Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:25 PM GMT

PDB ID	:	3ZEF
Title	:	Crystal structure of Prp8:Aar2 complex: second crystal form at 3.1 A resolution
Authors	:	Galej, W.P.; Oubridge, C.; Newman, A.J.; Nagai, K.
Deposited on	:	2012-12-05
Resolution	:	3.10 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:

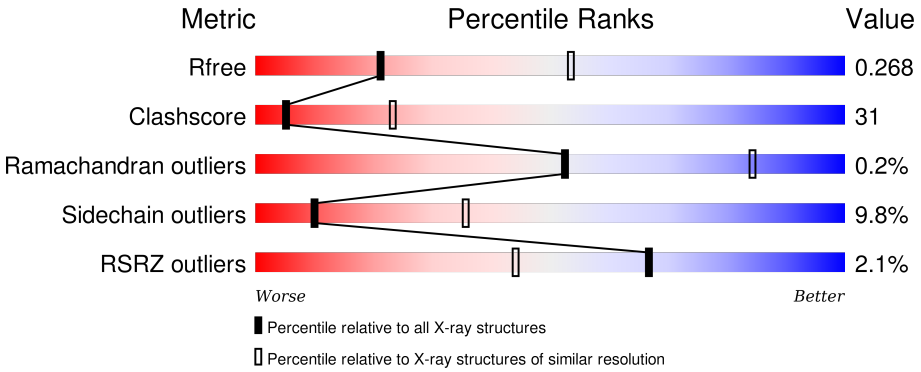
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	355	75% 15% • 8%
1	D	355	67% 18% • 11%
2	B	1531	3% 52% 33% 6% 9%
2	E	1531	2% 58% 29% 5% 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 28285 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 A1 CISTRON-SPLICING FACTOR AAR2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2684	1722	438	508	16			
1	D	317	Total	C	N	O	S	0	0	0
			2618	1682	426	493	17			

- Molecule 2 is a protein called PRE-MRNA-SPLICING FACTOR 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1398	Total	C	N	O	S	0	0	0
			11401	7329	1926	2109	37			
2	E	1420	Total	C	N	O	S	0	0	0
			11582	7445	1958	2142	37			

There are 8 discrepancies between the modelled and reference sequences:

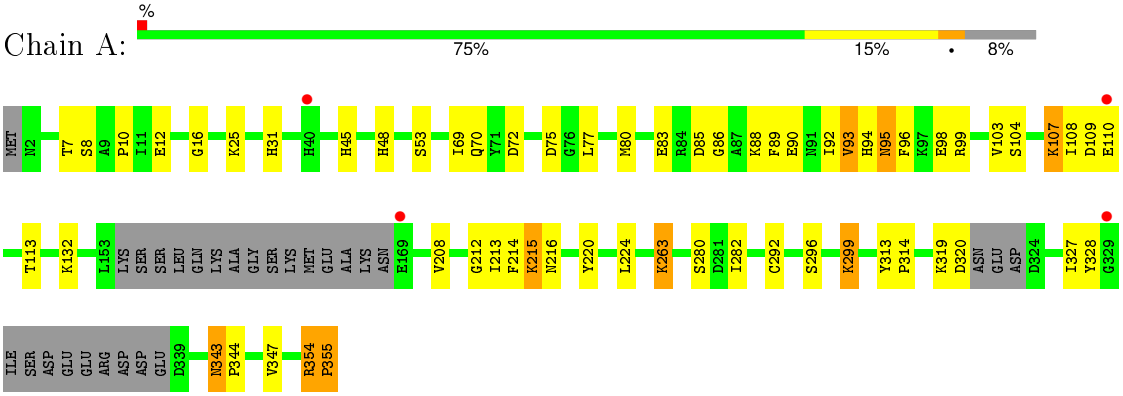
Chain	Residue	Modelled	Actual	Comment	Reference
B	883	SER	-	EXPRESSION TAG	UNP P33334
B	884	GLY	-	EXPRESSION TAG	UNP P33334
B	1961	ASN	LEU	ENGINEERED MUTATION	UNP P33334
B	1999	LEU	ILE	ENGINEERED MUTATION	UNP P33334
E	883	SER	-	EXPRESSION TAG	UNP P33334
E	884	GLY	-	EXPRESSION TAG	UNP P33334
E	1961	ASN	LEU	ENGINEERED MUTATION	UNP P33334
E	1999	LEU	ILE	ENGINEERED MUTATION	UNP P33334

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.

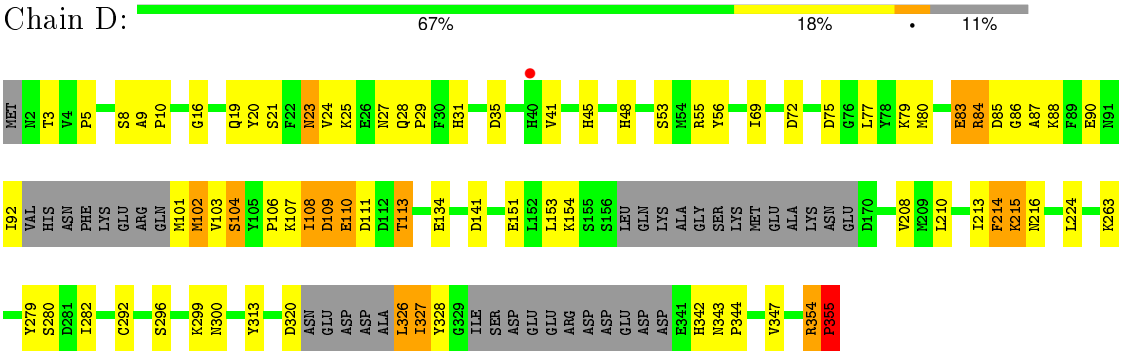
- Molecule 1: A1 CISTRON-SPLICING FACTOR AAR2

Chain A:



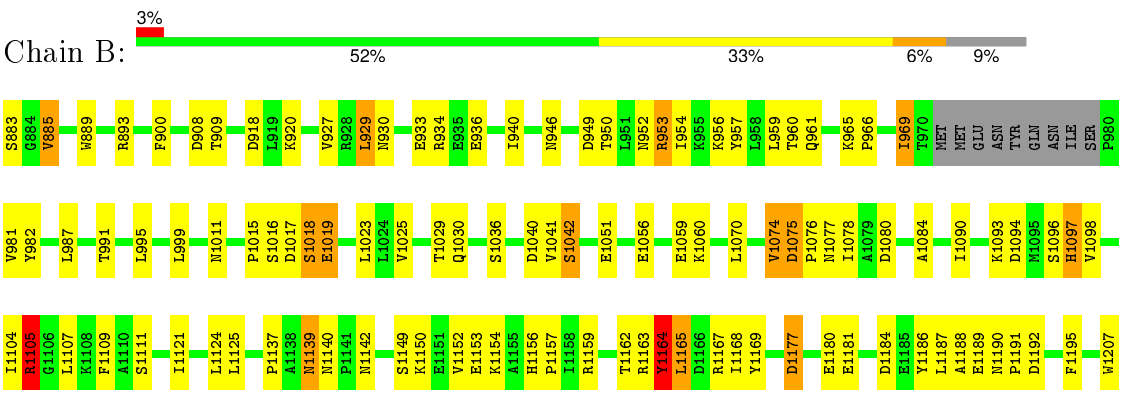
- Molecule 1: A1 CISTRON-SPLICING FACTOR AAR2

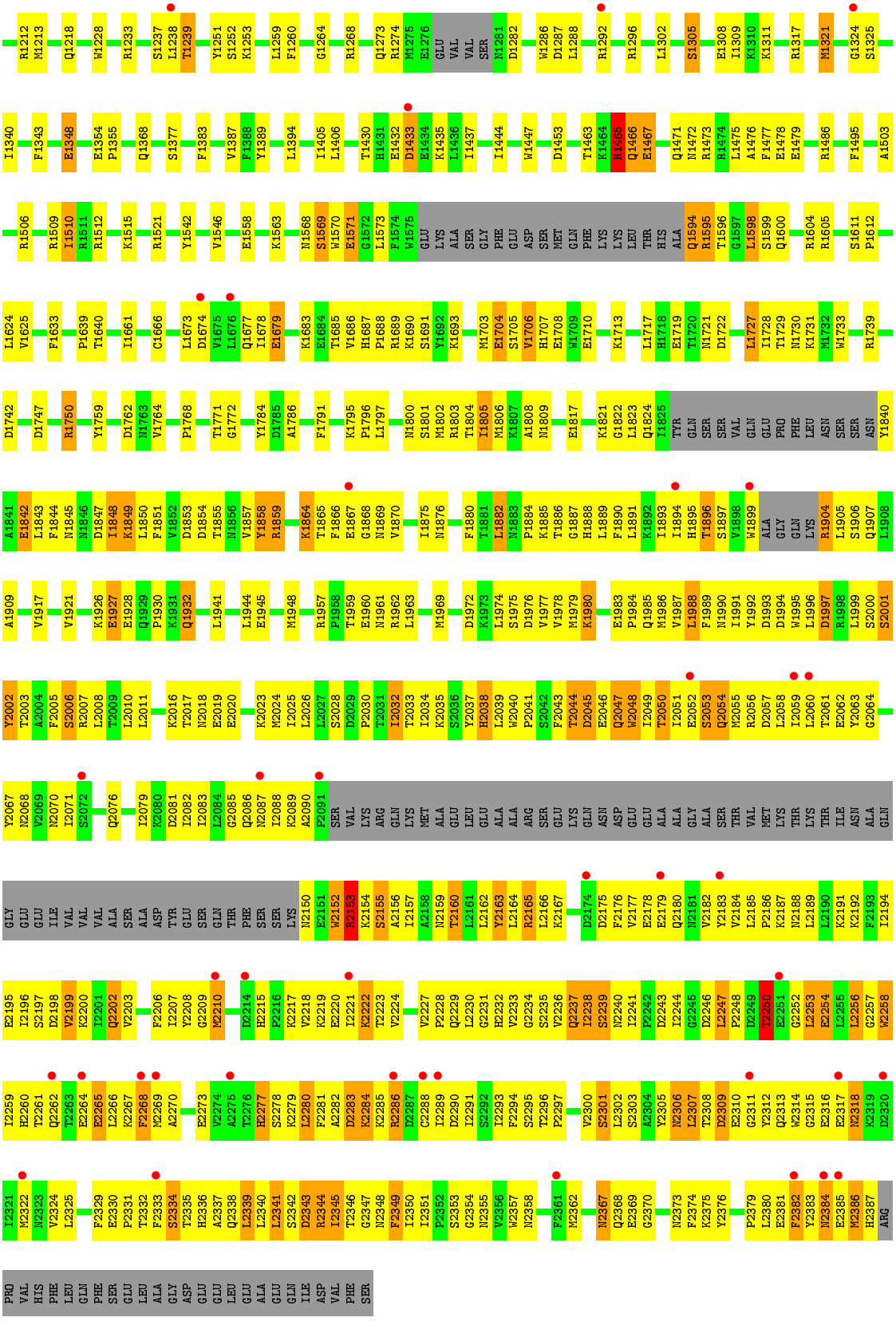
Chain D:



- Molecule 2: PRE-MRNA-SPLICING FACTOR 8

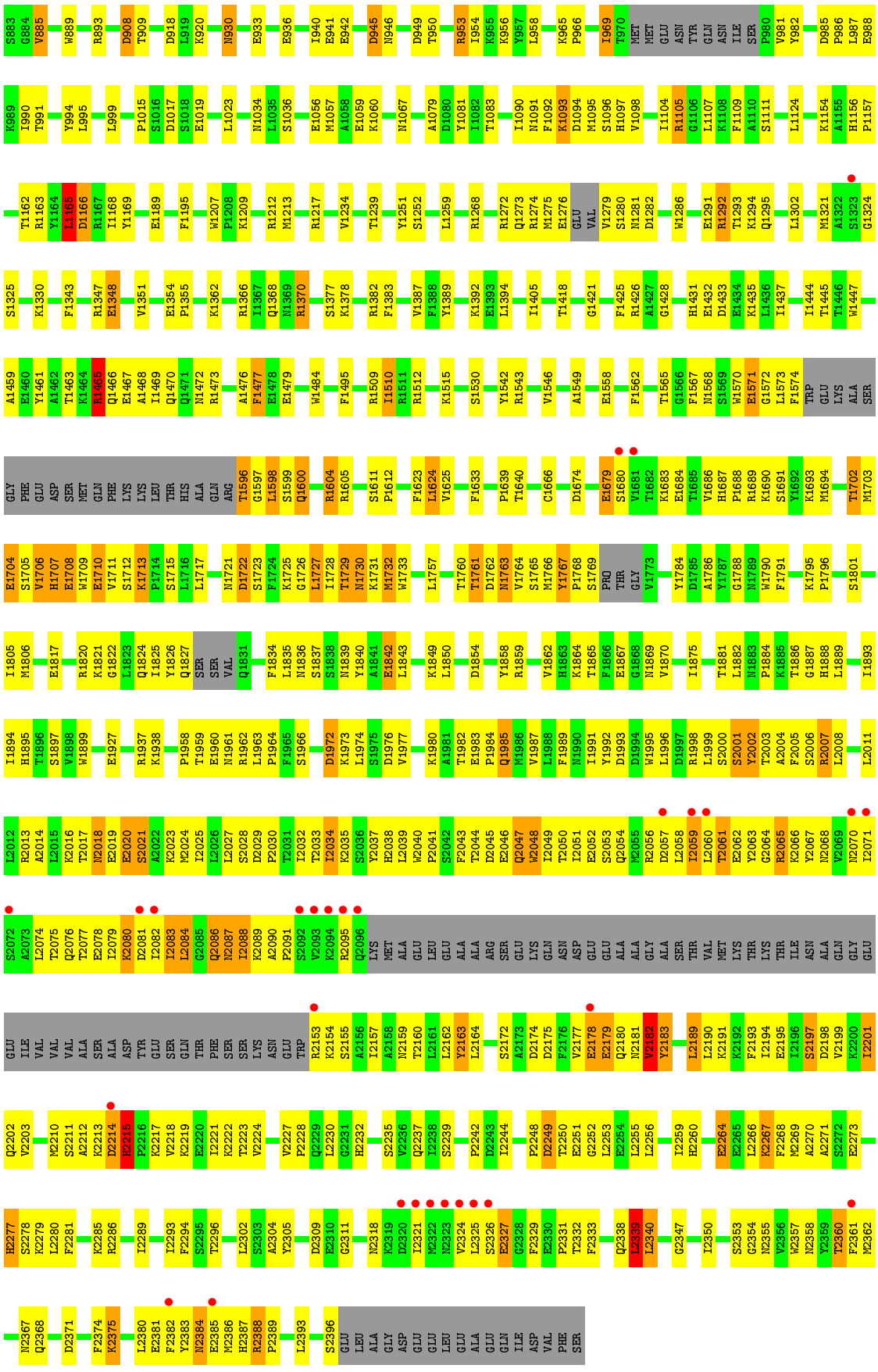
Chain B:





• Molecule 2: PRE-MRNA-SPLICING FACTOR 8

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	125.42Å 177.84Å 216.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	137.45 – 3.10 92.50 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (137.45-3.10) 99.8 (92.50-3.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0016	Depositor
R, R_{free}	0.220 , 0.267 0.221 , 0.268	Depositor DCC
R_{free} test set	4434 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	79.1	Xtriage
Anisotropy	0.449	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 67.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	2 of 97339 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	28285	wwPDB-VP
Average B, all atoms (Å^2)	96.0	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 20.50 % 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 8.5812e-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	0.55	0/2754	0.72	2/3725 (0.1%)
1	D	0.56	0/2685	0.75	4/3626 (0.1%)
2	B	0.59	1/11671 (0.0%)	0.79	5/15827 (0.0%)
2	E	0.58	3/11856 (0.0%)	0.77	8/16074 (0.0%)
All	All	0.58	4/28966 (0.0%)	0.77	19/39252 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	D	0	1
2	B	0	6
2	E	0	5
All	All	0	14

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1708	GLU	CD-OE1	8.75	1.35	1.25
2	E	1571	GLU	CD-OE1	7.11	1.33	1.25
2	B	1164	TYR	CE2-CZ	-6.19	1.30	1.38
2	E	1708	GLU	CD-OE2	6.10	1.32	1.25

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2339	LEU	CA-CB-CG	7.05	131.52	115.30
2	E	1105	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	D	355	PRO	CA-N-CD	-6.36	102.59	111.50
1	A	354	ARG	C-N-CD	6.34	141.71	128.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1465	ARG	NE-CZ-NH1	6.09	123.35	120.30
2	E	1963	LEU	CA-CB-CG	-6.00	101.50	115.30
1	D	354	ARG	C-N-CD	5.73	140.43	128.40
2	E	1165	LEU	CA-CB-CG	5.71	128.43	115.30
2	E	1604	ARG	NE-CZ-NH1	5.60	123.10	120.30
2	B	1988	LEU	CA-CB-CG	5.45	127.83	115.30
1	A	355	PRO	CA-N-CD	-5.42	103.91	111.50
2	E	1105	ARG	NE-CZ-NH2	-5.39	117.60	120.30
2	B	1105	ARG	NE-CZ-NH1	5.38	122.99	120.30
2	B	1075	ASP	C-N-CD	5.32	139.56	128.40
2	B	1465	ARG	NE-CZ-NH1	5.28	122.94	120.30
2	B	927	VAL	CB-CA-C	-5.25	101.43	111.40
1	D	41	VAL	N-CA-C	-5.23	96.88	111.00
2	E	2182	VAL	CB-CA-C	-5.23	101.47	111.40
1	D	214	PHE	N-CA-C	-5.16	97.06	111.00

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	LYS	Peptide
1	A	93	VAL	Peptide
2	B	1164	TYR	Peptide
2	B	1433	ASP	Peptide
2	B	1704	GLU	Peptide
2	B	2152	TRP	Peptide
2	B	2153	ARG	Peptide
2	B	2250	THR	Peptide
1	D	110	GLU	Peptide
2	E	1092	PHE	Peptide
2	E	1572	GLY	Peptide
2	E	1706	VAL	Peptide
2	E	2083	ILE	Peptide
2	E	2215	HIS	Peptide

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	2684	0	2530	54	0
1	D	2618	0	2494	81	0
2	B	11401	0	11345	879	1
2	E	11582	0	11528	721	1
All	All	28285	0	27897	1719	1

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 31.

