Full wwPDB X-ray Structure Validation Report (i)

Mar 9, 2024 – 04:08 PM EST

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
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:

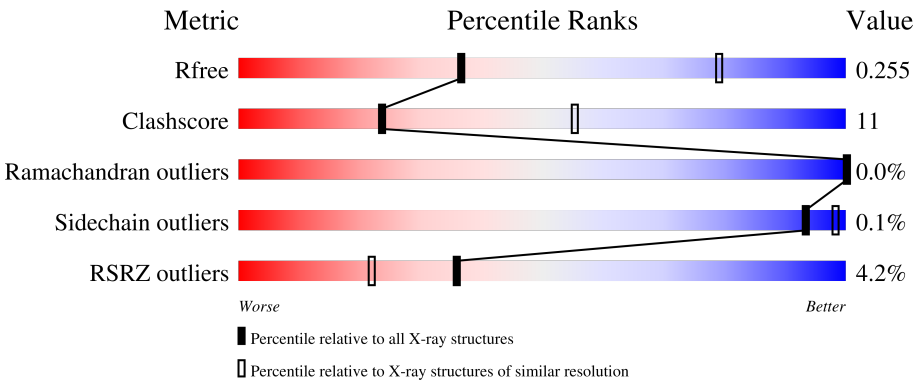
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 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}	130704	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)

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	.% 67% 21% 12%
1	B	526	2% 67% 20% 12%
1	C	526	73% 19% 8%
1	D	526	17% 61% 27% 12%
1	E	526	2% 67% 21% 12%

Continued on next page...

Continued from previous page...

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 (i)

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
			Total	C	N	O	S			
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
1	A	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
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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

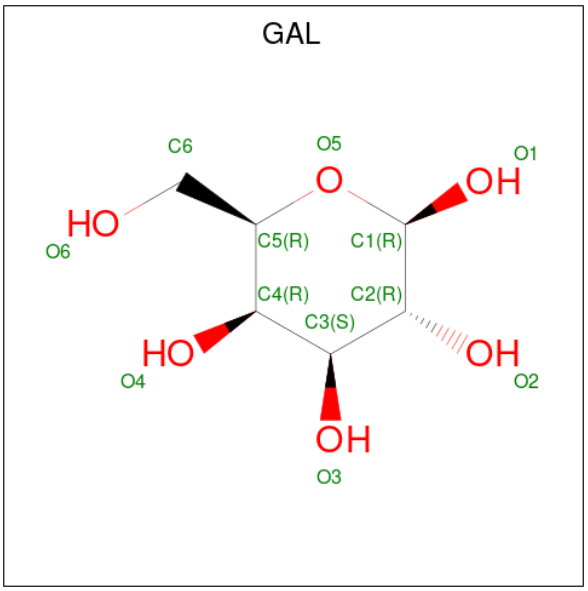
Chain	Residue	Modelled	Actual	Comment	Reference
E	0	PHE	-	expression tag	UNP A3DD67
F	-35	MET	-	expression tag	UNP A3DD67
F	-34	GLY	-	expression tag	UNP A3DD67
F	-33	SER	-	expression tag	UNP A3DD67
F	-32	SER	-	expression tag	UNP A3DD67
F	-31	HIS	-	expression tag	UNP A3DD67
F	-30	HIS	-	expression tag	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

Continued on next page...

Continued from previous page...

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 beta-D-galactopyranose (three-letter code: GAL) (formula: $C_6H_{12}O_6$).



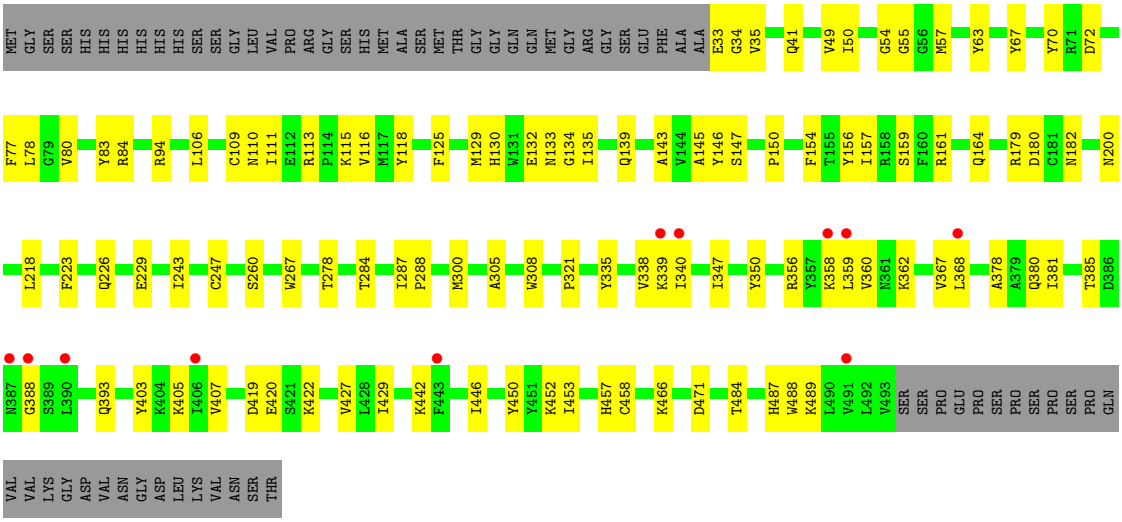
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	B	1	12	6	6	0	0
			Total	C	O		
2	C	1	12	6	6	0	0
			Total	C	O		
2	C	1	12	6	6	0	0
			Total	C	O		
2	E	1	12	6	6	0	0
			Total	C	O		
2	F	1	12	6	6	0	0
			Total	C	O		
2	F	1	12	6	6	0	0
			Total	C	O		
2	A	1	12	6	6	0	0

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.

