Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:02 PM GMT

PDB ID	:	3VT1
Title	:	Crystal structure of Ct1,3Gal43A in complex with galactose
Authors	:	Jiang, D.; Fan, J.; Wang, X.; Zhao, Y.; Huang, B.; Zhang, X.C.
Deposited on	:	2012-05-18
Resolution	:	3.19 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

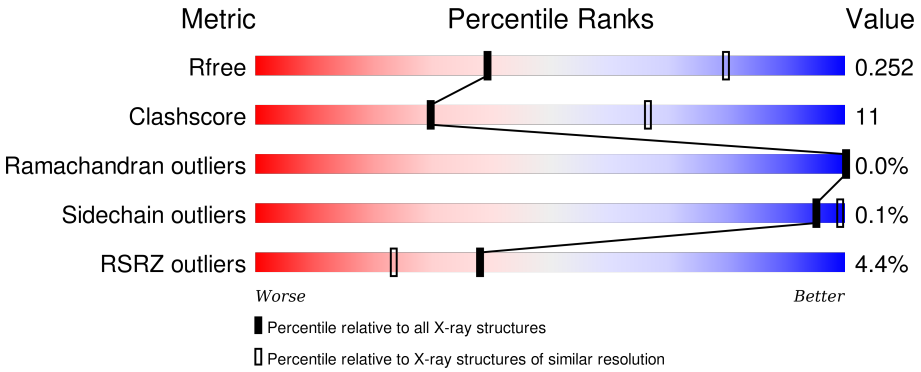
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.19 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1115 (3.22-3.14)
Clashscore	102246	1125 (3.20-3.16)
Ramachandran outliers	100387	1105 (3.20-3.16)
Sidechain outliers	100360	1104 (3.20-3.16)
RSRZ outliers	91569	1120 (3.22-3.14)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	67% 21% 12%
1	B	526	67% 20% 12%
1	C	526	73% 19% 8%
1	D	526	17% 61% 27% 12%
1	E	526	67% 21% 12%

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Mol	Chain	Length	Quality of chain
1	F	526	70% 17% 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	GAL	C	602	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22211 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ricin B lectin.

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

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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

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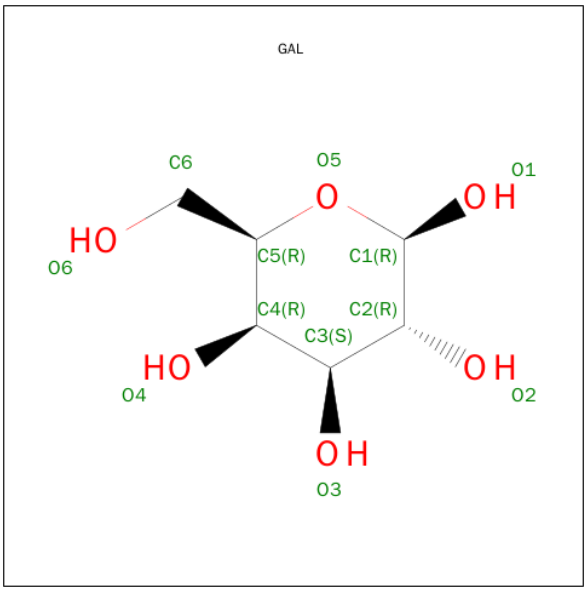
Chain	Residue	Modelled	Actual	Comment	Reference
A	-30	HIS	-	EXPRESSION TAG	UNP A3DD67
A	-29	HIS	-	EXPRESSION TAG	UNP A3DD67
A	-28	HIS	-	EXPRESSION TAG	UNP A3DD67
A	-27	HIS	-	EXPRESSION TAG	UNP A3DD67
A	-26	HIS	-	EXPRESSION TAG	UNP A3DD67
A	-25	SER	-	EXPRESSION TAG	UNP A3DD67
A	-24	SER	-	EXPRESSION TAG	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
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

- Molecule 2 is SUGAR (BETA-D-GALACTOSE) (three-letter code: GAL) (formula: $C_6H_{12}O_6$).



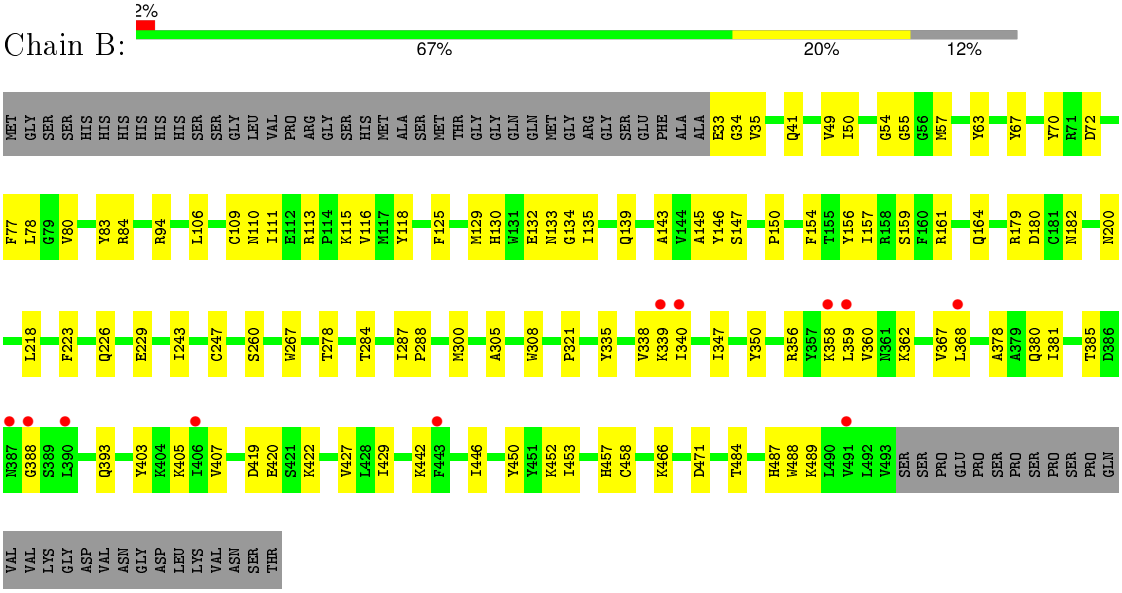
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 12 6 6	0	0
2	C	1	Total C O 12 6 6	0	0
2	C	1	Total C O 12 6 6	0	0
2	E	1	Total C O 12 6 6	0	0
2	F	1	Total C O 12 6 6	0	0
2	F	1	Total C O 12 6 6	0	0
2	A	1	Total C O 12 6 6	0	0

3 Residue-property plots

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

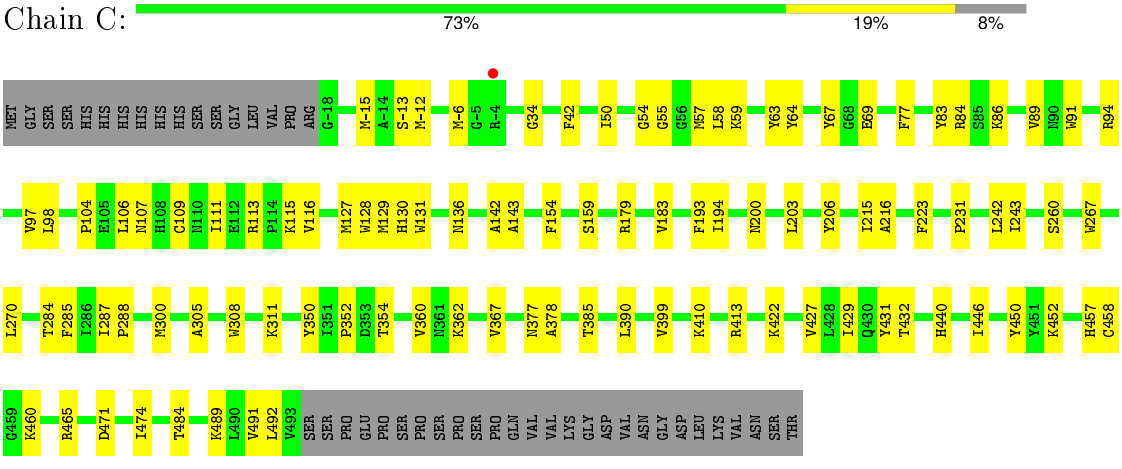
- Molecule 1: Ricin B lectin

Chain B:



