



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:25 PM UTC

PDB ID : 3VSF / pdb\_00003vsf  
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

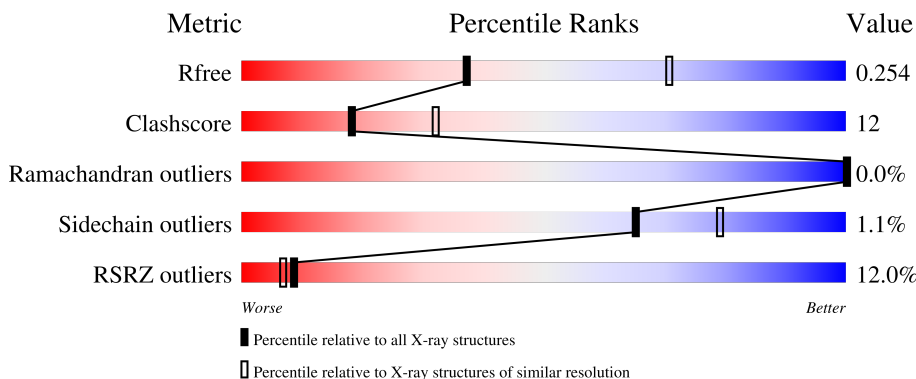
# 1 Overall quality at a glance

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.



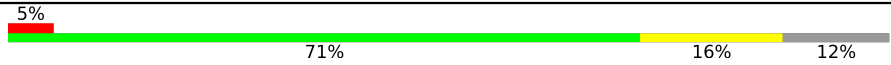
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	 8% 66% 21% 12%
1	B	526	 13% 65% 22% 12%
1	C	526	 2% 75% 17% 8%
1	D	526	 30% 56% 31% 12%
1	E	526	 5% 66% 21% 12%

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Mol	Chain	Length	Quality of chain
1	F	526	

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	-
2	GOL	C	601	-	-	X	-
2	GOL	F	601	-	-	X	-
2	GOL	F	603	-	-	X	-

## 2 Entry composition [i](#)

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

There are 216 discrepancies between the modelled and reference sequences:

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

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

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

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

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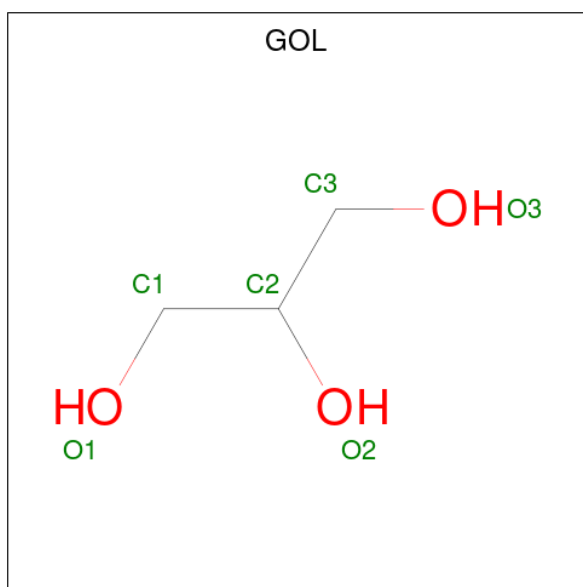
Chain	Residue	Modelled	Actual	Comment	Reference
D	0	PHE	-	expression tag	UNP A3DD67
E	-35	MET	-	expression tag	UNP A3DD67
E	-34	GLY	-	expression tag	UNP A3DD67
E	-33	SER	-	expression tag	UNP A3DD67
E	-32	SER	-	expression tag	UNP A3DD67
E	-31	HIS	-	expression tag	UNP A3DD67
E	-30	HIS	-	expression tag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

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

- Molecule 2 is GLYCEROL (CCD ID: 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 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	E	1	Total C O 6 3 3	0	0
2	F	1	Total C O 6 3 3	0	0
2	F	1	Total C O 6 3 3	0	0
2	F	1	Total C O 6 3 3	0	0
2	F	1	Total C O 6 3 3	0	0

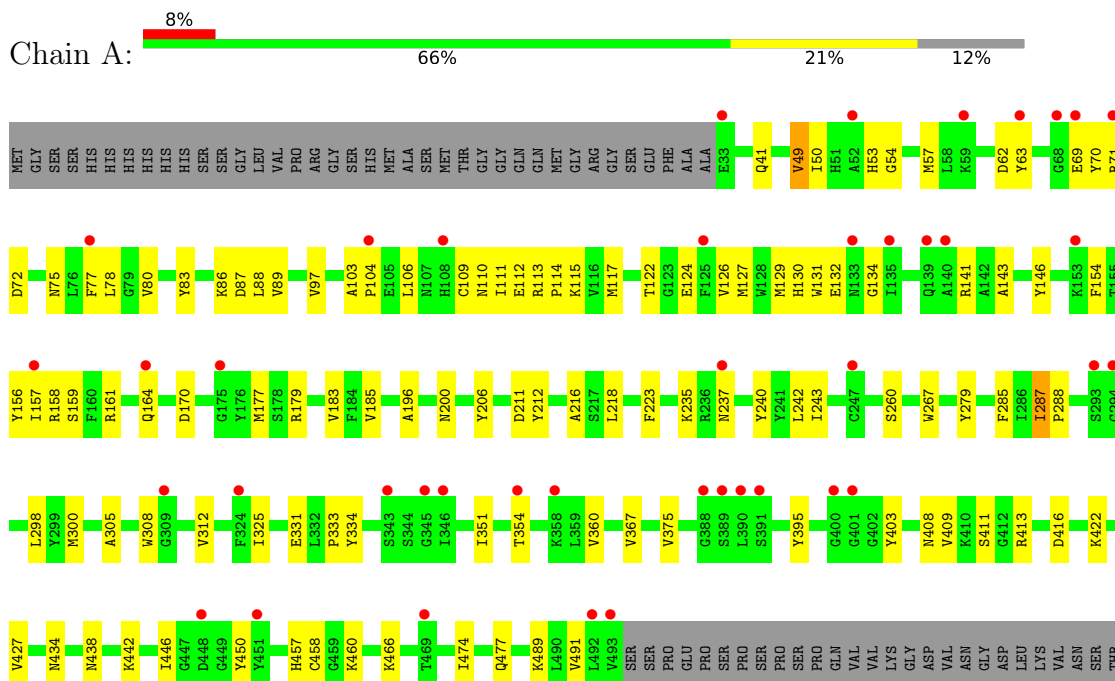
- Molecule 3 is water.