All (1719) 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)
2:B:2043:PHE:CE2	2:B:2051:ILE:HD11	1.31	1.63
2:B:2259:ILE:HD13	2:B:2291:ILE:CB	1.30	1.60
2:B:2183:TYR:CE1	2:B:2219:LYS:HD3	1.45	1.49
2:B:2183:TYR:HE1	2:B:2219:LYS:CD	1.26	1.47
2:B:2236:VAL:HG22	2:B:2238:ILE:CD1	1.44	1.47
2:E:2210:MET:HE1	2:E:2253:LEU:N	1.11	1.43
2:E:2210:MET:HE1	2:E:2252:GLY:C	1.06	1.41
2:B:2259:ILE:CD1	2:B:2291:ILE:HB	1.48	1.40
2:E:2034:ILE:HD12	2:E:2041:PRO:N	1.12	1.40
2:E:2210:MET:CE	2:E:2252:GLY:C	1.89	1.39
2:E:2034:ILE:CD1	2:E:2041:PRO:CA	1.99	1.39
2:E:2080:LYS:HD2	2:E:2083:ILE:CG1	1.49	1.38
2:B:2308:THR:HG23	2:B:2333:PHE:O	1.23	1.36
2:E:2304:ALA:HB2	2:E:2339:LEU:CD2	1.55	1.35
2:E:2011:LEU:HD13	2:E:2040:TRP:CZ3	1.59	1.34
2:E:1995:TRP:CZ3	2:E:2007:ARG:HG2	1.63	1.33
2:B:2044:THR:HG23	2:B:2047:GLN:NE2	1.40	1.33
2:E:2041:PRO:HB2	2:E:2043:PHE:CE1	1.61	1.32
2:B:2182:VAL:HG12	2:B:2338:GLN:CB	1.59	1.32
2:E:1998:ARG:CZ	2:E:2045:ASP:OD2	1.75	1.31
2:B:1125:LEU:O	2:B:1233:ARG:NH1	1.62	1.31
2:E:2018:ASN:ND2	2:E:2058:LEU:HD11	1.41	1.30
2:B:2210:MET:CE	2:B:2253:LEU:HA	1.61	1.29
2:B:2259:ILE:CD1	2:B:2291:ILE:CB	2.04	1.28
2:E:2046:GLU:O	2:E:2049:ILE:HG22	1.24	1.28
2:E:2210:MET:SD	2:E:2252:GLY:O	1.92	1.27
2:E:1392:LYS:NZ	2:E:1599:SER:O	1.67	1.27
2:E:2178:GLU:O	2:E:2217:LYS:NZ	1.68	1.26
2:B:900:PHE:HB2	2:B:1075:ASP:OD2	1.09	1.26
2:E:1472:ASN:O	2:E:2325:LEU:HB2	1.11	1.25

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1865:THR:HB	2:E:1867:GLU:OE1	1.20	1.25
2:E:2034:ILE:CD1	2:E:2041:PRO:N	1.98	1.25
2:B:2259:ILE:CD1	2:B:2291:ILE:CG2	2.15	1.24
2:E:2011:LEU:CD1	2:E:2040:TRP:CZ3	2.20	1.24
2:E:2043:PHE:CD2	2:E:2051:ILE:HG13	1.71	1.23
2:B:2043:PHE:CE2	2:B:2051:ILE:CD1	2.20	1.23
2:E:2034:ILE:HD11	2:E:2041:PRO:CG	1.68	1.23
2:E:2047:GLN:O	2:E:2050:THR:N	1.70	1.23
2:E:2080:LYS:CD	2:E:2083:ILE:CD1	2.17	1.23
2:B:2259:ILE:HD13	2:B:2291:ILE:CG2	1.68	1.22
2:B:2259:ILE:HD12	2:B:2291:ILE:O	1.39	1.22
2:B:2281:PHE:O	2:B:2286:ARG:HA	1.39	1.22
2:B:2236:VAL:CG2	2:B:2238:ILE:CD1	2.16	1.22
2:E:2018:ASN:HD21	2:E:2058:LEU:CD1	1.51	1.22
2:B:1604:ARG:NH2	2:B:1822:GLY:O	1.72	1.22
2:E:2210:MET:CE	2:E:2253:LEU:N	1.99	1.21
2:B:900:PHE:CB	2:B:1075:ASP:OD2	1.87	1.21
2:B:1993:ASP:OD2	2:B:2038:HIS:HB3	1.39	1.21
2:E:2080:LYS:CD	2:E:2083:ILE:HD11	1.69	1.21
2:E:2043:PHE:CE2	2:E:2051:ILE:HG13	1.74	1.20
2:E:2046:GLU:O	2:E:2049:ILE:CG2	1.90	1.20
2:E:2034:ILE:HD11	2:E:2041:PRO:HG3	1.19	1.19
2:E:2034:ILE:HG23	2:E:2040:TRP:O	1.04	1.18
2:B:1729:THR:HG21	2:B:1771:THR:CG2	1.74	1.18
1:D:86:GLY:O	1:D:90:GLU:HB2	1.43	1.18
2:B:2182:VAL:CG1	2:B:2338:GLN:HB3	1.74	1.18
2:E:2024:MET:CE	2:E:2157:ILE:CG2	2.21	1.18
1:D:19:GLN:NE2	1:D:110:GLU:HG2	1.58	1.17
2:B:2358:ASN:HB3	2:B:2387:HIS:ND1	1.57	1.17
2:E:2034:ILE:HD12	2:E:2040:TRP:C	1.64	1.16
2:E:2034:ILE:HG23	2:E:2040:TRP:C	1.62	1.16
2:B:1993:ASP:CG	2:B:2038:HIS:HB3	1.64	1.16
2:B:2259:ILE:HD11	2:B:2291:ILE:HG22	1.25	1.16
2:B:2281:PHE:O	2:B:2286:ARG:CA	1.93	1.16
2:B:2339:LEU:HD12	2:B:2340:LEU:N	1.57	1.16
2:B:1729:THR:CG2	2:B:1771:THR:HG21	1.75	1.15
2:B:2357:TRP:HH2	2:B:2382:PHE:CE1	1.63	1.15
2:B:2358:ASN:HB3	2:B:2387:HIS:CE1	1.82	1.14
2:B:2052:GLU:O	2:B:2056:ARG:HG3	1.48	1.14
2:E:2034:ILE:HD12	2:E:2041:PRO:CA	1.67	1.14
2:B:2034:ILE:CG1	2:B:2041:PRO:HA	1.75	1.14

