



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2017 – 03:44 PM EST

PDB ID : 4V6H  
Title : Crystal structure of succinate-semialdehyde dehydrogenase from Burkholderia pseudomallei  
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : unknown  
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

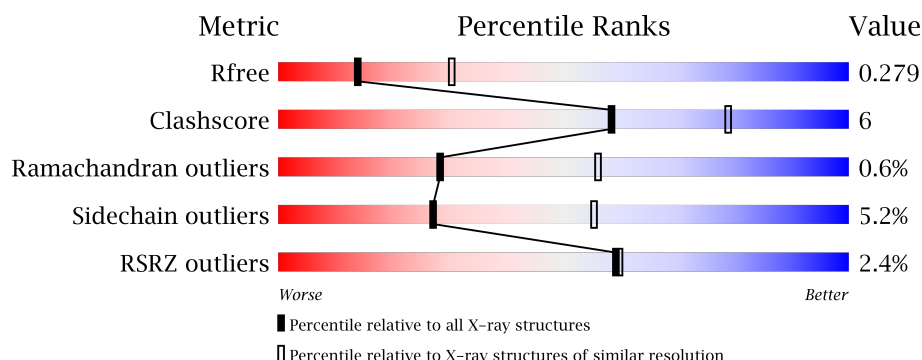
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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.













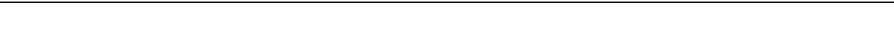

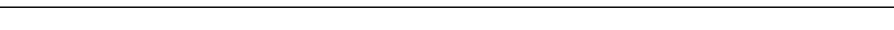
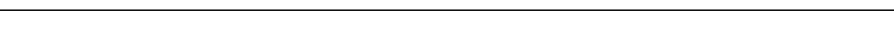











Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	1	484	<div> <div>11%</div> <div>79%</div> <div>19%</div> <div>.</div> </div>
1	2	484	<div> <div>%</div> <div>79%</div> <div>20%</div> <div>.</div> </div>
1	3	484	<div> <div>%</div> <div>82%</div> <div>17%</div> <div>.</div> </div>
1	4	484	<div> <div>%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>
1	5	484	<div> <div>%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	6	484	 89% 11%
1	A	484	 87% 11% .
1	B	484	 89% 10% .
1	C	484	 85% 13% .
1	D	484	 84% 15% .
1	E	484	 85% 13% .
1	F	484	 87% 11% .
1	G	484	 86% 12% .
1	H	484	 86% 13% .
1	I	484	 6% 80% 18% .
1	J	484	 83% 15% .
1	K	484	 % 88% 11% .
1	L	484	 86% 12% .
1	M	484	 83% 14% .
1	N	484	 87% 12% .
1	O	484	 87% 12% .
1	P	484	 87% 12% .
1	Q	484	 4% 83% 16% .
1	R	484	 3% 85% 13% .
1	S	484	 87% 12% .
1	T	484	 4% 82% 16% .
1	U	484	 12% 78% 20% .
1	V	484	 5% 82% 16% .
1	W	484	 88% 11%
1	X	484	 11% 78% 20% .

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Y	484	<div><div></div><div>3%</div><div>78%</div><div>20%</div><div></div></div>
1	Z	484	<div><div></div><div>11%</div><div>75%</div><div>24%</div><div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 114732 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 Succinate-semialdehyde dehydrogenase (NADP+).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3549	2259	607	669	14			
1	B	482	Total	C	N	O	S	0	0	0
			3553	2261	607	671	14			
1	C	482	Total	C	N	O	S	0	0	0
			3549	2259	607	669	14			
1	D	482	Total	C	N	O	S	0	0	0
			3549	2259	607	669	14			
1	E	482	Total	C	N	O	S	0	0	0
			3549	2259	607	669	14			
1	F	482	Total	C	N	O	S	0	0	0
			3549	2259	607	669	14			
1	G	482	Total	C	N	O	S	0	0	0
			3549	2259	607	669	14			
1	H	482	Total	C	N	O	S	0	0	0
			3549	2259	607	669	14			
1	I	482	Total	C	N	O	S	0	0	0
			3520	2242	597	667	14			
1	J	482	Total	C	N	O	S	0	0	0
			3549	2259	607	669	14			
1	K	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	L	482	Total	C	N	O	S	0	0	0
			3543	2255	607	667	14			
1	M	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	N	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	O	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	P	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	R	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	S	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	T	482	Total	C	N	O	S	0	0	0
			3535	2248	606	667	14			
1	U	482	Total	C	N	O	S	0	0	0
			3521	2241	601	665	14			
1	V	482	Total	C	N	O	S	0	0	0
			3532	2248	603	667	14			
1	W	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	X	482	Total	C	N	O	S	0	0	0
			3515	2235	603	663	14			
1	Y	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	Z	482	Total	C	N	O	S	0	0	0
			3532	2248	603	667	14			
1	1	482	Total	C	N	O	S	0	0	0
			3510	2235	595	666	14			
1	2	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	3	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	4	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	5	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			
1	6	482	Total	C	N	O	S	0	0	0
			3545	2257	607	667	14			

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
A	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
A	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
A	4	SER	-	EXPRESSION TAG	UNP Q3JS51
B	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
B	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
B	3	GLY	-	EXPRESSION TAG	UNP Q3JS51

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	4	SER	-	EXPRESSION TAG	UNP Q3JS51
C	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
C	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
C	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
C	4	SER	-	EXPRESSION TAG	UNP Q3JS51
D	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
D	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
D	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
D	4	SER	-	EXPRESSION TAG	UNP Q3JS51
E	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
E	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
E	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
E	4	SER	-	EXPRESSION TAG	UNP Q3JS51
F	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
F	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
F	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
F	4	SER	-	EXPRESSION TAG	UNP Q3JS51
G	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
G	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
G	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
G	4	SER	-	EXPRESSION TAG	UNP Q3JS51
H	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
H	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
H	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
H	4	SER	-	EXPRESSION TAG	UNP Q3JS51
I	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
I	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
I	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
I	4	SER	-	EXPRESSION TAG	UNP Q3JS51
J	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
J	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
J	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
J	4	SER	-	EXPRESSION TAG	UNP Q3JS51
K	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
K	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
K	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
K	4	SER	-	EXPRESSION TAG	UNP Q3JS51
L	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
L	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
L	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
L	4	SER	-	EXPRESSION TAG	UNP Q3JS51
M	1	GLY	-	EXPRESSION TAG	UNP Q3JS51

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
M	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
M	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
M	4	SER	-	EXPRESSION TAG	UNP Q3JS51
N	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
N	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
N	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
N	4	SER	-	EXPRESSION TAG	UNP Q3JS51
O	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
O	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
O	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
O	4	SER	-	EXPRESSION TAG	UNP Q3JS51
P	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
P	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
P	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
P	4	SER	-	EXPRESSION TAG	UNP Q3JS51
Q	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
Q	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
Q	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
Q	4	SER	-	EXPRESSION TAG	UNP Q3JS51
R	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
R	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
R	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
R	4	SER	-	EXPRESSION TAG	UNP Q3JS51
S	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
S	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
S	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
S	4	SER	-	EXPRESSION TAG	UNP Q3JS51
T	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
T	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
T	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
T	4	SER	-	EXPRESSION TAG	UNP Q3JS51
U	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
U	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
U	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
U	4	SER	-	EXPRESSION TAG	UNP Q3JS51
V	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
V	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
V	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
V	4	SER	-	EXPRESSION TAG	UNP Q3JS51
W	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
W	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
W	3	GLY	-	EXPRESSION TAG	UNP Q3JS51

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
W	4	SER	-	EXPRESSION TAG	UNP Q3JS51
X	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
X	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
X	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
X	4	SER	-	EXPRESSION TAG	UNP Q3JS51
Y	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
Y	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
Y	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
Y	4	SER	-	EXPRESSION TAG	UNP Q3JS51
Z	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
Z	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
Z	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
Z	4	SER	-	EXPRESSION TAG	UNP Q3JS51
1	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
1	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
1	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
1	4	SER	-	EXPRESSION TAG	UNP Q3JS51
2	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
2	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
2	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
2	4	SER	-	EXPRESSION TAG	UNP Q3JS51
3	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
3	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
3	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
3	4	SER	-	EXPRESSION TAG	UNP Q3JS51
4	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
4	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
4	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
4	4	SER	-	EXPRESSION TAG	UNP Q3JS51
5	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
5	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
5	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
5	4	SER	-	EXPRESSION TAG	UNP Q3JS51
6	1	GLY	-	EXPRESSION TAG	UNP Q3JS51
6	2	PRO	-	EXPRESSION TAG	UNP Q3JS51
6	3	GLY	-	EXPRESSION TAG	UNP Q3JS51
6	4	SER	-	EXPRESSION TAG	UNP Q3JS51

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	46	Total O 46 46	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	59	Total O 59 59	0	0
2	C	56	Total O 56 56	0	0
2	D	60	Total O 60 60	0	0
2	E	72	Total O 72 72	0	0
2	F	75	Total O 75 75	0	0
2	G	66	Total O 66 66	0	0
2	H	58	Total O 58 58	0	0
2	I	24	Total O 24 24	0	0
2	J	35	Total O 35 35	0	0
2	K	55	Total O 55 55	0	0
2	L	57	Total O 57 57	0	0
2	M	40	Total O 40 40	0	0
2	N	46	Total O 46 46	0	0
2	O	39	Total O 39 39	0	0
2	P	74	Total O 74 74	0	0
2	Q	22	Total O 22 22	0	0
2	R	35	Total O 35 35	0	0
2	S	55	Total O 55 55	0	0
2	T	13	Total O 13 13	0	0
2	U	13	Total O 13 13	0	0
2	V	29	Total O 29 29	0	0

*Continued on next page...*

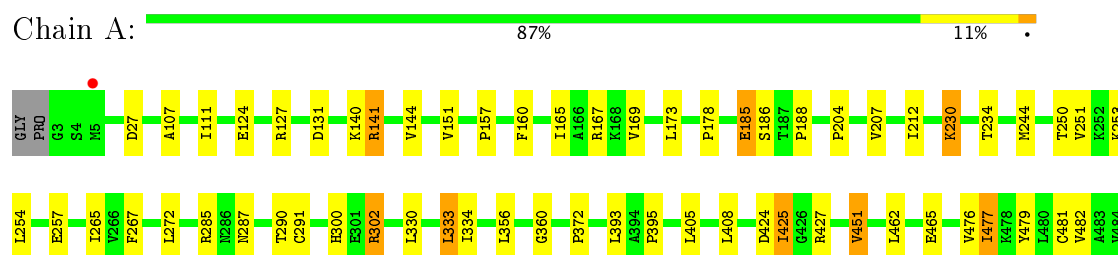
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	W	44	Total 44	O 44	0	0
2	X	8	Total 8	O 8	0	0
2	Y	36	Total 36	O 36	0	0
2	Z	20	Total 20	O 20	0	0
2	1	28	Total 28	O 28	0	0
2	2	37	Total 37	O 37	0	0
2	3	45	Total 45	O 45	0	0
2	4	46	Total 46	O 46	0	0
2	5	54	Total 54	O 54	0	0
2	6	57	Total 57	O 57	0	0

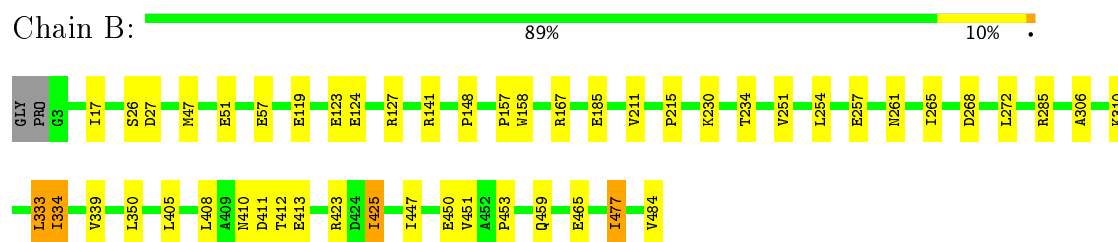
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

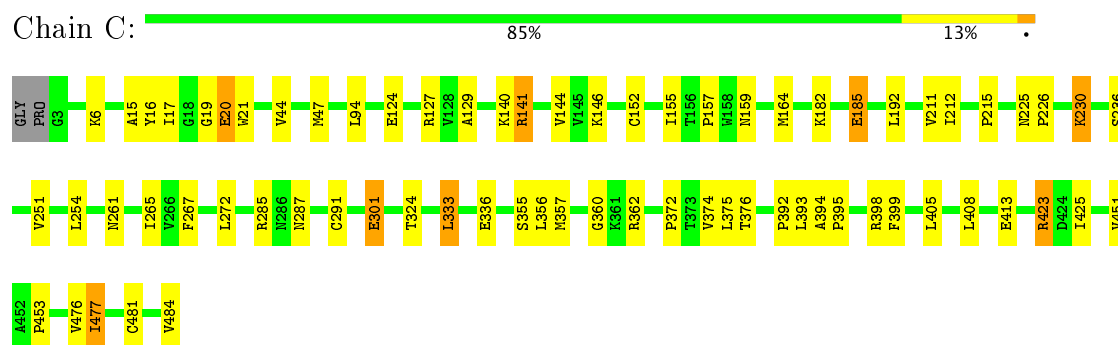
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



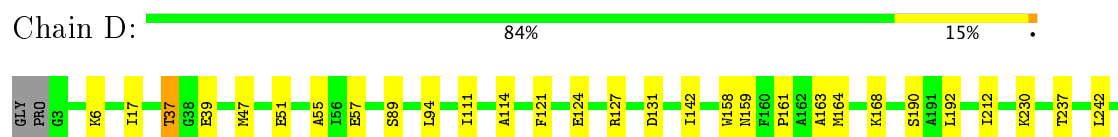
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

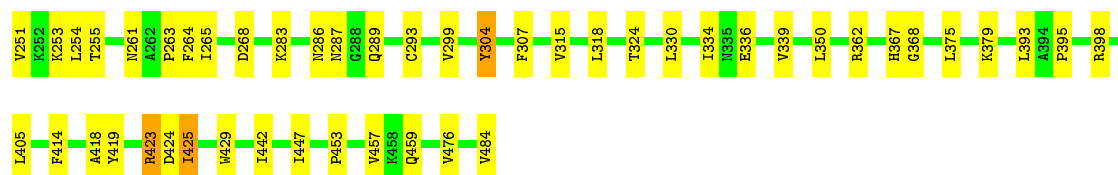


- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



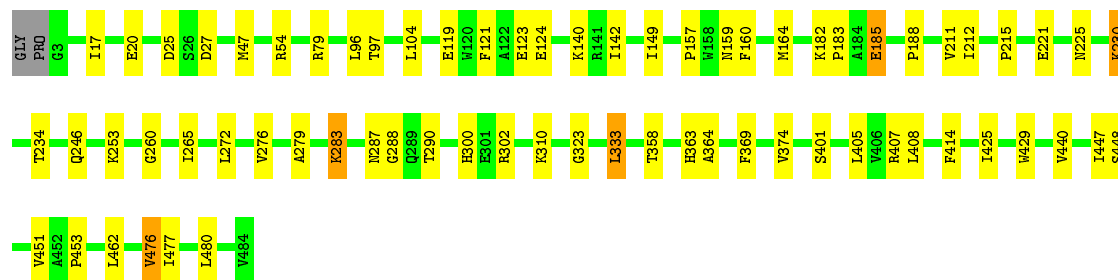
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)





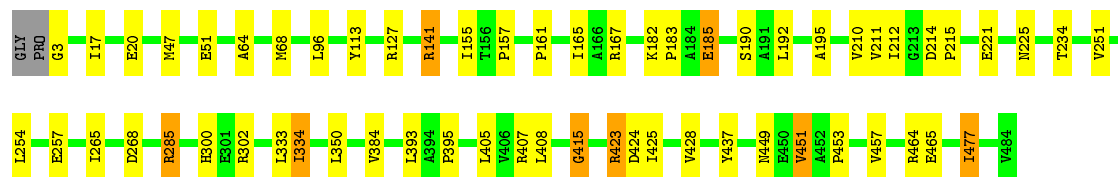
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

Chain E: 85% 13%



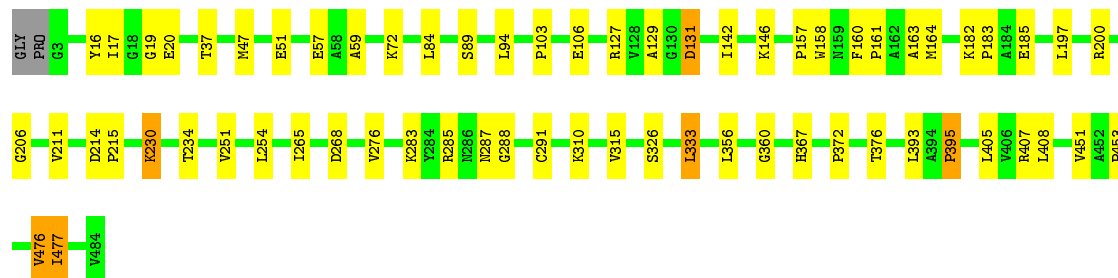
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

Chain F: 87% 11%



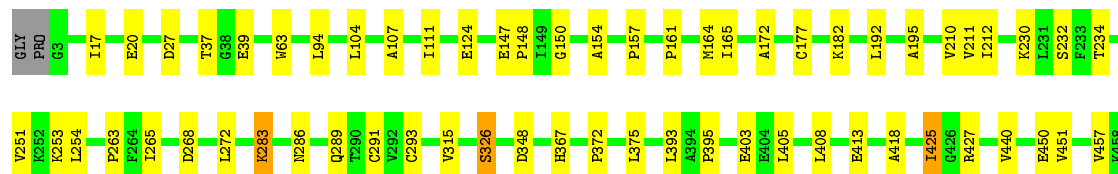
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

Chain G: 86% 12%



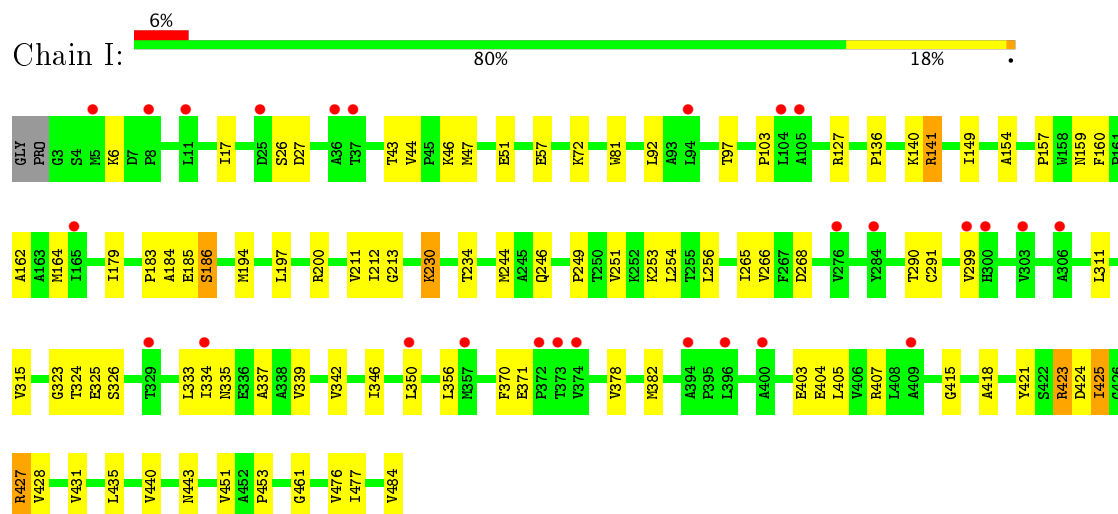
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

Chain H: 86% 13%

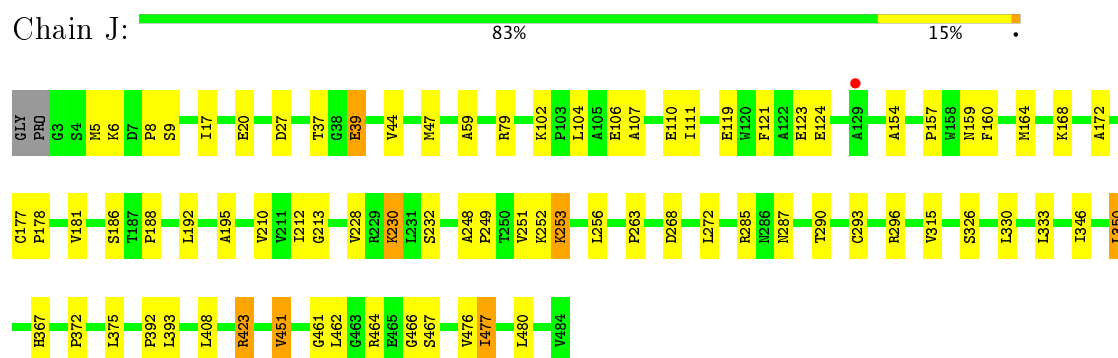




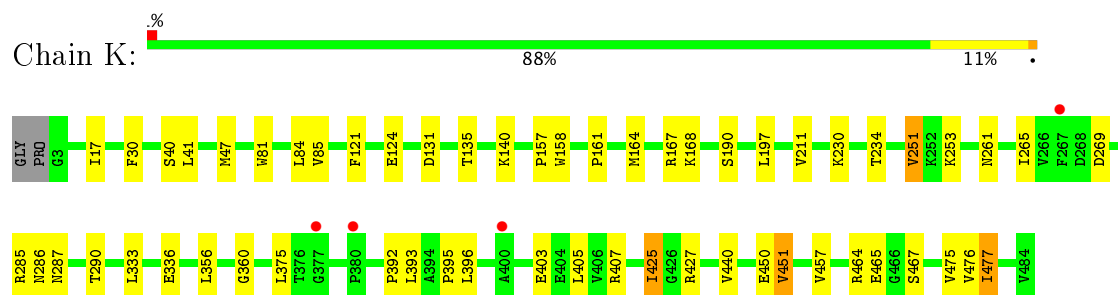
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



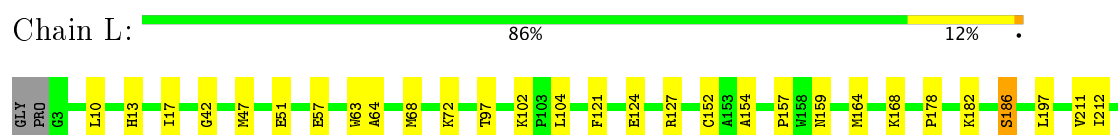
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

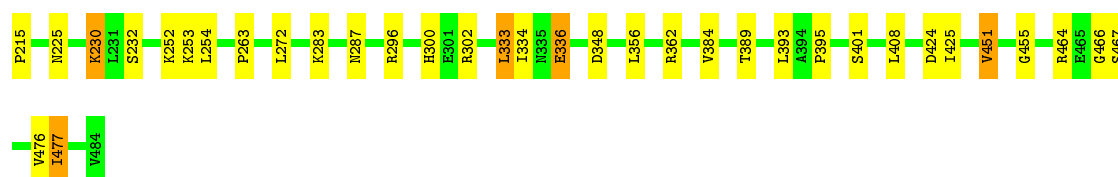


- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



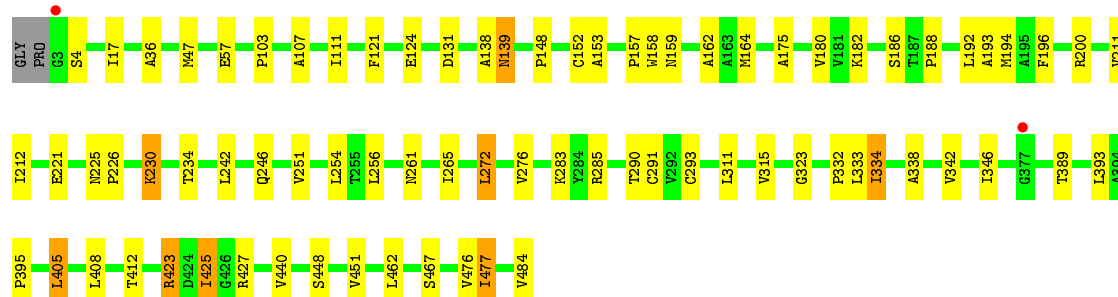
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)