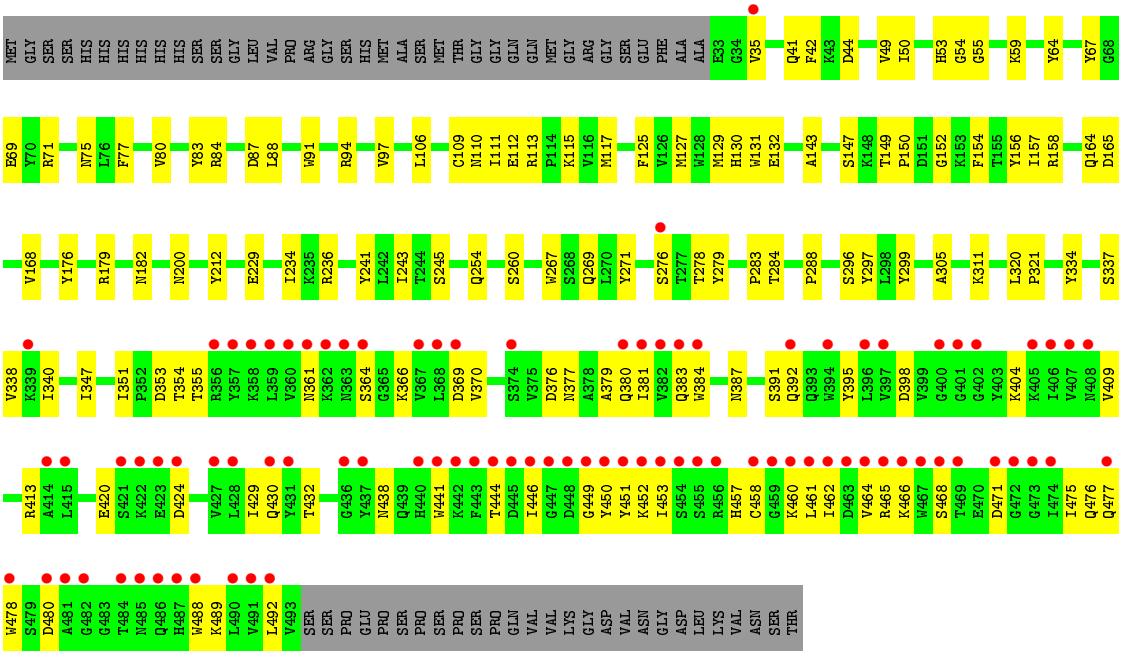
- Molecule 1: Ricin B lectin

Chain C:



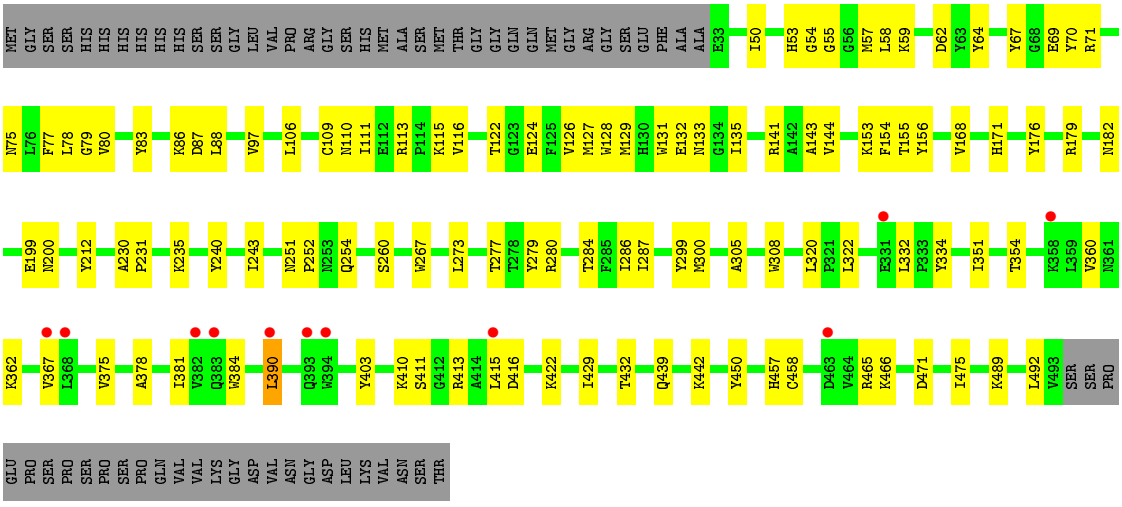
- Molecule 1: Ricin B lectin

Chain D:



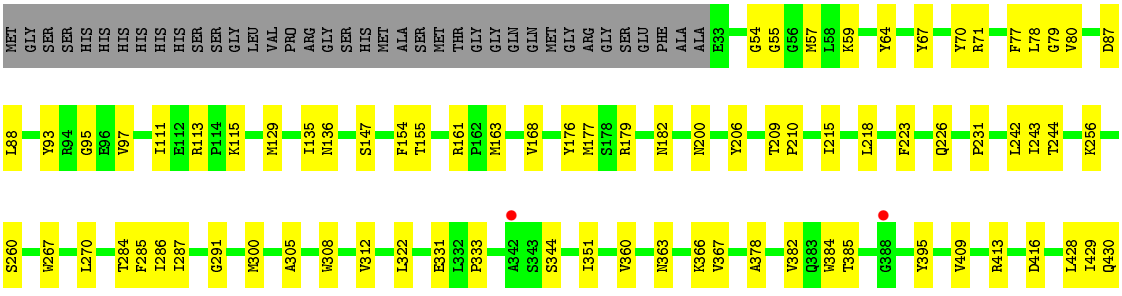
• Molecule 1: Ricin B lectin

Chain E:



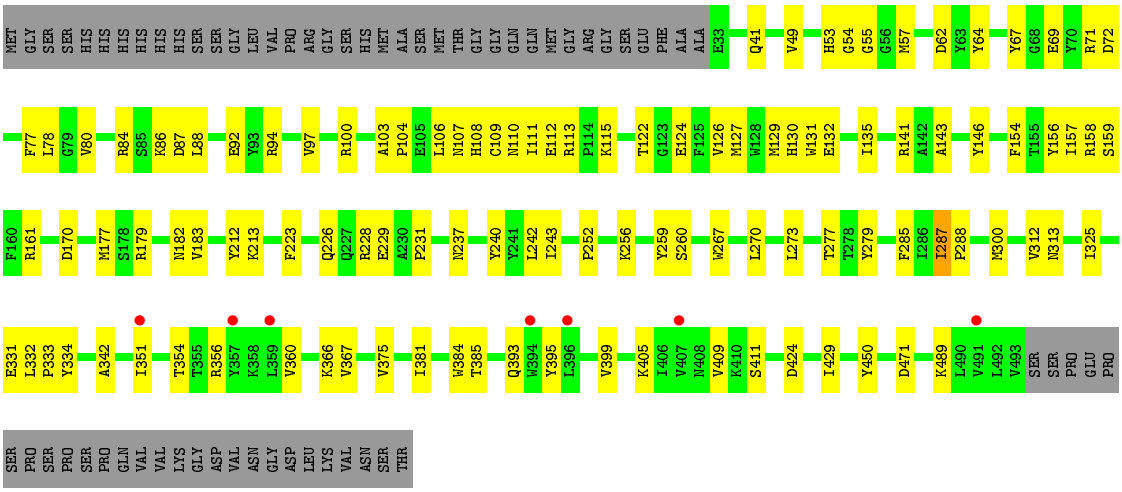
• Molecule 1: Ricin B lectin

Chain F:



• Molecule 1: Ricin B lectin

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	106.64Å 122.53Å 403.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.80 – 3.19 48.80 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.80-3.19) 99.3 (48.80-3.19)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.49 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.235 , 0.270 0.219 , 0.252	Depositor DCC
R_{free} test set	1595 reflections (1.80%)	DCC
Wilson B-factor (Å^2)	72.6	Xtriage
Anisotropy	0.752	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 32.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 88661 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	22211	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.20	0/3762	0.37	0/5104
1	B	0.21	0/3762	0.37	0/5104
1	C	0.21	0/3907	0.37	0/5295
1	D	0.22	0/3762	0.38	0/5104
1	E	0.21	0/3762	0.38	0/5104
1	F	0.21	0/3762	0.37	0/5104
All	All	0.21	0/22717	0.37	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

