE:HB3	1:D:226:GLN:HB2	2.02	0.41
1:A:129:MET:CG	1:A:143:ALA:HB3	2.49	0.40
1:E:223:PHE:CE2	1:E:242:LEU:HD23	2.55	0.40
1:C:236:ARG:HG3	1:C:297:TYR:OH	2.21	0.40
1:A:223:PHE:CE2	1:A:242:LEU:HD23	2.56	0.40
1:D:406:ILE:HD11	1:D:453:ILE:HD11	2.02	0.40
1:F:359:LEU:O	1:F:367:VAL:HA	2.21	0.40
1:B:359:LEU:O	1:B:367:VAL:HA	2.21	0.40
1:A:77:PHE:CZ	1:A:80:VAL:HG23	2.57	0.40
1:D:35:VAL:CG2	1:D:339:LYS:HE3	2.50	0.40
1:B:111:ILE:HA	1:B:130:HIS:O	2.21	0.40
1:D:418:LYS:HD2	1:D:429:ILE:HD13	2.03	0.40
1:D:42:PHE:HB2	1:D:50:ILE:CD1	2.51	0.40
1:E:305:ALA:HA	1:E:308:TRP:CH2	2.56	0.40
1:E:130:HIS:CE1	1:E:179:ARG:HD3	2.56	0.40
1:D:415:LEU:HD21	1:D:428:LEU:HD21	2.03	0.40
1:F:395:TYR:CE2	1:F:409:VAL:HG22	2.57	0.40
1:C:354:THR:O	1:C:354:THR:CG2	2.70	0.40
1:B:126:VAL:HG11	1:B:212:TYR:O	2.21	0.40
1:B:285:PHE:HD2	1:B:300:MET:CE	2.34	0.40
1:A:305:ALA:HA	1:A:308:TRP:CZ2	2.56	0.40
1:A:395:TYR:CE2	1:A:409:VAL:HG22	2.56	0.40
1:E:278:THR:HG22	1:E:278:THR:O	2.21	0.40
1:A:179:ARG:HD2	1:A:200:ASN:HD21	1.87	0.40
1:D:106:LEU:HA	1:D:109:CYS:SG	2.61	0.40
1:B:450:TYR:HA	1:B:488:TRP:O	2.22	0.40
1:B:57:MET:HE2	1:B:287:ILE:HG21	2.04	0.40
1:E:351:ILE:N	1:E:351:ILE:HD12	2.36	0.40
1:B:243:ILE:N	1:B:243:ILE:HD12	2.36	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%)	437 (95%)	22 (5%)	0	100	100
1	B	459/526 (87%)	435 (95%)	24 (5%)	0	100	100
1	C	480/526 (91%)	465 (97%)	15 (3%)	0	100	100
1	D	459/526 (87%)	429 (94%)	29 (6%)	1 (0%)	52	83
1	E	459/526 (87%)	436 (95%)	23 (5%)	0	100	100
1	F	459/526 (87%)	443 (96%)	16 (4%)	0	100	100
All	All	2775/3156 (88%)	2645 (95%)	129 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	450	TYR

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	389/442 (88%)	387 (100%)	2 (0%)	92	97
1	B	389/442 (88%)	385 (99%)	4 (1%)	82	95
1	C	402/442 (91%)	398 (99%)	4 (1%)	82	95
1	D	389/442 (88%)	385 (99%)	4 (1%)	82	95
1	E	389/442 (88%)	386 (99%)	3 (1%)	86	96
1	F	389/442 (88%)	387 (100%)	2 (0%)	92	97
All	All	2347/2652 (88%)	2328 (99%)	19 (1%)	86	96

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	287	ILE

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Mol	Chain	Res	Type
1	A	427	VAL
1	B	180	ASP
1	B	226	GLN
1	B	295	THR
1	B	448	ASP
1	C	42	PHE
1	C	69	GLU
1	C	427	VAL
1	C	432	THR
1	D	383	GLN
1	D	446	ILE
1	D	461	LEU
1	D	470	GLU
1	E	224	VAL
1	E	270	LEU
1	E	448	ASP
1	F	270	LEU
1	F	427	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	130	HIS
1	B	487	HIS
1	C	485	ASN
1	D	392	GLN
1	E	171	HIS
1	E	457	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

14 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	A	602	-	5,5,5	0.34	0	5,5,5	0.21	0
2	GOL	B	601	-	5,5,5	0.35	0	5,5,5	0.24	0
2	GOL	B	602	-	5,5,5	0.50	0	5,5,5	0.36	0
2	GOL	C	601	-	5,5,5	0.34	0	5,5,5	0.26	0
2	GOL	C	602	-	5,5,5	0.34	0	5,5,5	0.24	0
2	GOL	C	603	-	5,5,5	0.32	0	5,5,5	0.23	0
2	GOL	C	604	-	5,5,5	0.33	0	5,5,5	0.25	0
2	GOL	D	601	-	5,5,5	0.31	0	5,5,5	0.21	0
2	GOL	E	601	-	5,5,5	0.36	0	5,5,5	0.19	0
2	GOL	F	601	-	5,5,5	0.35	0	5,5,5	0.17	0
2	GOL	F	602	-	5,5,5	0.36	0	5,5,5	0.22	0
2	GOL	F	603	-	5,5,5	0.34	0	5,5,5	0.26	0
2	GOL	F	604	-	5,5,5	0.32	0	5,5,5	0.34	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	A	602	-	-	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	C	604	-	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	F	602	-	-	0/4/4/4	0/0/0/0
2	GOL	F	603	-	-	0/4/4/4	0/0/0/0
2	GOL	F	604	-	-	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.