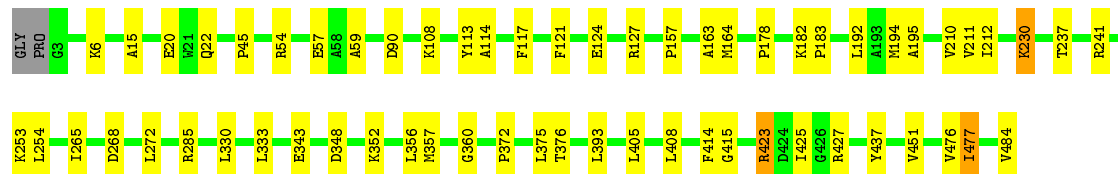
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

Chain M: 83% 14%



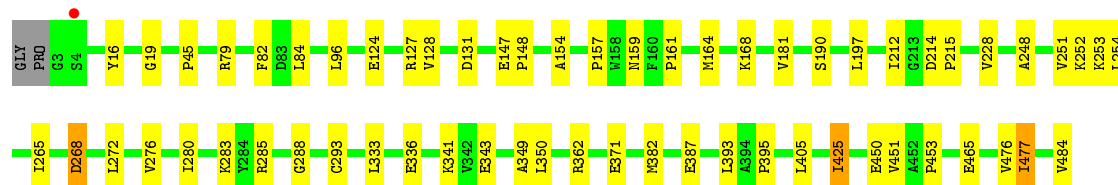
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

Chain N: 87% 12%



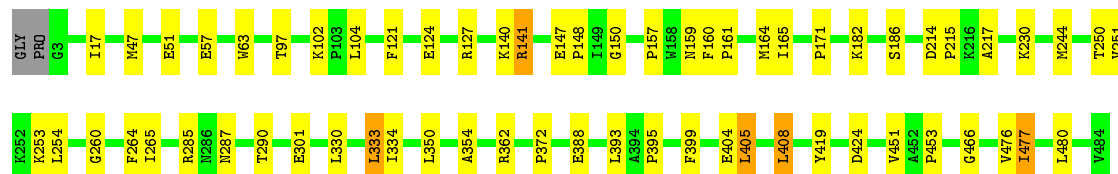
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

Chain O: 87% 12%

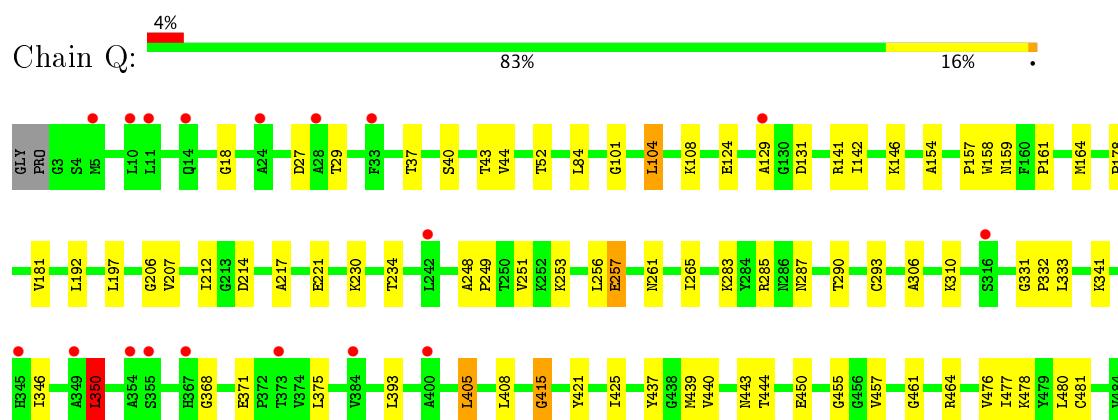


- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

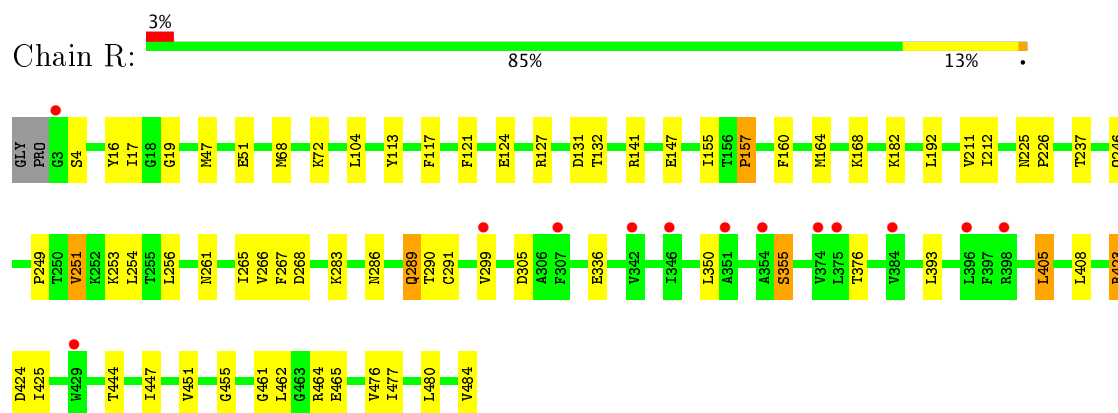
Chain P: 87% 12%



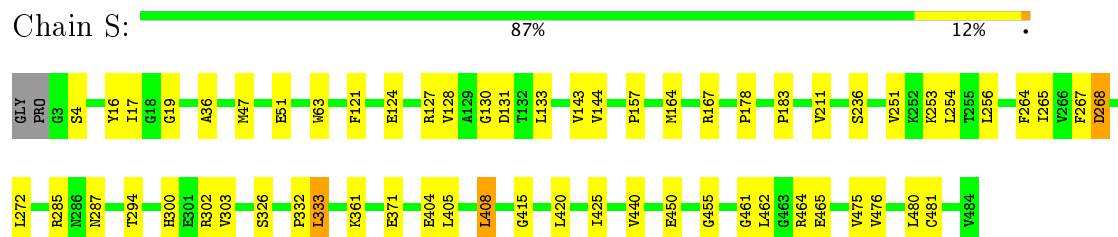
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



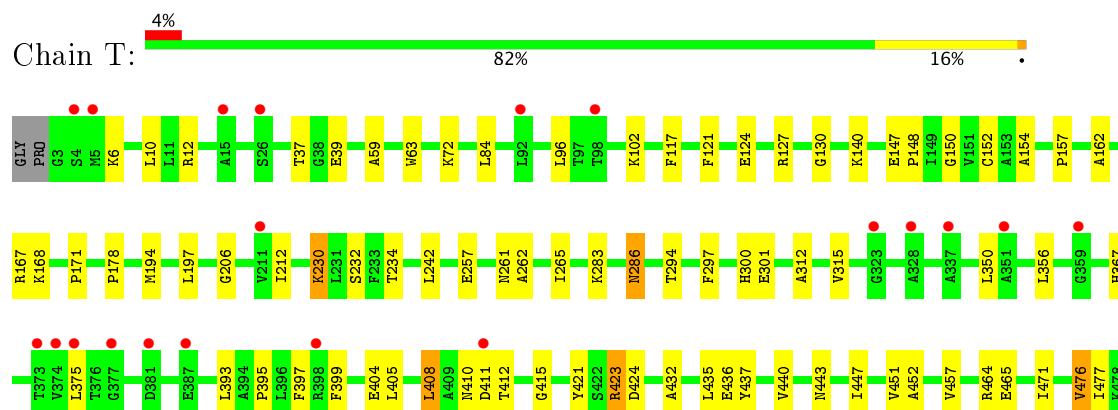
- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)




- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

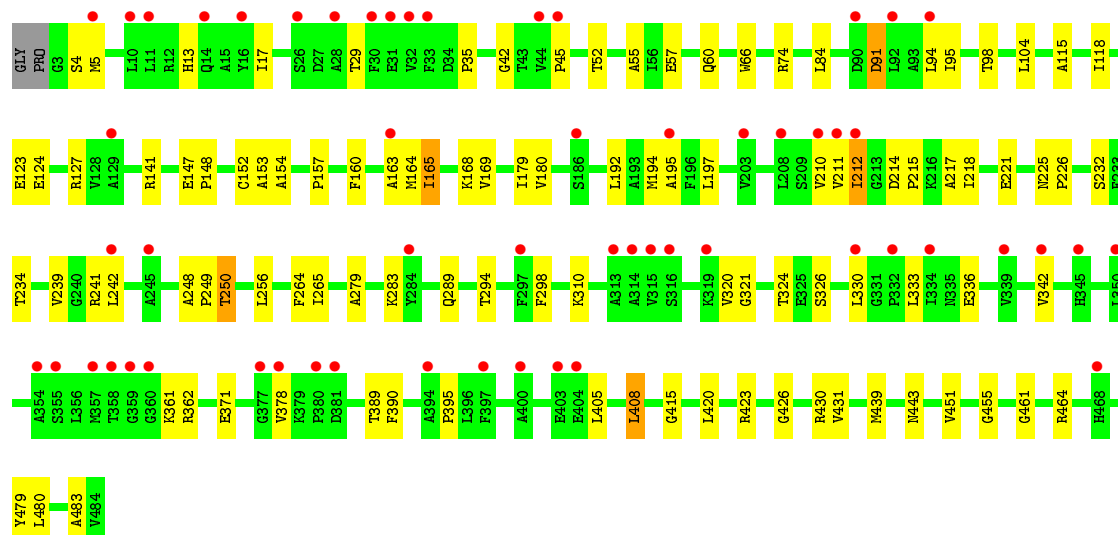







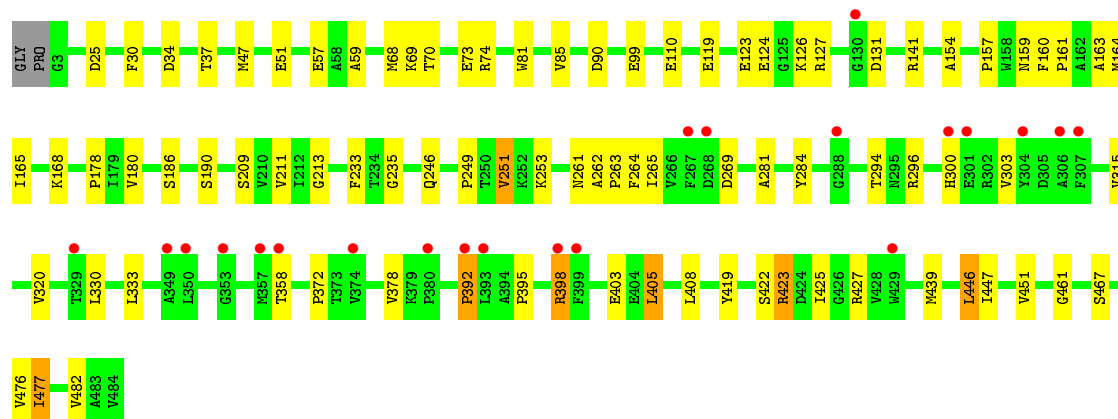
• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

Chain U: 



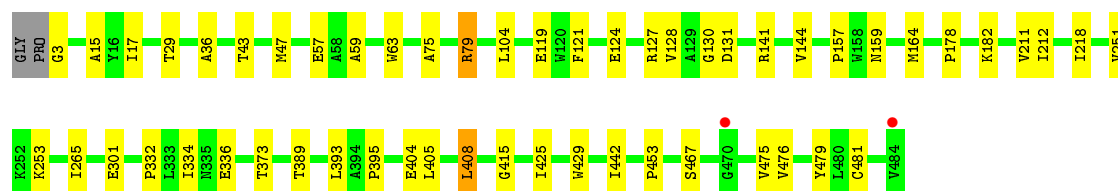
• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

Chain V: 

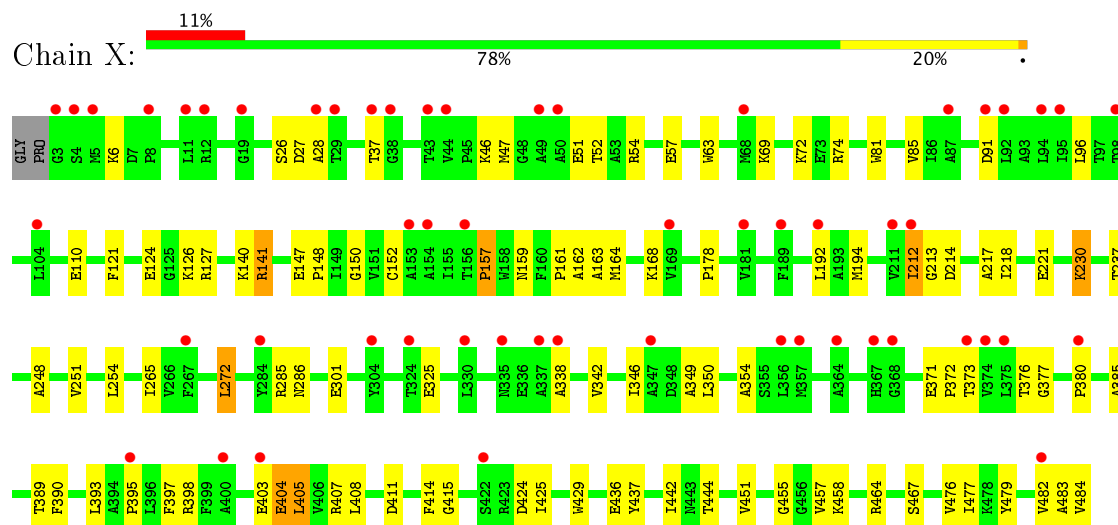


• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

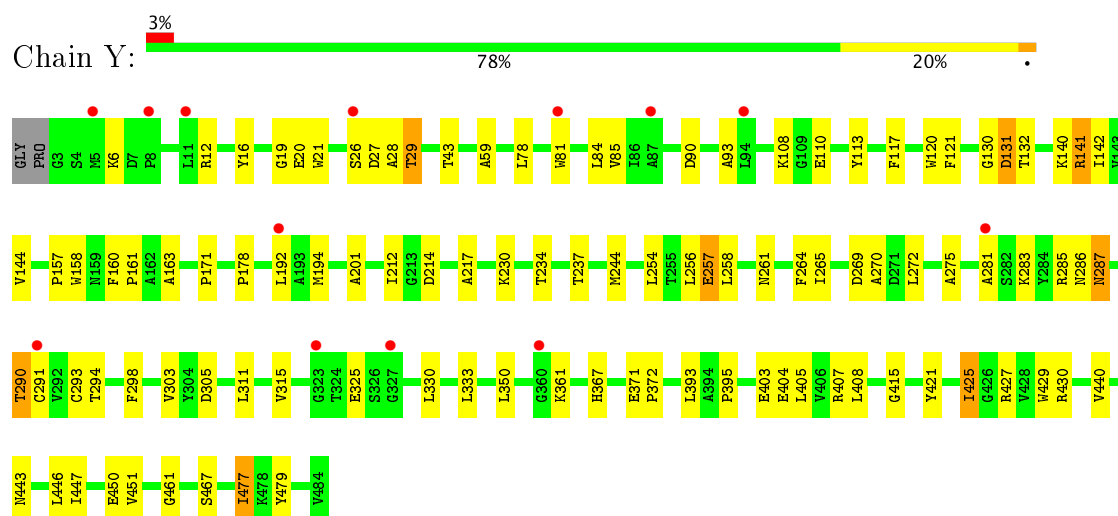
Chain W: 



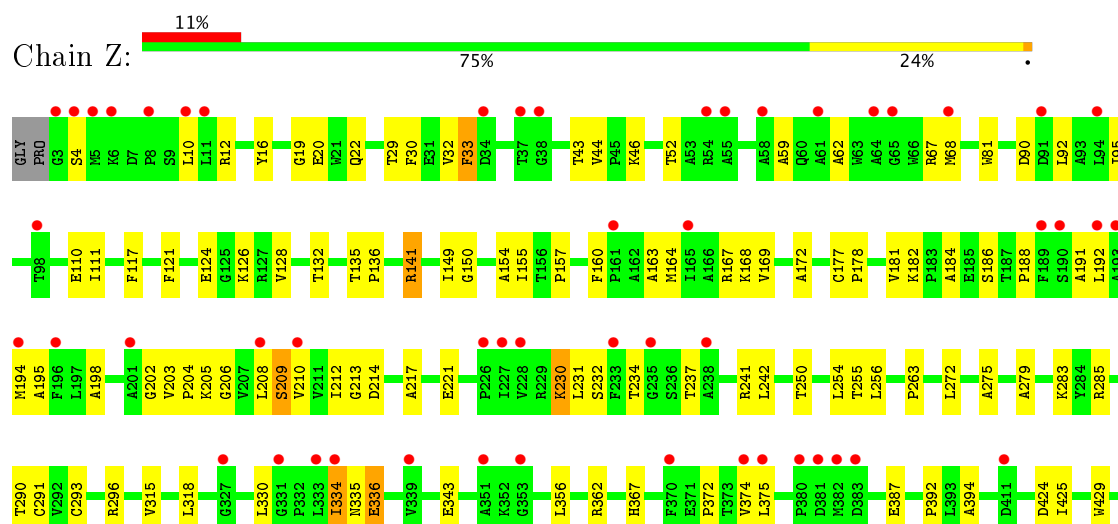
● Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



● Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

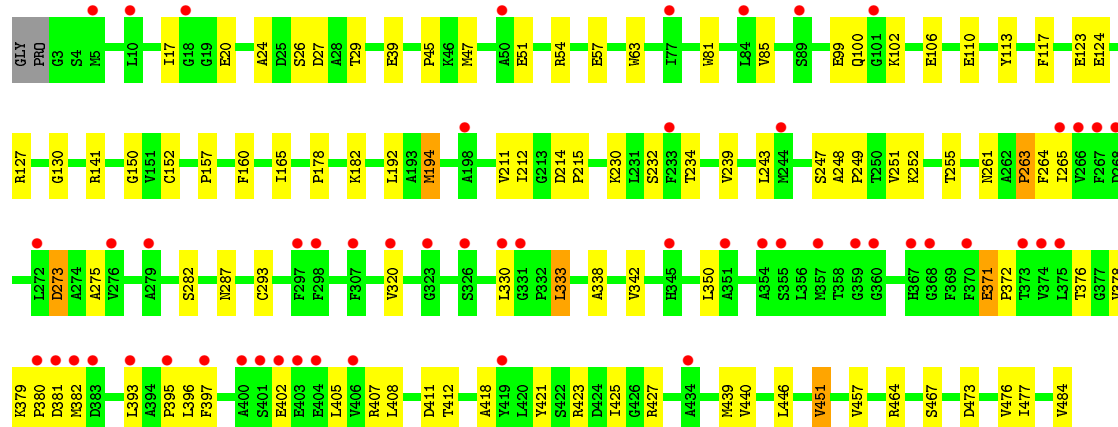


● Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

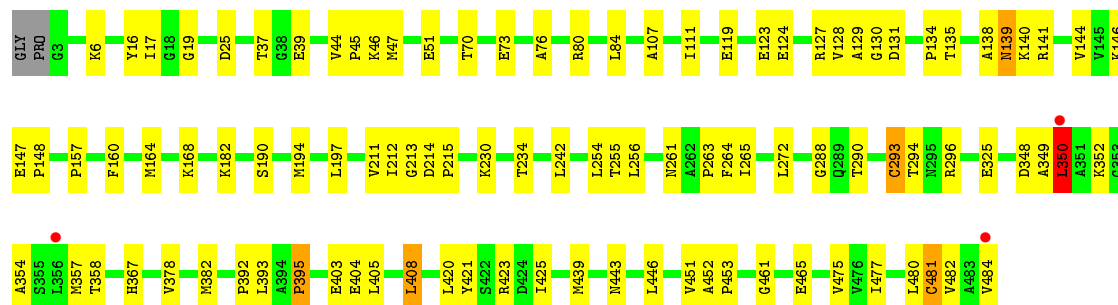
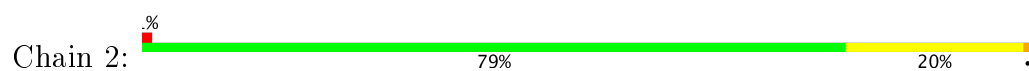




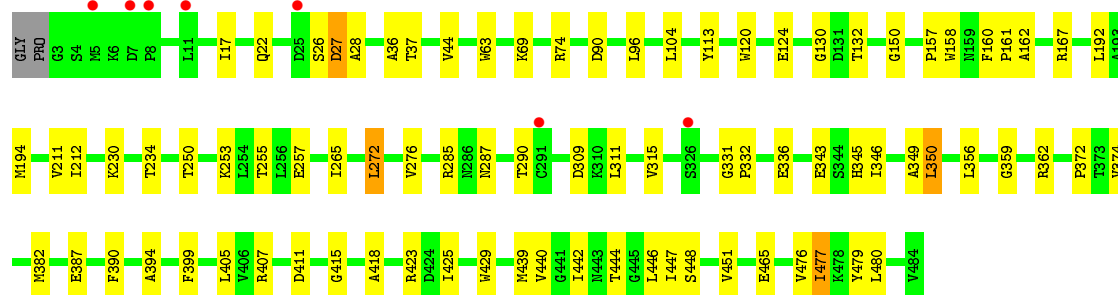
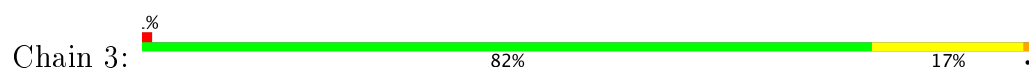
• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



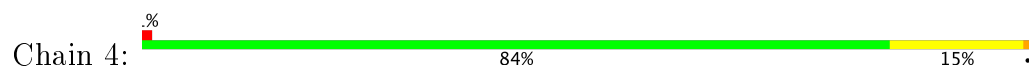
• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

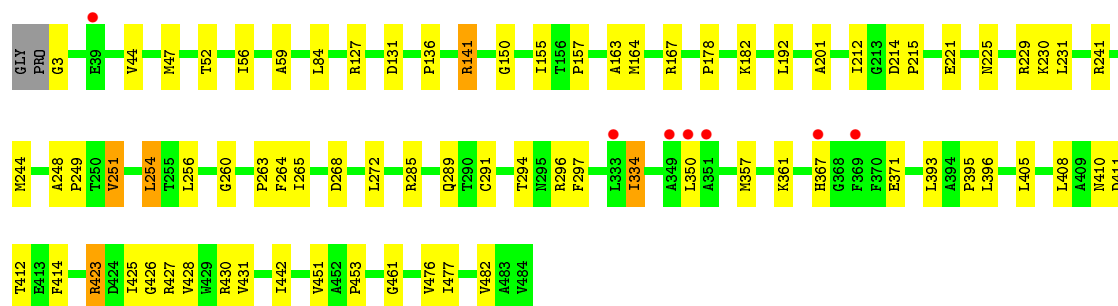


• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

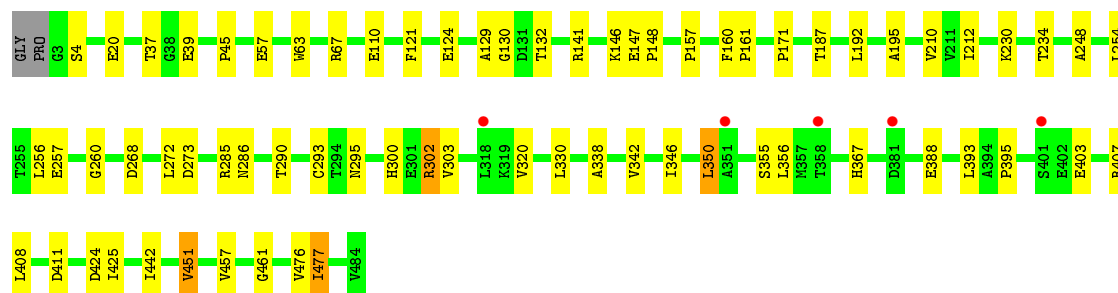
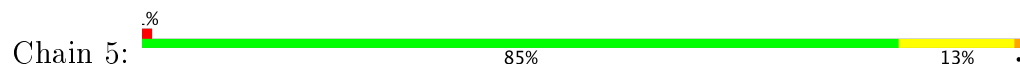


• Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)

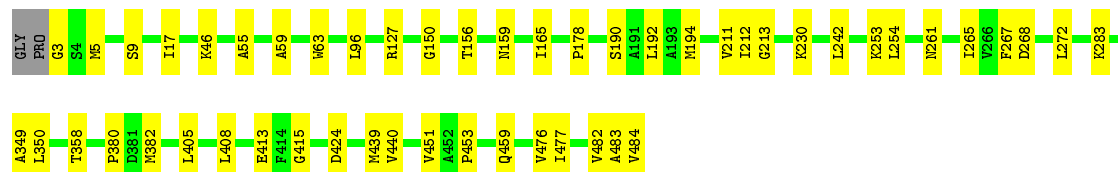
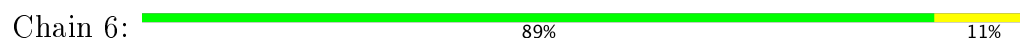




- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



- Molecule 1: Succinate-semialdehyde dehydrogenase (NADP+)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	185.66Å 164.87Å 278.90Å 90.00° 92.01° 90.00°	Depositor
Resolution (Å)	49.47 – 2.70 49.47 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.47-2.70) 98.3 (49.47-2.70)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.236 , 0.282 0.235 , 0.279	Depositor DCC
$R_{free}$ test set	22724 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.8	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 36.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	114732	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.06 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.8625e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	1	0.48	0/3584	0.56	0/4884
1	2	0.41	0/3619	0.56	1/4925 (0.0%)
1	3	0.42	0/3619	0.56	0/4925
1	4	0.41	0/3619	0.55	0/4925
1	5	0.41	0/3619	0.56	0/4925
1	6	0.41	0/3619	0.56	0/4925
1	A	0.39	0/3623	0.55	0/4930
1	B	0.40	0/3627	0.55	0/4935
1	C	0.41	0/3623	0.56	0/4930
1	D	0.41	0/3623	0.56	0/4930
1	E	0.40	0/3623	0.56	0/4930
1	F	0.41	0/3623	0.55	0/4930
1	G	0.41	0/3623	0.56	0/4930
1	H	0.41	0/3623	0.56	0/4930
1	I	0.44	0/3594	0.54	0/4896
1	J	0.41	0/3623	0.55	0/4930
1	K	0.41	0/3619	0.53	0/4925
1	L	0.40	0/3617	0.56	0/4922
1	M	0.41	0/3619	0.54	0/4925
1	N	0.39	0/3619	0.53	0/4925
1	O	0.41	0/3619	0.54	0/4925
1	P	0.39	0/3619	0.55	0/4925
1	Q	0.43	0/3619	0.54	1/4925 (0.0%)
1	R	0.41	0/3619	0.54	0/4925
1	S	0.39	0/3619	0.54	0/4925
1	T	0.43	0/3609	0.53	0/4913
1	U	0.47	0/3594	0.54	0/4894
1	V	0.44	0/3606	0.55	0/4910
1	W	0.42	0/3619	0.54	0/4925
1	X	0.47	0/3588	0.55	0/4885
1	Y	0.43	0/3619	0.57	0/4925
1	Z	0.46	0/3606	0.56	0/4910
All	All	0.42	0/115694	0.55	2/157464 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	6	0	1
1	U	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	350	LEU	CA-CB-CG	7.05	131.51	115.30
1	Q	350	LEU	CA-CB-CG	5.35	127.60	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	6	267	PHE	Peptide
1	U	4	SER	Peptide

## 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	1	3510	0	3426	54	0
1	2	3545	0	3503	61	0
1	3	3545	0	3503	52	0
1	4	3545	0	3503	44	0
1	5	3545	0	3503	40	0
1	6	3545	0	3503	21	0
1	A	3549	0	3507	37	0
1	B	3553	0	3511	34	0
1	C	3549	0	3507	41	0
1	D	3549	0	3507	47	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3549	0	3507	44	0
1	F	3549	0	3507	47	0
1	G	3549	0	3507	36	0
1	H	3549	0	3507	38	0
1	I	3520	0	3450	49	0
1	J	3549	0	3507	50	0
1	K	3545	0	3503	34	0
1	L	3543	0	3496	34	0
1	M	3545	0	3503	46	0
1	N	3545	0	3503	26	0
1	O	3545	0	3503	28	0
1	P	3545	0	3503	38	0
1	Q	3545	0	3503	46	0
1	R	3545	0	3503	33	0
1	S	3545	0	3503	38	0
1	T	3535	0	3474	51	0
1	U	3521	0	3463	50	0
1	V	3532	0	3472	47	0
1	W	3545	0	3503	37	0
1	X	3515	0	3438	62	0
1	Y	3545	0	3503	66	0
1	Z	3532	0	3472	77	0
2	1	28	0	0	0	0
2	2	37	0	0	2	0
2	3	45	0	0	1	0
2	4	46	0	0	2	0
2	5	54	0	0	1	0
2	6	57	0	0	1	0
2	A	46	0	0	0	0
2	B	59	0	0	1	0
2	C	56	0	0	1	0
2	D	60	0	0	3	0
2	E	72	0	0	2	0
2	F	75	0	0	4	0
2	G	66	0	0	1	0
2	H	58	0	0	1	0
2	I	24	0	0	1	0
2	J	35	0	0	2	0
2	K	55	0	0	2	0
2	L	57	0	0	2	0
2	M	40	0	0	1	0
2	N	46	0	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	O	39	0	0	0	0
2	P	74	0	0	1	0
2	Q	22	0	0	0	0
2	R	35	0	0	0	0
2	S	55	0	0	1	0
2	T	13	0	0	0	0
2	U	13	0	0	1	0
2	V	29	0	0	1	0
2	W	44	0	0	1	0
2	X	8	0	0	0	0
2	Y	36	0	0	2	0
2	Z	20	0	0	5	0
All	All	114732	0	111803	1241	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 6.