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	85	0
1	B	3664	0	3480	82	0
1	C	3807	0	3613	77	0
1	D	3664	0	3480	111	0
1	E	3664	0	3480	76	0
1	F	3664	0	3480	64	0
2	A	12	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	12	0	12	1	0
2	C	24	0	24	0	0
2	E	12	0	12	0	0
2	F	24	0	24	0	0
All	All	22211	0	21097	484	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (484) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:383:GLN:HG3	1:D:475:ILE:HD11	1.34	1.06
1:A:229:GLU:O	1:A:231:PRO:HD3	1.69	0.93
1:D:387:ASN:H	1:D:392:GLN:HE22	1.13	0.92
1:E:57:MET:HE2	1:E:287:ILE:HG21	1.53	0.91
1:B:84:ARG:HE	1:B:94:ARG:HE	1.16	0.90
1:D:450:TYR:HA	1:D:489:LYS:HB2	1.54	0.90
1:D:380:GLN:HA	1:D:429:ILE:HG22	1.53	0.88
1:C:57:MET:HE2	1:C:287:ILE:HD13	1.57	0.87
1:C:-12:MET:HG3	1:E:155:THR:HG22	1.59	0.83
1:D:461:LEU:HD21	1:D:480:ASP:HB3	1.61	0.82
1:D:254:GLN:HG2	1:D:276:SER:HA	1.61	0.82
1:D:340:ILE:HG22	1:D:347:ILE:HG22	1.62	0.81
1:D:321:PRO:HB3	1:D:347:ILE:HD13	1.62	0.81
1:C:42:PHE:CD2	1:C:50:ILE:HD12	2.16	0.81
1:C:42:PHE:HD2	1:C:50:ILE:HD12	1.47	0.80
1:F:461:LEU:HD11	1:F:486:GLN:HB3	1.63	0.79
1:C:34:GLY:HA2	1:C:89:VAL:HG21	1.65	0.78
1:D:449:GLY:C	1:D:489:LYS:HD2	2.05	0.76
1:F:360:VAL:HG22	1:F:367:VAL:HG12	1.67	0.76
1:B:356:ARG:HD3	1:B:393:GLN:NE2	2.00	0.75
1:C:260:SER:HB2	1:C:267:TRP:HA	1.69	0.74
1:B:133:ASN:HD22	1:B:139:GLN:HG2	1.52	0.74
1:A:366:LYS:HE2	1:A:385:THR:HG22	1.69	0.74
1:B:340:ILE:HG22	1:B:347:ILE:HG23	1.69	0.74
1:B:360:VAL:HG22	1:B:367:VAL:HG12	1.69	0.74
1:C:216:ALA:HA	1:D:164:GLN:HE22	1.52	0.74
1:E:422:LYS:HD3	1:E:458:CYS:HB3	1.70	0.74
1:D:420:GLU:HB3	1:D:457:HIS:CE1	2.25	0.72
1:D:465:ARG:HG2	1:D:466:LYS:HG3	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:HIS:CD2	1:D:179:ARG:HA	2.24	0.72
1:A:360:VAL:HG22	1:A:367:VAL:HG12	1.72	0.71
1:D:125:PHE:CZ	1:D:150:PRO:HG3	2.25	0.71
1:F:57:MET:HE2	1:F:287:ILE:HD13	1.73	0.70
1:C:360:VAL:HG22	1:C:367:VAL:HG12	1.73	0.70
1:C:-6:MET:CE	1:F:155:THR:HG21	2.23	0.69
1:E:416:ASP:HB3	1:E:439:GLN:HG2	1.74	0.69
1:E:381:ILE:HG22	1:E:475:ILE:HB	1.75	0.68
1:E:390:LEU:O	1:E:410:LYS:HB2	1.93	0.68
1:E:111:ILE:HD11	1:E:131:TRP:HD1	1.58	0.68
1:B:146:TYR:HD2	1:B:157:ILE:HD11	1.59	0.68
1:B:146:TYR:CD2	1:B:157:ILE:HD11	2.30	0.67
1:E:252:PRO:HB2	1:E:277:THR:HG23	1.76	0.67
1:B:57:MET:HE2	1:B:287:ILE:HG21	1.77	0.67
1:D:69:GLU:OE1	1:D:112:GLU:HA	1.95	0.66
1:A:72:ASP:HB3	1:A:78:LEU:HD12	1.77	0.66
1:E:129:MET:HG2	1:E:143:ALA:HB3	1.78	0.66
1:E:171:HIS:CE1	1:E:199:GLU:HB2	2.31	0.66
1:A:88:LEU:HD13	1:A:342:ALA:HB2	1.78	0.66
1:D:53:HIS:O	1:D:69:GLU:HG2	1.96	0.66
1:E:360:VAL:HG22	1:E:367:VAL:HG12	1.77	0.65
1:E:54:GLY:O	1:E:113:ARG:HA	1.97	0.65
1:D:395:TYR:CE2	1:D:409:VAL:HG22	2.32	0.65
1:F:71:ARG:HD3	1:F:312:VAL:HG11	1.78	0.65
1:D:71:ARG:HD3	1:D:75:ASN:OD1	1.97	0.65
1:D:381:ILE:HG22	1:D:475:ILE:HG13	1.79	0.65
1:B:179:ARG:HG3	1:B:200:ASN:OD1	1.96	0.65
1:A:110:ASN:HB2	1:A:132:GLU:HB2	1.78	0.65
1:B:133:ASN:OD1	1:B:135:ILE:HG13	1.97	0.64
1:D:115:LYS:HZ1	1:D:284:THR:HG22	1.62	0.64
1:A:260:SER:HB2	1:A:267:TRP:HA	1.79	0.64
1:C:98:LEU:HD22	1:C:127:MET:HE1	1.78	0.64
1:D:377:ASN:HD21	1:D:432:THR:HG23	1.61	0.64
1:C:422:LYS:HE3	1:C:457:HIS:CE1	2.31	0.64
1:F:260:SER:HB2	1:F:267:TRP:HA	1.80	0.63
1:A:157:ILE:HG22	1:A:158:ARG:HG2	1.80	0.63
1:C:422:LYS:HG2	1:C:458:CYS:HB3	1.81	0.63
1:B:129:MET:HG2	1:B:143:ALA:HB3	1.80	0.63
1:B:484:THR:HA	1:B:487:HIS:CD2	2.34	0.63
1:C:223:PHE:HE2	1:C:242:LEU:HD23	1.65	0.62
1:B:453:ILE:H	1:B:453:ILE:HD12	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:93:TYR:CZ	1:F:95:GLY:HA2	2.34	0.62
1:B:380:GLN:HE22	1:B:427:VAL:HG13	1.65	0.62
1:E:77:PHE:CD1	1:E:111:ILE:HB	2.33	0.62
1:D:260:SER:HB2	1:D:267:TRP:HA	1.81	0.62
1:F:168:VAL:HG11	1:F:176:TYR:CE1	2.34	0.62
1:C:77:PHE:CD1	1:C:111:ILE:HB	2.35	0.61
1:F:448:ASP:HA	1:A:237:ASN:HD21	1.65	0.61
1:E:422:LYS:HE2	1:E:457:HIS:CD2	2.36	0.61
1:A:62:ASP:O	1:A:86:LYS:HG3	2.01	0.61
1:F:223:PHE:HE2	1:F:242:LEU:HD23	1.64	0.60
1:A:80:VAL:HG11	1:A:127:MET:HE3	1.82	0.60
1:D:420:GLU:HB3	1:D:457:HIS:HE1	1.64	0.60
1:B:358:LYS:NZ	1:B:388:GLY:HA2	2.17	0.60
1:B:54:GLY:O	1:B:113:ARG:HA	2.02	0.59
1:C:84:ARG:HH21	1:C:94:ARG:NH1	2.00	0.59
1:C:450:TYR:CE1	1:C:489:LYS:HB2	2.36	0.59
1:B:161:ARG:O	1:B:164:GLN:HG3	2.02	0.59
1:E:179:ARG:HG3	1:E:200:ASN:OD1	2.03	0.59
1:C:50:ILE:HG23	1:C:83:TYR:CE1	2.37	0.59
1:A:228:ARG:NH2	1:A:256:LYS:HD2	2.18	0.59