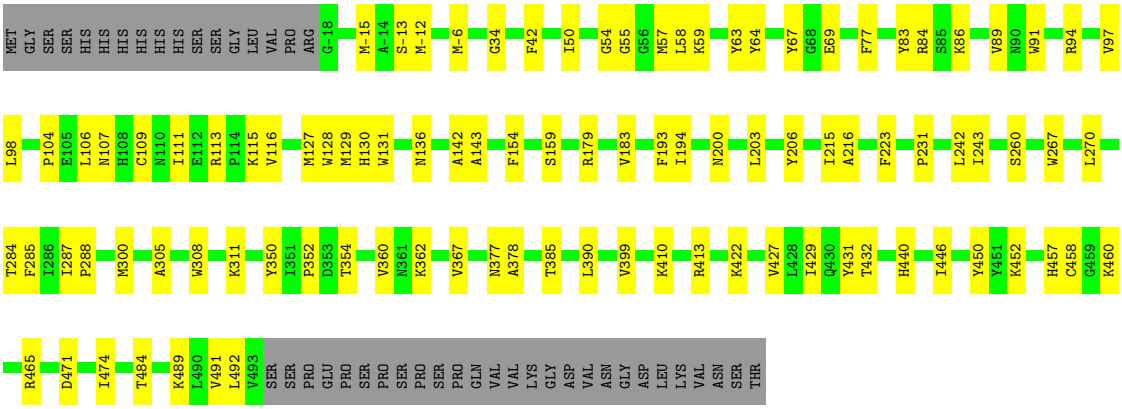
• Molecule 1: Ricin B lectin

Chain B:



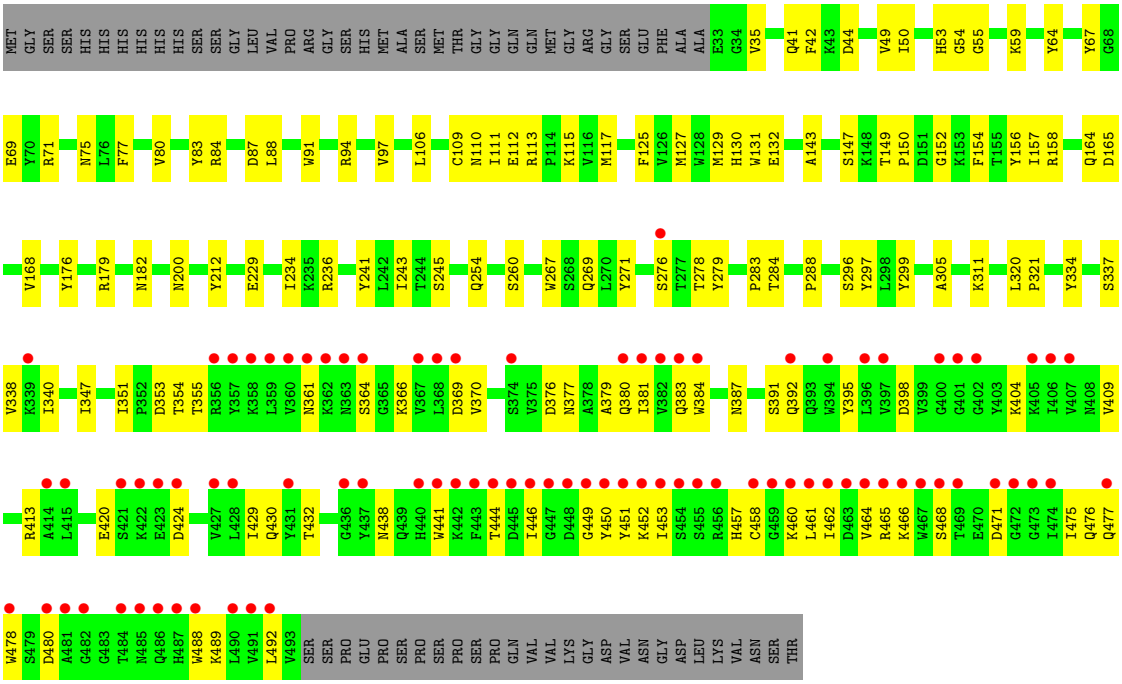
• Molecule 1: Ricin B lectin

Chain C:



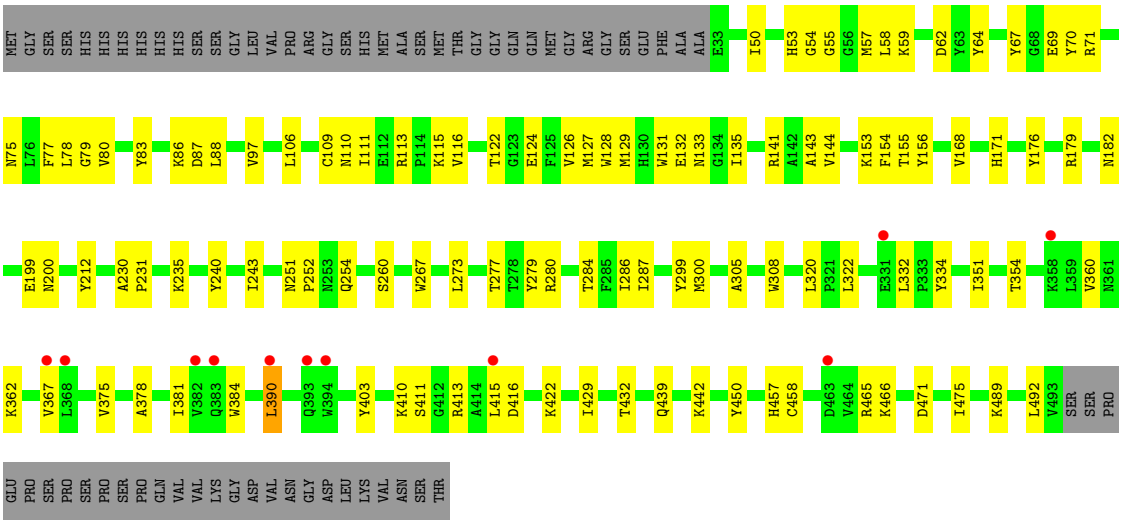
• Molecule 1: Ricin B lectin

Chain D:



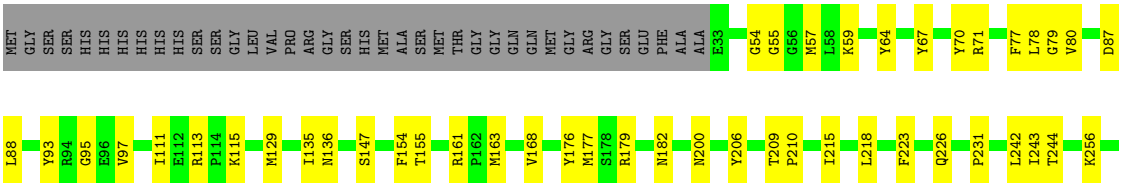
• Molecule 1: Ricin B lectin

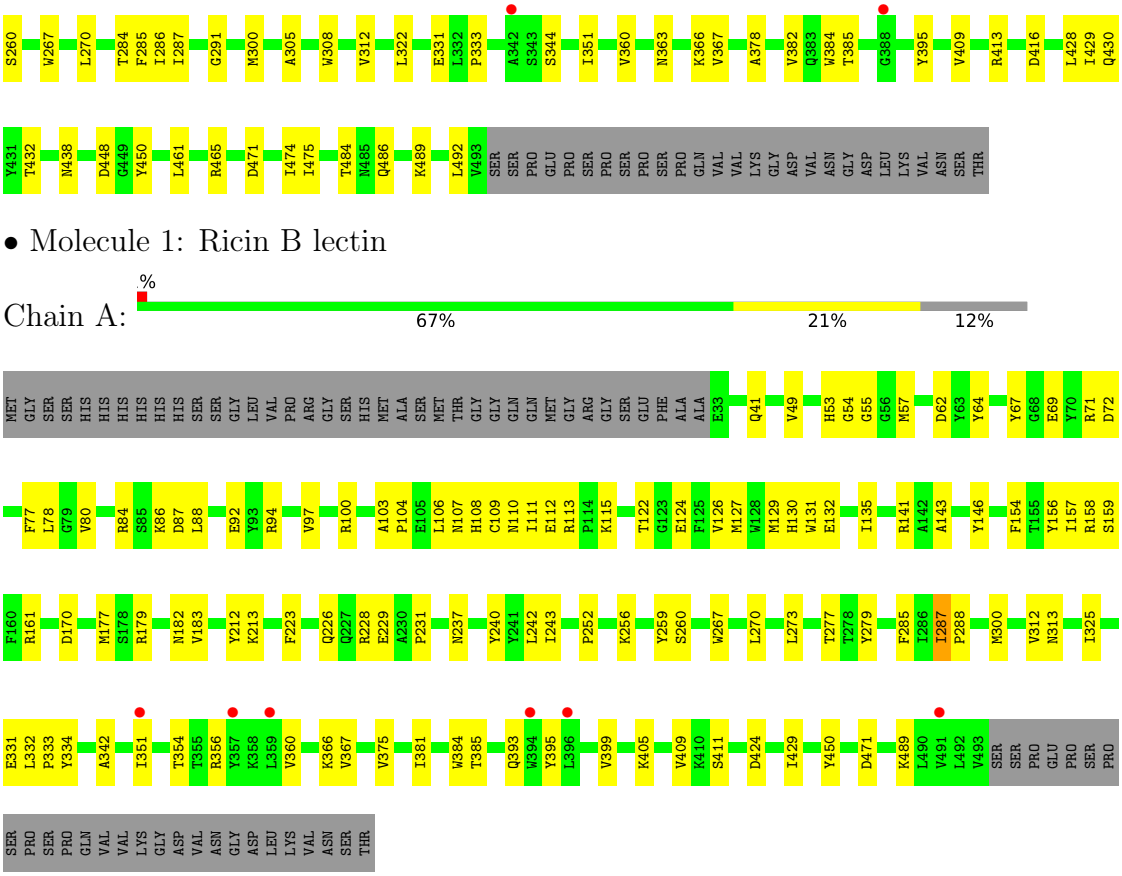
Chain E:



• Molecule 1: Ricin B lectin

Chain F:




S260 W267 L270 T284 F285 I286 I287 G291 M300 A305 W308 V312 L322 E331 L332 P333 A342 S343 S344 I351 V360 N363 K366 V367 A378 V382 Q383 W384 T385 G388 Y395 V409 R413 D416 L428 I429 Q430
Y431 T432 M438 D448 G449 Y450 L461 R465 D471 I474 I475 T484 N485 Q486 K489 L492 V493 SER SER PRO GLU PRO SER PRO SER PRO SER PRO GLN VAL VAL LYS GLY ASP VAL ASN GLY ASP LEU LYS VAL ASN SER THR
• Molecule 1: Ricin B lectin
Chain A:
%
67%
21%
12%
MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET ALA SER MET THR GLY GLY GLN GLN MET GLY ARG GLY SER GLU PHE ALA ALA E33 Q41 V49 H53 G54 G55 G56 M57 D62 Y63 Y64 Y67 G68 E69 Y70 R71 D72
F77 L78 G79 V80 R84 S85 K86 D87 L88 E92 Y93 R94 V97 R100 A103 P104 E105 L106 N107 H108 C109 N110 I111 E112 R113 P114 K115 T122 G123 E124 F125 V126 M127 W128 M129 H130 W131 E132 I135 R141 A142 A143 Y146 F154 T155 Y156 I157 R158 S159
F160 R161 D170 M177 S178 R179 N182 V183 Y212 K213 F223 Q226 Q227 R228 E229 A230 P231 N237 Y240 Y241 L242 I243 P252 K256 Y259 S260 W267 L270 L273 T277 T278 Y279 F285 I286 I287 P288 M300 V312 N313 I325
E331 L332 P333 Y334 A342 I351 T354 T355 R356 Y357 K358 L359 V360 K366 V367 V375 I381 W384 T385 Q393 W394 Y395 L396 V399 K405 V409 K410 S411 D424 I429 Y450 D471 K489 L490 V491 L492 V493 SER SER PRO GLU PRO SER PRO
SER PRO SER PRO GLN VAL VAL LYS GLY ASP VAL ASN GLY ASP LEU LYS VAL ASN SER THR

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 1.7_650	Depositor
R, R_{free}	0.235 , 0.270 0.222 , 0.255	Depositor DCC
R_{free} test set	1593 reflections (1.80%)	wwPDB-VP
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
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	0.91	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, 0.333 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: 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 (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	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

Continued on next page...

Continued from previous page...

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:B:133:ASN:HD22	1:B:139:GLN:HG2	1.52	0.74
1:C:260:SER:HB2	1:C:267:TRP:HA	1.69	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

Continued on next page...

Continued from previous page...

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:B:179:ARG:HG3	1:B:200:ASN:OD1	1.96	0.65
1:D:381:ILE:HG22	1:D:475:ILE:HG13	1.79	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:B:453:ILE:HD12	1:B:453:ILE:H	1.64	0.62
1:C:223:PHE:HE2	1:C:242:LEU:HD23	1.65	0.62

Continued on next page...

Continued from previous page...

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:D:260:SER:HB2	1:D:267:TRP:HA	1.81	0.62
1:E:77:PHE:CD1	1:E:111:ILE:HB	2.33	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:D:441:TRP:HZ3	1:D:477:GLN:HE22	1.50	0.58
1:F:223:PHE:HB3	1:F:226:GLN:HG3	1.86	0.58
1:A:100:ARG:HG2	1:A:107:ASN:HA	1.86	0.58
1:A:226:GLN:HE22	1:A:270:LEU:HD21	1.68	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:HD12	1:D:347:ILE:O	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

Continued on next page...

Continued from previous page...

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:77:PHE:CD1	1:D:111:ILE:HB	2.41	0.55
1:D:383:GLN:HE21	1:D:475:ILE:HD12	1.71	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:B:385:THR:HG23	1:B:471:ASP:OD1	2.06	0.55
1:D:157:ILE:HG22	1:D:158:ARG:HG2	1.88	0.55
1:F:223:PHE:CE2	1:F:242:LEU:HD23	2.41	0.55
1:B:55:GLY:HA3	1:B:67:TYR:O	2.07	0.55
1:B:362:LYS:HG3	1:B:484:THR:HB	1.88	0.55
1:D:97:VAL:HB	1:D:154:PHE:CD2	2.42	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: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:E:168:VAL:HG11	1:E:176:TYR:CE1	2.41	0.55
1:F:366:LYS:HE3	1:F:385:THR:HG22	1.89	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:E:260:SER:HB2	1:E:267:TRP:HA	1.90	0.54
1:F:428:LEU:HD12	1:F:475:ILE:HG22	1.90	0.54
1:C:55:GLY:HA3	1:C:67:TYR:O	2.07	0.54
1:C:458:CYS:SG	1:C:460:LYS:HG3	2.47	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:C:54:GLY:O	1:C:113:ARG:HA	2.08	0.53
1:F:135:ILE:HG22	1:F:136:ASN:HD22	1.73	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

Continued on next page...

Continued from previous page...