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

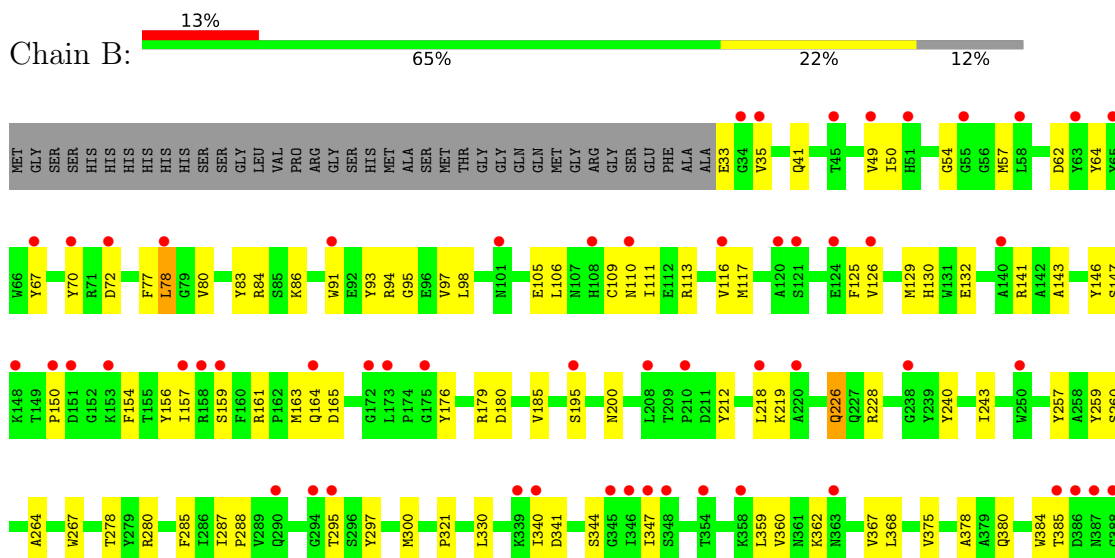
### 3 Residue-property plots

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

- Molecule 1: Ricin B lectin



- Molecule 1: Ricin B lectin







## 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) 98.0 (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)	Xtrriage
Refinement program	PHENIX 1.7_650	Depositor
R, $R_{free}$	0.236 , 0.257 0.233 , 0.254	Depositor DCC
$R_{free}$ test set	2469 reflections (1.81%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.5	Xtrriage
Anisotropy	0.463	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 33.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	22233	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtrriage'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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.23	0/3762	0.66	1/5104 (0.0%)
1	B	0.23	0/3762	0.63	0/5104
1	C	0.23	0/3907	0.65	0/5295
1	D	0.26	0/3762	0.66	1/5104 (0.0%)
1	E	0.23	0/3762	0.66	0/5104
1	F	0.23	0/3762	0.65	0/5104
All	All	0.23	0/22717	0.65	2/30815 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	461	LEU	N-CA-C	7.17	120.31	109.41
1	A	134	GLY	N-CA-C	-5.08	108.60	115.21