1:A:53:HIS:HE1	1:A:313:ASN:HA	1.68	0.59
1:A:375:VAL:HG12	1:A:411:SER:HB3	1.84	0.58
1:D:451:TYR:HB2	1:D:488:TRP:O	2.02	0.58
1:F:223:PHE:HB3	1:F:226:GLN:HG3	1.86	0.58
1:D:441:TRP:HZ3	1:D:477:GLN:HE22	1.50	0.58
1:A:226:GLN:HE22	1:A:270:LEU:HD21	1.68	0.58
1:A:100:ARG:HG2	1:A:107:ASN:HA	1.86	0.58
1:A:331:GLU:HG2	1:A:333:PRO:HD3	1.85	0.58
1:C:413:ARG:NH1	1:C:432:THR:HG22	2.18	0.58
1:F:77:PHE:CD1	1:F:111:ILE:HB	2.39	0.58
1:D:347:ILE:O	1:D:347:ILE:HD12	2.03	0.58
1:A:325:ILE:HD11	1:A:331:GLU:OE2	2.04	0.58
1:E:416:ASP:CB	1:E:439:GLN:HG2	2.33	0.57
1:A:285:PHE:CE2	1:A:287:ILE:HG23	2.40	0.57
1:C:413:ARG:HH12	1:C:432:THR:HG22	1.69	0.57
1:A:77:PHE:CD1	1:A:111:ILE:HB	2.40	0.57
1:B:145:ALA:HA	1:B:157:ILE:CD1	2.35	0.57
1:F:54:GLY:O	1:F:113:ARG:HA	2.03	0.57
1:C:129:MET:HG2	1:C:143:ALA:HB3	1.87	0.56
1:B:67:TYR:CE2	1:B:116:VAL:HG21	2.40	0.56
1:A:287:ILE:HD11	1:A:300:MET:HE3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:SER:HB3	1:D:283:PRO:HD2	1.86	0.56
1:D:115:LYS:NZ	1:D:284:THR:HG22	2.21	0.56
1:E:53:HIS:O	1:E:69:GLU:HG2	2.04	0.56
1:B:77:PHE:HE1	1:B:80:VAL:HG23	1.71	0.56
1:D:383:GLN:HE21	1:D:475:ILE:HD12	1.71	0.55
1:D:77:PHE:CD1	1:D:111:ILE:HB	2.41	0.55
1:F:231:PRO:HA	1:F:244:THR:HG22	1.89	0.55
1:B:339:LYS:HB2	1:B:350:TYR:HB2	1.87	0.55
1:D:157:ILE:HG22	1:D:158:ARG:HG2	1.88	0.55
1:B:385:THR:HG23	1:B:471:ASP:OD1	2.06	0.55
1:F:223:PHE:CE2	1:F:242:LEU:HD23	2.41	0.55
1:D:164:GLN:NE2	1:D:165:ASP:HB3	2.22	0.55
1:E:131:TRP:CE3	1:E:141:ARG:HD2	2.42	0.55
1:B:362:LYS:HG3	1:B:484:THR:HB	1.88	0.55
1:B:55:GLY:HA3	1:B:67:TYR:O	2.07	0.55
1:D:97:VAL:HB	1:D:154:PHE:CD2	2.42	0.55
1:B:453:ILE:HD12	1:B:453:ILE:N	2.21	0.55
1:A:103:ALA:HB3	1:A:106:LEU:HG	1.89	0.55
1:A:55:GLY:HA3	1:A:67:TYR:O	2.07	0.55
1:F:366:LYS:HE3	1:F:385:THR:HG22	1.89	0.55
1:E:168:VAL:HG11	1:E:176:TYR:CE1	2.41	0.55
1:D:384:TRP:CE3	1:D:471:ASP:HB3	2.42	0.55
1:A:100:ARG:HG3	1:A:106:LEU:O	2.06	0.54
1:D:424:ASP:OD2	1:D:460:LYS:HD2	2.07	0.54
1:F:305:ALA:HA	1:F:308:TRP:CZ2	2.43	0.54
1:D:80:VAL:HG11	1:D:127:MET:HE3	1.89	0.54
1:F:428:LEU:HD12	1:F:475:ILE:HG22	1.90	0.54
1:E:260:SER:HB2	1:E:267:TRP:HA	1.90	0.54
1:C:458:CYS:SG	1:C:460:LYS:HG3	2.47	0.54
1:C:55:GLY:HA3	1:C:67:TYR:O	2.07	0.54
1:A:84:ARG:HD2	1:A:94:ARG:HD3	1.89	0.54
1:B:260:SER:HB2	1:B:267:TRP:HA	1.90	0.54
1:F:384:TRP:CE3	1:F:471:ASP:HB3	2.43	0.54
1:A:84:ARG:HG2	1:A:92:GLU:HB3	1.89	0.54
1:A:129:MET:HG2	1:A:143:ALA:HB3	1.88	0.54
1:F:111:ILE:HG21	1:F:129:MET:HE2	1.90	0.53
1:F:135:ILE:HG22	1:F:136:ASN:HD22	1.73	0.53
1:C:54:GLY:O	1:C:113:ARG:HA	2.08	0.53
1:F:450:TYR:CE1	1:F:489:LYS:HB2	2.43	0.53
1:C:362:LYS:HE3	1:C:484:THR:HG22	1.91	0.53
1:C:-6:MET:HE2	1:F:155:THR:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:ARG:HE	1:C:94:ARG:NE	2.05	0.53
1:D:55:GLY:HA3	1:D:67:TYR:O	2.08	0.53
1:C:465:ARG:HH21	1:C:474:ILE:HG21	1.74	0.53
1:D:453:ILE:HG21	1:D:462:ILE:HD12	1.91	0.52
1:D:164:GLN:HE21	1:D:165:ASP:HB3	1.73	0.52
1:F:448:ASP:HA	1:A:237:ASN:ND2	2.23	0.52
1:B:77:PHE:CE1	1:B:80:VAL:HG23	2.44	0.52
1:E:80:VAL:HG21	1:E:127:MET:CE	2.40	0.52
1:E:252:PRO:HB2	1:E:277:THR:CG2	2.39	0.52
1:C:111:ILE:HD11	1:C:131:TRP:HD1	1.74	0.52
1:E:450:TYR:CE1	1:E:489:LYS:HB2	2.44	0.52
1:B:321:PRO:HB3	1:B:347:ILE:HG22	1.92	0.52
1:C:63:TYR:CE1	1:C:86:LYS:HE3	2.45	0.52
1:D:106:LEU:HD11	1:D:156:TYR:CD2	2.45	0.52
1:B:157:ILE:HD12	1:B:157:ILE:N	2.25	0.52
1:D:444:THR:OG1	1:D:452:LYS:HB3	2.10	0.52
1:A:279:TYR:CD2	1:A:334:TYR:HB2	2.45	0.52
1:C:97:VAL:HB	1:C:154:PHE:CD2	2.44	0.52
1:F:59:LYS:HD3	1:F:64:TYR:CE1	2.45	0.52
1:E:279:TYR:CD2	1:E:334:TYR:HB2	2.44	0.52
1:D:111:ILE:HD11	1:D:131:TRP:HD1	1.74	0.51
1:B:405:LYS:HE3	1:B:407:VAL:CG2	2.41	0.51
1:C:104:PRO:HA	1:C:107:ASN:ND2	2.25	0.51
1:D:383:GLN:HG3	1:D:475:ILE:CD1	2.24	0.51
1:D:379:ALA:HB3	1:D:430:GLN:HG2	1.93	0.51
1:B:218:LEU:O	1:B:218:LEU:HD12	2.10	0.51
1:B:57:MET:CE	1:B:287:ILE:HG21	2.40	0.51
1:D:117:MET:HE3	1:D:212:TYR:HB3	1.93	0.51
1:C:-13:SER:HA	1:C:492:LEU:HD11	1.93	0.51
1:B:70:TYR:CZ	1:B:78:LEU:HD11	2.45	0.51
1:B:223:PHE:HB3	1:B:226:GLN:HG3	1.93	0.51
1:B:110:ASN:HB2	1:B:132:GLU:HB2	1.92	0.51
1:D:42:PHE:HB2	1:D:50:ILE:HD11	1.93	0.51
1:A:53:HIS:CE1	1:A:313:ASN:HA	2.45	0.50
1:A:356:ARG:HD2	1:A:393:GLN:OE1	2.10	0.50
1:F:135:ILE:HD12	1:F:135:ILE:N	2.27	0.50
1:E:115:LYS:HG3	1:E:182:ASN:OD1	2.11	0.50
1:A:223:PHE:CE2	1:A:242:LEU:HD23	2.47	0.50
1:D:80:VAL:HG21	1:D:127:MET:HE1	1.94	0.50