All (1241) 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:242:LEU:HD22	1:1:26:SER:HA	1.18	1.18
1:4:476:VAL:HG21	1:5:457:VAL:HG12	1.36	1.04
1:Z:192:LEU:HD11	1:Z:212:ILE:HD11	1.39	1.02
1:X:237:THR:HG1	1:X:414:PHE:HE1	1.09	0.97
1:H:265:ILE:HG21	1:H:405:LEU:HD21	1.51	0.91
1:R:192:LEU:HD21	1:R:212:ILE:HD11	1.53	0.90
1:Y:265:ILE:HG21	1:Y:405:LEU:HD21	1.56	0.87
1:Y:26:SER:O	1:Y:28:ALA:N	2.09	0.85
1:J:160:PHE:HE2	1:J:290:THR:HG22	1.42	0.85
1:C:375:LEU:HD12	1:C:393:LEU:HD11	1.58	0.84
1:Z:192:LEU:HD11	1:Z:212:ILE:CD1	2.09	0.83
1:Y:192:LEU:HD21	1:Y:212:ILE:HD11	1.58	0.82
1:M:138:ALA:O	1:M:139:ASN:HB2	1.77	0.82
1:Y:265:ILE:CG2	1:Y:405:LEU:HD21	2.10	0.81
1:Y:477:ILE:HD11	1:2:453:PRO:HG2	1.62	0.81
1:H:251:VAL:O	1:H:251:VAL:HG12	1.83	0.79
1:3:272:LEU:O	1:3:276:VAL:HG23	1.83	0.78
1:X:385:ALA:HB2	1:X:397:PHE:HZ	1.46	0.78
1:4:476:VAL:CG2	1:5:457:VAL:HG12	2.14	0.78
1:Y:270:ALA:O	1:Y:272:LEU:HD12	1.83	0.78
1:F:407:ARG:HD3	2:F:516:HOH:O	1.84	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:47:MET:HE3	1:M:212:ILE:H	1.50	0.77
1:S:302:ARG:HD2	2:S:522:HOH:O	1.83	0.77
1:W:124:GLU:HG2	1:X:127:ARG:HH21	1.51	0.76
1:Z:334:ILE:HG23	1:Z:335:ASN:H	1.50	0.76
1:Z:110:GLU:HG3	1:Z:163:ALA:HB2	1.67	0.76
1:1:265:ILE:HG21	1:1:405:LEU:HD21	1.68	0.75
1:R:192:LEU:HD21	1:R:212:ILE:CD1	2.16	0.75
1:V:265:ILE:HG12	1:V:405:LEU:HD11	1.68	0.74
1:I:251:VAL:O	1:I:251:VAL:HG12	1.86	0.74
1:R:265:ILE:HG12	1:R:405:LEU:HD11	1.69	0.74
1:U:127:ARG:HH21	1:V:124:GLU:HG2	1.51	0.74
1:X:265:ILE:CG2	1:X:405:LEU:HD11	2.18	0.74
1:Q:375:LEU:HD12	1:Q:393:LEU:HD11	1.70	0.74
1:Q:265:ILE:HG23	1:Q:405:LEU:HD11	1.69	0.73
1:T:234:THR:HG23	1:T:257:GLU:HB2	1.69	0.73
1:J:480:LEU:HD23	1:K:440:VAL:HB	1.68	0.73
1:F:477:ILE:HD11	1:G:453:PRO:HB2	1.71	0.72
1:U:192:LEU:HD21	1:U:212:ILE:HD11	1.72	0.71
1:Y:265:ILE:HG12	1:Y:405:LEU:HD11	1.70	0.71
1:X:385:ALA:HB2	1:X:397:PHE:CZ	2.25	0.71
1:Z:62:ALA:HB2	1:Z:205:LYS:O	1.90	0.71
1:1:124:GLU:HG2	1:2:127:ARG:HH21	1.54	0.71
1:2:157:PRO:HD2	1:2:164:MET:HG3	1.72	0.71
1:I:418:ALA:HB3	1:I:440:VAL:HG22	1.73	0.71
1:C:127:ARG:HH21	1:D:124:GLU:HG2	1.56	0.70
1:3:26:SER:O	1:3:28:ALA:N	2.23	0.70
1:M:124:GLU:HG2	1:N:127:ARG:HH21	1.56	0.70
1:M:425:ILE:HG12	1:O:425:ILE:HG12	1.72	0.70
1:X:265:ILE:HG23	1:X:405:LEU:HD11	1.74	0.70
1:4:291:CYS:HB2	2:4:504:HOH:O	1.92	0.70
1:J:256:LEU:O	1:J:461:GLY:HA3	1.91	0.70
1:S:17:ILE:HD11	1:S:47:MET:CE	2.22	0.69
1:B:47:MET:HE2	1:B:51:GLU:CB	2.22	0.69
1:Q:332:PRO:HA	1:Q:368:GLY:O	1.92	0.69
1:R:251:VAL:O	1:R:251:VAL:HG12	1.93	0.69
1:2:37:THR:OG1	1:2:39:GLU:HG2	1.92	0.69
1:D:37:THR:HB	1:D:39:GLU:HG2	1.75	0.69
1:F:47:MET:CE	1:F:211:VAL:HG13	2.23	0.69
1:Z:10:LEU:HA	2:Z:520:HOH:O	1.93	0.69
1:S:127:ARG:HH21	1:T:124:GLU:HG2	1.57	0.69
1:3:124:GLU:HG2	1:4:127:ARG:HH21	1.57	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:265:ILE:HG23	1:M:405:LEU:HD11	1.75	0.68
1:1:378:VAL:HG13	1:1:382:MET:SD	2.32	0.68
1:M:251:VAL:O	1:M:251:VAL:HG12	1.91	0.68
1:3:120:TRP:CH2	1:3:451:VAL:HG23	2.28	0.68
1:Z:315:VAL:HG13	1:Z:372:PRO:HB2	1.75	0.68
1:B:413:GLU:HG2	1:B:459:GLN:HG3	1.75	0.68
1:I:200:ARG:HB2	2:I:514:HOH:O	1.94	0.68
1:T:265:ILE:HG23	1:T:405:LEU:HD11	1.75	0.68
1:Y:90:ASP:HA	1:Y:108:LYS:NZ	2.09	0.68
1:W:63:TRP:CD1	1:W:178:PRO:HD3	2.29	0.68
1:Q:192:LEU:HD21	1:Q:212:ILE:HD11	1.76	0.67
1:O:124:GLU:HG2	1:P:127:ARG:HH21	1.59	0.67
1:K:47:MET:HE3	1:K:211:VAL:HG13	1.75	0.67
1:F:192:LEU:HD11	1:F:212:ILE:HD11	1.76	0.67
1:Y:290:THR:OG1	1:Y:293:CYS:SG	2.47	0.67
1:W:429:TRP:CZ3	1:X:141:ARG:HG2	2.30	0.67
1:3:234:THR:HG23	1:3:257:GLU:HB2	1.77	0.66
1:6:192:LEU:HD21	1:6:212:ILE:HD11	1.77	0.66
1:F:47:MET:HE1	1:F:211:VAL:HG13	1.76	0.66
1:B:47:MET:CE	1:B:51:GLU:HB3	2.25	0.66
1:1:418:ALA:HB3	1:1:440:VAL:HG22	1.78	0.66
1:A:300:HIS:CE1	1:A:302:ARG:HG3	2.30	0.66
1:U:157:PRO:HD2	1:U:164:MET:HG3	1.78	0.66
1:G:251:VAL:HG12	1:G:251:VAL:O	1.95	0.66
1:M:138:ALA:O	1:M:139:ASN:CB	2.42	0.66
1:B:423:ARG:HG3	1:D:424:ASP:OD1	1.96	0.66
1:G:200:ARG:HD2	2:G:518:HOH:O	1.96	0.66
1:Z:458:LYS:HA	2:Z:504:HOH:O	1.96	0.66
1:P:265:ILE:HG23	1:P:405:LEU:HD11	1.78	0.65
1:5:110:GLU:HG3	1:5:160:PHE:HD1	1.61	0.65
1:Y:120:TRP:CZ3	1:Y:451:VAL:HG12	2.31	0.65
1:N:22:GLN:OE1	1:N:54:ARG:NH2	2.29	0.65
1:P:466:GLY:HA3	2:P:525:HOH:O	1.96	0.65
1:5:302:ARG:HD2	2:5:545:HOH:O	1.96	0.65
1:S:265:ILE:HG12	1:S:405:LEU:HD11	1.76	0.65
1:1:230:LYS:HE3	1:1:473:ASP:HB3	1.78	0.65
1:M:4:SER:HA	2:M:525:HOH:O	1.96	0.65
1:Z:476:VAL:HG21	1:1:457:VAL:HG12	1.78	0.65
1:S:450:GLU:OE2	1:T:72:LYS:HE2	1.97	0.65
1:V:251:VAL:O	1:V:251:VAL:HG13	1.97	0.65
1:O:341:LYS:HE2	1:O:387:GLU:OE2	1.97	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:VAL:HG13	1:C:477:ILE:HD12	1.79	0.65
1:T:157:PRO:HD3	1:T:234:THR:HB	1.79	0.64
1:V:447:ILE:HG22	1:W:481:CYS:HB3	1.80	0.64
1:B:251:VAL:O	1:B:251:VAL:HG12	1.98	0.64
1:H:265:ILE:CG2	1:H:405:LEU:HD21	2.26	0.64
1:E:300:HIS:CE1	1:E:302:ARG:HG3	2.33	0.64
1:K:41:LEU:CB	2:K:514:HOH:O	2.45	0.64
1:2:138:ALA:O	1:2:139:ASN:HB2	1.98	0.64
1:A:424:ASP:OD1	1:C:423:ARG:HG3	1.98	0.64
1:T:265:ILE:CG2	1:T:405:LEU:HD11	2.27	0.64
1:C:251:VAL:HG12	1:C:251:VAL:O	1.96	0.64
1:B:447:ILE:HG22	1:C:481:CYS:HB3	1.80	0.63
1:K:47:MET:CE	1:K:211:VAL:HG13	2.27	0.63
1:I:335:ASN:O	1:I:339:VAL:HG23	1.98	0.63
1:A:124:GLU:HG2	1:B:127:ARG:HH21	1.63	0.63
1:Q:478:LYS:NZ	1:T:432:ALA:O	2.29	0.63
1:F:192:LEU:HD11	1:F:212:ILE:CD1	2.28	0.63
1:K:393:LEU:O	1:K:395:PRO:HD3	1.99	0.63
1:M:157:PRO:HD2	1:M:164:MET:HG3	1.80	0.63
1:O:343:GLU:OE2	1:O:362:ARG:HD2	1.99	0.63
1:H:192:LEU:HD21	1:H:212:ILE:HD11	1.79	0.63
1:O:251:VAL:HG12	1:O:251:VAL:O	1.99	0.63
1:6:190:SER:O	1:6:194:MET:HG2	1.99	0.63
1:Z:52:THR:HB	1:Z:221:GLU:HG2	1.80	0.63
1:L:300:HIS:CE1	1:L:302:ARG:HG3	2.34	0.63
1:R:47:MET:HE1	1:R:211:VAL:HG13	1.79	0.63
1:5:320:VAL:HG22	1:5:330:LEU:HD12	1.81	0.62
1:3:250:THR:C	1:6:459:GLN:HE22	2.02	0.62
1:Y:16:TYR:CZ	1:Y:19:GLY:HA2	2.34	0.62
1:B:47:MET:HE3	1:B:51:GLU:HB3	1.81	0.62
1:B:453:PRO:HG2	1:C:477:ILE:HD11	1.82	0.62
1:H:107:ALA:O	1:H:111:ILE:HG12	1.99	0.62
1:Y:234:THR:OG1	1:Y:257:GLU:HG3	2.00	0.62
1:L:17:ILE:HD11	1:L:47:MET:HE1	1.80	0.62
1:M:251:VAL:O	1:M:251:VAL:CG1	2.47	0.62
1:Z:195:ALA:HA	1:Z:208:LEU:HD21	1.82	0.62
1:Z:457:VAL:HG12	1:1:476:VAL:HG21	1.82	0.62
1:L:157:PRO:HD2	1:L:164:MET:HG3	1.82	0.62
1:S:17:ILE:HD11	1:S:47:MET:HE1	1.82	0.62
1:U:195:ALA:HB2	1:U:210:VAL:HG21	1.80	0.62
1:Y:160:PHE:HE2	1:Y:290:THR:CG2	2.12	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:110:GLU:HG3	1:5:160:PHE:CD1	2.35	0.61
1:U:426:GLY:O	1:U:430:ARG:HG3	2.01	0.61
1:X:164:MET:O	1:X:168:LYS:HG2	2.00	0.61
1:C:124:GLU:HG2	1:D:127:ARG:HH21	1.65	0.61
1:I:26:SER:O	1:I:27:ASP:HB2	2.00	0.61
1:4:476:VAL:HG21	1:5:457:VAL:CG1	2.23	0.61
1:E:79:ARG:HH22	1:E:119:GLU:HG3	1.65	0.61
1:G:72:LYS:HE2	1:H:450:GLU:OE2	1.99	0.61
1:J:346:ILE:O	1:J:350:LEU:HB2	2.00	0.61
1:L:17:ILE:HD11	1:L:47:MET:CE	2.31	0.61
1:W:393:LEU:O	1:W:395:PRO:HD3	2.00	0.61
1:Q:476:VAL:HG21	1:T:457:VAL:HG12	1.82	0.61
1:Z:157:PRO:HD3	1:Z:234:THR:HB	1.82	0.61
1:V:477:ILE:HD11	1:W:453:PRO:HB2	1.82	0.61
1:1:265:ILE:HG21	1:1:405:LEU:CD2	2.31	0.60
1:J:160:PHE:CE2	1:J:290:THR:HG22	2.29	0.60
1:S:361:LYS:O	1:S:371:GLU:HB2	2.01	0.60
1:I:311:LEU:O	1:I:315:VAL:HG23	2.01	0.60
1:O:157:PRO:HD2	1:O:164:MET:HG3	1.84	0.60
1:F:3:GLY:HA3	2:F:519:HOH:O	2.01	0.60
1:S:287:ASN:ND2	1:S:333:LEU:HD13	2.16	0.60
1:V:119:GLU:O	1:V:123:GLU:HG3	2.01	0.60
1:V:47:MET:HE3	1:V:51:GLU:HB3	1.82	0.60
1:R:168:LYS:HE2	1:R:465:GLU:OE2	2.02	0.60
1:C:129:ALA:O	1:C:146:LYS:NZ	2.28	0.60
1:O:16:TYR:CZ	1:O:19:GLY:HA2	2.36	0.60
1:Z:315:VAL:CG1	1:Z:372:PRO:HB2	2.31	0.60
1:M:47:MET:CE	1:M:212:ILE:H	2.15	0.60
1:5:286:ASN:HB3	1:5:290:THR:HG23	1.82	0.60
1:P:157:PRO:HD2	1:P:164:MET:HG3	1.82	0.60
1:X:251:VAL:O	1:X:251:VAL:HG12	2.02	0.59
1:R:157:PRO:HD2	1:R:164:MET:HG3	1.84	0.59
1:B:453:PRO:CG	1:C:477:ILE:HD11	2.33	0.59
1:K:157:PRO:HD2	1:K:164:MET:HG3	1.85	0.59
1:2:265:ILE:HG12	1:2:405:LEU:HD11	1.84	0.59
1:5:346:ILE:O	1:5:350:LEU:HD22	2.02	0.59
1:6:265:ILE:HG21	1:6:405:LEU:HD21	1.84	0.59
1:F:453:PRO:HG2	1:G:477:ILE:HD11	1.85	0.59
1:U:17:ILE:HG23	1:U:55:ALA:HB2	1.84	0.59
1:3:311:LEU:O	1:3:315:VAL:HG23	2.02	0.59
1:D:287:ASN:HD22	1:D:330:LEU:HD22	1.66	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:47:MET:HB2	1:I:212:ILE:O	2.03	0.59
1:P:265:ILE:HG23	1:P:405:LEU:CD1	2.32	0.59
1:Q:142:ILE:HD13	1:T:452:ALA:HB2	1.83	0.59
1:1:393:LEU:O	1:1:395:PRO:HD3	2.03	0.59
1:Q:157:PRO:HD2	1:Q:164:MET:HG3	1.83	0.59
1:3:349:ALA:HA	1:3:382:MET:HG2	1.84	0.59
1:B:47:MET:HE2	1:B:51:GLU:HB2	1.85	0.59
1:J:251:VAL:O	1:J:251:VAL:HG12	2.03	0.58
1:K:121:PHE:HA	1:K:124:GLU:HB2	1.84	0.58
1:P:17:ILE:HD11	1:P:47:MET:HE1	1.84	0.58
1:X:214:ASP:HB3	1:X:217:ALA:HB3	1.83	0.58
1:I:425:ILE:HG12	1:K:425:ILE:HG12	1.86	0.58
1:U:124:GLU:HG2	1:V:127:ARG:HH21	1.68	0.58
1:Z:149:ILE:HG23	1:Z:150:GLY:H	1.69	0.58
1:1:192:LEU:HD21	1:1:212:ILE:HD11	1.86	0.58
1:X:6:LYS:HD2	1:X:6:LYS:H	1.68	0.58
1:Y:130:GLY:HA3	1:Y:144:VAL:O	2.04	0.58
1:G:47:MET:HE1	1:G:211:VAL:HG13	1.86	0.58
1:X:415:GLY:HA2	1:X:437:TYR:CD1	2.38	0.58
1:Q:84:LEU:HB3	1:Q:197:LEU:HD22	1.85	0.58
1:W:373:THR:HB	1:W:393:LEU:HD12	1.85	0.58
1:3:429:TRP:HZ3	1:4:141:ARG:HG2	1.69	0.58
1:3:192:LEU:HD21	1:3:212:ILE:HD11	1.85	0.58
1:4:453:PRO:HB2	1:5:477:ILE:HD11	1.86	0.57
1:T:393:LEU:O	1:T:395:PRO:HD3	2.04	0.57
1:H:251:VAL:CG1	1:H:251:VAL:O	2.52	0.57
1:S:157:PRO:HD2	1:S:164:MET:HG3	1.86	0.57
1:X:152:CYS:SG	1:X:230:LYS:HG2	2.44	0.57
1:D:47:MET:CE	1:D:51:GLU:HB3	2.34	0.57
1:P:244:MET:HA	1:P:254:LEU:HD21	1.85	0.57
1:Z:160:PHE:HB3	1:Z:163:ALA:HB3	1.85	0.57
1:Z:16:TYR:CZ	1:Z:19:GLY:HA2	2.38	0.57
1:R:256:LEU:HD12	1:S:251:VAL:HG13	1.84	0.57
1:E:260:GLY:HA2	1:E:414:PHE:HB3	1.85	0.57
1:1:113:TYR:CE1	1:1:117:PHE:HE2	2.22	0.57
1:5:147:GLU:HB2	1:5:148:PRO:HD2	1.85	0.57
1:N:330:LEU:HD13	1:N:372:PRO:HG3	1.87	0.57
1:A:140:LYS:O	1:A:141:ARG:HD3	2.04	0.56
1:L:47:MET:HB2	1:L:212:ILE:O	2.04	0.56
1:1:165:ILE:HG21	1:1:194:MET:HG2	1.87	0.56
1:A:356:LEU:HD21	1:A:360:GLY:HA3	1.88	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:286:ASN:C	1:T:286:ASN:HD22	2.09	0.56
1:X:159:ASN:HB2	1:X:286:ASN:HD21	1.70	0.56
1:M:283:LYS:HE2	1:M:393:LEU:O	2.05	0.56
1:M:477:ILE:HD11	1:P:453:PRO:HB2	1.87	0.56
1:Y:286:ASN:O	1:Y:287:ASN:HB2	2.05	0.56
1:E:182:LYS:HE2	1:E:215:PRO:HA	1.88	0.56
1:Y:81:TRP:O	1:Y:85:VAL:HG23	2.05	0.56
1:B:47:MET:CE	1:B:51:GLU:CB	2.84	0.56
1:W:127:ARG:HH21	1:X:124:GLU:HG2	1.69	0.56
1:3:157:PRO:HD3	1:3:234:THR:HB	1.87	0.56
1:A:476:VAL:HG21	1:D:457:VAL:HG12	1.87	0.56
1:Z:374:VAL:HG22	1:Z:394:ALA:HB3	1.88	0.56
1:4:150:GLY:HA3	1:4:229:ARG:HD2	1.88	0.56
1:E:276:VAL:HG21	1:E:310:LYS:HB3	1.87	0.56
1:N:195:ALA:HB2	1:N:210:VAL:HG21	1.88	0.56
1:Y:12:ARG:HG3	1:Y:21:TRP:CH2	2.40	0.56
1:M:290:THR:HG1	1:M:293:CYS:HG	1.53	0.56
1:T:154:ALA:HA	1:T:232:SER:O	2.05	0.56
1:U:115:ALA:HA	1:U:118:ILE:HD12	1.88	0.56
1:2:350:LEU:HA	1:2:354:ALA:HB3	1.88	0.56
1:I:162:ALA:HB1	1:I:194:MET:HE1	1.87	0.56
1:J:375:LEU:HD12	1:J:393:LEU:HD11	1.87	0.56
1:F:477:ILE:HD11	1:G:453:PRO:CB	2.35	0.55
1:I:265:ILE:HG12	1:I:405:LEU:HD11	1.88	0.55
1:D:251:VAL:O	1:D:251:VAL:HG12	2.05	0.55
1:Z:164:MET:O	1:Z:168:LYS:HG3	2.07	0.55
1:D:375:LEU:HD12	1:D:393:LEU:HD11	1.88	0.55
1:P:47:MET:CE	1:P:51:GLU:HB3	2.36	0.55
1:Q:104:LEU:HD22	1:Q:108:LYS:HE3	1.89	0.55
1:W:17:ILE:HD11	1:W:47:MET:CE	2.37	0.55
1:I:484:VAL:O	1:I:484:VAL:HG13	2.06	0.55
1:V:160:PHE:HB3	1:V:163:ALA:HB3	1.89	0.55
1:1:379:LYS:CB	1:1:380:PRO:HD2	2.36	0.55
1:E:185:GLU:CD	1:E:215:PRO:HG3	2.26	0.55
1:U:165:ILE:O	1:U:169:VAL:HB	2.07	0.55
1:X:272:LEU:H	1:X:272:LEU:HD13	1.72	0.55
1:Y:113:TYR:CE2	1:Y:117:PHE:HE2	2.25	0.55
1:1:407:ARG:O	1:1:411:ASP:HB2	2.07	0.55
1:I:103:PRO:HA	1:I:323:GLY:HA2	1.89	0.55
1:Z:212:ILE:HG22	1:Z:213:GLY:N	2.22	0.55
1:2:119:GLU:O	1:2:123:GLU:HG3	2.07	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:63:TRP:CZ2	1:1:150:GLY:HA2	2.41	0.55
1:H:427:ARG:CZ	2:H:532:HOH:O	2.54	0.55
1:U:160:PHE:HB3	1:U:163:ALA:HB3	1.87	0.55
1:1:275:ALA:HA	1:1:421:TYR:CE1	2.42	0.55
1:D:47:MET:HE3	1:D:51:GLU:HB3	1.88	0.55
1:E:47:MET:CE	1:E:211:VAL:HG13	2.37	0.55
1:G:16:TYR:CZ	1:G:19:GLY:HA2	2.41	0.55
1:5:286:ASN:HD22	1:5:290:THR:HG22	1.72	0.54
1:P:47:MET:HE3	1:P:51:GLU:HB3	1.89	0.54
1:3:343:GLU:OE1	1:3:362:ARG:NH1	2.40	0.54
1:D:265:ILE:HG12	1:D:405:LEU:HD11	1.88	0.54
1:E:123:GLU:HB2	1:F:127:ARG:NH2	2.22	0.54
1:B:265:ILE:HG12	1:B:405:LEU:HD11	1.88	0.54
1:H:192:LEU:HD21	1:H:212:ILE:CD1	2.37	0.54
1:A:477:ILE:HD11	1:D:453:PRO:HB2	1.89	0.54
1:F:251:VAL:HG12	1:F:251:VAL:O	2.07	0.54
1:Q:440:VAL:HB	1:T:480:LEU:HD23	1.89	0.54
1:W:59:ALA:HB1	1:W:178:PRO:HB2	1.89	0.54
1:B:447:ILE:HG22	1:C:481:CYS:CB	2.37	0.54
1:D:379:LYS:CB	2:D:522:HOH:O	2.55	0.54
1:E:364:ALA:HB3	1:J:9:SER:HB3	1.88	0.54
1:S:404:GLU:HG2	1:S:408:LEU:HD22	1.89	0.54
1:1:402:GLU:OE1	1:1:427:ARG:HG3	2.08	0.54
1:L:455:GLY:HA3	1:L:464:ARG:HD3	1.89	0.54
1:M:148:PRO:HG3	1:M:175:ALA:O	2.08	0.54
1:N:157:PRO:HD2	1:N:164:MET:HG3	1.88	0.54
1:X:265:ILE:HG21	1:X:405:LEU:HD11	1.87	0.54
1:Z:477:ILE:HG12	1:1:464:ARG:HE	1.72	0.54
1:A:167:ARG:NH2	1:A:465:GLU:OE1	2.41	0.54
1:I:251:VAL:CG1	1:I:251:VAL:O	2.56	0.54
1:R:113:TYR:CE1	1:R:117:PHE:HE2	2.26	0.54
1:F:161:PRO:O	1:F:165:ILE:HD13	2.08	0.54
1:Q:265:ILE:HG23	1:Q:405:LEU:CD1	2.38	0.54
1:S:124:GLU:HG2	1:T:127:ARG:HH21	1.72	0.54
1:Y:214:ASP:HB3	1:Y:217:ALA:HB3	1.89	0.54
1:F:300:HIS:CE1	1:F:302:ARG:HG3	2.43	0.54
1:I:81:TRP:HZ2	1:I:194:MET:HG3	1.71	0.54
1:2:393:LEU:O	1:2:395:PRO:HD3	2.08	0.53
1:3:477:ILE:HG23	2:3:504:HOH:O	2.08	0.53
1:5:290:THR:OG1	1:5:293:CYS:SG	2.62	0.53
1:V:378:VAL:HG11	1:V:395:PRO:HB2	1.90	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:346:ILE:HG22	1:3:350:LEU:HD22	1.89	0.53
1:J:248:ALA:HB3	1:J:249:PRO:HD3	1.90	0.53
1:Y:256:LEU:O	1:Y:461:GLY:HA3	2.08	0.53
1:B:477:ILE:HD11	1:C:453:PRO:HB2	1.90	0.53
1:E:440:VAL:HB	1:H:480:LEU:HD23	1.89	0.53
1:P:214:ASP:HB3	1:P:217:ALA:HB3	1.91	0.53
1:4:265:ILE:HG12	1:4:405:LEU:HD11	1.90	0.53
1:I:342:VAL:O	1:I:346:ILE:HG13	2.09	0.53
1:Q:332:PRO:CA	1:Q:368:GLY:O	2.56	0.53
1:Q:450:GLU:OE2	1:R:72:LYS:HE2	2.08	0.53
1:R:286:ASN:O	1:R:289:GLN:HG3	2.08	0.53
1:Y:132:THR:OG1	1:1:130:GLY:HA3	2.08	0.53
1:1:182:LYS:HE3	1:1:215:PRO:HA	1.91	0.53
1:4:264:PHE:HB2	1:4:294:THR:HG21	1.90	0.53
1:D:393:LEU:O	1:D:395:PRO:HD3	2.08	0.53
1:F:415:GLY:HA2	1:F:437:TYR:CD1	2.42	0.53
1:J:160:PHE:HE2	1:J:290:THR:CG2	2.18	0.53
1:T:312:ALA:HA	1:T:315:VAL:HB	1.91	0.53
1:V:69:LYS:O	1:V:74:ARG:NH1	2.41	0.53
1:X:162:ALA:HA	1:X:194:MET:HE1	1.90	0.53
1:5:260:GLY:O	1:5:388:GLU:HG3	2.09	0.53
1:A:265:ILE:HG12	1:A:405:LEU:HD11	1.91	0.53
1:D:263:PRO:HD2	1:D:418:ALA:HA	1.91	0.53
1:F:185:GLU:CD	1:F:185:GLU:H	2.10	0.53
1:I:431:VAL:O	1:I:435:LEU:HG	2.09	0.53
1:P:287:ASN:ND2	1:P:333:LEU:HD13	2.23	0.53
1:Y:264:PHE:HB2	1:Y:294:THR:CG2	2.38	0.53
1:Z:160:PHE:CE2	1:Z:290:THR:HG22	2.43	0.53
1:Y:479:TYR:HD2	1:2:439:MET:HG2	1.73	0.53
1:A:330:LEU:CD1	1:A:372:PRO:HG3	2.39	0.53
1:B:158:TRP:CD2	1:B:334:ILE:HD12	2.44	0.53
1:R:47:MET:HE3	1:R:51:GLU:HB3	1.91	0.53
1:4:393:LEU:O	1:4:395:PRO:HD3	2.08	0.53
1:E:429:TRP:CZ3	1:F:141:ARG:HG2	2.44	0.53
1:J:6:LYS:HD2	1:J:6:LYS:H	1.72	0.53
1:K:124:GLU:HG2	1:L:127:ARG:HH21	1.74	0.53
1:M:393:LEU:O	1:M:395:PRO:HD3	2.08	0.53
1:Q:52:THR:HB	1:Q:221:GLU:HG2	1.91	0.53
1:X:52:THR:OG1	1:X:218:ILE:HG23	2.09	0.53
1:X:28:ALA:O	1:X:46:LYS:HB3	2.08	0.53
1:J:157:PRO:HD2	1:J:164:MET:HG3	1.90	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:17:ILE:CD1	1:S:47:MET:HE3	2.39	0.53
1:Q:481:CYS:HB3	1:T:447:ILE:HG22	1.90	0.53
1:Z:336:GLU:OE1	1:Z:362:ARG:NH2	2.42	0.53
1:G:265:ILE:HG12	1:G:405:LEU:HD11	1.91	0.53
1:H:315:VAL:HG13	1:H:372:PRO:HB2	1.91	0.53
1:V:281:ALA:HB1	1:V:446:LEU:HD12	1.91	0.53
1:Y:158:TRP:O	1:Y:161:PRO:HD3	2.08	0.53
1:2:242:LEU:HD11	2:2:518:HOH:O	2.10	0.52
1:2:140:LYS:HA	1:2:482:VAL:O	2.08	0.52
1:K:286:ASN:HD22	1:K:290:THR:HG22	1.74	0.52
1:M:162:ALA:O	1:M:194:MET:HE1	2.09	0.52
1:V:47:MET:CE	1:V:51:GLU:HB3	2.39	0.52
1:Z:206:GLY:O	1:Z:208:LEU:N	2.40	0.52
1:M:121:PHE:HA	1:M:124:GLU:HB2	1.92	0.52
1:X:96:LEU:HD11	1:X:161:PRO:HD2	1.90	0.52
1:J:154:ALA:HB1	1:J:168:LYS:HD3	1.91	0.52
1:3:399:PHE:CZ	1:3:405:LEU:HD22	2.44	0.52
1:F:47:MET:HB2	1:F:212:ILE:O	2.09	0.52
1:W:47:MET:HE3	1:W:211:VAL:HG13	1.91	0.52
1:2:157:PRO:HD3	1:2:234:THR:HB	1.92	0.52
1:4:289:GLN:HE22	1:4:334:ILE:H	1.57	0.52
1:G:356:LEU:HD21	1:G:360:GLY:HA3	1.90	0.52
1:1:287:ASN:HD22	1:1:333:LEU:HD13	1.74	0.52
1:K:167:ARG:NH2	1:K:465:GLU:OE1	2.41	0.52
1:V:461:GLY:HA2	1:W:251:VAL:HG11	1.92	0.52
1:4:59:ALA:HB1	1:4:178:PRO:HB2	1.92	0.52
1:C:140:LYS:O	1:C:141:ARG:HD3	2.10	0.52
1:I:184:ALA:C	1:I:186:SER:H	2.11	0.52
1:X:26:SER:O	1:X:27:ASP:HB2	2.08	0.52
1:L:287:ASN:ND2	1:L:333:LEU:HD13	2.25	0.52
1:M:103:PRO:HA	1:M:323:GLY:HA2	1.92	0.52
1:T:152:CYS:SG	1:T:230:LYS:HG2	2.49	0.52
1:C:393:LEU:O	1:C:395:PRO:HD3	2.09	0.52
1:D:304:TYR:HE1	1:D:398:ARG:HB2	1.74	0.52
1:E:17:ILE:HD11	1:E:47:MET:HE1	1.92	0.52
1:K:157:PRO:HD3	1:K:234:THR:HB	1.91	0.52
1:3:265:ILE:CG2	1:3:405:LEU:HD21	2.39	0.52
1:A:477:ILE:HD11	1:D:453:PRO:CB	2.40	0.52
1:I:149:ILE:HD13	1:I:230:LYS:HB3	1.92	0.52
1:J:154:ALA:HB3	1:J:181:VAL:HG22	1.92	0.52
1:P:265:ILE:CG2	1:P:405:LEU:HD11	2.40	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:320:VAL:HG12	1:U:321:GLY:H	1.75	0.52
1:2:352:LYS:HD2	1:2:382:MET:HG2	1.92	0.51
1:3:477:ILE:HD11	1:6:453:PRO:HG3	1.92	0.51
1:F:424:ASP:O	1:F:428:VAL:HG23	2.10	0.51
1:Q:256:LEU:O	1:Q:461:GLY:HA3	2.09	0.51
1:Y:264:PHE:HB2	1:Y:294:THR:HG23	1.91	0.51
1:P:160:PHE:HE2	1:P:290:THR:HG22	1.75	0.51
1:W:429:TRP:HB2	1:X:484:VAL:HG21	1.92	0.51
1:1:338:ALA:O	1:1:342:VAL:HG23	2.11	0.51
1:5:256:LEU:O	1:5:461:GLY:HA3	2.10	0.51
1:B:47:MET:HE1	1:B:211:VAL:HG13	1.92	0.51
1:G:157:PRO:HD3	1:G:234:THR:HB	1.91	0.51
1:K:161:PRO:HB2	1:K:190:SER:HB2	1.91	0.51
1:R:47:MET:CE	1:R:211:VAL:HG13	2.39	0.51
1:U:265:ILE:HG12	1:U:405:LEU:HD11	1.91	0.51
1:X:63:TRP:CD1	1:X:178:PRO:HD3	2.46	0.51
1:1:273:ASP:OD1	1:1:273:ASP:N	2.43	0.51
1:1:127:ARG:HH21	1:2:124:GLU:HG2	1.75	0.51
1:T:37:THR:OG1	1:T:39:GLU:HG2	2.11	0.51
1:V:423:ARG:HG3	1:X:424:ASP:OD1	2.09	0.51
1:V:59:ALA:HB1	1:V:178:PRO:HB2	1.91	0.51
1:4:361:LYS:O	1:4:371:GLU:HB2	2.09	0.51
1:A:204:PRO:HG2	1:A:207:VAL:HG21	1.92	0.51
1:E:364:ALA:CB	1:J:9:SER:HB3	2.41	0.51
1:M:265:ILE:HG23	1:M:405:LEU:CD1	2.41	0.51
1:R:423:ARG:HG3	1:T:424:ASP:OD1	2.11	0.51
1:U:455:GLY:HA3	1:U:464:ARG:HD3	1.93	0.51
1:1:17:ILE:CD1	1:1:211:VAL:HG12	2.40	0.51
1:2:84:LEU:HB3	1:2:197:LEU:HD22	1.93	0.51
1:4:221:GLU:O	1:4:225:ASN:HB2	2.10	0.51
1:Q:464:ARG:HG3	1:T:477:ILE:HD11	1.93	0.51
1:Y:265:ILE:HG21	1:Y:405:LEU:CD2	2.36	0.51
1:A:476:VAL:CG2	1:D:457:VAL:HG12	2.40	0.51
1:B:234:THR:HG23	1:B:257:GLU:HB3	1.93	0.51
1:D:336:GLU:OE1	1:D:362:ARG:NH2	2.44	0.51
1:H:147:GLU:HB2	1:H:148:PRO:HD2	1.92	0.51
1:S:47:MET:HG2	1:S:51:GLU:HG2	1.92	0.51
1:Y:20:GLU:HG2	2:Y:519:HOH:O	2.10	0.51
1:2:190:SER:O	1:2:194:MET:HG2	2.10	0.51
1:O:84:LEU:HB3	1:O:197:LEU:HD22	1.92	0.51
1:U:214:ASP:HB3	1:U:217:ALA:HB3	1.92	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:241:ARG:NE	1:1:249:PRO:O	2.42	0.51
1:T:96:LEU:HD21	1:T:102:LYS:HE3	1.91	0.51
1:Z:476:VAL:CG2	1:1:457:VAL:HG12	2.41	0.51
1:B:425:ILE:HG12	1:D:425:ILE:HG12	1.93	0.51
1:H:37:THR:HB	1:H:39:GLU:HG2	1.92	0.51
1:M:311:LEU:O	1:M:315:VAL:HG23	2.11	0.51
1:V:157:PRO:HD2	1:V:164:MET:HG3	1.93	0.51
1:Y:283:LYS:HE2	1:Y:393:LEU:H	1.74	0.51
1:5:63:TRP:O	1:5:67:ARG:HG2	2.11	0.50
1:A:287:ASN:ND2	1:A:333:LEU:HD13	2.26	0.50
1:E:287:ASN:ND2	1:E:333:LEU:HD13	2.26	0.50
1:D:242:LEU:CD2	1:1:26:SER:HA	2.13	0.50
1:6:349:ALA:HA	1:6:382:MET:HG2	1.93	0.50
1:E:453:PRO:HB2	1:H:477:ILE:HD11	1.93	0.50
1:R:461:GLY:HA2	1:S:251:VAL:HG11	1.93	0.50
1:V:263:PRO:HA	1:V:296:ARG:O	2.11	0.50
1:Z:30:PHE:HD2	1:Z:46:LYS:HG3	1.76	0.50
1:A:230:LYS:HB2	1:A:253:LYS:HB3	1.93	0.50
1:O:147:GLU:HB2	1:O:148:PRO:HD2	1.93	0.50
1:U:310:LYS:HD2	2:U:513:HOH:O	2.11	0.50
1:2:76:ALA:O	1:2:80:ARG:HG3	2.11	0.50
1:4:482:VAL:HG22	1:5:442:ILE:HD12	1.92	0.50
1:C:17:ILE:CD1	1:C:211:VAL:HG12	2.42	0.50
1:E:79:ARG:NH2	1:E:119:GLU:HG3	2.26	0.50
1:L:336:GLU:OE1	1:L:362:ARG:NH1	2.30	0.50
1:M:186:SER:CB	1:M:334:ILE:HD11	2.42	0.50
1:2:47:MET:HE2	1:2:51:GLU:HB2	1.93	0.50
1:3:113:TYR:OH	1:3:448:SER:HB3	2.12	0.50
1:R:266:VAL:HB	1:R:299:VAL:HG13	1.93	0.50
1:U:289:GLN:HG2	1:U:390:PHE:O	2.12	0.50
1:W:121:PHE:HA	1:W:124:GLU:HB2	1.93	0.50
1:Y:281:ALA:HB1	1:Y:446:LEU:HD21	1.94	0.50
1:Z:126:LYS:C	1:2:134:PRO:HG2	2.32	0.50
1:B:306:ALA:O	1:B:310:LYS:HG3	2.12	0.50
1:L:168:LYS:HD3	1:L:232:SER:OG	2.11	0.50
1:P:182:LYS:HE3	1:P:215:PRO:HA	1.93	0.50
1:Q:444:THR:OG1	1:T:140:LYS:NZ	2.44	0.50
1:T:262:ALA:HB3	1:T:294:THR:HA	1.94	0.50
1:U:361:LYS:O	1:U:371:GLU:HB2	2.11	0.50
1:V:269:ASP:O	1:V:423:ARG:HB2	2.12	0.50
1:C:336:GLU:OE1	1:C:362:ARG:NH2	2.45	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:17:ILE:HD11	1:F:47:MET:CE	2.42	0.50
1:U:211:VAL:HG12	1:U:218:ILE:HD13	1.93	0.50
1:Y:90:ASP:HA	1:Y:108:LYS:HZ1	1.76	0.50
1:Z:424:ASP:OD1	1:2:423:ARG:HG3	2.12	0.50
1:2:45:PRO:O	1:2:212:ILE:HG22	2.11	0.50
1:4:453:PRO:CB	1:5:477:ILE:HD11	2.41	0.50
1:5:393:LEU:O	1:5:395:PRO:HD3	2.12	0.50
1:E:246:GLN:NE2	2:E:534:HOH:O	2.42	0.50
1:H:154:ALA:HA	1:H:232:SER:O	2.11	0.50
1:J:107:ALA:O	1:J:111:ILE:HG12	2.12	0.50
1:S:16:TYR:CZ	1:S:19:GLY:HA2	2.47	0.50
1:T:6:LYS:H	1:T:6:LYS:HD2	1.76	0.50
1:X:338:ALA:O	1:X:342:VAL:HG23	2.12	0.50
1:Y:141:ARG:HG3	1:Z:429:TRP:CZ3	2.47	0.50
1:4:410:ASN:O	1:4:412:THR:N	2.43	0.50
1:I:136:PRO:HG3	1:L:451:VAL:CG1	2.42	0.49
1:O:154:ALA:HB3	1:O:181:VAL:HG22	1.94	0.49
1:Y:311:LEU:O	1:Y:315:VAL:HG23	2.12	0.49
1:Z:184:ALA:C	1:Z:186:SER:H	2.14	0.49
1:Z:192:LEU:CD1	1:Z:212:ILE:HD11	2.26	0.49
1:1:17:ILE:HD11	1:1:211:VAL:HG12	1.94	0.49
1:2:160:PHE:HE2	1:2:290:THR:HG22	1.77	0.49
1:6:413:GLU:CB	1:6:459:GLN:HG3	2.42	0.49
1:C:152:CYS:SG	1:C:230:LYS:HG2	2.53	0.49
1:M:192:LEU:HD11	1:M:212:ILE:HD12	1.94	0.49
1:4:263:PRO:HA	1:4:296:ARG:O	2.11	0.49
1:6:265:ILE:HG12	1:6:405:LEU:HD11	1.93	0.49
1:A:169:VAL:HG13	1:A:173:LEU:HD13	1.93	0.49
1:A:330:LEU:HD13	1:A:372:PRO:HG3	1.93	0.49
1:B:119:GLU:O	1:B:123:GLU:HG3	2.11	0.49
1:E:123:GLU:HB2	1:F:127:ARG:HH22	1.77	0.49
1:K:168:LYS:HE2	1:K:465:GLU:OE2	2.13	0.49
1:U:152:CYS:HB2	1:U:179:ILE:HG13	1.94	0.49
1:O:288:GLY:HA2	1:O:293:CYS:SG	2.52	0.49
1:2:230:LYS:NZ	1:2:255:THR:OG1	2.44	0.49
1:K:265:ILE:HG12	1:K:405:LEU:HD11	1.95	0.49
1:X:451:VAL:O	1:X:467:SER:HB3	2.13	0.49
1:Z:198:ALA:HB1	1:Z:203:VAL:HG21	1.93	0.49
1:H:161:PRO:O	1:H:165:ILE:HD13	2.12	0.49
1:O:268:ASP:N	1:O:268:ASP:OD2	2.39	0.49
1:T:59:ALA:HA	1:T:206:GLY:O	2.12	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:404:GLU:HG2	1:T:408:LEU:HD22	1.94	0.49
1:K:17:ILE:CD1	1:K:211:VAL:HG22	2.42	0.49
1:O:276:VAL:O	1:O:280:ILE:HG12	2.13	0.49
1:R:17:ILE:HD11	1:R:47:MET:HE1	1.94	0.49
1:2:138:ALA:O	1:2:139:ASN:CB	2.61	0.49
1:S:63:TRP:CD1	1:S:178:PRO:HD3	2.47	0.49
1:X:342:VAL:O	1:X:346:ILE:HG13	2.13	0.49
1:3:429:TRP:CZ3	1:4:141:ARG:HG2	2.48	0.49
1:A:405:LEU:O	1:A:405:LEU:HG	2.09	0.49
1:F:451:VAL:HG22	1:G:142:ILE:HD13	1.95	0.49
1:Q:101:GLY:O	1:Q:332:PRO:HD2	2.13	0.49
1:W:429:TRP:CB	1:X:484:VAL:HG21	2.43	0.49
1:4:334:ILE:O	1:4:334:ILE:HD13	2.12	0.49
1:F:161:PRO:HB2	1:F:190:SER:HB2	1.93	0.49
1:H:375:LEU:HD12	1:H:393:LEU:HD11	1.94	0.49
1:I:421:TYR:HA	1:I:443:ASN:OD1	2.13	0.49
1:M:254:LEU:HD23	1:M:256:LEU:HD11	1.95	0.49
1:5:45:PRO:O	1:5:212:ILE:HG22	2.13	0.48
1:B:157:PRO:HD3	1:B:234:THR:HB	1.95	0.48
1:G:276:VAL:HG21	1:G:310:LYS:HB3	1.94	0.48
1:P:161:PRO:O	1:P:165:ILE:HD13	2.12	0.48
1:M:477:ILE:HD11	1:P:453:PRO:CB	2.43	0.48
1:Q:154:ALA:HB3	1:Q:181:VAL:HG22	1.95	0.48
1:V:422:SER:OG	1:V:427:ARG:HD2	2.13	0.48
1:W:15:ALA:CB	1:W:47:MET:HE1	2.43	0.48
1:Y:29:THR:OG1	1:Y:43:THR:HB	2.13	0.48
1:2:349:ALA:O	1:2:352:LYS:HB2	2.13	0.48
1:C:265:ILE:HG21	1:C:405:LEU:HD21	1.95	0.48
1:I:17:ILE:HD11	1:I:47:MET:HE1	1.95	0.48
1:K:269:ASP:CG	1:K:427:ARG:HH12	2.16	0.48
1:R:447:ILE:HG22	1:S:481:CYS:HB3	1.95	0.48
1:V:110:GLU:HG3	1:V:163:ALA:HB2	1.93	0.48
1:X:380:PRO:HA	1:X:397:PHE:HE1	1.79	0.48
1:2:47:MET:HB2	1:2:212:ILE:O	2.13	0.48
1:I:266:VAL:HB	1:I:299:VAL:HG13	1.95	0.48
1:M:342:VAL:O	1:M:346:ILE:HG13	2.13	0.48
1:N:182:LYS:NZ	1:N:183:PRO:O	2.44	0.48
1:N:375:LEU:HD12	1:N:393:LEU:HD11	1.95	0.48
1:Q:251:VAL:HG12	1:Q:251:VAL:O	2.12	0.48
1:Y:298:PHE:HE1	1:Y:408:LEU:HD23	1.77	0.48
1:J:315:VAL:HG13	1:J:372:PRO:HB2	1.94	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:154:ALA:HB1	1:L:168:LYS:HD2	1.95	0.48
1:N:192:LEU:HD11	1:N:212:ILE:CD1	2.43	0.48
1:P:147:GLU:HB2	1:P:148:PRO:HD2	1.95	0.48
1:Q:480:LEU:HD23	1:T:440:VAL:HB	1.94	0.48
1:F:265:ILE:HG12	1:F:405:LEU:HD11	1.94	0.48
1:M:36:ALA:HB2	1:M:332:PRO:HG3	1.96	0.48
1:S:128:VAL:HG11	1:S:475:VAL:HG11	1.96	0.48
1:V:47:MET:HE1	1:V:211:VAL:HG13	1.94	0.48
1:V:372:PRO:HA	1:V:392:PRO:HB2	1.95	0.48
1:X:407:ARG:O	1:X:411:ASP:HB2	2.13	0.48
1:3:17:ILE:CD1	1:3:211:VAL:HG12	2.44	0.48
1:J:172:ALA:O	1:J:177:CYS:HB2	2.13	0.48
1:K:465:GLU:HG2	2:K:505:HOH:O	2.12	0.48
1:Z:149:ILE:HG23	1:Z:150:GLY:N	2.28	0.48
1:D:304:TYR:CE1	1:D:398:ARG:HB2	2.49	0.48
1:X:415:GLY:HA2	1:X:437:TYR:CE1	2.49	0.48
1:5:37:THR:OG1	1:5:39:GLU:HG2	2.13	0.48
1:J:102:LYS:NZ	1:J:110:GLU:OE1	2.37	0.48
1:Q:421:TYR:HA	1:Q:443:ASN:OD1	2.13	0.48
1:Z:160:PHE:HE2	1:Z:290:THR:HG22	1.79	0.48
1:2:256:LEU:O	1:2:461:GLY:HA3	2.13	0.48
1:4:248:ALA:HB3	1:4:249:PRO:HD3	1.96	0.48
1:I:97:THR:HG23	1:I:323:GLY:HA3	1.96	0.48
1:J:47:MET:H	1:J:213:GLY:HA3	1.79	0.48
1:M:158:TRP:CD2	1:M:334:ILE:HD12	2.48	0.48
1:P:63:TRP:CZ2	1:P:150:GLY:HA2	2.49	0.48
1:X:52:THR:HB	1:X:221:GLU:HG2	1.95	0.48
1:4:264:PHE:HB2	1:4:294:THR:CG2	2.43	0.48
1:F:3:GLY:N	2:F:536:HOH:O	2.46	0.48
1:I:47:MET:HG2	1:I:51:GLU:HG2	1.96	0.48
1:M:157:PRO:HD3	1:M:234:THR:HB	1.96	0.48
1:H:37:THR:HG21	1:H:39:GLU:OE2	2.14	0.47
1:L:384:VAL:HG21	1:L:395:PRO:HG3	1.96	0.47
1:R:16:TYR:CZ	1:R:19:GLY:HA2	2.49	0.47
1:V:47:MET:HE2	1:V:51:GLU:HB2	1.95	0.47
1:Y:142:ILE:HD13	1:2:452:ALA:HB2	1.96	0.47
1:3:444:THR:HB	1:6:483:ALA:HB2	1.95	0.47
1:4:163:ALA:O	1:4:167:ARG:HB2	2.14	0.47
1:C:16:TYR:CZ	1:C:19:GLY:HA2	2.49	0.47
1:D:242:LEU:HB2	2:D:503:HOH:O	2.14	0.47
1:I:404:GLU:HA	1:I:407:ARG:HH12	1.79	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:287:ASN:ND2	1:K:333:LEU:HD12	2.29	0.47
1:U:439:MET:HG2	1:X:479:TYR:HD2	1.79	0.47
1:O:349:ALA:HA	1:O:382:MET:SD	2.55	0.47
1:V:70:THR:OG1	1:V:73:GLU:HB2	2.14	0.47
1:U:483:ALA:HB2	1:X:444:THR:HB	1.96	0.47
1:X:81:TRP:HZ2	1:X:194:MET:HB3	1.78	0.47
1:Y:429:TRP:CZ3	1:Z:141:ARG:HG2	2.49	0.47
1:2:147:GLU:HB2	1:2:148:PRO:HD2	1.97	0.47
1:F:425:ILE:HD12	1:H:425:ILE:HG12	1.97	0.47
1:H:157:PRO:HD3	1:H:234:THR:HB	1.96	0.47
1:J:372:PRO:HA	1:J:392:PRO:HB2	1.97	0.47
1:J:37:THR:OG1	1:J:39:GLU:HG3	2.15	0.47
1:T:162:ALA:HA	1:T:194:MET:HE1	1.96	0.47
1:A:160:PHE:HE2	1:A:290:THR:HG22	1.80	0.47
1:A:300:HIS:ND1	1:A:302:ARG:HG3	2.29	0.47
1:D:114:ALA:HB2	1:D:163:ALA:HA	1.97	0.47
1:G:127:ARG:HH21	1:H:124:GLU:HG2	1.79	0.47
1:O:393:LEU:O	1:O:395:PRO:HD3	2.15	0.47
1:4:251:VAL:HG13	1:4:251:VAL:O	2.14	0.47
1:B:167:ARG:NH2	1:B:465:GLU:OE1	2.48	0.47
1:P:186:SER:HB3	1:P:334:ILE:HD11	1.97	0.47
1:R:283:LYS:HE2	1:R:393:LEU:O	2.14	0.47
1:R:424:ASP:OD1	1:T:423:ARG:HG3	2.15	0.47
1:3:356:LEU:HD11	1:3:359:GLY:O	2.15	0.47
1:G:103:PRO:HG2	1:G:106:GLU:HG3	1.96	0.47
1:J:121:PHE:HA	1:J:124:GLU:HB2	1.95	0.47
1:J:462:LEU:HD21	1:K:251:VAL:O	2.15	0.47
1:S:167:ARG:NH2	1:S:465:GLU:OE1	2.48	0.47
1:U:91:ASP:OD2	1:U:91:ASP:N	2.46	0.47
1:2:47:MET:HE3	1:2:51:GLU:HB3	1.97	0.47
1:3:167:ARG:NH2	1:3:465:GLU:OE1	2.48	0.47
1:4:3:GLY:N	2:4:509:HOH:O	2.46	0.47
1:F:183:PRO:HD2	1:F:211:VAL:O	2.15	0.47
1:L:47:MET:HE3	1:L:51:GLU:HB3	1.97	0.47
1:R:121:PHE:HA	1:R:124:GLU:HB2	1.97	0.47
1:V:161:PRO:O	1:V:165:ILE:HD13	2.14	0.47
1:W:3:GLY:N	2:W:501:HOH:O	2.47	0.47
1:X:81:TRP:O	1:X:85:VAL:HG23	2.15	0.47
1:Z:334:ILE:HG23	1:Z:335:ASN:N	2.24	0.47
1:2:404:GLU:HG2	1:2:408:LEU:HD22	1.96	0.47