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:C:111:ILE:HD11	1:C:131:TRP:HD1	1.74	0.52
1:E:252:PRO:HB2	1:E:277:THR:CG2	2.39	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:N	1:B:157:ILE:HD12	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:E:279:TYR:CD2	1:E:334:TYR:HB2	2.44	0.52
1:F:59:LYS:HD3	1:F:64:TYR:CE1	2.45	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:379:ALA:HB3	1:D:430:GLN:HG2	1.93	0.51
1:D:383:GLN:HG3	1:D:475:ILE:CD1	2.24	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:B:70:TYR:CZ	1:B:78:LEU:HD11	2.45	0.51
1:C:-13:SER:HA	1:C:492:LEU:HD11	1.93	0.51
1:D:117:MET:HE3	1:D:212:TYR:HB3	1.93	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:E:115:LYS:HG3	1:E:182:ASN:OD1	2.11	0.50
1:F:135:ILE:HD12	1:F:135:ILE:N	2.27	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
1:A:223:PHE:CE2	1:A:242:LEU:HD23	2.47	0.50

Continued on next page...

Continued from previous page...

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:B:284:THR:HG22	1:B:300:MET:O	2.11	0.49
1:E:110:ASN:HB2	1:E:132:GLU:HB2	1.94	0.49
1:A:223:PHE:HB3	1:A:226:GLN:NE2	2.27	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:B:381:ILE:HG12	1:B:429:ILE:HA	1.94	0.49
1:E:284:THR:HG22	1:E:300:MET:O	2.13	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:F:363:ASN:HB2	1:F:484:THR:OG1	2.13	0.49
1:A:106:LEU:HA	1:A:109:CYS:SG	2.52	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:115:LYS:HE3	1:D:182:ASN:OD1	2.13	0.49
1:D:465:ARG:HD3	1:D:466:LYS:HE2	1.95	0.49
1:C:399:VAL:HG21	1:C:440:HIS:NE2	2.28	0.48
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:B:229:GLU:OE2	1:B:247:CYS:HB2	2.12	0.48
1:E:230:ALA:N	1:E:231:PRO:HD3	2.28	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:E:381:ILE:HD13	1:E:429:ILE:HA	1.95	0.48
1:B:33:GLU:HG2	1:B:35:VAL:HG12	1.95	0.48
1:B:84:ARG:HE	1:B:94:ARG:NE	1.96	0.48
1:C:98:LEU:HD22	1:C:127:MET:CE	2.42	0.48
1:D:420:GLU:HG2	1:D:438:ASN:ND2	2.28	0.48
1:F:284:THR:HG22	1:F:300:MET:O	2.13	0.48
1:F:395:TYR:CE2	1:F:409:VAL:HG22	2.49	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:B:106:LEU:HD22	1:B:111:ILE:HD11	1.95	0.48
1:F:413:ARG:NH1	1:F:432:THR:HG22	2.29	0.48
1:A:106:LEU:HD11	1:A:156:TYR:CD2	2.49	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:F:416:ASP:OD2	1:F:438:ASN:ND2	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:VAL:HB	1:A:154:PHE:CD2	2.48	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:B:125:PHE:CE2	1:B:150:PRO:HD3	2.49	0.48
1:A:146:TYR:CD2	1:A:157:ILE:HD11	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:C:446:ILE:HG21	1:C:452:LYS:HG3	1.97	0.47
1:D:54:GLY:O	1:D:113:ARG:HA	2.14	0.47
1:D:381:ILE:HG12	1:D:429:ILE:HA	1.96	0.47
1:A:54:GLY:O	1:A:113:ARG:HA	2.14	0.47
1:C:69:GLU:HG3	1:C:111:ILE:O	2.14	0.47
1:E:129:MET:CG	1:E:143:ALA:HB3	2.45	0.47
1:F:385:THR:HG23	1:F:471:ASP:OD1	2.14	0.47
1:A:385:THR:HG23	1:A:471:ASP:OD1	2.15	0.47
1:A:170:ASP:OD1	1:A:177:MET:HG3	2.14	0.47
1:B:335:TYR:HB2	1:B:338:VAL:HG22	1.97	0.47
1:E:80:VAL:HG21	1:E:127:MET:HE1	1.96	0.47
1:B:106:LEU:HD11	1:B:156:TYR:CD2	2.50	0.47
1:B:378:ALA:HA	1:B:429:ILE:HD12	1.97	0.47
1:C:-6:MET:HE1	1:F:155:THR:HG21	1.94	0.47
1:D:41:GLN:HB3	1:D:49:VAL:HG13	1.97	0.47
1:D:299:TYR:HB3	1:D:320:LEU:O	2.14	0.47
1:F:285:PHE:HE2	1:F:287:ILE:HB	1.80	0.47
1:A:161:ARG:NH2	1:A:177:MET:HG2	2.29	0.47
1:B:358:LYS:HZ1	1:B:388:GLY:HA2	1.79	0.47
1:C:385:THR:HG23	1:C:471:ASP:OD1	2.14	0.47
1:D:279:TYR:CD2	1:D:334:TYR:HB2	2.50	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:F:331:GLU:HG2	1:F:333:PRO:HD3	1.97	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:B:41:GLN:HB3	1:B:49:VAL:HG23	1.96	0.47
1:B:78:LEU:C	1:B:78:LEU:HD12	2.35	0.47
1:C:42:PHE:CE2	1:C:50:ILE:HD12	2.50	0.47
1:D:370:VAL:H	1:D:391:SER:HB3	1.80	0.47
1:A:129:MET:CG	1:A:143:ALA:HB3	2.45	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:492:LEU:H	1:D:492:LEU:HD12	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:HG13	1:D:464:VAL:O	2.15	0.46
1:F:209:THR:HB	1:F:210:PRO:HD2	1.98	0.46
1:D:353:ASP:OD1	1:D:355:THR:HG23	2.15	0.46
1:A:130:HIS:CD2	1:A:179:ARG:HA	2.51	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:106:LEU:HA	1:D:109:CYS:SG	2.56	0.46
1:D:296:SER:HB3	1:D:347:ILE:HD11	1.96	0.46
1:E:351:ILE:N	1:E:351:ILE:HD12	2.29	0.46
1:A:41:GLN:HB3	1:A:49:VAL:HG23	1.96	0.46
1:B:287:ILE:HA	1:B:288:PRO:HD3	1.85	0.46
1:D:446:ILE:HG13	1:D:450:TYR:O	2.15	0.46
1:A:64:TYR:CD2	1:A:88:LEU:HD11	2.51	0.46
1:B:130:HIS:CE1	1:B:179:ARG:HA	2.52	0.45
1:C:285:PHE:HE2	1:C:287:ILE:HB	1.81	0.45
1:D:87:ASP:O	1:D:88:LEU:HB2	2.16	0.45
1:E:70:TYR:O	1:E:78:LEU:HB3	2.16	0.45
1:A:77:PHE:CZ	1:A:80:VAL:HG23	2.51	0.45
1:A:111:ILE:HD11	1:A:131:TRP:HD1	1.81	0.45