1:D:398:ASP:HA	1:D:404:LYS:HG2	1.94	0.50
1:A:126:VAL:HG21	1:A:212:TYR:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:277:THR:HG22	1:E:277:THR:O	2.11	0.50
1:E:413:ARG:NH1	1:E:432:THR:HG22	2.27	0.50
1:F:286:ILE:HD13	1:F:322:LEU:HD22	1.94	0.49
1:A:223:PHE:HB3	1:A:226:GLN:NE2	2.27	0.49
1:E:110:ASN:HB2	1:E:132:GLU:HB2	1.94	0.49
1:B:284:THR:HG22	1:B:300:MET:O	2.11	0.49
1:D:147:SER:HB2	1:D:154:PHE:HA	1.94	0.49
1:D:200:ASN:HB3	1:D:229:GLU:OE2	2.11	0.49
1:E:284:THR:HG22	1:E:300:MET:O	2.13	0.49
1:B:381:ILE:HG12	1:B:429:ILE:HA	1.94	0.49
1:D:398:ASP:HB2	1:D:404:LYS:NZ	2.28	0.49
1:D:130:HIS:NE2	1:D:179:ARG:HA	2.27	0.49
1:A:106:LEU:HA	1:A:109:CYS:SG	2.52	0.49
1:F:363:ASN:HB2	1:F:484:THR:OG1	2.13	0.49
1:C:-12:MET:CG	1:E:155:THR:HG22	2.37	0.49
1:C:50:ILE:HG23	1:C:83:TYR:CZ	2.48	0.49
1:D:465:ARG:HD3	1:D:466:LYS:HE2	1.95	0.49
1:D:115:LYS:HE3	1:D:182:ASN:OD1	2.13	0.49
1:F:430:GLN:O	1:F:430:GLN:HG3	2.13	0.48
1:A:71:ARG:NH1	1:A:312:VAL:HG11	2.28	0.48
1:C:399:VAL:HG21	1:C:440:HIS:NE2	2.28	0.48
1:E:230:ALA:N	1:E:231:PRO:HD3	2.28	0.48
1:B:229:GLU:OE2	1:B:247:CYS:HB2	2.12	0.48
1:E:381:ILE:HD13	1:E:429:ILE:HA	1.95	0.48
1:D:84:ARG:HG2	1:D:94:ARG:HD3	1.95	0.48
1:E:97:VAL:HB	1:E:154:PHE:CD2	2.48	0.48
1:B:84:ARG:HE	1:B:94:ARG:NE	1.96	0.48
1:D:420:GLU:HG2	1:D:438:ASN:ND2	2.28	0.48
1:C:98:LEU:HD22	1:C:127:MET:CE	2.42	0.48
1:F:395:TYR:CE2	1:F:409:VAL:HG22	2.49	0.48
1:B:33:GLU:HG2	1:B:35:VAL:HG12	1.95	0.48
1:F:284:THR:HG22	1:F:300:MET:O	2.13	0.48
1:D:376:ASP:C	1:D:413:ARG:HH12	2.16	0.48
1:C:223:PHE:CE2	1:C:242:LEU:HD23	2.47	0.48
1:E:106:LEU:HD11	1:E:156:TYR:CD2	2.47	0.48
1:A:106:LEU:HD11	1:A:156:TYR:CD2	2.49	0.48
1:F:413:ARG:NH1	1:F:432:THR:HG22	2.29	0.48
1:B:106:LEU:HD22	1:B:111:ILE:HD11	1.95	0.48
1:A:381:ILE:HG12	1:A:429:ILE:HA	1.95	0.48
1:E:71:ARG:HH11	1:E:75:ASN:ND2	2.11	0.48
1:A:97:VAL:HB	1:A:154:PHE:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:416:ASP:OD2	1:F:438:ASN:ND2	2.47	0.48
1:E:305:ALA:HA	1:E:308:TRP:CZ2	2.49	0.48
1:A:115:LYS:HG3	1:A:182:ASN:HA	1.96	0.48
1:A:146:TYR:CD2	1:A:157:ILE:HD11	2.49	0.48
1:B:125:PHE:CE2	1:B:150:PRO:HD3	2.49	0.48
1:B:484:THR:HA	1:B:487:HIS:HD2	1.79	0.47
1:F:378:ALA:HA	1:F:429:ILE:HD12	1.96	0.47
1:D:381:ILE:HG12	1:D:429:ILE:HA	1.96	0.47
1:D:54:GLY:O	1:D:113:ARG:HA	2.14	0.47
1:C:446:ILE:HG21	1:C:452:LYS:HG3	1.97	0.47
1:A:54:GLY:O	1:A:113:ARG:HA	2.14	0.47
1:A:385:THR:HG23	1:A:471:ASP:OD1	2.15	0.47
1:E:129:MET:CG	1:E:143:ALA:HB3	2.45	0.47
1:C:69:GLU:HG3	1:C:111:ILE:O	2.14	0.47
1:F:385:THR:HG23	1:F:471:ASP:OD1	2.14	0.47
1:A:170:ASP:OD1	1:A:177:MET:HG3	2.14	0.47
1:E:80:VAL:HG21	1:E:127:MET:HE1	1.96	0.47
1:B:335:TYR:HB2	1:B:338:VAL:HG22	1.97	0.47
1:F:285:PHE:HE2	1:F:287:ILE:HB	1.80	0.47
1:C:-6:MET:HE1	1:F:155:THR:HG21	1.94	0.47
1:B:378:ALA:HA	1:B:429:ILE:HD12	1.97	0.47
1:B:106:LEU:HD11	1:B:156:TYR:CD2	2.50	0.47
1:A:161:ARG:NH2	1:A:177:MET:HG2	2.29	0.47
1:D:299:TYR:HB3	1:D:320:LEU:O	2.14	0.47
1:D:41:GLN:HB3	1:D:49:VAL:HG13	1.97	0.47
1:B:358:LYS:HZ1	1:B:388:GLY:HA2	1.79	0.47
1:A:161:ARG:HH22	1:A:177:MET:HG2	1.79	0.47
1:A:252:PRO:HB2	1:A:277:THR:HB	1.97	0.47
1:D:279:TYR:CD2	1:D:334:TYR:HB2	2.50	0.47
1:C:385:THR:HG23	1:C:471:ASP:OD1	2.14	0.47
1:F:331:GLU:HG2	1:F:333:PRO:HD3	1.97	0.47
1:D:464:VAL:HG21	1:D:468:SER:O	2.15	0.47
1:D:476:GLN:OE1	1:D:478:TRP:HE3	1.98	0.47
1:C:42:PHE:CE2	1:C:50:ILE:HD12	2.50	0.47
1:A:129:MET:CG	1:A:143:ALA:HB3	2.45	0.47
1:B:78:LEU:C	1:B:78:LEU:HD12	2.35	0.47
1:D:370:VAL:H	1:D:391:SER:HB3	1.80	0.47
1:B:41:GLN:HB3	1:B:49:VAL:HG23	1.96	0.47
1:B:450:TYR:HA	1:B:488:TRP:O	2.15	0.46
1:C:84:ARG:HE	1:C:94:ARG:CZ	2.28	0.46
1:D:168:VAL:HG21	1:D:176:TYR:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:492:LEU:HD12	1:D:492:LEU:H	1.79	0.46
1:E:70:TYR:HB3	1:E:79:GLY:O	2.15	0.46
1:A:69:GLU:HG2	1:A:112:GLU:HA	1.97	0.46
1:D:236:ARG:HA	1:D:297:TYR:OH	2.16	0.46
1:D:54:GLY:HA2	1:D:284:THR:HG21	1.98	0.46
1:D:369:ASP:OD1	1:D:391:SER:HB2	2.16	0.46
1:D:464:VAL:O	1:D:464:VAL:HG13	2.15	0.46
1:F:209:THR:HB	1:F:210:PRO:HD2	1.98	0.46
1:A:130:HIS:CD2	1:A:179:ARG:HA	2.51	0.46
1:D:353:ASP:OD1	1:D:355:THR:HG23	2.15	0.46
1:C:59:LYS:HD3	1:C:64:TYR:CE1	2.51	0.46
1:E:362:LYS:HD3	1:E:450:TYR:CZ	2.50	0.46
1:F:351:ILE:HD12	1:F:351:ILE:N	2.31	0.46
1:D:110:ASN:HB2	1:D:132:GLU:HB2	1.97	0.46
1:C:57:MET:CE	1:C:287:ILE:HG21	2.46	0.46
1:D:296:SER:HB3	1:D:347:ILE:HD11	1.96	0.46