1:F:195:ALA:HB2	1:F:210:VAL:HG21	1.97	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:84:LEU:HB3	1:K:197:LEU:HD22	1.97	0.47
1:P:121:PHE:CD2	1:P:171:PRO:HD3	2.50	0.47
1:Q:415:GLY:HA2	1:Q:437:TYR:CD1	2.50	0.47
1:Z:254:LEU:HD23	1:Z:256:LEU:HD11	1.96	0.47
1:2:358:THR:HA	1:3:309:ASP:OD1	2.15	0.47
1:3:423:ARG:HG3	1:5:424:ASP:OD1	2.15	0.47
1:3:477:ILE:HD11	1:6:453:PRO:CG	2.45	0.47
1:5:272:LEU:H	1:5:272:LEU:HD22	1.80	0.47
1:6:63:TRP:CZ2	1:6:150:GLY:HA2	2.50	0.47
1:A:127:ARG:HH21	1:B:124:GLU:HG2	1.80	0.47
1:T:421:TYR:HA	1:T:443:ASN:OD1	2.13	0.47
1:W:265:ILE:HG12	1:W:405:LEU:HD11	1.95	0.47
1:B:26:SER:O	1:B:27:ASP:HB2	2.15	0.47
1:H:413:GLU:CB	1:H:459:GLN:HG3	2.44	0.47
1:J:195:ALA:HB2	1:J:210:VAL:HG21	1.96	0.47
1:K:81:TRP:O	1:K:85:VAL:HG23	2.15	0.47
1:P:330:LEU:HD13	1:P:372:PRO:HG3	1.97	0.47
1:S:130:GLY:HA3	1:S:144:VAL:O	2.15	0.47
1:Y:93:ALA:CB	1:Y:108:LYS:HG2	2.45	0.47
1:Y:244:MET:HA	1:Y:254:LEU:HD21	1.97	0.47
1:3:130:GLY:HA3	1:5:132:THR:OG1	2.16	0.46
1:C:356:LEU:HD21	1:C:360:GLY:HA3	1.97	0.46
1:E:97:THR:HG23	1:E:323:GLY:HA3	1.95	0.46
1:Y:110:GLU:HG3	1:Y:163:ALA:HB2	1.98	0.46
1:Y:427:ARG:HG3	1:Y:430:ARG:NH2	2.29	0.46
1:2:107:ALA:O	1:2:111:ILE:HG12	2.15	0.46
1:D:158:TRP:CD2	1:D:334:ILE:HD12	2.50	0.46
1:L:186:SER:HB2	2:L:502:HOH:O	2.15	0.46
1:I:418:ALA:O	1:I:440:VAL:HA	2.15	0.46
1:L:466:GLY:HA3	2:L:513:HOH:O	2.16	0.46
1:M:107:ALA:O	1:M:111:ILE:HG12	2.16	0.46
1:Z:132:THR:OG1	1:2:130:GLY:HA3	2.14	0.46
1:1:63:TRP:CD1	1:1:178:PRO:HD3	2.51	0.46
1:F:234:THR:HG23	1:F:257:GLU:HB2	1.96	0.46
1:G:84:LEU:HB3	1:G:197:LEU:HD22	1.96	0.46
1:Q:265:ILE:CG2	1:Q:405:LEU:HD11	2.41	0.46
1:R:455:GLY:HA3	1:R:464:ARG:HD3	1.98	0.46
1:T:147:GLU:HB2	1:T:148:PRO:HD2	1.98	0.46
1:2:288:GLY:HA2	1:2:293:CYS:SG	2.56	0.46
1:3:442:ILE:HD12	1:6:482:VAL:HG22	1.96	0.46
1:4:182:LYS:HE2	1:4:215:PRO:HA	1.96	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:VAL:HA	1:A:178:PRO:HG2	1.96	0.46
1:I:335:ASN:HD21	1:I:337:ALA:HB3	1.81	0.46
1:L:152:CYS:SG	1:L:230:LYS:HG2	2.56	0.46
1:Q:146:LYS:HG2	1:Q:477:ILE:HG22	1.98	0.46
1:V:320:VAL:HG22	1:V:330:LEU:HB2	1.97	0.46
1:2:215:PRO:HG3	2:2:506:HOH:O	2.15	0.46
1:I:157:PRO:HD3	1:I:234:THR:HB	1.97	0.46
1:J:290:THR:OG1	1:J:293:CYS:SG	2.59	0.46
1:J:476:VAL:HG21	1:K:457:VAL:HG12	1.97	0.46
1:W:429:TRP:HZ3	1:X:141:ARG:HG2	1.80	0.46
1:Y:477:ILE:HG23	2:Y:510:HOH:O	2.16	0.46
1:U:84:LEU:HB3	1:U:197:LEU:HD22	1.97	0.46
1:X:455:GLY:HA3	1:X:464:ARG:HD3	1.97	0.46
1:Y:285:ARG:C	1:Y:287:ASN:H	2.19	0.46
1:Z:154:ALA:HB3	1:Z:181:VAL:HG22	1.98	0.46
1:G:17:ILE:HD11	1:G:47:MET:CE	2.46	0.46
1:I:404:GLU:HA	1:I:407:ARG:NH1	2.31	0.46
1:O:127:ARG:HH21	1:P:124:GLU:HG2	1.81	0.46
1:R:47:MET:CE	1:R:51:GLU:HB3	2.45	0.46
1:S:47:MET:CE	1:S:211:VAL:HG13	2.46	0.46
1:Y:131:ASP:OD1	1:Y:131:ASP:N	2.48	0.46
1:Z:387:GLU:HA	2:Z:519:HOH:O	2.15	0.46
1:2:47:MET:HE1	1:2:211:VAL:HG13	1.98	0.46
1:6:3:GLY:CA	2:6:550:HOH:O	2.63	0.46
1:D:89:SER:HB2	1:D:111:ILE:HG21	1.97	0.46
1:J:192:LEU:HD11	1:J:212:ILE:HD12	1.97	0.46
1:O:161:PRO:HB2	1:O:190:SER:HB2	1.96	0.46
1:P:160:PHE:CE2	1:P:290:THR:HG22	2.51	0.46
1:S:267:PHE:HE2	1:S:420:LEU:HD11	1.79	0.46
1:T:121:PHE:HA	1:T:124:GLU:HB2	1.98	0.46
1:U:123:GLU:HG2	1:V:123:GLU:CD	2.37	0.46
1:W:131:ASP:HB2	1:W:144:VAL:HB	1.97	0.46
1:Y:361:LYS:O	1:Y:371:GLU:HB2	2.16	0.46
1:Z:155:ILE:HG23	1:Z:182:LYS:HD2	1.98	0.46
1:G:158:TRP:O	1:G:161:PRO:HG3	2.16	0.46
1:H:172:ALA:O	1:H:177:CYS:HB2	2.16	0.46
1:R:480:LEU:HD23	1:S:440:VAL:HB	1.98	0.46
1:T:63:TRP:CD1	1:T:178:PRO:HD3	2.51	0.46
1:Z:214:ASP:HB3	1:Z:217:ALA:HB3	1.97	0.46
1:6:17:ILE:HG23	1:6:55:ALA:HB2	1.98	0.45
1:F:47:MET:HE3	1:F:51:GLU:HB3	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:127:ARG:HH22	1:J:123:GLU:HB2	1.80	0.45
1:E:401:SER:HB3	1:N:357:MET:HG3	1.98	0.45
1:N:477:ILE:HD11	1:O:453:PRO:HB2	1.98	0.45
1:S:268:ASP:N	1:S:268:ASP:OD2	2.47	0.45
1:V:482:VAL:HA	1:W:442:ILE:HB	1.96	0.45
1:5:234:THR:HA	1:5:257:GLU:O	2.15	0.45
1:B:450:GLU:HG2	1:B:451:VAL:HG12	1.98	0.45
1:D:423:ARG:HA	1:D:423:ARG:HD2	1.76	0.45
1:I:378:VAL:HG13	1:I:382:MET:SD	2.56	0.45
1:N:356:LEU:HD11	1:N:360:GLY:HA3	1.98	0.45
1:S:36:ALA:HB2	1:S:332:PRO:HG3	1.97	0.45
1:W:17:ILE:HD11	1:W:47:MET:HE3	1.98	0.45
1:X:301:GLU:HG2	1:X:398:ARG:HD3	1.98	0.45
1:G:283:LYS:O	1:G:288:GLY:HA2	2.15	0.45
1:W:404:GLU:HG2	1:W:408:LEU:HD22	1.97	0.45
1:Z:32:VAL:HG12	1:Z:33:PHE:H	1.81	0.45
1:2:157:PRO:CD	1:2:164:MET:HG3	2.45	0.45
1:A:234:THR:HG23	1:A:257:GLU:HB2	1.98	0.45
1:C:17:ILE:O	1:C:20:GLU:N	2.45	0.45
1:E:476:VAL:CG2	1:H:457:VAL:HG12	2.47	0.45
1:I:157:PRO:HD2	1:I:164:MET:HG3	1.97	0.45
1:T:10:LEU:O	1:T:12:ARG:HG2	2.16	0.45
1:U:336:GLU:OE1	1:U:362:ARG:NH2	2.47	0.45
1:U:443:ASN:HB2	1:X:483:ALA:HB3	1.98	0.45
1:2:129:ALA:O	1:2:146:LYS:HD2	2.17	0.45
1:R:155:ILE:HG12	1:R:182:LYS:HE3	1.98	0.45
1:U:420:LEU:HD13	1:U:431:VAL:HG11	1.98	0.45
1:X:72:LYS:HA	1:X:126:LYS:HD3	1.99	0.45
1:Y:275:ALA:HA	1:Y:421:TYR:CE1	2.52	0.45
1:1:81:TRP:O	1:1:85:VAL:HG23	2.17	0.45
1:2:70:THR:OG1	1:2:73:GLU:HB2	2.16	0.45
1:Q:287:ASN:ND2	1:Q:331:GLY:O	2.50	0.45
1:V:251:VAL:O	1:V:251:VAL:CG1	2.64	0.45
1:Y:440:VAL:HB	1:2:480:LEU:HD23	1.99	0.45
1:3:158:TRP:O	1:3:161:PRO:HD3	2.17	0.45
1:4:155:ILE:HD12	1:4:231:LEU:HD11	1.99	0.45
1:4:426:GLY:O	1:4:430:ARG:HG3	2.16	0.45
1:3:479:TYR:HD2	1:6:439:MET:HG2	1.81	0.45
1:F:415:GLY:HA2	1:F:437:TYR:CE1	2.51	0.45
1:I:46:LYS:HA	1:I:213:GLY:HA2	1.98	0.45
1:O:450:GLU:OE1	1:O:450:GLU:N	2.47	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:404:GLU:HG2	1:P:408:LEU:HD22	1.99	0.45
1:P:97:THR:HG23	1:P:102:LYS:O	2.17	0.45
1:V:47:MET:HE2	1:V:51:GLU:CB	2.47	0.45
1:Y:234:THR:HA	1:Y:257:GLU:O	2.17	0.45
1:E:157:PRO:HD3	1:E:234:THR:HB	1.99	0.45
1:O:168:LYS:HE2	1:O:465:GLU:OE2	2.15	0.45
1:N:423:ARG:HG3	1:P:424:ASP:OD1	2.15	0.45
1:V:300:HIS:HB3	1:V:303:VAL:HG22	1.99	0.45
1:W:47:MET:HE2	1:W:212:ILE:H	1.82	0.45
1:Y:269:ASP:OD1	1:Y:269:ASP:N	2.49	0.45
1:Y:451:VAL:O	1:Y:467:SER:HB3	2.17	0.45
1:Z:20:GLU:HB3	1:Z:22:GLN:NE2	2.31	0.45
1:1:287:ASN:ND2	1:1:333:LEU:HD13	2.32	0.45
1:F:64:ALA:O	1:F:68:MET:HB2	2.17	0.45
1:J:263:PRO:HA	1:J:296:ARG:O	2.16	0.45
1:L:225:ASN:O	1:L:252:LYS:NZ	2.50	0.45
1:Q:290:THR:O	1:Q:293:CYS:HB2	2.16	0.45
1:Y:90:ASP:HA	1:Y:108:LYS:HZ3	1.81	0.45
1:2:17:ILE:HD11	1:2:47:MET:HE1	1.98	0.45
1:3:69:LYS:O	1:3:74:ARG:NH1	2.49	0.45
1:H:157:PRO:HD2	1:H:164:MET:HG3	1.99	0.45
1:J:5:MET:CE	1:J:8:PRO:HA	2.47	0.45
1:N:59:ALA:HB1	1:N:178:PRO:HB2	1.99	0.45
1:U:157:PRO:HD3	1:U:234:THR:HB	1.98	0.45
1:E:358:THR:HG22	1:E:374:VAL:HB	1.99	0.44
1:E:265:ILE:HG12	1:E:405:LEU:HD11	1.99	0.44
1:G:129:ALA:O	1:G:146:LYS:NZ	2.37	0.44
1:I:246:GLN:O	1:I:249:PRO:HD2	2.17	0.44
1:J:287:ASN:HD22	1:J:330:LEU:HD22	1.82	0.44
1:J:451:VAL:O	1:J:467:SER:HB3	2.18	0.44
1:Y:26:SER:C	1:Y:28:ALA:H	2.09	0.44
1:4:428:VAL:HG13	1:4:442:ILE:HD13	1.99	0.44
1:G:47:MET:HE3	1:G:51:GLU:HB3	1.99	0.44
1:Q:18:GLY:HA2	1:Q:206:GLY:HA2	1.99	0.44
1:4:256:LEU:O	1:4:461:GLY:HA3	2.18	0.44
1:F:17:ILE:HD11	1:F:47:MET:HE3	1.99	0.44
1:M:153:ALA:HA	1:M:180:VAL:O	2.17	0.44
1:V:439:MET:HG2	1:W:479:TYR:HD2	1.82	0.44
1:X:157:PRO:HD2	1:X:164:MET:HG3	1.99	0.44
1:1:157:PRO:HD3	1:1:234:THR:HB	2.00	0.44
1:X:404:GLU:O	1:X:408:LEU:HB2	2.16	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:152:CYS:SG	1:1:230:LYS:HB3	2.58	0.44
1:3:162:ALA:HA	1:3:194:MET:HE1	2.00	0.44
1:A:107:ALA:O	1:A:111:ILE:HG12	2.18	0.44
1:A:157:PRO:HD3	1:A:234:THR:HB	1.99	0.44
1:D:237:THR:HG1	1:D:414:PHE:HE1	1.64	0.44
1:H:283:LYS:HD3	1:H:393:LEU:O	2.17	0.44
1:L:121:PHE:HA	1:L:124:GLU:HB2	2.00	0.44
1:L:389:THR:HG21	1:L:393:LEU:HB3	2.00	0.44
1:U:154:ALA:HB1	1:U:168:LYS:HD3	2.00	0.44
1:Z:46:LYS:HA	1:Z:213:GLY:HA2	1.99	0.44
1:J:17:ILE:HD11	1:J:47:MET:HE3	1.99	0.44
1:T:415:GLY:HA2	1:T:437:TYR:CE1	2.53	0.44
1:Z:263:PRO:HA	1:Z:296:ARG:O	2.17	0.44
1:2:46:LYS:HA	1:2:213:GLY:HA2	1.99	0.44
1:5:192:LEU:HD21	1:5:212:ILE:HD13	2.00	0.44
1:C:155:ILE:HG23	1:C:182:LYS:HD3	2.00	0.44
1:C:182:LYS:O	1:C:182:LYS:HD3	2.18	0.44
1:C:185:GLU:OE2	1:C:215:PRO:HB3	2.16	0.44
1:M:158:TRP:CG	1:M:334:ILE:HD12	2.53	0.44
1:Q:477:ILE:HD11	1:T:464:ARG:HG3	1.98	0.44
1:Q:457:VAL:HG12	1:T:476:VAL:HG21	1.98	0.44
1:W:128:VAL:HG11	1:W:475:VAL:HG11	2.00	0.44
1:Z:479:TYR:HB3	1:1:439:MET:HG2	1.99	0.44
1:Y:140:LYS:NZ	1:2:446:LEU:O	2.36	0.44
1:3:439:MET:HB3	1:3:447:ILE:HD12	2.00	0.44
1:4:260:GLY:HA2	1:4:414:PHE:HB3	2.00	0.44
1:4:136:PRO:HG3	1:5:451:VAL:HG13	2.00	0.44
1:C:17:ILE:HD11	1:C:47:MET:CE	2.47	0.44
1:F:285:ARG:HE	1:F:285:ARG:HB2	1.49	0.44
1:I:160:PHE:HE2	1:I:290:THR:HG22	1.83	0.44
1:M:272:LEU:H	1:M:272:LEU:HD22	1.83	0.44
1:M:389:THR:HG21	1:M:393:LEU:HB3	1.98	0.44
1:N:90:ASP:OD1	1:N:108:LYS:HE2	2.18	0.44
1:O:477:ILE:C	1:O:477:ILE:HD12	2.38	0.44
1:Z:356:LEU:HD12	1:Z:375:LEU:HD23	2.00	0.44
1:H:315:VAL:CG1	1:H:372:PRO:HB2	2.48	0.44
1:I:81:TRP:CZ2	1:I:194:MET:HG3	2.53	0.44
1:I:265:ILE:HD13	1:I:405:LEU:HD21	1.99	0.44
1:J:79:ARG:HH22	1:J:119:GLU:HG3	1.83	0.44
1:Q:439:MET:HG2	1:T:479:TYR:HD2	1.82	0.44
1:S:121:PHE:HA	1:S:124:GLU:HB2	2.00	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:254:LEU:HD12	1:S:256:LEU:HD21	2.00	0.44
1:T:168:LYS:HE2	1:T:465:GLU:OE2	2.18	0.44
1:U:153:ALA:HA	1:U:180:VAL:O	2.17	0.44
1:Y:405:LEU:HG	1:Y:405:LEU:O	2.18	0.44
1:Z:117:PHE:CE1	1:Z:167:ARG:HG3	2.52	0.44
1:Z:19:GLY:HA3	2:Z:510:HOH:O	2.18	0.44
1:D:121:PHE:HA	1:D:124:GLU:HB2	1.99	0.43
1:P:301:GLU:HG3	1:P:399:PHE:O	2.18	0.43
1:S:183:PRO:HD2	1:S:211:VAL:O	2.19	0.43
1:3:345:HIS:CE1	1:3:387:GLU:HB3	2.52	0.43
1:B:185:GLU:CD	1:B:215:PRO:HG3	2.39	0.43
1:I:325:GLU:HG2	1:I:326:SER:N	2.32	0.43
1:I:453:PRO:HB2	1:L:477:ILE:HD11	2.00	0.43
1:J:423:ARG:HG3	1:L:424:ASP:OD1	2.17	0.43
1:O:79:ARG:O	1:O:82:PHE:HB3	2.17	0.43
1:Z:81:TRP:CH2	1:Z:169:VAL:HG11	2.52	0.43
1:4:47:MET:HE2	1:4:212:ILE:H	1.83	0.43
1:5:129:ALA:O	1:5:146:LYS:HE3	2.19	0.43
1:D:299:VAL:HG21	1:D:307:PHE:CD2	2.53	0.43
1:D:339:VAL:HG21	1:D:368:GLY:HA2	2.00	0.43
1:F:47:MET:HB3	1:F:47:MET:HE2	1.82	0.43
1:I:421:TYR:CE1	1:I:443:ASN:HA	2.54	0.43
1:J:477:ILE:CD1	1:K:464:ARG:HG3	2.48	0.43
1:K:333:LEU:HD11	1:K:392:PRO:HD3	1.99	0.43
1:M:221:GLU:O	1:M:225:ASN:HB2	2.19	0.43
1:S:143:VAL:HB	1:S:480:LEU:HB2	2.01	0.43
1:T:410:ASN:O	1:T:412:THR:N	2.51	0.43
1:V:99:GLU:OE2	1:V:190:SER:OG	2.20	0.43
1:W:479:TYR:CZ	1:W:481:CYS:HB2	2.53	0.43
1:X:150:GLY:O	1:X:178:PRO:HD2	2.18	0.43
1:X:393:LEU:O	1:X:395:PRO:HD3	2.18	0.43
1:A:393:LEU:O	1:A:395:PRO:HD3	2.18	0.43
1:F:221:GLU:O	1:F:225:ASN:HB2	2.18	0.43
1:E:476:VAL:HG21	1:H:457:VAL:HG12	2.00	0.43
1:I:427:ARG:O	1:I:431:VAL:HG23	2.18	0.43
1:C:357:MET:HG3	1:L:401:SER:HB3	1.99	0.43
1:Q:306:ALA:O	1:Q:310:LYS:HG3	2.19	0.43
1:X:140:LYS:HA	1:X:482:VAL:O	2.19	0.43
1:Z:191:ALA:O	1:Z:210:VAL:HG21	2.17	0.43
1:Z:464:ARG:HE	1:1:477:ILE:HD11	1.82	0.43
1:2:139:ASN:O	1:2:484:VAL:HG12	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:265:ILE:HG23	1:3:405:LEU:HD21	2.00	0.43
1:5:124:GLU:HG2	1:6:127:ARG:HH21	1.84	0.43
1:A:185:GLU:H	1:A:185:GLU:CD	2.22	0.43
1:C:157:PRO:HD2	1:C:164:MET:HG3	1.99	0.43
1:C:251:VAL:O	1:C:251:VAL:CG1	2.66	0.43
1:F:334:ILE:HD13	1:F:334:ILE:O	2.18	0.43
1:F:113:TYR:HE1	1:F:449:ASN:HA	1.82	0.43
1:F:167:ARG:NH2	1:F:465:GLU:OE1	2.32	0.43
1:H:195:ALA:HB2	1:H:210:VAL:HG21	1.99	0.43
1:H:263:PRO:HD2	1:H:418:ALA:HA	1.99	0.43
1:J:106:GLU:HG3	2:J:515:HOH:O	2.19	0.43
1:L:97:THR:HG23	1:L:102:LYS:O	2.17	0.43
1:M:242:LEU:O	1:M:246:GLN:HG3	2.19	0.43
1:O:228:VAL:O	1:O:252:LYS:NZ	2.44	0.43
1:P:251:VAL:HG13	1:P:251:VAL:O	2.19	0.43
1:T:63:TRP:CZ2	1:T:150:GLY:HA2	2.53	0.43
1:U:52:THR:HB	1:U:221:GLU:HG2	1.99	0.43
1:X:47:MET:H	1:X:213:GLY:HA3	1.83	0.43
1:Y:234:THR:HG23	1:Y:257:GLU:HB2	2.00	0.43
1:Y:287:ASN:ND2	1:Y:333:LEU:HD12	2.33	0.43
1:Y:393:LEU:O	1:Y:395:PRO:HD3	2.19	0.43
1:1:102:LYS:HD3	1:1:106:GLU:HB3	2.00	0.43
1:2:404:GLU:HG2	1:2:408:LEU:CD2	2.48	0.43
1:A:131:ASP:HB2	1:A:144:VAL:HB	2.01	0.43
1:K:135:THR:HG21	1:K:140:LYS:O	2.18	0.43
1:U:29:THR:HG22	1:U:45:PRO:HA	1.99	0.43
1:V:47:MET:CE	1:V:51:GLU:CB	2.97	0.43
1:W:130:GLY:HA3	1:W:144:VAL:O	2.18	0.43
1:U:480:LEU:HD22	1:X:442:ILE:HD11	2.00	0.43
1:Y:404:GLU:HG3	1:Y:407:ARG:HH22	1.84	0.43
1:Y:450:GLU:HG2	1:Y:451:VAL:N	2.32	0.43
1:E:160:PHE:HE2	1:E:290:THR:HG22	1.83	0.43
1:E:25:ASP:CG	1:E:54:ARG:HH12	2.22	0.43
1:M:188:PRO:HB2	1:M:212:ILE:HD13	2.00	0.43
1:Q:234:THR:HG23	1:Q:257:GLU:HB2	2.01	0.43
1:W:157:PRO:HD2	1:W:164:MET:HG3	2.01	0.43
1:Z:241:ARG:O	1:1:248:ALA:HB1	2.18	0.43
1:2:16:TYR:CZ	1:2:19:GLY:HA2	2.54	0.43
1:J:228:VAL:O	1:J:252:LYS:NZ	2.46	0.43
1:L:300:HIS:ND1	1:L:302:ARG:HG3	2.34	0.43
1:V:262:ALA:HB3	1:V:294:THR:HA	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:121:PHE:CE2	1:5:171:PRO:HG3	2.54	0.43
1:A:481:CYS:HB3	1:D:447:ILE:HG22	2.01	0.43
1:E:188:PRO:HB2	1:E:212:ILE:HD13	2.00	0.43
1:G:17:ILE:HD11	1:G:47:MET:HE1	2.00	0.43
1:H:393:LEU:O	1:H:395:PRO:HD3	2.18	0.43
1:J:477:ILE:HD11	1:K:464:ARG:HG3	2.01	0.43
1:N:265:ILE:HD13	1:N:405:LEU:HD21	2.01	0.43
1:O:272:LEU:H	1:O:272:LEU:HD22	1.82	0.43
1:O:265:ILE:HG21	1:O:405:LEU:HD21	2.00	0.43
1:P:393:LEU:O	1:P:395:PRO:HD3	2.19	0.43
1:Q:124:GLU:HG2	1:R:127:ARG:HH21	1.84	0.43
1:V:246:GLN:O	1:V:249:PRO:HD2	2.19	0.43
1:W:36:ALA:HA	1:W:332:PRO:HG3	2.01	0.43
1:Z:202:GLY:O	1:Z:204:PRO:HD3	2.19	0.43
1:1:123:GLU:HG2	1:2:123:GLU:CD	2.40	0.43
1:2:131:ASP:HB2	1:2:144:VAL:HB	2.00	0.43
1:5:157:PRO:HD3	1:5:234:THR:HB	2.01	0.43
1:A:244:MET:HA	1:A:254:LEU:HD21	2.00	0.43
1:H:63:TRP:CZ2	1:H:150:GLY:HA2	2.54	0.43
1:Q:178:PRO:HB3	1:Q:207:VAL:HA	2.00	0.43
1:Q:29:THR:HB	1:Q:43:THR:HB	2.00	0.43
1:Z:181:VAL:N	1:Z:209:SER:O	2.51	0.43
1:Z:452:ALA:HA	1:Z:453:PRO:HD3	1.88	0.43
1:2:168:LYS:NZ	1:2:465:GLU:OE2	2.45	0.42
1:A:482:VAL:HA	1:D:442:ILE:HB	2.01	0.42
1:N:183:PRO:HD2	1:N:211:VAL:O	2.19	0.42
1:N:237:THR:HG1	1:N:414:PHE:HE1	1.67	0.42
1:T:121:PHE:CD2	1:T:171:PRO:HD3	2.54	0.42
1:U:35:PRO:HD2	1:U:98:THR:O	2.17	0.42
1:1:282:SER:O	1:1:293:CYS:HA	2.19	0.42
1:2:263:PRO:HA	1:2:296:ARG:O	2.19	0.42
1:3:315:VAL:CG1	1:3:372:PRO:HB2	2.49	0.42
1:E:17:ILE:HD11	1:E:47:MET:CE	2.48	0.42
1:I:423:ARG:NH1	1:I:443:ASN:ND2	2.67	0.42
1:K:158:TRP:O	1:K:161:PRO:HD3	2.19	0.42
1:M:423:ARG:HD2	1:M:423:ARG:HA	1.64	0.42
1:Y:265:ILE:HG23	1:Y:405:LEU:HD21	1.98	0.42
1:3:480:LEU:HD23	1:6:440:VAL:HB	2.00	0.42
1:4:192:LEU:HD11	1:4:212:ILE:CD1	2.49	0.42
1:6:46:LYS:HA	1:6:213:GLY:HA2	2.01	0.42
1:A:250:THR:O	1:D:459:GLN:NE2	2.47	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:LEU:HD21	1:D:212:ILE:CD1	2.50	0.42
1:F:453:PRO:HG2	1:G:477:ILE:CD1	2.49	0.42
1:G:182:LYS:NZ	1:G:183:PRO:O	2.51	0.42
1:G:37:THR:O	1:G:367:HIS:NE2	2.53	0.42
1:I:424:ASP:O	1:I:428:VAL:HG23	2.19	0.42
1:M:17:ILE:HD12	1:M:211:VAL:HG22	2.01	0.42
1:M:272:LEU:O	1:M:276:VAL:HG23	2.20	0.42
1:P:350:LEU:HD13	1:P:354:ALA:O	2.19	0.42
1:P:260:GLY:O	1:P:388:GLU:HG3	2.20	0.42
1:Q:248:ALA:N	1:Q:249:PRO:HD2	2.34	0.42
1:Q:129:ALA:HB2	1:S:133:LEU:HD23	2.02	0.42
1:T:435:LEU:O	1:T:437:TYR:N	2.51	0.42
1:U:225:ASN:HA	1:U:226:PRO:HD3	1.92	0.42
1:W:17:ILE:HD11	1:W:47:MET:HE1	2.02	0.42
1:X:192:LEU:HD11	1:X:212:ILE:HD11	2.00	0.42
1:X:371:GLU:HA	1:X:372:PRO:HD2	1.82	0.42
1:Y:84:LEU:HD12	1:Y:201:ALA:HB2	2.01	0.42
1:Z:318:LEU:HB3	1:Z:330:LEU:HD11	2.01	0.42
1:5:295:ASN:OD1	1:5:388:GLU:HA	2.19	0.42
1:B:158:TRP:CE3	1:B:334:ILE:HD12	2.55	0.42
1:C:399:PHE:CD1	1:C:405:LEU:HB2	2.54	0.42
1:E:183:PRO:HD2	1:E:211:VAL:O	2.19	0.42
1:K:375:LEU:O	1:K:396:LEU:HG	2.19	0.42
1:M:440:VAL:HB	1:P:480:LEU:HD23	2.02	0.42
1:Y:421:TYR:CE1	1:Y:443:ASN:HA	2.54	0.42
1:Y:59:ALA:HB1	1:Y:178:PRO:HB2	2.02	0.42
1:2:214:ASP:HA	1:2:215:PRO:HD3	1.90	0.42
1:5:300:HIS:HB3	1:5:303:VAL:HG22	2.01	0.42
1:G:59:ALA:HA	1:G:206:GLY:O	2.19	0.42
1:J:17:ILE:HD11	1:J:47:MET:CE	2.49	0.42
1:K:356:LEU:HD21	1:K:360:GLY:HA3	2.01	0.42
1:L:63:TRP:CD1	1:L:178:PRO:HD3	2.55	0.42
1:Q:214:ASP:HB3	1:Q:217:ALA:HB3	2.01	0.42
1:S:131:ASP:H	1:S:144:VAL:HB	1.85	0.42
1:T:297:PHE:HB2	1:T:395:PRO:O	2.19	0.42
1:X:121:PHE:HA	1:X:124:GLU:HB2	2.01	0.42
1:1:51:GLU:HG3	1:1:54:ARG:HH12	1.84	0.42
1:3:132:THR:OG1	1:5:130:GLY:HA3	2.20	0.42
1:4:157:PRO:HD2	1:4:164:MET:HG3	2.00	0.42
1:D:264:PHE:HA	1:D:419:TYR:HB2	2.00	0.42
1:J:464:ARG:HE	1:K:477:ILE:HG13	1.84	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:477:ILE:C	1:P:477:ILE:HD12	2.39	0.42
1:U:239:VAL:HA	1:U:242:LEU:HD12	2.01	0.42
1:2:378:VAL:HG13	1:2:382:MET:SD	2.59	0.42
1:2:128:VAL:HG11	1:2:475:VAL:HG11	2.02	0.42
1:4:214:ASP:HA	1:4:215:PRO:HD2	1.85	0.42
1:5:195:ALA:HB2	1:5:210:VAL:HG21	2.00	0.42
1:B:47:MET:HE2	1:B:47:MET:HB3	1.80	0.42
1:C:192:LEU:HD21	1:C:212:ILE:CD1	2.49	0.42
1:D:315:VAL:HA	1:D:318:LEU:HD12	2.01	0.42
1:G:157:PRO:HD2	1:G:164:MET:HG3	2.01	0.42
1:I:256:LEU:O	1:I:461:GLY:HA3	2.19	0.42
1:J:423:ARG:HD2	1:J:423:ARG:HA	1.88	0.42
1:K:450:GLU:HG2	1:K:451:VAL:HG12	2.02	0.42
1:L:64:ALA:O	1:L:68:MET:HB2	2.18	0.42
1:Z:343:GLU:OE1	1:Z:362:ARG:NH1	2.52	0.42
1:1:371:GLU:HA	1:1:372:PRO:HD2	1.90	0.42
1:3:345:HIS:HE1	1:3:387:GLU:HB3	1.85	0.42
1:A:267:PHE:CE1	1:A:427:ARG:HD3	2.53	0.42
1:N:114:ALA:HB2	1:N:163:ALA:HA	2.00	0.42
1:P:160:PHE:O	1:P:164:MET:HG2	2.20	0.42
1:U:241:ARG:O	1:X:248:ALA:HB1	2.20	0.42
1:U:342:VAL:HG22	1:U:389:THR:HG22	2.02	0.42
1:V:30:PHE:HE2	1:V:213:GLY:HA2	1.83	0.42
1:X:230:LYS:O	1:X:230:LYS:HG3	2.19	0.42
1:1:214:ASP:HA	1:1:215:PRO:HD2	1.90	0.42
1:4:427:ARG:O	1:4:431:VAL:HG23	2.20	0.42
1:A:451:VAL:HG22	1:D:142:ILE:HD13	2.02	0.42
1:F:155:ILE:HG23	1:F:182:LYS:HE3	2.01	0.42
1:G:214:ASP:HA	1:G:215:PRO:HD3	1.93	0.42
1:G:393:LEU:O	1:G:395:PRO:HD3	2.19	0.42
1:K:450:GLU:OE2	1:L:72:LYS:HE3	2.20	0.42
1:T:84:LEU:HB3	1:T:197:LEU:HD22	2.02	0.42
1:2:47:MET:HE2	1:2:51:GLU:CB	2.50	0.42
1:5:338:ALA:O	1:5:342:VAL:HG23	2.19	0.42
1:E:480:LEU:HD23	1:H:440:VAL:HB	2.02	0.42
1:F:393:LEU:O	1:F:395:PRO:HD3	2.20	0.42
1:I:154:ALA:HB2	1:I:179:ILE:HD11	2.02	0.42
1:L:10:LEU:HD21	1:L:197:LEU:HD21	2.02	0.42
1:L:263:PRO:HA	1:L:296:ARG:O	2.20	0.42
1:M:225:ASN:HA	1:M:226:PRO:HD3	1.94	0.42
1:S:17:ILE:CD1	1:S:47:MET:CE	2.92	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:117:PHE:CE1	1:T:167:ARG:HG2	2.55	0.42
1:V:284:TYR:HB3	1:V:330:LEU:HD21	2.02	0.42
1:X:110:GLU:HG3	1:X:163:ALA:HB2	2.00	0.42
1:X:389:THR:O	1:X:390:PHE:HB2	2.19	0.42
1:X:69:LYS:O	1:X:74:ARG:NH1	2.52	0.42
1:Y:447:ILE:HG22	1:2:481:CYS:HB2	2.02	0.42
1:2:264:PHE:HB2	1:2:294:THR:CG2	2.50	0.41
1:3:160:PHE:HE2	1:3:290:THR:HG22	1.85	0.41
1:3:36:ALA:HB2	1:3:332:PRO:HG3	2.01	0.41
1:3:374:VAL:HG22	1:3:394:ALA:HB3	2.01	0.41
1:4:52:THR:O	1:4:56:ILE:HD12	2.20	0.41
1:C:225:ASN:HA	1:C:226:PRO:HD3	1.86	0.41
1:J:5:MET:HE3	1:J:8:PRO:HA	2.02	0.41
1:N:121:PHE:HA	1:N:124:GLU:HB2	2.02	0.41
1:S:455:GLY:HA3	1:S:464:ARG:HD3	2.02	0.41
1:U:147:GLU:HB2	1:U:148:PRO:HD2	2.02	0.41
1:U:264:PHE:HB2	1:U:294:THR:HG21	2.01	0.41
1:U:320:VAL:HG22	1:U:330:LEU:HD23	2.02	0.41
1:Z:232:SER:HA	1:Z:255:THR:O	2.20	0.41
1:3:160:PHE:CE2	1:3:290:THR:HG22	2.55	0.41
1:4:244:MET:HA	1:4:254:LEU:HD21	2.02	0.41
1:4:297:PHE:HB2	1:4:396:LEU:HD23	2.02	0.41
1:B:333:LEU:HD23	1:B:339:VAL:HA	2.01	0.41
1:E:279:ALA:O	1:E:283:LYS:HB3	2.21	0.41
1:J:466:GLY:HA3	2:J:509:HOH:O	2.19	0.41
1:M:193:ALA:O	1:M:196:PHE:HB3	2.20	0.41
1:Q:158:TRP:O	1:Q:161:PRO:HD3	2.21	0.41
1:S:256:LEU:O	1:S:461:GLY:HA3	2.20	0.41
1:T:356:LEU:HA	1:T:375:LEU:HD23	2.00	0.41
1:U:248:ALA:N	1:U:249:PRO:CD	2.82	0.41
1:V:154:ALA:HB1	1:V:168:LYS:HD3	2.00	0.41
1:1:110:GLU:HG3	1:1:160:PHE:HD1	1.86	0.41
1:Z:135:THR:HG23	1:2:70:THR:HG22	2.03	0.41
1:B:251:VAL:CG1	1:B:251:VAL:O	2.67	0.41
1:C:374:VAL:HG22	1:C:394:ALA:HB3	2.02	0.41
1:H:37:THR:O	1:H:367:HIS:CE1	2.73	0.41
1:J:230:LYS:HB2	1:J:253:LYS:HB3	2.02	0.41
1:K:403:GLU:OE2	1:K:407:ARG:NH1	2.53	0.41
1:R:160:PHE:HE2	1:R:290:THR:HG21	1.85	0.41
1:S:300:HIS:HB3	1:S:303:VAL:HG22	2.02	0.41
1:U:66:TRP:CZ2	1:U:74:ARG:HD2	2.55	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:315:VAL:HG13	1:V:372:PRO:HB2	2.02	0.41
1:Y:121:PHE:CD2	1:Y:171:PRO:HD3	2.55	0.41
1:Z:81:TRP:HH2	1:Z:169:VAL:HG11	1.85	0.41
1:Z:59:ALA:HB1	1:Z:178:PRO:HB2	2.02	0.41
1:Z:212:ILE:CG2	1:Z:213:GLY:N	2.84	0.41
1:Z:275:ALA:O	1:Z:279:ALA:N	2.54	0.41
1:1:320:VAL:HG22	1:1:330:LEU:HD12	2.01	0.41
1:5:161:PRO:HB3	1:5:187:THR:OG1	2.20	0.41
1:5:407:ARG:O	1:5:411:ASP:HB2	2.21	0.41
1:A:165:ILE:O	1:A:169:VAL:HB	2.20	0.41
1:E:283:LYS:O	1:E:288:GLY:HA2	2.21	0.41
1:G:160:PHE:HB3	1:G:163:ALA:HB3	2.02	0.41
1:G:251:VAL:CG1	1:G:251:VAL:O	2.66	0.41
1:L:287:ASN:HD22	1:L:333:LEU:HD13	1.84	0.41
1:N:348:ASP:OD1	1:N:352:LYS:NZ	2.38	0.41
1:3:287:ASN:ND2	1:3:331:GLY:O	2.53	0.41
1:C:301:GLU:OE2	1:C:398:ARG:HD3	2.20	0.41
1:D:484:VAL:HG13	1:D:484:VAL:O	2.20	0.41
1:G:230:LYS:HE2	1:G:230:LYS:HB2	1.94	0.41
1:I:140:LYS:O	1:I:141:ARG:HD3	2.20	0.41
1:P:264:PHE:HA	1:P:419:TYR:HB2	2.01	0.41
1:R:132:THR:OG1	1:T:130:GLY:HA3	2.21	0.41
1:6:59:ALA:O	1:6:178:PRO:HG3	2.19	0.41
1:C:267:PHE:CZ	1:C:405:LEU:HD22	2.55	0.41
1:D:164:MET:O	1:D:168:LYS:HG3	2.21	0.41
1:E:363:HIS:HB3	1:E:369:PHE:HB3	2.03	0.41
1:E:407:ARG:HD3	2:E:546:HOH:O	2.20	0.41
1:N:241:ARG:O	1:O:248:ALA:HB1	2.19	0.41
1:Q:455:GLY:HA3	1:Q:464:ARG:HD3	2.03	0.41
1:R:355:SER:HB2	1:R:376:THR:OG1	2.20	0.41
1:T:300:HIS:HD2	1:T:399:PHE:CE1	2.39	0.41
1:U:298:PHE:HE1	1:U:408:LEU:HD23	1.86	0.41
1:U:378:VAL:HG11	1:U:395:PRO:HB2	2.02	0.41
1:V:180:VAL:HG22	1:V:209:SER:HB2	2.02	0.41
1:Z:121:PHE:HA	1:Z:124:GLU:HB2	2.03	0.41
1:1:24:ALA:HA	1:1:47:MET:HG2	2.02	0.41
1:3:285:ARG:HH21	1:3:446:LEU:HD21	1.85	0.41
1:3:96:LEU:HG	1:3:161:PRO:HG2	2.03	0.41
1:6:156:THR:HG21	1:6:165:ILE:HD13	2.02	0.41
1:C:141:ARG:HG3	1:D:429:TRP:CZ3	2.55	0.41
1:F:457:VAL:HG11	1:G:476:VAL:HG11	2.03	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:315:VAL:CG1	1:G:372:PRO:HB2	2.51	0.41
1:H:17:ILE:CD1	1:H:211:VAL:HG22	2.51	0.41
1:J:168:LYS:HE2	1:J:232:SER:OG	2.21	0.41
1:J:188:PRO:HB3	1:J:212:ILE:HD13	2.02	0.41
1:L:182:LYS:HE2	1:L:215:PRO:HA	2.02	0.41
1:M:152:CYS:SG	1:M:230:LYS:HG2	2.60	0.41
1:W:75:ALA:O	1:W:79:ARG:HB2	2.20	0.41
1:X:147:GLU:HB2	1:X:148:PRO:HD2	2.02	0.41
1:Z:136:PRO:HD3	1:1:451:VAL:HG11	2.03	0.41
1:4:241:ARG:O	1:5:248:ALA:HB1	2.21	0.41
1:A:188:PRO:HB2	1:A:212:ILE:HD13	2.01	0.41
1:N:230:LYS:HB2	1:N:253:LYS:HB3	2.03	0.41
1:U:479:TYR:CD1	1:U:480:LEU:N	2.89	0.41
1:V:398:ARG:HG3	2:V:524:HOH:O	2.20	0.41
1:V:81:TRP:O	1:V:85:VAL:HG23	2.20	0.41
1:W:141:ARG:HG2	1:X:429:TRP:CZ3	2.54	0.41
1:Y:237:THR:HA	1:Y:258:LEU:HD13	2.02	0.41
1:Z:12:ARG:HD3	2:Z:520:HOH:O	2.20	0.41
1:Z:372:PRO:HA	1:Z:392:PRO:HB2	2.03	0.41
1:1:239:VAL:HG12	1:1:243:LEU:CD1	2.51	0.41
1:A:251:VAL:HG12	1:A:251:VAL:O	2.21	0.41
1:C:413:GLU:CB	2:C:508:HOH:O	2.69	0.41
1:D:255:THR:HG21	2:D:511:HOH:O	2.21	0.41
1:E:182:LYS:NZ	1:E:185:GLU:OE1	2.45	0.41
1:I:92:LEU:HD21	1:I:197:LEU:HD11	2.02	0.41
1:J:59:ALA:HB1	1:J:178:PRO:HB2	2.02	0.41
1:N:15:ALA:H	1:N:45:PRO:HG2	1.84	0.41
1:O:45:PRO:O	1:O:212:ILE:HG22	2.21	0.41
1:S:264:PHE:HB2	1:S:294:THR:CG2	2.50	0.41
1:T:283:LYS:HA	1:T:283:LYS:HD2	1.90	0.41
1:U:13:HIS:HE1	1:U:42:GLY:HA3	1.86	0.41
1:U:279:ALA:O	1:U:283:LYS:HB3	2.21	0.41
1:V:233:PHE:CZ	1:V:235:GLY:HA3	2.56	0.41
1:Y:371:GLU:HA	1:Y:372:PRO:HD2	1.80	0.41
1:1:232:SER:HA	1:1:255:THR:O	2.21	0.41
1:1:381:ASP:O	1:1:382:MET:HG3	2.21	0.41
1:3:265:ILE:HG21	1:3:405:LEU:HD21	2.01	0.41
1:3:407:ARG:O	1:3:411:ASP:HB2	2.21	0.41
1:5:300:HIS:CE1	1:5:302:ARG:HG3	2.55	0.41
1:C:287:ASN:ND2	1:C:333:LEU:HD13	2.36	0.41
1:E:149:ILE:HD13	1:E:230:LYS:HB3	2.03	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:287:ASN:ND2	1:G:333:LEU:HD13	2.36	0.41
1:L:13:HIS:CE1	1:L:42:GLY:HA3	2.56	0.41
1:R:225:ASN:HA	1:R:226:PRO:HD2	1.97	0.41
1:W:29:THR:HB	1:W:43:THR:HB	2.03	0.41
1:1:247:SER:HB3	1:1:252:LYS:HG3	2.03	0.41
1:1:29:THR:HG22	1:1:45:PRO:HA	2.03	0.41
1:3:418:ALA:O	1:3:440:VAL:HA	2.20	0.41
1:4:423:ARG:HG3	1:6:424:ASP:OD1	2.21	0.41
1:B:465:GLU:HG2	2:B:502:HOH:O	2.21	0.41
1:C:372:PRO:HA	1:C:392:PRO:HB2	2.03	0.41
1:F:384:VAL:HG21	1:F:395:PRO:HG3	2.03	0.41
1:F:423:ARG:HA	1:F:423:ARG:HD2	1.87	0.41
1:F:464:ARG:NE	2:F:560:HOH:O	2.48	0.41
1:H:286:ASN:O	1:H:289:GLN:HB2	2.21	0.41
1:E:142:ILE:CD1	1:H:451:VAL:HG22	2.51	0.41
1:Q:476:VAL:CG2	1:T:457:VAL:HG12	2.50	0.41
1:X:349:ALA:O	1:X:354:ALA:HB3	2.21	0.41
1:Z:111:ILE:HD13	1:Z:111:ILE:HA	1.77	0.41
1:3:63:TRP:CZ2	1:3:150:GLY:HA2	2.56	0.40
1:2:357:MET:O	1:3:309:ASP:HB3	2.21	0.40
1:B:17:ILE:HG13	1:B:47:MET:HE3	2.03	0.40
1:E:25:ASP:OD2	1:E:54:ARG:NH1	2.53	0.40
1:R:246:GLN:O	1:R:249:PRO:HD2	2.20	0.40
1:W:79:ARG:NH2	1:W:119:GLU:HG3	2.36	0.40
1:X:51:GLU:HA	1:X:54:ARG:NH1	2.36	0.40
1:Z:67:ARG:HG3	1:Z:68:MET:N	2.36	0.40
1:Z:10:LEU:HB3	1:Z:95:ILE:CD1	2.50	0.40
1:L:47:MET:HE2	1:L:51:GLU:HB2	2.04	0.40
1:R:283:LYS:CE	1:R:393:LEU:O	2.69	0.40
1:B:410:ASN:O	1:B:412:THR:N	2.51	0.40
1:C:15:ALA:O	1:C:21:TRP:HA	2.21	0.40
1:D:161:PRO:HB2	1:D:190:SER:HB2	2.03	0.40
1:D:17:ILE:HG23	1:D:55:ALA:HB2	2.03	0.40
1:F:157:PRO:HD3	1:F:234:THR:HB	2.03	0.40
1:I:183:PRO:HD2	1:I:211:VAL:O	2.21	0.40
1:O:214:ASP:HA	1:O:215:PRO:HD2	1.92	0.40
1:P:140:LYS:O	1:P:141:ARG:HD3	2.22	0.40
1:U:226:PRO:HA	1:U:250:THR:CG2	2.51	0.40
1:X:436:GLU:HB3	1:X:458:LYS:HD2	2.04	0.40
1:Z:172:ALA:O	1:Z:177:CYS:HB2	2.21	0.40
1:Z:230:LYS:HG3	1:Z:231:LEU:N	2.37	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:MET:HE2	1:C:47:MET:HB2	1.91	0.40
1:E:121:PHE:HA	1:E:124:GLU:HB2	2.02	0.40
1:E:157:PRO:HD2	1:E:164:MET:HG3	2.03	0.40
1:E:447:ILE:HG22	1:H:481:CYS:HB3	2.04	0.40
1:G:131:ASP:N	1:G:131:ASP:OD1	2.53	0.40
1:M:484:VAL:O	1:M:484:VAL:HG13	2.22	0.40
1:N:423:ARG:HD2	1:N:423:ARG:HA	1.80	0.40
1:P:17:ILE:CD1	1:P:47:MET:HE1	2.50	0.40
1:S:300:HIS:CE1	1:S:302:ARG:HG3	2.56	0.40
1:U:256:LEU:O	1:U:461:GLY:HA3	2.21	0.40
1:V:264:PHE:CD1	1:V:419:TYR:HB2	2.56	0.40
1:1:263:PRO:HD2	1:1:418:ALA:HA	2.03	0.40
1:2:421:TYR:HA	1:2:443:ASN:OD1	2.22	0.40
1:3:234:THR:HA	1:3:257:GLU:O	2.22	0.40
1:4:84:LEU:HD12	1:4:201:ALA:HB2	2.04	0.40
1:C:141:ARG:CG	1:D:429:TRP:CZ3	3.05	0.40
1:D:286:ASN:O	1:D:289:GLN:HG3	2.22	0.40
1:E:221:GLU:O	1:E:225:ASN:HB2	2.21	0.40
1:E:230:LYS:HB2	1:E:253:LYS:HB3	2.03	0.40
1:F:214:ASP:HA	1:F:215:PRO:HD2	1.97	0.40
1:I:244:MET:HA	1:I:254:LEU:HD21	2.04	0.40
1:J:287:ASN:O	1:J:392:PRO:HD3	2.21	0.40
1:M:338:ALA:O	1:M:342:VAL:HG23	2.21	0.40
1:N:113:TYR:CZ	1:N:117:PHE:HE2	2.39	0.40
1:N:415:GLY:HA2	1:N:437:TYR:CD1	2.56	0.40
1:Q:346:ILE:O	1:Q:350:LEU:HD22	2.21	0.40
1:Q:415:GLY:HA2	1:Q:437:TYR:CE1	2.56	0.40
1:V:477:ILE:HD11	1:W:453:PRO:CB	2.49	0.40
1:W:182:LYS:HG3	1:W:218:ILE:HG21	2.03	0.40
1:Z:237:THR:O	1:Z:241:ARG:HG3	2.22	0.40
1:Z:29:THR:HB	1:Z:43:THR:HB	2.03	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	1	480/484 (99%)	441 (92%)	33 (7%)	6 (1%)	14	35
1	2	480/484 (99%)	443 (92%)	31 (6%)	6 (1%)	14	35
1	3	480/484 (99%)	451 (94%)	27 (6%)	2 (0%)	38	66
1	4	480/484 (99%)	459 (96%)	18 (4%)	3 (1%)	28	56
1	5	480/484 (99%)	459 (96%)	18 (4%)	3 (1%)	28	56
1	6	480/484 (99%)	463 (96%)	13 (3%)	4 (1%)	22	49
1	A	480/484 (99%)	457 (95%)	21 (4%)	2 (0%)	38	66
1	B	480/484 (99%)	464 (97%)	13 (3%)	3 (1%)	28	56
1	C	480/484 (99%)	465 (97%)	14 (3%)	1 (0%)	51	79
1	D	480/484 (99%)	450 (94%)	27 (6%)	3 (1%)	28	56
1	E	480/484 (99%)	456 (95%)	24 (5%)	0	100	100
1	F	480/484 (99%)	463 (96%)	15 (3%)	2 (0%)	38	66
1	G	480/484 (99%)	462 (96%)	16 (3%)	2 (0%)	38	66
1	H	480/484 (99%)	454 (95%)	24 (5%)	2 (0%)	38	66
1	I	480/484 (99%)	445 (93%)	32 (7%)	3 (1%)	28	56
1	J	480/484 (99%)	451 (94%)	27 (6%)	2 (0%)	38	66
1	K	480/484 (99%)	459 (96%)	19 (4%)	2 (0%)	38	66
1	L	480/484 (99%)	460 (96%)	19 (4%)	1 (0%)	51	79
1	M	480/484 (99%)	458 (95%)	19 (4%)	3 (1%)	28	56
1	N	480/484 (99%)	463 (96%)	16 (3%)	1 (0%)	51	79
1	O	480/484 (99%)	460 (96%)	19 (4%)	1 (0%)	51	79
1	P	480/484 (99%)	458 (95%)	22 (5%)	0	100	100
1	Q	480/484 (99%)	456 (95%)	21 (4%)	3 (1%)	28	56
1	R	480/484 (99%)	458 (95%)	17 (4%)	5 (1%)	18	43
1	S	480/484 (99%)	462 (96%)	17 (4%)	1 (0%)	51	79
1	T	480/484 (99%)	447 (93%)	29 (6%)	4 (1%)	22	49
1	U	480/484 (99%)	438 (91%)	41 (8%)	1 (0%)	51	79
1	V	480/484 (99%)	443 (92%)	33 (7%)	4 (1%)	22	49
1	W	480/484 (99%)	456 (95%)	21 (4%)	3 (1%)	28	56
1	X	480/484 (99%)	429 (89%)	48 (10%)	3 (1%)	28	56

