Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:25 PM GMT

PDB ID	:	4EQV
Title	:	Structure of Saccharomyces cerevisiae invertase
Authors	:	Sainz-Polo, M.A.; Sanz-Aparicio, J.
Deposited on	:	2012-04-19
Resolution	:	3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

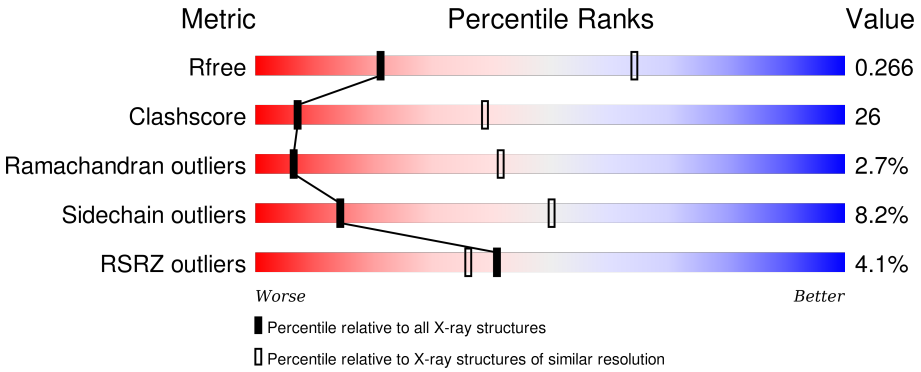
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 Å.

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



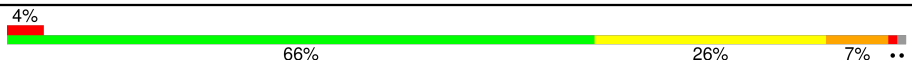
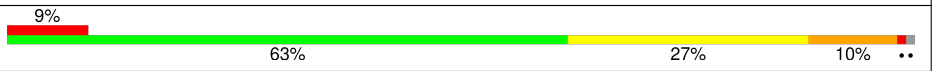
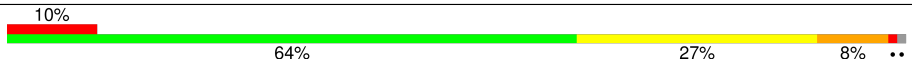
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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

Mol	Chain	Length	Quality of chain
1	A	512	71% 22% 6%
1	B	512	70% 24% 5%
1	C	512	2% 68% 25% 6%
1	D	512	3% 70% 22% 7%
1	E	512	4% 64% 27% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	512	
1	G	512	
1	H	512	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 33016 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 Invertase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	509	Total	C	N	O	S	0	0	0
			4124	2646	658	809	11			
1	B	509	Total	C	N	O	S	0	0	0
			4124	2646	658	809	11			
1	C	509	Total	C	N	O	S	0	0	0
			4124	2646	658	809	11			
1	D	509	Total	C	N	O	S	0	0	0
			4124	2646	658	809	11			
1	E	509	Total	C	N	O	S	0	0	0
			4124	2646	658	809	11			
1	F	509	Total	C	N	O	S	0	0	0
			4124	2646	658	809	11			
1	G	509	Total	C	N	O	S	0	0	0
			4124	2646	658	809	11			
1	H	509	Total	C	N	O	S	0	0	0
			4124	2646	658	809	11			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total	O	0	0
			6	6		
2	B	2	Total	O	0	0
			2	2		
2	C	4	Total	O	0	0
			4	4		
2	D	2	Total	O	0	0
			2	2		
2	E	1	Total	O	0	0
			1	1		
2	F	4	Total	O	0	0
			4	4		

Continued on next page...

Continued from previous page...

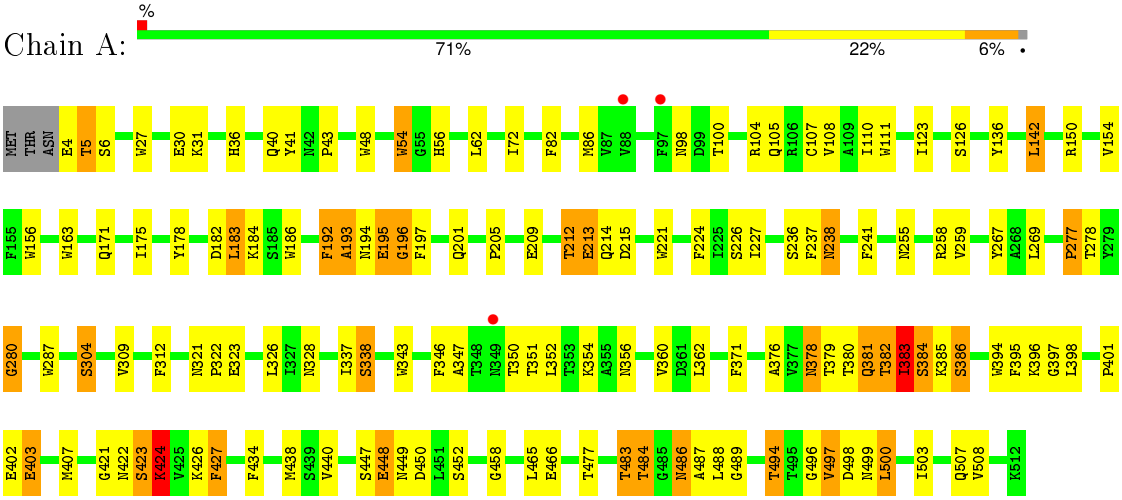
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total O 2 2	0	0
2	H	3	Total O 3 3	0	0

3 Residue-property plots (i)

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

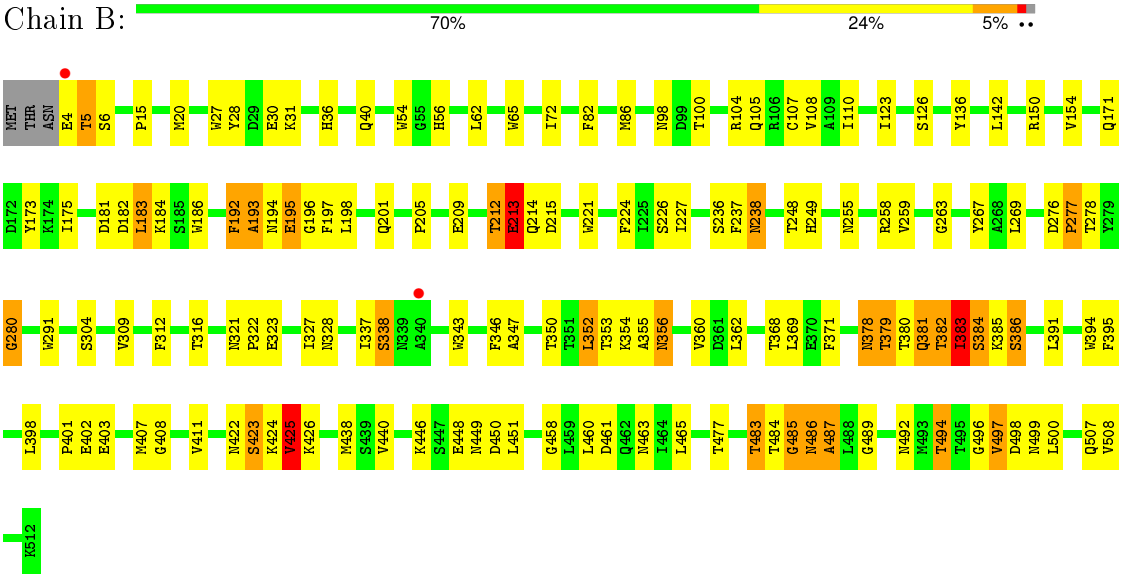
- Molecule 1: Invertase 2

Chain A:



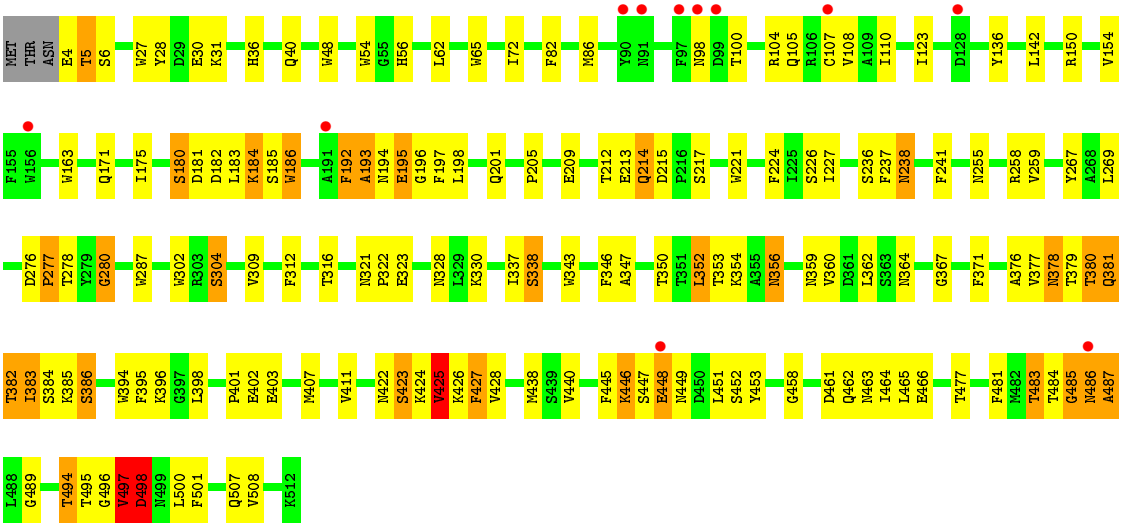
- Molecule 1: Invertase 2

Chain B:



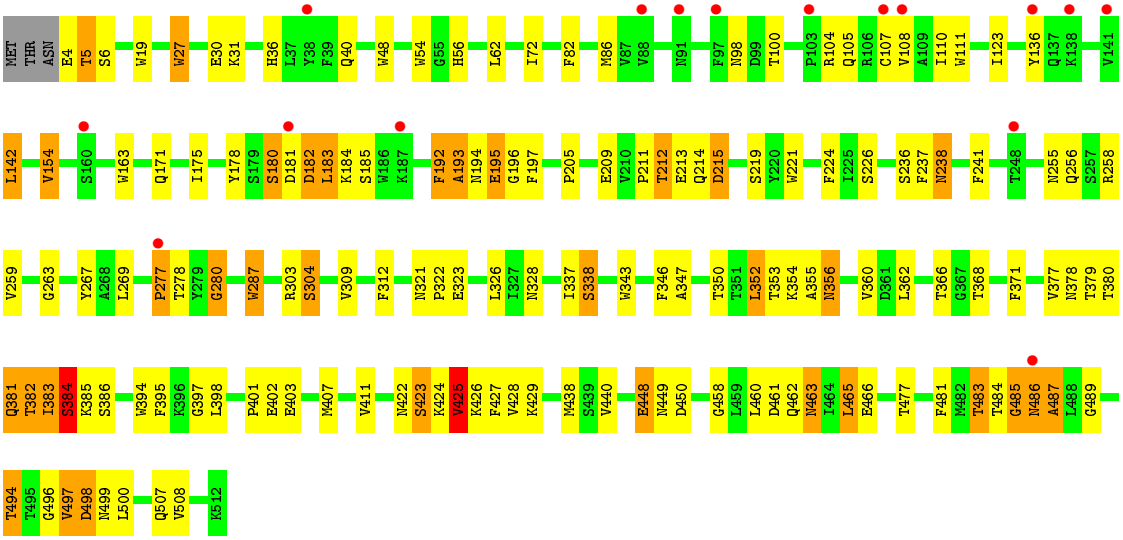
- Molecule 1: Invertase 2

Chain C:



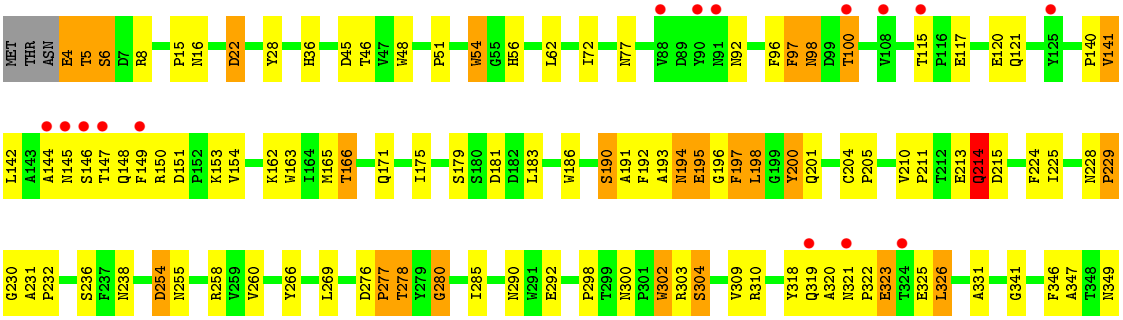
• Molecule 1: Invertase 2

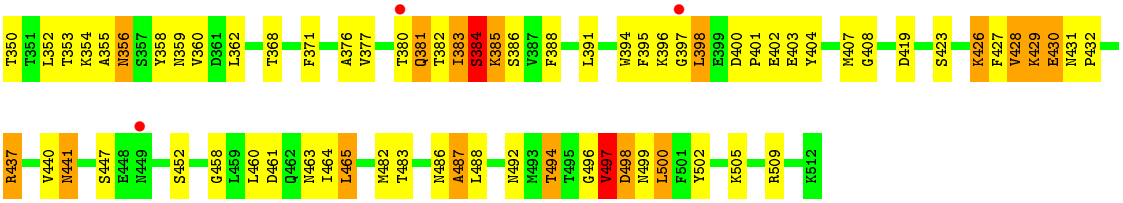
Chain D:



• Molecule 1: Invertase 2

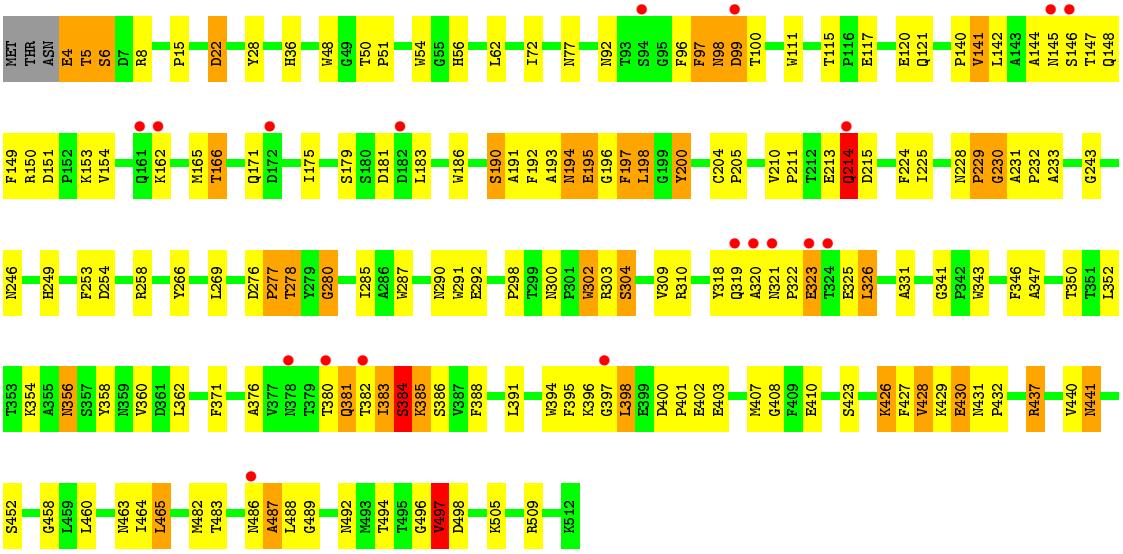
Chain E:





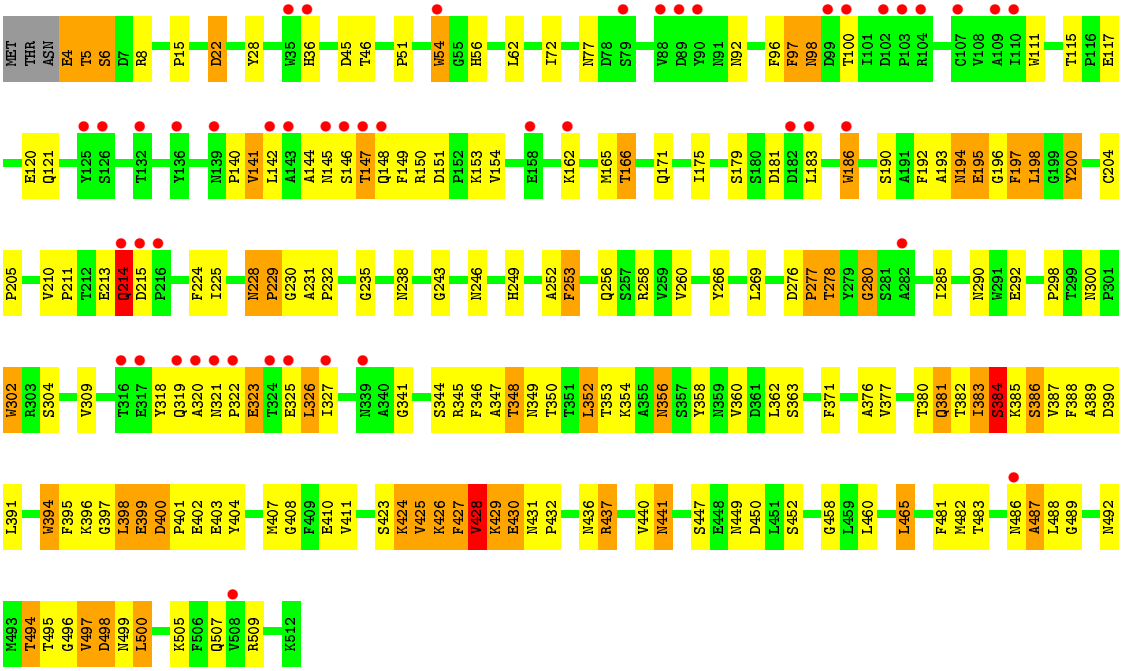
• Molecule 1: Invertase 2

Chain F:



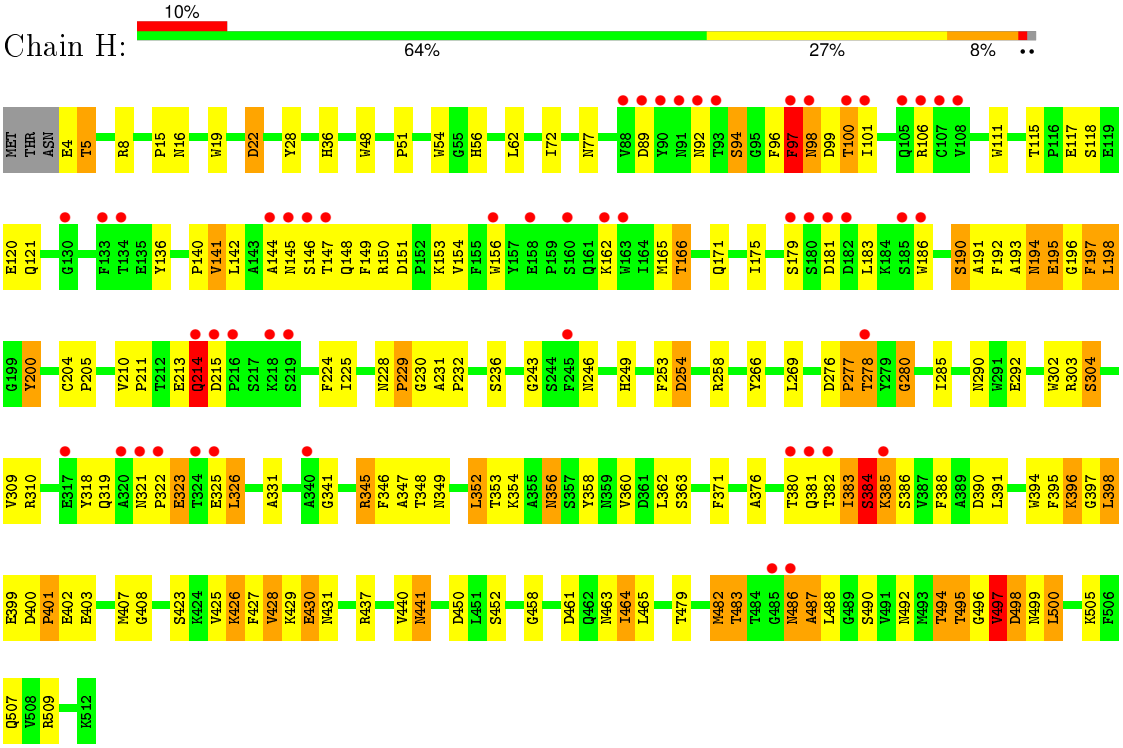
• Molecule 1: Invertase 2

Chain G:



• Molecule 1: Invertase 2

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	268.66Å 268.66Å 224.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	56.31 – 3.40 56.31 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.8 (56.31-3.40) 99.3 (56.31-3.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.92 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.221 , 0.239 0.247 , 0.266	Depositor DCC
R_{free} test set	6376 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	57.1	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.0	EDS
Estimated twinning fraction	0.730 for H, K, L 0.270 for -H, -K, L 0.000 for -h,-k,l	Xtriage
Reported twinning fraction	0.730 for H, K, L 0.270 for -H, -K, L	Depositor
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	1 of 127516 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	33016	wwPDB-VP
Average B, all atoms (Å^2)	51.0	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 21.37 % 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 7.1077e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.60	6/4252 (0.1%)	0.61	0/5798
1	B	0.58	2/4252 (0.0%)	0.62	2/5798 (0.0%)
1	C	0.56	4/4252 (0.1%)	0.59	1/5798 (0.0%)
1	D	0.57	7/4252 (0.2%)	0.60	2/5798 (0.0%)
1	E	0.55	5/4252 (0.1%)	0.59	0/5798
1	F	0.55	6/4252 (0.1%)	0.59	0/5798
1	G	0.58	7/4252 (0.2%)	0.59	1/5798 (0.0%)
1	H	0.60	6/4252 (0.1%)	0.59	0/5798
All	All	0.57	43/34016 (0.1%)	0.60	6/46384 (0.0%)

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	403	GLU	CD-OE1	10.25	1.36	1.25
1	H	385	LYS	CD-CE	9.87	1.75	1.51
1	H	385	LYS	CE-NZ	-9.31	1.25	1.49
1	G	4	GLU	CD-OE1	-7.78	1.17	1.25
1	G	4	GLU	CD-OE2	-7.65	1.17	1.25
1	E	302	TRP	CD2-CE2	5.36	1.47	1.41
1	F	287	TRP	CD2-CE2	5.33	1.47	1.41
1	B	65	TRP	CD2-CE2	5.32	1.47	1.41
1	D	111	TRP	CD2-CE2	5.28	1.47	1.41
1	C	186	TRP	CD2-CE2	5.27	1.47	1.41
1	A	48	TRP	CD2-CE2	5.20	1.47	1.41
1	D	27	TRP	CD2-CE2	5.18	1.47	1.41
1	H	48	TRP	CD2-CE2	5.18	1.47	1.41
1	A	54	TRP	CD2-CE2	5.18	1.47	1.41
1	D	353	THR	CB-CG2	-5.18	1.35	1.52
1	E	54	TRP	CD2-CE2	5.17	1.47	1.41
1	H	156	TRP	CD2-CE2	5.17	1.47	1.41
1	A	156	TRP	CD2-CE2	5.16	1.47	1.41
1	G	394	TRP	CD2-CE2	5.15	1.47	1.41
1	D	287	TRP	CD2-CE2	5.14	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	291	TRP	CD2-CE2	5.13	1.47	1.41
1	D	163	TRP	CD2-CE2	5.12	1.47	1.41
1	E	48	TRP	CD2-CE2	5.12	1.47	1.41
1	C	65	TRP	CD2-CE2	5.11	1.47	1.41
1	F	111	TRP	CD2-CE2	5.11	1.47	1.41
1	C	302	TRP	CD2-CE2	5.10	1.47	1.41
1	H	19	TRP	CD2-CE2	5.09	1.47	1.41
1	E	163	TRP	CD2-CE2	5.09	1.47	1.41
1	F	291	TRP	CD2-CE2	5.07	1.47	1.41
1	F	48	TRP	CD2-CE2	5.07	1.47	1.41
1	A	111	TRP	CD2-CE2	5.06	1.47	1.41
1	G	186	TRP	CD2-CE2	5.06	1.47	1.41
1	F	343	TRP	CD2-CE2	5.05	1.47	1.41
1	H	111	TRP	CD2-CE2	5.05	1.47	1.41
1	C	48	TRP	CD2-CE2	5.05	1.47	1.41
1	D	48	TRP	CD2-CE2	5.05	1.47	1.41
1	A	163	TRP	CD2-CE2	5.04	1.47	1.41
1	G	54	TRP	CD2-CE2	5.03	1.47	1.41
1	F	302	TRP	CD2-CE2	5.03	1.47	1.41
1	G	111	TRP	CD2-CE2	5.01	1.47	1.41
1	E	4	GLU	CD-OE2	-5.01	1.20	1.25
1	D	19	TRP	CD2-CE2	5.01	1.47	1.41
1	G	302	TRP	CD2-CE2	5.01	1.47	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	352	LEU	CA-CB-CG	5.84	128.74	115.30
1	D	352	LEU	CA-CB-CG	5.65	128.31	115.30
1	C	498	ASP	CB-CG-OD1	5.17	122.96	118.30
1	G	228	ASN	C-N-CD	-5.08	109.43	120.60
1	B	213	GLU	N-CA-C	-5.05	97.35	111.00
1	D	215	ASP	N-CA-CB	5.04	119.68	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4124	0	3831	176	0
1	B	4124	0	3831	156	0
1	C	4124	0	3831	187	0
1	D	4124	0	3831	178	0
1	E	4124	0	3831	243	0
1	F	4124	0	3831	232	0
1	G	4124	0	3831	282	0
1	H	4124	0	3831	271	0
2	A	6	0	0	1	0
2	B	2	0	0	0	0
2	C	4	0	0	1	0
2	D	2	0	0	0	0
2	E	1	0	0	0	0
2	F	4	0	0	0	0
2	G	2	0	0	0	0
2	H	3	0	0	0	0
All	All	33016	0	30648	1670	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 26.