1:D:106:LEU:HA	1:D:109:CYS:SG	2.56	0.46
1:A:41:GLN:HB3	1:A:49:VAL:HG23	1.96	0.46
1:E:351:ILE:N	1:E:351:ILE:HD12	2.29	0.46
1:D:446:ILE:HG13	1:D:450:TYR:O	2.15	0.46
1:B:287:ILE:HA	1:B:288:PRO:HD3	1.85	0.46
1:A:64:TYR:CD2	1:A:88:LEU:HD11	2.51	0.46
1:C:285:PHE:HE2	1:C:287:ILE:HB	1.81	0.45
1:B:130:HIS:CE1	1:B:179:ARG:HA	2.52	0.45
1:A:111:ILE:HD11	1:A:131:TRP:HD1	1.81	0.45
1:A:77:PHE:CZ	1:A:80:VAL:HG23	2.51	0.45
1:E:70:TYR:O	1:E:78:LEU:HB3	2.16	0.45
1:D:87:ASP:O	1:D:88:LEU:HB2	2.16	0.45
1:A:273:LEU:HD21	1:A:332:LEU:CB	2.46	0.45
1:F:465:ARG:HE	1:F:474:ILE:HG21	1.81	0.45
1:C:203:LEU:HD21	1:C:231:PRO:HB3	1.97	0.45
1:E:320:LEU:HB2	1:E:332:LEU:HD11	1.98	0.45
1:C:130:HIS:CE1	1:C:179:ARG:HA	2.52	0.45
1:A:351:ILE:N	1:A:351:ILE:HD12	2.32	0.45
1:E:465:ARG:HG2	1:E:466:LYS:HG2	1.98	0.45
1:D:449:GLY:CA	1:D:489:LYS:HD2	2.46	0.45
1:C:179:ARG:HG3	1:C:200:ASN:OD1	2.17	0.45
1:C:354:THR:O	1:C:354:THR:HG22	2.15	0.45
1:C:63:TYR:CE1	1:C:84:ARG:NH1	2.85	0.45
1:B:115:LYS:HG3	1:B:182:ASN:HA	1.97	0.45
1:C:223:PHE:CD1	1:C:270:LEU:HD11	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:ASP:HA	1:B:78:LEU:HD23	1.99	0.45
1:D:149:THR:OG1	1:D:152:GLY:HA3	2.17	0.45
1:A:395:TYR:CE2	1:A:409:VAL:HG22	2.52	0.45
1:C:287:ILE:HA	1:C:288:PRO:HD3	1.83	0.45
1:F:382:VAL:HA	1:F:475:ILE:HG12	1.99	0.45
1:E:133:ASN:OD1	1:E:135:ILE:HG13	2.17	0.45
1:C:-15:MET:HE3	1:E:153:LYS:HE2	1.99	0.45
1:D:398:ASP:HB2	1:D:404:LYS:HZ2	1.81	0.45
1:D:129:MET:CG	1:D:143:ALA:HB3	2.47	0.45
1:F:55:GLY:HA3	1:F:67:TYR:O	2.17	0.45
1:B:129:MET:CG	1:B:143:ALA:HB3	2.46	0.44
1:A:131:TRP:CE3	1:A:141:ARG:HD2	2.52	0.44
1:B:50:ILE:HG23	1:B:83:TYR:CE1	2.52	0.44
1:D:451:TYR:CD2	1:D:489:LYS:HG3	2.52	0.44
1:C:64:TYR:O	1:C:84:ARG:HA	2.17	0.44
1:D:384:TRP:CZ3	1:D:471:ASP:HB3	2.52	0.44
1:A:84:ARG:HD2	1:A:94:ARG:CD	2.48	0.44
1:A:130:HIS:NE2	1:A:179:ARG:HA	2.33	0.44
1:C:284:THR:HG22	1:C:300:MET:O	2.17	0.44
1:E:55:GLY:HA3	1:E:67:TYR:O	2.18	0.44
1:B:466:LYS:HA	1:B:466:LYS:HE2	1.98	0.44
1:F:97:VAL:HB	1:F:154:PHE:CD2	2.52	0.44
1:B:106:LEU:HD21	1:B:156:TYR:CE2	2.53	0.44
1:F:256:LYS:HD3	1:F:270:LEU:HB3	2.00	0.44
1:E:50:ILE:HG23	1:E:83:TYR:CE1	2.52	0.44
1:C:378:ALA:HA	1:C:429:ILE:HD12	2.00	0.44
1:C:42:PHE:CE2	1:C:91:TRP:CD1	3.05	0.44
1:B:358:LYS:HZ3	1:B:388:GLY:HA2	1.82	0.44
1:D:129:MET:HG2	1:D:143:ALA:HB3	1.99	0.44
1:D:305:ALA:HB3	1:D:311:LYS:O	2.18	0.44
1:A:124:GLU:OE1	1:A:213:LYS:HE3	2.18	0.44
1:B:63:TYR:CZ	1:B:84:ARG:NH1	2.86	0.44
1:E:299:TYR:HB3	1:E:320:LEU:O	2.17	0.44
1:F:179:ARG:HD2	1:F:200:ASN:OD1	2.18	0.44
1:D:243:ILE:N	1:D:243:ILE:HD12	2.32	0.44
1:D:35:VAL:HG21	1:D:337:SER:HB3	1.98	0.44
1:B:118:TYR:HD2	1:B:125:PHE:CE1	2.35	0.44
1:E:122:THR:OG1	1:E:124:GLU:HG2	2.17	0.44
1:A:243:ILE:N	1:A:243:ILE:HD12	2.33	0.44
1:F:163:MET:HE2	1:F:218:LEU:N	2.33	0.44
1:B:403:TYR:CD1	1:B:442:LYS:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:361:ASN:HB3	1:D:364:SER:OG	2.18	0.44
1:D:269:GLN:HG3	1:D:271:TYR:CE1	2.52	0.44
1:D:383:GLN:HE21	1:D:475:ILE:CD1	2.31	0.43
1:F:461:LEU:CD1	1:F:486:GLN:HB3	2.40	0.43
1:B:356:ARG:HD3	1:B:393:GLN:HE22	1.80	0.43
1:D:377:ASN:HD21	1:D:432:THR:H	1.66	0.43
1:C:194:ILE:HD11	1:C:203:LEU:HD23	2.00	0.43
1:F:243:ILE:HD12	1:F:243:ILE:N	2.32	0.43
1:D:383:GLN:NE2	1:D:488:TRP:CH2	2.86	0.43
1:A:228:ARG:HH22	1:A:256:LYS:HE3	1.83	0.43
1:D:429:ILE:HD12	1:D:429:ILE:C	2.38	0.43
1:E:378:ALA:HA	1:E:429:ILE:HD12	1.99	0.43
1:B:362:LYS:CG	1:B:484:THR:HB	2.48	0.43
1:C:270:LEU:N	1:C:270:LEU:HD12	2.33	0.43
1:B:156:TYR:OH	1:B:159:SER:HB3	2.18	0.43
1:B:446:ILE:HD13	1:B:452:LYS:HG3	1.99	0.43
1:E:492:LEU:HD12	1:E:492:LEU:N	2.33	0.43
1:B:362:LYS:HE2	1:B:450:TYR:CZ	2.53	0.43
1:A:279:TYR:CE2	1:A:334:TYR:HB2	2.53	0.43
1:E:109:CYS:HB2	1:E:132:GLU:O	2.18	0.43
1:C:136:ASN:HB2	1:A:424:ASP:O	2.18	0.43
1:C:390:LEU:HB3	1:C:410:LYS:HB2	1.99	0.43
1:C:350:TYR:O	1:C:352:PRO:HD3	2.19	0.43
1:D:420:GLU:O	1:D:457:HIS:CE1	2.72	0.43
1:F:448:ASP:CA	1:A:237:ASN:HD21	2.32	0.43
1:A:450:TYR:CE2	1:A:489:LYS:HE3	2.53	0.43
1:E:403:TYR:CE1	1:E:442:LYS:HB2	2.54	0.43
1:E:111:ILE:HD11	1:E:131:TRP:CD1	2.47	0.43
1:D:395:TYR:CZ	1:D:409:VAL:HG22	2.54	0.43
1:D:351:ILE:HD12	1:D:351:ILE:N	2.34	0.43
1:B:305:ALA:HA	1:B:308:TRP:CZ2	2.54	0.43
1:C:58:LEU:HD22	1:C:116:VAL:HG12	2.01	0.43
1:A:57:MET:CB	1:A:300:MET:HE1	2.48	0.43
1:F:115:LYS:HG3	1:F:182:ASN:HA	2.00	0.43
1:E:58:LEU:HD22	1:E:116:VAL:HG12	2.01	0.43
1:E:235:LYS:HD2	1:E:240:TYR:CE2	2.54	0.43