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	93	0
1	B	3664	0	3480	87	0
1	C	3807	0	3613	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3664	0	3480	136	0
1	E	3664	0	3480	74	0
1	F	3664	0	3480	72	0
2	A	12	0	16	5	0
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	523	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 (523) 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:57:MET:HE2	1:C:287:ILE:HG21	1.48	0.96
1:F:57:MET:HE2	1:F:287:ILE:HG21	1.51	0.91
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:422:LYS:HD3	1:A:458:CYS:HB3	1.73	0.70
1:D:454:SER:HA	1:D:461:LEU:HD21	1.72	0.70
1:E:416:ASP:HB3	1:E:439:GLN:HG2	1.73	0.70
1:F:111:ILE:HG12	1:F:129:MET:HE2	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:C:-18:GLY:HA3	1:C:-15:MET:HE2	1.75	0.69
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:A:72:ASP:HB3	1:A:78:LEU:HD12	1.76	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: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:E:80:VAL:HG21	1:E:127:MET:HE1	1.77	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:C:98:LEU:HD22	1:C:127:MET:HE1	1.79	0.63
1:C:54:GLY:O	1:C:113:ARG:HA	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:450:TYR:HA	1:D:489:LYS:HA	1.81	0.63
1:D:80:VAL:HG21	1:D:127:MET:HE1	1.81	0.63
1:E:77:PHE:CD1	1:E:111:ILE:HB	2.33	0.63
1:D:347:ILE:HD12	1:D:347:ILE:O	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:F:98:LEU:HD23	1:F:129:MET:HE1	1.81	0.62
1:D:467:TRP:HH2	1:D:484:THR:HG1	1.47	0.62
1:D:380:GLN:NE2	1:D:474:ILE:HG13	2.15	0.62
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:97:VAL:HB	1:A:154:PHE:CD2	2.36	0.61
1:E:416:ASP:CB	1:E:439:GLN:HG2	2.30	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:A:287:ILE:HD11	1:A:300:MET:HE3	1.81	0.61
1:B:340:ILE:HG22	1:B:347:ILE:HG23	1.82	0.61
1:B:161:ARG:O	1:B:164:GLN:HG3	2.01	0.61
1:C:438:ASN:HD21	2:C:602:GOL:H11	1.66	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: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: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:117:MET:HE3	1:B:185:VAL:HG22	1.85	0.58
1:B:163:MET:HE2	1:B:176:TYR:HE2	1.69	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:C:-13:SER:HA	1:C:492:LEU:HD11	1.86	0.58
1:F:358:LYS:HZ2	1:F:388:GLY:HA2	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:168:VAL:HG11	1:E:176:TYR:CE1	2.40	0.57
1:F:428:LEU:HD12	1:F:475:ILE:HG22	1.87	0.57
1:B:449:GLY:O	1:B:489:LYS:HA	2.04	0.57
1:E:111:ILE:HD11	1:E:131:TRP:HD1	1.68	0.57
1:D:444:THR:OG1	1:D:452:LYS:HB2	2.05	0.56
1:A:279:TYR:CD2	1:A:334:TYR:HB2	2.40	0.56
1:B:97:VAL:HB	1:B:154:PHE:CD2	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:F:416:ASP:CG	2:F:601:GOL:H11	2.30	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:80:VAL:HG21	1:E:127:MET:CE	2.36	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:D:454:SER:C	1:D:461:LEU:HD11	2.30	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:D:163:MET:HE3	1:D:166:THR:HG21	1.88	0.55
1:F:285:PHE:HB3	1:F:300:MET:HE3	1.89	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:F:57:MET:HE3	1:F:64:TYR:CD1	2.42	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:E:163:MET:HE3	1:E:166:THR:HG21	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:226:GLN:HB3	1:B:228:ARG:HG2	1.90	0.54
1:C:106:LEU:HD22	1:C:111:ILE:HD11	1.89	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:E:97:VAL:HB	1:E:154:PHE:CD2	2.42	0.53
1:F:325:ILE:HD11	1:F:331:GLU:OE1	2.08	0.53
1:A:106:LEU:HD11	1:A:156:TYR:CD2	2.43	0.53
1:A:331:GLU:HG2	1:A:333:PRO:HD3	1.89	0.53
1:D:441:TRP:HA	1:D:454:SER:O	2.07	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
1:A:63:TYR:CE1	1:A:86:LYS:HE3	2.44	0.53
1:B:130:HIS:CE1	1:B:179:ARG:HD3	2.43	0.53
1:B:422:LYS:HE3	1:B:457:HIS:NE2	2.24	0.53
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:122:THR:OG1	1:A:124:GLU:HG2	2.10	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:D:454:SER:HA	1:D:461:LEU:CD2	2.39	0.52
1:B:466:LYS:N	2:B:602:GOL:O2	2.42	0.52
1:D:460:LYS:O	1:D:461:LEU:HD13	2.10	0.52
1:E:383:GLN:O	1:E:383:GLN:HG3	2.09	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:B:67:TYR:CE2	1:B:116:VAL:HG21	2.45	0.52
1:C:434:ASN:ND2	2:C:602:GOL:H12	2.24	0.52
1:F:223:PHE:HE2	1:F:242:LEU:HD23	1.74	0.51
1:B:54:GLY:O	1:B:113:ARG:HA	2.10	0.51
1:E:422:LYS:CD	1:E:458:CYS:HB3	2.41	0.51
1:B:72:ASP:CA	1:B:78:LEU:HD23	2.40	0.51
