Full wwPDB X-ray Structure Validation Report (i)

Mar 9, 2024 – 09:05 AM EST

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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

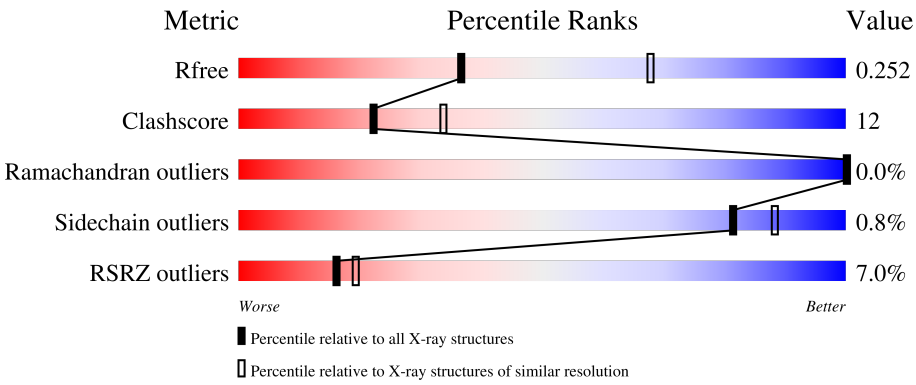
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	526	5% 67% 20% 12%
1	B	526	9% 66% 21% 12%
1	C	526	% 76% 15% 8%
1	D	526	20% 57% 30% • 12%
1	E	526	2% 67% 20% 12%

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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	-
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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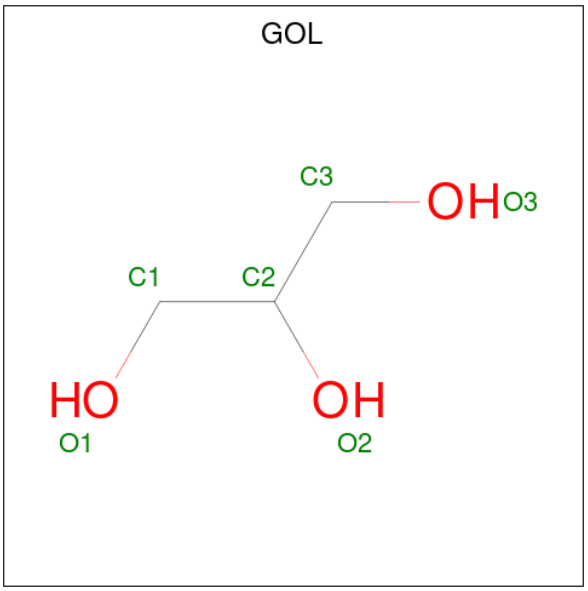
Chain	Residue	Modelled	Actual	Comment	Reference
F	-30	HIS	-	expression tag	UNP A3DD67
F	-29	HIS	-	expression tag	UNP A3DD67
F	-28	HIS	-	expression tag	UNP A3DD67
F	-27	HIS	-	expression tag	UNP A3DD67
F	-26	HIS	-	expression tag	UNP A3DD67
F	-25	SER	-	expression tag	UNP A3DD67
F	-24	SER	-	expression tag	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 (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is water.

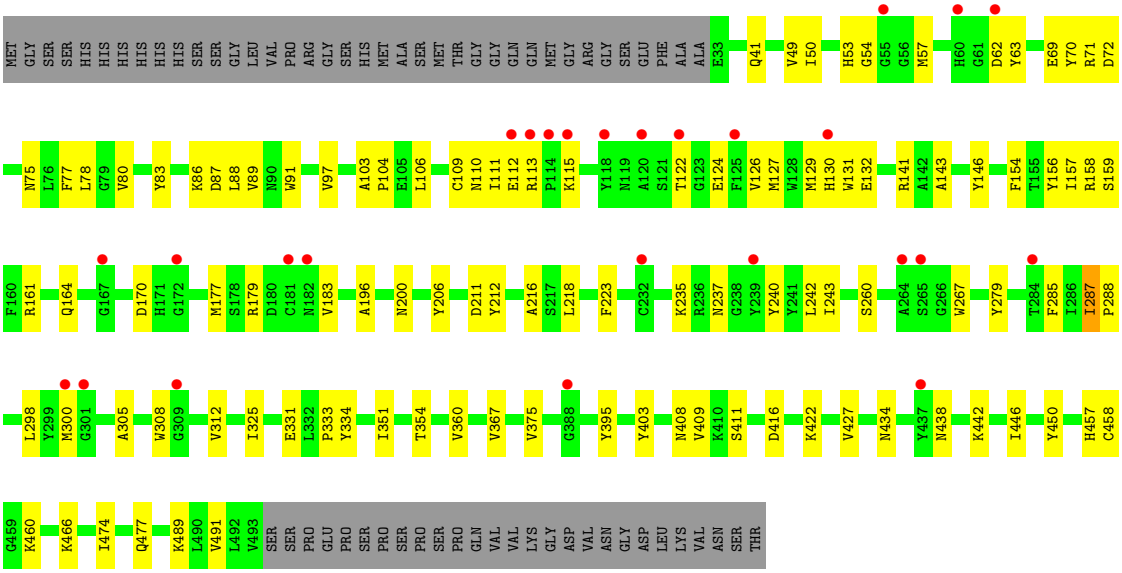
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	4	4	4	0	0
			Total	O		
3	C	12	12	12	0	0
			Total	O		
3	E	2	2	2	0	0
			Total	O		
3	F	4	4	4	0	0