1:C:243:ILE:N	1:C:243:ILE:HD12	2.34	0.43
1:D:338:VAL:HG12	1:D:340:ILE:HG23	2.01	0.42
1:E:131:TRP:CZ3	1:E:141:ARG:HD2	2.54	0.42
1:F:492:LEU:N	1:F:492:LEU:HD12	2.34	0.42
1:A:226:GLN:NE2	1:A:270:LEU:HD21	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:278:THR:HG22	1:D:278:THR:O	2.19	0.42
1:F:59:LYS:HD3	1:F:64:TYR:CD1	2.54	0.42
1:E:59:LYS:HD3	1:E:64:TYR:CE1	2.54	0.42
1:B:450:TYR:CE1	1:B:489:LYS:HB2	2.54	0.42
1:B:359:LEU:HD12	1:B:368:LEU:HD22	2.02	0.42
1:A:240:TYR:O	1:A:259:TYR:HA	2.18	0.42
1:B:147:SER:HB2	1:B:154:PHE:HA	2.01	0.42
1:F:70:TYR:O	1:F:78:LEU:HB2	2.19	0.42
1:E:251:ASN:HA	1:E:252:PRO:HD3	1.92	0.42
1:A:270:LEU:N	1:A:270:LEU:HD22	2.35	0.42
1:E:384:TRP:CE3	1:E:471:ASP:HB3	2.54	0.42
1:E:286:ILE:HD13	1:E:322:LEU:HD22	2.02	0.42
1:E:254:GLN:NE2	1:E:273:LEU:H	2.17	0.42
1:E:57:MET:CE	1:E:287:ILE:HD13	2.49	0.42
1:B:34:GLY:O	1:B:339:LYS:HA	2.19	0.42
1:D:83:TYR:HB3	1:D:91:TRP:HB3	2.02	0.42
1:A:115:LYS:HB3	1:A:183:VAL:HG22	2.02	0.42
1:C:106:LEU:HA	1:C:109:CYS:SG	2.59	0.42
1:F:57:MET:CE	1:F:287:ILE:HG21	2.50	0.42
1:D:458:CYS:SG	1:D:460:LYS:HE3	2.60	0.42
1:C:491:VAL:HG12	1:C:492:LEU:O	2.20	0.42
1:F:80:VAL:O	1:F:97:VAL:HG22	2.20	0.42
1:E:381:ILE:HG12	1:E:415:LEU:CD1	2.50	0.42
1:F:70:TYR:HB3	1:F:79:GLY:O	2.19	0.42
1:F:161:ARG:HH22	1:F:177:MET:HG2	1.83	0.42
1:C:42:PHE:HE2	1:C:91:TRP:CD1	2.38	0.41
1:A:87:ASP:O	1:A:88:LEU:HB2	2.20	0.41
1:D:97:VAL:HB	1:D:154:PHE:HD2	1.84	0.41
1:A:135:ILE:N	1:A:135:ILE:HD12	2.35	0.41
1:D:420:GLU:O	1:D:457:HIS:HE1	2.03	0.41
1:F:64:TYR:CG	1:F:88:LEU:HD21	2.55	0.41
1:D:377:ASN:ND2	1:D:432:THR:HG23	2.31	0.41
1:F:87:ASP:O	1:F:88:LEU:HB2	2.20	0.41
1:A:103:ALA:HB1	1:A:104:PRO:HD2	2.01	0.41
1:C:130:HIS:CE1	1:C:179:ARG:HD3	2.56	0.41
1:C:142:ALA:O	1:C:159:SER:HA	2.20	0.41
1:B:278:THR:O	1:B:278:THR:HG22	2.21	0.41
1:B:321:PRO:HB3	1:B:347:ILE:CG2	2.50	0.41
1:D:288:PRO:HB3	1:D:297:TYR:CE1	2.56	0.41
1:C:128:TRP:HB3	1:C:193:PHE:CE1	2.56	0.41
1:B:419:ASP:OD1	2:B:601:GAL:H62	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:THR:O	1:A:354:THR:HG22	2.20	0.41
1:E:422:LYS:HE2	1:E:457:HIS:NE2	2.36	0.41
1:F:147:SER:HB2	1:F:154:PHE:HA	2.02	0.41
1:C:305:ALA:HA	1:C:308:TRP:CZ2	2.55	0.41
1:F:206:TYR:HB3	1:F:215:ILE:HG23	2.01	0.41
1:D:234:ILE:HD11	1:D:241:TYR:HB2	2.02	0.41
1:D:59:LYS:HD3	1:D:64:TYR:CD1	2.56	0.41
1:B:110:ASN:OD1	1:B:134:GLY:HA2	2.19	0.41
1:E:62:ASP:O	1:E:86:LYS:HG2	2.21	0.41
1:E:277:THR:HG22	1:E:280:ARG:HA	2.02	0.41
1:A:100:ARG:HD2	1:A:107:ASN:O	2.21	0.41
1:D:44:ASP:HB3	1:D:50:ILE:HG22	2.03	0.41
1:A:122:THR:OG1	1:A:124:GLU:HG2	2.20	0.41
1:C:305:ALA:HB3	1:C:311:LYS:O	2.20	0.41
1:B:422:LYS:HG2	1:B:458:CYS:HB3	2.01	0.41
1:D:354:THR:HG22	1:D:354:THR:O	2.21	0.41
1:E:243:ILE:HD12	1:E:243:ILE:N	2.35	0.41
1:A:156:TYR:OH	1:A:159:SER:HB3	2.20	0.41
1:D:376:ASP:O	1:D:379:ALA:HB2	2.21	0.41
1:E:50:ILE:HG23	1:E:83:TYR:CZ	2.55	0.41
1:C:377:ASN:OD1	1:C:431:TYR:HA	2.21	0.41
1:A:53:HIS:N	1:A:53:HIS:CD2	2.88	0.41
1:F:161:ARG:HH22	1:F:177:MET:CG	2.34	0.41
1:A:108:HIS:CD2	1:A:135:ILE:HD11	2.56	0.41
1:E:87:ASP:O	1:E:88:LEU:HB2	2.20	0.41
1:A:384:TRP:CZ3	1:A:471:ASP:HB3	2.56	0.40
1:D:111:ILE:HA	1:D:130:HIS:O	2.21	0.40
1:A:360:VAL:HG22	1:A:367:VAL:CG1	2.48	0.40
1:A:287:ILE:HA	1:A:288:PRO:HD3	1.91	0.40
1:B:109:CYS:HB2	1:B:132:GLU:O	2.21	0.40
1:E:305:ALA:HA	1:E:308:TRP:CH2	2.56	0.40
1:B:50:ILE:HG23	1:B:83:TYR:CZ	2.56	0.40
1:B:305:ALA:HA	1:B:308:TRP:CH2	2.56	0.40
1:E:128:TRP:CZ3	1:E:144:VAL:HG22	2.56	0.40
1:F:291:GLY:HA3	1:F:344:SER:C	2.42	0.40
1:D:366:LYS:HB3	1:D:384:TRP:O	2.21	0.40
1:C:-13:SER:HA	1:C:492:LEU:CD1	2.51	0.40
1:B:420:GLU:HB3	1:B:457:HIS:CE1	2.56	0.40
1:E:126:VAL:HG21	1:E:212:TYR:HB2	2.03	0.40
1:E:354:THR:O	1:E:354:THR:HG22	2.21	0.40
1:C:115:LYS:HB3	1:C:183:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:VAL:HG11	1:A:405:LYS:HG3	2.03	0.40
1:C:206:TYR:HB3	1:C:215:ILE:HG23	2.03	0.40
1:E:375:VAL:HG12	1:E:411:SER:HB3	2.04	0.40
1:B:243:ILE:N	1:B:243:ILE:HD12	2.37	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%)	431 (94%)	28 (6%)	0	100	100
1	B	459/526 (87%)	432 (94%)	27 (6%)	0	100	100
1	C	480/526 (91%)	461 (96%)	19 (4%)	0	100	100
1	D	459/526 (87%)	431 (94%)	28 (6%)	0	100	100
1	E	459/526 (87%)	436 (95%)	22 (5%)	1 (0%)	52	88
1	F	459/526 (87%)	441 (96%)	18 (4%)	0	100	100
All	All	2775/3156 (88%)	2632 (95%)	142 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	390	LEU