1:A:117:MET:HE3	1:A:185:VAL:HG22	1.91	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:376:ASP:C	1:D:413:ARG:HH12	2.18	0.51
1:B:97:VAL:HB	1:B:154:PHE:HD2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:GLY:O	1:D:113:ARG:HA	2.11	0.51
1:D:453:ILE:C	1:D:461:LEU:HG	2.36	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:A:57:MET:CB	1:A:300:MET:HE1	2.42	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
1:D:126:VAL:HG21	1:D:212:TYR:HB2	1.93	0.50
1:D:338:VAL:HG12	1:D:340:ILE:HG23	1.93	0.50
1:D:425:GLY:HA2	1:D:476:GLN:CD	2.35	0.50
1:A:438:ASN:HD21	2:A:602:GOL:H11	1.75	0.50
1:C:321:PRO:HB3	1:C:347:ILE:HG22	1.93	0.50
1:F:431:TYR:CD2	2:F:601:GOL:H12	2.47	0.50
1:A:57:MET:HE3	1:A:300:MET:HE1	1.94	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:A:161:ARG:NH2	1:A:177:MET:HG2	2.27	0.49
1:C:57:MET:HE3	1:C:64:TYR:CD1	2.48	0.49
1:D:71:ARG:HG2	1:D:75:ASN:C	2.38	0.49
1:D:364:SER:HA	1:D:469:THR:OG1	2.12	0.49
1:F:93:TYR:CZ	1:F:95:GLY:HA2	2.47	0.49
1:C:84:ARG:HE	1:C:94:ARG:NE	2.10	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: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:B:78:LEU:C	1:B:78:LEU:HD12	2.38	0.49
1:D:285:PHE:HB3	1:D:300:MET:HE3	1.93	0.49
1:D:376:ASP:O	1:D:379:ALA:HB2	2.12	0.49
1:D:87:ASP:O	1:D:88:LEU:HB2	2.13	0.49
1:D:369:ASP:OD1	1:D:391:SER: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:D:97:VAL:HB	1:D:154:PHE:CD2	2.47	0.48
1:F:59:LYS:HD3	1:F:64:TYR:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:MET:HB2	1:A:300:MET:HE1	1.93	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:A:62:ASP:O	1:A:86:LYS:HG2	2.14	0.48
1:B:465:ARG:HG2	1:B:466:LYS:HG2	1.95	0.48
1:C:284:THR:HG22	1:C:300:MET:O	2.12	0.48
1:E:465:ARG:HG2	1:E:466:LYS:HG2	1.96	0.48
1:A:375:VAL:HG12	1:A:411:SER:HB3	1.94	0.48
1:B:288:PRO:HG3	1:B:297:TYR:CE1	2.48	0.48
1:D:55:GLY:HA3	1:D:67:TYR:O	2.13	0.48
1:D:377:ASN:HD21	1:D:432:THR:H	1.61	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:A:80:VAL:HG21	1:A:127:MET:HE1	1.96	0.47
1:B:93:TYR:CZ	1:B:95:GLY:HA2	2.49	0.47
1:D:296:SER:HB2	1:D:347:ILE:HD11	1.95	0.47
1:B:50:ILE:HG23	1:B:83:TYR:CE1	2.49	0.47
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:D:278:THR:HG22	1:D:278:THR:O	2.13	0.47
1:E:305:ALA:HA	1:E:308:TRP:CZ2	2.50	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:A:422:LYS:HE2	1:A:457:HIS:ND1	2.29	0.47
1:D:381:ILE:HG22	1:D:475:ILE:HG13	1.96	0.47
1:E:492:LEU:HD12	1:E:492:LEU:H	1.79	0.47
1:F:446:ILE:HG12	1:F:450:TYR:O	2.15	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:B:399:VAL:HG11	1:B:405:LYS:HG3	1.97	0.47
1:C:366:LYS:HE3	1:C:385:THR:HG22	1.97	0.47
1:C:399:VAL:HG21	1:C:440:HIS:NE2	2.29	0.47
1:D:35:VAL:HG11	1:D:337:SER:HB3	1.96	0.47
1:D:357:TYR:O	1:D:393:GLN:HA	2.15	0.47
1:D:454:SER:HA	1:D:461:LEU:CG	2.45	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: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:D:450:TYR:N	1:D:489:LYS:HG2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:131:TRP:CE3	1:A:141:ARG:HD2	2.49	0.46
1:D:305:ALA:HB3	1:D:311:LYS:O	2.15	0.46
1:D:461:LEU:HD13	1:D:461:LEU:HA	1.54	0.46
1:C:465:ARG:NH2	1:C:474:ILE:HG21	2.26	0.46
1:D:394:TRP:CE3	1:D:406:ILE:HG22	2.50	0.46
1:A:87:ASP:O	1:A:88:LEU:HB2	2.14	0.46
1:E:390:LEU:HA	1:E:393:GLN:OE1	2.15	0.46
1:F:98:LEU:CD2	1:F:129:MET:HE1	2.46	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: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:C:463:ASP:OD1	2:C:601:GOL:H12	2.15	0.46
1:C:485:ASN:HD21	2:C:601:GOL:C1	2.18	0.46
1:A:408:ASN:HB3	1:A:411:SER:O	2.16	0.46
1:A:466:LYS:HB3	1:C:250:TRP:CD1	2.52	0.45
1:A:161:ARG:HH22	1:A:177:MET:HG2	1.82	0.45
1:A:434:ASN:HD21	2:A:602:GOL:H12	1.81	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:F:382:VAL:HA	1:F:475:ILE:HG12	1.96	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: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: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:A:434:ASN:HD21	2:A:602:GOL:C1	2.29	0.45
1:B:130:HIS:CE1	1:B:179:ARG:HA	2.51	0.45
1:C:350:TYR:O	1:C:352:PRO:HD3	2.17	0.45
1:E:492:LEU:HD12	1:E:492:LEU:N	2.32	0.45
1:A:354:THR:HG22	1:A:354:THR:O	2.16	0.45
1:B:33:GLU:HG2	1:B:35:VAL:HG12	1.98	0.45
1:B:141:ARG:HB3	1:B:161:ARG:HG3	1.98	0.45
1:D:59:LYS:HD3	1:D:64:TYR:CD1	2.51	0.45
1:D:243:ILE:N	1:D:243:ILE:HD12	2.32	0.45
1:F:351:ILE:HD12	1:F:351:ILE:N	2.31	0.45