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2037:TYR:CD1	2:E:2038:HIS:CD2	2.36	1.13
2:B:2224:VAL:CG1	2:B:2349:PHE:CZ	2.32	1.13
2:B:2210:MET:HG3	2:B:2222:LYS:HD2	1.15	1.13
2:E:1731:LYS:CE	2:E:1768:PRO:HB2	1.77	1.12
2:B:1729:THR:HG21	2:B:1771:THR:HG21	1.19	1.12
2:E:2034:ILE:HD13	2:E:2041:PRO:HA	1.13	1.12
2:E:1472:ASN:O	2:E:2325:LEU:CB	1.96	1.12
2:E:1998:ARG:NE	2:E:2045:ASP:OD2	1.84	1.11
2:E:2018:ASN:HD22	2:E:2058:LEU:HD21	1.10	1.11
2:B:2182:VAL:HG13	2:B:2338:GLN:OE1	1.49	1.10
2:E:2034:ILE:CG2	2:E:2040:TRP:O	1.98	1.10
2:E:1763:ASN:C	2:E:1766:MET:CE	2.20	1.10
2:B:2208:TYR:HB3	2:B:2253:LEU:CD2	1.82	1.10
2:E:1865:THR:CB	2:E:1867:GLU:OE1	1.98	1.10
2:B:2236:VAL:HG22	2:B:2238:ILE:HD13	1.26	1.09
2:E:2080:LYS:HD3	2:E:2083:ILE:HD11	1.10	1.09
2:B:2191:LYS:O	2:B:2195:GLU:HG3	1.51	1.09
2:E:1998:ARG:NH1	2:E:2045:ASP:OD2	1.86	1.08
2:E:2048:TRP:O	2:E:2052:GLU:HB3	1.51	1.08
2:E:2385:GLU:O	2:E:2388:ARG:HB2	1.53	1.08
2:B:2224:VAL:O	2:B:2349:PHE:CD1	2.06	1.08
2:B:2358:ASN:N	2:B:2387:HIS:HE1	1.51	1.08
2:E:2037:TYR:HD1	2:E:2038:HIS:CD2	1.71	1.08
2:B:2339:LEU:O	2:B:2340:LEU:HD12	1.51	1.08
2:B:2357:TRP:CH2	2:B:2382:PHE:CE1	2.42	1.08
2:E:1763:ASN:C	2:E:1766:MET:HE2	1.73	1.07
2:B:2314:TRP:O	2:B:2318:ASN:ND2	1.87	1.07
2:E:2080:LYS:CD	2:E:2083:ILE:CG1	2.33	1.06
2:B:2183:TYR:CE1	2:B:2219:LYS:CD	2.15	1.06
2:E:2080:LYS:CD	2:E:2083:ILE:HG13	1.84	1.06
2:B:2208:TYR:HB3	2:B:2253:LEU:HD21	1.34	1.06
2:B:2159:ASN:OD1	2:B:2199:VAL:HG13	1.56	1.06
2:E:2018:ASN:ND2	2:E:2058:LEU:CD1	2.11	1.05
2:B:2210:MET:CE	2:B:2253:LEU:CA	2.34	1.05
2:B:2150:ASN:HA	2:B:2152:TRP:CZ3	1.90	1.05
2:E:1604:ARG:NH2	2:E:1822:GLY:O	1.90	1.05
2:B:2157:ILE:O	2:B:2160:THR:OG1	1.75	1.05
2:E:2064:GLY:O	2:E:2067:TYR:N	1.89	1.05
2:E:1291:GLU:O	2:E:1294:LYS:HE3	1.55	1.05
2:B:2043:PHE:CZ	2:B:2051:ILE:HD11	1.92	1.04
2:B:2307:LEU:HD12	2:B:2308:THR:N	1.72	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2039:LEU:HB2	2:E:2040:TRP:NE1	1.71	1.04
2:B:2281:PHE:O	2:B:2286:ARG:N	1.90	1.04
2:B:2358:ASN:H	2:B:2387:HIS:CE1	1.74	1.04
2:B:2358:ASN:CB	2:B:2387:HIS:CE1	2.41	1.04
2:E:2255:LEU:O	2:E:2285:LYS:NZ	1.91	1.04
2:B:2034:ILE:HG12	2:B:2041:PRO:HA	1.36	1.04
2:B:2210:MET:HE3	2:B:2253:LEU:CA	1.87	1.03
2:B:2210:MET:SD	2:B:2222:LYS:HD3	1.99	1.03
2:E:1597:GLY:HA2	2:E:1598:LEU:HB3	1.37	1.03
2:E:2039:LEU:HB2	2:E:2040:TRP:CD1	1.94	1.02
2:B:1859:ARG:HD2	2:B:1876:ASN:O	1.59	1.02
2:B:2268:PHE:HD2	2:B:2331:PRO:HB3	1.23	1.02
2:E:2034:ILE:CD1	2:E:2041:PRO:HA	1.71	1.02
2:E:2024:MET:HE3	2:E:2157:ILE:CG2	1.86	1.02
2:E:1465:ARG:HG2	2:E:1465:ARG:HH11	1.24	1.02
2:E:1727:LEU:C	2:E:1728:ILE:HD13	1.81	1.01
2:E:2048:TRP:O	2:E:2052:GLU:CB	2.08	1.01
2:B:1885:LYS:O	2:B:2001:SER:OG	1.76	1.01
2:B:2224:VAL:HB	2:B:2349:PHE:CZ	1.96	1.00
2:E:1731:LYS:HE2	2:E:1768:PRO:HB2	1.02	1.00
2:E:2024:MET:HE1	2:E:2157:ILE:HG22	1.44	1.00
1:D:109:ASP:OD1	1:D:111:ASP:N	1.94	1.00
2:E:2230:LEU:HD12	2:E:2360:THR:HA	1.42	0.99
2:E:1995:TRP:CZ3	2:E:2007:ARG:CG	2.45	0.99
2:E:1995:TRP:CH2	2:E:2007:ARG:HG2	1.96	0.99
2:B:2350:ILE:HD13	2:B:2376:TYR:HA	1.44	0.99
2:E:2304:ALA:HB2	2:E:2339:LEU:HD23	1.44	0.99
2:E:1705:SER:OG	2:E:1730:ASN:O	1.80	0.99
2:E:2353:SER:O	2:E:2375:LYS:NZ	1.95	0.99
2:E:2041:PRO:CB	2:E:2043:PHE:CE1	2.44	0.99
2:B:2030:PRO:O	2:B:2033:THR:OG1	1.79	0.99
2:B:2037:TYR:HB2	2:B:2038:HIS:CD2	1.96	0.99
2:B:2381:GLU:OE1	2:B:2381:GLU:N	1.95	0.99
2:E:2304:ALA:HB2	2:E:2339:LEU:HD22	1.42	0.99
2:B:2024:MET:O	2:B:2028:SER:HB2	1.63	0.99
2:B:2210:MET:CG	2:B:2222:LYS:HD2	1.93	0.98
2:B:2182:VAL:HA	2:B:2338:GLN:HB2	1.43	0.98
2:B:2224:VAL:HG12	2:B:2349:PHE:CE1	1.97	0.98
2:E:2018:ASN:HD21	2:E:2058:LEU:CG	1.76	0.98
2:E:2304:ALA:CB	2:E:2339:LEU:CD2	2.41	0.98
2:B:2224:VAL:HB	2:B:2349:PHE:CE1	1.99	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2294:PHE:HD2	2:B:2301:SER:OG	1.45	0.98
2:E:2034:ILE:CG2	2:E:2040:TRP:C	2.32	0.98
2:B:1011:ASN:ND2	2:B:1142:ASN:O	1.97	0.98
2:E:2024:MET:HE1	2:E:2157:ILE:CG2	1.90	0.97
2:E:2213:LYS:HA	2:E:2215:HIS:H	1.30	0.97
2:B:2236:VAL:CG2	2:B:2238:ILE:HD11	1.94	0.97
2:B:2358:ASN:H	2:B:2387:HIS:HE1	0.98	0.97
2:E:1207:TRP:O	2:E:1212:ARG:NH1	1.96	0.97
2:E:2080:LYS:HD2	2:E:2083:ILE:CD1	1.86	0.97
2:E:1834:PHE:CE2	2:E:1960:GLU:OE2	2.17	0.97
2:B:2236:VAL:HG22	2:B:2238:ILE:HD11	1.41	0.97
2:E:1067:ASN:HD22	2:E:1083:THR:HG21	1.27	0.97
2:E:2024:MET:HE3	2:E:2157:ILE:HG23	1.47	0.96
1:D:327:ILE:HB	1:D:328:TYR:HD1	1.27	0.96
2:B:2259:ILE:CD1	2:B:2291:ILE:HG22	1.84	0.96
2:E:2154:LYS:O	2:E:2157:ILE:N	1.98	0.96
2:E:1324:GLY:HA2	2:E:1325:SER:OG	1.62	0.96
2:B:2224:VAL:CB	2:B:2349:PHE:CE1	2.49	0.96
2:E:2034:ILE:CD1	2:E:2041:PRO:CG	2.44	0.96
2:E:1966:SER:OG	2:E:2016:LYS:HE3	1.66	0.95
2:B:1568:ASN:OD1	2:B:1569:SER:OG	1.84	0.95
2:E:1702:THR:CG2	2:E:1768:PRO:HG3	1.97	0.95
2:E:1762:ASP:OD1	2:E:1763:ASN:ND2	1.99	0.95
2:B:1887:GLY:HA3	2:B:1992:TYR:CD2	2.01	0.95
2:B:2224:VAL:CB	2:B:2349:PHE:CZ	2.50	0.95
2:B:2210:MET:HG3	2:B:2222:LYS:CD	1.96	0.95
2:E:2278:SER:O	2:E:2281:PHE:N	1.98	0.95
2:B:1707:HIS:CD2	2:B:1708:GLU:HB2	2.01	0.95
2:B:2034:ILE:HG12	2:B:2041:PRO:CA	1.97	0.95
2:B:2230:LEU:O	2:B:2236:VAL:HG23	1.66	0.95
2:E:2018:ASN:ND2	2:E:2058:LEU:CG	2.29	0.95
2:B:2043:PHE:HE2	2:B:2051:ILE:HD11	1.24	0.94
2:B:2357:TRP:CH2	2:B:2382:PHE:CD1	2.55	0.94
1:D:151:GLU:OE2	1:D:154:LYS:HE3	1.67	0.94
2:E:2011:LEU:HD13	2:E:2040:TRP:CE3	2.03	0.94
2:B:2210:MET:HE3	2:B:2253:LEU:HA	0.95	0.94
2:E:2041:PRO:HB2	2:E:2043:PHE:HE1	1.23	0.94
2:E:1567:PHE:CZ	2:E:1820:ARG:NH1	2.36	0.94
1:D:107:LYS:HB3	1:D:108:ILE:HG22	1.50	0.94
2:E:1711:VAL:HG12	2:E:1790:TRP:O	1.68	0.94
2:B:2310:GLU:OE1	2:B:2310:GLU:N	2.00	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2043:PHE:CD2	2:E:2051:ILE:CG1	2.50	0.93
2:B:1252:SER:O	2:B:1274:ARG:NH1	1.99	0.93
2:E:2011:LEU:HD13	2:E:2040:TRP:HZ3	1.23	0.93
2:E:1826:TYR:OH	2:E:1938:LYS:NZ	1.99	0.93
2:B:2224:VAL:CG1	2:B:2349:PHE:CE1	2.50	0.93
2:E:1998:ARG:CD	2:E:2045:ASP:OD2	2.16	0.93
2:E:1709:TRP:O	2:E:1729:THR:N	2.01	0.93
2:B:2011:LEU:HD13	2:B:2040:TRP:CZ3	2.04	0.93
1:A:86:GLY:O	1:A:90:GLU:HG2	1.66	0.93
2:E:1684:GLU:OE2	2:E:1702:THR:OG1	1.85	0.93
2:E:2267:LYS:O	2:E:2305:TYR:OH	1.86	0.93
1:D:19:GLN:HE21	1:D:110:GLU:HG2	1.25	0.93
2:B:2192:LYS:O	2:B:2195:GLU:N	2.02	0.92
2:E:2034:ILE:CD1	2:E:2041:PRO:CB	2.46	0.92
2:B:1993:ASP:OD2	2:B:2038:HIS:CB	2.17	0.92
2:E:2210:MET:CE	2:E:2253:LEU:CA	2.47	0.92
2:E:1731:LYS:HE2	2:E:1768:PRO:CB	1.97	0.92
2:E:2034:ILE:HG21	2:E:2040:TRP:N	1.84	0.92
2:E:2304:ALA:CB	2:E:2339:LEU:HD23	2.00	0.92
2:E:2210:MET:HE1	2:E:2253:LEU:CA	1.99	0.92
2:B:1961:ASN:OD1	2:B:2079:ILE:HD11	1.68	0.92
2:E:1826:TYR:H	2:E:1827:GLN:HG3	1.35	0.92
2:E:2210:MET:CE	2:E:2252:GLY:O	2.14	0.92
2:B:2315:GLY:O	2:B:2318:ASN:N	2.03	0.92
2:B:1887:GLY:HA3	2:B:1992:TYR:HD2	1.33	0.92
2:B:2183:TYR:HE1	2:B:2219:LYS:HD2	1.34	0.91
2:E:2041:PRO:CB	2:E:2043:PHE:HE1	1.80	0.91
2:B:2339:LEU:CD1	2:B:2340:LEU:N	2.33	0.91
2:E:2028:SER:O	2:E:2030:PRO:HD3	1.70	0.91
2:E:2030:PRO:HB2	2:E:2153:ARG:NH2	1.85	0.91
2:E:2019:GLU:O	2:E:2023:LYS:HG3	1.68	0.91
2:B:2282:ALA:HB2	2:B:2316:GLU:OE2	1.70	0.91
2:B:2034:ILE:HG13	2:B:2041:PRO:HA	1.51	0.91
2:B:2182:VAL:HG12	2:B:2338:GLN:HB3	0.92	0.90
2:B:2286:ARG:HD3	2:B:2312:TYR:CZ	2.07	0.90
2:E:2202:GLN:HE22	2:E:2235:SER:CA	1.84	0.90
2:B:2357:TRP:HH2	2:B:2382:PHE:CD1	1.87	0.90
2:B:2259:ILE:HD11	2:B:2291:ILE:CG2	1.91	0.90
2:B:2183:TYR:HE1	2:B:2219:LYS:HD3	0.77	0.90
2:B:2182:VAL:CG1	2:B:2338:GLN:CB	2.42	0.90
2:B:2237:GLN:C	2:B:2238:ILE:HD13	1.92	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2224:VAL:HG11	2:B:2349:PHE:HZ	1.35	0.89
2:E:1292:ARG:HD3	2:E:1293:THR:HG23	1.54	0.89
2:B:2339:LEU:CD1	2:B:2340:LEU:H	1.85	0.89
2:E:2050:THR:O	2:E:2053:SER:OG	1.90	0.89
2:B:1961:ASN:OD1	2:B:2079:ILE:CD1	2.20	0.89
2:B:2044:THR:OG1	2:B:2047:GLN:HG3	1.72	0.89
2:E:2014:ALA:HA	2:E:2059:ILE:CD1	2.03	0.89
2:E:1834:PHE:HE2	2:E:1960:GLU:OE2	1.51	0.89
2:B:2236:VAL:CG2	2:B:2238:ILE:HD12	2.02	0.89
2:B:1983:GLU:HB2	2:B:1984:PRO:HD2	1.52	0.89
2:E:2210:MET:HE1	2:E:2252:GLY:O	1.72	0.89
2:B:950:THR:O	2:B:954:ILE:HG13	1.72	0.89
2:E:2011:LEU:HD12	2:E:2040:TRP:CZ3	2.06	0.89
2:B:1848:ILE:HD13	2:B:1928:GLU:O	1.72	0.89
2:B:2182:VAL:CA	2:B:2338:GLN:HB2	2.03	0.88
2:E:1324:GLY:CA	2:E:1325:SER:OG	2.21	0.88
2:B:2259:ILE:HD12	2:B:2291:ILE:C	1.93	0.88
2:B:2019:GLU:O	2:B:2023:LYS:HG3	1.74	0.88
1:D:106:PRO:O	1:D:107:LYS:HG2	1.71	0.88
2:B:1594:GLN:OE1	2:B:1595:ARG:N	2.06	0.88
2:E:2037:TYR:CD1	2:E:2038:HIS:NE2	2.42	0.88
1:D:31:HIS:O	1:D:102:MET:SD	2.31	0.88
2:B:1016:SER:OG	2:B:1018:SER:OG	1.92	0.87
2:B:2282:ALA:CB	2:B:2316:GLU:OE2	2.21	0.87
2:E:2018:ASN:HD22	2:E:2058:LEU:CD2	1.86	0.87
2:E:2018:ASN:ND2	2:E:2058:LEU:HD21	1.87	0.87
2:E:1762:ASP:OD2	2:E:1764:VAL:HG22	1.75	0.87
1:A:347:VAL:HG21	2:B:1875:ILE:HD11	1.56	0.87
2:E:941:GLU:O	2:E:945:ASP:OD1	1.93	0.87
2:B:1849:LYS:O	2:B:1850:LEU:HD23	1.75	0.87
2:E:1998:ARG:HD2	2:E:2045:ASP:OD2	1.74	0.86
2:B:1015:PRO:HD2	2:B:1165:LEU:HD23	1.54	0.86
2:E:2080:LYS:HD2	2:E:2083:ILE:HG13	0.88	0.86
2:B:2286:ARG:HD3	2:B:2312:TYR:CE2	2.11	0.86
2:B:2358:ASN:HB3	2:B:2387:HIS:HD1	1.37	0.86
2:E:1466:GLN:O	2:E:1469:ILE:N	2.09	0.86
2:E:1992:TYR:OH	2:E:2005:PHE:HB2	1.76	0.86
2:B:2020:GLU:OE1	2:B:2165:ARG:NH2	2.07	0.86
2:E:2014:ALA:CA	2:E:2059:ILE:HD11	2.06	0.85
2:E:2030:PRO:HB2	2:E:2153:ARG:HH21	1.41	0.85
2:B:1137:PRO:HG2	2:B:1140:ASN:O	1.76	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2207:ILE:N	2:B:2257:GLY:O	2.09	0.85
1:D:106:PRO:C	1:D:107:LYS:HG2	1.93	0.85
2:B:2203:VAL:CG2	2:B:2382:PHE:CE1	2.59	0.85
1:A:94:HIS:O	1:A:98:GLU:CB	2.24	0.85
2:B:1868:GLY:O	2:B:1870:VAL:HG23	1.75	0.85
2:B:2182:VAL:CG1	2:B:2338:GLN:OE1	2.24	0.85
2:E:2177:VAL:HG23	2:E:2180:GLN:H	1.41	0.85
2:E:1252:SER:O	2:E:1274:ARG:NH1	2.08	0.85
2:B:2350:ILE:HG23	2:B:2375:LYS:O	1.76	0.85
2:B:2256:LEU:O	2:B:2288:CYS:SG	2.34	0.85
2:E:2011:LEU:CD1	2:E:2040:TRP:CE3	2.59	0.85
2:E:2037:TYR:CD1	2:E:2038:HIS:HD2	1.95	0.85
2:B:2357:TRP:HH2	2:B:2382:PHE:HE1	1.18	0.85
2:E:1757:LEU:O	2:E:1761:THR:HG23	1.77	0.84
2:B:2034:ILE:CG1	2:B:2041:PRO:CA	2.55	0.84
2:B:2178:GLU:O	2:B:2217:LYS:CD	2.24	0.84
2:B:2210:MET:SD	2:B:2222:LYS:CD	2.65	0.84
1:D:327:ILE:HB	1:D:328:TYR:CD1	2.12	0.84
2:E:2065:ARG:NH1	2:E:2065:ARG:HB3	1.93	0.84
2:B:2281:PHE:CE1	2:B:2288:CYS:HB2	2.13	0.84
2:B:2157:ILE:O	2:B:2160:THR:N	2.08	0.84
2:B:1887:GLY:CA	2:B:1992:TYR:CD2	2.60	0.84
2:B:2049:ILE:O	2:B:2053:SER:OG	1.93	0.84
2:B:1994:ASP:O	2:B:1997:ASP:HB2	1.78	0.84
2:E:1763:ASN:CA	2:E:1766:MET:HE2	2.08	0.83
2:E:2174:ASP:OD1	2:E:2175:ASP:N	2.10	0.83
2:B:1686:VAL:HG11	2:B:1690:LYS:HD2	1.60	0.83
2:B:1895:HIS:CD2	2:B:1896:THR:H	1.94	0.83
2:B:2203:VAL:HG22	2:B:2382:PHE:HE1	1.43	0.83
2:B:2208:TYR:CD2	2:B:2253:LEU:HD13	2.12	0.83
2:B:2183:TYR:CE1	2:B:2219:LYS:HD2	2.09	0.83
2:E:2034:ILE:HD13	2:E:2041:PRO:CA	1.80	0.83
2:E:1763:ASN:O	2:E:1766:MET:CE	2.25	0.83
2:E:2064:GLY:O	2:E:2068:ASN:N	2.11	0.83
2:B:2294:PHE:CZ	2:B:2296:THR:CG2	2.61	0.83
2:E:1712:SER:OG	2:E:1713:LYS:O	1.94	0.83
2:E:2210:MET:HE2	2:E:2253:LEU:HA	1.59	0.83
2:B:2182:VAL:HA	2:B:2338:GLN:CB	2.08	0.83
2:E:2034:ILE:HD12	2:E:2041:PRO:CD	2.09	0.83
2:B:2210:MET:CG	2:B:2222:LYS:CD	2.54	0.83
2:B:1999:LEU:HD12	2:B:2000:SER:H	1.43	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2294:PHE:CZ	2:B:2296:THR:HG21	2.13	0.83
2:E:2381:GLU:OE1	2:E:2381:GLU:N	2.10	0.83
2:B:2256:LEU:C	2:B:2288:CYS:SG	2.58	0.82
2:E:2189:LEU:CD1	2:E:2224:VAL:HG23	2.09	0.82
2:B:1853:ASP:OD1	2:B:1855:THR:OG1	1.97	0.82
2:E:1711:VAL:CG1	2:E:1790:TRP:O	2.28	0.82
2:B:2380:LEU:HD13	2:B:2384:ASN:OD1	1.77	0.82
2:B:2224:VAL:C	2:B:2349:PHE:CE1	2.53	0.82
2:B:2224:VAL:O	2:B:2349:PHE:HD1	1.63	0.82
2:E:2034:ILE:HD11	2:E:2041:PRO:CB	2.07	0.82
2:B:1999:LEU:HD21	2:B:2003:THR:HG22	1.60	0.82
2:B:1848:ILE:CD1	2:B:1928:GLU:O	2.27	0.82
2:B:1999:LEU:HD11	2:B:2003:THR:HB	1.60	0.82
2:B:1568:ASN:OD1	2:B:1569:SER:N	2.13	0.82
2:B:2339:LEU:HD12	2:B:2340:LEU:H	1.35	0.82
2:E:1705:SER:OG	2:E:1730:ASN:CA	2.28	0.82
2:E:1987:VAL:HG12	2:E:1989:PHE:CE1	2.15	0.82
2:E:2083:ILE:HG22	2:E:2084:LEU:HD13	1.62	0.81