1:A:273:LEU:HD21	1:A:332:LEU:CB	2.46	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:F:465:ARG:HE	1:F:474:ILE:HG21	1.81	0.45
1:C:130:HIS:CE1	1:C:179:ARG:HA	2.52	0.45
1:E:465:ARG:HG2	1:E:466:LYS:HG2	1.98	0.45
1:A:351:ILE:HD12	1:A:351:ILE:N	2.32	0.45
1:C:179:ARG:HG3	1:C:200:ASN:OD1	2.17	0.45
1:C:354:THR:HG22	1:C:354:THR:O	2.15	0.45
1:D:449:GLY:CA	1:D:489:LYS:HD2	2.46	0.45
1:B:115:LYS:HG3	1:B:182:ASN:HA	1.97	0.45
1:C:63:TYR:CE1	1:C:84:ARG:NH1	2.85	0.45
1:B:72:ASP:HA	1:B:78:LEU:HD23	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:PHE:CD1	1:C:270:LEU:HD11	2.51	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:-15:MET:HE3	1:E:153:LYS:HE2	1.99	0.45
1:C:287:ILE:HA	1:C:288:PRO:HD3	1.83	0.45
1:E:133:ASN:OD1	1:E:135:ILE:HG13	2.17	0.45
1:F:382:VAL:HA	1:F:475:ILE:HG12	1.99	0.45
1:D:129:MET:CG	1:D:143:ALA:HB3	2.47	0.45
1:D:398:ASP:HB2	1:D:404:LYS:HZ2	1.81	0.45
1:F:55:GLY:HA3	1:F:67:TYR:O	2.17	0.45
1:B:50:ILE:HG23	1:B:83:TYR:CE1	2.52	0.44
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:C:64:TYR:O	1:C:84:ARG:HA	2.17	0.44
1:C:284:THR:HG22	1:C:300:MET:O	2.17	0.44
1:D:384:TRP:CZ3	1:D:471:ASP:HB3	2.52	0.44
1:D:451:TYR:CD2	1:D:489:LYS:HG3	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:B:466:LYS:HE2	1:B:466:LYS:HA	1.98	0.44
1:E:55:GLY:HA3	1:E:67:TYR:O	2.18	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:C:378:ALA:HA	1:C:429:ILE:HD12	2.00	0.44
1:E:50:ILE:HG23	1:E:83:TYR:CE1	2.52	0.44
1:F:256:LYS:HD3	1:F:270:LEU:HB3	2.00	0.44
1:B:358:LYS:HZ3	1:B:388:GLY:HA2	1.82	0.44
1:C:42:PHE:CE2	1:C:91:TRP:CD1	3.05	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:D:35:VAL:HG21	1:D:337:SER:HB3	1.98	0.44
1:D:243:ILE:N	1:D:243:ILE:HD12	2.32	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: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:F:163:MET:HE2	1:F:218:LEU:N	2.33	0.44
1:A:243:ILE:N	1:A:243:ILE:HD12	2.33	0.44
1:B:403:TYR:CD1	1:B:442:LYS:HB2	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:269:GLN:HG3	1:D:271:TYR:CE1	2.52	0.44
1:D:361:ASN:HB3	1:D:364:SER:OG	2.18	0.44
1:B:356:ARG:HD3	1:B:393:GLN:HE22	1.80	0.43
1:C:194:ILE:HD11	1:C:203:LEU:HD23	2.00	0.43
1:D:377:ASN:HD21	1:D:432:THR:H	1.66	0.43
1:D:383:GLN:HE21	1:D:475:ILE:CD1	2.31	0.43
1:F:243:ILE:N	1:F:243:ILE:HD12	2.32	0.43
1:F:461:LEU:CD1	1:F:486:GLN:HB3	2.40	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:C	1:D:429:ILE:HD12	2.38	0.43
1:E:378:ALA:HA	1:E:429:ILE:HD12	1.99	0.43
1:B:156:TYR:OH	1:B:159:SER:HB3	2.18	0.43
1:B:362:LYS:CG	1:B:484:THR:HB	2.48	0.43
1:B:446:ILE:HD13	1:B:452:LYS:HG3	1.99	0.43
1:C:270:LEU:HD12	1:C:270:LEU:N	2.33	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: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:E:109:CYS:HB2	1:E:132:GLU:O	2.18	0.43
1:A:279:TYR:CE2	1:A:334:TYR:HB2	2.53	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:E:403:TYR:CE1	1:E:442:LYS:HB2	2.54	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:B:305:ALA:HA	1:B:308:TRP:CZ2	2.54	0.43
1:D:351:ILE:N	1:D:351:ILE:HD12	2.34	0.43
1:D:395:TYR:CZ	1:D:409:VAL:HG22	2.54	0.43
1:E:111:ILE:HD11	1:E:131:TRP:CD1	2.47	0.43
1:C:58:LEU:HD22	1:C:116:VAL:HG12	2.01	0.43
1:C:243:ILE:N	1:C:243:ILE:HD12	2.34	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:F:115:LYS:HG3	1:F:182:ASN:HA	2.00	0.43
1:A:57:MET:CB	1:A:300:MET:HE1	2.48	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:D:278:THR:HG22	1:D:278:THR:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:GLN:NE2	1:A:270:LEU:HD21	2.32	0.42
1:E:59:LYS:HD3	1:E:64:TYR:CE1	2.54	0.42
1:F:59:LYS:HD3	1:F:64:TYR:CD1	2.54	0.42
1:B:359:LEU:HD12	1:B:368:LEU:HD22	2.02	0.42
1:B:450:TYR:CE1	1:B:489:LYS:HB2	2.54	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:E:254:GLN:NE2	1:E:273:LEU:H	2.17	0.42
1:E:286:ILE:HD13	1:E:322:LEU:HD22	2.02	0.42
1:E:384:TRP:CE3	1:E:471:ASP:HB3	2.54	0.42
1:A:270:LEU:N	1:A:270:LEU:HD22	2.35	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:E:57:MET:CE	1:E:287:ILE:HD13	2.49	0.42
1:C:106:LEU:HA	1:C:109:CYS:SG	2.59	0.42
1:A:115:LYS:HB3	1:A:183:VAL:HG22	2.02	0.42
1:C:491:VAL:HG12	1:C:492:LEU:O	2.20	0.42
1:D:458:CYS:SG	1:D:460:LYS:HE3	2.60	0.42
1:F:57:MET:CE	1:F:287:ILE:HG21	2.50	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:D:97:VAL:HB	1:D:154:PHE:HD2	1.84	0.41
1:A:87:ASP:O	1:A:88:LEU:HB2	2.20	0.41
1:A:135:ILE:HD12	1:A:135:ILE:N	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:B:278:THR:HG22	1:B:278:THR:O	2.21	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:A:103:ALA:HB1	1:A:104:PRO:HD2	2.01	0.41
1:B:321:PRO:HB3	1:B:347:ILE:CG2	2.50	0.41
1:B:419:ASP:OD1	2:B:601:GAL:H62	2.20	0.41
1:C:128:TRP:HB3	1:C:193:PHE:CE1	2.56	0.41
1:D:288:PRO:HB3	1:D:297:TYR:CE1	2.56	0.41