3 Residue-property plots (i)

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

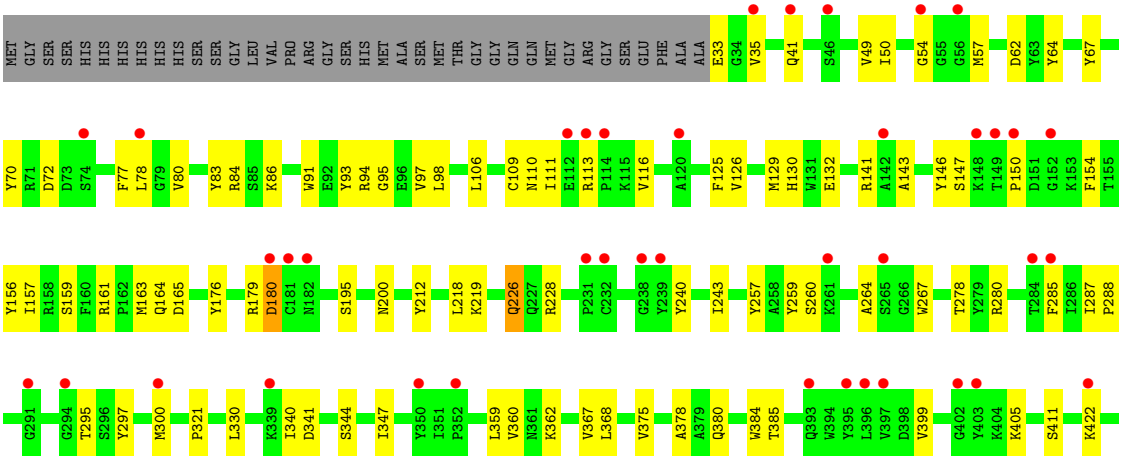
• Molecule 1: Ricin B lectin

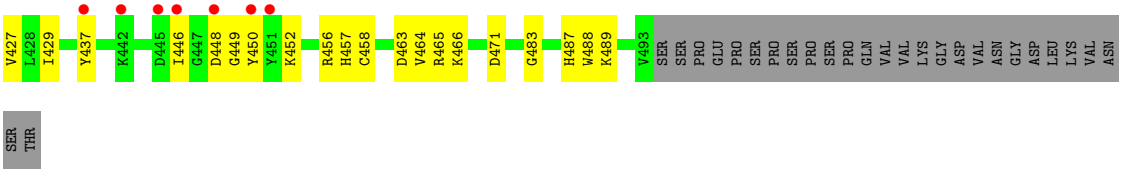
Chain A:



• Molecule 1: Ricin B lectin

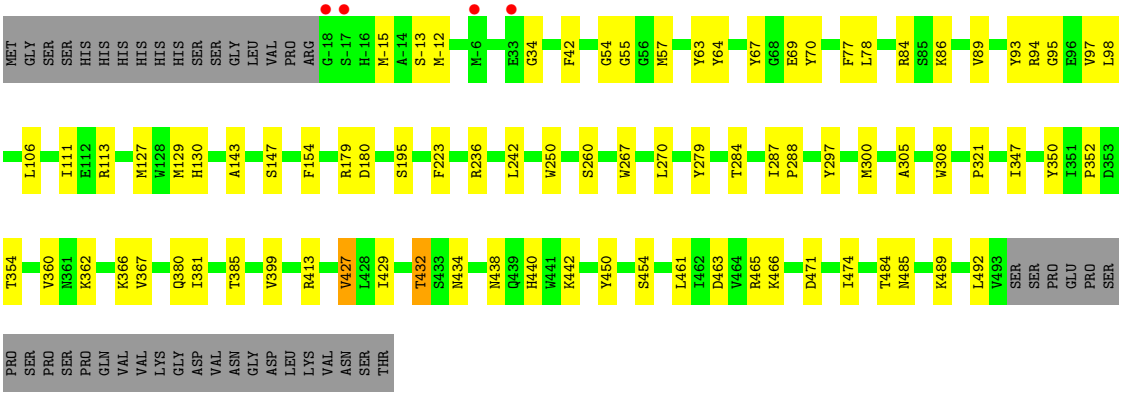
Chain B:





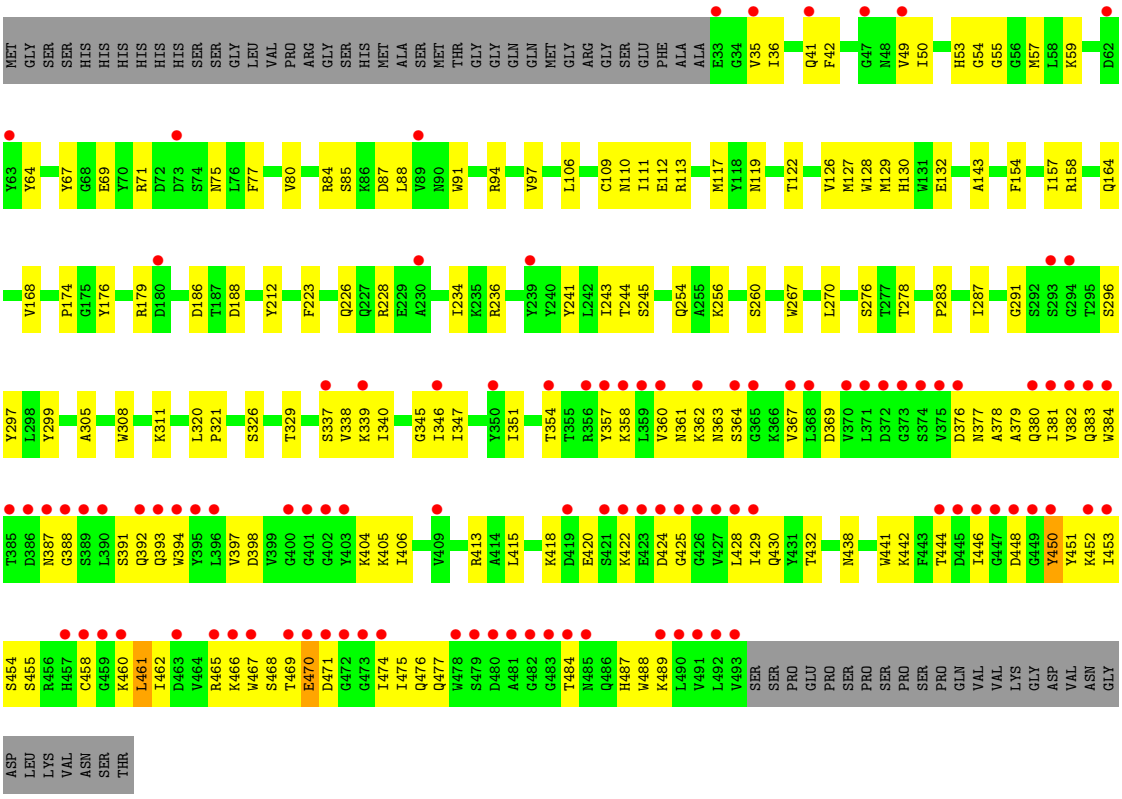
- Molecule 1: Ricin B lectin

Chain C:



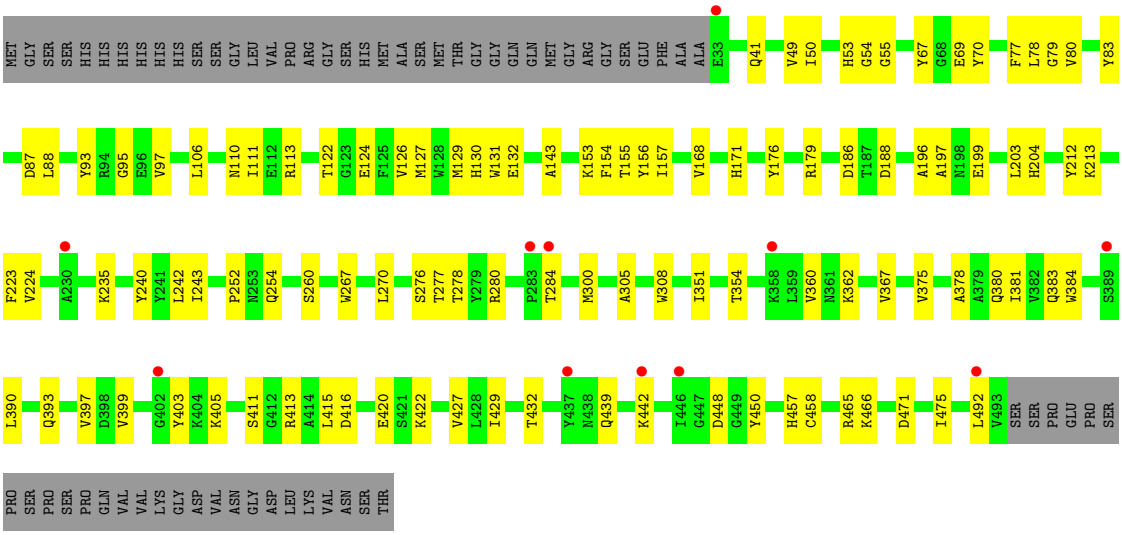
- Molecule 1: Ricin B lectin

Chain D:



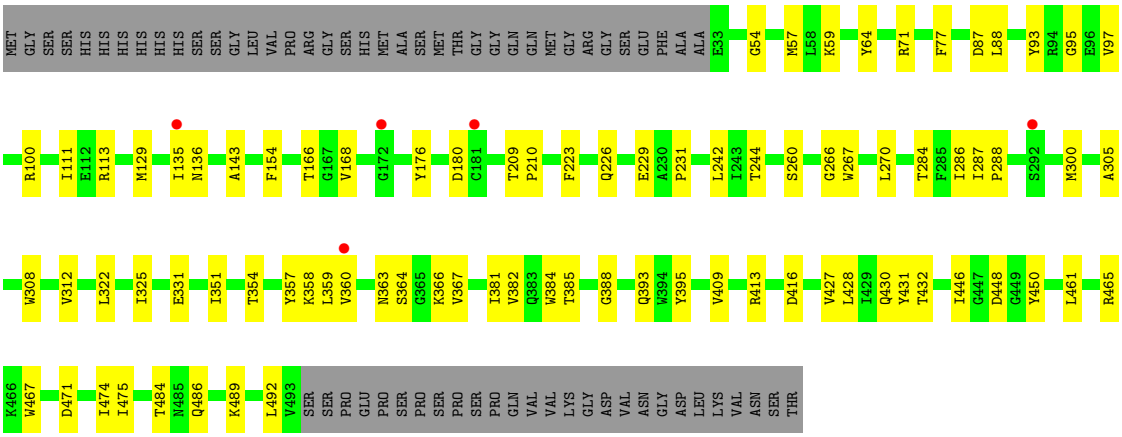
- Molecule 1: Ricin B lectin

Chain E:



- Molecule 1: Ricin B lectin

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	107.60Å 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
$< I/\sigma(I) >$ [1]	4.16 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.7_650	Depositor
R, R_{free}	0.236 , 0.257 0.231 , 0.252	Depositor DCC
R_{free} test set	2469 reflections (1.81%)	wwPDB-VP
Wilson B-factor (Å^2)	60.5	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 37.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	22233	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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: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: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: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: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:54:GLY:O	1:C:113:ARG:HA	1.98	0.63
1:D:450:TYR:HA	1:D:489:LYS:HA	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: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: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: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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:80:VAL:HG11	1:D:127:MET:HE3	1.90	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:383:GLN:O	1:E:383:GLN:HG3	2.09	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: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: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: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:F:416:ASP:CG	2:F:601:GOL:H11	2.30	0.51
1:B:54:GLY:O	1:B:113:ARG:HA	2.10	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: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: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:D:454:SER:C	1:D:461:LEU:HD11	2.30	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: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:A:438:ASN:HD21	2:A:602:GOL:H11	1.75	0.50
1:C:-15:MET:HE3	1:E:153:LYS:HE2	1.92	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: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: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: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:F:57:MET:HE2	1:F:287:ILE:HD13	1.95	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
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:117:MET:HE3	1:D:128:TRP:CD1	2.47	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:376:ASP:C	1:D:413:ARG:HH12	2.18	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:F:57:MET:CE	1:F:287:ILE:HG21	2.40	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:F:430:GLN:O	1:F:430:GLN:HG3	2.17	0.45
1:D:129:MET:HG2	1:D:143:ALA:HB3	1.98	0.45
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:D:71:ARG:HG2	1:D:75:ASN:C	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:78:LEU:C	1:B:78:LEU:HD12	2.38	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:A:57:MET:HE2	1:A:91:TRP:CH2	2.52	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: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: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: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:111:ILE:HG21	1:F:129:MET:HE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:57:MET:HB3	1:A:300:MET:HE1	1.99	0.43
1:F:461:LEU:CD1	1:F:486:GLN:HB3	2.42	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
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:N	1:D:351:ILE:HD12	2.35	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:87:ASP:O	1:E:88:LEU:HB2	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
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: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: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:E:127:MET:HG2	1:E:129:MET:HE2	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:57:MET:HE2	1:D:287:ILE:HD13	2.02	0.41
1:D:168:VAL:HG21	1:D:176:TYR:CE1	2.56	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:156:TYR:HH	1:B:159:SER:HB3	1.84	0.41
1:B:437:TYR:CD1	1:B:456:ARG:HD3	2.55	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

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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: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: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
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:57:MET:HE2	1:B:287:ILE:HG21	2.04	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: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%)	47	69
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%)	387 (100%)	2 (0%)	88	92
1	B	389/442 (88%)	385 (99%)	4 (1%)	76	85
1	C	402/442 (91%)	398 (99%)	4 (1%)	76	85
1	D	389/442 (88%)	385 (99%)	4 (1%)	76	85
1	E	389/442 (88%)	386 (99%)	3 (1%)	81	88
1	F	389/442 (88%)	387 (100%)	2 (0%)	88	92
All	All	2347/2652 (88%)	2328 (99%)	19 (1%)	81	88

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

Sometimes 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 (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 monosaccharides 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	C	602	-	5,5,5	0.36	0	5,5,5	0.28	0
2	GOL	B	602	-	5,5,5	0.51	0	5,5,5	0.32	0
2	GOL	F	602	-	5,5,5	0.38	0	5,5,5	0.27	0
2	GOL	B	601	-	5,5,5	0.37	0	5,5,5	0.28	0
2	GOL	F	601	-	5,5,5	0.37	0	5,5,5	0.19	0
2	GOL	C	601	-	5,5,5	0.36	0	5,5,5	0.30	0
2	GOL	F	603	-	5,5,5	0.36	0	5,5,5	0.32	0
2	GOL	C	603	-	5,5,5	0.35	0	5,5,5	0.25	0
2	GOL	D	601	-	5,5,5	0.33	0	5,5,5	0.24	0
2	GOL	E	601	-	5,5,5	0.37	0	5,5,5	0.23	0
2	GOL	F	604	-	5,5,5	0.36	0	5,5,5	0.37	0
2	GOL	C	604	-	5,5,5	0.36	0	5,5,5	0.29	0
2	GOL	A	601	-	5,5,5	0.38	0	5,5,5	0.26	0
2	GOL	A	602	-	5,5,5	0.36	0	5,5,5	0.26	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	C	602	-	-	2/4/4/4	-
2	GOL	B	602	-	-	4/4/4/4	-
2	GOL	F	602	-	-	2/4/4/4	-
2	GOL	B	601	-	-	2/4/4/4	-
2	GOL	F	601	-	-	1/4/4/4	-
2	GOL	C	601	-	-	2/4/4/4	-
2	GOL	F	603	-	-	2/4/4/4	-
2	GOL	C	603	-	-	0/4/4/4	-
2	GOL	D	601	-	-	2/4/4/4	-

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (25) torsion outliers are listed below:

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

There are no ring outliers.