All (1670) 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:H:385:LYS:CE	1:H:385:LYS:CD	1.75	1.58
1:E:228:ASN:ND2	1:E:229:PRO:HB3	1.35	1.40
1:F:228:ASN:ND2	1:F:229:PRO:HB3	1.35	1.37
1:H:486:ASN:HA	1:H:487:ALA:CB	1.41	1.35
1:H:97:PHE:CE2	1:H:106:ARG:HB3	1.62	1.34
1:E:228:ASN:CG	1:E:229:PRO:HB3	1.47	1.33
1:E:192:PHE:CG	1:E:193:ALA:HB2	1.68	1.28
1:D:496:GLY:O	1:D:497:VAL:HG22	1.12	1.28
1:F:194:ASN:HA	1:F:195:GLU:CB	1.63	1.28
1:G:98:ASN:CB	1:G:100:THR:HG22	1.61	1.28
1:G:256:GLN:OE1	1:G:327:ILE:HD12	1.17	1.27
1:F:192:PHE:CG	1:F:193:ALA:HB2	1.70	1.27
1:H:194:ASN:HA	1:H:195:GLU:CB	1.62	1.27
1:G:423:SER:OG	1:G:425:VAL:HG23	1.35	1.27
1:G:192:PHE:CG	1:G:193:ALA:HB2	1.69	1.26