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:TYR:HB3	1:C:215:ILE:HG23	2.03	0.40
1:A:399:VAL:HG11	1:A:405:LYS:HG3	2.03	0.40
1:B:243:ILE:N	1:B:243:ILE:HD12	2.37	0.40
1:E:375:VAL:HG12	1:E:411:SER:HB3	2.04	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%)	47	78
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%)	92 97
1	B	389/442 (88%)	388 (100%)	1 (0%)	92 97
1	C	402/442 (91%)	401 (100%)	1 (0%)	93 98
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%)	93 98

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

Sometimes 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	430	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	F	601	-	12,12,12	0.55	0	17,17,17	0.55	0
2	GAL	A	601	-	12,12,12	0.54	0	17,17,17	0.56	0
2	GAL	C	602	-	12,12,12	0.53	0	17,17,17	0.55	0
2	GAL	C	601	-	12,12,12	0.55	0	17,17,17	0.58	0
2	GAL	B	601	-	12,12,12	0.54	0	17,17,17	0.53	0
2	GAL	F	602	-	12,12,12	0.55	0	17,17,17	0.52	0
2	GAL	E	601	-	12,12,12	0.52	0	17,17,17	0.53	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	F	601	-	-	0/2/22/22	0/1/1/1
2	GAL	A	601	-	-	1/2/22/22	0/1/1/1
2	GAL	C	602	-	-	0/2/22/22	0/1/1/1
2	GAL	C	601	-	-	1/2/22/22	0/1/1/1
2	GAL	B	601	-	-	1/2/22/22	0/1/1/1
2	GAL	F	602	-	-	0/2/22/22	0/1/1/1
2	GAL	E	601	-	-	1/2/22/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GAL	O5-C5-C6-O6
2	E	601	GAL	O5-C5-C6-O6
2	C	601	GAL	O5-C5-C6-O6
2	B	601	GAL	O5-C5-C6-O6