9 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	602	GOL	3	0
2	B	602	GOL	3	0
2	B	601	GOL	1	0
2	F	601	GOL	4	0
2	C	601	GOL	5	0
2	F	603	GOL	4	0
2	C	603	GOL	1	0
2	F	604	GOL	1	0
2	A	602	GOL	5	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	461/526 (87%)	0.45	26 (5%) 24 29	48, 73, 88, 100	0
1	B	461/526 (87%)	0.68	47 (10%) 6 7	59, 82, 101, 106	0
1	C	482/526 (91%)	-0.01	4 (0%) 86 90	39, 50, 65, 93	0
1	D	461/526 (87%)	1.27	103 (22%) 0 0	46, 77, 140, 145	0
1	E	461/526 (87%)	0.28	11 (2%) 59 68	45, 60, 76, 88	0
1	F	461/526 (87%)	0.19	5 (1%) 80 86	38, 56, 74, 93	0
All	All	2787/3156 (88%)	0.47	196 (7%) 16 19	38, 65, 106, 145	0

All (196) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	390	LEU	8.3
1	D	484	THR	7.9
1	D	481	ALA	7.3
1	D	382	VAL	7.0
1	D	374	SER	7.0
1	D	426	GLY	6.8
1	D	371	LEU	6.7
1	D	380	GLN	6.6
1	D	425	GLY	6.0
1	D	474	ILE	6.0
1	D	384	TRP	5.8
1	D	383	GLN	5.5
1	D	375	VAL	5.5
1	D	401	GLY	5.4
1	D	427	VAL	5.3
1	D	466	LYS	5.3
1	D	402	GLY	5.1
1	D	422	LYS	5.0
1	D	392	GLN	4.9