1:D:129:MET:HG2	1:D:143:ALA:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:378:ALA:HA	1:E:429:ILE:HD12	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:A:50:ILE:HG23	1:A:83:TYR:CE1	2.52	0.45
1:C:163:MET:HE3	1:C:166:THR:HG21	1.99	0.45
1:D:114:PRO:HB2	1:D:127:MET:HE3	1.99	0.45
1:E:106:LEU:HD11	1:E:156:TYR:CD2	2.51	0.45
1:F:325:ILE:N	1:F:325:ILE:HD12	2.32	0.45
1:F:465:ARG:NH2	1:F:474:ILE:HG21	2.29	0.45
1:B:106:LEU:HD11	1:B:156:TYR:CD2	2.52	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
1:D:36:ILE:HD12	1:D:42:PHE:CZ	2.51	0.45
1:D:460:LYS:C	1:D:461:LEU:HD22	2.41	0.45
1:B:341:ASP:HB3	1:B:344:SER:HB2	1.99	0.44
1:B:384:TRP:CZ3	1:B:471:ASP:HB3	2.51	0.44
1:B:466:LYS:HE2	1:B:466:LYS:HA	1.98	0.44
1:D:236:ARG:HA	1:D:297:TYR:OH	2.17	0.44
1:E:354:THR:O	1:E:354:THR:HG22	2.17	0.44
1:C:270:LEU:HD12	1:C:270:LEU:N	2.33	0.44
1:D:397:VAL:HB	1:D:405:LYS:HG3	1.97	0.44
1:A:235:LYS:HD2	1:A:240:TYR:CE2	2.52	0.44
1:B:375:VAL:HG12	1:B:411:SER:HB3	1.98	0.44
1:D:363:ASN:HB2	1:D:467:TRP:HZ3	1.80	0.44
1:D:381:ILE:HD11	1:D:430:GLN:HB3	2.00	0.44
1:B:257:TYR:CE2	1:B:330:LEU:HD13	2.52	0.44
1:F:166:THR:OG1	1:F:168:VAL:HG23	2.18	0.44
1:D:345:GLY:O	1:D:346:ILE:HD12	2.18	0.44
1:D:360:VAL:O	1:D:488:TRP:HA	2.17	0.44
1:E:93:TYR:CZ	1:E:95:GLY:HA2	2.53	0.44
1:A:103:ALA:HB1	1:A:104:PRO:HD2	1.98	0.44
1:A:196:ALA:HB1	1:A:200:ASN:HA	1.99	0.44
1:B:483:GLY:O	1:B:487:HIS:CD2	2.70	0.44
1:D:382:VAL:HA	1:D:475:ILE:HG12	1.98	0.44
1:E:55:GLY:HA3	1:E:67:TYR:O	2.17	0.44
1:F:111:ILE:CG1	1:F:129:MET:HE2	2.43	0.44
1:A:146:TYR:HH	1:B:105:GLU:HB2	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:425:GLY:HA2	1:C:476:GLN:CD	2.43	0.44
1:F:284:THR:HG22	1:F:300:MET:O	2.18	0.44
1:B:147:SER:HB2	1:B:154:PHE:HA	1.99	0.43
1:D:387:ASN:H	1:D:392:GLN:NE2	2.11	0.43
1:E:384:TRP:CZ3	1:E:471:ASP:HB3	2.53	0.43
1:F:286:ILE:HD13	1:F:322:LEU:HD22	2.00	0.43
1:F:430:GLN:O	1:F:430:GLN:HG3	2.17	0.43
1:A:411:SER:C	1:A:413:ARG:H	2.27	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:F:57:MET:HB2	1:F:300:MET:HE1	2.00	0.43
1:F:287:ILE:HA	1:F:288:PRO:HD3	1.87	0.43
1:A:109:CYS:HB2	1:A:132:GLU:O	2.19	0.43
1:A:460:LYS:HB2	1:A:477:GLN:HG2	2.01	0.43
1:C:130:HIS:CE1	1:C:179:ARG:HD3	2.53	0.43
1:D:234:ILE:HD11	1:D:241:TYR:HB2	1.99	0.43
1:E:380:GLN:HE22	1:E:427:VAL:CG2	2.32	0.43
1:F:325:ILE:HD12	1:F:325:ILE:H	1.83	0.43
1:F:363:ASN:ND2	1:F:467:TRP:HE3	2.17	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:80:VAL:HG11	1:A:127:MET:HE1	2.01	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:474:ILE:HD12	1:D:474:ILE:N	2.33	0.43
1:C:381:ILE:HG12	1:C:429:ILE:HA	2.00	0.43
1:D:84:ARG:HG2	1:D:94:ARG:HD3	2.00	0.43
1:D:129:MET:CG	1:D:143:ALA:HB3	2.48	0.43
1:F:492:LEU:HD12	1:F:492:LEU:N	2.34	0.43
1:B:146:TYR:CD2	1:B:157:ILE:HD11	2.53	0.43
1:C:362:LYS:HB2	1:C:450:TYR:CE1	2.53	0.43
1:D:362:LYS:HB3	1:D:484:THR:O	2.19	0.43
1:E:252:PRO:HB2	1:E:277:THR:CG2	2.46	0.43
1:E:375:VAL:HG12	1:E:411:SER:HB3	2.01	0.43
1:A:351:ILE:HD12	1:A:351:ILE:N	2.34	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:B:422:LYS:HG2	1:B:458:CYS:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:448:ASP:C	1:D:450:TYR:H	2.27	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:B:57:MET:HE3	1:B:287:ILE:HG21	2.01	0.42
1:D:351:ILE:N	1:D:351:ILE:HD12	2.35	0.42
1:E:73:ASP:C	1:E:75:ASN:H	2.27	0.42
1:A:156:TYR:OH	1:A:159:SER:HB3	2.20	0.42
1:B:359:LEU:HD12	1:B:368:LEU:CD2	2.49	0.42
1:D:451:TYR:H	1:D:488:TRP:H	1.67	0.42
1:A:474:ILE:HD12	1:A:474:ILE:N	2.34	0.42
1:E:130:HIS:CE1	1:E:179:ARG:HA	2.54	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:97:VAL:HB	1:F:154:PHE:CD2	2.54	0.42
1:F:354:THR:HG22	1:F:354:THR:O	2.20	0.42
1:A:438:ASN:HD21	2:A:602:GOL:C1	2.33	0.42
1:E:126:VAL:HG21	1:E:212:TYR:HB2	2.00	0.42
1:F:223:PHE:CE2	1:F:242:LEU:HD23	2.54	0.42
1:F:413:ARG:NH1	1:F:432:THR:HG22	2.35	0.42
1:A:115:LYS:HB3	1:A:183:VAL:HG22	2.01	0.42
1:C:130:HIS:CE1	1:C:179:ARG:HA	2.55	0.42
1:C:492:LEU:HD12	1:C:492:LEU:N	2.35	0.42
1:D:57:MET:HE2	1:D:287:ILE:HD13	2.02	0.42
1:A:287:ILE:HD12	1:A:298:LEU:HB3	2.01	0.42
1:A:450:TYR:CE2	1:A:489:LYS:HE3	2.54	0.42
1:B:278:THR:HG22	1:B:278:THR:O	2.20	0.42
1:C:223:PHE:CE2	1:C:242:LEU:HD23	2.53	0.42
1:D:85:SER:HB3	1:D:91:TRP:HA	2.00	0.42
1:D:354:THR:HG22	1:D:354:THR:O	2.20	0.42
1:D:377:ASN:O	1:D:378:ALA:HB3	2.19	0.42
1:E:243:ILE:HD12	1:E:243:ILE:N	2.34	0.42
1:F:135:ILE:HD12	1:F:135:ILE:H	1.84	0.42
1:A:211:ASP:O	1:A:212:TYR:HB2	2.19	0.42