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Y	480/484 (99%)	427 (89%)	45 (9%)	8 (2%)	11	27
1	Z	480/484 (99%)	430 (90%)	45 (9%)	5 (1%)	18	43
All	All	15360/15488 (99%)	14487 (94%)	784 (5%)	89 (1%)	28	56

All (89) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	268	ASP
1	D	261	ASN
1	D	268	ASP
1	G	268	ASP
1	H	268	ASP
1	I	268	ASP
1	J	268	ASP
1	J	367	HIS
1	N	268	ASP
1	Y	27	ASP
1	Y	287	ASN
1	3	27	ASP
1	5	268	ASP
1	6	268	ASP
1	I	185	GLU
1	T	367	HIS
1	T	411	ASP
1	Y	330	LEU
1	Y	425	ILE
1	Z	128	VAL
1	Z	334	ILE
1	Z	367	HIS
1	2	139	ASN
1	2	261	ASN
1	F	268	ASP
1	M	261	ASN
1	R	261	ASN
1	T	261	ASN
1	V	25	ASP
1	Y	261	ASN
1	Y	367	HIS
1	1	261	ASN
1	1	264	PHE
1	1	423	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	6	261	ASN
1	A	27	ASP
1	C	261	ASN
1	D	367	HIS
1	K	261	ASN
1	L	467	SER
1	M	139	ASN
1	M	467	SER
1	Q	27	ASP
1	R	268	ASP
1	V	467	SER
1	W	301	GLU
1	X	377	GLY
1	Z	4	SER
1	2	25	ASP
1	2	367	HIS
1	2	392	PRO
1	4	268	ASP
1	4	411	ASP
1	5	367	HIS
1	B	261	ASN
1	B	411	ASP
1	V	261	ASN
1	W	467	SER
1	1	467	SER
1	4	367	HIS
1	5	4	SER
1	H	326	SER
1	K	467	SER
1	Q	261	ASN
1	Q	415	GLY
1	R	4	SER
1	T	436	GLU
1	X	157	PRO
1	Z	188	PRO
1	U	415	GLY
1	V	392	PRO
1	Y	157	PRO
1	Y	415	GLY
1	1	263	PRO
1	A	425	ILE
1	F	415	GLY