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Mol	Chain	Res	Type	RSRZ
1	D	479	SER	4.9
1	D	358	LYS	4.9
1	D	480	ASP	4.8
1	D	492	LEU	4.7
1	C	-18	GLY	4.7
1	D	458	CYS	4.7
1	D	423	GLU	4.6
1	D	444	THR	4.5
1	D	33	GLU	4.5
1	D	47	GLY	4.4
1	D	471	ASP	4.4
1	D	450	TYR	4.4
1	D	372	ASP	4.4
1	D	478	TRP	4.4
1	C	-6	MET	4.3
1	B	402	GLY	4.3
1	D	469	THR	4.3
1	D	491	VAL	4.2
1	D	367	VAL	4.2
1	D	370	VAL	4.1
1	D	472	GLY	4.1
1	A	181	CYS	4.0
1	D	467	TRP	4.0
1	D	473	GLY	4.0
1	D	470	GLU	4.0
1	D	389	SER	3.9
1	D	446	ILE	3.9
1	D	387	ASN	3.9
1	B	148	LYS	3.8
1	D	447	GLY	3.8
1	D	400	GLY	3.7
1	A	284	THR	3.7
1	B	446	ILE	3.7
1	D	459	GLY	3.6
1	D	453	ILE	3.6
1	B	437	TYR	3.6
1	D	63	TYR	3.6
1	B	294	GLY	3.5
1	D	354	THR	3.5
1	D	388	GLY	3.4
1	D	463	ASP	3.4
1	D	359	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	35	VAL	3.3
1	D	49	VAL	3.3
1	D	452	LYS	3.3
1	D	424	ASP	3.3
1	D	381	ILE	3.3
1	D	385	THR	3.2
1	F	172	GLY	3.2
1	D	465	ARG	3.2
1	D	409	VAL	3.2
1	D	460	LYS	3.1
1	D	368	LEU	3.1
1	A	113	ARG	3.1
1	D	356	ARG	3.1
1	A	114	PRO	3.1
1	D	448	ASP	3.0
1	D	490	LEU	3.0
1	D	493	VAL	3.0
1	E	33	GLU	2.9
1	D	445	ASP	2.9
1	B	232	CYS	2.9
1	B	239	TYR	2.9
1	F	135	ILE	2.9
1	B	442	LYS	2.9
1	D	35	VAL	2.8
1	A	437	TYR	2.8
1	A	300	MET	2.8
1	D	403	TYR	2.8
1	D	421	SER	2.8
1	D	457	HIS	2.8
1	F	292	SER	2.8
1	D	350	TYR	2.8
1	D	483	GLY	2.8
1	D	239	TYR	2.7
1	D	364	SER	2.7
1	E	358	LYS	2.7
1	D	62	ASP	2.7
1	B	285	PHE	2.7
1	D	489	LYS	2.7
1	A	55	GLY	2.7
1	B	152	GLY	2.7
1	B	238	GLY	2.7
1	B	114	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	231	PRO	2.6
1	D	294	GLY	2.6
1	B	74	SER	2.6
1	D	376	ASP	2.6
1	B	284	THR	2.6
1	B	181	CYS	2.6
1	D	346	ILE	2.6
1	D	89	VAL	2.6
1	B	56	GLY	2.6
1	D	449	GLY	2.6
1	B	339	LYS	2.5
1	D	482	GLY	2.5
1	D	419	ASP	2.5
1	B	445	ASP	2.5
1	E	446	ILE	2.5
1	B	78	LEU	2.5
1	D	357	TYR	2.5
1	A	182	ASN	2.5
1	A	112	GLU	2.5
1	B	182	ASN	2.5
1	A	239	TYR	2.5
1	A	309	GLY	2.5
1	B	150	PRO	2.5
1	E	437	TYR	2.4
1	B	120	ALA	2.4
1	E	492	LEU	2.4
1	B	261	LYS	2.4
1	E	389	SER	2.4
1	A	388	GLY	2.4
1	A	265	SER	2.4
1	D	429	ILE	2.4
1	B	395	TYR	2.4
1	B	352	PRO	2.4
1	D	337	SER	2.4
1	A	172	GLY	2.4
1	A	120	ALA	2.4
1	D	360	VAL	2.4
1	D	41	GLN	2.3
1	A	115	LYS	2.3
1	D	293	SER	2.3
1	D	339	LYS	2.3
1	B	450	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	451	TYR	2.3
1	E	402	GLY	2.3
1	E	284	THR	2.3
1	B	149	THR	2.3
1	A	60	HIS	2.3
1	A	167	GLY	2.3
1	B	291	GLY	2.3
1	A	130	HIS	2.3
1	D	393	GLN	2.3
1	B	41	GLN	2.2
1	B	393	GLN	2.2
1	B	403	TYR	2.2
1	B	54	GLY	2.2
1	B	180	ASP	2.2
1	B	396	LEU	2.2
1	E	283	PRO	2.2
1	D	396	LEU	2.2
1	B	142	ALA	2.2
1	D	73	ASP	2.2
1	B	46	SER	2.2
1	F	360	VAL	2.2
1	D	362	LYS	2.2
1	A	301	GLY	2.2
1	D	373	GLY	2.2
1	D	395	TYR	2.2
1	B	397	VAL	2.2
1	D	365	GLY	2.2
1	E	230	ALA	2.2
1	D	230	ALA	2.1
1	B	113	ARG	2.1
1	A	118	TYR	2.1
1	D	180	ASP	2.1
1	B	300	MET	2.1
1	B	265	SER	2.1
1	B	112	GLU	2.1
1	C	-17	SER	2.1
1	D	394	TRP	2.1
1	B	422	LYS	2.1
1	D	428	LEU	2.0
1	A	122	THR	2.0
1	B	448	ASP	2.0
1	B	350	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	386	ASP	2.0
1	E	442	LYS	2.0
1	F	181	CYS	2.0
1	C	33	GLU	2.0
1	D	485	ASN	2.0
1	A	62	ASP	2.0
1	A	264	ALA	2.0
1	A	125	PHE	2.0
1	A	232	CYS	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 monosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	F	604	6/6	0.75	0.38	46,50,63,67	0
2	GOL	C	602	6/6	0.83	0.34	52,54,60,64	0
2	GOL	F	601	6/6	0.85	0.18	55,61,63,63	0
2	GOL	B	602	6/6	0.85	0.22	62,63,67,72	0
2	GOL	B	601	6/6	0.88	0.31	67,69,74,75	0
2	GOL	F	603	6/6	0.89	0.20	51,53,56,59	0
2	GOL	C	603	6/6	0.89	0.23	44,51,54,57	0
2	GOL	D	601	6/6	0.90	0.20	67,74,75,75	0
2	GOL	A	602	6/6	0.90	0.25	58,60,61,63	0
2	GOL	E	601	6/6	0.93	0.23	60,63,64,66	0
2	GOL	C	601	6/6	0.93	0.21	46,51,51,53	0
2	GOL	C	604	6/6	0.94	0.19	48,51,52,56	0
2	GOL	A	601	6/6	0.94	0.20	47,51,53,57	0
2	GOL	F	602	6/6	0.95	0.22	55,59,60,60	0

6.5 Other polymers (i)

There are no such residues in this entry.