1:B:287:ILE:HA	1:B:288:PRO:HD3	1.91	0.42
1:D:126:VAL:HG11	1:D:212:TYR:O	2.20	0.42
1:D:186:ASP:HB3	1:D:188:ASP:OD1	2.19	0.42
1:B:180:ASP:O	1:B:195:SER:HA	2.20	0.42
1:B:280:ARG:NH2	2:B:601:GOL:H11	2.35	0.42
1:D:454:SER:CA	1:D:461:LEU:HD11	2.50	0.42
1:E:186:ASP:HB3	1:E:188:ASP:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:GLN:HB3	1:A:49:VAL:HG23	2.02	0.41
1:D:42:PHE:N	1:D:42:PHE:CD1	2.85	0.41
1:E:381:ILE:HG13	1:E:415:LEU:CD1	2.50	0.41
1:A:114:PRO:HB2	1:A:127:MET:HE3	2.01	0.41
1:D:228:ARG:HB3	1:D:244:THR:HB	2.01	0.41
1:F:209:THR:HB	1:F:210:PRO:HD2	2.03	0.41
1:B:129:MET:CG	1:B:143:ALA:HB3	2.49	0.41
1:B:446:ILE:HD11	1:B:487:HIS:ND1	2.35	0.41
1:D:245:SER:HB3	1:D:283:PRO:HD2	2.01	0.41
1:D:358:LYS:NZ	1:D:388:GLY:HA2	2.35	0.41
1:E:122:THR:OG1	1:E:124:GLU:HG2	2.19	0.41
1:F:113:ARG:NE	2:F:603:GOL:H31	2.31	0.41
1:C:-13:SER:HA	1:C:492:LEU:CD1	2.49	0.41
1:C:70:TYR:CE2	1:C:78:LEU:HD23	2.56	0.41
1:C:180:ASP:O	1:C:195:SER:HA	2.21	0.41
1:D:305:ALA:HA	1:D:308:TRP:CZ2	2.55	0.41
1:E:77:PHE:HB2	1:E:111:ILE:H	1.84	0.41
1:F:87:ASP:O	1:F:88:LEU:HB2	2.20	0.41
1:F:416:ASP:OD1	2:F:601:GOL:H11	2.19	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:A:287:ILE:HA	1:A:288:PRO:HD3	1.90	0.41
1:B:321:PRO:HB3	1:B:347:ILE:CG2	2.50	0.41
1:B:362:LYS:HB2	1:B:450:TYR:CE1	2.55	0.41
1:B:464:VAL:O	2:B:602:GOL:O2	2.37	0.41
1:D:35:VAL:HG23	1:D:339:LYS:HE3	2.02	0.41
1:D:117:MET:HE3	1:D:128:TRP:HD1	1.86	0.41
1:D:164:GLN:OE1	1:D:174:PRO:HB2	2.20	0.41
1:A:71:ARG:HG2	1:A:75:ASN:OD1	2.21	0.41
1:A:216:ALA:O	1:B:165:ASP:HA	2.20	0.41
1:A:243:ILE:HD12	1:A:243:ILE:N	2.36	0.41
1:A:474:ILE:HD12	1:A:474:ILE:H	1.84	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:F:381:ILE:HG22	1:F:475:ILE:HG13	2.02	0.41
1:A:53:HIS:HD2	1:A:312:VAL:HG12	1.84	0.41
1:A:206:TYR:CE1	1:A:218:LEU:HD23	2.56	0.41
1:C:147:SER:HB2	1:C:154:PHE:HA	2.02	0.41
1:C:287:ILE:HA	1:C:288:PRO:HD3	1.86	0.41
1:C:380:GLN:HE22	1:C:427:VAL:HG22	1.86	0.41
1:D:130:HIS:CE1	1:D:179:ARG:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:ASP:CG	1:D:177:MET:HG3	2.45	0.41
1:F:129:MET:CG	1:F:143:ALA:HB3	2.50	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: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:E:57:MET:HE3	1:E:287:ILE:HG21	2.01	0.41
1:E:277:THR:HG22	1:E:280:ARG:HA	2.03	0.41
1:A:111:ILE:HA	1:A:130:HIS:O	2.20	0.41
1:A:170:ASP:OD1	1:A:177:MET:HG3	2.20	0.41
1:A:279:TYR:CE2	1:A:334:TYR:HB2	2.56	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:C:71:ARG:HG2	1:C:75:ASN:C	2.46	0.41
1:D:451:TYR:HB2	1:D:488:TRP:O	2.21	0.41
1:E:196:ALA:HA	1:E:203:LEU:HD23	2.02	0.41
1:E:399:VAL:HG11	1:E:405:LYS:HG3	2.03	0.41
1:E:403:TYR:CE1	1:E:442:LYS:HB2	2.56	0.41
1:F:113:ARG:NH2	2:F:603:GOL:H31	2.31	0.41
1:B:64:TYR:O	1:B:84:ARG:HA	2.21	0.41
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:E:87:ASP:O	1:E:88:LEU:HB2	2.19	0.41
1:A:129:MET:CG	1:A:143:ALA:HB3	2.49	0.40
1:A:223:PHE:CE2	1:A:242:LEU:HD23	2.56	0.40
1:C:236:ARG:HG3	1:C:297:TYR:OH	2.21	0.40
1:E:223:PHE:CE2	1:E:242:LEU:HD23	2.55	0.40
1:A:77:PHE:CZ	1:A:80:VAL:HG23	2.57	0.40
1:B:111:ILE:HA	1:B:130:HIS:O	2.21	0.40
1:B:359:LEU:O	1:B:367:VAL:HA	2.21	0.40
1:D:35:VAL:CG2	1:D:339:LYS:HE3	2.50	0.40
1:D:406:ILE:HD11	1:D:453:ILE:HD11	2.02	0.40
1:E:127:MET:HG2	1:E:129:MET:HE2	2.03	0.40
1:F:359:LEU:O	1:F:367:VAL:HA	2.21	0.40
1:C:354:THR:O	1:C:354:THR:CG2	2.70	0.40
1:D:42:PHE:HB2	1:D:50:ILE:CD1	2.51	0.40
1:D:415:LEU:HD21	1:D:428:LEU:HD21	2.03	0.40
1:D:418:LYS:HD2	1:D:429:ILE:HD13	2.03	0.40
1:E:130:HIS:CE1	1:E:179:ARG:HD3	2.56	0.40
1:E:305:ALA:HA	1:E:308:TRP:CH2	2.56	0.40
1:F:395:TYR:CE2	1:F:409:VAL:HG22	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:243:ILE:N	1:B:243:ILE:HD12	2.36	0.40
1:B:450:TYR:HA	1:B:488:TRP:O	2.22	0.40
1:D:66:TRP:CD1	1:D:66:TRP:C	2.99	0.40
1:D:106:LEU:HA	1:D:109:CYS:SG	2.61	0.40
1:E:351:ILE:N	1:E:351:ILE:HD12	2.36	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	459/526 (87%)	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%)	43	64
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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	389/442 (88%)	386 (99%)	3 (1%)	73	84
1	B	389/442 (88%)	384 (99%)	5 (1%)	61	76
1	C	402/442 (91%)	399 (99%)	3 (1%)	76	86
1	D	389/442 (88%)	381 (98%)	8 (2%)	47	67
1	E	389/442 (88%)	385 (99%)	4 (1%)	68	81
1	F	389/442 (88%)	386 (99%)	3 (1%)	73	84
All	All	2347/2652 (88%)	2321 (99%)	26 (1%)	65	79