2:E:2080:LYS:HD3	2:E:2083:ILE:CD1	1.92	0.81
2:E:2024:MET:CE	2:E:2157:ILE:HG23	2.01	0.81
2:B:2192:LYS:O	2:B:2195:GLU:HB2	1.80	0.81
2:B:2224:VAL:HG12	2:B:2349:PHE:HE1	1.45	0.81
2:E:1711:VAL:CB	2:E:1790:TRP:O	2.28	0.81
2:E:2074:LEU:O	2:E:2075:THR:OG1	1.98	0.81
2:B:2044:THR:HG23	2:B:2047:GLN:CD	2.00	0.81
2:B:2224:VAL:HG11	2:B:2349:PHE:CZ	2.09	0.81
2:E:2177:VAL:CG2	2:E:2180:GLN:HB2	2.09	0.81
2:B:2358:ASN:CA	2:B:2387:HIS:CE1	2.63	0.81
2:E:1974:LEU:O	2:E:1977:VAL:HG22	1.80	0.81
2:B:1895:HIS:CD2	2:B:1896:THR:OG1	2.33	0.81
2:B:2060:LEU:O	2:B:2063:TYR:HB3	1.80	0.81
2:B:1941:LEU:O	2:B:1945:GLU:HG3	1.81	0.81
2:B:2047:GLN:O	2:B:2051:ILE:N	2.13	0.81
2:E:2018:ASN:HD21	2:E:2058:LEU:HD11	1.07	0.81
1:D:107:LYS:HB3	1:D:108:ILE:CG2	2.10	0.81
2:E:1727:LEU:O	2:E:1728:ILE:HD13	1.80	0.81
2:E:2030:PRO:HG2	2:E:2153:ARG:NE	1.95	0.81
1:D:210:LEU:O	1:D:214:PHE:O	1.99	0.81
2:B:2259:ILE:HD12	2:B:2291:ILE:HB	1.63	0.81
2:B:2182:VAL:HG12	2:B:2338:GLN:CG	2.11	0.81
2:B:2198:ASP:OD1	2:B:2200:LYS:N	2.14	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2178:GLU:O	2:B:2217:LYS:HD3	1.79	0.80
2:E:1849:LYS:O	2:E:1850:LEU:HD23	1.81	0.80
2:B:2259:ILE:HD13	2:B:2291:ILE:HB	0.81	0.80
2:E:1711:VAL:CG1	2:E:1791:PHE:HB3	2.11	0.80
2:B:1707:HIS:NE2	2:B:1708:GLU:HB2	1.97	0.80
2:E:2202:GLN:NE2	2:E:2235:SER:C	2.34	0.80
2:B:900:PHE:CA	2:B:1075:ASP:OD2	2.28	0.80
2:B:2367:ASN:OD1	2:B:2370:GLY:N	2.15	0.80
2:E:2384:ASN:HD22	2:E:2386:MET:H	1.30	0.80
2:B:2308:THR:CG2	2:B:2333:PHE:O	2.19	0.80
2:E:2037:TYR:HD1	2:E:2038:HIS:NE2	1.77	0.80
2:B:2279:LYS:HZ3	2:B:2368:GLN:HE22	1.30	0.80
2:E:2034:ILE:CD1	2:E:2041:PRO:CD	2.59	0.80
2:E:2084:LEU:HD22	2:E:2084:LEU:O	1.81	0.80
2:E:1995:TRP:CE2	2:E:2007:ARG:HD2	2.17	0.80
2:B:2044:THR:CG2	2:B:2047:GLN:NE2	2.36	0.80
2:E:1995:TRP:CH2	2:E:2007:ARG:CG	2.62	0.80
2:B:2358:ASN:CA	2:B:2387:HIS:HE1	1.95	0.79
2:B:1843:LEU:HD11	2:B:1884:PRO:CG	2.12	0.79
2:E:1987:VAL:CG1	2:E:1989:PHE:CE1	2.65	0.79
2:B:1961:ASN:CG	2:B:2079:ILE:HD11	2.03	0.79
2:B:2176:PHE:HA	2:B:2338:GLN:NE2	1.97	0.79
2:E:2065:ARG:HB3	2:E:2065:ARG:CZ	2.12	0.79
2:B:1976:ASP:O	2:B:1980:LYS:HG3	1.83	0.79
2:B:2035:LYS:HD2	2:B:2037:TYR:CE1	2.17	0.79
2:B:2176:PHE:HA	2:B:2338:GLN:HE21	1.47	0.79
2:E:2202:GLN:NE2	2:E:2235:SER:CA	2.46	0.79
1:D:75:ASP:OD2	1:D:79:LYS:CE	2.31	0.79
2:B:2184:VAL:HG23	2:B:2219:LYS:O	1.83	0.79
2:E:1995:TRP:CD2	2:E:2007:ARG:HD2	2.17	0.79
2:E:2353:SER:HA	2:E:2375:LYS:CD	2.13	0.79
2:B:2224:VAL:CG1	2:B:2349:PHE:HZ	1.86	0.78
2:E:2384:ASN:ND2	2:E:2386:MET:H	1.81	0.78
2:B:1895:HIS:CD2	2:B:1896:THR:N	2.51	0.78
2:E:1703:MET:N	2:E:1732:MET:O	2.17	0.78
2:B:2183:TYR:CD2	2:B:2289:ILE:HD13	2.19	0.78
2:E:2034:ILE:CG2	2:E:2040:TRP:N	2.47	0.78
2:B:2154:LYS:O	2:B:2157:ILE:HB	1.82	0.78
2:B:1843:LEU:HD12	2:B:1843:LEU:O	1.84	0.78
2:E:2043:PHE:HB3	2:E:2047:GLN:HG3	1.66	0.78
2:B:2358:ASN:N	2:B:2387:HIS:CE1	2.39	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:ARG:NH2	1:D:279:TYR:CE1	2.51	0.78
2:E:1727:LEU:HD23	2:E:1728:ILE:H	1.49	0.78
2:B:1111:SER:HB2	2:B:1510:ILE:HG12	1.65	0.78
2:B:1348:GLU:OE1	2:B:1447:TRP:N	2.15	0.78
2:B:1797:LEU:O	2:B:1801:SER:OG	2.00	0.77
2:B:2224:VAL:O	2:B:2349:PHE:CE1	2.36	0.77
2:B:1503:ALA:O	2:B:1506:ARG:NH1	2.17	0.77
2:E:2087:ASN:HD22	2:E:2089:LYS:H	1.31	0.77
2:B:2236:VAL:HG21	2:B:2238:ILE:HD12	1.65	0.77
2:B:2279:LYS:NZ	2:B:2368:GLN:NE2	2.33	0.77
1:D:108:ILE:HD13	1:D:109:ASP:H	1.48	0.77
2:B:2268:PHE:CD2	2:B:2331:PRO:HB3	2.15	0.77
2:B:1983:GLU:HB2	2:B:1984:PRO:CD	2.14	0.77
2:E:2210:MET:CE	2:E:2253:LEU:HA	2.14	0.77
2:E:1562:PHE:O	2:E:1565:THR:OG1	2.02	0.77
2:E:1565:THR:O	2:E:1820:ARG:NH2	2.17	0.77
2:E:2078:GLU:C	2:E:2079:ILE:HD13	2.05	0.77
2:B:2157:ILE:C	2:B:2160:THR:HG1	1.85	0.77
2:E:2080:LYS:CE	2:E:2083:ILE:CD1	2.63	0.77
2:B:2283:ASP:OD1	2:B:2284:LYS:HA	1.84	0.77
2:E:1163:ARG:HG3	2:E:1168:ILE:HG22	1.67	0.77
2:E:2201:ILE:HG21	2:E:2382:PHE:CZ	2.20	0.77
2:B:2357:TRP:CH2	2:B:2382:PHE:HE1	1.95	0.77
2:B:1999:LEU:HD21	2:B:2003:THR:CG2	2.15	0.77
2:E:2087:ASN:HD22	2:E:2089:LYS:N	1.83	0.77
2:B:2294:PHE:HD2	2:B:2301:SER:HG	0.78	0.76
2:B:2247:LEU:HD12	2:B:2248:PRO:CD	2.16	0.76
2:E:2201:ILE:HG21	2:E:2382:PHE:HZ	1.49	0.76
2:B:2286:ARG:CD	2:B:2312:TYR:CE2	2.68	0.76
2:B:2281:PHE:C	2:B:2286:ARG:HA	2.04	0.76
2:E:1111:SER:HB2	2:E:1510:ILE:HG12	1.66	0.76
2:E:2057:ASP:O	2:E:2061:THR:N	2.17	0.76
2:B:2244:ILE:O	2:B:2250:THR:HG21	1.85	0.76
1:A:344:PRO:HB3	2:B:1858:TYR:CE1	2.21	0.76
2:B:2280:LEU:HD12	2:B:2281:PHE:CE2	2.21	0.76
2:E:2039:LEU:C	2:E:2040:TRP:CD1	2.59	0.76
2:E:2080:LYS:HE3	2:E:2083:ILE:HD12	1.68	0.76
2:E:2018:ASN:ND2	2:E:2058:LEU:CD2	2.44	0.76
2:E:1348:GLU:OE1	2:E:1447:TRP:N	2.19	0.76
2:E:2210:MET:HE2	2:E:2253:LEU:CA	2.16	0.76
2:B:1729:THR:HG22	2:B:1771:THR:HG21	1.67	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1843:LEU:O	2:B:1849:LYS:HE3	1.86	0.75
1:A:292:CYS:O	1:A:296:SER:OG	2.03	0.75
2:B:2177:VAL:H	2:B:2338:GLN:NE2	1.84	0.75
2:B:1605:ARG:NH2	2:B:1824:GLN:OE1	2.17	0.75
2:B:2309:ASP:HA	2:B:2312:TYR:HB2	1.66	0.75
2:E:1995:TRP:CH2	2:E:2007:ARG:CD	2.69	0.75
2:B:2227:VAL:O	2:B:2229:GLN:HG2	1.87	0.75
2:E:2189:LEU:HD13	2:E:2224:VAL:HG23	1.66	0.75
1:D:292:CYS:O	1:D:296:SER:OG	2.04	0.75
2:B:1477:PHE:CD2	2:B:1495:PHE:CD2	2.73	0.75
2:E:1292:ARG:HD3	2:E:1293:THR:CG2	2.16	0.75
2:E:2041:PRO:CG	2:E:2043:PHE:HE1	1.98	0.75
2:B:1207:TRP:O	2:B:1212:ARG:NH1	2.19	0.75
2:B:1287:ASP:OD2	2:B:1296:ARG:NH2	2.18	0.75
2:B:2183:TYR:CD1	2:B:2219:LYS:HD3	2.20	0.75
2:E:1702:THR:HG21	2:E:1768:PRO:HG3	1.66	0.75
2:E:1964:PRO:HG3	2:E:2013:ARG:NH1	2.02	0.75
2:E:1324:GLY:HA2	2:E:1325:SER:CB	2.16	0.75
2:E:1093:LYS:HG3	2:E:1094:ASP:OD1	1.87	0.74
2:E:1570:TRP:O	2:E:1571:GLU:CD	2.25	0.74
2:E:2047:GLN:O	2:E:2050:THR:CA	2.34	0.74
2:B:1895:HIS:HD2	2:B:1896:THR:H	1.32	0.74
2:B:2232:HIS:N	2:B:2235:SER:O	2.20	0.74
2:B:2236:VAL:CG1	2:B:2238:ILE:HD11	2.17	0.74
2:E:1995:TRP:CE3	2:E:2007:ARG:HD2	2.22	0.74
2:B:1859:ARG:CD	2:B:1876:ASN:O	2.35	0.74
1:A:212:GLY:O	1:A:215:LYS:NZ	2.19	0.74
2:E:2157:ILE:O	2:E:2160:THR:CB	2.34	0.74
2:E:2227:VAL:CG1	2:E:2239:SER:OG	2.35	0.74
2:E:2034:ILE:HG21	2:E:2040:TRP:CA	2.17	0.74
2:B:2203:VAL:HG22	2:B:2382:PHE:CE1	2.20	0.74
2:E:2066:LYS:HB2	2:E:2067:TYR:CD1	2.21	0.74
2:E:1570:TRP:O	2:E:1571:GLU:OE2	2.04	0.74
2:E:2041:PRO:HB2	2:E:2043:PHE:CD1	2.23	0.74
2:B:2210:MET:HE1	2:B:2253:LEU:CA	2.16	0.74
2:E:2162:LEU:CD1	2:E:2194:ILE:O	2.36	0.74
2:E:1418:THR:OG1	2:E:1421:GLY:O	2.05	0.74
2:B:1999:LEU:HG	2:B:2000:SER:O	1.87	0.74
2:B:2309:ASP:OD1	2:B:2309:ASP:N	2.18	0.74
2:B:2185:LEU:HG	2:B:2186:PRO:N	2.00	0.73
2:E:1834:PHE:CD1	2:E:1958:PRO:HG2	2.23	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1932:GLN:OE1	2:B:1957:ARG:NH1	2.21	0.73
2:E:1597:GLY:CA	2:E:1598:LEU:HB3	2.18	0.73
2:B:2238:ILE:HD13	2:B:2238:ILE:N	2.03	0.73
2:E:2230:LEU:CD1	2:E:2360:THR:HA	2.17	0.73
2:B:2309:ASP:HA	2:B:2312:TYR:HD2	1.54	0.73
2:E:2047:GLN:C	2:E:2050:THR:H	1.92	0.73
2:B:2034:ILE:HG12	2:B:2040:TRP:C	2.09	0.73
2:B:2209:GLY:HA3	2:B:2256:LEU:HD21	1.70	0.73
2:E:2202:GLN:HE22	2:E:2235:SER:HA	1.53	0.73
2:E:1705:SER:OG	2:E:1730:ASN:C	2.27	0.73
2:E:1987:VAL:HG11	2:E:1989:PHE:CZ	2.23	0.73
2:B:1993:ASP:OD1	2:B:2038:HIS:HB3	1.88	0.73
2:B:2306:ASN:N	2:B:2335:THR:O	2.17	0.72
1:A:88:LYS:O	1:A:92:ILE:HD13	1.89	0.72
2:E:2177:VAL:HG21	2:E:2180:GLN:HG3	1.70	0.72
2:E:2024:MET:CE	2:E:2157:ILE:HG21	2.18	0.72
2:E:1733:TRP:CE2	2:E:1767:TYR:HD2	2.07	0.72
2:B:2045:ASP:N	2:B:2045:ASP:OD1	2.21	0.72
2:B:1679:GLU:N	2:B:1704:GLU:O	2.22	0.72
2:E:1973:LYS:O	2:E:1977:VAL:HG13	1.89	0.72
2:E:2277:HIS:HD1	2:E:2281:PHE:HD2	1.35	0.72
1:D:75:ASP:OD2	1:D:79:LYS:NZ	2.23	0.72
2:E:1711:VAL:HG12	2:E:1791:PHE:HB3	1.70	0.72
2:E:2084:LEU:H	2:E:2084:LEU:HD13	1.55	0.72
2:E:2021:SER:O	2:E:2024:MET:N	2.22	0.72
2:E:1428:GLY:N	2:E:1433:ASP:OD2	2.19	0.72
2:B:2011:LEU:HD13	2:B:2040:TRP:CE3	2.24	0.72
2:B:2230:LEU:HD23	2:B:2237:GLN:HG3	1.72	0.72
2:B:2037:TYR:HB2	2:B:2038:HIS:HD2	1.55	0.72
1:D:19:GLN:NE2	1:D:110:GLU:CG	2.49	0.72
2:B:2034:ILE:HG12	2:B:2040:TRP:O	1.88	0.72
2:E:2178:GLU:C	2:E:2217:LYS:HZ2	1.87	0.72
2:B:2046:GLU:O	2:B:2049:ILE:HG22	1.89	0.71
2:B:2165:ARG:O	2:B:2300:VAL:HG13	1.90	0.71
2:B:2247:LEU:HG	2:B:2375:LYS:HA	1.72	0.71
2:B:2279:LYS:HZ3	2:B:2368:GLN:NE2	1.87	0.71
2:B:1308:GLU:OE2	2:B:1311:LYS:HE3	1.90	0.71
2:E:2162:LEU:HD13	2:E:2194:ILE:O	1.89	0.71
2:B:1996:LEU:HA	2:B:1999:LEU:O	1.89	0.71
2:E:2017:THR:HG22	2:E:2018:ASN:OD1	1.91	0.71
2:E:2048:TRP:O	2:E:2052:GLU:HB2	1.91	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2014:ALA:HA	2:E:2059:ILE:HD11	1.68	0.71
2:E:2043:PHE:CE2	2:E:2051:ILE:CG1	2.64	0.71
1:D:19:GLN:HE22	1:D:110:GLU:HG2	1.52	0.71
2:E:1763:ASN:CA	2:E:1766:MET:CE	2.68	0.71
2:B:2159:ASN:OD1	2:B:2199:VAL:CG1	2.37	0.71
2:E:1291:GLU:O	2:E:1294:LYS:CE	2.37	0.71
2:E:1465:ARG:NH1	2:E:1465:ARG:HG2	1.97	0.71
2:B:1983:GLU:HG3	2:B:1985:GLN:HE21	1.56	0.71
2:B:1731:LYS:HE3	2:B:1768:PRO:HB2	1.73	0.70
2:B:1927:GLU:N	2:B:1927:GLU:OE1	2.24	0.70
2:B:2207:ILE:HB	2:B:2221:ILE:HG23	1.71	0.70
2:E:2210:MET:SD	2:E:2252:GLY:C	2.57	0.70
2:B:1180:GLU:O	2:B:1184:ASP:OD1	2.09	0.70
2:B:2247:LEU:HD12	2:B:2248:PRO:HD2	1.73	0.70
2:E:1679:GLU:HB2	2:E:1706:VAL:HG13	1.74	0.70
2:B:1729:THR:HG21	2:B:1771:THR:HG23	1.73	0.70
2:B:2048:TRP:O	2:B:2052:GLU:HG3	1.92	0.70
1:D:48:HIS:CD2	1:D:53:SER:OG	2.45	0.70
2:B:2044:THR:OG1	2:B:2047:GLN:CG	2.39	0.70
2:B:2307:LEU:HD12	2:B:2308:THR:H	1.55	0.70
2:B:2224:VAL:HG12	2:B:2349:PHE:CZ	2.17	0.70
2:B:2230:LEU:HB3	2:B:2237:GLN:CG	2.22	0.70
2:E:1093:LYS:CG	2:E:1094:ASP:HA	2.21	0.70
2:B:2188:ASN:HD21	2:B:2346:THR:HB	1.56	0.70
2:B:1974:LEU:O	2:B:1977:VAL:HG12	1.91	0.70
2:B:2236:VAL:HG13	2:B:2238:ILE:HD11	1.73	0.70
2:E:2024:MET:HE3	2:E:2157:ILE:HG21	1.74	0.70
2:E:1731:LYS:CE	2:E:1768:PRO:CB	2.64	0.70
2:E:1995:TRP:CZ2	2:E:2007:ARG:HD2	2.27	0.70
2:E:1763:ASN:O	2:E:1766:MET:HE1	1.91	0.70
2:B:1704:GLU:HG3	2:B:1730:ASN:O	1.92	0.70
2:B:2044:THR:HG23	2:B:2047:GLN:HE21	1.50	0.69
2:E:2030:PRO:HG2	2:E:2153:ARG:CZ	2.21	0.69
2:B:1687:HIS:ND1	2:B:1688:PRO:HD2	2.06	0.69
2:E:1093:LYS:HG3	2:E:1094:ASP:HA	1.74	0.69
2:E:1687:HIS:ND1	2:E:1688:PRO:HD2	2.07	0.69
2:E:1711:VAL:HB	2:E:1790:TRP:O	1.92	0.69
2:B:1722:ASP:OD1	2:B:1722:ASP:N	2.26	0.69
2:B:2223:THR:HG23	2:B:2348:ASN:O	1.92	0.69
2:B:2314:TRP:O	2:B:2317:GLU:HB2	1.93	0.69
2:E:2213:LYS:HA	2:E:2215:HIS:N	2.05	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2084:LEU:CD1	2:E:2084:LEU:H	2.05	0.69
2:E:2157:ILE:O	2:E:2160:THR:HB	1.92	0.69
2:E:1763:ASN:HA	2:E:1766:MET:HE2	1.75	0.69
2:E:1705:SER:HG	2:E:1730:ASN:C	1.93	0.69
2:B:954:ILE:HG23	2:B:991:THR:HG22	1.73	0.69
2:B:2281:PHE:CD1	2:B:2288:CYS:HB2	2.27	0.69
2:E:1274:ARG:O	2:E:1276:GLU:HB3	1.93	0.69
2:B:1017:ASP:HA	2:B:1509:ARG:HG3	1.75	0.69
2:B:2210:MET:HE2	2:B:2252:GLY:O	1.93	0.69
2:B:2152:TRP:HA	2:B:2154:LYS:N	2.07	0.69
2:E:2327:GLU:HA	2:E:2327:GLU:OE1	1.93	0.69
2:B:2207:ILE:HG22	2:B:2224:VAL:HG22	1.75	0.69
2:B:2286:ARG:HD3	2:B:2312:TYR:CE1	2.28	0.69
2:B:2182:VAL:CG1	2:B:2338:GLN:CD	2.62	0.69
2:E:1472:ASN:C	2:E:2325:LEU:HB2	2.09	0.69
2:E:2201:ILE:CG2	2:E:2382:PHE:CZ	2.76	0.69
2:B:2268:PHE:HD2	2:B:2331:PRO:CB	2.03	0.68
2:B:1704:GLU:HG2	2:B:1705:SER:H	1.58	0.68
2:B:1475:LEU:HD12	2:B:1479:GLU:OE2	1.94	0.68
2:E:1705:SER:OG	2:E:1730:ASN:HA	1.92	0.68
2:B:2294:PHE:CZ	2:B:2296:THR:HG23	2.29	0.68
2:B:2350:ILE:HD11	2:B:2376:TYR:CD1	2.29	0.68
2:E:2189:LEU:HD13	2:E:2224:VAL:CG2	2.23	0.68
2:B:2339:LEU:HD12	2:B:2340:LEU:O	1.94	0.68
2:B:2198:ASP:OD1	2:B:2199:VAL:N	2.27	0.68
2:B:1961:ASN:CG	2:B:2079:ILE:CD1	2.63	0.68
2:B:1192:ASP:OD2	2:B:1195:PHE:HA	1.94	0.67
2:E:2018:ASN:HD21	2:E:2058:LEU:HG	1.57	0.67
2:E:1763:ASN:HA	2:E:1766:MET:CE	2.24	0.67
2:B:1163:ARG:HG3	2:B:1168:ILE:HG22	1.77	0.67
2:B:2309:ASP:HA	2:B:2312:TYR:CD2	2.29	0.67
2:E:1834:PHE:CD2	2:E:1960:GLU:HG2	2.28	0.67
2:E:1573:LEU:HD22	2:E:1826:TYR:HD2	1.60	0.67
2:B:1858:TYR:HB2	2:B:1899:TRP:CZ2	2.29	0.67
2:B:1880:PHE:CE2	2:B:1889:LEU:HD11	2.30	0.67
2:E:2385:GLU:O	2:E:2388:ARG:CB	2.36	0.67
2:E:1995:TRP:CZ3	2:E:2007:ARG:HD2	2.29	0.67