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:192:PHE:CG	1:H:193:ALA:HB2	1.70	1.25
1:E:194:ASN:HA	1:E:195:GLU:CB	1.63	1.24
1:G:194:ASN:HA	1:G:195:GLU:CB	1.63	1.22
1:E:500:LEU:O	1:E:500:LEU:HD12	1.39	1.22
1:E:486:ASN:HA	1:E:487:ALA:CB	1.65	1.21
1:F:486:ASN:HA	1:F:487:ALA:CB	1.63	1.20
1:G:486:ASN:HA	1:G:487:ALA:CB	1.66	1.20
1:G:98:ASN:HB2	1:G:100:THR:CG2	1.69	1.19
1:G:385:LYS:HG3	1:G:386:SER:H	1.09	1.18
1:H:228:ASN:CG	1:H:229:PRO:HG3	1.61	1.18
1:D:213:GLU:O	1:D:214:GLN:CD	1.82	1.18
1:C:378:ASN:O	1:C:379:THR:HG22	1.43	1.18
1:D:378:ASN:O	1:D:379:THR:HG22	1.43	1.17
1:H:383:ILE:HD12	1:H:383:ILE:N	1.57	1.15
1:A:398:LEU:CB	1:A:487:ALA:HB3	1.77	1.15
1:D:496:GLY:O	1:D:497:VAL:CG2	1.95	1.15
1:H:97:PHE:HE2	1:H:106:ARG:CB	1.59	1.14
1:F:228:ASN:CG	1:F:229:PRO:HB3	1.67	1.14
1:A:378:ASN:O	1:A:379:THR:HG22	1.45	1.14
1:E:98:ASN:HB2	1:E:100:THR:HG23	1.14	1.13
1:B:424:LYS:C	1:B:425:VAL:HG23	1.63	1.13
1:H:98:ASN:HB2	1:H:100:THR:HG22	1.13	1.13
1:C:496:GLY:O	1:C:497:VAL:HG22	1.46	1.13
1:H:97:PHE:CE2	1:H:106:ARG:CB	2.30	1.12
1:G:243:GLY:HA2	1:G:253:PHE:CE1	1.84	1.12
1:F:194:ASN:CA	1:F:195:GLU:HB3	1.80	1.12
1:E:194:ASN:CA	1:E:195:GLU:HB3	1.79	1.12
1:D:180:SER:HB2	1:D:185:SER:O	1.46	1.12
1:H:194:ASN:CA	1:H:195:GLU:HB3	1.79	1.11
1:G:243:GLY:HA2	1:G:253:PHE:CD1	1.85	1.11
1:G:194:ASN:CA	1:G:195:GLU:HB3	1.80	1.10
1:A:213:GLU:O	1:A:214:GLN:CD	1.90	1.10
1:G:423:SER:OG	1:G:425:VAL:CG2	1.99	1.10
1:G:228:ASN:CG	1:G:229:PRO:HG3	1.71	1.10
1:E:398:LEU:CD1	1:E:487:ALA:O	2.00	1.10
1:H:228:ASN:OD1	1:H:229:PRO:HG3	1.52	1.10
1:E:144:ALA:HB1	1:E:145:ASN:HA	1.32	1.10
1:A:449:ASN:ND2	1:A:450:ASP:H	1.48	1.09
1:F:144:ALA:HB1	1:F:145:ASN:HA	1.30	1.09
1:A:398:LEU:HB2	1:A:487:ALA:HB3	1.11	1.09
1:B:496:GLY:O	1:B:497:VAL:HG22	1.50	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:398:LEU:HD13	1:F:398:LEU:H	1.12	1.09
1:F:5:THR:O	1:F:6:SER:HB2	1.47	1.09
1:B:449:ASN:ND2	1:B:450:ASP:H	1.50	1.08
1:H:228:ASN:ND2	1:H:229:PRO:HB3	1.68	1.08
1:C:192:PHE:CE2	1:C:195:GLU:HG2	1.89	1.08
1:G:486:ASN:HA	1:G:487:ALA:HB2	1.34	1.07
1:C:352:LEU:CD1	1:C:352:LEU:H	1.67	1.07
1:H:486:ASN:CA	1:H:487:ALA:CB	2.30	1.07
1:E:398:LEU:HD12	1:E:487:ALA:O	1.55	1.07
1:C:352:LEU:HD12	1:C:352:LEU:N	1.66	1.07
1:H:383:ILE:H	1:H:383:ILE:HD12	1.07	1.07
1:H:228:ASN:ND2	1:H:229:PRO:HG3	1.71	1.06
1:H:486:ASN:HA	1:H:487:ALA:HB2	1.37	1.06
1:F:486:ASN:HA	1:F:487:ALA:HB2	1.29	1.05
1:D:379:THR:HG22	1:D:450:ASP:O	1.56	1.05
1:E:486:ASN:HA	1:E:487:ALA:HB2	1.33	1.05
1:G:228:ASN:ND2	1:G:229:PRO:HG3	1.72	1.05
1:A:423:SER:O	1:A:424:LYS:HB2	1.52	1.05
1:H:144:ALA:HB1	1:H:145:ASN:HA	1.33	1.05
1:C:362:LEU:HA	1:E:356:ASN:HB3	1.34	1.05
1:E:398:LEU:CD1	1:E:398:LEU:H	1.70	1.05
1:B:378:ASN:O	1:B:379:THR:HG22	1.54	1.04
1:E:398:LEU:HD12	1:E:398:LEU:N	1.72	1.04
1:H:144:ALA:HB1	1:H:145:ASN:CA	1.87	1.04
1:D:213:GLU:C	1:D:214:GLN:OE1	1.95	1.04
1:D:379:THR:CG2	1:D:450:ASP:O	2.06	1.04
1:G:256:GLN:OE1	1:G:327:ILE:CD1	2.06	1.03
1:F:398:LEU:HD13	1:F:398:LEU:N	1.69	1.03
1:F:144:ALA:HB1	1:F:145:ASN:CA	1.89	1.03
1:G:385:LYS:HG3	1:G:386:SER:N	1.72	1.03
1:A:496:GLY:O	1:A:497:VAL:HG22	1.59	1.03
1:H:97:PHE:CD2	1:H:106:ARG:HG2	1.94	1.02
1:E:144:ALA:HB1	1:E:145:ASN:CA	1.88	1.02
1:B:424:LYS:O	1:B:425:VAL:HG23	1.58	1.02
1:D:403:GLU:OE2	1:D:424:LYS:HG3	1.58	1.02
1:A:422:ASN:HA	1:A:423:SER:HB2	1.40	1.02
1:E:385:LYS:HG3	1:E:386:SER:N	1.74	1.02
1:A:212:THR:HG22	1:A:215:ASP:O	1.60	1.01
1:G:144:ALA:HB1	1:G:145:ASN:CA	1.91	1.01
1:H:147:THR:HB	1:H:171:GLN:NE2	1.75	1.01
1:F:147:THR:HB	1:F:171:GLN:NE2	1.75	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:192:PHE:CD2	1:G:193:ALA:HB2	1.96	1.01
1:G:228:ASN:ND2	1:G:229:PRO:HB3	1.74	1.01
1:E:419:ASP:OD2	1:E:437:ARG:NH1	1.93	1.01
1:H:486:ASN:HA	1:H:487:ALA:HB3	1.02	1.00
1:A:403:GLU:OE2	1:A:424:LYS:CG	2.09	1.00
1:B:212:THR:HG23	1:B:213:GLU:O	1.57	1.00
1:A:500:LEU:HD12	1:A:500:LEU:O	1.59	1.00
1:A:213:GLU:C	1:A:214:GLN:OE1	1.99	1.00
1:E:192:PHE:CD2	1:E:193:ALA:HB2	1.96	1.00
1:G:228:ASN:OD1	1:G:229:PRO:HG3	1.62	1.00
1:E:147:THR:HB	1:E:171:GLN:NE2	1.76	1.00
1:H:192:PHE:CD2	1:H:193:ALA:HB2	1.98	0.99
1:G:98:ASN:N	1:G:98:ASN:HD22	1.58	0.99
1:H:486:ASN:CA	1:H:487:ALA:HB3	1.92	0.99
1:F:147:THR:HB	1:F:171:GLN:HE21	1.28	0.98
1:F:192:PHE:CD2	1:F:193:ALA:HB2	1.98	0.98
1:A:362:LEU:HA	1:F:356:ASN:HB3	1.42	0.98
1:E:228:ASN:CG	1:E:229:PRO:CB	2.31	0.98
1:A:352:LEU:CD1	1:A:503:ILE:HG12	1.94	0.98
1:C:352:LEU:HD12	1:C:352:LEU:H	0.83	0.97
1:C:422:ASN:HA	1:C:423:SER:HB2	1.46	0.97
1:E:228:ASN:OD1	1:E:229:PRO:HG3	1.63	0.97
1:A:496:GLY:O	1:A:497:VAL:HG13	1.64	0.97
1:G:228:ASN:CG	1:G:229:PRO:CG	2.32	0.97
1:H:228:ASN:CG	1:H:229:PRO:CG	2.32	0.97
1:F:385:LYS:HG3	1:F:386:SER:N	1.78	0.97
1:E:98:ASN:HB2	1:E:100:THR:CG2	1.94	0.96
1:H:147:THR:HB	1:H:171:GLN:HE21	1.30	0.96
1:G:98:ASN:HD22	1:G:98:ASN:H	1.03	0.96
1:A:212:THR:HG23	1:A:213:GLU:O	1.66	0.96
1:G:147:THR:HB	1:G:171:GLN:NE2	1.81	0.96
1:D:182:ASP:OD2	1:D:184:LYS:HG3	1.64	0.96
1:B:212:THR:CG2	1:B:213:GLU:O	2.14	0.96
1:G:194:ASN:HA	1:G:195:GLU:HB3	0.96	0.96
1:G:232:PRO:HG2	1:H:441:ASN:HB2	1.47	0.95
1:E:428:VAL:O	1:F:437:ARG:NH2	1.99	0.95
1:B:379:THR:CG2	1:B:380:THR:N	2.28	0.95
1:E:194:ASN:ND2	1:E:196:GLY:H	1.64	0.95
1:H:228:ASN:ND2	1:H:229:PRO:CB	2.29	0.95
1:E:147:THR:HB	1:E:171:GLN:HE21	1.31	0.95
1:H:194:ASN:ND2	1:H:196:GLY:H	1.65	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:145:ASN:N	1:H:146:SER:HA	1.81	0.95
1:G:144:ALA:HB1	1:G:145:ASN:HA	1.45	0.95
1:G:194:ASN:ND2	1:G:196:GLY:H	1.65	0.95
1:F:228:ASN:ND2	1:F:229:PRO:CB	2.29	0.94
1:G:383:ILE:O	1:G:384:SER:HB2	1.65	0.94
1:G:228:ASN:ND2	1:G:229:PRO:CB	2.29	0.94
1:H:194:ASN:HA	1:H:195:GLU:HB3	0.94	0.94
1:F:398:LEU:HD13	1:F:487:ALA:O	1.67	0.94
1:F:145:ASN:N	1:F:146:SER:HA	1.80	0.94
1:E:486:ASN:HA	1:E:487:ALA:HB3	1.50	0.93
1:F:486:ASN:HA	1:F:487:ALA:HB3	1.50	0.93
1:H:98:ASN:CB	1:H:100:THR:HG22	1.98	0.93
1:H:97:PHE:HD2	1:H:106:ARG:HG2	1.29	0.93
1:F:398:LEU:CD1	1:F:398:LEU:N	2.32	0.93
1:E:228:ASN:ND2	1:E:229:PRO:CB	2.29	0.93
1:A:422:ASN:HA	1:A:423:SER:CB	1.99	0.93
1:C:448:GLU:HA	1:C:448:GLU:OE1	1.67	0.93
1:F:194:ASN:ND2	1:F:196:GLY:H	1.65	0.92
1:F:194:ASN:HA	1:F:195:GLU:HB3	0.96	0.92
1:G:228:ASN:ND2	1:G:229:PRO:CG	2.32	0.92
1:E:145:ASN:N	1:E:146:SER:HA	1.82	0.92
1:E:326:LEU:H	1:E:326:LEU:HD12	1.34	0.92
1:A:192:PHE:HD2	1:A:192:PHE:O	1.53	0.92
1:H:228:ASN:ND2	1:H:229:PRO:CG	2.32	0.92
1:G:144:ALA:HB1	1:G:145:ASN:C	1.90	0.92
1:D:385:LYS:O	1:D:386:SER:HB3	1.68	0.92
1:G:437:ARG:NH2	1:H:428:VAL:O	2.03	0.91
1:G:385:LYS:CG	1:G:386:SER:N	2.30	0.91
1:F:400:ASP:OD1	1:F:401:PRO:O	1.89	0.91
1:E:194:ASN:HA	1:E:195:GLU:HB3	0.95	0.90
1:E:437:ARG:NH2	1:F:428:VAL:O	2.04	0.90
1:A:379:THR:CG2	1:A:450:ASP:O	2.20	0.90
1:A:449:ASN:HD22	1:A:450:ASP:H	1.15	0.90
1:G:486:ASN:HA	1:G:487:ALA:HB3	1.50	0.90
1:E:98:ASN:CB	1:E:100:THR:HG23	2.02	0.89
1:G:437:ARG:NH1	1:H:431:ASN:O	2.04	0.89
1:H:352:LEU:HB3	1:H:495:THR:HG21	1.55	0.89
1:D:213:GLU:O	1:D:214:GLN:OE1	1.91	0.89
1:F:496:GLY:O	1:F:497:VAL:HG12	1.72	0.89
1:H:97:PHE:CD2	1:H:106:ARG:CG	2.55	0.89
1:F:326:LEU:H	1:F:326:LEU:HD12	1.35	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:423:SER:O	1:C:425:VAL:HG23	1.73	0.89
1:B:449:ASN:HD22	1:B:450:ASP:H	1.15	0.89
1:H:326:LEU:HD12	1:H:326:LEU:H	1.36	0.89
1:F:394:TRP:HE1	1:F:494:THR:HB	1.38	0.89
1:E:192:PHE:CD1	1:E:193:ALA:HB2	2.09	0.88
1:H:383:ILE:CD1	1:H:383:ILE:N	2.33	0.88
1:A:496:GLY:C	1:A:497:VAL:HG13	1.94	0.88
1:F:98:ASN:HB2	1:F:100:THR:HG22	1.54	0.88
1:F:192:PHE:CD1	1:F:193:ALA:HB2	2.07	0.88
1:C:192:PHE:CZ	1:C:195:GLU:CG	2.57	0.88
1:B:446:LYS:NZ	1:B:448:GLU:OE2	2.04	0.88
1:C:192:PHE:CZ	1:C:195:GLU:HG2	2.09	0.88
1:H:323:GLU:OE2	1:H:323:GLU:HA	1.74	0.88
1:H:192:PHE:CD1	1:H:193:ALA:HB2	2.08	0.88
1:G:192:PHE:CD1	1:G:193:ALA:HB2	2.09	0.87
1:B:424:LYS:C	1:B:425:VAL:CG2	2.38	0.87
1:A:213:GLU:HB3	1:A:214:GLN:OE1	1.74	0.87
1:C:182:ASP:O	1:C:183:LEU:HB2	1.74	0.87
1:F:397:GLY:O	1:F:487:ALA:O	1.92	0.87
1:A:403:GLU:OE2	1:A:424:LYS:CB	2.22	0.87
1:G:5:THR:O	1:G:6:SER:HB2	1.75	0.86
1:G:326:LEU:HD12	1:G:326:LEU:H	1.37	0.86
1:B:422:ASN:HA	1:B:423:SER:HB2	1.56	0.86
1:D:403:GLU:OE2	1:D:424:LYS:CG	2.24	0.86
1:F:323:GLU:HA	1:F:323:GLU:OE2	1.74	0.86
1:E:323:GLU:OE2	1:E:323:GLU:HA	1.74	0.86
1:H:346:PHE:CE1	1:H:360:VAL:HG23	2.10	0.86
1:F:228:ASN:CG	1:F:229:PRO:CB	2.43	0.86
1:G:147:THR:HB	1:G:171:GLN:HE21	1.36	0.86
1:G:323:GLU:HA	1:G:323:GLU:OE2	1.75	0.86
1:H:92:ASN:OD1	1:H:96:PHE:O	1.93	0.86
1:E:194:ASN:HD22	1:E:196:GLY:H	1.24	0.86
1:D:212:THR:HG22	1:D:215:ASP:O	1.76	0.86
1:G:194:ASN:CA	1:G:195:GLU:CB	2.49	0.85
1:H:427:PHE:O	1:H:427:PHE:CD2	2.29	0.85
1:E:398:LEU:H	1:E:398:LEU:HD12	1.28	0.85
1:C:380:THR:HG22	1:C:380:THR:O	1.75	0.85
1:A:379:THR:CG2	1:A:380:THR:N	2.40	0.85
1:G:441:ASN:HB2	1:H:232:PRO:HG2	1.59	0.85
1:B:192:PHE:O	1:B:192:PHE:CD2	2.30	0.85
1:E:398:LEU:CD1	1:E:398:LEU:N	2.35	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:THR:HG23	1:A:380:THR:N	1.91	0.84
1:B:379:THR:HG22	1:B:380:THR:H	1.41	0.84
1:E:427:PHE:CD2	1:E:427:PHE:O	2.30	0.84
1:E:394:TRP:HE1	1:E:494:THR:HB	1.42	0.84
1:F:194:ASN:CA	1:F:195:GLU:CB	2.48	0.84
1:H:385:LYS:NZ	1:H:385:LYS:CD	2.41	0.84
1:G:396:LYS:HG2	1:G:404:TYR:HB3	1.60	0.84
1:E:497:VAL:O	1:E:497:VAL:HG12	1.78	0.84
1:A:192:PHE:CD2	1:A:192:PHE:O	2.31	0.84
1:B:238:ASN:HD21	1:B:269:LEU:H	1.25	0.84
1:D:422:ASN:HA	1:D:423:SER:HB2	1.59	0.84
1:F:427:PHE:CD2	1:F:427:PHE:O	2.31	0.83
1:D:195:GLU:OE2	1:D:195:GLU:HA	1.76	0.83
1:F:194:ASN:HD22	1:F:196:GLY:H	1.25	0.83
1:G:243:GLY:CA	1:G:253:PHE:CE1	2.60	0.83
1:D:238:ASN:HD21	1:D:269:LEU:H	1.26	0.83
1:G:394:TRP:HE1	1:G:494:THR:HB	1.41	0.83
1:C:378:ASN:C	1:C:378:ASN:HD22	1.81	0.83
1:C:238:ASN:HD21	1:C:269:LEU:H	1.26	0.82
1:H:198:LEU:HD12	1:H:198:LEU:C	1.99	0.82
1:E:194:ASN:CA	1:E:195:GLU:CB	2.48	0.82
1:B:379:THR:HG22	1:B:380:THR:N	1.93	0.82
1:H:353:THR:HB	1:H:498:ASP:OD1	1.79	0.82
1:B:382:THR:C	1:B:383:ILE:HG12	2.00	0.82
1:G:318:TYR:HD2	1:G:319:GLN:O	1.63	0.82
1:F:398:LEU:HD11	1:F:489:GLY:HA3	1.62	0.82
1:H:194:ASN:HD22	1:H:196:GLY:H	1.25	0.81
1:E:198:LEU:HD12	1:E:198:LEU:C	2.00	0.81
1:C:496:GLY:O	1:C:497:VAL:CG2	2.28	0.81
1:F:326:LEU:N	1:F:326:LEU:HD12	1.96	0.81
1:F:198:LEU:HD12	1:F:198:LEU:C	2.01	0.81
1:A:496:GLY:O	1:A:497:VAL:CG2	2.28	0.81
1:F:318:TYR:HD2	1:F:319:GLN:O	1.63	0.81
1:A:238:ASN:HD21	1:A:269:LEU:H	1.26	0.81
1:B:356:ASN:HB3	1:G:362:LEU:HA	1.62	0.81
1:E:318:TYR:HD2	1:E:319:GLN:O	1.63	0.81
1:E:326:LEU:HD12	1:E:326:LEU:N	1.95	0.81
1:C:323:GLU:HG2	1:D:171:GLN:HE21	1.46	0.81
1:H:318:TYR:HD2	1:H:319:GLN:O	1.62	0.81
1:H:97:PHE:HE2	1:H:106:ARG:CA	1.93	0.81
1:D:379:THR:HG23	1:D:380:THR:N	1.95	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:347:ALA:HB1	1:E:350:THR:HG21	1.63	0.81
1:H:383:ILE:H	1:H:383:ILE:CD1	1.78	0.80
1:E:5:THR:O	1:E:300:ASN:O	2.00	0.80
1:A:192:PHE:CZ	1:A:195:GLU:HG2	2.16	0.80
1:H:231:ALA:H	1:H:232:PRO:HD2	1.46	0.80
1:A:403:GLU:OE2	1:A:424:LYS:HG3	1.80	0.80
1:F:496:GLY:O	1:F:497:VAL:CB	2.30	0.80
1:G:198:LEU:HD12	1:G:198:LEU:C	2.01	0.80
1:C:213:GLU:O	1:C:214:GLN:CG	2.30	0.80
1:G:346:PHE:CE1	1:G:360:VAL:HG23	2.17	0.80
1:H:228:ASN:OD1	1:H:229:PRO:CG	2.30	0.80
1:F:228:ASN:OD1	1:F:229:PRO:CG	2.30	0.80
1:B:497:VAL:HG23	1:B:497:VAL:O	1.82	0.80
1:D:195:GLU:CA	1:D:195:GLU:OE2	2.30	0.80
1:G:92:ASN:OD1	1:G:96:PHE:O	1.98	0.80
1:H:385:LYS:CG	1:H:385:LYS:CE	2.60	0.79
1:D:497:VAL:HG23	1:D:497:VAL:O	1.82	0.79
1:F:427:PHE:O	1:F:428:VAL:HG23	1.82	0.79
1:F:347:ALA:HB1	1:F:350:THR:HG21	1.62	0.79
1:A:500:LEU:HD12	1:A:500:LEU:C	1.99	0.79
1:H:144:ALA:HB1	1:H:145:ASN:C	2.01	0.79
1:H:144:ALA:CB	1:H:145:ASN:HA	2.13	0.79
1:C:379:THR:CG2	1:C:380:THR:N	2.46	0.79
1:A:378:ASN:C	1:A:378:ASN:HD22	1.84	0.79
1:H:98:ASN:ND2	1:H:98:ASN:N	2.31	0.79
1:G:194:ASN:HD22	1:G:196:GLY:H	1.26	0.79
1:A:379:THR:HG22	1:A:450:ASP:O	1.81	0.79
1:B:449:ASN:ND2	1:B:450:ASP:N	2.31	0.79
1:B:192:PHE:O	1:B:192:PHE:HD2	1.65	0.79
1:B:362:LEU:HA	1:G:356:ASN:HB3	1.65	0.79
1:E:228:ASN:OD1	1:E:229:PRO:CG	2.30	0.79
1:G:145:ASN:N	1:G:146:SER:HA	1.97	0.79
1:E:96:PHE:O	1:E:97:PHE:CD1	2.36	0.79
1:E:497:VAL:O	1:E:497:VAL:CG1	2.30	0.79
1:D:394:TRP:HE1	1:D:494:THR:HB	1.48	0.79
1:F:290:ASN:OD1	1:F:292:GLU:HG2	1.83	0.79
1:E:353:THR:HA	1:E:498:ASP:O	1.83	0.79
1:C:445:PHE:CE1	1:C:446:LYS:HD3	2.18	0.79
1:E:144:ALA:HB1	1:E:145:ASN:C	2.03	0.78
1:H:147:THR:CB	1:H:171:GLN:NE2	2.47	0.78
1:F:228:ASN:OD1	1:F:229:PRO:HD3	1.83	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:228:ASN:OD1	1:G:229:PRO:CG	2.31	0.78
1:H:326:LEU:HD12	1:H:326:LEU:N	1.97	0.78
1:C:180:SER:HB2	1:C:185:SER:O	1.83	0.78
1:G:486:ASN:CA	1:G:487:ALA:CB	2.58	0.78
1:E:98:ASN:CB	1:E:100:THR:CG2	2.61	0.78
1:E:427:PHE:O	1:E:427:PHE:CG	2.34	0.78
1:H:98:ASN:N	1:H:98:ASN:HD22	1.79	0.78
1:B:496:GLY:O	1:B:497:VAL:CG2	2.30	0.78
1:C:192:PHE:O	1:C:192:PHE:HD2	1.67	0.78
1:G:326:LEU:N	1:G:326:LEU:HD12	1.97	0.78
1:F:228:ASN:OD1	1:F:229:PRO:CD	2.32	0.78
1:G:423:SER:HG	1:G:425:VAL:CG2	1.92	0.78
1:B:212:THR:HG22	1:B:215:ASP:O	1.84	0.78
1:D:385:LYS:HG3	1:D:386:SER:H	1.48	0.78
1:G:5:THR:HG22	1:G:6:SER:O	1.83	0.78
1:E:5:THR:O	1:E:6:SER:CB	2.30	0.78
1:E:192:PHE:CD2	1:E:193:ALA:CB	2.67	0.78
1:E:92:ASN:OD1	1:E:96:PHE:O	2.02	0.78
1:A:449:ASN:ND2	1:A:450:ASP:N	2.30	0.78
1:F:144:ALA:CB	1:F:145:ASN:HA	2.11	0.78
1:C:394:TRP:HE1	1:C:494:THR:HB	1.48	0.78
1:A:394:TRP:HE1	1:A:494:THR:HB	1.47	0.78
1:F:147:THR:CB	1:F:171:GLN:NE2	2.47	0.77
1:F:496:GLY:O	1:F:497:VAL:CG1	2.31	0.77
1:A:171:GLN:HE21	1:B:323:GLU:HG2	1.49	0.77
1:H:97:PHE:HD2	1:H:106:ARG:CG	1.94	0.77
1:A:403:GLU:OE2	1:A:483:THR:HB	1.84	0.77
1:E:290:ASN:OD1	1:E:292:GLU:HG2	1.83	0.77
1:C:497:VAL:CG2	1:C:497:VAL:O	2.31	0.77
1:A:496:GLY:O	1:A:497:VAL:CG1	2.32	0.77
1:E:144:ALA:CB	1:E:145:ASN:HA	2.12	0.77
1:G:232:PRO:CG	1:H:441:ASN:HB2	2.14	0.77
1:G:192:PHE:CD2	1:G:193:ALA:CB	2.67	0.77
1:D:379:THR:HG21	1:D:450:ASP:O	1.84	0.77
1:G:427:PHE:O	1:G:428:VAL:HG23	1.84	0.77
1:C:485:GLY:O	1:C:486:ASN:HB2	1.85	0.77
1:H:290:ASN:OD1	1:H:292:GLU:HG2	1.84	0.77
1:B:394:TRP:HE1	1:B:494:THR:HB	1.48	0.77
1:E:147:THR:CB	1:E:171:GLN:NE2	2.47	0.77
1:E:298:PRO:HD3	1:E:427:PHE:CD2	2.19	0.77
1:G:290:ASN:OD1	1:G:292:GLU:HG2	1.85	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:496:GLY:C	1:D:497:VAL:HG22	2.03	0.76
1:H:427:PHE:O	1:H:428:VAL:HG23	1.84	0.76
1:H:96:PHE:C	1:H:97:PHE:HD1	1.87	0.76
1:G:5:THR:O	1:G:300:ASN:O	2.04	0.76
1:F:347:ALA:CB	1:F:350:THR:HG21	2.15	0.76
1:C:379:THR:HG23	1:C:380:THR:N	1.98	0.76
1:G:231:ALA:H	1:G:232:PRO:HD2	1.49	0.76
1:B:403:GLU:OE2	1:B:483:THR:HB	1.85	0.76
1:G:428:VAL:HG12	1:G:429:LYS:N	1.99	0.76
1:D:485:GLY:O	1:D:486:ASN:HB2	1.84	0.76
1:D:356:ASN:HB3	1:H:362:LEU:HA	1.67	0.76
1:G:381:GLN:O	1:G:382:THR:C	2.23	0.76
1:D:378:ASN:O	1:D:379:THR:CG2	2.31	0.76
1:D:379:THR:CG2	1:D:380:THR:N	2.48	0.76
1:G:147:THR:HA	1:G:171:GLN:HE22	1.51	0.76
1:C:403:GLU:OE2	1:C:483:THR:HB	1.86	0.76
1:F:4:GLU:CD	1:F:4:GLU:N	2.37	0.76
1:C:214:GLN:HG2	1:C:215:ASP:H	1.51	0.75
1:H:192:PHE:CD2	1:H:193:ALA:CB	2.69	0.75
1:B:277:PRO:HB3	1:B:280:GLY:HA2	1.67	0.75
1:G:388:PHE:CE2	1:G:390:ASP:HB3	2.21	0.75
1:A:378:ASN:O	1:A:379:THR:CG2	2.31	0.75
1:B:378:ASN:O	1:B:379:THR:CG2	2.34	0.75
1:C:403:GLU:OE2	1:C:424:LYS:HG3	1.86	0.75
1:H:231:ALA:HB3	1:H:232:PRO:HD3	1.68	0.75
1:H:488:LEU:N	1:H:488:LEU:HD23	2.01	0.75
1:C:192:PHE:CZ	1:C:195:GLU:HG3	2.21	0.75
1:G:121:GLN:HG3	1:G:149:PHE:HE2	1.52	0.75
1:C:352:LEU:CD1	1:C:501:PHE:O	2.35	0.75
1:G:496:GLY:O	1:G:497:VAL:HG22	1.85	0.75
1:B:424:LYS:O	1:B:425:VAL:CG2	2.32	0.75
1:E:347:ALA:CB	1:E:350:THR:HG21	2.16	0.74
1:C:496:GLY:C	1:C:497:VAL:HG13	2.05	0.74
1:G:383:ILE:O	1:G:384:SER:CB	2.35	0.74
1:F:460:LEU:HG	1:F:465:LEU:HD12	1.68	0.74
1:C:380:THR:O	1:C:380:THR:CG2	2.35	0.74
1:D:403:GLU:OE2	1:D:483:THR:HB	1.87	0.74
1:G:231:ALA:HB3	1:G:232:PRO:HD3	1.70	0.74
1:D:277:PRO:HB3	1:D:280:GLY:HA2	1.67	0.74
1:F:147:THR:HA	1:F:171:GLN:HE22	1.53	0.74
1:F:96:PHE:O	1:F:97:PHE:HB2	1.87	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:GLY:O	1:B:486:ASN:HB2	1.85	0.74
1:D:362:LEU:HA	1:H:356:ASN:HB3	1.69	0.74
1:G:397:GLY:O	1:G:487:ALA:O	2.05	0.74
1:F:144:ALA:HB1	1:F:145:ASN:C	2.08	0.74
1:B:379:THR:HG23	1:B:380:THR:N	2.01	0.74
1:G:147:THR:CB	1:G:171:GLN:NE2	2.50	0.74
1:F:148:GLN:HE21	1:F:150:ARG:CZ	2.01	0.74
1:G:194:ASN:HD22	1:G:196:GLY:N	1.86	0.74
1:C:277:PRO:HB3	1:C:280:GLY:HA2	1.69	0.74
1:C:192:PHE:C	1:C:192:PHE:CD2	2.60	0.74
1:H:194:ASN:HD22	1:H:196:GLY:N	1.85	0.73
1:G:144:ALA:HB1	1:G:145:ASN:O	1.88	0.73
1:G:496:GLY:C	1:G:497:VAL:HG13	2.07	0.73
1:E:194:ASN:HD22	1:E:196:GLY:N	1.85	0.73
1:C:378:ASN:O	1:C:379:THR:CG2	2.29	0.73
1:B:98:ASN:HB2	1:B:100:THR:HG22	1.69	0.73
1:H:121:GLN:HG3	1:H:149:PHE:HE2	1.52	0.73
1:H:97:PHE:CE2	1:H:106:ARG:CG	2.69	0.73
1:F:192:PHE:CD2	1:F:193:ALA:CB	2.69	0.73
1:G:228:ASN:CG	1:G:229:PRO:HB3	2.09	0.73
1:B:136:TYR:CE1	1:B:184:LYS:HD3	2.24	0.73
1:F:194:ASN:HD22	1:F:196:GLY:N	1.85	0.73
1:D:98:ASN:HB2	1:D:100:THR:HG22	1.71	0.73
1:A:277:PRO:HB3	1:A:280:GLY:HA2	1.69	0.73
1:A:422:ASN:CA	1:A:423:SER:HB2	2.17	0.73
1:G:395:PHE:HE2	1:G:407:MET:HE2	1.53	0.73
1:H:486:ASN:CA	1:H:487:ALA:HB2	2.08	0.73
1:F:147:THR:CB	1:F:171:GLN:HE21	2.01	0.73
1:A:31:LYS:HB3	1:A:104:ARG:HE	1.54	0.73
1:A:192:PHE:CD2	1:A:192:PHE:C	2.62	0.72
1:G:497:VAL:CG2	1:G:497:VAL:O	2.36	0.72
1:A:212:THR:CG2	1:A:215:ASP:O	2.36	0.72
1:A:379:THR:HG21	1:A:450:ASP:O	1.87	0.72
1:H:147:THR:HA	1:H:171:GLN:HE22	1.53	0.72
1:A:352:LEU:CD1	1:A:503:ILE:CG1	2.66	0.72
1:F:229:PRO:HG2	1:F:230:GLY:H	1.53	0.72
1:H:400:ASP:O	1:H:401:PRO:O	2.07	0.72
1:F:395:PHE:HE2	1:F:407:MET:HE2	1.54	0.72
1:A:378:ASN:C	1:A:378:ASN:ND2	2.42	0.72
1:E:231:ALA:HB3	1:E:232:PRO:HD3	1.70	0.72
1:B:353:THR:HB	1:B:498:ASP:OD2	1.88	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:GLU:O	1:C:214:GLN:HG2	1.88	0.72
1:H:400:ASP:OD1	1:H:401:PRO:O	2.08	0.72
1:E:147:THR:HA	1:E:171:GLN:HE22	1.53	0.72
1:F:497:VAL:O	1:F:497:VAL:CG1	2.38	0.72