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	VAL
1	A	287	ILE
1	A	427	VAL
1	B	78	LEU
1	B	226	GLN
1	B	295	THR
1	B	423	GLU
1	B	448	ASP
1	C	69	GLU
1	C	427	VAL
1	C	432	THR
1	D	164	GLN
1	D	339	LYS
1	D	346	ILE
1	D	347	ILE
1	D	383	GLN
1	D	446	ILE
1	D	461	LEU
1	D	470	GLU
1	E	144	VAL
1	E	224	VAL
1	E	270	LEU

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Mol	Chain	Res	Type
1	E	448	ASP
1	F	270	LEU
1	F	427	VAL
1	F	432	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	227	GLN
1	A	361	ASN
1	B	48	ASN
1	B	130	HIS
1	B	361	ASN
1	B	487	HIS
1	C	53	HIS
1	C	75	ASN
1	C	485	ASN
1	D	392	GLN
1	D	477	GLN
1	E	110	ASN
1	E	130	HIS
1	E	171	HIS
1	E	269	GLN
1	E	361	ASN
1	E	457	HIS
1	F	171	HIS
1	F	457	HIS
1	F	476	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	F	604	-	5,5,5	0.38	0	5,5,5	0.41	0
2	GOL	A	601	-	5,5,5	0.39	0	5,5,5	0.29	0
2	GOL	C	601	-	5,5,5	0.37	0	5,5,5	0.33	0
2	GOL	C	602	-	5,5,5	0.37	0	5,5,5	0.31	0
2	GOL	F	601	-	5,5,5	0.38	0	5,5,5	0.21	0
2	GOL	B	602	-	5,5,5	0.53	0	5,5,5	0.33	0
2	GOL	B	601	-	5,5,5	0.38	0	5,5,5	0.32	0
2	GOL	C	604	-	5,5,5	0.37	0	5,5,5	0.32	0
2	GOL	D	601	-	5,5,5	0.33	0	5,5,5	0.28	0
2	GOL	E	601	-	5,5,5	0.38	0	5,5,5	0.27	0
2	GOL	A	602	-	5,5,5	0.36	0	5,5,5	0.30	0
2	GOL	C	603	-	5,5,5	0.35	0	5,5,5	0.28	0
2	GOL	F	603	-	5,5,5	0.37	0	5,5,5	0.36	0
2	GOL	F	602	-	5,5,5	0.38	0	5,5,5	0.31	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	F	604	-	-	0/4/4/4	-
2	GOL	A	601	-	-	2/4/4/4	-
2	GOL	C	601	-	-	2/4/4/4	-
2	GOL	C	602	-	-	2/4/4/4	-
2	GOL	F	601	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	602	-	-	4/4/4/4	-
2	GOL	B	601	-	-	2/4/4/4	-
2	GOL	C	604	-	-	2/4/4/4	-
2	GOL	D	601	-	-	2/4/4/4	-
2	GOL	E	601	-	-	2/4/4/4	-
2	GOL	A	602	-	-	2/4/4/4	-
2	GOL	C	603	-	-	0/4/4/4	-
2	GOL	F	603	-	-	2/4/4/4	-
2	GOL	F	602	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GOL	O1-C1-C2-C3
2	B	601	GOL	O1-C1-C2-C3
2	B	602	GOL	O1-C1-C2-C3
2	B	602	GOL	C1-C2-C3-O3
2	B	602	GOL	O2-C2-C3-O3
2	C	601	GOL	O1-C1-C2-C3
2	C	602	GOL	O1-C1-C2-C3
2	C	604	GOL	C1-C2-C3-O3
2	F	602	GOL	O1-C1-C2-C3
2	C	604	GOL	O2-C2-C3-O3
2	A	602	GOL	O1-C1-C2-C3
2	D	601	GOL	O1-C1-C2-C3
2	E	601	GOL	O1-C1-C2-C3
2	F	603	GOL	O1-C1-C2-C3
2	B	602	GOL	O1-C1-C2-O2
2	C	602	GOL	O1-C1-C2-O2
2	F	602	GOL	O1-C1-C2-O2
2	B	601	GOL	O1-C1-C2-O2
2	C	601	GOL	O1-C1-C2-O2
2	D	601	GOL	O1-C1-C2-O2
2	F	603	GOL	O1-C1-C2-O2
2	A	601	GOL	O1-C1-C2-O2
2	A	602	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	E	601	GOL	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	604	GOL	1	0
2	C	601	GOL	5	0
2	C	602	GOL	3	0
2	F	601	GOL	4	0
2	B	602	GOL	3	0
2	B	601	GOL	1	0
2	A	602	GOL	5	0
2	C	603	GOL	1	0
2	F	603	GOL	4	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%)	0.91	41 (8%) 15 15	48, 73, 88, 100	0
1	B	461/526 (87%)	1.17	70 (15%) 5 4	59, 82, 101, 106	0
1	C	482/526 (91%)	0.26	11 (2%) 61 59	39, 50, 65, 93	0
1	D	461/526 (87%)	1.72	159 (34%) 1 0	46, 77, 140, 145	0
1	E	461/526 (87%)	0.53	25 (5%) 31 31	45, 60, 76, 88	0
1	F	461/526 (87%)	0.55	28 (6%) 27 27	38, 56, 74, 93	0
All	All	2787/3156 (88%)	0.85	334 (11%) 9 7	38, 65, 106, 145	0