2:E:1976:ASP:O	2:E:1980:LYS:HG2	1.94	0.67
2:E:2179:GLU:O	2:E:2217:LYS:HD3	1.93	0.67
2:B:2044:THR:N	2:B:2047:GLN:OE1	2.27	0.67
2:E:2056:ARG:O	2:E:2060:LEU:HG	1.94	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1188:ALA:O	2:B:1191:PRO:HD3	1.95	0.67
2:E:1727:LEU:CD2	2:E:1728:ILE:H	2.06	0.67
2:B:1686:VAL:HG11	2:B:1690:LYS:CD	2.25	0.67
2:B:2192:LYS:O	2:B:2195:GLU:CB	2.43	0.67
2:E:1707:HIS:HB3	2:E:1730:ASN:HB3	1.76	0.67
1:D:110:GLU:HB2	1:D:113:THR:H	1.59	0.67
2:E:2049:ILE:O	2:E:2053:SER:N	2.28	0.66
2:B:1187:LEU:O	2:B:1191:PRO:HG3	1.95	0.66
2:E:1017:ASP:HA	2:E:1509:ARG:HG3	1.76	0.66
1:D:347:VAL:HG21	2:E:1875:ILE:HD11	1.76	0.66
2:B:2277:HIS:HB3	2:B:2307:LEU:HD23	1.75	0.66
2:E:2025:ILE:HG23	2:E:2054:GLN:NE2	2.10	0.66
2:B:2343:ASP:HB3	2:B:2344:ARG:NH2	2.11	0.66
2:B:1987:VAL:HG12	2:B:1989:PHE:CE2	2.29	0.66
2:E:1995:TRP:CH2	2:E:2007:ARG:HD2	2.31	0.66
1:D:327:ILE:HD12	1:D:327:ILE:H	1.59	0.66
2:E:2014:ALA:HB2	2:E:2059:ILE:HD11	1.78	0.66
2:B:1040:ASP:OD1	2:B:1042:SER:OG	2.13	0.66
2:E:1597:GLY:CA	2:E:1599:SER:H	2.08	0.66
2:B:2178:GLU:O	2:B:2217:LYS:CE	2.43	0.66
2:B:2277:HIS:NE2	2:B:2288:CYS:O	2.28	0.66
2:B:2192:LYS:HA	2:B:2195:GLU:HB2	1.78	0.66
2:E:2202:GLN:NE2	2:E:2235:SER:N	2.43	0.66
2:B:909:THR:OG1	2:B:2175:ASP:OD1	2.13	0.66
2:E:2039:LEU:CB	2:E:2040:TRP:CD1	2.77	0.66
2:E:2014:ALA:CB	2:E:2059:ILE:HD11	2.26	0.66
2:B:1886:THR:OG1	2:B:1888:HIS:CE1	2.48	0.66
2:B:946:ASN:HB3	2:B:949:ASP:OD2	1.96	0.66
2:B:2306:ASN:OD1	2:B:2337:ALA:HB2	1.95	0.66
2:B:2259:ILE:HD12	2:B:2291:ILE:CB	2.17	0.66
2:E:1987:VAL:CG1	2:E:1989:PHE:CZ	2.79	0.66
2:E:2159:ASN:ND2	2:E:2197:SER:O	2.29	0.66
2:B:2208:TYR:CB	2:B:2253:LEU:HD21	2.22	0.66
2:B:2379:PRO:O	2:B:2380:LEU:HD23	1.96	0.66
2:B:1727:LEU:HD23	2:B:1728:ILE:H	1.59	0.66
2:B:2230:LEU:O	2:B:2237:GLN:N	2.27	0.65
2:E:2221:ILE:HD13	2:E:2256:LEU:HD12	1.76	0.65
1:D:84:ARG:HG3	1:D:84:ARG:HH11	1.60	0.65
2:E:1711:VAL:HG12	2:E:1790:TRP:C	2.17	0.65
2:E:2381:GLU:CD	2:E:2381:GLU:H	1.99	0.65
2:B:2203:VAL:CG2	2:B:2382:PHE:HE1	2.00	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1186:TYR:HB2	2:B:1228:TRP:CE3	2.30	0.65
1:A:319:LYS:O	1:A:320:ASP:OD1	2.14	0.65
2:B:2177:VAL:O	2:B:2180:GLN:O	2.14	0.65
2:B:2260:HIS:CD2	2:B:2290:ASP:OD1	2.50	0.65
2:B:2368:GLN:HB3	2:B:2369:GLU:OE2	1.95	0.65
2:B:2087:ASN:HB3	2:B:2089:LYS:HG3	1.78	0.65
2:B:2182:VAL:CA	2:B:2338:GLN:CB	2.71	0.65
2:E:2087:ASN:C	2:E:2088:ILE:HG12	2.16	0.65
1:D:25:LYS:O	1:D:28:GLN:N	2.30	0.65
2:B:2259:ILE:CD1	2:B:2291:ILE:C	2.63	0.65
2:E:1709:TRP:O	2:E:1728:ILE:HA	1.97	0.65
2:E:2034:ILE:CG2	2:E:2040:TRP:CA	2.73	0.65
2:E:1763:ASN:C	2:E:1766:MET:HE1	2.17	0.65
2:E:1097:HIS:HD2	2:E:1098:VAL:O	1.80	0.65
2:E:1886:THR:HB	2:E:1888:HIS:CE1	2.32	0.65
1:A:327:ILE:HG23	2:B:1340:ILE:HD11	1.79	0.65
2:E:1995:TRP:CZ3	2:E:2007:ARG:CD	2.80	0.64
2:B:2182:VAL:CB	2:B:2338:GLN:HB3	2.25	0.64
2:E:1836:ASN:HB2	2:E:1839:ASN:OD1	1.98	0.64
2:B:1598:LEU:HD22	2:B:1598:LEU:O	1.97	0.64
2:E:2080:LYS:CE	2:E:2083:ILE:HD12	2.25	0.64
2:E:2178:GLU:O	2:E:2217:LYS:CE	2.46	0.64
2:B:2192:LYS:O	2:B:2195:GLU:CA	2.44	0.64
2:E:2037:TYR:CE1	2:E:2038:HIS:NE2	2.66	0.64
2:B:2203:VAL:HG21	2:B:2382:PHE:CE1	2.32	0.64
2:B:1605:ARG:NE	2:B:1824:GLN:OE1	2.30	0.64
2:B:2044:THR:H	2:B:2047:GLN:CD	2.01	0.64
2:E:1763:ASN:ND2	2:E:1763:ASN:H	1.93	0.64
2:B:1162:THR:HG22	2:B:1169:TYR:HB2	1.79	0.64
2:E:1867:GLU:H	2:E:1867:GLU:CD	2.01	0.64
1:D:108:ILE:HD13	1:D:109:ASP:N	2.12	0.64
2:B:2007:ARG:HG2	2:B:2052:GLU:OE2	1.98	0.63
2:B:2339:LEU:CD1	2:B:2340:LEU:O	2.46	0.63
2:B:1961:ASN:OD1	2:B:2079:ILE:HD12	1.96	0.63
2:B:2035:LYS:HB3	2:B:2037:TYR:HD1	1.62	0.63
2:B:1149:SER:OG	2:B:1152:VAL:HG12	1.97	0.63
2:B:2230:LEU:HB3	2:B:2237:GLN:HG3	1.79	0.63
2:E:2384:ASN:HD22	2:E:2385:GLU:N	1.96	0.63
1:D:134:GLU:N	1:D:134:GLU:OE1	2.22	0.63
2:B:2208:TYR:HB3	2:B:2253:LEU:CD1	2.29	0.63
2:E:2277:HIS:ND1	2:E:2281:PHE:CD2	2.66	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1091:ASN:HB3	2:E:1093:LYS:CE	2.28	0.63
2:B:1105:ARG:HG3	2:B:1105:ARG:HH11	1.62	0.63
2:B:1999:LEU:HD12	2:B:2000:SER:N	2.12	0.63
2:B:1886:THR:OG1	2:B:1888:HIS:ND1	2.32	0.63
2:E:2177:VAL:HG22	2:E:2180:GLN:HB2	1.80	0.63
2:B:2159:ASN:ND2	2:B:2198:ASP:HA	2.13	0.63
2:B:1999:LEU:HD11	2:B:2003:THR:CB	2.28	0.63
2:E:1995:TRP:CZ2	2:E:2007:ARG:CD	2.82	0.62
2:E:1961:ASN:OD1	2:E:2079:ILE:HD12	1.98	0.62
2:E:1972:ASP:OD1	2:E:1972:ASP:N	2.32	0.62
2:B:2177:VAL:H	2:B:2338:GLN:HE22	1.47	0.62
2:B:2247:LEU:HD12	2:B:2248:PRO:HD3	1.82	0.62
2:E:1887:GLY:HA3	2:E:1992:TYR:CD2	2.34	0.62
2:B:2037:TYR:C	2:B:2038:HIS:HD2	2.03	0.62
1:D:110:GLU:HB3	1:D:113:THR:OG1	1.99	0.62
2:E:1573:LEU:HD22	2:E:1826:TYR:CD2	2.33	0.62
2:E:1707:HIS:HB2	2:E:1708:GLU:HG3	1.79	0.62
2:B:1477:PHE:CE2	2:B:1495:PHE:HD2	2.17	0.62
2:B:2206:PHE:O	2:B:2224:VAL:HA	2.00	0.62
1:D:109:ASP:O	1:D:110:GLU:HB2	1.99	0.62
2:B:2153:ARG:HH11	2:B:2153:ARG:CG	2.12	0.62
1:A:94:HIS:O	1:A:98:GLU:N	2.28	0.62
2:E:1834:PHE:CE1	2:E:1958:PRO:HG2	2.35	0.62
2:E:1826:TYR:N	2:E:1827:GLN:HG3	2.11	0.62
2:E:2090:ALA:HB1	2:E:2091:PRO:HD2	1.82	0.62
2:E:950:THR:O	2:E:954:ILE:HG13	2.00	0.62
2:E:1991:ILE:CG2	2:E:2008:LEU:HD22	2.29	0.62
2:B:2286:ARG:CD	2:B:2312:TYR:CD2	2.83	0.62
2:B:918:ASP:OD1	2:B:1515:LYS:NZ	2.27	0.62
2:E:1162:THR:HG22	2:E:1169:TYR:HB2	1.82	0.62
2:B:2294:PHE:HZ	2:B:2296:THR:HG21	1.63	0.61
2:E:1839:ASN:O	2:E:1842:GLU:HG3	2.00	0.61
2:B:1983:GLU:CB	2:B:1984:PRO:HD2	2.27	0.61
2:B:1324:GLY:HA2	2:B:1325:SER:CB	2.29	0.61
2:B:2046:GLU:O	2:B:2050:THR:N	2.33	0.61
2:E:2157:ILE:O	2:E:2160:THR:OG1	2.18	0.61
2:B:2278:SER:OG	2:B:2316:GLU:HG3	2.00	0.61
2:E:1834:PHE:CD2	2:E:1960:GLU:CG	2.84	0.61
1:D:83:GLU:HA	1:D:83:GLU:OE1	1.99	0.61
2:B:2043:PHE:CD2	2:B:2051:ILE:CD1	2.82	0.61
2:B:2286:ARG:HD3	2:B:2312:TYR:CD2	2.35	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2039:LEU:HB2	2:E:2040:TRP:HE1	1.59	0.61
2:B:1853:ASP:OD1	2:B:1855:THR:N	2.19	0.61
2:B:2224:VAL:C	2:B:2349:PHE:HE1	2.04	0.61
2:E:2353:SER:HA	2:E:2375:LYS:HD3	1.82	0.61
2:E:2028:SER:O	2:E:2030:PRO:CD	2.46	0.61
2:B:2185:LEU:O	2:B:2341:LEU:HA	2.00	0.61
2:B:2011:LEU:HD13	2:B:2040:TRP:CH2	2.35	0.61
2:E:2084:LEU:N	2:E:2084:LEU:HD13	2.14	0.61
2:E:1709:TRP:N	2:E:1729:THR:O	2.32	0.61
2:B:2154:LYS:O	2:B:2157:ILE:HD13	2.01	0.61
2:B:1759:TYR:HA	2:B:1762:ASP:HB2	1.82	0.61
2:E:1710:GLU:OE2	2:E:1725:LYS:HA	2.01	0.60
2:E:1324:GLY:CA	2:E:1325:SER:CB	2.76	0.60
2:E:2177:VAL:HG21	2:E:2180:GLN:CG	2.31	0.60
2:E:2358:ASN:HB3	2:E:2387:HIS:ND1	2.15	0.60
2:E:1966:SER:OG	2:E:2016:LYS:CE	2.46	0.60
2:B:2305:TYR:HB3	2:B:2334:SER:HB3	1.82	0.60
2:B:1137:PRO:CG	2:B:1140:ASN:O	2.48	0.60
2:B:1849:LYS:C	2:B:1850:LEU:HD23	2.22	0.60
1:A:354:ARG:HB2	1:A:355:PRO:HD3	1.83	0.60
2:E:1056:GLU:O	2:E:1060:LYS:HG2	2.01	0.60
2:E:2304:ALA:CB	2:E:2339:LEU:HD22	2.20	0.60
2:B:1858:TYR:HB2	2:B:1899:TRP:CH2	2.37	0.60
2:B:1823:LEU:O	2:B:1824:GLN:HB2	2.01	0.60
2:B:2277:HIS:HB3	2:B:2307:LEU:CD2	2.31	0.60
2:E:2177:VAL:CG2	2:E:2180:GLN:CB	2.80	0.60
2:B:2152:TRP:HA	2:B:2154:LYS:H	1.67	0.60
2:E:2214:ASP:OD1	2:E:2214:ASP:N	2.34	0.60
2:E:1468:ALA:HB1	2:E:1473:ARG:O	2.02	0.60
2:B:1705:SER:HB2	2:B:1730:ASN:O	2.00	0.60
2:E:1467:GLU:OE1	2:E:1470:GLN:NE2	2.35	0.60
2:B:1030:GLN:HE22	2:B:1288:LEU:HA	1.64	0.60
2:B:2236:VAL:HG21	2:B:2238:ILE:CD1	2.16	0.60
1:D:342:HIS:O	1:D:343:ASN:ND2	2.31	0.60
2:E:1999:LEU:HD11	2:E:2004:ALA:HB2	1.84	0.60
2:B:2227:VAL:HG12	2:B:2239:SER:HB3	1.84	0.60
2:E:1706:VAL:O	2:E:1706:VAL:HG23	2.01	0.60
2:E:1639:PRO:C	2:E:1640:THR:HG23	2.22	0.60
2:E:1476:ALA:HB3	2:E:1479:GLU:HG3	1.84	0.60
2:B:2182:VAL:HG12	2:B:2338:GLN:CD	2.21	0.59
2:B:2034:ILE:HG12	2:B:2041:PRO:N	2.18	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2309:ASP:O	2:B:2312:TYR:HB2	2.02	0.59
2:B:900:PHE:N	2:B:1075:ASP:OD2	2.35	0.59
2:B:2353:SER:O	2:B:2375:LYS:NZ	2.30	0.59
1:A:319:LYS:N	1:A:319:LYS:HD2	2.18	0.59
1:A:95:ASN:O	1:A:99:ARG:CB	2.51	0.59
2:E:1731:LYS:NZ	2:E:1768:PRO:HB2	2.17	0.59
1:A:314:PRO:HB2	1:A:319:LYS:HB2	1.84	0.59
2:B:1840:TYR:HH	2:B:2005:PHE:HD2	1.50	0.59
2:B:1747:ASP:CG	2:B:1750:ARG:HG3	2.23	0.59
2:E:1702:THR:CG2	2:E:1768:PRO:CG	2.77	0.59
2:B:2268:PHE:HA	2:B:2305:TYR:CE2	2.37	0.59
1:A:86:GLY:O	1:A:90:GLU:CG	2.46	0.59
2:E:1761:THR:O	2:E:1761:THR:OG1	2.21	0.59
2:B:2269:MET:HE3	2:B:2273:GLU:HB3	1.82	0.59
2:B:2309:ASP:O	2:B:2313:GLN:N	2.34	0.59
2:E:2080:LYS:CE	2:E:2083:ILE:HD11	2.30	0.59
2:E:2353:SER:HA	2:E:2375:LYS:HD2	1.84	0.59
2:B:1887:GLY:O	2:B:1991:ILE:HG22	2.03	0.59
2:B:1843:LEU:HD11	2:B:1884:PRO:HG2	1.84	0.59
2:B:1070:LEU:O	2:B:1074:VAL:HG22	2.03	0.59
2:B:2209:GLY:N	2:B:2254:GLU:O	2.35	0.59
2:B:1733:TRP:NE1	2:B:1771:THR:O	2.35	0.59
2:B:1324:GLY:HA2	2:B:1325:SER:OG	2.03	0.59
2:E:1034:ASN:OD1	2:E:1291:GLU:N	2.27	0.59
2:B:2350:ILE:HG23	2:B:2375:LYS:C	2.23	0.59
2:B:2302:LEU:HD12	2:B:2302:LEU:N	2.18	0.59
2:E:1067:ASN:HD22	2:E:1083:THR:CG2	2.11	0.59
2:B:1690:LYS:HA	2:B:1693:LYS:HG3	1.85	0.58
2:B:1453:ASP:OD2	2:B:1486:ARG:HD2	2.03	0.58
2:B:2230:LEU:O	2:B:2236:VAL:CG2	2.47	0.58
2:E:2039:LEU:C	2:E:2040:TRP:CG	2.76	0.58
2:E:1893:ILE:HG12	2:E:1985:GLN:O	2.03	0.58
2:B:2041:PRO:HG2	2:B:2043:PHE:CD1	2.38	0.58
2:B:2227:VAL:CG1	2:B:2239:SER:HB3	2.34	0.58
2:B:2265:GLU:O	2:B:2266:LEU:HD23	2.03	0.58
2:E:889:TRP:O	2:E:893:ARG:HG2	2.04	0.58
2:E:1015:PRO:HD2	2:E:1165:LEU:HD23	1.85	0.58
2:E:2267:LYS:O	2:E:2305:TYR:CZ	2.56	0.58
2:B:1687:HIS:HE1	2:B:1689:ARG:HG3	1.68	0.58
1:A:214:PHE:O	1:A:215:LYS:HB2	2.04	0.58
2:B:2183:TYR:HD2	2:B:2289:ILE:HD13	1.67	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1727:LEU:CD2	2:B:1728:ILE:H	2.15	0.58
2:E:2268:PHE:CD2	2:E:2331:PRO:HB3	2.38	0.58
2:E:1999:LEU:HD13	2:E:2003:THR:HB	1.85	0.58
2:B:2221:ILE:HD13	2:B:2256:LEU:HD12	1.85	0.58
2:B:1983:GLU:CB	2:B:1984:PRO:CD	2.80	0.58
2:B:2053:SER:HA	2:B:2056:ARG:HD2	1.86	0.58
2:B:1731:LYS:O	2:B:1771:THR:OG1	2.21	0.58
2:B:1476:ALA:O	2:B:1479:GLU:HB2	2.03	0.58
2:B:2038:HIS:N	2:B:2038:HIS:CD2	2.72	0.58
2:E:1091:ASN:HB3	2:E:1093:LYS:HE3	1.84	0.58
2:B:1056:GLU:O	2:B:1060:LYS:HG2	2.03	0.58
2:B:1025:VAL:O	2:B:1029:THR:HG23	2.04	0.58
1:D:344:PRO:HB3	2:E:1858:TYR:CE2	2.39	0.57
2:E:2041:PRO:CG	2:E:2043:PHE:CE1	2.80	0.57
2:E:2304:ALA:HB2	2:E:2339:LEU:HD21	1.73	0.57
2:E:2066:LYS:HB2	2:E:2067:TYR:HD1	1.69	0.57
2:E:1709:TRP:HB2	2:E:1729:THR:O	2.04	0.57
2:E:1834:PHE:O	2:E:1839:ASN:ND2	2.34	0.57
2:B:1186:TYR:HB2	2:B:1228:TRP:CZ3	2.39	0.57
2:E:1704:GLU:HA	2:E:1704:GLU:OE1	2.05	0.57
2:E:2021:SER:O	2:E:2024:MET:CB	2.53	0.57
2:B:2268:PHE:O	2:B:2268:PHE:HD1	1.88	0.57
2:B:2309:ASP:CA	2:B:2312:TYR:HB2	2.35	0.57
2:E:1826:TYR:HA	2:E:1827:GLN:HB2	1.86	0.57
2:E:1251:TYR:OH	2:E:1274:ARG:HD3	2.05	0.57
2:E:2162:LEU:HD21	2:E:2199:VAL:HG12	1.86	0.57
1:D:8:SER:OG	1:D:10:PRO:HD3	2.04	0.57
2:B:1019:GLU:HB2	2:B:1023:LEU:HD23	1.87	0.57
2:B:1015:PRO:CD	2:B:1165:LEU:HD23	2.29	0.57
2:B:2185:LEU:HG	2:B:2186:PRO:CD	2.33	0.57
1:A:327:ILE:HG23	2:B:1340:ILE:CD1	2.34	0.57
2:B:2194:ILE:HA	2:B:2197:SER:OG	2.04	0.57
2:B:2259:ILE:CD1	2:B:2291:ILE:O	2.33	0.57
2:B:1639:PRO:C	2:B:1640:THR:HG23	2.25	0.57
2:B:1251:TYR:OH	2:B:1274:ARG:HD3	2.04	0.57
1:A:8:SER:OG	1:A:10:PRO:HD3	2.05	0.57
2:B:2221:ILE:HD13	2:B:2256:LEU:CD1	2.35	0.57
1:D:87:ALA:O	1:D:90:GLU:HB3	2.04	0.57
2:B:2152:TRP:CA	2:B:2154:LYS:H	2.18	0.57
2:E:1324:GLY:HA3	2:E:1325:SER:OG	2.02	0.57
2:B:889:TRP:O	2:B:893:ARG:HG2	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1721:ASN:OD1	2:E:1722:ASP:N	2.38	0.57
2:B:2228:PRO:O	2:B:2239:SER:HB3	2.05	0.57
2:B:1477:PHE:CE2	2:B:1495:PHE:CD2	2.93	0.57
2:E:1687:HIS:HE1	2:E:1689:ARG:HG3	1.69	0.57
2:B:2046:GLU:O	2:B:2049:ILE:N	2.38	0.56
2:E:2018:ASN:CG	2:E:2058:LEU:HD11	2.20	0.56
2:B:2307:LEU:HD11	2:B:2311:GLY:HA3	1.88	0.56
2:B:2191:LYS:C	2:B:2195:GLU:HG3	2.25	0.56
2:E:2358:ASN:H	2:E:2387:HIS:CE1	2.22	0.56
2:B:1976:ASP:OD1	2:B:1980:LYS:HG3	2.05	0.56
2:B:1977:VAL:HG13	2:B:1978:VAL:N	2.19	0.56
2:E:930:ASN:HD22	2:E:933:GLU:HB2	1.70	0.56
2:B:2281:PHE:CE1	2:B:2288:CYS:CB	2.87	0.56
2:E:1468:ALA:O	2:E:1472:ASN:N	2.38	0.56
2:B:2035:LYS:HD2	2:B:2037:TYR:HE1	1.68	0.56