1:H:98:ASN:ND2	1:H:98:ASN:H	1.88	0.72
1:D:321:ASN:HB2	1:D:322:PRO:HD2	1.72	0.72
1:A:98:ASN:HB2	1:A:100:THR:HG22	1.71	0.72
1:D:212:THR:HG23	1:D:213:GLU:O	1.90	0.72
1:H:383:ILE:O	1:H:384:SER:HB2	1.88	0.72
1:B:31:LYS:HB3	1:B:104:ARG:HE	1.55	0.72
1:C:255:ASN:O	1:D:194:ASN:O	2.08	0.72
1:D:192:PHE:O	1:D:192:PHE:CD2	2.43	0.72
1:E:232:PRO:HG2	1:F:441:ASN:HB2	1.71	0.71
1:D:192:PHE:HA	1:D:193:ALA:HB2	1.71	0.71
1:D:180:SER:CB	1:D:185:SER:O	2.32	0.71
1:G:346:PHE:CE1	1:G:360:VAL:CG2	2.73	0.71
1:G:353:THR:HA	1:G:498:ASP:O	1.91	0.71
1:E:228:ASN:OD1	1:E:229:PRO:HB3	1.90	0.71
1:G:398:LEU:N	1:G:487:ALA:O	2.24	0.71
1:E:147:THR:CB	1:E:171:GLN:HE21	2.01	0.71
1:A:422:ASN:CA	1:A:423:SER:CB	2.68	0.71
1:E:5:THR:O	1:E:6:SER:HB2	1.91	0.71
1:H:423:SER:OG	1:H:425:VAL:HG23	1.91	0.71
1:H:147:THR:CB	1:H:171:GLN:HE21	2.01	0.71
1:G:148:GLN:HE21	1:G:150:ARG:CZ	2.03	0.71
1:A:195:GLU:CA	1:A:195:GLU:OE2	2.38	0.71
1:E:228:ASN:HD21	1:E:229:PRO:HB3	1.49	0.71
1:C:171:GLN:HE21	1:D:323:GLU:HG2	1.55	0.71
1:G:229:PRO:CG	1:G:230:GLY:H	2.02	0.70
1:H:96:PHE:CB	1:H:97:PHE:HD1	2.04	0.70
1:G:401:PRO:O	1:G:402:GLU:CB	2.38	0.70
1:G:147:THR:CB	1:G:171:GLN:HE21	2.04	0.70
1:F:121:GLN:HG3	1:F:149:PHE:HE2	1.54	0.70
1:A:352:LEU:HD11	1:A:503:ILE:CG1	2.22	0.70
1:G:228:ASN:CG	1:G:229:PRO:CB	2.57	0.70
1:F:144:ALA:CB	1:F:145:ASN:CA	2.67	0.70
1:F:5:THR:O	1:F:300:ASN:O	2.10	0.70
1:F:231:ALA:HB3	1:F:232:PRO:HD3	1.73	0.70
1:D:31:LYS:HB3	1:D:104:ARG:HE	1.56	0.70
1:H:148:GLN:HE21	1:H:150:ARG:CZ	2.03	0.70
1:B:378:ASN:ND2	1:B:380:THR:O	2.23	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:318:TYR:CD2	1:G:319:GLN:O	2.45	0.70
1:E:121:GLN:HG3	1:E:149:PHE:HE2	1.54	0.70
1:H:96:PHE:C	1:H:97:PHE:CD1	2.64	0.70
1:C:31:LYS:HB3	1:C:104:ARG:HE	1.55	0.70
1:F:298:PRO:HD3	1:F:427:PHE:CD2	2.26	0.70
1:G:144:ALA:CB	1:G:145:ASN:CA	2.67	0.70
1:E:419:ASP:CG	1:E:437:ARG:HH11	1.93	0.70
1:B:346:PHE:CE1	1:B:360:VAL:HG23	2.26	0.70
1:F:397:GLY:HA2	1:F:400:ASP:O	1.91	0.69
1:F:318:TYR:CD2	1:F:319:GLN:O	2.45	0.69
1:F:4:GLU:OE2	1:F:4:GLU:N	2.25	0.69
1:A:381:GLN:O	1:A:382:THR:OG1	2.09	0.69
1:D:385:LYS:HG3	1:D:386:SER:N	2.05	0.69
1:D:195:GLU:HB3	1:D:241:PHE:CZ	2.27	0.69
1:H:318:TYR:CD2	1:H:319:GLN:O	2.45	0.69
1:A:195:GLU:OE2	1:A:195:GLU:HA	1.91	0.69
1:C:213:GLU:O	1:C:214:GLN:CD	2.30	0.69
1:B:403:GLU:OE2	1:B:424:LYS:HG3	1.92	0.69
1:G:62:LEU:HD22	1:G:309:VAL:HG21	1.74	0.69
1:A:213:GLU:O	1:A:214:GLN:OE1	2.02	0.69
1:B:383:ILE:O	1:B:384:SER:CB	2.41	0.69
1:G:400:ASP:OD1	1:G:400:ASP:C	2.30	0.69
1:F:486:ASN:CA	1:F:487:ALA:CB	2.55	0.69
1:G:229:PRO:HG2	1:G:230:GLY:H	1.58	0.69
1:G:256:GLN:NE2	1:G:326:LEU:HB2	2.07	0.69
1:A:381:GLN:C	1:A:382:THR:OG1	2.30	0.69
1:G:243:GLY:C	1:G:253:PHE:HE1	1.95	0.69
1:D:182:ASP:OD2	1:D:182:ASP:C	2.30	0.69
1:A:195:GLU:HB3	1:A:241:PHE:CZ	2.28	0.69
1:G:5:THR:O	1:G:6:SER:CB	2.40	0.69
1:C:346:PHE:CE1	1:C:360:VAL:HG23	2.28	0.69
1:C:215:ASP:OD1	1:C:215:ASP:C	2.31	0.69
1:F:4:GLU:OE2	1:F:4:GLU:C	2.31	0.69
1:F:96:PHE:O	1:F:97:PHE:CB	2.41	0.69
1:C:98:ASN:HB2	1:C:100:THR:HG22	1.73	0.69
1:H:194:ASN:CA	1:H:195:GLU:CB	2.48	0.69
1:A:212:THR:HG22	1:A:215:ASP:C	2.14	0.69
1:E:194:ASN:ND2	1:E:196:GLY:N	2.41	0.68
1:F:62:LEU:HD22	1:F:309:VAL:HG21	1.73	0.68
1:D:346:PHE:CE1	1:D:360:VAL:HG23	2.28	0.68
1:D:192:PHE:CE1	1:D:195:GLU:CG	2.77	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:144:ALA:CB	1:G:145:ASN:HA	2.22	0.68
1:G:411:VAL:HG21	1:G:500:LEU:CD2	2.23	0.68
1:G:427:PHE:CD2	1:G:427:PHE:O	2.45	0.68
1:H:497:VAL:CG1	1:H:497:VAL:O	2.42	0.68
1:E:318:TYR:CD2	1:E:319:GLN:O	2.45	0.68
1:C:321:ASN:HB2	1:C:322:PRO:HD2	1.76	0.68
1:C:192:PHE:HA	1:C:193:ALA:HB2	1.76	0.68
1:D:423:SER:O	1:D:425:VAL:HG23	1.94	0.68
1:D:192:PHE:CZ	1:D:195:GLU:CG	2.77	0.68
1:A:346:PHE:CE1	1:A:360:VAL:HG23	2.29	0.68
1:E:4:GLU:CG	1:E:4:GLU:O	2.42	0.68
1:A:323:GLU:HG2	1:B:171:GLN:HE21	1.56	0.68
1:F:98:ASN:ND2	1:F:98:ASN:N	2.41	0.68
1:B:183:LEU:HD23	1:B:186:TRP:HZ2	1.59	0.68
1:G:228:ASN:HD21	1:G:229:PRO:HG3	1.53	0.68
1:F:496:GLY:O	1:F:497:VAL:HB	1.92	0.68
1:H:346:PHE:HE1	1:H:360:VAL:HG23	1.58	0.68
1:C:195:GLU:HB3	1:C:241:PHE:CZ	2.28	0.68
1:A:352:LEU:HD13	1:A:503:ILE:HG12	1.73	0.68
1:E:298:PRO:HD3	1:E:427:PHE:HD2	1.58	0.68
1:C:214:GLN:HG2	1:C:215:ASP:N	2.06	0.68
1:F:141:VAL:HG23	1:F:186:TRP:CD1	2.29	0.68
1:A:398:LEU:CB	1:A:487:ALA:CB	2.65	0.67
1:E:395:PHE:HB3	1:E:488:LEU:HB3	1.75	0.67
1:D:213:GLU:O	1:D:214:GLN:CG	2.42	0.67
1:H:198:LEU:O	1:H:198:LEU:HD12	1.93	0.67
1:D:175:ILE:HD13	1:D:205:PRO:HB3	1.75	0.67
1:G:98:ASN:ND2	1:G:98:ASN:N	2.30	0.67
1:G:441:ASN:HB2	1:H:232:PRO:CG	2.23	0.67
1:G:96:PHE:O	1:G:97:PHE:CD1	2.47	0.67
1:E:62:LEU:HD22	1:E:309:VAL:HG21	1.76	0.67
1:H:62:LEU:HD22	1:H:309:VAL:HG21	1.75	0.67
1:F:228:ASN:OD1	1:F:229:PRO:HG3	1.94	0.67
1:H:228:ASN:HD22	1:H:229:PRO:HB3	1.54	0.67
1:E:98:ASN:HD22	1:E:98:ASN:N	1.91	0.67
1:H:141:VAL:HG23	1:H:186:TRP:CD1	2.29	0.67
1:C:497:VAL:HG23	1:C:497:VAL:O	1.94	0.67
1:B:448:GLU:O	1:B:449:ASN:CG	2.32	0.67
1:H:96:PHE:CB	1:H:97:PHE:CD1	2.77	0.67
1:H:97:PHE:CE2	1:H:106:ARG:HG2	2.30	0.67
1:D:423:SER:OG	1:D:424:LYS:N	2.27	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:198:LEU:O	1:E:198:LEU:HD12	1.95	0.67
1:A:421:GLY:O	1:A:422:ASN:HB2	1.94	0.67
1:H:346:PHE:CE1	1:H:360:VAL:CG2	2.78	0.67
1:A:321:ASN:HB2	1:A:322:PRO:HD2	1.75	0.67
1:A:182:ASP:O	1:A:183:LEU:HB2	1.93	0.67
1:A:213:GLU:O	1:A:214:GLN:CG	2.43	0.67
1:D:449:ASN:O	1:D:449:ASN:ND2	2.28	0.67
1:C:212:THR:HG22	1:C:213:GLU:O	1.95	0.67
1:F:141:VAL:HG21	1:F:186:TRP:HE1	1.60	0.67
1:C:378:ASN:HA	1:C:451:LEU:CD2	2.25	0.67
1:C:183:LEU:HD23	1:C:186:TRP:CZ2	2.30	0.67
1:E:96:PHE:O	1:E:97:PHE:HB2	1.94	0.67
1:E:141:VAL:HG23	1:E:186:TRP:CD1	2.30	0.66
1:F:427:PHE:O	1:F:427:PHE:CG	2.48	0.66
1:A:496:GLY:O	1:A:497:VAL:CB	2.43	0.66
1:F:148:GLN:NE2	1:F:150:ARG:CZ	2.58	0.66
1:A:192:PHE:HA	1:A:193:ALA:HB2	1.76	0.66
1:F:92:ASN:OD1	1:F:96:PHE:O	2.14	0.66
1:G:231:ALA:N	1:G:232:PRO:HD2	2.10	0.66
1:G:141:VAL:HG23	1:G:186:TRP:CD1	2.30	0.66
1:C:378:ASN:C	1:C:378:ASN:ND2	2.46	0.66
1:D:422:ASN:HA	1:D:423:SER:CB	2.26	0.66
1:C:175:ILE:HD13	1:C:205:PRO:HB3	1.76	0.66
1:B:321:ASN:HB2	1:B:322:PRO:HD2	1.76	0.66
1:H:464:ILE:HG13	1:H:479:THR:HG22	1.76	0.66
1:B:175:ILE:HD13	1:B:205:PRO:HB3	1.77	0.66
1:D:424:LYS:C	1:D:425:VAL:HG23	2.15	0.66
1:F:198:LEU:HD12	1:F:198:LEU:O	1.96	0.66
1:G:380:THR:HG23	1:G:381:GLN:N	2.11	0.66
1:E:254:ASP:O	1:E:255:ASN:HB2	1.95	0.66
1:F:194:ASN:ND2	1:F:196:GLY:N	2.41	0.66
1:G:194:ASN:HA	1:G:195:GLU:HB2	1.75	0.66
1:A:378:ASN:O	1:A:378:ASN:ND2	2.29	0.66
1:D:136:TYR:CE1	1:D:184:LYS:HD3	2.31	0.65
1:B:182:ASP:O	1:B:183:LEU:HB2	1.94	0.65
1:B:213:GLU:HB3	1:B:214:GLN:OE1	1.96	0.65
1:D:192:PHE:CZ	1:D:195:GLU:HG2	2.31	0.65
1:G:198:LEU:O	1:G:198:LEU:HD12	1.96	0.65
1:D:449:ASN:O	1:D:450:ASP:HB2	1.95	0.65
1:F:5:THR:HG22	1:F:6:SER:O	1.96	0.65
1:D:398:LEU:HB2	1:D:487:ALA:HB3	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:496:GLY:O	1:D:497:VAL:CB	2.43	0.65
1:G:401:PRO:O	1:G:402:GLU:HB3	1.96	0.65
1:G:194:ASN:ND2	1:G:196:GLY:N	2.41	0.65
1:C:194:ASN:O	1:D:255:ASN:O	2.14	0.65
1:E:441:ASN:HB2	1:F:232:PRO:HG2	1.78	0.65
1:A:175:ILE:HD13	1:A:205:PRO:HB3	1.79	0.65
1:G:98:ASN:ND2	1:G:98:ASN:H	1.82	0.65
1:D:195:GLU:N	1:D:195:GLU:OE2	2.30	0.65
1:G:345:ARG:NH1	1:G:507:GLN:NE2	2.45	0.65
1:H:401:PRO:C	1:H:403:GLU:H	2.01	0.65
1:F:486:ASN:CA	1:F:487:ALA:HB2	2.17	0.65
1:B:195:GLU:OE2	1:B:195:GLU:N	2.30	0.65
1:A:497:VAL:CG2	1:A:497:VAL:O	2.44	0.65
1:B:183:LEU:HD23	1:B:186:TRP:CZ2	2.31	0.65
1:E:141:VAL:HG21	1:E:186:TRP:HE1	1.61	0.65
1:F:398:LEU:HD11	1:F:489:GLY:CA	2.27	0.64
1:E:96:PHE:O	1:E:97:PHE:HD1	1.78	0.64
1:D:366:THR:O	1:D:462:GLN:NE2	2.18	0.64
1:E:228:ASN:OD1	1:E:229:PRO:CB	2.45	0.64
1:E:398:LEU:H	1:E:398:LEU:HD13	1.60	0.64
1:H:96:PHE:O	1:H:97:PHE:HB2	1.98	0.64
1:A:403:GLU:OE2	1:A:424:LYS:HB2	1.96	0.64
1:G:141:VAL:HG21	1:G:186:TRP:HE1	1.62	0.64
1:A:398:LEU:HD13	1:A:487:ALA:CB	2.28	0.64
1:D:62:LEU:HD22	1:D:309:VAL:HG21	1.79	0.64
1:H:148:GLN:NE2	1:H:150:ARG:CZ	2.61	0.64
1:F:383:ILE:O	1:F:384:SER:HB2	1.95	0.64
1:C:195:GLU:N	1:C:195:GLU:OE2	2.30	0.64
1:G:231:ALA:N	1:G:232:PRO:CD	2.60	0.64
1:A:195:GLU:OE2	1:A:195:GLU:N	2.31	0.64
1:A:277:PRO:HA	1:A:278:THR:C	2.19	0.64
1:A:192:PHE:CZ	1:A:195:GLU:CG	2.81	0.64
1:G:411:VAL:HG21	1:G:500:LEU:HD21	1.79	0.64
1:C:62:LEU:HD22	1:C:309:VAL:HG21	1.78	0.64
1:E:380:THR:HG23	1:E:381:GLN:N	2.13	0.64
1:F:397:GLY:O	1:F:487:ALA:C	2.35	0.63
1:G:243:GLY:C	1:G:253:PHE:CE1	2.70	0.63
1:C:352:LEU:CD1	1:C:352:LEU:N	2.42	0.63
1:E:96:PHE:O	1:E:97:PHE:CB	2.43	0.63
1:H:96:PHE:HB2	1:H:97:PHE:CD1	2.33	0.63
1:H:194:ASN:HA	1:H:195:GLU:HB2	1.74	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:148:GLN:NE2	1:G:150:ARG:CZ	2.60	0.63
1:H:353:THR:HA	1:H:498:ASP:O	1.98	0.63
1:H:243:GLY:HA2	1:H:253:PHE:CE1	2.34	0.63
1:F:397:GLY:C	1:F:487:ALA:O	2.36	0.63
1:C:193:ALA:HB3	1:C:195:GLU:OE2	1.98	0.63
1:G:326:LEU:HD13	1:G:326:LEU:O	1.98	0.63
1:G:175:ILE:N	1:G:192:PHE:O	2.31	0.63
1:G:147:THR:CA	1:G:171:GLN:NE2	2.62	0.63
1:B:192:PHE:C	1:B:192:PHE:CD2	2.71	0.63
1:C:398:LEU:HB2	1:C:487:ALA:HB3	1.79	0.63
1:G:397:GLY:C	1:G:487:ALA:O	2.37	0.63
1:D:182:ASP:OD2	1:D:184:LYS:N	2.31	0.63
1:B:212:THR:HG22	1:B:213:GLU:O	1.99	0.63
1:H:228:ASN:ND2	1:H:236:SER:OG	2.31	0.63
1:C:378:ASN:O	1:C:378:ASN:ND2	2.31	0.63
1:E:147:THR:CA	1:E:171:GLN:NE2	2.61	0.63
1:H:141:VAL:HG21	1:H:186:TRP:HE1	1.61	0.63
1:F:380:THR:HG23	1:F:381:GLN:N	2.13	0.63
1:E:147:THR:CA	1:E:171:GLN:HE22	2.12	0.63
1:E:277:PRO:HB3	1:E:280:GLY:HA2	1.81	0.63
1:F:277:PRO:HA	1:F:278:THR:C	2.19	0.63
1:D:4:GLU:OE1	1:D:4:GLU:HA	1.99	0.63
1:H:147:THR:CA	1:H:171:GLN:NE2	2.62	0.62
1:H:326:LEU:HD13	1:H:326:LEU:O	1.99	0.62
1:B:277:PRO:HA	1:B:278:THR:C	2.19	0.62
1:D:180:SER:OG	1:D:183:LEU:N	2.30	0.62
1:F:147:THR:CA	1:F:171:GLN:NE2	2.61	0.62
1:H:426:LYS:CD	1:H:430:GLU:OE2	2.47	0.62
1:A:62:LEU:HD22	1:A:309:VAL:HG21	1.80	0.62
1:E:500:LEU:C	1:E:500:LEU:HD12	2.06	0.62
1:H:231:ALA:N	1:H:232:PRO:HD2	2.13	0.62
1:E:401:PRO:C	1:E:403:GLU:H	2.02	0.62
1:D:425:VAL:HG21	1:D:481:PHE:O	2.00	0.62
1:E:385:LYS:HG3	1:E:386:SER:H	1.64	0.62
1:D:238:ASN:ND2	1:D:269:LEU:H	1.98	0.62
1:F:229:PRO:CG	1:F:230:GLY:H	2.11	0.62
1:B:62:LEU:HD22	1:B:309:VAL:HG21	1.81	0.62
1:A:4:GLU:HA	1:A:4:GLU:OE1	2.00	0.62
1:B:4:GLU:OE1	1:B:4:GLU:HA	1.98	0.62
1:A:379:THR:CG2	1:A:380:THR:H	2.11	0.62
1:A:383:ILE:O	1:A:384:SER:CB	2.48	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:228:ASN:OD1	1:G:229:PRO:CD	2.48	0.62
1:D:424:LYS:O	1:D:425:VAL:C	2.37	0.62
1:E:326:LEU:HD13	1:E:326:LEU:O	2.00	0.62
1:F:326:LEU:HD13	1:F:326:LEU:O	2.00	0.62
1:E:277:PRO:HA	1:E:278:THR:C	2.19	0.62
1:G:398:LEU:HD21	1:G:489:GLY:HA3	1.81	0.62
1:A:343:TRP:CE3	1:A:507:GLN:HB3	2.34	0.62
1:G:253:PHE:HD1	1:G:253:PHE:N	1.98	0.62
1:F:228:ASN:HD21	1:F:229:PRO:HB3	1.55	0.62
1:B:497:VAL:CG2	1:B:497:VAL:O	2.48	0.62
1:G:323:GLU:OE2	1:G:323:GLU:CA	2.48	0.62
1:H:496:GLY:O	1:H:497:VAL:HG12	2.00	0.62
1:F:277:PRO:HB3	1:F:280:GLY:HA2	1.82	0.62
1:A:396:LYS:HE2	2:A:602:HOH:O	1.99	0.62
1:C:192:PHE:CD2	1:C:192:PHE:O	2.51	0.61
1:H:354:LYS:HA	1:H:495:THR:O	2.00	0.61
1:E:323:GLU:CA	1:E:323:GLU:OE2	2.48	0.61
1:B:195:GLU:OE2	1:B:195:GLU:CA	2.48	0.61
1:C:238:ASN:ND2	1:C:269:LEU:H	1.96	0.61
1:C:323:GLU:HG2	1:D:171:GLN:NE2	2.15	0.61
1:C:277:PRO:HA	1:C:278:THR:C	2.20	0.61
1:B:343:TRP:CE3	1:B:507:GLN:HB3	2.36	0.61
1:F:147:THR:CA	1:F:171:GLN:HE22	2.13	0.61
1:F:326:LEU:N	1:F:326:LEU:CD1	2.63	0.61
1:A:497:VAL:HG23	1:A:497:VAL:O	2.00	0.61
1:A:352:LEU:HD11	1:A:503:ILE:HG13	1.80	0.61
1:E:326:LEU:CD1	1:E:326:LEU:N	2.62	0.61
1:C:4:GLU:OE1	1:C:4:GLU:HA	1.99	0.61
1:D:463:ASN:OD1	1:D:463:ASN:C	2.39	0.61
1:F:401:PRO:C	1:F:403:GLU:H	2.02	0.61
1:G:228:ASN:HD22	1:G:229:PRO:HB3	1.64	0.61
1:H:326:LEU:N	1:H:326:LEU:CD1	2.64	0.61
1:B:192:PHE:HA	1:B:193:ALA:HB2	1.82	0.61
1:F:383:ILE:O	1:F:384:SER:CB	2.47	0.61
1:D:499:ASN:OD1	1:D:499:ASN:C	2.37	0.61
1:G:147:THR:CA	1:G:171:GLN:HE22	2.13	0.61
1:F:497:VAL:O	1:F:497:VAL:HG13	1.99	0.61
1:F:194:ASN:HA	1:F:195:GLU:HB2	1.73	0.61
1:H:194:ASN:ND2	1:H:196:GLY:N	2.41	0.61
1:C:383:ILE:N	1:C:383:ILE:HD13	2.16	0.61
1:C:448:GLU:OE1	1:C:448:GLU:CA	2.42	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:99:ASP:N	1:F:99:ASP:OD1	2.30	0.61
1:E:231:ALA:N	1:E:232:PRO:CD	2.64	0.61
1:G:277:PRO:HA	1:G:278:THR:C	2.21	0.61
1:H:380:THR:HG23	1:H:381:GLN:N	2.15	0.61
1:G:326:LEU:N	1:G:326:LEU:CD1	2.64	0.61
1:D:381:GLN:C	1:D:382:THR:OG1	2.38	0.61
1:G:115:THR:HG22	1:G:117:GLU:H	1.66	0.61
1:E:395:PHE:HE2	1:E:407:MET:HE2	1.66	0.60
1:D:379:THR:CG2	1:D:380:THR:H	2.12	0.60
1:H:147:THR:CA	1:H:171:GLN:HE22	2.14	0.60
1:A:194:ASN:O	1:B:255:ASN:O	2.19	0.60
1:F:4:GLU:OE2	1:F:4:GLU:CA	2.48	0.60
1:F:98:ASN:HD22	1:F:98:ASN:N	1.99	0.60
1:B:238:ASN:ND2	1:B:269:LEU:H	1.96	0.60
1:A:36:HIS:HD2	1:A:56:HIS:NE2	1.98	0.60
1:G:400:ASP:OD2	1:G:424:LYS:NZ	2.35	0.60
1:F:398:LEU:CD1	1:F:489:GLY:H	2.14	0.60
1:G:228:ASN:OD1	1:G:229:PRO:HD3	2.00	0.60
1:A:192:PHE:CE2	1:A:195:GLU:HG2	2.36	0.60
1:H:346:PHE:HE1	1:H:360:VAL:CG2	2.14	0.60
1:A:238:ASN:ND2	1:A:269:LEU:H	1.98	0.60
1:F:381:GLN:O	1:F:382:THR:C	2.40	0.60
1:F:115:THR:HG22	1:F:117:GLU:H	1.67	0.60
1:G:398:LEU:CD2	1:G:489:GLY:HA3	2.32	0.60
1:E:326:LEU:H	1:E:326:LEU:CD1	2.12	0.60
1:A:171:GLN:NE2	1:B:323:GLU:HG2	2.15	0.60
1:B:401:PRO:C	1:B:403:GLU:H	2.04	0.60
1:H:277:PRO:HB3	1:H:280:GLY:HA2	1.82	0.60
1:D:277:PRO:HA	1:D:278:THR:C	2.22	0.60
1:G:371:PHE:CZ	1:G:407:MET:HE3	2.36	0.60
1:C:36:HIS:HD2	1:C:56:HIS:NE2	1.99	0.60
1:B:182:ASP:C	1:B:182:ASP:OD2	2.40	0.60
1:A:401:PRO:C	1:A:403:GLU:H	2.04	0.60
1:D:192:PHE:CZ	1:D:195:GLU:HG3	2.35	0.60
1:E:441:ASN:HB2	1:F:232:PRO:CG	2.32	0.60
1:H:141:VAL:HG23	1:H:186:TRP:HD1	1.67	0.60
1:H:277:PRO:HA	1:H:278:THR:C	2.22	0.60
1:B:36:HIS:HD2	1:B:56:HIS:NE2	2.00	0.60
1:F:398:LEU:N	1:F:487:ALA:O	2.34	0.59
1:A:398:LEU:HB3	1:A:487:ALA:HB3	1.80	0.59
1:C:401:PRO:C	1:C:403:GLU:H	2.04	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:115:THR:HG22	1:E:117:GLU:H	1.67	0.59
1:C:343:TRP:CE3	1:C:507:GLN:HB3	2.36	0.59
1:D:343:TRP:CE3	1:D:507:GLN:HB3	2.37	0.59
1:E:175:ILE:N	1:E:192:PHE:O	2.33	0.59
1:H:198:LEU:CD1	1:H:198:LEU:C	2.70	0.59
1:D:401:PRO:C	1:D:403:GLU:H	2.05	0.59
1:E:381:GLN:O	1:E:382:THR:C	2.40	0.59
1:H:115:THR:HG22	1:H:117:GLU:H	1.67	0.59
1:H:323:GLU:OE2	1:H:323:GLU:CA	2.48	0.59
1:F:141:VAL:HG23	1:F:186:TRP:HD1	1.67	0.59
1:F:385:LYS:CG	1:F:386:SER:N	2.62	0.59
1:G:277:PRO:HB3	1:G:280:GLY:HA2	1.83	0.59
1:G:253:PHE:CD1	1:G:253:PHE:N	2.70	0.59
1:F:231:ALA:N	1:F:232:PRO:HD2	2.17	0.59
1:F:346:PHE:CE1	1:F:360:VAL:HG23	2.38	0.59
1:F:98:ASN:H	1:F:98:ASN:ND2	2.00	0.59
1:A:183:LEU:HD23	1:A:186:TRP:HZ2	1.68	0.59
1:D:460:LEU:HG	1:D:465:LEU:HD12	1.85	0.59
1:F:463:ASN:C	1:F:463:ASN:OD1	2.41	0.58
1:B:398:LEU:HB2	1:B:487:ALA:HB3	1.84	0.58
1:D:36:HIS:HD2	1:D:56:HIS:NE2	2.00	0.58
1:E:194:ASN:HA	1:E:195:GLU:HB2	1.74	0.58
1:A:213:GLU:CB	1:A:214:GLN:OE1	2.50	0.58
1:A:423:SER:OG	1:A:424:LYS:N	2.36	0.58
1:F:148:GLN:HE21	1:F:150:ARG:NE	2.00	0.58
1:H:427:PHE:CG	1:H:427:PHE:O	2.55	0.58
1:H:97:PHE:CD2	1:H:106:ARG:HD3	2.38	0.58
1:E:395:PHE:O	1:E:404:TYR:HB2	2.04	0.58
1:H:228:ASN:HD21	1:H:229:PRO:HG3	1.59	0.58
1:A:398:LEU:HD12	1:A:489:GLY:HA3	1.86	0.58
1:G:231:ALA:H	1:G:232:PRO:CD	2.16	0.58
1:G:347:ALA:HB2	1:G:358:TYR:CE1	2.38	0.58
1:E:231:ALA:N	1:E:232:PRO:HD2	2.18	0.58
1:D:354:LYS:HB3	1:D:498:ASP:OD2	2.04	0.58
1:E:228:ASN:ND2	1:E:236:SER:OG	2.36	0.58
1:F:5:THR:O	1:F:6:SER:CB	2.30	0.58
1:A:423:SER:O	1:A:424:LYS:CB	2.36	0.58
1:F:323:GLU:CA	1:F:323:GLU:OE2	2.48	0.58
1:E:141:VAL:HG23	1:E:186:TRP:HD1	1.68	0.58
1:H:400:ASP:C	1:H:401:PRO:O	2.41	0.58
1:G:401:PRO:C	1:G:403:GLU:H	2.05	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:403:GLU:HG2	1:F:482:MET:HG3	1.86	0.58
1:B:424:LYS:O	1:B:425:VAL:CB	2.49	0.58
1:E:148:GLN:HE21	1:E:150:ARG:CZ	2.16	0.58
1:E:486:ASN:CA	1:E:487:ALA:HB2	2.20	0.58
1:A:212:THR:O	1:A:212:THR:HG22	2.02	0.58
1:B:209:GLU:HG3	1:B:221:TRP:CE2	2.39	0.58
1:A:197:PHE:CE1	1:B:258:ARG:HA	2.39	0.58
1:C:258:ARG:HA	1:D:197:PHE:CE1	2.39	0.58
1:D:425:VAL:O	1:D:426:LYS:C	2.43	0.57
1:G:298:PRO:HD3	1:G:427:PHE:CD2	2.39	0.57
1:C:398:LEU:HD12	1:C:489:GLY:HA3	1.85	0.57
1:C:427:PHE:CD2	1:C:427:PHE:C	2.77	0.57
1:E:346:PHE:CE1	1:E:360:VAL:HG23	2.39	0.57
1:F:198:LEU:C	1:F:198:LEU:CD1	2.73	0.57
1:C:381:GLN:C	1:C:382:THR:OG1	2.41	0.57
1:G:486:ASN:CA	1:G:487:ALA:HB2	2.21	0.57
1:C:379:THR:CG2	1:C:380:THR:H	2.16	0.57
1:A:381:GLN:C	1:A:383:ILE:H	2.07	0.57
1:G:148:GLN:HE21	1:G:150:ARG:NE	2.02	0.57
1:E:96:PHE:C	1:E:97:PHE:CD1	2.78	0.57
1:G:497:VAL:HG22	1:G:497:VAL:O	2.04	0.57
1:F:175:ILE:N	1:F:192:PHE:O	2.34	0.57
1:H:175:ILE:N	1:H:192:PHE:O	2.32	0.57
1:A:379:THR:HG22	1:A:380:THR:H	1.69	0.57
1:B:381:GLN:O	1:B:383:ILE:N	2.31	0.57
1:G:426:LYS:O	1:G:430:GLU:HB2	2.05	0.57
1:E:403:GLU:HG2	1:E:482:MET:HG3	1.85	0.57
1:H:228:ASN:CG	1:H:229:PRO:CB	2.71	0.57
1:G:144:ALA:CB	1:G:145:ASN:C	2.69	0.57
1:H:426:LYS:HD2	1:H:430:GLU:OE2	2.03	0.57
1:A:500:LEU:CD1	1:A:500:LEU:C	2.72	0.57
1:H:148:GLN:HE21	1:H:150:ARG:NE	2.03	0.57
1:D:497:VAL:CG2	1:D:497:VAL:O	2.52	0.57
1:F:482:MET:HG2	1:F:488:LEU:HD21	1.87	0.57
1:F:145:ASN:N	1:F:146:SER:CA	2.63	0.57
1:G:96:PHE:O	1:G:97:PHE:CB	2.52	0.57
1:G:141:VAL:HG23	1:G:186:TRP:HD1	1.69	0.57
1:E:497:VAL:HG11	1:E:500:LEU:CB	2.34	0.56
1:H:145:ASN:N	1:H:146:SER:CA	2.63	0.56
1:G:387:VAL:HG13	1:G:388:PHE:N	2.19	0.56
1:A:209:GLU:HG3	1:A:221:TRP:CE2	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:400:ASP:OD1	1:E:401:PRO:O	2.23	0.56
1:C:378:ASN:HD22	1:C:380:THR:N	2.02	0.56
1:E:148:GLN:H	1:E:171:GLN:NE2	2.02	0.56
1:C:424:LYS:O	1:C:425:VAL:C	2.42	0.56
1:C:448:GLU:HB2	1:C:453:TYR:HE2	1.70	0.56
1:G:395:PHE:CE2	1:G:407:MET:HE2	2.39	0.56
1:G:285:ILE:HD12	1:G:309:VAL:HG22	1.87	0.56
1:C:258:ARG:NH2	1:C:328:ASN:OD1	2.39	0.56
1:C:395:PHE:CE2	1:C:407:MET:HE2	2.40	0.56
1:G:98:ASN:HB2	1:G:100:THR:HG22	0.73	0.56
1:G:121:GLN:CG	1:G:149:PHE:HE2	2.18	0.56