All (334) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	390	LEU	11.0
1	D	427	VAL	8.2
1	D	493	VAL	8.1
1	D	446	ILE	7.6
1	D	375	VAL	7.6
1	D	492	LEU	6.8
1	D	453	ILE	6.4
1	D	484	THR	6.4
1	D	472	GLY	5.8
1	D	474	ILE	5.7
1	D	380	GLN	5.6
1	D	384	TRP	5.5
1	F	493	VAL	5.5
1	C	-6	MET	5.4
1	B	469	THR	5.3
1	D	347	ILE	5.3
1	D	389	SER	5.1
1	F	388	GLY	4.9
1	D	383	GLN	4.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	374	SER	4.8
1	D	358	LYS	4.5
1	D	415	LEU	4.5
1	D	482	GLY	4.5
1	D	490	LEU	4.4
1	D	392	GLN	4.3
1	D	452	LYS	4.3
1	D	414	ALA	4.3
1	D	481	ALA	4.3
1	D	483	GLY	4.2
1	D	473	GLY	4.2
1	D	428	LEU	4.2
1	D	396	LEU	4.2
1	D	449	GLY	4.1
1	F	492	LEU	4.1
1	D	480	ASP	4.1
1	D	443	PHE	4.1
1	F	491	VAL	4.1
1	D	399	VAL	4.1
1	B	395	TYR	4.0
1	D	337	SER	4.0
1	D	421	SER	4.0
1	F	449	GLY	3.9
1	D	491	VAL	3.9
1	D	359	LEU	3.9
1	D	464	VAL	3.9
1	C	-18	GLY	3.9
1	B	493	VAL	3.9
1	D	95	GLY	3.8
1	D	371	LEU	3.8
1	D	462	ILE	3.8
1	C	-7	GLN	3.8
1	D	478	TRP	3.8
1	D	468	SER	3.8
1	A	133	ASN	3.7
1	D	450	TYR	3.7
1	F	360	VAL	3.7
1	D	63	TYR	3.7
1	D	486	GLN	3.7
1	D	402	GLY	3.6
1	D	346	ILE	3.6
1	D	441	TRP	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	463	ASP	3.6
1	A	401	GLY	3.5
1	D	436	GLY	3.5
1	D	385	THR	3.5
1	A	492	LEU	3.5
1	D	367	VAL	3.5
1	D	467	TRP	3.4
1	B	491	VAL	3.4
1	D	400	GLY	3.4
1	D	393	GLN	3.4
1	D	466	LYS	3.4
1	D	108	HIS	3.4
1	D	422	LYS	3.3
1	A	469	THR	3.3
1	F	328	THR	3.3
1	D	340	ILE	3.3
1	D	488	TRP	3.3
1	D	395	TYR	3.3
1	D	430	GLN	3.3
1	B	340	ILE	3.3
1	B	78	LEU	3.3
1	D	379	ALA	3.3
1	D	85	SER	3.3
1	D	429	ILE	3.3
1	B	148	LYS	3.2
1	D	410	LYS	3.2
1	D	457	HIS	3.2
1	D	360	VAL	3.2
1	D	237	ASN	3.2
1	D	295	THR	3.2
1	E	449	GLY	3.2
1	A	493	VAL	3.2
1	B	55	GLY	3.2
1	D	475	ILE	3.2
1	D	485	ASN	3.2
1	D	487	HIS	3.2
1	B	45	THR	3.2
1	D	426	GLY	3.2
1	E	389	SER	3.2
1	D	50	ILE	3.2
1	D	432	THR	3.1
1	E	391	SER	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	220	ALA	3.1
1	A	237	ASN	3.1
1	A	354	THR	3.1
1	D	470	GLU	3.1
1	D	338	VAL	3.1
1	D	110	ASN	3.0
1	B	153	LYS	3.0
1	A	108	HIS	3.0
1	D	36	ILE	3.0
1	D	444	THR	3.0
1	D	378	ALA	3.0
1	D	438	ASN	3.0
1	D	398	ASP	3.0
1	D	447	GLY	3.0
1	E	110	ASN	2.9
1	F	354	THR	2.9
1	D	489	LYS	2.9
1	A	345	GLY	2.9
1	D	401	GLY	2.9
1	B	358	LYS	2.9
1	F	134	GLY	2.9
1	E	358	LYS	2.9
1	C	-4	ARG	2.8
1	D	394	TRP	2.8
1	B	218	LEU	2.8
1	D	411	SER	2.8
1	A	358	LYS	2.8
1	B	388	GLY	2.8
1	D	368	LEU	2.8
1	B	35	VAL	2.8
1	D	164	GLN	2.8
1	D	455	SER	2.8
1	B	126	VAL	2.8
1	A	247	CYS	2.8
1	D	442	LYS	2.8
1	D	391	SER	2.8
1	D	382	VAL	2.8
1	B	164	GLN	2.7
1	B	346	ILE	2.7
1	A	388	GLY	2.7
1	D	448	ASP	2.7
1	E	492	LEU	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	172	GLY	2.7
1	D	370	VAL	2.7
1	D	471	ASP	2.7
1	E	226	GLN	2.7
1	D	381	ILE	2.7
1	A	294	GLY	2.7
1	B	175	GLY	2.7
1	E	326	SER	2.7
1	A	69	GLU	2.7
1	D	354	THR	2.7
1	D	351	ILE	2.7
1	F	396	LEU	2.7
1	F	172	GLY	2.7
1	B	159	SER	2.7
1	A	140	ALA	2.7
1	B	65	TYR	2.6
1	F	358	LYS	2.6
1	B	294	GLY	2.6
1	B	402	GLY	2.6
1	B	348	SER	2.6
1	D	469	THR	2.6
1	C	70	TYR	2.6
1	A	68	GLY	2.6
1	B	116	VAL	2.6
1	C	-17	SER	2.6
1	B	67	TYR	2.6
1	A	59	LYS	2.6
1	D	49	VAL	2.6
1	D	251	ASN	2.6
1	D	324	PHE	2.6
1	A	139	GLN	2.5
1	D	439	GLN	2.5
1	B	150	PRO	2.5
1	B	363	ASN	2.5
1	D	387	ASN	2.5
1	A	391	SER	2.5
1	D	296	SER	2.5
1	F	364	SER	2.5
1	B	158	ARG	2.5
1	B	492	LEU	2.5
1	F	359	LEU	2.5
1	D	397	VAL	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	383	GLN	2.5
1	B	195	SER	2.5
1	D	406	ILE	2.5
1	D	403	TYR	2.5
1	D	57	MET	2.4
1	D	451	TYR	2.4
1	F	357	TYR	2.4
1	D	366	LYS	2.4
1	D	418	LYS	2.4
1	D	62	ASP	2.4
1	A	309	GLY	2.4
1	B	63	TYR	2.4
1	B	70	TYR	2.4
1	B	446	ILE	2.4
1	F	133	ASN	2.4
1	D	460	LYS	2.4
1	C	-5	GLY	2.4
1	E	491	VAL	2.4
1	F	390	LEU	2.4
1	B	386	ASP	2.4
1	D	34	GLY	2.4
1	D	225	GLY	2.4
1	D	236	ARG	2.4
1	E	367	VAL	2.4
1	E	70	TYR	2.3
1	C	-13	SER	2.3
1	A	77	PHE	2.3
1	D	350	TYR	2.3
1	E	489	LYS	2.3
1	B	72	ASP	2.3
1	D	445	ASP	2.3
1	D	373	GLY	2.3
1	D	459	GLY	2.3
1	E	412	GLY	2.3
1	F	412	GLY	2.3
1	B	51	HIS	2.3
1	B	385	THR	2.3
1	D	239	TYR	2.3
1	B	110	ASN	2.3
1	B	151	ASP	2.3
1	B	210	PRO	2.3
1	D	416	ASP	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	34	GLY	2.3
1	B	447	GLY	2.3
1	D	388	GLY	2.3
1	D	409	VAL	2.3
1	A	324	PHE	2.3
1	B	461	LEU	2.3
1	E	247	CYS	2.3
1	B	451	TYR	2.3
1	D	69	GLU	2.3
1	E	331	GLU	2.3
1	D	454	SER	2.3
1	F	490	LEU	2.3
1	A	52	ALA	2.2
1	A	135	ILE	2.2
1	F	446	ILE	2.2
1	E	69	GLU	2.2
1	D	437	TYR	2.2
1	A	71	ARG	2.2
1	E	73	ASP	2.2
1	F	165	ASP	2.2
1	A	390	LEU	2.2
1	D	458	CYS	2.2
1	A	343	SER	2.2
1	B	250	TRP	2.2
1	B	339	LYS	2.2
1	D	339	LYS	2.2
1	D	407	VAL	2.2
1	E	493	VAL	2.2
1	B	295	THR	2.2
1	B	354	THR	2.2
1	F	33	GLU	2.2
1	F	331	GLU	2.2
1	A	153	LYS	2.2
1	B	445	ASP	2.2
1	E	366	LYS	2.2
1	A	157	ILE	2.2
1	B	91	TRP	2.2
1	D	243	ILE	2.2
1	B	124	GLU	2.2
1	D	124	GLU	2.2
1	D	357	TYR	2.2
1	B	393	GLN	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	400	GLY	2.2
1	B	58	LEU	2.2
1	B	345	GLY	2.2
1	D	47	GLY	2.2
1	D	58	LEU	2.2
1	D	435	GLY	2.2
1	A	448	ASP	2.2
1	A	104	PRO	2.1
1	B	290	GLN	2.1
1	F	489	LYS	2.1
1	E	390	LEU	2.1
1	B	238	GLY	2.1
1	D	326	SER	2.1
1	F	389	SER	2.1
1	D	43	LYS	2.1
1	D	64	TYR	2.1
1	D	259	TYR	2.1
1	B	108	HIS	2.1
1	D	336	ASP	2.1
1	D	372	ASP	2.1
1	D	343	SER	2.1
1	D	348	SER	2.1
1	B	173	LEU	2.1
1	B	101	ASN	2.1
1	D	408	ASN	2.1
1	A	451	TYR	2.1
1	B	172	GLY	2.1
1	B	450	TYR	2.1
1	D	365	GLY	2.1
1	A	346	ILE	2.1
1	B	347	ILE	2.1
1	B	140	ALA	2.1
1	D	33	GLU	2.1
1	D	258	ALA	2.1
1	A	164	GLN	2.1
1	B	208	LEU	2.1
1	D	273	LEU	2.1
1	E	359	LEU	2.1
1	B	387	ASN	2.1
1	E	34	GLY	2.1
1	D	234	ILE	2.1
1	E	137	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	35	VAL	2.1
1	D	376	ASP	2.0
1	A	33	GLU	2.0
1	A	389	SER	2.0
1	B	121	SER	2.0
1	C	237	ASN	2.0
1	F	108	HIS	2.0
1	A	175	GLY	2.0
1	B	157	ILE	2.0
1	A	63	TYR	2.0
1	B	49	VAL	2.0
1	F	367	VAL	2.0
1	F	397	VAL	2.0
1	A	125	PHE	2.0
1	C	33	GLU	2.0
1	B	120	ALA	2.0
1	C	358	LYS	2.0
1	D	342	ALA	2.0
1	A	293	SER	2.0
1	D	117	MET	2.0
1	D	330	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	GOL	F	604	6/6	0.61	0.22	46,50,63,67	0
2	GOL	B	602	6/6	0.79	0.20	62,63,67,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	C	602	6/6	0.80	0.28	52,54,60,64	0
2	GOL	B	601	6/6	0.82	0.18	67,69,74,75	0
2	GOL	F	603	6/6	0.83	0.15	51,53,56,59	0
2	GOL	A	602	6/6	0.84	0.17	58,60,61,63	0
2	GOL	C	601	6/6	0.85	0.19	46,51,51,53	0
2	GOL	F	601	6/6	0.87	0.15	55,61,63,63	0
2	GOL	C	603	6/6	0.87	0.14	44,51,54,57	0
2	GOL	D	601	6/6	0.87	0.17	67,74,75,75	0
2	GOL	E	601	6/6	0.91	0.12	60,63,64,66	0
2	GOL	F	602	6/6	0.93	0.15	55,59,60,60	0
2	GOL	C	604	6/6	0.94	0.13	48,51,52,56	0
2	GOL	A	601	6/6	0.95	0.12	47,51,53,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.