2:B:1887:GLY:HA2	2:B:1992:TYR:CE2	2.40	0.56
2:E:1826:TYR:OH	2:E:1938:LYS:CE	2.53	0.56
2:E:1687:HIS:CE1	2:E:1688:PRO:HD2	2.41	0.56
2:B:2210:MET:CE	2:B:2253:LEU:N	2.69	0.56
2:E:2277:HIS:CE1	2:E:2281:PHE:CD2	2.94	0.56
2:B:2060:LEU:O	2:B:2064:GLY:N	2.38	0.56
2:B:1995:TRP:HH2	2:B:2011:LEU:HD11	1.71	0.56
2:B:1075:ASP:OD1	2:B:1076:PRO:HD2	2.05	0.56
2:B:1605:ARG:CZ	2:B:1824:GLN:OE1	2.53	0.56
2:E:2162:LEU:HD12	2:E:2194:ILE:O	2.06	0.56
2:E:1431:HIS:C	2:E:1433:ASP:H	2.07	0.56
2:B:1264:GLY:O	2:B:1305:SER:OG	2.24	0.56
1:A:108:ILE:HG22	1:A:109:ASP:O	2.04	0.56
2:B:2235:SER:HB3	2:B:2322:MET:HA	1.88	0.56
2:B:2208:TYR:CB	2:B:2253:LEU:HD11	2.35	0.56
2:E:1973:LYS:HE3	2:E:2038:HIS:O	2.06	0.56
2:B:2315:GLY:C	2:B:2318:ASN:H	2.08	0.56
2:E:2182:VAL:HG12	2:E:2338:GLN:CB	2.36	0.56
2:B:2282:ALA:HB1	2:B:2316:GLU:OE2	2.03	0.56
2:E:2210:MET:HE1	2:E:2252:GLY:CA	2.22	0.56
2:B:2208:TYR:HB3	2:B:2253:LEU:HD22	1.84	0.56
2:B:2037:TYR:CB	2:B:2038:HIS:CD2	2.79	0.56
2:E:1711:VAL:HG12	2:E:1791:PHE:CB	2.34	0.56
2:E:1711:VAL:HG12	2:E:1791:PHE:CA	2.36	0.56
2:B:2024:MET:SD	2:B:2157:ILE:HG22	2.46	0.56
2:E:1826:TYR:CZ	2:E:1938:LYS:NZ	2.72	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2043:PHE:CD2	2:B:2047:GLN:OE1	2.59	0.55
2:B:2247:LEU:CG	2:B:2375:LYS:HA	2.35	0.55
2:B:2258:TRP:HD1	2:B:2258:TRP:H	1.52	0.55
2:B:2358:ASN:CB	2:B:2387:HIS:ND1	2.47	0.55
2:B:2003:THR:O	2:B:2006:SER:N	2.38	0.55
2:E:1293:THR:O	2:E:1295:GLN:N	2.39	0.55
1:A:31:HIS:HB3	1:A:96:PHE:CD2	2.41	0.55
2:E:2178:GLU:O	2:E:2217:LYS:CD	2.55	0.55
2:E:1731:LYS:NZ	2:E:1768:PRO:CB	2.68	0.55
2:B:1598:LEU:HD13	2:B:1598:LEU:C	2.26	0.55
2:E:2025:ILE:HG23	2:E:2054:GLN:CD	2.26	0.55
2:E:2213:LYS:CA	2:E:2215:HIS:H	2.12	0.55
2:B:1887:GLY:CA	2:B:1992:TYR:CE2	2.90	0.55
2:E:1293:THR:OG1	2:E:1293:THR:O	2.24	0.55
2:B:1687:HIS:CE1	2:B:1688:PRO:HD2	2.41	0.55
2:E:2087:ASN:HD22	2:E:2088:ILE:N	2.04	0.55
1:A:85:ASP:OD1	1:A:88:LYS:N	2.22	0.55
2:B:2183:TYR:HD1	2:B:2219:LYS:HB2	1.71	0.55
2:E:1998:ARG:HD2	2:E:2045:ASP:CG	2.27	0.55
2:E:2278:SER:OG	2:E:2279:LYS:N	2.39	0.55
2:B:1795:LYS:HB3	2:B:1796:PRO:HD3	1.89	0.55
2:E:1259:LEU:HD23	2:E:1268:ARG:HG3	1.89	0.55
2:B:2037:TYR:CB	2:B:2038:HIS:HD2	2.15	0.55
2:B:1895:HIS:NE2	2:B:1896:THR:OG1	2.38	0.55
1:D:69:ILE:HD13	1:D:80:MET:HA	1.89	0.55
2:B:1866:PHE:H	2:B:1866:PHE:HD1	1.53	0.55
2:B:2024:MET:SD	2:B:2157:ILE:CG2	2.95	0.55
2:E:2232:HIS:HE1	2:E:2237:GLN:HE21	1.55	0.55
2:E:1991:ILE:HG23	2:E:2008:LEU:HD22	1.89	0.55
1:A:48:HIS:CE1	1:A:53:SER:HG	2.25	0.55
2:B:2017:THR:CG2	2:B:2062:GLU:HG3	2.37	0.55
2:B:2208:TYR:CG	2:B:2253:LEU:HD13	2.42	0.55
2:E:2193:PHE:CZ	2:E:2203:VAL:HG12	2.42	0.55
2:E:2244:ILE:O	2:E:2250:THR:HG21	2.06	0.55
2:B:2002:TYR:CD1	2:B:2002:TYR:C	2.80	0.54
2:E:2034:ILE:CD1	2:E:2040:TRP:C	2.58	0.54
2:B:2037:TYR:C	2:B:2038:HIS:CD2	2.80	0.54
2:B:1733:TRP:CE2	2:B:1772:GLY:HA3	2.41	0.54
2:B:2386:MET:HE2	2:B:2387:HIS:N	2.22	0.54
2:B:1679:GLU:HB3	2:B:1704:GLU:O	2.07	0.54
2:B:2182:VAL:N	2:B:2338:GLN:HB2	2.22	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2061:THR:O	2:B:2064:GLY:N	2.41	0.54
2:B:2259:ILE:CD1	2:B:2291:ILE:CA	2.84	0.54
2:B:2209:GLY:HA3	2:B:2256:LEU:CD2	2.35	0.54
2:B:2183:TYR:HD1	2:B:2219:LYS:CB	2.20	0.54
2:E:1598:LEU:HD22	2:E:1598:LEU:C	2.28	0.54
2:E:2179:GLU:HG2	2:E:2180:GLN:N	2.22	0.54
2:B:2037:TYR:N	2:B:2037:TYR:CD1	2.76	0.54
2:B:2382:PHE:HB3	2:B:2383:TYR:HD1	1.72	0.54
2:B:1704:GLU:CG	2:B:1705:SER:H	2.20	0.54
2:B:2262:GLN:N	2:B:2293:ILE:O	2.41	0.54
2:B:934:ARG:HG2	2:B:934:ARG:HH11	1.73	0.54
2:B:2192:LYS:HA	2:B:2195:GLU:CG	2.37	0.54
2:E:1710:GLU:HA	2:E:1728:ILE:HA	1.90	0.54
2:B:2192:LYS:CA	2:B:2195:GLU:HB2	2.37	0.54
1:A:347:VAL:HG21	2:B:1875:ILE:CD1	2.33	0.54
2:B:1259:LEU:HD23	2:B:1268:ARG:HG3	1.90	0.54
2:E:1624:LEU:HD23	2:E:1625:VAL:N	2.22	0.54
1:D:35:ASP:OD2	1:D:104:SER:OG	2.25	0.54
2:E:1825:ILE:O	2:E:1826:TYR:HB3	2.08	0.54
2:E:1466:GLN:O	2:E:1469:ILE:HB	2.07	0.54
2:B:885:VAL:HG21	2:B:1124:LEU:HD21	1.90	0.54
1:A:12:GLU:HG3	1:A:25:LYS:HA	1.89	0.54
2:B:2208:TYR:HB3	2:B:2253:LEU:HD11	1.90	0.54
2:E:2079:ILE:HD13	2:E:2079:ILE:N	2.23	0.54
2:B:1139:ASN:H	2:B:1139:ASN:ND2	2.05	0.54
2:B:2050:THR:HA	2:B:2053:SER:OG	2.06	0.54
2:B:2209:GLY:O	2:B:2254:GLU:O	2.25	0.54
2:B:2358:ASN:O	2:B:2387:HIS:ND1	2.41	0.54
2:E:1292:ARG:HG2	2:E:1292:ARG:HH11	1.72	0.54
2:B:1598:LEU:H	2:B:1598:LEU:HD12	1.72	0.54
1:D:354:ARG:HB2	1:D:355:PRO:HD3	1.89	0.54
2:B:1882:LEU:CD1	2:B:1991:ILE:HG21	2.37	0.54
2:B:1801:SER:O	2:B:1805:ILE:HG23	2.08	0.54
2:B:2007:ARG:HG2	2:B:2052:GLU:CD	2.28	0.53
2:B:2278:SER:HB3	2:B:2316:GLU:CG	2.38	0.53
2:B:2210:MET:HE2	2:B:2252:GLY:C	2.27	0.53
2:B:1961:ASN:HA	2:B:2079:ILE:HD12	1.89	0.53
2:B:2188:ASN:ND2	2:B:2346:THR:HB	2.20	0.53
2:B:1070:LEU:O	2:B:1074:VAL:CG2	2.56	0.53
2:B:2386:MET:HE2	2:B:2387:HIS:H	1.73	0.53
2:E:1702:THR:HG23	2:E:1768:PRO:HG3	1.85	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2296:THR:O	2:B:2297:PRO:C	2.44	0.53
2:B:1190:ASN:N	2:B:1191:PRO:HD3	2.22	0.53
2:B:1866:PHE:N	2:B:1866:PHE:CD1	2.76	0.53
2:E:1899:TRP:CE3	2:E:1899:TRP:HA	2.43	0.53
2:B:2007:ARG:NE	2:B:2052:GLU:OE2	2.41	0.53
2:B:2184:VAL:O	2:B:2221:ILE:HG12	2.08	0.53
2:B:2256:LEU:C	2:B:2288:CYS:HG	2.03	0.53
1:D:347:VAL:HG21	2:E:1875:ILE:CD1	2.38	0.53
1:A:208:VAL:O	1:A:213:ILE:HD12	2.08	0.53
2:E:2202:GLN:NE2	2:E:2235:SER:O	2.37	0.53
2:E:1259:LEU:CD2	2:E:1268:ARG:HG3	2.38	0.53
2:B:2202:GLN:HG2	2:B:2261:THR:O	2.09	0.53
2:E:1801:SER:O	2:E:1805:ILE:HG12	2.09	0.53
2:B:950:THR:O	2:B:954:ILE:N	2.40	0.53
2:E:2227:VAL:HG13	2:E:2228:PRO:HD2	1.91	0.53
2:B:2233:VAL:HG23	2:B:2234:GLY:N	2.24	0.53
1:D:109:ASP:OD1	1:D:110:GLU:N	2.42	0.53
1:A:109:ASP:OD2	1:A:113:THR:OG1	2.27	0.53
2:E:2003:THR:O	2:E:2006:SER:N	2.42	0.53
2:B:2035:LYS:HB3	2:B:2037:TYR:CD1	2.43	0.53
2:B:2185:LEU:O	2:B:2342:SER:N	2.37	0.53
2:B:2202:GLN:CG	2:B:2261:THR:O	2.57	0.53
2:B:1624:LEU:HD23	2:B:1624:LEU:C	2.29	0.53
2:B:2339:LEU:C	2:B:2339:LEU:HD12	2.26	0.53
2:B:2339:LEU:HD13	2:B:2340:LEU:H	1.68	0.53
2:E:2384:ASN:ND2	2:E:2385:GLU:N	2.57	0.53
2:B:1598:LEU:H	2:B:1598:LEU:CD1	2.21	0.53
2:E:1104:ILE:CG2	2:E:1107:LEU:HD13	2.39	0.53
1:A:69:ILE:HD13	1:A:80:MET:HA	1.90	0.53
2:B:2339:LEU:C	2:B:2340:LEU:HD12	2.24	0.52
2:B:1259:LEU:CD2	2:B:1268:ARG:HG3	2.39	0.52
2:B:2294:PHE:CD2	2:B:2301:SER:OG	2.36	0.52
1:A:214:PHE:CE1	1:A:220:TYR:HA	2.44	0.52
2:B:2273:GLU:OE2	2:B:2290:ASP:OD2	2.26	0.52
2:B:1107:LEU:HD23	2:B:1109:PHE:CE1	2.44	0.52
2:E:2024:MET:O	2:E:2027:LEU:N	2.42	0.52
2:B:2350:ILE:HD13	2:B:2376:TYR:CA	2.30	0.52
2:E:1279:VAL:HG12	2:E:1280:SER:O	2.09	0.52
2:B:1719:GLU:HA	2:B:1719:GLU:OE1	2.09	0.52
2:B:1466:GLN:OE1	2:B:1466:GLN:HA	2.08	0.52
2:E:2014:ALA:HA	2:E:2059:ILE:HD12	1.87	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2083:ILE:HG22	2:E:2084:LEU:CD1	2.38	0.52
2:B:2223:THR:OG1	2:B:2348:ASN:OD1	2.08	0.52
2:E:1966:SER:HG	2:E:2016:LYS:HE3	1.72	0.52
2:B:1599:SER:C	2:B:1600:GLN:HG2	2.29	0.52
2:B:1721:ASN:CB	2:E:1463:THR:HB	2.39	0.52
2:B:1383:PHE:HE2	2:B:1387:VAL:HG21	1.75	0.52
2:E:2043:PHE:HA	2:E:2047:GLN:OE1	2.10	0.52
2:B:2183:TYR:CE2	2:B:2289:ILE:HD13	2.44	0.52
2:E:1324:GLY:HA2	2:E:1325:SER:HG	1.71	0.52
2:E:2267:LYS:O	2:E:2305:TYR:CE1	2.63	0.52
2:E:2182:VAL:HG12	2:E:2338:GLN:HB2	1.91	0.52
2:B:1104:ILE:CG2	2:B:1107:LEU:HD13	2.39	0.52
2:E:1864:LYS:HG3	2:E:1870:VAL:HG22	1.90	0.52
2:E:1767:TYR:CD1	2:E:1767:TYR:N	2.77	0.52
2:E:2060:LEU:O	2:E:2063:TYR:HB3	2.09	0.52
2:B:2280:LEU:CD1	2:B:2281:PHE:CE2	2.91	0.52
1:D:106:PRO:C	1:D:107:LYS:CG	2.72	0.52
2:E:2384:ASN:HD22	2:E:2386:MET:N	2.02	0.52
2:B:1848:ILE:O	2:B:1930:PRO:HA	2.09	0.52
2:B:2060:LEU:O	2:B:2063:TYR:CB	2.53	0.52
2:E:918:ASP:OD1	2:E:1515:LYS:NZ	2.39	0.52
2:E:1286:TRP:CE2	2:E:1302:LEU:HD11	2.45	0.52
1:D:88:LYS:O	1:D:92:ILE:HG13	2.10	0.52
2:E:1666:CYS:SG	2:E:1683:LYS:HE3	2.50	0.52
2:B:2357:TRP:CH2	2:B:2382:PHE:HD1	2.22	0.52
2:E:1212:ARG:HG2	2:E:1212:ARG:HH11	1.74	0.52
2:B:1595:ARG:HG3	2:B:1596:THR:N	2.24	0.52
2:E:2074:LEU:C	2:E:2075:THR:HG1	2.09	0.52
2:B:2233:VAL:CG2	2:B:2234:GLY:N	2.73	0.52
2:E:2011:LEU:O	2:E:2014:ALA:HB3	2.09	0.51
1:A:296:SER:O	1:A:299:LYS:HG2	2.10	0.51
2:B:1093:LYS:HE2	2:B:1094:ASP:OD1	2.10	0.51
2:E:2302:LEU:HD12	2:E:2302:LEU:N	2.24	0.51
2:B:2182:VAL:HG13	2:B:2338:GLN:CD	2.23	0.51
2:B:2286:ARG:HD2	2:B:2312:TYR:CE2	2.45	0.51
2:B:2035:LYS:CD	2:B:2037:TYR:HE1	2.22	0.51
2:B:2152:TRP:HA	2:B:2153:ARG:C	2.29	0.51
2:E:1093:LYS:CD	2:E:1094:ASP:HA	2.41	0.51
1:D:20:TYR:CZ	1:D:106:PRO:HG2	2.44	0.51
2:E:1107:LEU:HD23	2:E:1109:PHE:CE1	2.45	0.51
2:E:1763:ASN:H	2:E:1763:ASN:HD22	1.58	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2064:GLY:O	2:E:2067:TYR:CA	2.58	0.51
2:B:2162:LEU:HD23	2:B:2165:ARG:NE	2.24	0.51
2:E:2062:GLU:OE2	2:E:2065:ARG:NH2	2.34	0.51
2:E:1991:ILE:HG21	2:E:2008:LEU:HD22	1.92	0.51
2:B:2189:LEU:HD21	2:B:2347:GLY:CA	2.40	0.51
2:E:2361:PHE:CZ	2:E:2383:TYR:CE1	2.98	0.51
2:E:1097:HIS:CD2	2:E:1098:VAL:O	2.63	0.51
2:E:1899:TRP:HE3	2:E:1899:TRP:HA	1.75	0.51
2:E:1767:TYR:N	2:E:1767:TYR:HD1	2.09	0.51
2:B:959:LEU:HD12	2:B:1077:ASN:OD1	2.11	0.51
2:B:2037:TYR:HB2	2:B:2038:HIS:NE2	2.26	0.51
2:E:2357:TRP:H	2:E:2387:HIS:CE1	2.28	0.51
2:B:2017:THR:HG23	2:B:2062:GLU:OE2	2.11	0.51
2:B:1041:VAL:HG21	2:B:1253:LYS:HA	1.91	0.51
2:E:1843:LEU:HD22	2:E:1884:PRO:HG3	1.93	0.51
2:B:2155:SER:O	2:B:2156:ALA:HB3	2.10	0.51
2:E:1292:ARG:NH1	2:E:1292:ARG:HG2	2.26	0.51
2:E:920:LYS:HG3	2:E:940:ILE:HG21	1.92	0.51
2:E:2050:THR:HA	2:E:2053:SER:HB3	1.93	0.51
2:E:2025:ILE:CG2	2:E:2054:GLN:CD	2.79	0.51
2:B:2210:MET:HE1	2:B:2253:LEU:CB	2.40	0.51
2:E:1472:ASN:C	2:E:2325:LEU:CB	2.75	0.51
2:B:2019:GLU:OE2	2:B:2167:LYS:NZ	2.44	0.51
2:B:1105:ARG:HG3	2:B:1105:ARG:NH1	2.25	0.51
2:B:1029:THR:HG22	2:B:1260:PHE:CZ	2.46	0.51
2:B:1029:THR:HG22	2:B:1260:PHE:HZ	1.75	0.51
2:E:2041:PRO:HG2	2:E:2043:PHE:CE1	2.46	0.50
2:E:2049:ILE:O	2:E:2053:SER:HB3	2.11	0.50
2:B:2208:TYR:CB	2:B:2253:LEU:CD1	2.88	0.50
2:B:1687:HIS:CE1	2:B:1689:ARG:HG3	2.46	0.50
2:B:2236:VAL:CB	2:B:2238:ILE:HD11	2.41	0.50
2:E:2034:ILE:CG2	2:E:2040:TRP:H	2.22	0.50
2:B:1075:ASP:HB3	2:B:1078:ILE:HD12	1.93	0.50
2:B:2157:ILE:HA	2:B:2160:THR:OG1	2.10	0.50
2:B:1661:ILE:HG23	2:B:1805:ILE:CD1	2.41	0.50
2:E:1605:ARG:NH2	2:E:1824:GLN:OE1	2.44	0.50
2:B:1317:ARG:O	2:B:1321:MET:HB2	2.12	0.50
2:E:1599:SER:C	2:E:1600:GLN:HG2	2.31	0.50
2:B:1999:LEU:CD1	2:B:2003:THR:HB	2.36	0.50
2:B:2350:ILE:CD1	2:B:2376:TYR:HA	2.31	0.50
2:B:2194:ILE:O	2:B:2197:SER:OG	2.28	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2183:TYR:OH	2:B:2219:LYS:NZ	2.37	0.50
2:B:2247:LEU:CD1	2:B:2248:PRO:HD3	2.41	0.50
1:D:55:ARG:NH2	1:D:279:TYR:CZ	2.79	0.50
2:E:2227:VAL:HG13	2:E:2239:SER:OG	2.10	0.50
2:E:1687:HIS:CE1	2:E:1689:ARG:HG3	2.46	0.50
2:E:1057:MET:CE	2:E:1166:ASP:HB2	2.41	0.50
2:E:1795:LYS:HB3	2:E:1796:PRO:HD3	1.94	0.50
2:E:1343:PHE:HB3	2:E:1444:ILE:CD1	2.40	0.50
2:E:2040:TRP:N	2:E:2040:TRP:CD1	2.80	0.50
2:B:2157:ILE:CA	2:B:2160:THR:OG1	2.60	0.50
2:B:2162:LEU:CD2	2:B:2165:ARG:NE	2.74	0.50
2:B:1854:ASP:HA	2:B:1857:VAL:HG23	1.94	0.50
2:E:885:VAL:HG21	2:E:1124:LEU:HD21	1.94	0.50
2:E:1983:GLU:HB2	2:E:1984:PRO:HD2	1.94	0.50
2:B:2032:ILE:CD1	2:B:2047:GLN:HE22	2.24	0.50
2:E:2018:ASN:ND2	2:E:2058:LEU:HG	2.17	0.50
2:B:2350:ILE:CD1	2:B:2376:TYR:CD1	2.95	0.50
1:A:327:ILE:HB	1:A:328:TYR:CD2	2.47	0.50
2:B:1969:MET:O	2:B:1975:SER:OG	2.30	0.50
2:E:1764:VAL:N	2:E:1766:MET:HE2	2.24	0.50
1:D:280:SER:HB2	1:D:313:TYR:CE1	2.47	0.50
1:D:153:LEU:C	1:D:153:LEU:HD23	2.32	0.50
2:B:2278:SER:CB	2:B:2316:GLU:HG3	2.42	0.50
2:E:945:ASP:N	2:E:945:ASP:OD1	2.45	0.50
1:A:215:LYS:O	1:A:216:ASN:OD1	2.29	0.50
2:B:1036:SER:HB3	2:B:1154:LYS:HE2	1.93	0.50
2:E:2051:ILE:N	2:E:2051:ILE:HD13	2.27	0.49
2:E:2083:ILE:HG22	2:E:2084:LEU:H	1.77	0.49
2:E:2177:VAL:CG2	2:E:2180:GLN:HG3	2.42	0.49
1:D:19:GLN:HE22	1:D:110:GLU:CG	2.18	0.49
2:E:2182:VAL:HA	2:E:2338:GLN:HB2	1.92	0.49
2:E:1854:ASP:OD1	2:E:1937:ARG:HD3	2.11	0.49
2:E:2311:GLY:HA2	2:E:2333:PHE:CD1	2.46	0.49
2:B:2182:VAL:O	2:B:2182:VAL:HG23	2.11	0.49
2:E:2083:ILE:HG22	2:E:2084:LEU:N	2.27	0.49
2:E:2064:GLY:C	2:E:2067:TYR:H	2.11	0.49