1:H:497:VAL:O	1:H:497:VAL:HG12	2.05	0.56
1:G:403:GLU:HG2	1:G:482:MET:HG3	1.87	0.56
1:A:448:GLU:O	1:A:449:ASN:CG	2.44	0.56
1:C:182:ASP:OD2	1:C:184:LYS:HG3	2.05	0.56
1:B:496:GLY:C	1:B:497:VAL:HG22	2.25	0.56
1:G:96:PHE:O	1:G:97:PHE:HB2	2.06	0.56
1:H:285:ILE:HD12	1:H:309:VAL:HG22	1.88	0.56
1:H:97:PHE:CD2	1:H:106:ARG:CD	2.89	0.56
1:B:195:GLU:OE2	1:B:195:GLU:HA	2.05	0.56
1:E:383:ILE:O	1:E:384:SER:CB	2.54	0.56
1:C:378:ASN:HD22	1:C:380:THR:H	1.54	0.56
1:H:98:ASN:HB2	1:H:100:THR:CG2	2.09	0.56
1:A:212:THR:CG2	1:A:215:ASP:H	2.19	0.56
1:H:383:ILE:O	1:H:384:SER:CB	2.52	0.56
1:B:395:PHE:CE2	1:B:407:MET:HE2	2.40	0.56
1:A:362:LEU:HD23	1:F:356:ASN:ND2	2.20	0.55
1:H:96:PHE:O	1:H:97:PHE:CB	2.54	0.55
1:H:253:PHE:CD1	1:H:253:PHE:N	2.73	0.55
1:F:229:PRO:HG2	1:F:230:GLY:N	2.21	0.55
1:C:182:ASP:O	1:C:183:LEU:CB	2.52	0.55
1:G:496:GLY:C	1:G:497:VAL:CG1	2.74	0.55
1:B:258:ARG:NH2	1:B:328:ASN:OD1	2.40	0.55
1:A:110:ILE:HG13	1:A:123:ILE:HG22	1.88	0.55
1:H:96:PHE:HB2	1:H:97:PHE:CE1	2.41	0.55
1:D:496:GLY:O	1:D:497:VAL:HG13	2.06	0.55
1:D:377:VAL:HG12	1:D:379:THR:N	2.22	0.55
1:G:396:LYS:HG2	1:G:404:TYR:CB	2.33	0.55
1:E:486:ASN:CA	1:E:487:ALA:CB	2.57	0.55
1:F:398:LEU:CD1	1:F:489:GLY:N	2.70	0.55
1:G:326:LEU:H	1:G:326:LEU:CD1	2.14	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:198:LEU:CD1	1:G:198:LEU:C	2.72	0.55
1:G:98:ASN:C	1:G:100:THR:H	2.08	0.55
1:H:231:ALA:N	1:H:232:PRO:CD	2.68	0.55
1:E:198:LEU:CD1	1:E:198:LEU:C	2.72	0.55
1:C:209:GLU:HG3	1:C:221:TRP:CE2	2.41	0.55
1:B:499:ASN:OD1	1:B:499:ASN:C	2.45	0.55
1:H:400:ASP:OD1	1:H:400:ASP:C	2.45	0.55
1:C:396:LYS:HE2	2:C:601:HOH:O	2.06	0.55
1:G:341:GLY:HA2	1:G:509:ARG:HD2	1.89	0.55
1:G:148:GLN:H	1:G:171:GLN:NE2	2.05	0.55
1:H:321:ASN:C	1:H:323:GLU:N	2.61	0.55
1:D:398:LEU:HD12	1:D:489:GLY:HA3	1.88	0.55
1:D:209:GLU:HG3	1:D:221:TRP:CE2	2.42	0.55
1:B:398:LEU:HD12	1:B:489:GLY:HA3	1.87	0.55
1:H:121:GLN:CG	1:H:149:PHE:HE2	2.18	0.55
1:F:285:ILE:HD12	1:F:309:VAL:HG22	1.89	0.55
1:F:141:VAL:HG21	1:F:186:TRP:NE1	2.21	0.55
1:G:497:VAL:HG23	1:G:497:VAL:O	2.06	0.54
1:E:285:ILE:HD12	1:E:309:VAL:HG22	1.88	0.54
1:H:99:ASP:O	1:H:101:ILE:N	2.40	0.54
1:A:395:PHE:HE2	1:A:407:MET:HE2	1.72	0.54
1:A:213:GLU:C	1:A:214:GLN:CD	2.50	0.54
1:E:460:LEU:HG	1:E:465:LEU:HD12	1.88	0.54
1:A:196:GLY:HA2	1:A:197:PHE:C	2.28	0.54
1:A:27:TRP:CZ2	1:A:107:CYS:SG	3.00	0.54
1:H:141:VAL:HG21	1:H:186:TRP:NE1	2.22	0.54
1:E:141:VAL:HG21	1:E:186:TRP:NE1	2.22	0.54
1:C:383:ILE:HG22	1:C:384:SER:N	2.22	0.54
1:A:398:LEU:CD1	1:A:487:ALA:CB	2.85	0.54
1:B:381:GLN:C	1:B:382:THR:OG1	2.46	0.54
1:C:425:VAL:HG21	1:C:481:PHE:O	2.07	0.54
1:C:398:LEU:CB	1:C:487:ALA:HB3	2.38	0.54
1:B:27:TRP:CZ2	1:B:107:CYS:SG	3.00	0.54
1:H:399:GLU:CG	1:H:486:ASN:HD22	2.21	0.54
1:E:482:MET:HG2	1:E:488:LEU:HD21	1.90	0.54
1:F:398:LEU:CD1	1:F:487:ALA:O	2.50	0.54
1:C:379:THR:HG22	1:C:380:THR:H	1.73	0.54
1:E:96:PHE:HB2	1:E:97:PHE:CE1	2.42	0.54
1:F:15:PRO:HG2	1:F:302:TRP:HB2	1.89	0.54
1:F:229:PRO:CG	1:F:230:GLY:N	2.69	0.54
1:F:321:ASN:C	1:F:323:GLU:N	2.60	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:321:ASN:C	1:G:323:GLU:N	2.60	0.54
1:H:15:PRO:HG2	1:H:302:TRP:HB2	1.90	0.54
1:F:200:TYR:N	1:F:200:TYR:CD2	2.76	0.54
1:H:97:PHE:HE2	1:H:106:ARG:HA	1.73	0.54
1:E:401:PRO:O	1:E:402:GLU:HB3	2.08	0.54
1:H:381:GLN:NE2	1:H:381:GLN:HA	2.23	0.54
1:H:380:THR:CG2	1:H:381:GLN:N	2.70	0.54
1:H:341:GLY:HA2	1:H:509:ARG:HD2	1.89	0.54
1:H:254:ASP:OD1	1:H:254:ASP:N	2.40	0.54
1:E:98:ASN:N	1:E:98:ASN:ND2	2.54	0.54
1:C:110:ILE:HG13	1:C:123:ILE:HG22	1.89	0.54
1:G:120:GLU:HB3	1:G:140:PRO:HB3	1.90	0.54
1:H:96:PHE:HZ	1:H:136:TYR:CD1	2.26	0.53
1:E:321:ASN:C	1:E:323:GLU:N	2.62	0.53
1:G:380:THR:CG2	1:G:381:GLN:N	2.71	0.53
1:D:196:GLY:HA2	1:D:197:PHE:C	2.28	0.53
1:A:395:PHE:CE2	1:A:407:MET:HE2	2.43	0.53
1:G:482:MET:HG2	1:G:488:LEU:HD21	1.89	0.53
1:H:98:ASN:OD1	1:H:100:THR:HG21	2.07	0.53
1:D:182:ASP:O	1:D:183:LEU:CB	2.56	0.53
1:H:148:GLN:H	1:H:171:GLN:NE2	2.07	0.53
1:C:445:PHE:CE1	1:C:446:LYS:CD	2.92	0.53
1:H:426:LYS:O	1:H:430:GLU:HB2	2.08	0.53
1:B:110:ILE:HG13	1:B:123:ILE:HG22	1.89	0.53
1:H:399:GLU:HG2	1:H:486:ASN:HD22	1.73	0.53
1:G:397:GLY:O	1:G:487:ALA:C	2.45	0.53
1:E:149:PHE:HZ	1:E:165:MET:HE1	1.74	0.53
1:D:212:THR:CG2	1:D:213:GLU:O	2.55	0.53
1:D:385:LYS:CG	1:D:386:SER:N	2.71	0.53
1:G:394:TRP:HB2	1:G:492:ASN:HB2	1.90	0.53
1:B:411:VAL:HG21	1:B:500:LEU:HD21	1.90	0.53
1:C:197:PHE:CE1	1:D:258:ARG:HA	2.43	0.53
1:B:196:GLY:HA2	1:B:197:PHE:C	2.28	0.53
1:H:399:GLU:HG3	1:H:486:ASN:ND2	2.24	0.53
1:D:213:GLU:HG2	1:D:214:GLN:N	2.23	0.53
1:C:352:LEU:HD12	1:C:501:PHE:O	2.08	0.53
1:G:354:LYS:H	1:G:498:ASP:HA	1.74	0.53
1:H:482:MET:HG2	1:H:488:LEU:HD21	1.90	0.53
1:G:98:ASN:C	1:G:100:THR:N	2.62	0.53
1:C:497:VAL:HG22	1:C:497:VAL:O	2.08	0.53
1:C:214:GLN:NE2	1:C:316:THR:OG1	2.40	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:ASP:O	1:B:183:LEU:CB	2.56	0.53
1:E:15:PRO:HG2	1:E:302:TRP:HB2	1.90	0.53
1:A:212:THR:CG2	1:A:213:GLU:O	2.50	0.53
1:H:231:ALA:HB3	1:H:232:PRO:CD	2.35	0.53
1:E:380:THR:CG2	1:E:381:GLN:N	2.72	0.53
1:D:110:ILE:HG13	1:D:123:ILE:HG22	1.89	0.53
1:A:136:TYR:CE1	1:A:184:LYS:HD3	2.43	0.53
1:H:231:ALA:H	1:H:232:PRO:CD	2.21	0.53
1:F:141:VAL:CG2	1:F:186:TRP:CD1	2.91	0.53
1:C:196:GLY:HA2	1:C:197:PHE:C	2.28	0.53
1:H:345:ARG:NH1	1:H:507:GLN:NE2	2.57	0.53
1:D:383:ILE:O	1:D:384:SER:CB	2.56	0.53
1:A:183:LEU:HD23	1:A:186:TRP:CZ2	2.43	0.53
1:D:192:PHE:C	1:D:192:PHE:CD2	2.82	0.52
1:E:121:GLN:CG	1:E:149:PHE:HE2	2.20	0.52
1:H:380:THR:HB	1:H:450:ASP:HB3	1.90	0.52
1:B:40:GLN:HE22	1:B:82:PHE:HA	1.74	0.52
1:G:400:ASP:OD1	1:G:401:PRO:O	2.27	0.52
1:D:383:ILE:C	1:D:384:SER:OG	2.47	0.52
1:H:383:ILE:HD13	1:H:384:SER:H	1.74	0.52
1:C:448:GLU:HB2	1:C:453:TYR:CE2	2.43	0.52
1:H:326:LEU:H	1:H:326:LEU:CD1	2.13	0.52
1:F:121:GLN:CG	1:F:149:PHE:HE2	2.21	0.52
1:H:141:VAL:CG2	1:H:186:TRP:CD1	2.92	0.52
1:G:54:TRP:HB2	1:G:72:ILE:HB	1.92	0.52
1:E:341:GLY:HA2	1:E:509:ARG:HD2	1.91	0.52
1:E:497:VAL:HG11	1:E:500:LEU:HB3	1.91	0.52
1:F:394:TRP:HB2	1:F:492:ASN:HB2	1.91	0.52
1:G:141:VAL:HG21	1:G:186:TRP:NE1	2.23	0.52
1:A:86:MET:HG3	1:A:108:VAL:O	2.10	0.52
1:H:120:GLU:HB3	1:H:140:PRO:HB3	1.92	0.52
1:A:382:THR:C	1:A:383:ILE:HG12	2.30	0.52
1:F:148:GLN:H	1:F:171:GLN:NE2	2.08	0.52
1:C:136:TYR:CE1	1:C:184:LYS:HD3	2.44	0.52
1:B:192:PHE:CZ	1:B:195:GLU:HG3	2.44	0.52
1:F:380:THR:CG2	1:F:381:GLN:N	2.72	0.52
1:F:376:ALA:HA	1:F:452:SER:O	2.09	0.52
1:G:200:TYR:N	1:G:200:TYR:CD2	2.77	0.52
1:H:200:TYR:N	1:H:200:TYR:CD2	2.78	0.52
1:B:401:PRO:O	1:B:402:GLU:HB3	2.10	0.52
1:B:449:ASN:CG	1:B:450:ASP:H	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:ALA:HB1	1:C:350:THR:OG1	2.10	0.52
1:B:486:ASN:CB	1:B:487:ALA:HB2	2.39	0.52
1:H:394:TRP:HE1	1:H:494:THR:HB	1.75	0.52
1:D:381:GLN:O	1:D:382:THR:OG1	2.27	0.52
1:G:229:PRO:CG	1:G:230:GLY:N	2.71	0.52
1:G:256:GLN:NE2	1:G:326:LEU:CB	2.71	0.52
1:F:401:PRO:O	1:F:402:GLU:HB3	2.10	0.52
1:C:486:ASN:CB	1:C:487:ALA:HB2	2.40	0.52
1:H:394:TRP:HB2	1:H:492:ASN:HB2	1.90	0.52
1:G:15:PRO:HG2	1:G:302:TRP:HB2	1.90	0.52
1:H:228:ASN:OD1	1:H:229:PRO:CD	2.58	0.52
1:E:354:LYS:H	1:E:498:ASP:HA	1.75	0.52
1:D:395:PHE:HE2	1:D:407:MET:HE2	1.75	0.52
1:A:449:ASN:CG	1:A:450:ASP:H	2.08	0.52
1:E:148:GLN:NE2	1:E:150:ARG:CZ	2.72	0.52
1:D:398:LEU:CB	1:D:487:ALA:HB3	2.39	0.52
1:A:258:ARG:NH2	1:A:328:ASN:OD1	2.40	0.52
1:G:200:TYR:HD2	1:G:200:TYR:N	2.08	0.52
1:A:356:ASN:HB3	1:F:362:LEU:HA	1.91	0.52
1:E:120:GLU:HB3	1:E:140:PRO:HB3	1.90	0.52
1:F:120:GLU:HB3	1:F:140:PRO:HB3	1.91	0.51
1:F:175:ILE:HG13	1:F:225:ILE:HD12	1.92	0.51
1:D:378:ASN:O	1:D:450:ASP:O	2.29	0.51
1:B:424:LYS:O	1:B:425:VAL:O	2.27	0.51
1:G:145:ASN:HB3	1:G:147:THR:H	1.75	0.51
1:F:326:LEU:H	1:F:326:LEU:CD1	2.13	0.51
1:F:347:ALA:HB2	1:F:358:TYR:CZ	2.45	0.51
1:C:171:GLN:NE2	1:D:323:GLU:HG2	2.24	0.51
1:F:341:GLY:HA2	1:F:509:ARG:HD2	1.91	0.51
1:F:371:PHE:CZ	1:F:407:MET:HE3	2.45	0.51
1:C:377:VAL:HG12	1:C:379:THR:H	1.75	0.51
1:E:347:ALA:HB2	1:E:358:TYR:CZ	2.46	0.51
1:C:381:GLN:O	1:C:382:THR:OG1	2.29	0.51
1:D:347:ALA:HB1	1:D:350:THR:OG1	2.10	0.51
1:H:98:ASN:OD1	1:H:100:THR:CG2	2.59	0.51
1:B:448:GLU:O	1:B:449:ASN:C	2.46	0.51
1:G:141:VAL:CG2	1:G:186:TRP:CD1	2.93	0.51
1:C:383:ILE:H	1:C:383:ILE:HD13	1.74	0.51
1:H:144:ALA:HB1	1:H:145:ASN:O	2.11	0.51
1:D:192:PHE:O	1:D:192:PHE:HD2	1.94	0.51
1:A:182:ASP:O	1:A:183:LEU:CB	2.58	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:141:VAL:CG2	1:E:186:TRP:CD1	2.92	0.51
1:H:243:GLY:HA2	1:H:253:PHE:CD1	2.45	0.51
1:D:182:ASP:O	1:D:183:LEU:HB2	2.11	0.51
1:D:27:TRP:CZ2	1:D:107:CYS:SG	3.03	0.51
1:E:376:ALA:HA	1:E:452:SER:O	2.10	0.51
1:H:500:LEU:HD12	1:H:500:LEU:O	2.10	0.51
1:D:486:ASN:CB	1:D:487:ALA:HB2	2.41	0.51
1:D:40:GLN:HE22	1:D:82:PHE:HA	1.75	0.51
1:F:54:TRP:HB2	1:F:72:ILE:HB	1.92	0.51
1:D:321:ASN:HB2	1:D:322:PRO:CD	2.40	0.51
1:E:4:GLU:HG3	1:E:4:GLU:O	2.11	0.51
1:C:27:TRP:CZ2	1:C:107:CYS:SG	3.04	0.51
1:B:381:GLN:O	1:B:382:THR:OG1	2.28	0.51
1:D:395:PHE:CE2	1:D:407:MET:HE2	2.45	0.51
1:D:411:VAL:HG21	1:D:500:LEU:HD21	1.93	0.51
1:H:54:TRP:HB2	1:H:72:ILE:HB	1.93	0.51
1:F:398:LEU:CD1	1:F:489:GLY:HA3	2.39	0.50
1:G:230:GLY:O	1:G:235:GLY:HA2	2.10	0.50
1:D:192:PHE:CE1	1:D:195:GLU:HG3	2.45	0.50
1:B:395:PHE:HE2	1:B:407:MET:HE2	1.74	0.50
1:F:200:TYR:N	1:F:200:TYR:HD2	2.08	0.50
1:H:97:PHE:HD2	1:H:106:ARG:CD	2.22	0.50
1:H:175:ILE:HG13	1:H:225:ILE:HD12	1.93	0.50
1:C:192:PHE:C	1:C:192:PHE:HD2	2.06	0.50
1:C:377:VAL:O	1:C:451:LEU:HD22	2.11	0.50
1:B:378:ASN:O	1:B:379:THR:CB	2.60	0.50
1:E:368:THR:HG23	1:E:461:ASP:OD1	2.11	0.50
1:A:258:ARG:HA	1:B:197:PHE:CE1	2.46	0.50
1:E:391:LEU:O	1:E:408:GLY:HA3	2.11	0.50
1:B:347:ALA:HB1	1:B:350:THR:OG1	2.12	0.50
1:B:369:LEU:HD12	1:B:460:LEU:HD13	1.94	0.50
1:D:496:GLY:O	1:D:497:VAL:CG1	2.59	0.50
1:E:371:PHE:CZ	1:E:407:MET:HE3	2.47	0.50
1:E:145:ASN:N	1:E:146:SER:CA	2.64	0.50
1:F:231:ALA:N	1:F:232:PRO:CD	2.72	0.50
1:G:391:LEU:O	1:G:408:GLY:HA3	2.12	0.50
1:E:175:ILE:HG13	1:E:225:ILE:HD12	1.93	0.50
1:D:401:PRO:O	1:D:402:GLU:HB3	2.11	0.50
1:C:395:PHE:HE2	1:C:407:MET:HE2	1.75	0.50
1:C:367:GLY:C	1:C:462:GLN:NE2	2.65	0.50
1:H:401:PRO:O	1:H:402:GLU:HB3	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:ILE:O	1:B:384:SER:HB2	2.11	0.50
1:A:193:ALA:O	1:A:194:ASN:OD1	2.30	0.50
1:B:193:ALA:O	1:B:194:ASN:OD1	2.30	0.50
1:C:212:THR:CG2	1:C:213:GLU:O	2.59	0.50
1:F:231:ALA:HB3	1:F:232:PRO:CD	2.41	0.50
1:G:175:ILE:HG13	1:G:225:ILE:HD12	1.93	0.50
1:C:193:ALA:O	1:C:194:ASN:OD1	2.30	0.50
1:B:182:ASP:O	1:B:182:ASP:OD2	2.30	0.50
1:E:154:VAL:HG22	1:E:165:MET:HB2	1.93	0.50
1:E:54:TRP:HB2	1:E:72:ILE:HB	1.94	0.50
1:H:488:LEU:N	1:H:488:LEU:CD2	2.73	0.50
1:C:496:GLY:O	1:C:497:VAL:HG13	2.11	0.50
1:A:362:LEU:HD23	1:F:356:ASN:HD22	1.76	0.50
1:F:347:ALA:HB2	1:F:358:TYR:CE1	2.47	0.50
1:H:391:LEU:O	1:H:408:GLY:HA3	2.12	0.50
1:E:394:TRP:HB2	1:E:492:ASN:HB2	1.94	0.49
1:B:499:ASN:OD1	1:B:499:ASN:O	2.30	0.49
1:E:200:TYR:N	1:E:200:TYR:CD2	2.77	0.49
1:F:192:PHE:CD1	1:F:193:ALA:CB	2.91	0.49
1:G:192:PHE:CE2	1:G:193:ALA:CB	2.95	0.49
1:C:182:ASP:OD2	1:C:182:ASP:O	2.30	0.49
1:D:192:PHE:CE1	1:D:195:GLU:HG2	2.46	0.49
1:D:258:ARG:NH2	1:D:328:ASN:OD1	2.45	0.49
1:G:376:ALA:HA	1:G:452:SER:O	2.12	0.49
1:H:371:PHE:CZ	1:H:407:MET:HE3	2.46	0.49
1:H:36:HIS:HD2	1:H:56:HIS:NE2	2.10	0.49
1:A:269:LEU:HD11	1:A:312:PHE:CZ	2.48	0.49
1:H:381:GLN:HA	1:H:381:GLN:HE21	1.77	0.49
1:B:483:THR:HG23	1:B:483:THR:O	2.11	0.49
1:C:195:GLU:CA	1:C:195:GLU:OE2	2.60	0.49
1:D:424:LYS:C	1:D:425:VAL:CG2	2.81	0.49
1:D:193:ALA:O	1:D:194:ASN:OD1	2.29	0.49
1:F:154:VAL:HG22	1:F:165:MET:HB2	1.94	0.49
1:D:499:ASN:OD1	1:D:499:ASN:O	2.29	0.49
1:E:192:PHE:CE2	1:E:193:ALA:CB	2.95	0.49
1:C:215:ASP:OD1	1:C:217:SER:N	2.45	0.49
1:E:200:TYR:N	1:E:200:TYR:HD2	2.09	0.49
1:H:347:ALA:HB2	1:H:358:TYR:CE1	2.47	0.49
1:C:353:THR:HA	1:C:498:ASP:O	2.12	0.49
1:A:40:GLN:HE22	1:A:82:PHE:HA	1.76	0.49
1:H:97:PHE:CD1	1:H:97:PHE:N	2.81	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:TRP:HE1	1:A:494:THR:CB	2.23	0.49
1:C:354:LYS:HA	1:C:495:THR:HG23	1.95	0.49
1:D:355:ALA:O	1:H:363:SER:HB2	2.12	0.49
1:E:398:LEU:HD13	1:E:487:ALA:O	2.05	0.49
1:B:398:LEU:CB	1:B:487:ALA:HB3	2.42	0.49
1:H:200:TYR:HD2	1:H:200:TYR:N	2.10	0.49
1:H:395:PHE:HE2	1:H:407:MET:HE2	1.77	0.49
1:G:213:GLU:O	1:G:214:GLN:HG2	2.13	0.49
1:F:213:GLU:O	1:F:214:GLN:HG2	2.13	0.49
1:H:192:PHE:CE2	1:H:193:ALA:CB	2.96	0.49
1:C:378:ASN:ND2	1:C:380:THR:N	2.61	0.49
1:D:424:LYS:O	1:D:425:VAL:O	2.31	0.49
1:A:269:LEU:HD11	1:A:312:PHE:HZ	1.77	0.49
1:H:499:ASN:O	1:H:499:ASN:OD1	2.30	0.49
1:E:499:ASN:OD1	1:E:499:ASN:O	2.30	0.49
1:E:398:LEU:N	1:E:487:ALA:O	2.46	0.49
1:E:213:GLU:O	1:E:214:GLN:HG2	2.12	0.49
1:G:499:ASN:C	1:G:499:ASN:OD1	2.51	0.49
1:G:499:ASN:O	1:G:499:ASN:OD1	2.30	0.49
1:G:256:GLN:HE22	1:G:326:LEU:CB	2.25	0.49
1:F:192:PHE:CE2	1:F:193:ALA:CB	2.96	0.49
1:E:144:ALA:CB	1:E:145:ASN:CA	2.66	0.49
1:G:389:ALA:O	1:G:410:GLU:HA	2.13	0.49
1:F:426:LYS:O	1:F:430:GLU:HB2	2.12	0.49
1:F:395:PHE:CE2	1:F:407:MET:HE2	2.42	0.48
1:D:382:THR:O	1:D:384:SER:OG	2.30	0.48
1:B:422:ASN:CA	1:B:423:SER:HB2	2.35	0.48
1:G:253:PHE:HD1	1:G:253:PHE:H	1.59	0.48
1:E:148:GLN:HE21	1:E:150:ARG:NE	2.11	0.48
1:F:440:VAL:O	1:F:441:ASN:HB3	2.13	0.48
1:D:346:PHE:HE1	1:D:360:VAL:HG23	1.78	0.48
1:F:388:PHE:CE1	1:F:410:GLU:HG3	2.48	0.48
1:C:401:PRO:O	1:C:402:GLU:HB3	2.13	0.48
1:C:461:ASP:HB3	1:C:464:ILE:HG22	1.94	0.48
1:E:395:PHE:O	1:E:404:TYR:CB	2.61	0.48
1:D:383:ILE:O	1:D:384:SER:OG	2.31	0.48
1:A:383:ILE:O	1:A:384:SER:OG	2.30	0.48
1:G:36:HIS:HD2	1:G:56:HIS:NE2	2.11	0.48
1:D:368:THR:CG2	1:D:461:ASP:OD1	2.62	0.48
1:H:213:GLU:C	1:H:215:ASP:H	2.17	0.48
1:H:400:ASP:OD1	1:H:400:ASP:O	2.31	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:401:PRO:C	1:H:403:GLU:N	2.67	0.48
1:H:96:PHE:HB3	1:H:97:PHE:HD1	1.79	0.48
1:D:483:THR:O	1:D:483:THR:HG23	2.13	0.48
1:G:149:PHE:HZ	1:G:165:MET:CE	2.27	0.48
1:F:213:GLU:C	1:F:215:ASP:H	2.17	0.48
1:H:213:GLU:O	1:H:214:GLN:HG2	2.13	0.48
1:C:364:ASN:OD1	1:E:355:ALA:HB1	2.12	0.48
1:G:427:PHE:O	1:G:428:VAL:CG2	2.59	0.48
1:E:149:PHE:HZ	1:E:165:MET:CE	2.27	0.48
1:E:36:HIS:HD2	1:E:56:HIS:NE2	2.12	0.48
1:F:228:ASN:CG	1:F:229:PRO:CG	2.79	0.48
1:F:398:LEU:HD11	1:F:489:GLY:N	2.28	0.48
1:A:401:PRO:O	1:A:402:GLU:HB3	2.13	0.48
1:C:483:THR:HG23	1:C:483:THR:O	2.13	0.48
1:G:154:VAL:HG22	1:G:165:MET:HB2	1.95	0.48
1:B:425:VAL:O	1:B:426:LYS:C	2.50	0.48
1:E:144:ALA:HB1	1:E:145:ASN:O	2.12	0.48
1:B:213:GLU:C	1:B:214:GLN:OE1	2.52	0.48
1:E:432:PRO:O	1:F:437:ARG:HB3	2.13	0.48
1:A:255:ASN:O	1:B:194:ASN:O	2.32	0.48
1:G:352:LEU:HB3	1:G:495:THR:HG21	1.96	0.48
1:B:378:ASN:O	1:B:380:THR:N	2.39	0.48
1:C:163:TRP:CD1	1:C:183:LEU:HG	2.49	0.48
1:B:269:LEU:HD11	1:B:312:PHE:HZ	1.78	0.48
1:E:347:ALA:HB2	1:E:358:TYR:CE1	2.48	0.48
1:E:500:LEU:O	1:E:500:LEU:CD1	2.33	0.48
1:C:496:GLY:O	1:C:497:VAL:CB	2.61	0.48
1:B:346:PHE:HE1	1:B:360:VAL:HG23	1.77	0.48
1:E:383:ILE:O	1:E:384:SER:HB2	2.14	0.48
1:H:499:ASN:OD1	1:H:499:ASN:C	2.51	0.48
1:H:376:ALA:HA	1:H:452:SER:O	2.13	0.48
1:A:397:GLY:O	1:A:486:ASN:ND2	2.47	0.48
1:H:96:PHE:HB3	1:H:97:PHE:CD1	2.48	0.48
1:E:403:GLU:HG3	1:E:423:SER:HA	1.96	0.48
1:A:448:GLU:O	1:A:449:ASN:OD1	2.32	0.48
1:F:5:THR:HG22	1:F:6:SER:N	2.29	0.48
1:H:354:LYS:H	1:H:498:ASP:HA	1.78	0.48
1:F:394:TRP:NE1	1:F:494:THR:HB	2.18	0.48
1:E:440:VAL:O	1:E:441:ASN:HB3	2.14	0.48
1:F:391:LEU:O	1:F:408:GLY:HA3	2.14	0.48
1:F:486:ASN:CA	1:F:487:ALA:HB3	2.35	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:377:VAL:CG1	1:D:379:THR:H	2.26	0.47
1:A:403:GLU:OE2	1:A:424:LYS:HG2	2.08	0.47
1:E:96:PHE:C	1:E:97:PHE:CG	2.86	0.47
1:H:464:ILE:CG2	1:H:464:ILE:O	2.61	0.47
1:G:347:ALA:CB	1:G:350:THR:HG21	2.44	0.47
1:F:36:HIS:HD2	1:F:56:HIS:NE2	2.11	0.47
1:C:449:ASN:O	1:C:449:ASN:OD1	2.30	0.47
1:G:397:GLY:HA2	1:G:400:ASP:O	2.14	0.47
1:B:383:ILE:O	1:B:384:SER:OG	2.31	0.47
1:D:269:LEU:HD11	1:D:312:PHE:CZ	2.49	0.47
1:G:352:LEU:O	1:G:498:ASP:O	2.32	0.47
1:E:213:GLU:C	1:E:215:ASP:H	2.18	0.47
1:C:411:VAL:HG21	1:C:500:LEU:HD21	1.96	0.47
1:C:377:VAL:HG12	1:C:379:THR:N	2.29	0.47
1:B:269:LEU:HD11	1:B:312:PHE:CZ	2.49	0.47
1:D:269:LEU:HD11	1:D:312:PHE:HZ	1.79	0.47
1:C:269:LEU:HD11	1:C:312:PHE:HZ	1.79	0.47
1:G:387:VAL:CG1	1:G:388:PHE:N	2.75	0.47
1:G:213:GLU:C	1:G:215:ASP:H	2.17	0.47
1:B:86:MET:HG3	1:B:108:VAL:O	2.14	0.47
1:H:97:PHE:HD1	1:H:97:PHE:N	2.13	0.47
1:D:379:THR:HG21	1:D:450:ASP:C	2.34	0.47
1:H:440:VAL:O	1:H:441:ASN:HB3	2.14	0.47
1:C:183:LEU:CD2	1:C:186:TRP:HZ2	2.27	0.47
1:E:96:PHE:O	1:E:97:PHE:CG	2.67	0.47
1:G:381:GLN:C	1:G:382:THR:OG1	2.51	0.47
1:D:86:MET:HG3	1:D:108:VAL:O	2.13	0.47
1:B:226:SER:HB2	1:B:267:TYR:CE1	2.50	0.47
1:G:346:PHE:CE1	1:G:360:VAL:HG22	2.48	0.47
1:H:154:VAL:HG22	1:H:165:MET:HB2	1.96	0.47
1:F:149:PHE:HZ	1:F:165:MET:CE	2.27	0.47
1:C:321:ASN:HB2	1:C:322:PRO:CD	2.43	0.47
1:G:348:THR:O	1:G:349:ASN:C	2.52	0.47
1:C:463:ASN:C	1:C:463:ASN:OD1	2.53	0.47
1:C:378:ASN:HA	1:C:451:LEU:HD21	1.97	0.47
1:E:5:THR:O	1:E:6:SER:OG	2.31	0.47
1:B:54:TRP:HB2	1:B:72:ILE:HB	1.97	0.47
1:H:400:ASP:CG	1:H:400:ASP:O	2.53	0.47
1:E:192:PHE:CD1	1:E:193:ALA:CB	2.91	0.47
1:G:256:GLN:OE1	1:G:327:ILE:CG1	2.61	0.47
1:C:378:ASN:ND2	1:C:380:THR:H	2.12	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:258:ARG:HH21	1:E:326:LEU:HD21	1.79	0.47
1:G:440:VAL:O	1:G:441:ASN:HB3	2.14	0.47
1:C:205:PRO:HA	1:C:224:PHE:O	2.14	0.47
1:B:369:LEU:CD1	1:B:460:LEU:HD13	2.44	0.47
1:G:436:ASN:OD1	1:H:437:ARG:NH1	2.47	0.47
1:H:396:LYS:O	1:H:490:SER:HB3	2.14	0.47
1:B:448:GLU:O	1:B:449:ASN:OD1	2.32	0.47
1:H:144:ALA:CB	1:H:145:ASN:C	2.80	0.47
1:C:360:VAL:HG22	1:E:358:TYR:CD1	2.50	0.47
1:C:394:TRP:HE1	1:C:494:THR:CB	2.25	0.47
1:F:383:ILE:H	1:F:383:ILE:HG13	1.44	0.47
1:A:347:ALA:HB1	1:A:350:THR:OG1	2.15	0.47
1:H:399:GLU:CG	1:H:486:ASN:ND2	2.78	0.47
1:A:323:GLU:HG2	1:B:171:GLN:NE2	2.25	0.47
1:E:464:ILE:O	1:E:464:ILE:HG23	2.15	0.47
1:G:258:ARG:HH21	1:G:326:LEU:HD21	1.79	0.47
1:E:437:ARG:HD2	1:F:432:PRO:HA	1.96	0.47