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	I	415	GLY
1	O	128	VAL
1	W	415	GLY
1	X	457	VAL
1	6	415	GLY
1	R	251	VAL
1	1	251	VAL
1	3	415	GLY
1	G	395	PRO
1	R	157	PRO
1	S	415	GLY
1	2	395	PRO
1	6	380	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	341/363 (94%)	320 (94%)	21 (6%)	21	46
1	2	349/363 (96%)	331 (95%)	18 (5%)	27	55
1	3	349/363 (96%)	333 (95%)	16 (5%)	31	61
1	4	349/363 (96%)	333 (95%)	16 (5%)	31	61
1	5	349/363 (96%)	332 (95%)	17 (5%)	29	58
1	6	349/363 (96%)	331 (95%)	18 (5%)	27	55
1	A	350/363 (96%)	334 (95%)	16 (5%)	31	61
1	B	351/363 (97%)	337 (96%)	14 (4%)	36	67
1	C	350/363 (96%)	325 (93%)	25 (7%)	17	39
1	D	350/363 (96%)	333 (95%)	17 (5%)	29	58
1	E	350/363 (96%)	332 (95%)	18 (5%)	28	56
1	F	350/363 (96%)	337 (96%)	13 (4%)	39	70
1	G	350/363 (96%)	332 (95%)	18 (5%)	28	56
1	H	350/363 (96%)	331 (95%)	19 (5%)	26	54

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	344/363 (95%)	319 (93%)	25 (7%)	16	38
1	J	350/363 (96%)	332 (95%)	18 (5%)	28	56
1	K	349/363 (96%)	336 (96%)	13 (4%)	39	70
1	L	348/363 (96%)	328 (94%)	20 (6%)	24	51
1	M	349/363 (96%)	327 (94%)	22 (6%)	21	46
1	N	349/363 (96%)	330 (95%)	19 (5%)	26	54
1	O	349/363 (96%)	332 (95%)	17 (5%)	29	58
1	P	349/363 (96%)	334 (96%)	15 (4%)	33	64
1	Q	349/363 (96%)	330 (95%)	19 (5%)	26	54
1	R	349/363 (96%)	324 (93%)	25 (7%)	17	39
1	S	349/363 (96%)	337 (97%)	12 (3%)	42	73
1	T	346/363 (95%)	334 (96%)	12 (4%)	41	72
1	U	344/363 (95%)	324 (94%)	20 (6%)	23	50
1	V	346/363 (95%)	322 (93%)	24 (7%)	18	41
1	W	349/363 (96%)	338 (97%)	11 (3%)	44	75
1	X	340/363 (94%)	321 (94%)	19 (6%)	25	51
1	Y	349/363 (96%)	332 (95%)	17 (5%)	29	58
1	Z	346/363 (95%)	326 (94%)	20 (6%)	23	50
All	All	11141/11616 (96%)	10567 (95%)	574 (5%)	27	55