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 (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%)	0.18	6 (1%) 77 65	57, 86, 108, 120	0
1	B	461/526 (87%)	0.25	11 (2%) 59 44	66, 96, 121, 129	0
1	C	482/526 (91%)	0.05	0 100 100	47, 66, 86, 125	0
1	D	461/526 (87%)	0.90	87 (18%) 1 0	58, 104, 174, 183	0
1	E	461/526 (87%)	0.17	11 (2%) 59 44	50, 73, 94, 111	0
1	F	461/526 (87%)	0.09	2 (0%) 92 89	45, 68, 88, 115	0
All	All	2787/3156 (88%)	0.27	117 (4%) 36 22	45, 80, 133, 183	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	490	LEU	9.7
1	D	448	ASP	8.3
1	D	394	TRP	7.1
1	D	383	GLN	7.0
1	D	359	LEU	6.1
1	D	491	VAL	5.7
1	D	382	VAL	5.6
1	D	450	TYR	5.5
1	D	443	PHE	5.5
1	D	444	THR	5.4
1	D	484	THR	5.4
1	D	374	SER	5.1
1	D	453	ILE	5.0
1	D	452	LYS	5.0
1	D	380	GLN	4.9
1	D	368	LEU	4.7
1	D	481	ALA	4.6
1	D	401	GLY	4.3
1	D	492	LEU	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	367	VAL	4.3
1	D	357	TYR	4.0
1	B	358	LYS	4.0
1	D	449	GLY	4.0
1	D	427	VAL	3.9
1	D	477	GLN	3.9
1	D	473	GLY	3.9
1	D	442	LYS	3.8
1	D	421	SER	3.8
1	D	360	VAL	3.7
1	D	396	LEU	3.7
1	D	440	HIS	3.7
1	D	405	LYS	3.7
1	D	445	ASP	3.6
1	A	396	LEU	3.6
1	D	402	GLY	3.6
1	D	466	LYS	3.6
1	D	474	ILE	3.6
1	E	390	LEU	3.5
1	D	369	ASP	3.5
1	D	461	LEU	3.5
1	D	488	TRP	3.5
1	D	462	ILE	3.4
1	D	423	GLU	3.4
1	D	406	ILE	3.3
1	D	471	ASP	3.3
1	D	392	GLN	3.2
1	B	443	PHE	3.2
1	D	447	GLY	3.1
1	E	368	LEU	3.1
1	D	451	TYR	3.0
1	D	486	GLN	3.0
1	D	436	GLY	3.0
1	D	428	LEU	3.0
1	D	441	TRP	3.0
1	D	358	LYS	3.0
1	D	422	LYS	2.9
1	D	458	CYS	2.9
1	D	482	GLY	2.9
1	B	339	LYS	2.9
1	B	388	GLY	2.9
1	E	383	GLN	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	472	GLY	2.8
1	D	381	ILE	2.7
1	E	394	TRP	2.7
1	D	400	GLY	2.7
1	D	480	ASP	2.7
1	D	463	ASP	2.6
1	B	340	ILE	2.6
1	D	467	TRP	2.6
1	D	454	SER	2.6
1	D	424	ASP	2.6
1	D	485	ASN	2.6
1	D	415	LEU	2.5
1	A	357	TYR	2.5
1	D	465	ARG	2.5
1	B	491	VAL	2.5
1	D	478	TRP	2.5
1	A	394	TRP	2.5
1	B	406	ILE	2.5
1	B	368	LEU	2.4
1	B	390	LEU	2.4
1	D	363	ASN	2.4
1	D	276	SER	2.4
1	E	358	LYS	2.4
1	D	356	ARG	2.3
1	D	456	ARG	2.3
1	A	359	LEU	2.3
1	D	407	VAL	2.3
1	D	487	HIS	2.3
1	D	364	SER	2.3
1	E	415	LEU	2.2
1	D	455	SER	2.2
1	A	491	VAL	2.2
1	E	331	GLU	2.2
1	B	387	ASN	2.2
1	D	468	SER	2.2
1	D	469	THR	2.2
1	D	339	LYS	2.2
1	D	361	ASN	2.2
1	E	393	GLN	2.1
1	E	382	VAL	2.1
1	D	397	VAL	2.1
1	D	437	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	431	TYR	2.1
1	E	367	VAL	2.1
1	B	359	LEU	2.1
1	D	459	GLY	2.1
1	D	362	LYS	2.1
1	D	464	VAL	2.1
1	D	414	ALA	2.1
1	D	460	LYS	2.1
1	A	351	ILE	2.1
1	F	388	GLY	2.0
1	D	446	ILE	2.0
1	D	384	TRP	2.0
1	E	463	ASP	2.0
1	F	342	ALA	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	GAL	C	602	12/12	0.79	0.40	80,96,102,105	0
2	GAL	E	601	12/12	0.91	0.21	68,77,83,84	0
2	GAL	A	601	12/12	0.92	0.22	64,68,72,83	0
2	GAL	C	601	12/12	0.94	0.23	67,74,80,90	0
2	GAL	F	601	12/12	0.94	0.18	57,69,75,75	0
2	GAL	F	602	12/12	0.94	0.18	62,66,71,73	0
2	GAL	B	601	12/12	0.94	0.16	74,86,88,99	0

6.5 Other polymers (i)

There are no such residues in this entry.