1:C:226:SER:HB2	1:C:267:TYR:CE1	2.50	0.47
1:H:228:ASN:OD1	1:H:229:PRO:HD3	2.14	0.46
1:A:496:GLY:C	1:A:497:VAL:CG1	2.66	0.46
1:E:96:PHE:HB2	1:E:97:PHE:CD1	2.50	0.46
1:G:347:ALA:HB1	1:G:350:THR:HG21	1.96	0.46
1:G:400:ASP:OD1	1:G:400:ASP:O	2.32	0.46
1:H:192:PHE:CD1	1:H:193:ALA:CB	2.92	0.46
1:G:321:ASN:C	1:G:323:GLU:H	2.18	0.46
1:C:269:LEU:HD11	1:C:312:PHE:CZ	2.50	0.46
1:G:346:PHE:HE1	1:G:360:VAL:CG2	2.24	0.46
1:G:388:PHE:CE1	1:G:410:GLU:HG3	2.50	0.46
1:H:149:PHE:HZ	1:H:165:MET:CE	2.28	0.46
1:C:40:GLN:HE22	1:C:82:PHE:HA	1.80	0.46
1:E:497:VAL:CG1	1:E:500:LEU:HB3	2.45	0.46
1:G:149:PHE:HZ	1:G:165:MET:HE1	1.80	0.46
1:G:395:PHE:CE2	1:G:407:MET:CE	2.98	0.46
1:B:316:THR:HA	1:B:327:ILE:HA	1.96	0.46
1:E:228:ASN:HA	1:E:229:PRO:HA	1.58	0.46
1:F:397:GLY:HA2	1:F:400:ASP:C	2.36	0.46
1:E:368:THR:CG2	1:E:461:ASP:OD1	2.63	0.46
1:G:403:GLU:HG3	1:G:423:SER:HA	1.97	0.46
1:D:213:GLU:CB	1:D:214:GLN:OE1	2.63	0.46
1:B:394:TRP:HE1	1:B:494:THR:CB	2.26	0.46
1:G:496:GLY:O	1:G:497:VAL:O	2.33	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:SER:HB2	1:A:267:TYR:CE1	2.51	0.46
1:C:385:LYS:CG	1:C:386:SER:H	2.29	0.46
1:H:403:GLU:HG3	1:H:423:SER:HA	1.97	0.46
1:G:192:PHE:CD1	1:G:193:ALA:CB	2.92	0.46
1:F:258:ARG:HH21	1:F:326:LEU:HD21	1.81	0.46
1:G:389:ALA:HA	1:G:497:VAL:CG1	2.45	0.46
1:D:463:ASN:O	1:D:463:ASN:OD1	2.34	0.46
1:H:348:THR:O	1:H:349:ASN:C	2.54	0.46
1:B:385:LYS:CG	1:B:386:SER:H	2.29	0.46
1:F:401:PRO:C	1:F:403:GLU:N	2.69	0.46
1:E:428:VAL:HG12	1:E:429:LYS:N	2.30	0.46
1:F:321:ASN:C	1:F:323:GLU:H	2.18	0.46
1:F:231:ALA:O	1:F:233:ALA:O	2.32	0.46
1:A:205:PRO:HA	1:A:224:PHE:O	2.16	0.46
1:H:371:PHE:CE2	1:H:458:GLY:HA3	2.51	0.46
1:G:98:ASN:CB	1:G:100:THR:CG2	2.55	0.46
1:G:194:ASN:CB	1:G:195:GLU:HB3	2.45	0.46
1:D:379:THR:HG22	1:D:380:THR:H	1.79	0.46
1:D:425:VAL:O	1:D:428:VAL:N	2.48	0.46
1:B:182:ASP:OD2	1:B:184:LYS:HG3	2.16	0.46
1:A:385:LYS:CG	1:A:386:SER:H	2.29	0.46
1:C:451:LEU:HD23	1:C:451:LEU:HA	1.80	0.46
1:C:422:ASN:CA	1:C:423:SER:HB2	2.32	0.46
1:E:232:PRO:HG2	1:F:441:ASN:CB	2.45	0.46
1:G:377:VAL:HG13	1:G:500:LEU:CD2	2.46	0.46
1:A:371:PHE:CE2	1:A:458:GLY:HA3	2.51	0.46
1:F:403:GLU:HG3	1:F:423:SER:HA	1.97	0.46
1:A:382:THR:O	1:A:384:SER:OG	2.31	0.46
1:C:195:GLU:HB3	1:C:241:PHE:CE1	2.51	0.46
1:F:386:SER:OG	1:F:386:SER:O	2.32	0.46
1:G:96:PHE:C	1:G:97:PHE:CG	2.88	0.46
1:B:205:PRO:HA	1:B:224:PHE:O	2.16	0.46
1:G:162:LYS:HD3	1:G:179:SER:HB2	1.98	0.46
1:E:463:ASN:C	1:E:463:ASN:OD1	2.53	0.46
1:D:448:GLU:O	1:D:449:ASN:OD1	2.33	0.45
1:G:145:ASN:HB3	1:G:147:THR:N	2.31	0.45
1:C:346:PHE:HB3	1:C:347:ALA:H	1.40	0.45
1:G:429:LYS:HB3	1:G:429:LYS:HE2	1.68	0.45
1:G:496:GLY:O	1:G:497:VAL:HG13	2.16	0.45
1:H:321:ASN:C	1:H:323:GLU:H	2.19	0.45
1:A:427:PHE:CZ	1:A:434:PHE:CD1	3.05	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:PRO:HA	1:D:219:SER:HB3	1.99	0.45
1:A:150:ARG:HH22	1:A:201:GLN:NE2	2.14	0.45
1:C:383:ILE:HG22	1:C:384:SER:H	1.80	0.45
1:A:351:THR:HG21	1:A:499:ASN:OD1	2.16	0.45
1:F:398:LEU:HD12	1:F:489:GLY:H	1.82	0.45
1:D:183:LEU:O	1:D:183:LEU:HD23	2.17	0.45
1:E:321:ASN:HB3	1:E:322:PRO:HD2	1.98	0.45
1:E:321:ASN:C	1:E:323:GLU:H	2.20	0.45
1:D:226:SER:HB2	1:D:267:TYR:CE1	2.51	0.45
1:A:378:ASN:HD22	1:A:380:THR:N	2.15	0.45
1:A:383:ILE:C	1:A:384:SER:OG	2.55	0.45
1:F:497:VAL:HG12	1:F:497:VAL:O	2.16	0.45
1:H:321:ASN:HB3	1:H:322:PRO:HD2	1.99	0.45
1:C:183:LEU:CD2	1:C:186:TRP:CZ2	2.99	0.45
1:C:382:THR:O	1:C:383:ILE:C	2.55	0.45
1:E:205:PRO:HA	1:E:224:PHE:O	2.17	0.45
1:F:22:ASP:N	1:F:22:ASP:OD1	2.50	0.45
1:H:403:GLU:HG2	1:H:482:MET:HG3	1.99	0.45
1:E:395:PHE:O	1:E:404:TYR:HA	2.17	0.45
1:E:397:GLY:HA2	1:E:400:ASP:C	2.37	0.45
1:F:397:GLY:HA3	1:F:398:LEU:HA	1.81	0.45
1:C:427:PHE:CD2	1:C:428:VAL:N	2.85	0.45
1:E:401:PRO:C	1:E:403:GLU:N	2.69	0.45
1:F:398:LEU:CD1	1:F:489:GLY:CA	2.94	0.45
1:D:195:GLU:HB3	1:D:241:PHE:CE1	2.52	0.45
1:E:162:LYS:HD3	1:E:179:SER:HB2	1.99	0.45
1:H:487:ALA:C	1:H:488:LEU:HD23	2.37	0.45
1:H:229:PRO:CD	1:H:230:GLY:H	2.30	0.45
1:G:228:ASN:CB	1:G:229:PRO:HB3	2.47	0.45
1:F:96:PHE:O	1:F:97:PHE:CD1	2.69	0.45
1:H:89:ASP:OD2	1:H:94:SER:OG	2.25	0.45
1:E:8:ARG:NH2	1:E:16:ASN:O	2.50	0.45
1:C:54:TRP:HB2	1:C:72:ILE:HB	1.99	0.45
1:F:195:GLU:C	1:F:195:GLU:OE1	2.55	0.44
1:E:497:VAL:CG1	1:E:500:LEU:CB	2.94	0.44
1:E:148:GLN:N	1:E:171:GLN:NE2	2.65	0.44
1:D:426:LYS:O	1:D:427:PHE:C	2.55	0.44
1:H:121:GLN:CG	1:H:149:PHE:CE2	3.00	0.44
1:G:121:GLN:CG	1:G:149:PHE:CE2	3.00	0.44
1:A:346:PHE:HE1	1:A:360:VAL:HG23	1.81	0.44
1:H:380:THR:HB	1:H:450:ASP:CB	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:162:LYS:HD3	1:H:179:SER:HB2	1.99	0.44
1:G:28:TYR:CE2	1:G:276:ASP:HB2	2.52	0.44
1:H:22:ASP:OD1	1:H:22:ASP:N	2.50	0.44
1:F:145:ASN:O	1:F:145:ASN:OD1	2.36	0.44
1:F:321:ASN:HB3	1:F:322:PRO:HD2	1.99	0.44
1:G:389:ALA:O	1:G:410:GLU:HG2	2.18	0.44
1:D:205:PRO:HA	1:D:224:PHE:O	2.17	0.44
1:H:253:PHE:N	1:H:253:PHE:HD1	2.13	0.44
1:E:346:PHE:CE1	1:E:360:VAL:CG2	3.01	0.44
1:C:86:MET:HG3	1:C:108:VAL:O	2.17	0.44
1:C:378:ASN:HD21	1:C:380:THR:C	2.18	0.44
1:C:496:GLY:O	1:C:497:VAL:O	2.35	0.44
1:F:147:THR:O	1:F:148:GLN:C	2.56	0.44
1:B:213:GLU:O	1:B:215:ASP:N	2.50	0.44
1:C:422:ASN:HA	1:C:423:SER:CB	2.28	0.44
1:G:371:PHE:CE2	1:G:458:GLY:HA3	2.52	0.44
1:A:30:GLU:HB3	1:A:104:ARG:HD2	1.99	0.44
1:A:321:ASN:HB2	1:A:322:PRO:CD	2.43	0.44
1:C:354:LYS:HA	1:C:495:THR:CG2	2.48	0.44
1:F:303:ARG:O	1:F:304:SER:HB2	2.18	0.44
1:H:51:PRO:HB3	1:H:77:ASN:HA	1.99	0.44
1:D:213:GLU:O	1:D:214:GLN:NE2	2.46	0.44
1:A:483:THR:O	1:A:483:THR:HG23	2.18	0.44
1:F:346:PHE:CE1	1:F:360:VAL:CG2	3.00	0.44
1:F:28:TYR:CE2	1:F:276:ASP:HB2	2.52	0.44
1:A:41:TYR:CE2	1:A:43:PRO:HB3	2.53	0.44
1:C:378:ASN:ND2	1:C:380:THR:O	2.41	0.44
1:C:424:LYS:C	1:C:425:VAL:HG23	2.37	0.44
1:C:258:ARG:HA	1:D:197:PHE:HE1	1.83	0.44
1:G:460:LEU:HG	1:G:465:LEU:HD12	2.00	0.44
1:E:228:ASN:CG	1:E:229:PRO:CG	2.81	0.44
1:G:192:PHE:HZ	1:G:252:ALA:HB2	1.82	0.44
1:C:182:ASP:C	1:C:182:ASP:OD2	2.54	0.44
1:C:381:GLN:C	1:C:383:ILE:H	2.21	0.44
1:E:461:ASP:HB3	1:E:464:ILE:HG22	2.00	0.44
1:A:484:THR:HG22	1:A:484:THR:O	2.18	0.44
1:E:394:TRP:NE1	1:E:494:THR:HB	2.21	0.44
1:H:28:TYR:CE2	1:H:276:ASP:HB2	2.52	0.44
1:G:45:ASP:OD1	1:G:46:THR:N	2.47	0.44
1:E:371:PHE:CE2	1:E:458:GLY:HA3	2.52	0.44
1:E:28:TYR:CE2	1:E:276:ASP:HB2	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:THR:OG1	1:D:6:SER:N	2.51	0.44
1:E:401:PRO:O	1:E:402:GLU:CB	2.65	0.43
1:E:98:ASN:HB3	1:E:100:THR:CG2	2.48	0.43
1:H:147:THR:O	1:H:148:GLN:C	2.56	0.43
1:G:321:ASN:HB3	1:G:322:PRO:HD2	1.99	0.43
1:F:246:ASN:HD21	1:F:249:HIS:HB2	1.83	0.43
1:H:403:GLU:OE1	1:H:483:THR:OG1	2.33	0.43
1:E:194:ASN:CB	1:E:195:GLU:HB3	2.44	0.43
1:D:377:VAL:CG1	1:D:378:ASN:N	2.76	0.43
1:H:145:ASN:HB3	1:H:147:THR:H	1.83	0.43
1:B:382:THR:O	1:B:383:ILE:HG12	2.17	0.43
1:E:386:SER:OG	1:E:386:SER:O	2.32	0.43
1:C:425:VAL:O	1:C:426:LYS:C	2.57	0.43
1:C:346:PHE:HE1	1:C:360:VAL:HG23	1.81	0.43
1:D:394:TRP:HE1	1:D:494:THR:CB	2.24	0.43
1:D:371:PHE:CE2	1:D:458:GLY:HA3	2.52	0.43
1:E:197:PHE:HB2	1:E:200:TYR:CG	2.53	0.43
1:G:432:PRO:HA	1:H:437:ARG:HE	1.81	0.43
1:A:54:TRP:HB2	1:A:72:ILE:HB	2.00	0.43
1:H:423:SER:HG	1:H:425:VAL:HG23	1.83	0.43
1:G:423:SER:CB	1:G:425:VAL:HG23	2.40	0.43
1:A:401:PRO:C	1:A:403:GLU:N	2.71	0.43
1:B:378:ASN:HA	1:B:451:LEU:HD23	2.00	0.43
1:G:96:PHE:O	1:G:97:PHE:CG	2.71	0.43
1:G:246:ASN:HD21	1:G:249:HIS:HB2	1.83	0.43
1:C:359:ASN:HB3	1:E:359:ASN:HB3	2.00	0.43
1:G:151:ASP:HB3	1:G:204:CYS:HA	2.00	0.43
1:B:173:TYR:O	1:B:193:ALA:O	2.36	0.43
1:B:192:PHE:CZ	1:B:195:GLU:CG	3.01	0.43
1:B:486:ASN:CA	1:B:487:ALA:HB2	2.48	0.43
1:G:426:LYS:HB2	1:G:426:LYS:HE3	1.94	0.43
1:H:388:PHE:CD2	1:H:390:ASP:HB3	2.53	0.43
1:F:151:ASP:HB3	1:F:204:CYS:HA	2.00	0.43
1:C:424:LYS:O	1:C:425:VAL:O	2.37	0.43
1:H:258:ARG:HH21	1:H:326:LEU:HD21	1.84	0.43
1:G:22:ASP:N	1:G:22:ASP:OD1	2.51	0.43
1:H:151:ASP:HB3	1:H:204:CYS:HA	2.00	0.43
1:C:5:THR:OG1	1:C:6:SER:N	2.52	0.43
1:H:403:GLU:OE2	1:H:483:THR:OG1	2.36	0.43
1:D:213:GLU:C	1:D:214:GLN:CD	2.49	0.43
1:D:448:GLU:O	1:D:449:ASN:C	2.56	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:354:LYS:HD2	1:F:497:VAL:H	1.82	0.43
1:E:151:ASP:HB3	1:E:204:CYS:HA	2.00	0.43
1:E:238:ASN:HD22	1:E:260:VAL:HG21	1.84	0.43
1:E:195:GLU:C	1:E:195:GLU:OE1	2.57	0.43
1:E:497:VAL:HG11	1:E:500:LEU:HB2	2.01	0.43
1:H:197:PHE:HB2	1:H:200:TYR:CG	2.54	0.43
1:G:210:VAL:HA	1:G:211:PRO:HD2	1.89	0.43
1:F:162:LYS:HD3	1:F:179:SER:HB2	1.99	0.43
1:D:54:TRP:HB2	1:D:72:ILE:HB	2.00	0.43
1:E:22:ASP:N	1:E:22:ASP:OD1	2.52	0.43
1:B:463:ASN:C	1:B:463:ASN:OD1	2.57	0.43
1:F:253:PHE:CD1	1:F:253:PHE:N	2.85	0.43
1:G:228:ASN:CA	1:G:229:PRO:CB	2.97	0.43
1:G:147:THR:O	1:G:148:GLN:C	2.57	0.43
1:H:99:ASP:C	1:H:101:ILE:N	2.72	0.43
1:C:371:PHE:CE2	1:C:458:GLY:HA3	2.54	0.43
1:D:449:ASN:O	1:D:449:ASN:CG	2.52	0.43
1:B:30:GLU:HB3	1:B:104:ARG:HD2	2.01	0.43
1:E:383:ILE:HG13	1:E:383:ILE:H	1.46	0.43
1:G:51:PRO:HB3	1:G:77:ASN:HA	2.00	0.43
1:H:386:SER:OG	1:H:386:SER:O	2.30	0.43
1:G:205:PRO:HA	1:G:224:PHE:O	2.19	0.43
1:G:397:GLY:HA3	1:G:398:LEU:HA	1.78	0.43
1:F:371:PHE:CE2	1:F:458:GLY:HA3	2.54	0.43
1:D:449:ASN:O	1:D:450:ASP:CB	2.63	0.43
1:D:422:ASN:CA	1:D:423:SER:CB	2.96	0.43
1:G:394:TRP:NE1	1:G:494:THR:HB	2.19	0.43
1:G:346:PHE:HE1	1:G:360:VAL:HG22	1.84	0.43
1:H:497:VAL:HG13	1:H:497:VAL:O	2.18	0.43
1:G:8:ARG:NH2	1:G:15:PRO:O	2.49	0.43
1:E:51:PRO:HB3	1:E:77:ASN:HA	2.01	0.43
1:E:349:ASN:HA	1:E:502:TYR:OH	2.19	0.43
1:B:5:THR:OG1	1:B:6:SER:N	2.51	0.43
1:E:153:LYS:HB3	1:E:166:THR:HG23	2.01	0.43
1:F:194:ASN:CB	1:F:195:GLU:HB3	2.44	0.42
1:G:256:GLN:HE22	1:G:326:LEU:HB2	1.76	0.42
1:E:321:ASN:CB	1:E:322:PRO:HD2	2.50	0.42
1:G:428:VAL:HG12	1:G:429:LYS:H	1.81	0.42
1:G:389:ALA:HA	1:G:497:VAL:HG11	2.01	0.42
1:D:30:GLU:HB3	1:D:104:ARG:HD2	2.00	0.42
1:B:15:PRO:HD3	1:B:20:MET:SD	2.59	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:ASN:HB3	1:E:362:LEU:HA	2.02	0.42
1:A:424:LYS:HA	1:A:424:LYS:HD3	1.51	0.42
1:B:383:ILE:HB	1:B:384:SER:H	1.60	0.42
1:D:401:PRO:C	1:D:403:GLU:N	2.72	0.42
1:G:148:GLN:N	1:G:171:GLN:NE2	2.67	0.42
1:F:96:PHE:C	1:F:97:PHE:CG	2.92	0.42
1:F:121:GLN:CG	1:F:149:PHE:CE2	3.02	0.42
1:D:395:PHE:CE2	1:D:407:MET:CE	3.01	0.42
1:F:464:ILE:O	1:F:464:ILE:HG23	2.17	0.42
1:E:266:TYR:HE2	1:E:269:LEU:HD12	1.84	0.42
1:D:425:VAL:O	1:D:427:PHE:N	2.51	0.42
1:G:377:VAL:HG13	1:G:500:LEU:HD23	2.00	0.42
1:C:383:ILE:CG2	1:C:384:SER:H	2.32	0.42
1:D:371:PHE:CZ	1:D:407:MET:HE3	2.55	0.42
1:F:205:PRO:HA	1:F:224:PHE:O	2.19	0.42
1:H:429:LYS:HB3	1:H:429:LYS:HE3	1.45	0.42
1:D:466:GLU:HG2	1:D:477:THR:HG23	2.01	0.42
1:H:210:VAL:HA	1:H:211:PRO:HD2	1.89	0.42
1:H:228:ASN:CG	1:H:229:PRO:HB3	2.31	0.42
1:A:380:THR:HG22	1:A:380:THR:O	2.19	0.42
1:D:426:LYS:O	1:D:429:LYS:N	2.52	0.42
1:G:383:ILE:H	1:G:383:ILE:HG13	1.46	0.42
1:A:395:PHE:CE2	1:A:407:MET:CE	3.01	0.42
1:E:190:SER:OG	1:E:191:ALA:N	2.51	0.42
1:E:210:VAL:HA	1:E:211:PRO:HD2	1.88	0.42
1:E:377:VAL:HG13	1:E:500:LEU:HD11	2.00	0.42
1:H:229:PRO:HD2	1:H:230:GLY:H	1.85	0.42
1:C:213:GLU:OE1	1:C:330:LYS:CD	2.68	0.42
1:H:205:PRO:HA	1:H:224:PHE:O	2.19	0.42
1:H:303:ARG:O	1:H:304:SER:HB2	2.19	0.42
1:E:201:GLN:HB2	1:E:228:ASN:O	2.20	0.42
1:B:394:TRP:HB2	1:B:492:ASN:HB2	2.01	0.42
1:G:347:ALA:HB2	1:G:358:TYR:CZ	2.55	0.42
1:A:197:PHE:HE1	1:B:258:ARG:HA	1.81	0.42
1:F:197:PHE:HB2	1:F:200:TYR:CG	2.54	0.42
1:H:195:GLU:OE1	1:H:195:GLU:C	2.58	0.42
1:G:401:PRO:C	1:G:403:GLU:N	2.67	0.42
1:F:401:PRO:O	1:F:402:GLU:CB	2.67	0.42
1:D:212:THR:O	1:D:212:THR:HG22	2.19	0.42
1:B:423:SER:C	1:B:424:LYS:HG2	2.40	0.42
1:E:441:ASN:CB	1:F:232:PRO:HG2	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:ASN:HB2	1:B:322:PRO:CD	2.44	0.42
1:C:236:SER:HB2	1:C:267:TYR:CD1	2.55	0.42
1:H:246:ASN:HD21	1:H:249:HIS:HB2	1.84	0.42
1:H:5:THR:O	1:H:5:THR:HG22	2.19	0.42
1:H:397:GLY:H	1:H:401:PRO:HA	1.83	0.42
1:E:145:ASN:HB3	1:E:147:THR:H	1.84	0.42
1:B:380:THR:HA	1:B:381:GLN:HA	1.36	0.42
1:D:394:TRP:NE1	1:D:494:THR:HB	2.27	0.42
1:H:395:PHE:CE2	1:H:407:MET:HE2	2.55	0.42
1:F:51:PRO:HB3	1:F:77:ASN:HA	2.02	0.42
1:C:287:TRP:HE1	1:C:304:SER:HB3	1.84	0.42
1:H:266:TYR:HE2	1:H:269:LEU:HD12	1.84	0.42
1:C:425:VAL:O	1:C:428:VAL:N	2.53	0.42
1:B:337:ILE:O	1:B:338:SER:HB3	2.20	0.42
1:D:337:ILE:O	1:D:338:SER:HB3	2.20	0.42
1:G:425:VAL:HG21	1:G:481:PHE:O	2.20	0.42
1:E:385:LYS:CG	1:E:386:SER:N	2.61	0.42
1:F:200:TYR:H	1:F:200:TYR:HD2	1.67	0.42
1:F:266:TYR:HE2	1:F:269:LEU:HD12	1.85	0.42
1:H:153:LYS:HB3	1:H:166:THR:HG23	2.02	0.42
1:A:466:GLU:HG2	1:A:477:THR:HG23	2.01	0.42
1:C:378:ASN:HA	1:C:451:LEU:HD23	2.01	0.41
1:A:378:ASN:H	1:A:500:LEU:CD1	2.32	0.41
1:A:378:ASN:O	1:A:450:ASP:O	2.38	0.41
1:G:231:ALA:HB3	1:G:232:PRO:CD	2.46	0.41
1:G:388:PHE:HE2	1:G:390:ASP:HB3	1.79	0.41
1:C:30:GLU:HB3	1:C:104:ARG:HD2	2.01	0.41
1:H:381:GLN:O	1:H:382:THR:C	2.58	0.41
1:D:256:GLN:OE1	1:D:258:ARG:HD2	2.19	0.41
1:H:200:TYR:HD2	1:H:200:TYR:H	1.68	0.41
1:B:355:ALA:O	1:G:363:SER:HB2	2.19	0.41
1:B:28:TYR:CZ	1:B:276:ASP:HB2	2.54	0.41
1:A:380:THR:HA	1:A:381:GLN:HA	1.37	0.41
1:B:449:ASN:CG	1:B:450:ASP:N	2.66	0.41
1:C:362:LEU:HD23	1:E:356:ASN:ND2	2.35	0.41
1:E:368:THR:HA	1:E:460:LEU:O	2.20	0.41
1:A:337:ILE:O	1:A:338:SER:HB3	2.20	0.41
1:B:248:THR:OG1	1:B:249:HIS:HD2	2.04	0.41
1:G:449:ASN:HB3	1:G:450:ASP:H	1.67	0.41
1:C:337:ILE:O	1:C:338:SER:HB3	2.20	0.41
1:A:227:ILE:O	1:A:227:ILE:HG13	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:496:GLY:C	1:D:497:VAL:HG13	2.41	0.41
1:G:228:ASN:HA	1:G:229:PRO:HB3	2.02	0.41
1:B:448:GLU:O	1:B:450:ASP:N	2.53	0.41
1:C:486:ASN:CA	1:C:487:ALA:HB2	2.50	0.41
1:H:310:ARG:HB3	1:H:331:ALA:HB1	2.01	0.41
1:D:303:ARG:O	1:D:304:SER:HB2	2.20	0.41
1:G:399:GLU:HG3	1:G:486:ASN:ND2	2.35	0.41
1:B:401:PRO:C	1:B:403:GLU:N	2.72	0.41
1:E:147:THR:O	1:E:148:GLN:C	2.58	0.41
1:B:192:PHE:HA	1:B:193:ALA:CB	2.47	0.41
1:H:190:SER:OG	1:H:191:ALA:N	2.52	0.41
1:C:376:ALA:HA	1:C:452:SER:O	2.20	0.41
1:G:321:ASN:CB	1:G:322:PRO:HD2	2.50	0.41
1:A:394:TRP:NE1	1:A:494:THR:HB	2.26	0.41
1:E:266:TYR:CE2	1:E:269:LEU:HD12	2.55	0.41
1:A:142:LEU:HD11	1:A:178:TYR:CD1	2.56	0.41
1:H:321:ASN:CB	1:H:322:PRO:HD2	2.50	0.41
1:G:197:PHE:HB2	1:G:200:TYR:CG	2.56	0.41
1:D:287:TRP:HE1	1:D:304:SER:HB3	1.86	0.41
1:E:45:ASP:OD1	1:E:46:THR:N	2.48	0.41
1:A:376:ALA:HA	1:A:452:SER:O	2.20	0.41
1:F:395:PHE:HB3	1:F:488:LEU:HB3	2.03	0.41
1:G:228:ASN:CA	1:G:229:PRO:HB3	2.51	0.41
1:F:321:ASN:CB	1:F:322:PRO:HD2	2.50	0.41
1:F:96:PHE:O	1:F:97:PHE:CG	2.73	0.41
1:A:287:TRP:HE1	1:A:304:SER:HB3	1.86	0.41
1:E:426:LYS:HG2	1:E:430:GLU:OE2	2.20	0.41
1:B:150:ARG:HH22	1:B:201:GLN:NE2	2.18	0.41
1:F:153:LYS:HB3	1:F:166:THR:HG23	2.02	0.41
1:E:4:GLU:O	1:E:4:GLU:HG2	2.21	0.41
1:G:345:ARG:HH11	1:G:507:GLN:NE2	2.19	0.41
1:G:200:TYR:HD2	1:G:200:TYR:H	1.69	0.41
1:F:50:THR:HA	1:F:51:PRO:C	2.41	0.41
1:G:195:GLU:OE1	1:G:195:GLU:C	2.59	0.41
1:C:378:ASN:ND2	1:C:380:THR:C	2.73	0.41
1:A:213:GLU:CA	1:A:214:GLN:OE1	2.68	0.41
1:D:401:PRO:O	1:D:402:GLU:CB	2.68	0.41
1:E:437:ARG:HB3	1:F:432:PRO:O	2.21	0.41
1:C:394:TRP:NE1	1:C:494:THR:HB	2.26	0.41
1:B:354:LYS:H	1:B:498:ASP:HA	1.86	0.41
1:H:426:LYS:HG2	1:H:430:GLU:OE2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:396:LYS:C	1:H:490:SER:HB3	2.41	0.41
1:G:238:ASN:HD22	1:G:260:VAL:HG21	1.85	0.41
1:C:150:ARG:HH22	1:C:201:GLN:NE2	2.19	0.41
1:B:368:THR:CG2	1:B:461:ASP:OD1	2.69	0.41
1:C:227:ILE:HG13	1:C:227:ILE:O	2.20	0.41
1:E:496:GLY:O	1:E:497:VAL:O	2.39	0.41
1:B:401:PRO:O	1:B:402:GLU:CB	2.68	0.41
1:A:107:CYS:HB2	1:A:126:SER:HB3	2.02	0.41
1:G:153:LYS:HB3	1:G:166:THR:HG23	2.03	0.41
1:C:198:LEU:HD23	1:D:326:LEU:HD11	2.03	0.41
1:B:391:LEU:O	1:B:408:GLY:HA3	2.21	0.41
1:H:461:ASP:O	1:H:463:ASN:N	2.51	0.41
1:F:210:VAL:HA	1:F:211:PRO:HD2	1.88	0.41
1:C:28:TYR:CZ	1:C:276:ASP:HB2	2.56	0.41
1:F:310:ARG:HB3	1:F:331:ALA:HB1	2.03	0.41
1:G:144:ALA:CB	1:G:145:ASN:O	2.65	0.40
1:H:381:GLN:HE21	1:H:381:GLN:CA	2.33	0.40
1:H:8:ARG:NH2	1:H:16:ASN:O	2.50	0.40
1:B:371:PHE:CE2	1:B:458:GLY:HA3	2.56	0.40
1:E:397:GLY:HA3	1:E:398:LEU:HA	1.83	0.40
1:A:398:LEU:HB3	1:A:487:ALA:CB	2.46	0.40
1:A:448:GLU:O	1:A:449:ASN:C	2.59	0.40
1:F:318:TYR:HE2	1:F:320:ALA:O	2.04	0.40
1:G:381:GLN:C	1:G:382:THR:HG1	2.25	0.40
1:F:243:GLY:HA2	1:F:253:PHE:CD1	2.55	0.40
1:F:266:TYR:CE2	1:F:269:LEU:HD12	2.56	0.40
1:A:337:ILE:H	1:A:337:ILE:HD12	1.86	0.40
1:G:266:TYR:HE2	1:G:269:LEU:HD12	1.86	0.40
1:F:190:SER:OG	1:F:191:ALA:N	2.53	0.40
1:E:303:ARG:O	1:E:304:SER:HB2	2.21	0.40
1:A:5:THR:OG1	1:A:6:SER:N	2.53	0.40
1:H:397:GLY:HA3	1:H:398:LEU:HA	1.82	0.40
1:H:228:ASN:HA	1:H:229:PRO:HA	1.80	0.40
1:D:377:VAL:HG12	1:D:379:THR:H	1.85	0.40
1:B:383:ILE:C	1:B:384:SER:OG	2.59	0.40
1:E:319:GLN:HB3	1:E:320:ALA:H	1.74	0.40
1:E:232:PRO:CG	1:F:441:ASN:HB2	2.44	0.40
1:B:236:SER:HB2	1:B:267:TYR:CD1	2.55	0.40
1:D:263:GLY:HA3	1:D:477:THR:H	1.87	0.40
1:H:266:TYR:CE2	1:H:269:LEU:HD12	2.56	0.40
1:D:142:LEU:HD11	1:D:178:TYR:CD1	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:ILE:HG13	1:B:227:ILE:O	2.21	0.40
1:D:397:GLY:HA3	1:D:398:LEU:HA	1.91	0.40
1:H:115:THR:HB	1:H:118:SER:H	1.87	0.40
1:D:236:SER:HB2	1:D:267:TYR:CD1	2.56	0.40
1:C:466:GLU:HG2	1:C:477:THR:HG23	2.04	0.40
1:E:310:ARG:HB3	1:E:331:ALA:HB1	2.03	0.40
1:A:326:LEU:HD11	1:B:198:LEU:HD23	2.03	0.40
1:B:263:GLY:HA3	1:B:477:THR:H	1.87	0.40
1:D:380:THR:HA	1:D:381:GLN:HA	1.30	0.40
1:C:180:SER:HG	1:C:183:LEU:H	1.62	0.40
1:G:318:TYR:HE2	1:G:320:ALA:O	2.05	0.40
1:G:96:PHE:C	1:G:97:PHE:CD1	2.95	0.40
1:B:107:CYS:HB2	1:B:126:SER:HB3	2.04	0.40
1:D:110:ILE:HD13	1:D:154:VAL:CG1	2.51	0.40
1:A:236:SER:HB2	1:A:267:TYR:CD1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	507/512 (99%)	452 (89%)	44 (9%)	11 (2%)	8	46
1	B	507/512 (99%)	448 (88%)	46 (9%)	13 (3%)	7	42
1	C	507/512 (99%)	448 (88%)	47 (9%)	12 (2%)	7	44
1	D	507/512 (99%)	446 (88%)	48 (10%)	13 (3%)	7	42
1	E	507/512 (99%)	446 (88%)	46 (9%)	15 (3%)	5	39
1	F	507/512 (99%)	447 (88%)	45 (9%)	15 (3%)	5	39
1	G	507/512 (99%)	452 (89%)	41 (8%)	14 (3%)	6	41
1	H	507/512 (99%)	448 (88%)	44 (9%)	15 (3%)	5	39