All (574) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	ARG
1	A	185	GLU
1	A	186	SER
1	A	230	LYS
1	A	272	LEU
1	A	285	ARG
1	A	291	CYS
1	A	302	ARG
1	A	333	LEU
1	A	334	ILE
1	A	408	LEU
1	A	425	ILE
1	A	451	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	462	LEU
1	A	477	ILE
1	A	479	TYR
1	B	57	GLU
1	B	141	ARG
1	B	148	PRO
1	B	230	LYS
1	B	254	LEU
1	B	272	LEU
1	B	285	ARG
1	B	333	LEU
1	B	334	ILE
1	B	350	LEU
1	B	408	LEU
1	B	425	ILE
1	B	477	ILE
1	B	484	VAL
1	C	6	LYS
1	C	20	GLU
1	C	44	VAL
1	C	94	LEU
1	C	141	ARG
1	C	159	ASN
1	C	185	GLU
1	C	230	LYS
1	C	236	SER
1	C	254	LEU
1	C	272	LEU
1	C	285	ARG
1	C	291	CYS
1	C	301	GLU
1	C	324	THR
1	C	333	LEU
1	C	355	SER
1	C	376	THR
1	C	408	LEU
1	C	423	ARG
1	C	425	ILE
1	C	451	VAL
1	C	476	VAL
1	C	477	ILE
1	C	484	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	6	LYS
1	D	37	THR
1	D	57	GLU
1	D	94	LEU
1	D	131	ASP
1	D	159	ASN
1	D	230	LYS
1	D	253	LYS
1	D	254	LEU
1	D	283	LYS
1	D	293	CYS
1	D	304	TYR
1	D	324	THR
1	D	350	LEU
1	D	423	ARG
1	D	425	ILE
1	D	476	VAL
1	E	20	GLU
1	E	27	ASP
1	E	96	LEU
1	E	104	LEU
1	E	140	LYS
1	E	159	ASN
1	E	185	GLU
1	E	230	LYS
1	E	272	LEU
1	E	283	LYS
1	E	333	LEU
1	E	408	LEU
1	E	425	ILE
1	E	448	SER
1	E	451	VAL
1	E	462	LEU
1	E	476	VAL
1	E	477	ILE
1	F	20	GLU
1	F	96	LEU
1	F	141	ARG
1	F	185	GLU
1	F	254	LEU
1	F	285	ARG
1	F	333	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	334	ILE
1	F	350	LEU
1	F	408	LEU
1	F	423	ARG
1	F	451	VAL
1	F	477	ILE
1	G	20	GLU
1	G	57	GLU
1	G	89	SER
1	G	94	LEU
1	G	131	ASP
1	G	185	GLU
1	G	230	LYS
1	G	254	LEU
1	G	285	ARG
1	G	291	CYS
1	G	326	SER
1	G	333	LEU
1	G	376	THR
1	G	407	ARG
1	G	408	LEU
1	G	451	VAL
1	G	476	VAL
1	G	477	ILE
1	H	20	GLU
1	H	27	ASP
1	H	94	LEU
1	H	104	LEU
1	H	182	LYS
1	H	230	LYS
1	H	253	LYS
1	H	254	LEU
1	H	272	LEU
1	H	283	LYS
1	H	291	CYS
1	H	293	CYS
1	H	326	SER
1	H	348	ASP
1	H	403	GLU
1	H	408	LEU
1	H	425	ILE
1	H	476	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	H	477	ILE
1	I	6	LYS
1	I	43	THR
1	I	44	VAL
1	I	57	GLU
1	I	72	LYS
1	I	141	ARG
1	I	159	ASN
1	I	186	SER
1	I	230	LYS
1	I	253	LYS
1	I	291	CYS
1	I	324	THR
1	I	333	LEU
1	I	334	ILE
1	I	350	LEU
1	I	356	LEU
1	I	370	PHE
1	I	371	GLU
1	I	403	GLU
1	I	423	ARG
1	I	425	ILE
1	I	427	ARG
1	I	451	VAL
1	I	476	VAL
1	I	477	ILE
1	J	20	GLU
1	J	27	ASP
1	J	39	GLU
1	J	44	VAL
1	J	104	LEU
1	J	159	ASN
1	J	186	SER
1	J	230	LYS
1	J	253	LYS
1	J	272	LEU
1	J	285	ARG
1	J	326	SER
1	J	333	LEU
1	J	350	LEU
1	J	408	LEU
1	J	423	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	J	451	VAL
1	J	477	ILE
1	K	30	PHE
1	K	40	SER
1	K	131	ASP
1	K	230	LYS
1	K	251	VAL
1	K	253	LYS
1	K	285	ARG
1	K	336	GLU
1	K	425	ILE
1	K	451	VAL
1	K	475	VAL
1	K	476	VAL
1	K	477	ILE
1	L	57	GLU
1	L	104	LEU
1	L	159	ASN
1	L	186	SER
1	L	211	VAL
1	L	230	LYS
1	L	253	LYS
1	L	254	LEU
1	L	272	LEU
1	L	283	LYS
1	L	333	LEU
1	L	334	ILE
1	L	336	GLU
1	L	348	ASP
1	L	356	LEU
1	L	408	LEU
1	L	425	ILE
1	L	451	VAL
1	L	476	VAL
1	L	477	ILE
1	M	57	GLU
1	M	131	ASP
1	M	159	ASN
1	M	182	LYS
1	M	200	ARG
1	M	230	LYS
1	M	272	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	M	285	ARG
1	M	291	CYS
1	M	333	LEU
1	M	334	ILE
1	M	405	LEU
1	M	408	LEU
1	M	412	THR
1	M	423	ARG
1	M	425	ILE
1	M	427	ARG
1	M	448	SER
1	M	451	VAL
1	M	462	LEU
1	M	476	VAL
1	M	477	ILE
1	N	6	LYS
1	N	20	GLU
1	N	57	GLU
1	N	194	MET
1	N	230	LYS
1	N	254	LEU
1	N	272	LEU
1	N	285	ARG
1	N	333	LEU
1	N	343	GLU
1	N	376	THR
1	N	408	LEU
1	N	423	ARG
1	N	425	ILE
1	N	427	ARG
1	N	451	VAL
1	N	476	VAL
1	N	477	ILE
1	N	484	VAL
1	O	96	LEU
1	O	131	ASP
1	O	159	ASN
1	O	253	LYS
1	O	254	LEU
1	O	268	ASP
1	O	283	LYS
1	O	285	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	O	333	LEU
1	O	336	GLU
1	O	350	LEU
1	O	371	GLU
1	O	425	ILE
1	O	451	VAL
1	O	476	VAL
1	O	477	ILE
1	O	484	VAL
1	P	57	GLU
1	P	104	LEU
1	P	141	ARG
1	P	159	ASN
1	P	230	LYS
1	P	250	THR
1	P	253	LYS
1	P	285	ARG
1	P	333	LEU
1	P	362	ARG
1	P	405	LEU
1	P	408	LEU
1	P	451	VAL
1	P	476	VAL
1	P	477	ILE
1	Q	37	THR
1	Q	40	SER
1	Q	44	VAL
1	Q	104	LEU
1	Q	131	ASP
1	Q	141	ARG
1	Q	159	ASN
1	Q	230	LYS
1	Q	253	LYS
1	Q	257	GLU
1	Q	283	LYS
1	Q	285	ARG
1	Q	333	LEU
1	Q	341	LYS
1	Q	350	LEU
1	Q	371	GLU
1	Q	405	LEU
1	Q	408	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	Q	425	ILE
1	R	68	MET
1	R	104	LEU
1	R	131	ASP
1	R	141	ARG
1	R	147	GLU
1	R	237	THR
1	R	253	LYS
1	R	254	LEU
1	R	267	PHE
1	R	289	GLN
1	R	291	CYS
1	R	305	ASP
1	R	336	GLU
1	R	350	LEU
1	R	355	SER
1	R	405	LEU
1	R	408	LEU
1	R	423	ARG
1	R	425	ILE
1	R	444	THR
1	R	451	VAL
1	R	462	LEU
1	R	476	VAL
1	R	477	ILE
1	R	484	VAL
1	S	4	SER
1	S	236	SER
1	S	253	LYS
1	S	268	ASP
1	S	272	LEU
1	S	285	ARG
1	S	326	SER
1	S	333	LEU
1	S	408	LEU
1	S	425	ILE
1	S	462	LEU
1	S	476	VAL
1	T	212	ILE
1	T	230	LYS
1	T	242	LEU
1	T	286	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	T	301	GLU
1	T	350	LEU
1	T	397	PHE
1	T	408	LEU
1	T	423	ARG
1	T	451	VAL
1	T	471	ILE
1	T	476	VAL
1	U	5	MET
1	U	57	GLU
1	U	60	GLN
1	U	91	ASP
1	U	94	LEU
1	U	95	ILE
1	U	104	LEU
1	U	141	ARG
1	U	165	ILE
1	U	194	MET
1	U	212	ILE
1	U	215	PRO
1	U	232	SER
1	U	250	THR
1	U	324	THR
1	U	326	SER
1	U	333	LEU
1	U	408	LEU
1	U	423	ARG
1	U	451	VAL
1	V	34	ASP
1	V	37	THR
1	V	57	GLU
1	V	68	MET
1	V	90	ASP
1	V	126	LYS
1	V	131	ASP
1	V	141	ARG
1	V	159	ASN
1	V	186	SER
1	V	251	VAL
1	V	253	LYS
1	V	333	LEU
1	V	358	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	V	398	ARG
1	V	403	GLU
1	V	405	LEU
1	V	408	LEU
1	V	423	ARG
1	V	425	ILE
1	V	446	LEU
1	V	451	VAL
1	V	476	VAL
1	V	477	ILE
1	W	57	GLU
1	W	79	ARG
1	W	104	LEU
1	W	159	ASN
1	W	253	LYS
1	W	334	ILE
1	W	336	GLU
1	W	389	THR
1	W	408	LEU
1	W	425	ILE
1	W	476	VAL
1	X	37	THR
1	X	57	GLU
1	X	91	ASP
1	X	141	ARG
1	X	212	ILE
1	X	230	LYS
1	X	254	LEU
1	X	272	LEU
1	X	285	ARG
1	X	325	GLU
1	X	350	LEU
1	X	373	THR
1	X	376	THR
1	X	403	GLU
1	X	404	GLU
1	X	405	LEU
1	X	425	ILE
1	X	476	VAL
1	X	477	ILE
1	Y	6	LYS
1	Y	29	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	Y	78	LEU
1	Y	131	ASP
1	Y	141	ARG
1	Y	194	MET
1	Y	230	LYS
1	Y	257	GLU
1	Y	290	THR
1	Y	291	CYS
1	Y	303	VAL
1	Y	305	ASP
1	Y	325	GLU
1	Y	350	LEU
1	Y	403	GLU
1	Y	425	ILE
1	Y	477	ILE
1	Z	33	PHE
1	Z	44	VAL
1	Z	90	ASP
1	Z	92	LEU
1	Z	141	ARG
1	Z	194	MET
1	Z	209	SER
1	Z	230	LYS
1	Z	242	LEU
1	Z	250	THR
1	Z	272	LEU
1	Z	283	LYS
1	Z	285	ARG
1	Z	291	CYS
1	Z	293	CYS
1	Z	336	GLU
1	Z	425	ILE
1	Z	448	SER
1	Z	451	VAL
1	Z	477	ILE
1	1	20	GLU
1	1	27	ASP
1	1	39	GLU
1	1	57	GLU
1	1	99	GLU
1	1	100	GLN
1	1	141	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1	194	MET
1	1	273	ASP
1	1	333	LEU
1	1	350	LEU
1	1	371	GLU
1	1	376	THR
1	1	396	LEU
1	1	397	PHE
1	1	408	LEU
1	1	412	THR
1	1	425	ILE
1	1	446	LEU
1	1	451	VAL
1	1	484	VAL
1	2	6	LYS
1	2	44	VAL
1	2	135	THR
1	2	141	ARG
1	2	182	LYS
1	2	254	LEU
1	2	272	LEU
1	2	293	CYS
1	2	325	GLU
1	2	348	ASP
1	2	350	LEU
1	2	403	GLU
1	2	408	LEU
1	2	420	LEU
1	2	425	ILE
1	2	451	VAL
1	2	477	ILE
1	2	481	CYS
1	3	22	GLN
1	3	27	ASP
1	3	37	THR
1	3	44	VAL
1	3	90	ASP
1	3	104	LEU
1	3	230	LYS
1	3	253	LYS
1	3	255	THR
1	3	272	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	3	336	GLU
1	3	350	LEU
1	3	390	PHE
1	3	425	ILE
1	3	476	VAL
1	3	477	ILE
1	4	44	VAL
1	4	131	ASP
1	4	141	ARG
1	4	230	LYS
1	4	251	VAL
1	4	254	LEU
1	4	272	LEU
1	4	285	ARG
1	4	334	ILE
1	4	350	LEU
1	4	357	MET
1	4	408	LEU
1	4	423	ARG
1	4	425	ILE
1	4	451	VAL
1	4	477	ILE
1	5	20	GLU
1	5	57	GLU
1	5	141	ARG
1	5	230	LYS
1	5	254	LEU
1	5	273	ASP
1	5	285	ARG
1	5	302	ARG
1	5	350	LEU
1	5	355	SER
1	5	356	LEU
1	5	403	GLU
1	5	408	LEU
1	5	425	ILE
1	5	451	VAL
1	5	476	VAL
1	5	477	ILE
1	6	5	MET
1	6	9	SER
1	6	96	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	6	159	ASN
1	6	211	VAL
1	6	230	LYS
1	6	242	LEU
1	6	253	LYS
1	6	254	LEU
1	6	272	LEU
1	6	283	LYS
1	6	350	LEU
1	6	358	THR
1	6	408	LEU
1	6	451	VAL
1	6	476	VAL
1	6	477	ILE
1	6	484	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	287	ASN
1	J	159	ASN
1	J	287	ASN
1	J	443	ASN
1	J	468	HIS
1	Q	468	HIS
1	X	286	ASN
1	Z	13	HIS
1	Z	22	GLN
1	1	100	GLN
1	1	286	ASN
1	1	443	ASN
1	4	289	GLN
1	6	459	GLN

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	1	482/484 (99%)	0.71	54 (11%) 6 4	36, 52, 63, 68	1 (0%)
1	2	482/484 (99%)	-0.04	3 (0%) 89 90	28, 42, 57, 62	1 (0%)
1	3	482/484 (99%)	0.11	7 (1%) 74 75	27, 43, 56, 64	1 (0%)
1	4	482/484 (99%)	-0.00	7 (1%) 74 75	33, 44, 57, 64	1 (0%)
1	5	482/484 (99%)	0.02	5 (1%) 82 82	31, 44, 58, 63	1 (0%)
1	6	482/484 (99%)	-0.18	0 100 100	26, 37, 51, 55	1 (0%)
1	A	482/484 (99%)	-0.14	1 (0%) 94 96	29, 41, 52, 64	1 (0%)
1	B	482/484 (99%)	-0.19	0 100 100	26, 38, 49, 59	1 (0%)
1	C	482/484 (99%)	-0.17	0 100 100	25, 38, 51, 62	1 (0%)
1	D	482/484 (99%)	-0.03	0 100 100	25, 40, 54, 63	1 (0%)
1	E	482/484 (99%)	-0.14	0 100 100	24, 37, 47, 59	1 (0%)
1	F	482/484 (99%)	-0.14	0 100 100	25, 36, 47, 58	1 (0%)
1	G	482/484 (99%)	-0.18	0 100 100	26, 38, 51, 61	1 (0%)
1	H	482/484 (99%)	-0.11	0 100 100	25, 39, 53, 62	1 (0%)
1	I	482/484 (99%)	0.36	27 (5%) 25 23	33, 49, 62, 67	1 (0%)
1	J	482/484 (99%)	-0.09	1 (0%) 94 96	29, 43, 54, 63	1 (0%)
1	K	482/484 (99%)	-0.08	4 (0%) 86 86	28, 41, 57, 60	1 (0%)
1	L	482/484 (99%)	-0.25	0 100 100	28, 39, 47, 54	1 (0%)
1	M	482/484 (99%)	-0.02	2 (0%) 92 93	32, 43, 55, 63	1 (0%)
1	N	482/484 (99%)	-0.13	0 100 100	29, 41, 51, 62	1 (0%)
1	O	482/484 (99%)	-0.05	1 (0%) 94 96	28, 42, 56, 61	1 (0%)
1	P	482/484 (99%)	-0.22	0 100 100	28, 36, 46, 54	1 (0%)
1	Q	482/484 (99%)	0.21	18 (3%) 42 41	38, 50, 61, 67	1 (0%)
1	R	482/484 (99%)	0.06	13 (2%) 55 55	31, 43, 57, 60	1 (0%)

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	S	482/484 (99%)	-0.20	0 100 100	32, 40, 49, 58	1 (0%)
1	T	482/484 (99%)	0.32	20 (4%) 38 36	39, 51, 62, 68	1 (0%)
1	U	482/484 (99%)	0.74	57 (11%) 5 4	43, 53, 64, 69	1 (0%)
1	V	482/484 (99%)	0.20	22 (4%) 33 31	38, 47, 60, 64	1 (0%)
1	W	482/484 (99%)	-0.07	2 (0%) 92 93	35, 44, 52, 59	1 (0%)
1	X	482/484 (99%)	0.77	55 (11%) 6 4	43, 54, 63, 69	1 (0%)
1	Y	482/484 (99%)	0.31	13 (2%) 55 55	30, 48, 59, 67	1 (0%)
1	Z	482/484 (99%)	0.68	52 (10%) 6 5	40, 52, 62, 71	1 (0%)
All	All	15424/15488 (99%)	0.07	364 (2%) 59 60	24, 43, 59, 71	32 (0%)

All (364) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	2	484	VAL	5.6
1	Z	8	PRO	5.4
1	Y	8	PRO	5.1
1	U	32	VAL	5.0
1	X	211	VAL	5.0
1	X	189	PHE	5.0
1	X	373	THR	4.8
1	Y	11	LEU	4.8
1	X	337	ALA	4.6
1	Z	4	SER	4.5
1	Z	227	ILE	4.5
1	U	11	LEU	4.5
1	M	3	GLY	4.4
1	X	400	ALA	4.4
1	1	101	GLY	4.4
1	1	406	VAL	4.3
1	Z	331	GLY	4.2
1	1	298	PHE	4.2
1	X	98	THR	4.1
1	X	95	ILE	4.0
1	Z	196	PHE	4.0
1	Z	65	GLY	4.0
1	U	33	PHE	3.9
1	1	373	THR	3.8
1	R	307	PHE	3.8
1	1	381	ASP	3.8

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	Z	193	ALA	3.8
1	X	44	VAL	3.8
1	1	84	LEU	3.7
1	1	5	MET	3.7
1	T	26	SER	3.7
1	I	374	VAL	3.7
1	U	381	ASP	3.7
1	Z	189	PHE	3.6
1	U	211	VAL	3.6
1	1	434	ALA	3.6
1	Q	349	ALA	3.5
1	U	314	ALA	3.5
1	I	372	PRO	3.5
1	U	332	PRO	3.5
1	X	181	VAL	3.5
1	Q	24	ALA	3.5
1	Z	351	ALA	3.5
1	U	377	GLY	3.4
1	X	5	MET	3.4
1	Z	10	LEU	3.4
1	I	373	THR	3.3
1	X	335	ASN	3.3
1	U	16	TYR	3.3
1	I	299	VAL	3.3
1	I	357	MET	3.3
1	1	351	ALA	3.3
1	Z	94	LEU	3.3
1	V	392	PRO	3.3
1	X	94	LEU	3.3
1	Z	6	LYS	3.2
1	R	375	LEU	3.2
1	X	92	LEU	3.2
1	U	210	VAL	3.2
1	U	92	LEU	3.2
1	U	359	GLY	3.2
1	V	307	PHE	3.2
1	V	374	VAL	3.2
1	Z	228	VAL	3.2
1	1	360	GLY	3.2
1	Z	382	MET	3.2
1	X	28	ALA	3.1
1	Z	334	ILE	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	1	397	PHE	3.1
1	U	212	ILE	3.1
1	X	3	GLY	3.1
1	X	49	ALA	3.1
1	Z	61	ALA	3.1
1	1	345	HIS	3.1
1	X	50	ALA	3.1
1	1	368	GLY	3.1
1	X	347	ALA	3.1
1	Z	208	LEU	3.1
1	U	45	PRO	3.1
1	Z	54	ARG	3.1
1	Z	201	ALA	3.0
1	T	375	LEU	3.0
1	Z	58	ALA	3.0
1	I	300	HIS	3.0
1	U	242	LEU	3.0
1	1	400	ALA	3.0
1	I	104	LEU	3.0
1	U	315	VAL	3.0
1	1	198	ALA	3.0
1	U	5	MET	3.0
1	T	359	GLY	2.9
1	U	357	MET	2.9
1	U	94	LEU	2.9
1	Z	37	THR	2.9
1	T	15	ALA	2.9
1	X	43	THR	2.9
1	X	192	LEU	2.9
1	R	342	VAL	2.9
1	Z	374	VAL	2.9
1	1	279	ALA	2.9
1	Z	5	MET	2.9
1	I	394	ALA	2.9
1	Z	91	ASP	2.9
1	T	373	THR	2.9
1	T	381	ASP	2.9
1	X	422	SER	2.9
1	X	104	LEU	2.9
1	U	284	TYR	2.9
1	U	380	PRO	2.8
1	Q	33	PHE	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	Q	5	MET	2.8
1	1	357	MET	2.8
1	1	297	PHE	2.8
1	Z	192	LEU	2.8
1	U	31	GLU	2.8
1	T	5	MET	2.8
1	1	419	TYR	2.8
1	A	5	MET	2.8
1	U	358	THR	2.8
1	U	360	GLY	2.8
1	K	400	ALA	2.8
1	R	374	VAL	2.8
1	V	306	ALA	2.8
1	3	326	SER	2.8
1	I	11	LEU	2.8
1	I	276	VAL	2.8
1	Z	238	ALA	2.8
1	Q	14	GLN	2.8
1	T	411	ASP	2.8
1	Z	161	PRO	2.7
1	V	399	PHE	2.7
1	I	306	ALA	2.7
1	T	351	ALA	2.7
1	1	276	VAL	2.7
1	I	94	LEU	2.7
1	1	375	LEU	2.7
1	4	350	LEU	2.7
1	Q	384	VAL	2.7
1	U	245	ALA	2.7
1	Z	381	ASP	2.7
1	1	307	PHE	2.7
1	4	351	ALA	2.7
1	V	380	PRO	2.7
1	Z	226	PRO	2.7
1	X	19	GLY	2.7
1	3	5	MET	2.7
1	X	11	LEU	2.7
1	1	265	ILE	2.7
1	5	381	ASP	2.7
1	V	300	HIS	2.6
1	V	304	TYR	2.6
1	X	4	SER	2.6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	X	29	THR	2.6
1	1	380	PRO	2.6
1	Y	5	MET	2.6
1	Q	242	LEU	2.6
1	4	39	GLU	2.6
1	Q	316	SER	2.6
1	V	398	ARG	2.6
1	U	397	PHE	2.6
1	T	377	GLY	2.6
1	Z	190	SER	2.6
1	R	398	ARG	2.6
1	U	297	PHE	2.6
1	1	233	PHE	2.6
1	Y	87	ALA	2.6
1	U	378	VAL	2.6
1	1	370	PHE	2.6
1	I	165	ILE	2.6
1	V	358	THR	2.6
1	X	212	ILE	2.6
1	X	324	THR	2.6
1	Q	28	ALA	2.6
1	I	5	MET	2.6
1	1	382	MET	2.6
1	U	186	SER	2.6
1	R	396	LEU	2.5
1	Y	94	LEU	2.5
1	4	333	LEU	2.5
1	V	353	GLY	2.5
1	X	482	VAL	2.5
1	V	357	MET	2.5
1	1	326	SER	2.5
1	1	404	GLU	2.5
1	3	291	CYS	2.5
1	Z	339	VAL	2.5
1	U	334	ILE	2.5
1	Z	98	THR	2.5
1	R	299	VAL	2.5
1	I	105	ALA	2.5
1	1	401	SER	2.5
1	U	26	SER	2.5
1	Z	353	GLY	2.5
1	X	368	GLY	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	U	355	SER	2.4
1	T	92	LEU	2.4
1	1	393	LEU	2.4
1	1	267	PHE	2.4
1	Q	400	ALA	2.4
1	U	129	ALA	2.4
1	U	354	ALA	2.4
1	U	468	HIS	2.4
1	X	37	THR	2.4
1	X	156	THR	2.4
1	I	396	LEU	2.4
1	T	398	ARG	2.4
1	U	330	LEU	2.4
1	1	89	SER	2.4
1	U	342	VAL	2.4
1	R	346	ILE	2.4
1	M	377	GLY	2.4
1	V	288	GLY	2.4
1	Z	210	VAL	2.4
1	Z	370	PHE	2.4
1	Z	383	ASP	2.4
1	K	267	PHE	2.4
1	V	267	PHE	2.4
1	I	37	THR	2.4
1	I	409	ALA	2.4
1	Q	11	LEU	2.4
1	Y	281	ALA	2.4
1	Y	360	GLY	2.4
1	Z	327	GLY	2.4
1	1	395	PRO	2.3
1	5	401	SER	2.3
1	U	203	VAL	2.3
1	I	400	ALA	2.3
1	U	400	ALA	2.3
1	X	375	LEU	2.3
1	Y	323	GLY	2.3
1	R	384	VAL	2.3
1	X	169	VAL	2.3
1	1	320	VAL	2.3
1	U	14	GLN	2.3
1	U	404	GLU	2.3
1	Z	11	LEU	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	1	331	GLY	2.3
1	1	354	ALA	2.3
1	U	403	GLU	2.3
1	Y	291	CYS	2.3
1	Q	367	HIS	2.3
1	X	367	HIS	2.3
1	Z	235	GLY	2.3
1	3	8	PRO	2.3
1	T	323	GLY	2.3
1	X	380	PRO	2.3
1	U	163	ALA	2.3
1	U	44	VAL	2.3
1	1	403	GLU	2.3
1	O	4	SER	2.3
1	T	328	ALA	2.3
1	Z	55	ALA	2.3
1	1	50	ALA	2.3
1	U	30	PHE	2.3
1	I	25	ASP	2.3
1	I	36	ALA	2.3
1	Z	411	ASP	2.3
1	1	266	VAL	2.3
1	X	395	PRO	2.2
1	V	301	GLU	2.2
1	X	338	ALA	2.2
1	T	4	SER	2.2
1	U	345	HIS	2.2
1	X	357	MET	2.2
1	Q	373	THR	2.2
1	T	98	THR	2.2
1	3	7	ASP	2.2
1	T	374	VAL	2.2
1	3	11	LEU	2.2
1	1	383	ASP	2.2
1	I	334	ILE	2.2
1	Z	165	ILE	2.2
1	1	330	LEU	2.2
1	V	429	TRP	2.2
1	U	313	ALA	2.2
1	I	329	THR	2.2
1	V	329	THR	2.2
1	Z	34	ASP	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	X	403	GLU	2.2
1	I	284	TYR	2.2
1	X	374	VAL	2.2
1	5	318	LEU	2.2
1	T	337	ALA	2.2
1	R	3	GLY	2.2
1	Y	327	GLY	2.2
1	1	268	ASP	2.2
1	T	211	VAL	2.2
1	1	77	ILE	2.2
1	U	350	LEU	2.2
1	Z	194	MET	2.2
1	U	316	SER	2.2
1	Y	192	LEU	2.2
1	Z	380	PRO	2.2
1	1	367	HIS	2.2
1	Z	3	GLY	2.2
1	3	25	ASP	2.2
1	R	354	ALA	2.2
1	U	28	ALA	2.2
1	U	90	ASP	2.1
1	X	91	ASP	2.1
1	X	364	ALA	2.1
1	Z	68	MET	2.1
1	T	387	GLU	2.1
1	1	402	GLU	2.1
1	1	10	LEU	2.1
1	K	377	GLY	2.1
1	V	130	GLY	2.1
1	V	350	LEU	2.1
1	1	272	LEU	2.1
1	U	319	LYS	2.1
1	X	12	ARG	2.1
1	Q	354	ALA	2.1
1	U	195	ALA	2.1
1	Z	64	ALA	2.1
1	Z	233	PHE	2.1
1	U	208	LEU	2.1
1	X	284	TYR	2.1
1	X	356	LEU	2.1
1	1	374	VAL	2.1
1	R	351	ALA	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	Y	81	TRP	2.1
1	1	355	SER	2.1
1	V	268	ASP	2.1
1	I	303	VAL	2.1
1	U	10	LEU	2.1
1	U	339	VAL	2.1
1	X	38	GLY	2.1
1	1	359	GLY	2.1
1	2	350	LEU	2.1
1	4	367	HIS	2.1
1	J	129	ALA	2.1
1	X	154	ALA	2.1
1	5	358	THR	2.1
1	W	470	GLY	2.1
1	Z	38	GLY	2.1
1	V	393	LEU	2.1
1	2	356	LEU	2.1
1	X	304	TYR	2.1
1	X	153	ALA	2.1
1	R	429	TRP	2.1
1	1	323	GLY	2.1
1	U	394	ALA	2.1
1	4	349	ALA	2.1
1	I	350	LEU	2.0
1	X	330	LEU	2.0
1	X	8	PRO	2.0
1	V	349	ALA	2.0
1	X	87	ALA	2.0
1	Y	26	SER	2.0
1	1	244	MET	2.0
1	Z	333	LEU	2.0
1	Z	375	LEU	2.0
1	Q	345	HIS	2.0
1	K	380	PRO	2.0
1	5	351	ALA	2.0
1	X	267	PHE	2.0
1	4	369	PHE	2.0
1	Q	10	LEU	2.0
1	I	8	PRO	2.0
1	Q	129	ALA	2.0
1	Q	355	SER	2.0
1	1	18	GLY	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	X	68	MET	2.0
1	W	484	VAL	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.