9 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	602	GOL	5	0
2	B	601	GOL	1	0
2	B	602	GOL	3	0
2	C	601	GOL	5	0
2	C	602	GOL	3	0
2	C	603	GOL	1	0
2	F	601	GOL	4	0
2	F	603	GOL	4	0
2	F	604	GOL	1	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%)	0.48	27 (5%) 26 19	48, 73, 88, 100	0
1	B	461/526 (87%)	0.73	48 (10%) 8 5	59, 82, 101, 106	0
1	C	482/526 (91%)	0.03	4 (0%) 87 83	39, 50, 65, 93	0
1	D	461/526 (87%)	1.31	108 (23%) 1 1	46, 77, 140, 145	0
1	E	461/526 (87%)	0.31	13 (2%) 56 50	45, 60, 76, 88	0
1	F	461/526 (87%)	0.23	6 (1%) 79 75	38, 56, 74, 93	0
All	All	2787/3156 (88%)	0.51	206 (7%) 17 12	38, 65, 106, 145	0

All (206) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	390	LEU	8.4
1	D	484	THR	8.0
1	D	481	ALA	7.4
1	D	382	VAL	7.2
1	D	374	SER	7.0
1	D	426	GLY	6.9
1	D	371	LEU	6.8
1	D	380	GLN	6.7
1	D	425	GLY	6.2
1	D	474	ILE	6.0
1	D	384	TRP	5.8
1	D	383	GLN	5.6
1	D	375	VAL	5.6
1	D	466	LYS	5.4
1	D	401	GLY	5.4
1	D	427	VAL	5.4
1	D	422	LYS	5.1
1	D	402	GLY	5.1
1	D	392	GLN	5.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	358	LYS	5.0
1	D	479	SER	4.9
1	D	480	ASP	4.9
1	D	458	CYS	4.8
1	D	423	GLU	4.8
1	C	-18	GLY	4.8
1	D	492	LEU	4.7
1	D	444	THR	4.7
1	D	471	ASP	4.6
1	D	47	GLY	4.5
1	D	33	GLU	4.5
1	D	372	ASP	4.5
1	C	-6	MET	4.5
1	D	450	TYR	4.4
1	D	478	TRP	4.4
1	B	402	GLY	4.4
1	D	469	THR	4.4
1	D	367	VAL	4.2
1	D	491	VAL	4.2
1	D	370	VAL	4.2
1	A	181	CYS	4.2
1	D	472	GLY	4.1
1	D	470	GLU	4.0
1	D	467	TRP	4.0
1	D	473	GLY	4.0
1	D	446	ILE	4.0
1	D	389	SER	4.0
1	D	387	ASN	4.0
1	D	447	GLY	3.9
1	B	148	LYS	3.9
1	D	400	GLY	3.8
1	A	284	THR	3.8
1	D	459	GLY	3.8
1	B	446	ILE	3.7
1	B	437	TYR	3.7
1	D	63	TYR	3.6
1	B	294	GLY	3.6
1	D	453	ILE	3.6
1	D	354	THR	3.6
1	D	463	ASP	3.5
1	D	388	GLY	3.5
1	D	424	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	359	LEU	3.4
1	D	452	LYS	3.4
1	D	49	VAL	3.4
1	B	35	VAL	3.4
1	D	381	ILE	3.3
1	D	385	THR	3.3
1	F	172	GLY	3.3
1	D	409	VAL	3.3
1	D	465	ARG	3.3
1	D	460	LYS	3.2
1	A	113	ARG	3.2
1	D	356	ARG	3.1
1	D	368	LEU	3.1
1	A	114	PRO	3.1
1	D	448	ASP	3.1
1	D	445	ASP	3.0
1	D	490	LEU	3.0
1	E	33	GLU	3.0
1	B	232	CYS	3.0
1	D	493	VAL	3.0
1	B	239	TYR	2.9
1	A	300	MET	2.9
1	F	135	ILE	2.9
1	D	35	VAL	2.9
1	A	437	TYR	2.9
1	B	442	LYS	2.9
1	D	457	HIS	2.9
1	D	403	TYR	2.9
1	D	62	ASP	2.8
1	D	421	SER	2.8
1	F	292	SER	2.8
1	E	358	LYS	2.8
1	D	483	GLY	2.8
1	D	350	TYR	2.8
1	D	239	TYR	2.8
1	A	55	GLY	2.8
1	B	152	GLY	2.8
1	D	489	LYS	2.8
1	B	285	PHE	2.8
1	B	238	GLY	2.8
1	D	364	SER	2.7
1	B	181	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	231	PRO	2.7