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4056/4096 (99%)	3587 (88%)	361 (9%)	108 (3%)	6 41

All (108) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	423	SER
1	A	424	LYS
1	D	423	SER
1	E	229	PRO
1	E	487	ALA
1	F	229	PRO
1	F	487	ALA
1	G	229	PRO
1	G	428	VAL
1	G	487	ALA
1	H	100	THR
1	H	229	PRO
1	H	401	PRO
1	H	487	ALA
1	A	497	VAL
1	C	423	SER
1	D	497	VAL
1	E	6	SER
1	E	97	PHE
1	E	195	GLU
1	E	230	GLY
1	E	277	PRO
1	E	384	SER
1	E	428	VAL
1	F	6	SER
1	F	97	PHE
1	F	195	GLU
1	F	230	GLY
1	F	428	VAL
1	F	497	VAL
1	G	6	SER
1	G	97	PHE
1	G	195	GLU
1	H	97	PHE
1	H	195	GLU
1	H	428	VAL
1	A	193	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	277	PRO
1	A	384	SER
1	B	193	ALA
1	B	277	PRO
1	B	383	ILE
1	B	384	SER
1	B	486	ASN
1	B	487	ALA
1	C	193	ALA
1	C	277	PRO
1	C	486	ASN
1	C	487	ALA
1	D	193	ALA
1	D	277	PRO
1	D	384	SER
1	D	486	ASN
1	E	214	GLN
1	E	280	GLY
1	F	214	GLN
1	F	277	PRO
1	F	280	GLY
1	F	384	SER
1	G	214	GLN
1	G	277	PRO
1	G	280	GLY
1	G	384	SER
1	H	214	GLN
1	H	277	PRO
1	H	280	GLY
1	H	441	ASN
1	H	486	ASN
1	A	383	ILE
1	B	338	SER
1	B	423	SER
1	B	497	VAL
1	C	383	ILE
1	C	497	VAL
1	D	383	ILE
1	D	487	ALA
1	E	381	GLN
1	E	441	ASN
1	E	497	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	381	GLN
1	F	441	ASN
1	G	381	GLN
1	G	441	ASN
1	G	497	VAL
1	H	384	SER
1	H	497	VAL
1	A	338	SER
1	B	425	VAL
1	C	338	SER
1	C	425	VAL
1	C	485	GLY
1	D	338	SER
1	D	485	GLY
1	A	304	SER
1	B	304	SER
1	B	485	GLY
1	C	304	SER
1	D	304	SER
1	E	304	SER
1	F	304	SER
1	G	304	SER
1	H	304	SER
1	C	280	GLY
1	D	425	VAL
1	A	196	GLY
1	A	280	GLY
1	B	280	GLY
1	D	280	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	450/453 (99%)	416 (92%)	34 (8%)	16 54
1	B	450/453 (99%)	421 (94%)	29 (6%)	22 62