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%)	388 (100%)	1 (0%)	94 98
1	B	389/442 (88%)	388 (100%)	1 (0%)	94 98
1	C	402/442 (91%)	401 (100%)	1 (0%)	95 99
1	D	389/442 (88%)	389 (100%)	0	100 100
1	E	389/442 (88%)	389 (100%)	0	100 100
1	F	389/442 (88%)	389 (100%)	0	100 100
All	All	2347/2652 (88%)	2344 (100%)	3 (0%)	95 99

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	180	ASP
1	C	427	VAL
1	A	287	ILE

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

Mol	Chain	Res	Type
1	B	171	HIS
1	B	430	GLN
1	B	487	HIS
1	C	107	ASN
1	C	198	ASN
1	C	457	HIS
1	D	164	GLN
1	D	377	ASN
1	D	383	GLN
1	D	392	GLN
1	D	430	GLN
1	D	457	HIS
1	E	53	HIS
1	E	75	ASN
1	E	171	HIS
1	E	269	GLN
1	E	457	HIS
1	F	171	HIS
1	A	53	HIS
1	A	226	GLN

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Mol	Chain	Res	Type
1	A	430	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

7 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	GAL	A	601	-	12,12,12	0.54	0	17,17,17	0.54	0
2	GAL	B	601	-	12,12,12	0.55	0	17,17,17	0.51	0
2	GAL	C	601	-	12,12,12	0.56	0	17,17,17	0.55	0
2	GAL	C	602	-	12,12,12	0.53	0	17,17,17	0.52	0
2	GAL	E	601	-	12,12,12	0.52	0	17,17,17	0.52	0
2	GAL	F	601	-	12,12,12	0.56	0	17,17,17	0.53	0
2	GAL	F	602	-	12,12,12	0.56	0	17,17,17	0.50	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	GAL	A	601	-	-	0/2/22/22	0/1/1/1
2	GAL	B	601	-	-	0/2/22/22	0/1/1/1
2	GAL	C	601	-	-	0/2/22/22	0/1/1/1
2	GAL	C	602	-	-	0/2/22/22	0/1/1/1
2	GAL	E	601	-	-	0/2/22/22	0/1/1/1
2	GAL	F	601	-	-	0/2/22/22	0/1/1/1
2	GAL	F	602	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	GAL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.20	7 (1%) 76 63	57, 86, 108, 120	0
1	B	461/526 (87%)	0.28	11 (2%) 62 47	66, 96, 121, 129	0
1	C	482/526 (91%)	0.08	1 (0%) 95 94	47, 66, 86, 125	0
1	D	461/526 (87%)	0.94	90 (19%) 1 1	58, 104, 174, 183	0
1	E	461/526 (87%)	0.20	11 (2%) 62 47	50, 73, 94, 111	0
1	F	461/526 (87%)	0.11	2 (0%) 93 90	45, 68, 88, 115	0
All	All	2787/3156 (88%)	0.30	122 (4%) 38 23	45, 80, 133, 183	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	490	LEU	10.0
1	D	448	ASP	8.5
1	D	394	TRP	7.3
1	D	383	GLN	7.2
1	D	359	LEU	6.2
1	D	491	VAL	5.9
1	D	382	VAL	5.7
1	D	450	TYR	5.7
1	D	443	PHE	5.6
1	D	444	THR	5.6
1	D	484	THR	5.5
1	D	374	SER	5.3
1	D	452	LYS	5.2
1	D	453	ILE	5.2
1	D	380	GLN	5.0
1	D	368	LEU	4.8
1	D	481	ALA	4.7
1	D	492	LEU	4.4
1	D	401	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	367	VAL	4.4
1	D	357	TYR	4.2
1	B	358	LYS	4.1
1	D	449	GLY	4.1
1	D	427	VAL	4.0
1	D	473	GLY	4.0
1	D	477	GLN	4.0
1	D	442	LYS	3.9
1	D	421	SER	3.9
1	D	360	VAL	3.8
1	D	396	LEU	3.8
1	D	405	LYS	3.8
1	D	440	HIS	3.7
1	D	445	ASP	3.7
1	A	396	LEU	3.7
1	D	466	LYS	3.7
1	D	402	GLY	3.7
1	D	474	ILE	3.7
1	D	461	LEU	3.6
1	E	390	LEU	3.6
1	D	369	ASP	3.6
1	D	488	TRP	3.6
1	D	462	ILE	3.5
1	D	423	GLU	3.5
1	D	406	ILE	3.4
1	D	471	ASP	3.4
1	B	443	PHE	3.3
1	D	392	GLN	3.3
1	D	451	TYR	3.2
1	D	447	GLY	3.2
1	E	368	LEU	3.2
1	D	428	LEU	3.1
1	D	436	GLY	3.1
1	D	441	TRP	3.1
1	D	486	GLN	3.1
1	D	358	LYS	3.1
1	D	422	LYS	3.0
1	D	458	CYS	3.0
1	D	482	GLY	3.0
1	B	339	LYS	3.0
1	B	388	GLY	2.9
1	D	472	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	383	GLN	2.9
1	E	394	TRP	2.8
1	D	400	GLY	2.8
1	D	381	ILE	2.8
1	D	480	ASP	2.7
1	D	467	TRP	2.7
1	D	463	ASP	2.7
1	D	454	SER	2.7
1	D	424	ASP	2.7
1	B	340	ILE	2.7
1	A	357	TYR	2.7
1	D	415	LEU	2.6
1	D	485	ASN	2.6
1	D	465	ARG	2.6
1	B	491	VAL	2.6
1	D	478	TRP	2.6
1	A	394	TRP	2.6
1	B	368	LEU	2.5
1	B	406	ILE	2.5
1	B	390	LEU	2.5
1	D	276	SER	2.5
1	D	363	ASN	2.5
1	E	358	LYS	2.5
1	D	356	ARG	2.4
1	D	456	ARG	2.4
1	D	407	VAL	2.4
1	A	359	LEU	2.4
1	D	364	SER	2.3
1	D	487	HIS	2.3
1	E	415	LEU	2.3
1	D	455	SER	2.3
1	D	468	SER	2.3
1	D	469	THR	2.3
1	E	331	GLU	2.3
1	A	491	VAL	2.3
1	D	339	LYS	2.3
1	B	387	ASN	2.3
1	D	431	TYR	2.3
1	D	361	ASN	2.2
1	D	437	TYR	2.2
1	D	397	VAL	2.2
1	E	382	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	393	GLN	2.2
1	E	367	VAL	2.2
1	B	359	LEU	2.2
1	D	459	GLY	2.2
1	D	414	ALA	2.2
1	D	362	LYS	2.2
1	D	460	LYS	2.2
1	D	464	VAL	2.1
1	F	388	GLY	2.1
1	A	351	ILE	2.1
1	D	384	TRP	2.1
1	F	342	ALA	2.1
1	E	463	ASP	2.1
1	D	446	ILE	2.1
1	A	407	VAL	2.1
1	D	430	GLN	2.0
1	D	35	VAL	2.0
1	C	-4	ARG	2.0
1	D	408	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	GAL	C	602	12/12	0.79	0.40	6.69	80,96,102,105	0
2	GAL	C	601	12/12	0.94	0.22	0.15	67,74,80,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	GAL	A	601	12/12	0.92	0.22	-0.23	64,68,72,83	0
2	GAL	E	601	12/12	0.91	0.21	-0.87	68,77,83,84	0
2	GAL	F	602	12/12	0.94	0.18	-0.88	62,66,71,73	0
2	GAL	B	601	12/12	0.94	0.17	-1.08	74,86,88,99	0
2	GAL	F	601	12/12	0.94	0.18	-1.32	57,69,75,75	0

6.5 Other polymers

There are no such residues in this entry.