1	D	376	ASP	2.7
1	B	114	PRO	2.7
1	D	294	GLY	2.7
1	B	445	ASP	2.6
1	B	74	SER	2.6
1	D	419	ASP	2.6
1	D	449	GLY	2.6
1	B	284	THR	2.6
1	B	339	LYS	2.6
1	D	346	ILE	2.6
1	B	56	GLY	2.6
1	D	482	GLY	2.6
1	D	89	VAL	2.6
1	A	112	GLU	2.6
1	A	182	ASN	2.6
1	B	182	ASN	2.6
1	D	357	TYR	2.6
1	E	446	ILE	2.6
1	B	78	LEU	2.5
1	B	150	PRO	2.5
1	A	239	TYR	2.5
1	E	437	TYR	2.5
1	A	309	GLY	2.5
1	B	261	LYS	2.5
1	A	388	GLY	2.5
1	E	492	LEU	2.5
1	A	120	ALA	2.5
1	B	120	ALA	2.5
1	A	172	GLY	2.4
1	E	389	SER	2.4
1	D	339	LYS	2.4
1	B	395	TYR	2.4
1	D	41	GLN	2.4
1	D	429	ILE	2.4
1	B	149	THR	2.4
1	A	115	LYS	2.4
1	A	265	SER	2.4
1	B	352	PRO	2.4
1	D	360	VAL	2.4
1	E	402	GLY	2.4
1	D	293	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	337	SER	2.4
1	B	451	TYR	2.4
1	E	284	THR	2.4
1	B	393	GLN	2.4
1	A	167	GLY	2.3
1	B	450	TYR	2.3
1	A	60	HIS	2.3
1	B	291	GLY	2.3
1	A	130	HIS	2.3
1	B	180	ASP	2.3
1	B	41	GLN	2.3
1	D	73	ASP	2.3
1	B	403	TYR	2.3
1	B	54	GLY	2.3
1	D	373	GLY	2.3
1	B	142	ALA	2.3
1	D	362	LYS	2.3
1	D	393	GLN	2.3
1	B	396	LEU	2.2
1	D	180	ASP	2.2
1	B	46	SER	2.2
1	E	283	PRO	2.2
1	A	301	GLY	2.2
1	E	230	ALA	2.2
1	F	360	VAL	2.2
1	D	365	GLY	2.2
1	D	395	TYR	2.2
1	D	230	ALA	2.2
1	A	118	TYR	2.2
1	D	396	LEU	2.2
1	B	113	ARG	2.2
1	B	300	MET	2.2
1	B	112	GLU	2.2
1	B	397	VAL	2.2
1	B	448	ASP	2.2
1	B	422	LYS	2.1
1	D	394	TRP	2.1
1	D	386	ASP	2.1
1	B	265	SER	2.1
1	B	350	TYR	2.1
1	A	62	ASP	2.1
1	D	379	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	33	GLU	2.1
1	E	442	LYS	2.1
1	F	181	CYS	2.1
1	C	-17	SER	2.1
1	D	428	LEU	2.1
1	A	232	CYS	2.1
1	A	122	THR	2.1
1	A	264	ALA	2.1
1	A	86	LYS	2.0
1	B	358	LYS	2.0
1	F	293	SER	2.0
1	D	485	ASN	2.0
1	A	125	PHE	2.0
1	D	284	THR	2.0
1	E	181	CYS	2.0
1	D	48	ASN	2.0
1	D	113	ARG	2.0
1	D	398	ASP	2.0
1	E	285	PHE	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	GOL	F	604	6/6	0.75	0.38	15.11	46,50,63,67	0
2	GOL	C	602	6/6	0.83	0.34	6.56	52,54,60,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	B	601	6/6	0.88	0.31	4.32	67,69,74,75	0
2	GOL	A	602	6/6	0.90	0.26	3.18	58,60,61,63	0
2	GOL	C	603	6/6	0.89	0.23	2.55	44,51,54,57	0
2	GOL	E	601	6/6	0.93	0.23	2.37	60,63,64,66	0
2	GOL	C	601	6/6	0.93	0.21	1.90	46,51,51,53	0
2	GOL	B	602	6/6	0.85	0.22	1.75	62,63,67,72	0
2	GOL	A	601	6/6	0.94	0.20	1.32	47,51,53,57	0
2	GOL	F	602	6/6	0.95	0.22	1.15	55,59,60,60	0
2	GOL	F	601	6/6	0.85	0.18	0.48	55,61,63,63	0
2	GOL	F	603	6/6	0.89	0.20	0.34	51,53,56,59	0
2	GOL	D	601	6/6	0.90	0.20	0.02	67,74,75,75	0
2	GOL	C	604	6/6	0.94	0.19	-0.36	48,51,52,56	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.