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	450/453 (99%)	416 (92%)	34 (8%)	16 54
1	D	450/453 (99%)	420 (93%)	30 (7%)	20 60
1	E	450/453 (99%)	409 (91%)	41 (9%)	12 44
1	F	450/453 (99%)	411 (91%)	39 (9%)	13 47
1	G	450/453 (99%)	403 (90%)	47 (10%)	9 37
1	H	450/453 (99%)	409 (91%)	41 (9%)	12 44
All	All	3600/3624 (99%)	3305 (92%)	295 (8%)	14 50

All (295) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	105	GLN
1	A	142	LEU
1	A	154	VAL
1	A	183	LEU
1	A	192	PHE
1	A	195	GLU
1	A	212	THR
1	A	213	GLU
1	A	237	PHE
1	A	238	ASN
1	A	259	VAL
1	A	354	LYS
1	A	378	ASN
1	A	381	GLN
1	A	382	THR
1	A	383	ILE
1	A	386	SER
1	A	424	LYS
1	A	426	LYS
1	A	427	PHE
1	A	438	MET
1	A	440	VAL
1	A	447	SER
1	A	448	GLU
1	A	465	LEU
1	A	483	THR
1	A	484	THR
1	A	486	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	488	LEU
1	A	494	THR
1	A	498	ASP
1	A	500	LEU
1	A	508	VAL
1	B	5	THR
1	B	105	GLN
1	B	142	LEU
1	B	154	VAL
1	B	181	ASP
1	B	183	LEU
1	B	192	PHE
1	B	195	GLU
1	B	212	THR
1	B	213	GLU
1	B	237	PHE
1	B	238	ASN
1	B	259	VAL
1	B	352	LEU
1	B	356	ASN
1	B	378	ASN
1	B	379	THR
1	B	381	GLN
1	B	382	THR
1	B	383	ILE
1	B	386	SER
1	B	425	VAL
1	B	438	MET
1	B	440	VAL
1	B	465	LEU
1	B	483	THR
1	B	484	THR
1	B	494	THR
1	B	508	VAL
1	C	5	THR
1	C	105	GLN
1	C	142	LEU
1	C	154	VAL
1	C	180	SER
1	C	181	ASP
1	C	184	LYS
1	C	192	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	195	GLU
1	C	214	GLN
1	C	237	PHE
1	C	238	ASN
1	C	259	VAL
1	C	352	LEU
1	C	356	ASN
1	C	378	ASN
1	C	380	THR
1	C	381	GLN
1	C	382	THR
1	C	386	SER
1	C	425	VAL
1	C	427	PHE
1	C	438	MET
1	C	440	VAL
1	C	446	LYS
1	C	447	SER
1	C	448	GLU
1	C	465	LEU
1	C	483	THR
1	C	484	THR
1	C	494	THR
1	C	497	VAL
1	C	498	ASP
1	C	508	VAL
1	D	5	THR
1	D	105	GLN
1	D	142	LEU
1	D	154	VAL
1	D	180	SER
1	D	181	ASP
1	D	182	ASP
1	D	183	LEU
1	D	192	PHE
1	D	195	GLU
1	D	212	THR
1	D	237	PHE
1	D	238	ASN
1	D	259	VAL
1	D	352	LEU
1	D	356	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	381	GLN
1	D	382	THR
1	D	384	SER
1	D	425	VAL
1	D	438	MET
1	D	440	VAL
1	D	448	GLU
1	D	463	ASN
1	D	465	LEU
1	D	483	THR
1	D	484	THR
1	D	494	THR
1	D	498	ASP
1	D	508	VAL
1	E	5	THR
1	E	22	ASP
1	E	98	ASN
1	E	100	THR
1	E	141	VAL
1	E	142	LEU
1	E	166	THR
1	E	181	ASP
1	E	183	LEU
1	E	190	SER
1	E	194	ASN
1	E	197	PHE
1	E	198	LEU
1	E	200	TYR
1	E	214	GLN
1	E	254	ASP
1	E	278	THR
1	E	323	GLU
1	E	325	GLU
1	E	326	LEU
1	E	352	LEU
1	E	356	ASN
1	E	383	ILE
1	E	384	SER
1	E	385	LYS
1	E	388	PHE
1	E	396	LYS
1	E	398	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	426	LYS
1	E	429	LYS
1	E	430	GLU
1	E	431	ASN
1	E	437	ARG
1	E	447	SER
1	E	465	LEU
1	E	483	THR
1	E	494	THR
1	E	497	VAL
1	E	498	ASP
1	E	500	LEU
1	E	505	LYS
1	F	4	GLU
1	F	5	THR
1	F	8	ARG
1	F	22	ASP
1	F	98	ASN
1	F	99	ASP
1	F	141	VAL
1	F	142	LEU
1	F	166	THR
1	F	181	ASP
1	F	183	LEU
1	F	190	SER
1	F	194	ASN
1	F	197	PHE
1	F	198	LEU
1	F	200	TYR
1	F	214	GLN
1	F	254	ASP
1	F	278	THR
1	F	323	GLU
1	F	325	GLU
1	F	326	LEU
1	F	352	LEU
1	F	356	ASN
1	F	383	ILE
1	F	384	SER
1	F	385	LYS
1	F	396	LYS
1	F	398	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	426	LYS
1	F	429	LYS
1	F	430	GLU
1	F	431	ASN
1	F	437	ARG
1	F	465	LEU
1	F	483	THR
1	F	497	VAL
1	F	498	ASP
1	F	505	LYS
1	G	4	GLU
1	G	5	THR
1	G	22	ASP
1	G	98	ASN
1	G	141	VAL
1	G	142	LEU
1	G	147	THR
1	G	166	THR
1	G	181	ASP
1	G	183	LEU
1	G	190	SER
1	G	194	ASN
1	G	197	PHE
1	G	198	LEU
1	G	200	TYR
1	G	214	GLN
1	G	253	PHE
1	G	278	THR
1	G	323	GLU
1	G	325	GLU
1	G	326	LEU
1	G	344	SER
1	G	348	THR
1	G	352	LEU
1	G	356	ASN
1	G	383	ILE
1	G	384	SER
1	G	386	SER
1	G	398	LEU
1	G	399	GLU
1	G	400	ASP
1	G	424	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	425	VAL
1	G	426	LYS
1	G	427	PHE
1	G	428	VAL
1	G	429	LYS
1	G	430	GLU
1	G	431	ASN
1	G	437	ARG
1	G	447	SER
1	G	465	LEU
1	G	483	THR
1	G	494	THR
1	G	498	ASP
1	G	500	LEU
1	G	505	LYS
1	H	4	GLU
1	H	5	THR
1	H	22	ASP
1	H	94	SER
1	H	97	PHE
1	H	98	ASN
1	H	141	VAL
1	H	142	LEU
1	H	166	THR
1	H	181	ASP
1	H	183	LEU
1	H	190	SER
1	H	194	ASN
1	H	197	PHE
1	H	198	LEU
1	H	200	TYR
1	H	214	GLN
1	H	254	ASP
1	H	278	THR
1	H	323	GLU
1	H	325	GLU
1	H	326	LEU
1	H	345	ARG
1	H	352	LEU
1	H	356	ASN
1	H	383	ILE
1	H	384	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	396	LYS
1	H	398	LEU
1	H	426	LYS
1	H	430	GLU
1	H	464	ILE
1	H	465	LEU
1	H	482	MET
1	H	483	THR
1	H	494	THR
1	H	495	THR
1	H	497	VAL
1	H	498	ASP
1	H	500	LEU
1	H	505	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	36	HIS
1	A	40	GLN
1	A	105	GLN
1	A	171	GLN
1	A	194	ASN
1	A	201	GLN
1	A	238	ASN
1	A	249	HIS
1	A	270	GLN
1	A	319	GLN
1	A	378	ASN
1	A	422	ASN
1	A	431	ASN
1	A	449	ASN
1	A	486	ASN
1	B	24	ASN
1	B	36	HIS
1	B	40	GLN
1	B	105	GLN
1	B	171	GLN
1	B	238	ASN
1	B	249	HIS
1	B	270	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	319	GLN
1	B	378	ASN
1	B	431	ASN
1	B	449	ASN
1	C	24	ASN
1	C	36	HIS
1	C	40	GLN
1	C	105	GLN
1	C	171	GLN
1	C	194	ASN
1	C	214	GLN
1	C	238	ASN
1	C	249	HIS
1	C	270	GLN
1	C	319	GLN
1	C	359	ASN
1	C	378	ASN
1	C	431	ASN
1	C	462	GLN
1	D	24	ASN
1	D	36	HIS
1	D	40	GLN
1	D	171	GLN
1	D	194	ASN
1	D	238	ASN
1	D	249	HIS
1	D	270	GLN
1	D	319	GLN
1	D	431	ASN
1	E	36	HIS
1	E	98	ASN
1	E	121	GLN
1	E	148	GLN
1	E	171	GLN
1	E	194	ASN
1	E	228	ASN
1	E	249	HIS
1	E	270	GLN
1	E	349	ASN
1	E	356	ASN
1	E	431	ASN
1	E	507	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	36	HIS
1	F	98	ASN
1	F	121	GLN
1	F	148	GLN
1	F	171	GLN
1	F	194	ASN
1	F	249	HIS
1	F	270	GLN
1	F	356	ASN
1	F	431	ASN
1	F	507	GLN
1	G	36	HIS
1	G	92	ASN
1	G	98	ASN
1	G	121	GLN
1	G	148	GLN
1	G	171	GLN
1	G	194	ASN
1	G	249	HIS
1	G	270	GLN
1	G	431	ASN
1	G	507	GLN
1	H	36	HIS
1	H	92	ASN
1	H	98	ASN
1	H	121	GLN
1	H	148	GLN
1	H	171	GLN
1	H	194	ASN
1	H	228	ASN
1	H	249	HIS
1	H	270	GLN
1	H	349	ASN
1	H	381	GLN
1	H	507	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	509/512 (99%)	0.01	3 (0%) 90 86	29, 37, 51, 70	0
1	B	509/512 (99%)	-0.04	2 (0%) 93 91	29, 38, 49, 72	0
1	C	509/512 (99%)	0.16	11 (2%) 65 60	38, 50, 66, 79	0
1	D	509/512 (99%)	0.16	16 (3%) 52 48	37, 51, 68, 78	0
1	E	509/512 (99%)	0.20	18 (3%) 48 42	33, 47, 71, 114	0
1	F	509/512 (99%)	0.25	19 (3%) 45 40	31, 48, 75, 132	0
1	G	509/512 (99%)	0.60	47 (9%) 11 11	39, 59, 89, 130	0
1	H	509/512 (99%)	0.57	52 (10%) 9 9	40, 62, 93, 140	0
All	All	4072/4096 (99%)	0.24	168 (4%) 41 36	29, 48, 81, 140	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	146	SER	5.7
1	F	324	THR	5.5
1	H	145	ASN	4.8
1	H	162	LYS	4.4
1	H	107	CYS	4.4
1	H	98	ASN	4.2
1	H	146	SER	4.2
1	H	216	PRO	4.0
1	G	162	LYS	3.9
1	G	99	ASP	3.9
1	H	325	GLU	3.9
1	F	146	SER	3.9
1	E	321	ASN	3.7
1	G	88	VAL	3.7
1	H	321	ASN	3.7
1	H	486	ASN	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	145	ASN	3.7
1	G	324	THR	3.6
1	G	35	TRP	3.5
1	H	156	TRP	3.5
1	H	163	TRP	3.5
1	H	182	ASP	3.4
1	F	486	ASN	3.4
1	H	89	ASP	3.4
1	F	319	GLN	3.4
1	G	216	PRO	3.4
1	F	99	ASP	3.3
1	D	103	PRO	3.3
1	D	97	PHE	3.3
1	E	319	GLN	3.3
1	H	101	ILE	3.3
1	G	145	ASN	3.2
1	G	147	THR	3.2
1	F	320	ALA	3.2
1	G	36	HIS	3.2
1	H	214	GLN	3.2
1	A	88	VAL	3.1
1	F	378	ASN	3.1
1	H	324	THR	3.1
1	E	146	SER	3.1
1	F	382	THR	3.1
1	H	130	GLY	3.1
1	F	321	ASN	3.1
1	G	319	GLN	3.0
1	G	90	TYR	3.0
1	G	100	THR	3.0
1	F	214	GLN	3.0
1	G	110	ILE	3.0
1	G	142	LEU	2.9
1	H	91	ASN	2.9
1	H	93	THR	2.9
1	F	162	LYS	2.9
1	H	147	THR	2.9
1	G	158	GLU	2.9
1	G	102	ASP	2.9
1	H	322	PRO	2.9
1	G	320	ALA	2.9
1	G	182	ASP	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	148	GLN	2.8
1	C	97	PHE	2.8
1	H	179	SER	2.8
1	F	380	THR	2.7
1	G	104	ARG	2.7
1	F	182	ASP	2.7
1	E	115	THR	2.7
1	H	97	PHE	2.7
1	G	89	ASP	2.7
1	G	109	ALA	2.7
1	H	340	ALA	2.7
1	G	486	ASN	2.7
1	G	327	ILE	2.6
1	D	136	TYR	2.6
1	C	486	ASN	2.6
1	G	325	GLU	2.6
1	C	156	TRP	2.6
1	E	88	VAL	2.6
1	H	278	THR	2.6
1	C	91	ASN	2.6
1	H	385	LYS	2.6
1	E	90	TYR	2.6
1	H	90	TYR	2.6
1	H	180	SER	2.6
1	H	134	THR	2.6
1	H	382	THR	2.6
1	E	397	GLY	2.6
1	H	381	GLN	2.5
1	G	183	LEU	2.5
1	D	160	SER	2.5
1	G	339	ASN	2.5
1	H	181	ASP	2.5
1	C	448	GLU	2.5
1	G	214	GLN	2.5
1	G	322	PRO	2.5
1	H	317	GLU	2.5
1	H	92	ASN	2.5
1	H	144	ALA	2.5
1	E	324	THR	2.4
1	G	126	SER	2.4
1	H	320	ALA	2.4
1	F	323	GLU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	186	TRP	2.4
1	H	88	VAL	2.4
1	E	100	THR	2.4
1	H	380	THR	2.4
1	H	245	PHE	2.4
1	D	277	PRO	2.4
1	G	79	SER	2.4
1	D	181	ASP	2.4
1	H	106	ARG	2.3
1	G	321	ASN	2.3
1	H	158	GLU	2.3
1	D	141	VAL	2.3
1	D	486	ASN	2.3
1	C	128	ASP	2.3
1	D	248	THR	2.3
1	F	94	SER	2.3
1	H	185	SER	2.3
1	D	88	VAL	2.3
1	H	100	THR	2.3
1	C	99	ASP	2.3
1	C	191	ALA	2.2
1	E	144	ALA	2.2
1	D	107	CYS	2.2
1	G	316	THR	2.2
1	A	97	PHE	2.2
1	G	132	THR	2.2
1	E	91	ASN	2.2
1	G	139	ASN	2.2
1	E	147	THR	2.2
1	G	103	PRO	2.2
1	G	282	ALA	2.2
1	G	215	ASP	2.2
1	G	136	TYR	2.2
1	F	397	GLY	2.2
1	D	108	VAL	2.2
1	B	340	ALA	2.2
1	H	219	SER	2.2
1	B	4	GLU	2.1
1	H	218	LYS	2.1
1	G	107	CYS	2.1
1	D	38	TYR	2.1
1	D	91	ASN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	317	GLU	2.1
1	H	108	VAL	2.1
1	C	90	TYR	2.1
1	E	125	TYR	2.1
1	A	349	ASN	2.1
1	C	98	ASN	2.1
1	G	143	ALA	2.1
1	F	161	GLN	2.1
1	H	485	GLY	2.1
1	C	107	CYS	2.1
1	G	54	TRP	2.1
1	E	149	PHE	2.1
1	E	449	ASN	2.1
1	F	145	ASN	2.1
1	H	105	GLN	2.1
1	G	125	TYR	2.1
1	H	160	SER	2.1
1	H	186	TRP	2.1
1	H	215	ASP	2.1
1	D	187	LYS	2.1
1	G	508	VAL	2.1
1	F	172	ASP	2.0
1	H	133	PHE	2.0
1	E	380	THR	2.0
1	D	138	LYS	2.0
1	E	108	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.