2:E:1705:SER:OG	2:E:1730:ASN:CB	2.60	0.49
2:E:1015:PRO:CD	2:E:1165:LEU:HD23	2.42	0.49
2:B:969:ILE:HA	2:B:981:VAL:O	2.12	0.49
2:B:1890:PHE:HB3	2:B:1986:MET:SD	2.52	0.49
2:B:1666:CYS:SG	2:B:1683:LYS:HE3	2.52	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1604:ARG:HH22	2:B:1822:GLY:C	2.14	0.49
2:B:2192:LYS:HA	2:B:2195:GLU:CB	2.41	0.49
1:D:151:GLU:OE2	1:D:154:LYS:CE	2.49	0.49
1:A:280:SER:HB2	1:A:313:TYR:CE1	2.48	0.49
2:B:2041:PRO:CG	2:B:2043:PHE:CE1	2.96	0.49
2:B:2052:GLU:O	2:B:2056:ARG:CG	2.40	0.49
2:E:1711:VAL:CA	2:E:1790:TRP:O	2.60	0.49
2:B:1015:PRO:CD	2:B:1165:LEU:CD2	2.90	0.49
2:E:2201:ILE:HG22	2:E:2382:PHE:CZ	2.48	0.49
2:E:988:GLU:O	2:E:991:THR:HG22	2.12	0.49
1:D:77:LEU:C	1:D:77:LEU:HD12	2.33	0.49
2:B:2208:TYR:C	2:B:2253:LEU:HD21	2.33	0.49
2:B:2247:LEU:CD1	2:B:2375:LYS:HA	2.42	0.49
2:E:1394:LEU:HD23	2:E:1570:TRP:CZ2	2.47	0.49
2:E:2163:TYR:CE1	2:E:2164:LEU:CD2	2.96	0.49
2:B:1463:THR:O	2:B:1467:GLU:HG2	2.12	0.49
2:E:1766:MET:C	2:E:1767:TYR:HD1	2.16	0.49
2:B:2153:ARG:HA	2:B:2155:SER:O	2.12	0.49
1:D:88:LYS:NZ	1:D:92:ILE:HD11	2.27	0.49
1:D:326:LEU:O	1:D:326:LEU:HG	2.13	0.49
2:B:2055:MET:O	2:B:2058:LEU:N	2.45	0.49
1:D:110:GLU:O	1:D:111:ASP:CB	2.60	0.49
2:B:1687:HIS:ND1	2:B:1688:PRO:CD	2.76	0.49
2:B:2064:GLY:O	2:B:2068:ASN:N	2.45	0.49
2:E:1368:GLN:NE2	2:E:1389:TYR:OH	2.44	0.49
2:E:1383:PHE:HE2	2:E:1387:VAL:HG21	1.75	0.49
1:A:72:ASP:OD2	1:A:75:ASP:HB2	2.13	0.49
2:E:1036:SER:HB3	2:E:1154:LYS:HE2	1.95	0.49
1:A:83:GLU:CG	1:A:89:PHE:HB2	2.42	0.49
2:B:2182:VAL:CB	2:B:2338:GLN:CB	2.89	0.49
2:B:2183:TYR:N	2:B:2338:GLN:O	2.40	0.49
2:E:2177:VAL:HG23	2:E:2180:GLN:N	2.19	0.49
2:E:1461:TYR:O	2:E:1465:ARG:N	2.44	0.49
2:B:1137:PRO:CD	2:B:1140:ASN:O	2.61	0.49
2:B:2284:LYS:HE2	2:B:2285:LYS:CA	2.42	0.49
2:B:1324:GLY:CA	2:B:1325:SER:CB	2.91	0.49
2:B:1097:HIS:ND1	2:B:1098:VAL:N	2.60	0.49
2:E:2251:GLU:N	2:E:2251:GLU:OE1	2.46	0.49
2:B:930:ASN:N	2:B:933:GLU:OE1	2.46	0.49
2:B:1624:LEU:HD21	2:B:1633:PHE:CD1	2.48	0.49
2:B:920:LYS:HG3	2:B:940:ILE:HG21	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1993:ASP:CG	2:B:2038:HIS:CB	2.58	0.49
2:B:2381:GLU:CD	2:B:2381:GLU:H	2.00	0.49
2:E:2087:ASN:ND2	2:E:2088:ILE:N	2.61	0.49
2:B:1808:ALA:O	2:B:1809:ASN:C	2.51	0.49
2:B:2044:THR:H	2:B:2047:GLN:NE2	2.11	0.48
2:B:2259:ILE:HD12	2:B:2291:ILE:CA	2.42	0.48
2:B:2259:ILE:HD13	2:B:2291:ILE:HG21	1.82	0.48
2:B:1729:THR:CG2	2:B:1771:THR:CG2	2.54	0.48
2:E:2384:ASN:C	2:E:2384:ASN:HD22	2.16	0.48
2:B:2379:PRO:C	2:B:2380:LEU:HD23	2.33	0.48
2:E:2163:TYR:CD1	2:E:2164:LEU:N	2.81	0.48
2:B:1465:ARG:HG3	2:B:1465:ARG:NH1	2.28	0.48
2:B:2282:ALA:O	2:B:2286:ARG:HG2	2.14	0.48
2:E:2177:VAL:CG2	2:E:2180:GLN:CG	2.91	0.48
2:E:1733:TRP:CE2	2:E:1767:TYR:CD2	2.97	0.48
2:E:2163:TYR:CE1	2:E:2164:LEU:HD23	2.48	0.48
2:E:2183:TYR:CD1	2:E:2289:ILE:HD13	2.48	0.48
2:B:2342:SER:HG	2:B:2344:ARG:H	1.59	0.48
2:B:2307:LEU:C	2:B:2307:LEU:HD12	2.28	0.48
2:B:2208:TYR:OH	2:B:2244:ILE:HG23	2.13	0.48
2:E:1209:LYS:HG2	2:E:1212:ARG:NH2	2.27	0.48
2:E:2270:ALA:HB1	2:E:2324:VAL:HA	1.95	0.48
2:E:2269:MET:HE3	2:E:2273:GLU:HB3	1.95	0.48
2:B:2044:THR:O	2:B:2048:TRP:CD1	2.66	0.48
2:E:1709:TRP:O	2:E:1728:ILE:CA	2.62	0.48
2:B:2284:LYS:HE3	2:B:2284:LYS:C	2.34	0.48
2:E:2183:TYR:CE1	2:E:2289:ILE:HG21	2.48	0.48
2:B:1432:GLU:O	2:B:1433:ASP:CB	2.61	0.48
1:D:224:LEU:C	1:D:224:LEU:HD23	2.33	0.48
2:B:2280:LEU:HD12	2:B:2281:PHE:CD2	2.49	0.48
2:B:2386:MET:CE	2:B:2387:HIS:N	2.76	0.48
2:B:930:ASN:O	2:B:934:ARG:HB2	2.14	0.48
2:B:2210:MET:CE	2:B:2252:GLY:C	2.82	0.48
2:E:1762:ASP:CG	2:E:1763:ASN:N	2.66	0.48
2:E:1343:PHE:HB3	2:E:1444:ILE:HD13	1.96	0.48
2:E:2271:ALA:HA	2:E:2329:PHE:CE1	2.48	0.48
2:B:2278:SER:HB3	2:B:2316:GLU:HG2	1.96	0.48
2:E:1865:THR:OG1	2:E:1867:GLU:OE1	2.31	0.48
2:E:2019:GLU:HG2	2:E:2019:GLU:O	2.14	0.48
2:B:1687:HIS:CG	2:B:1688:PRO:HD2	2.49	0.48
2:B:2384:ASN:HD22	2:B:2385:GLU:N	2.11	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1899:TRP:HB3	2:B:1905:LEU:HD21	1.95	0.48
1:D:280:SER:CB	1:D:313:TYR:CE1	2.97	0.48
1:A:77:LEU:C	1:A:77:LEU:HD12	2.33	0.48
1:A:77:LEU:O	1:A:77:LEU:HD12	2.14	0.48
2:B:2183:TYR:HE2	2:B:2289:ILE:HG21	1.79	0.48
2:B:2307:LEU:CD1	2:B:2308:THR:O	2.62	0.48
2:B:2358:ASN:CB	2:B:2387:HIS:HE1	2.04	0.48
2:E:2037:TYR:C	2:E:2038:HIS:CD2	2.88	0.48
2:E:2066:LYS:HB2	2:E:2067:TYR:CE1	2.49	0.48
2:B:1188:ALA:O	2:B:1191:PRO:CD	2.62	0.48
2:B:1164:TYR:O	2:B:1167:ARG:N	2.42	0.48
2:B:1368:GLN:NE2	2:B:1389:TYR:OH	2.47	0.48
2:B:1959:THR:OG1	2:B:1960:GLU:N	2.47	0.48
2:B:2177:VAL:N	2:B:2338:GLN:NE2	2.59	0.47
2:E:2268:PHE:C	2:E:2268:PHE:CD1	2.87	0.47
1:A:108:ILE:N	1:A:108:ILE:HD12	2.29	0.47
2:B:1041:VAL:O	2:B:1041:VAL:HG23	2.13	0.47
2:B:936:GLU:O	2:B:940:ILE:CD1	2.61	0.47
2:B:1570:TRP:O	2:B:1571:GLU:HG3	2.14	0.47
2:B:2267:LYS:O	2:B:2305:TYR:HE2	1.96	0.47
2:E:2277:HIS:O	2:E:2281:PHE:HD2	1.96	0.47
2:B:2186:PRO:HG3	2:B:2345:ILE:HD12	1.95	0.47
2:B:1759:TYR:O	2:B:1762:ASP:CB	2.62	0.47
2:B:2350:ILE:HD11	2:B:2376:TYR:CE1	2.49	0.47
2:B:2294:PHE:CE1	2:B:2296:THR:HG23	2.48	0.47
2:B:1895:HIS:CD2	2:B:1896:THR:HG1	2.26	0.47
2:B:1624:LEU:HD23	2:B:1625:VAL:N	2.30	0.47
2:B:2058:LEU:O	2:B:2059:ILE:C	2.52	0.47
2:B:1394:LEU:HD23	2:B:1570:TRP:CZ2	2.49	0.47
2:B:1558:GLU:CD	2:B:1563:LYS:HZ1	2.17	0.47
2:B:1677:GLN:OE1	2:B:1706:VAL:HG11	2.15	0.47
1:D:108:ILE:H	1:D:108:ILE:HD13	1.78	0.47
2:B:2268:PHE:CE2	2:B:2331:PRO:HG3	2.49	0.47
2:B:1189:GLU:C	2:B:1191:PRO:HD3	2.35	0.47
2:E:936:GLU:O	2:E:940:ILE:CD1	2.61	0.47
2:B:2025:ILE:O	2:B:2025:ILE:HG22	2.12	0.47
2:E:2053:SER:OG	2:E:2054:GLN:N	2.48	0.47
2:E:1472:ASN:HB3	2:E:2325:LEU:O	2.14	0.47
2:B:2302:LEU:CD1	2:B:2302:LEU:N	2.77	0.47
2:E:1791:PHE:CD1	2:E:1791:PHE:C	2.87	0.47
2:B:953:ARG:HG3	2:B:953:ARG:HH11	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2230:LEU:CD2	2:B:2237:GLN:HG3	2.44	0.47
2:E:2339:LEU:O	2:E:2340:LEU:HD12	2.14	0.47
2:E:2004:ALA:O	2:E:2007:ARG:HB3	2.14	0.47
2:B:1075:ASP:CB	2:B:1078:ILE:HD12	2.45	0.47
2:B:2192:LYS:O	2:B:2196:ILE:N	2.46	0.47
2:B:2247:LEU:HA	2:B:2247:LEU:HD13	1.74	0.47
2:E:1079:ALA:O	2:E:1083:THR:HG22	2.15	0.47
2:B:2163:TYR:CD1	2:B:2164:LEU:N	2.83	0.47
2:B:2306:ASN:HB2	2:B:2335:THR:OG1	2.14	0.47
2:E:1886:THR:CB	2:E:1888:HIS:CE1	2.96	0.47
1:D:77:LEU:O	1:D:77:LEU:HD12	2.14	0.47
2:B:1097:HIS:ND1	2:B:1098:VAL:O	2.48	0.47
2:E:1686:VAL:HG11	2:E:1690:LYS:HD2	1.95	0.47
2:B:2215:HIS:HB3	2:B:2218:VAL:HB	1.97	0.47
1:D:320:ASP:OD1	2:E:1330:LYS:HE2	2.15	0.47
2:E:969:ILE:HA	2:E:981:VAL:O	2.15	0.47
1:D:215:LYS:HD2	1:D:215:LYS:N	2.29	0.47
2:E:2177:VAL:HG23	2:E:2180:GLN:HB2	1.93	0.47
2:E:2037:TYR:C	2:E:2038:HIS:HD2	2.17	0.47
2:B:2178:GLU:O	2:B:2217:LYS:CG	2.62	0.47
2:B:1857:VAL:HG13	2:B:1894:ILE:HG13	1.97	0.47
2:E:1687:HIS:ND1	2:E:1688:PRO:CD	2.78	0.47
2:E:1019:GLU:HB2	2:E:1023:LEU:HD23	1.97	0.47
2:B:1471:GLN:O	2:B:1473:ARG:HG3	2.15	0.47
2:B:1791:PHE:C	2:B:1791:PHE:CD1	2.87	0.47
2:B:2208:TYR:CE2	2:B:2244:ILE:HD13	2.50	0.47
2:B:1984:PRO:O	2:B:1985:GLN:NE2	2.48	0.47
2:E:1680:SER:OG	2:E:1704:GLU:HB2	2.15	0.47
2:B:2007:ARG:CG	2:B:2052:GLU:OE2	2.62	0.47
2:E:2210:MET:CE	2:E:2252:GLY:CA	2.85	0.47
2:E:2011:LEU:HD12	2:E:2040:TRP:CH2	2.49	0.47
2:E:1067:ASN:ND2	2:E:1083:THR:HG21	2.11	0.47
2:B:1721:ASN:HB2	2:E:1463:THR:HB	1.96	0.47
2:B:2184:VAL:CG2	2:B:2219:LYS:O	2.60	0.46
2:E:1999:LEU:HD12	2:E:2000:SER:O	2.15	0.46
2:B:1733:TRP:CD1	2:B:1771:THR:O	2.68	0.46
2:E:2056:ARG:O	2:E:2060:LEU:N	2.42	0.46
2:B:1707:HIS:CG	2:B:1708:GLU:N	2.83	0.46
2:B:1840:TYR:OH	2:B:2005:PHE:HD2	1.98	0.46
2:E:2260:HIS:HE1	2:E:2273:GLU:OE2	1.97	0.46
1:D:208:VAL:O	1:D:213:ILE:HD12	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2032:ILE:HD11	2:B:2047:GLN:HE22	1.80	0.46
2:B:2034:ILE:HG23	2:B:2040:TRP:O	2.15	0.46
2:B:2210:MET:CE	2:B:2253:LEU:CB	2.93	0.46
2:E:1760:THR:C	2:E:1762:ASP:H	2.19	0.46
1:D:75:ASP:OD2	1:D:79:LYS:HE2	2.11	0.46
2:E:1687:HIS:CG	2:E:1688:PRO:HD2	2.50	0.46
1:A:108:ILE:H	1:A:108:ILE:HD12	1.80	0.46
2:B:2007:ARG:CD	2:B:2052:GLU:OE2	2.63	0.46
2:B:2153:ARG:NH1	2:B:2153:ARG:CG	2.74	0.46
2:E:1728:ILE:HD13	2:E:1728:ILE:N	2.26	0.46
2:E:1834:PHE:HD2	2:E:1960:GLU:CG	2.28	0.46
2:E:1405:ILE:HB	2:E:1437:ILE:HB	1.98	0.46
2:E:2044:THR:H	2:E:2047:GLN:CD	2.18	0.46
2:E:2047:GLN:O	2:E:2051:ILE:N	2.48	0.46
2:E:1730:ASN:N	2:E:1730:ASN:OD1	2.49	0.46
1:D:327:ILE:CB	1:D:328:TYR:HD1	2.13	0.46
1:A:292:CYS:HA	1:A:296:SER:OG	2.15	0.46
2:B:1679:GLU:HB3	2:B:1704:GLU:C	2.36	0.46
2:B:1570:TRP:C	2:B:1571:GLU:HG3	2.36	0.46
2:E:965:LYS:HB3	2:E:966:PRO:HD2	1.98	0.46
2:E:1370:ARG:CG	2:E:1370:ARG:HH11	2.28	0.46
2:B:1059:GLU:N	2:B:1059:GLU:OE1	2.48	0.46
2:B:2227:VAL:CG1	2:B:2239:SER:CB	2.94	0.46
2:E:1733:TRP:CZ2	2:E:1767:TYR:CD2	3.04	0.46
2:B:2247:LEU:CD1	2:B:2248:PRO:CD	2.91	0.46
2:B:1324:GLY:CA	2:B:1325:SER:OG	2.64	0.46
1:D:354:ARG:HB2	1:D:355:PRO:CD	2.45	0.46
2:E:1378:LYS:HE3	2:E:1623:PHE:CE2	2.50	0.46
2:B:2198:ASP:CG	2:B:2199:VAL:N	2.68	0.46
2:E:1679:GLU:HB3	2:E:1704:GLU:O	2.16	0.46
2:E:2159:ASN:HD21	2:E:2198:ASP:HA	1.81	0.46
2:B:929:LEU:HA	2:B:933:GLU:OE1	2.16	0.46
2:B:1104:ILE:HG22	2:B:1107:LEU:HD13	1.97	0.46
2:B:1465:ARG:HG3	2:B:1465:ARG:HH11	1.81	0.46
2:E:1895:HIS:CD2	2:E:1982:THR:C	2.89	0.46
2:E:1565:THR:O	2:E:1820:ARG:CZ	2.64	0.46
2:B:2163:TYR:CE1	2:B:2164:LEU:CD2	2.99	0.46
2:E:2182:VAL:CG1	2:E:2338:GLN:HB2	2.46	0.46
2:E:1104:ILE:HG22	2:E:1107:LEU:HD13	1.97	0.46
2:B:936:GLU:O	2:B:940:ILE:HD13	2.15	0.46
2:B:1286:TRP:CE2	2:B:1302:LEU:HD11	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1763:ASN:N	2:E:1763:ASN:HD22	2.13	0.46
2:B:2265:GLU:HG3	2:B:2294:PHE:CG	2.50	0.46
2:B:1991:ILE:HD11	2:B:2008:LEU:HD11	1.98	0.46
2:B:1137:PRO:HD2	2:B:1140:ASN:O	2.14	0.46
2:B:2367:ASN:OD1	2:B:2370:GLY:CA	2.64	0.46
2:B:1156:HIS:ND1	2:B:1157:PRO:HD2	2.31	0.46
2:E:2354:GLY:O	2:E:2355:ASN:HB2	2.16	0.46
2:E:2081:ASP:CG	2:E:2082:ILE:HG23	2.37	0.46
2:B:2209:GLY:HA2	2:B:2220:GLU:O	2.16	0.46
2:B:2081:ASP:CG	2:B:2082:ILE:HG23	2.36	0.46
2:E:1961:ASN:OD1	2:E:2079:ILE:CD1	2.63	0.46
2:B:1188:ALA:O	2:B:1191:PRO:CG	2.64	0.46
2:E:1542:TYR:CE2	2:E:1546:VAL:HG21	2.51	0.46
2:B:1611:SER:N	2:B:1612:PRO:CD	2.79	0.46
2:B:2282:ALA:HA	2:B:2286:ARG:HG2	1.98	0.46
2:E:2014:ALA:N	2:E:2059:ILE:HD11	2.31	0.46
2:B:2208:TYR:N	2:B:2223:THR:O	2.40	0.46
2:E:1887:GLY:CA	2:E:1992:TYR:CD2	2.98	0.46
1:A:327:ILE:HG21	1:A:328:TYR:CE2	2.51	0.46
2:E:936:GLU:O	2:E:940:ILE:HD13	2.16	0.46
2:E:2212:ALA:HB3	2:E:2218:VAL:HB	1.97	0.46
2:E:2211:SER:HA	2:E:2219:LYS:HA	1.97	0.46
1:A:103:VAL:HG22	1:A:104:SER:N	2.30	0.46
2:E:1425:PHE:CD1	2:E:1425:PHE:N	2.84	0.46
2:E:1597:GLY:CA	2:E:1599:SER:N	2.78	0.45
2:B:1121:ILE:HD13	2:B:1239:THR:HG21	1.96	0.45
2:B:1121:ILE:HD13	2:B:1239:THR:CG2	2.46	0.45
2:B:1177:ASP:O	2:B:1181:GLU:HB2	2.16	0.45
2:B:2041:PRO:CG	2:B:2043:PHE:CD1	2.99	0.45
2:B:2308:THR:HG23	2:B:2333:PHE:C	2.19	0.45
2:B:1996:LEU:HD21	2:B:2001:SER:HA	1.99	0.45
1:A:86:GLY:O	1:A:90:GLU:N	2.43	0.45
2:B:2178:GLU:C	2:B:2217:LYS:HZ3	2.18	0.45
2:B:1976:ASP:OD1	2:B:1980:LYS:HD2	2.16	0.45
1:D:84:ARG:CG	1:D:84:ARG:HH11	2.27	0.45
1:A:280:SER:CB	1:A:313:TYR:CE1	2.98	0.45
2:E:2002:TYR:C	2:E:2002:TYR:CD1	2.89	0.45
2:B:2176:PHE:CA	2:B:2338:GLN:NE2	2.73	0.45
2:B:2182:VAL:HA	2:B:2338:GLN:O	2.16	0.45
2:E:1999:LEU:CD1	2:E:2004:ALA:HB2	2.45	0.45
2:B:2339:LEU:HD12	2:B:2340:LEU:CA	2.41	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2277:HIS:ND1	2:E:2281:PHE:HD2	2.07	0.45
2:B:1727:LEU:C	2:B:1728:ILE:HG12	2.36	0.45
2:E:1459:ALA:O	2:E:1463:THR:HG23	2.17	0.45
2:B:2070:ASN:O	2:B:2071:ILE:HG23	2.16	0.45
2:E:2264:GLU:C	2:E:2294:PHE:CD1	2.89	0.45
2:B:957:TYR:HD2	2:B:991:THR:HG21	1.80	0.45
2:B:1238:LEU:O	2:B:1239:THR:HG22	2.16	0.45
2:E:2047:GLN:HA	2:E:2050:THR:HB	1.97	0.45
2:B:2247:LEU:HD23	2:B:2374:PHE:HB2	1.99	0.45
2:B:1707:HIS:NE2	2:B:1708:GLU:OE1	2.50	0.45
2:B:1843:LEU:HD21	2:B:1851:PHE:HE2	1.82	0.45
2:E:2061:THR:CG2	2:E:2062:GLU:N	2.79	0.45
1:D:72:ASP:OD2	1:D:75:ASP:HB2	2.17	0.45
2:B:1090:ILE:HD11	2:B:1104:ILE:HD11	1.99	0.45
2:B:2286:ARG:HD3	2:B:2312:TYR:CD1	2.52	0.45
2:B:2177:VAL:N	2:B:2338:GLN:HE22	2.13	0.45
2:B:2208:TYR:OH	2:B:2244:ILE:CG2	2.65	0.45
2:B:2208:TYR:CG	2:B:2253:LEU:CD1	3.00	0.45
2:B:1977:VAL:CG1	2:B:1978:VAL:N	2.78	0.45
1:A:354:ARG:CB	1:A:355:PRO:HD3	2.44	0.45
2:B:1097:HIS:CE1	2:B:1098:VAL:O	2.70	0.45
2:E:2070:ASN:O	2:E:2071:ILE:HG23	2.16	0.45
2:E:1059:GLU:OE1	2:E:1059:GLU:N	2.49	0.45
2:B:1844:PHE:CD1	2:B:1844:PHE:N	2.84	0.45
2:B:2210:MET:SD	2:B:2222:LYS:HD2	2.47	0.45
2:B:2386:MET:H	2:B:2386:MET:HG3	1.63	0.45
2:B:2215:HIS:HB3	2:B:2218:VAL:CG2	2.46	0.45
2:B:2208:TYR:CZ	2:B:2244:ILE:HG21	2.52	0.45
1:D:103:VAL:HG22	1:D:104:SER:N	2.31	0.45
2:E:1987:VAL:HB	2:E:1989:PHE:HE1	1.81	0.45
2:B:2081:ASP:OD1	2:B:2082:ILE:HG23	2.16	0.45
2:B:2343:ASP:CB	2:B:2344:ARG:NH2	2.79	0.45
2:B:1886:THR:HG1	2:B:1888:HIS:CE1	2.31	0.45
2:B:2260:HIS:NE2	2:B:2273:GLU:OE2	2.50	0.45
2:B:1104:ILE:CG2	2:B:1107:LEU:CD1	2.95	0.45
2:E:2223:THR:HG21	2:E:2350:ILE:HG12	1.99	0.45
2:E:1881:THR:O	2:E:1889:LEU:HD12	2.16	0.45
2:B:1472:ASN:HB3	2:B:2325:LEU:O	2.17	0.45
1:D:108:ILE:CD1	1:D:108:ILE:H	2.30	0.45
2:E:1763:ASN:N	2:E:1763:ASN:ND2	2.61	0.45
2:B:2192:LYS:HA	2:B:2195:GLU:HG3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2159:ASN:HD21	2:B:2198:ASP:HA	1.77	0.45
2:E:1826:TYR:O	2:E:1826:TYR:CG	2.70	0.45
2:E:2183:TYR:CE1	2:E:2289:ILE:HD13	2.52	0.45
2:E:1837:SER:O	2:E:1840:TYR:HB2	2.17	0.45
2:B:2278:SER:HG	2:B:2316:GLU:HG3	1.80	0.45
2:B:2192:LYS:C	2:B:2195:GLU:HB2	2.35	0.45
2:B:2185:LEU:HA	2:B:2186:PRO:HD3	1.57	0.45
2:E:2081:ASP:OD1	2:E:2082:ILE:HG23	2.17	0.45
2:E:1156:HIS:ND1	2:E:1157:PRO:HD2	2.32	0.45
1:A:263:LYS:HD2	1:A:263:LYS:HA	1.60	0.45
2:E:2037:TYR:CE1	2:E:2038:HIS:CD2	3.01	0.44
2:E:1684:GLU:CD	2:E:1702:THR:OG1	2.52	0.44
2:B:2264:GLU:HG2	2:B:2265:GLU:O	2.16	0.44
2:E:2089:LYS:HA	2:E:2090:ALA:HA	1.66	0.44
2:E:1195:PHE:CD1	2:E:1217:ARG:HD2	2.52	0.44
1:A:343:ASN:HD22	1:A:343:ASN:HA	1.64	0.44
2:E:1996:LEU:CD2	2:E:2001:SER:HA	2.47	0.44
2:E:2039:LEU:CA	2:E:2040:TRP:CD1	3.00	0.44
2:E:1710:GLU:HA	2:E:1727:LEU:O	2.17	0.44
2:E:1093:LYS:HD3	2:E:1094:ASP:HA	2.00	0.44
2:E:1370:ARG:CG	2:E:1370:ARG:NH1	2.79	0.44
2:B:2354:GLY:O	2:B:2355:ASN:HB2	2.17	0.44
1:A:224:LEU:C	1:A:224:LEU:HD23	2.37	0.44
2:B:2240:ASN:O	2:B:2241:ILE:C	2.56	0.44
2:B:2210:MET:HE1	2:B:2253:LEU:N	2.31	0.44
2:B:2305:TYR:HB3	2:B:2334:SER:CB	2.47	0.44
2:B:1999:LEU:HD21	2:B:2003:THR:CB	2.48	0.44
2:E:958:LEU:HA	2:E:1081:TYR:CD2	2.52	0.44
2:B:2277:HIS:CE1	2:B:2288:CYS:O	2.70	0.44
2:E:2003:THR:O	2:E:2007:ARG:N	2.50	0.44
2:E:1825:ILE:HG22	2:E:1825:ILE:O	2.16	0.44
2:E:2227:VAL:HG12	2:E:2239:SER:OG	2.14	0.44
2:E:1347:ARG:HD3	2:E:1445:THR:O	2.17	0.44
2:B:2043:PHE:CZ	2:B:2051:ILE:CD1	2.78	0.44
2:B:2277:HIS:ND1	2:B:2307:LEU:HD23	2.32	0.44
2:E:1763:ASN:CA	2:E:1766:MET:HE1	2.46	0.44
2:B:2178:GLU:O	2:B:2217:LYS:HG2	2.17	0.44
2:B:2284:LYS:CE	2:B:2285:LYS:HA	2.47	0.44
2:E:1347:ARG:NH1	2:E:1445:THR:O	2.38	0.44
2:E:2190:LEU:O	2:E:2190:LEU:HG	2.17	0.44
2:B:2048:TRP:CE3	2:B:2048:TRP:HA	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2232:HIS:HB2	2:B:2235:SER:O	2.17	0.44
2:E:2046:GLU:O	2:E:2049:ILE:HG23	2.04	0.44
2:E:2357:TRP:H	2:E:2387:HIS:HE1	1.64	0.44
2:E:2174:ASP:CG	2:E:2175:ASP:H	2.14	0.44
2:E:1431:HIS:C	2:E:1433:ASP:N	2.71	0.44
2:B:2262:GLN:HG2	2:B:2293:ILE:O	2.18	0.44
2:E:1362:LYS:O	2:E:1366:ARG:HG3	2.17	0.44
2:E:2248:PRO:C	2:E:2249:ASP:OD1	2.56	0.44
1:D:263:LYS:HD2	1:D:263:LYS:HA	1.80	0.44
2:E:1558:GLU:HG3	2:E:1558:GLU:O	2.18	0.44
2:B:2183:TYR:CD1	2:B:2219:LYS:CD	2.90	0.44
2:E:2202:GLN:HE22	2:E:2235:SER:N	2.10	0.44
2:B:2163:TYR:CE1	2:B:2164:LEU:HD23	2.53	0.44
2:E:2191:LYS:HE2	2:E:2195:GLU:OE2	2.17	0.44
2:B:1343:PHE:HB3	2:B:1444:ILE:CD1	2.48	0.44
2:E:2043:PHE:HD2	2:E:2051:ILE:CG1	2.21	0.44
2:B:2301:SER:C	2:B:2302:LEU:HD12	2.39	0.44
2:B:1887:GLY:HA2	2:B:1992:TYR:CD2	2.44	0.44
1:A:109:ASP:O	1:A:109:ASP:OD1	2.35	0.44
2:E:1104:ILE:CG2	2:E:1107:LEU:CD1	2.96	0.44
2:B:965:LYS:HB3	2:B:966:PRO:HD2	1.98	0.44
2:E:1431:HIS:O	2:E:1433:ASP:N	2.51	0.44
1:A:48:HIS:CG	1:A:53:SER:HG	2.32	0.44
2:E:1090:ILE:HD11	2:E:1104:ILE:HD11	1.99	0.44
2:B:2067:TYR:CD1	2:B:2067:TYR:N	2.86	0.44
2:B:2040:TRP:CD1	2:B:2040:TRP:N	2.86	0.43
2:B:2011:LEU:HB3	2:B:2040:TRP:CZ3	2.53	0.43
2:B:2044:THR:CG2	2:B:2047:GLN:CD	2.80	0.43
2:E:1992:TYR:O	2:E:1993:ASP:HB2	2.18	0.43
2:E:1093:LYS:HD3	2:E:1093:LYS:HA	1.79	0.43
2:E:1624:LEU:HD21	2:E:1633:PHE:HB3	2.00	0.43
2:E:1059:GLU:OE2	2:E:1105:ARG:NH2	2.51	0.43
2:B:1784:TYR:CD1	2:B:1806:MET:HG3	2.53	0.43
2:E:2029:ASP:OD2	2:E:2032:ILE:CD1	2.65	0.43
2:E:908:ASP:OD1	2:E:994:TYR:OH	2.25	0.43
2:B:2024:MET:SD	2:B:2157:ILE:HG21	2.58	0.43
2:E:2066:LYS:CB	2:E:2067:TYR:CD1	2.97	0.43
2:B:1305:SER:O	2:B:1309:ILE:HG13	2.18	0.43
2:B:1354:GLU:N	2:B:1355:PRO:CD	2.81	0.43
2:E:2242:PRO:CB	2:E:2374:PHE:CE2	3.01	0.43
2:B:2045:ASP:O	2:B:2048:TRP:HB2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2083:ILE:CG2	2:E:2084:LEU:H	2.32	0.43
1:D:20:TYR:CE2	1:D:106:PRO:HG2	2.53	0.43
2:E:1292:ARG:NH1	2:E:1293:THR:HG22	2.33	0.43
2:B:2179:GLU:HA	2:B:2217:LYS:HE2	2.01	0.43
2:B:1894:ILE:HD13	2:B:1894:ILE:HA	1.86	0.43
2:B:953:ARG:CG	2:B:953:ARG:HH11	2.31	0.43
2:B:1842:GLU:O	2:B:1844:PHE:N	2.51	0.43
2:E:2223:THR:HG21	2:E:2350:ILE:CG1	2.48	0.43
2:B:2358:ASN:CB	2:B:2387:HIS:HD1	2.18	0.43
2:B:2020:GLU:HG3	2:B:2164:LEU:HD12	2.00	0.43
2:B:2342:SER:OG	2:B:2344:ARG:N	2.37	0.43
1:D:25:LYS:O	1:D:28:GLN:CB	2.66	0.43
2:E:930:ASN:ND2	2:E:933:GLU:HB2	2.32	0.43
2:B:2017:THR:HG21	2:B:2062:GLU:HG3	1.99	0.43
2:B:2054:GLN:HE21	2:B:2054:GLN:HB3	1.64	0.43
2:E:1788:GLY:O	2:E:1790:TRP:CD1	2.71	0.43
2:B:2166:LEU:O	2:B:2167:LYS:C	2.56	0.43
2:B:2087:ASN:CB	2:B:2089:LYS:HG3	2.46	0.43
2:E:2181:ASN:O	2:E:2338:GLN:HG3	2.18	0.43
2:B:1906:SER:O	2:B:1909:ALA:HB3	2.19	0.43
2:E:1354:GLU:N	2:E:1355:PRO:CD	2.81	0.43
2:E:2154:LYS:O	2:E:2157:ILE:HB	2.18	0.43
1:D:35:ASP:O	1:D:107:LYS:NZ	2.34	0.43
2:E:2063:TYR:O	2:E:2067:TYR:CD1	2.71	0.43
2:B:1853:ASP:OD1	2:B:1854:ASP:N	2.51	0.43
2:B:2270:ALA:HB1	2:B:2324:VAL:HA	2.00	0.43
2:E:1784:TYR:CD1	2:E:1806:MET:HG3	2.53	0.43
2:E:953:ARG:HG3	2:E:953:ARG:HH11	1.83	0.43
2:B:2281:PHE:HB3	2:B:2286:ARG:O	2.19	0.43
2:E:2253:LEU:HA	2:E:2253:LEU:HD23	1.90	0.43
2:E:2384:ASN:HB3	2:E:2387:HIS:HD2	1.83	0.43
2:B:1542:TYR:CE2	2:B:1546:VAL:HG21	2.53	0.43
2:B:1864:LYS:NZ	2:B:1865:THR:O	2.44	0.43
2:B:2231:GLY:O	2:B:2232:HIS:CD2	2.71	0.43
2:B:2357:TRP:CZ3	2:B:2382:PHE:CE1	3.04	0.43
2:B:2153:ARG:HH11	2:B:2153:ARG:HG3	1.82	0.43
2:B:2178:GLU:HB3	2:B:2217:LYS:HZ2	1.84	0.43
2:B:1187:LEU:O	2:B:1191:PRO:CG	2.66	0.43
1:D:9:ALA:N	1:D:10:PRO:HD3	2.34	0.43
2:B:2085:GLY:HA3	2:B:2086:GLN:HA	1.79	0.43
2:B:2329:PHE:C	2:B:2330:GLU:HG2	2.39	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1091:ASN:HB3	2:E:1093:LYS:HE2	2.00	0.43
2:B:2185:LEU:HG	2:B:2186:PRO:HD2	2.00	0.43
2:E:2318:ASN:HB3	2:E:2321:ILE:HD11	2.01	0.43
1:D:327:ILE:HG21	1:D:328:TYR:HE1	1.84	0.43
2:B:1707:HIS:CE1	2:B:1708:GLU:CD	2.92	0.43
2:B:1704:GLU:CG	2:B:1705:SER:N	2.81	0.43
2:E:2065:ARG:HH11	2:E:2065:ARG:HB3	1.81	0.42
2:E:2302:LEU:CD1	2:E:2302:LEU:N	2.82	0.42
2:E:1835:LEU:HB3	2:E:1959:THR:HB	2.00	0.42
2:B:2230:LEU:CB	2:B:2237:GLN:HG3	2.47	0.42
2:B:1961:ASN:HA	2:B:2079:ILE:CD1	2.49	0.42
2:E:2086:GLN:O	2:E:2088:ILE:HG12	2.20	0.42
2:B:1051:GLU:HG3	2:B:1169:TYR:CE2	2.54	0.42
2:B:1721:ASN:HB3	2:E:1463:THR:HB	2.00	0.42
2:B:1383:PHE:CE2	2:B:1387:VAL:HG21	2.54	0.42
2:E:2155:SER:HB3	2:E:2383:TYR:CE2	2.53	0.42
2:B:2076:GLN:OE1	2:B:2076:GLN:HA	2.19	0.42
2:E:1596:THR:O	2:E:1598:LEU:HB3	2.19	0.42
2:E:1763:ASN:HD22	2:E:1764:VAL:N	2.17	0.42
2:B:1847:ASP:O	2:B:1849:LYS:HD2	2.19	0.42
2:E:2061:THR:HG22	2:E:2062:GLU:N	2.34	0.42
2:B:2189:LEU:HD21	2:B:2347:GLY:HA3	2.01	0.42
2:E:958:LEU:HD23	2:E:1081:TYR:CD2	2.55	0.42
2:B:1917:VAL:O	2:B:1921:VAL:HG23	2.19	0.42
2:B:2373:ASN:O	2:B:2374:PHE:CG	2.72	0.42
2:E:1567:PHE:CE2	2:E:1820:ARG:NH1	2.84	0.42
2:B:2064:GLY:O	2:B:2068:ASN:HA	2.19	0.42
2:E:2087:ASN:O	2:E:2088:ILE:HG12	2.19	0.42
2:B:1321:MET:HA	2:B:1321:MET:CE	2.49	0.42
2:E:1837:SER:O	2:E:1840:TYR:CB	2.68	0.42
2:E:2075:THR:HG22	2:E:2076:GLN:N	2.34	0.42
2:B:2063:TYR:CE1	2:B:2081:ASP:O	2.73	0.42
2:E:2086:GLN:HG2	2:E:2086:GLN:O	2.19	0.42
2:B:1097:HIS:ND1	2:B:1097:HIS:C	2.73	0.42
2:E:1435:LYS:HD3	2:E:1549:ALA:O	2.19	0.42
2:E:1596:THR:O	2:E:1598:LEU:CB	2.67	0.42
2:E:1604:ARG:HH22	2:E:1822:GLY:C	2.23	0.42
2:B:957:TYR:O	2:B:961:GLN:N	2.48	0.42
2:B:1848:ILE:HD11	2:B:1928:GLU:O	2.14	0.42
2:B:1894:ILE:HG22	2:B:1894:ILE:O	2.18	0.42
2:E:1964:PRO:HG3	2:E:2013:ARG:CZ	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2020:GLU:HG3	2:E:2164:LEU:HD12	2.02	0.42
2:E:2259:ILE:HD11	2:E:2293:ILE:HD11	2.01	0.42
2:E:1234:VAL:HG11	2:E:1239:THR:CG2	2.49	0.42
2:E:1674:ASP:OD1	2:E:1674:ASP:N	2.52	0.42
2:E:1717:LEU:HB2	2:E:1786:ALA:HB3	2.02	0.42
2:B:2035:LYS:O	2:B:2037:TYR:N	2.53	0.42
2:B:1015:PRO:HD2	2:B:1165:LEU:CD2	2.36	0.42
2:B:1661:ILE:HG12	2:B:1805:ILE:CD1	2.50	0.42
1:D:23:ASN:ND2	1:D:23:ASN:N	2.68	0.42
2:B:2232:HIS:HE1	2:B:2237:GLN:HE21	1.68	0.42
2:B:2208:TYR:HB3	2:B:2253:LEU:CG	2.45	0.42
2:B:1854:ASP:CA	2:B:1857:VAL:HG23	2.49	0.42
1:D:3:THR:HG22	1:D:5:PRO:HD3	2.01	0.42
2:B:1800:ASN:OD1	2:B:1803:ARG:NH1	2.53	0.42
2:B:1944:LEU:O	2:B:1948:MET:HG2	2.20	0.42
2:E:2388:ARG:HD3	2:E:2389:PRO:HD2	2.02	0.42
2:B:2063:TYR:HE1	2:B:2081:ASP:O	2.02	0.42
2:B:969:ILE:HG22	2:B:982:TYR:CD2	2.55	0.42
2:E:1484:TRP:CH2	2:E:1495:PHE:HB2	2.55	0.42
2:E:2021:SER:O	2:E:2024:MET:HB3	2.20	0.42
2:B:2229:GLN:NE2	2:B:2357:TRP:CE3	2.88	0.42
1:D:282:ILE:HD13	2:E:1604:ARG:HD2	2.02	0.42
1:A:214:PHE:CD1	1:A:220:TYR:HA	2.55	0.42
2:B:1904:ARG:HD3	2:B:1907:GLN:OE1	2.20	0.42
2:B:1893:ILE:CG2	2:B:1978:VAL:HG13	2.50	0.41
2:B:2010:LEU:HA	2:B:2010:LEU:HD12	1.82	0.41
2:B:2230:LEU:HD12	2:B:2230:LEU:HA	1.84	0.41
2:E:1712:SER:OG	2:E:1713:LYS:N	2.51	0.41
2:E:2078:GLU:O	2:E:2079:ILE:HD13	2.20	0.41
1:D:48:HIS:HE1	1:D:56:TYR:OH	2.03	0.41
2:E:1370:ARG:HG2	2:E:1370:ARG:NH1	2.36	0.41
2:E:1611:SER:N	2:E:1612:PRO:CD	2.83	0.41
2:B:2309:ASP:O	2:B:2312:TYR:N	2.53	0.41
2:B:2082:ILE:O	2:B:2083:ILE:CG1	2.69	0.41
2:E:1849:LYS:C	2:E:1850:LEU:HD23	2.40	0.41
2:B:1717:LEU:HB2	2:B:1786:ALA:HB3	2.02	0.41
2:B:2183:TYR:CD1	2:B:2219:LYS:CB	3.01	0.41
2:B:2309:ASP:N	2:B:2310:GLU:OE1	2.54	0.41
2:E:2386:MET:C	2:E:2388:ARG:N	2.74	0.41
2:B:1990:ASN:OD1	2:B:1992:TYR:N	2.52	0.41
2:B:1843:LEU:HD11	2:B:1884:PRO:HG3	1.94	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1853:ASP:CG	2:B:1855:THR:OG1	2.57	0.41
2:B:2351:ILE:HG21	2:B:2379:PRO:HA	2.02	0.41
2:E:2070:ASN:O	2:E:2071:ILE:CG2	2.69	0.41
2:B:1674:ASP:OD1	2:B:1674:ASP:N	2.53	0.41
2:B:2278:SER:OG	2:B:2312:TYR:O	2.38	0.41
2:E:2304:ALA:HB3	2:E:2339:LEU:HD23	1.98	0.41
2:B:2318:ASN:ND2	2:B:2318:ASN:N	2.68	0.41
1:D:328:TYR:CD2	2:E:1543:ARG:NH1	2.89	0.41
1:D:84:ARG:NH1	1:D:84:ARG:CG	2.84	0.41
2:B:2258:TRP:N	2:B:2258:TRP:CD1	2.82	0.41
2:E:965:LYS:HE3	2:E:985:ASP:CG	2.41	0.41
2:E:995:LEU:O	2:E:999:LEU:HG	2.21	0.41
2:E:2084:LEU:C	2:E:2084:LEU:HD22	2.37	0.41
1:A:282:ILE:HD13	2:B:1604:ARG:HD2	2.03	0.41
2:E:1762:ASP:CG	2:E:1763:ASN:H	2.23	0.41
2:E:1705:SER:HB3	2:E:1709:TRP:CE3	2.55	0.41
2:E:2280:LEU:HB2	2:E:2281:PHE:CD2	2.56	0.41
2:E:2182:VAL:HG12	2:E:2338:GLN:HB3	2.02	0.41
2:E:986:PRO:O	2:E:990:ILE:HD12	2.20	0.41
2:B:1686:VAL:HG12	2:B:1687:HIS:N	2.36	0.41
2:E:1624:LEU:CD2	2:E:1625:VAL:N	2.83	0.41
2:E:1996:LEU:HD21	2:E:2001:SER:HA	2.02	0.41
1:A:16:GLY:HA3	1:A:45:HIS:CE1	2.54	0.41
2:B:1963:LEU:HD23	2:B:1963:LEU:HA	1.95	0.41
2:B:1673:LEU:HA	2:B:1678:ILE:HB	2.03	0.41
2:B:1435:LYS:NZ	2:E:1351:VAL:HG13	2.36	0.41
2:B:2307:LEU:HD12	2:B:2308:THR:O	2.21	0.41
2:E:2014:ALA:CA	2:E:2059:ILE:CD1	2.72	0.41
2:E:2157:ILE:HD12	2:E:2157:ILE:HA	1.74	0.41
2:B:2386:MET:CE	2:B:2387:HIS:CD2	3.03	0.41
2:E:1763:ASN:O	2:E:1766:MET:HE3	2.18	0.41
2:B:1137:PRO:O	2:B:1140:ASN:C	2.59	0.41
2:E:2189:LEU:HD21	2:E:2347:GLY:C	2.41	0.41
2:B:1889:LEU:HD23	2:B:1891:LEU:HB2	2.03	0.41
2:E:1865:THR:OG1	2:E:1869:ASN:HB2	2.20	0.41
2:E:1826:TYR:CA	2:E:1827:GLN:HB2	2.50	0.41
2:E:2267:LYS:C	2:E:2305:TYR:OH	2.58	0.41
2:E:2030:PRO:CG	2:E:2153:ARG:NE	2.77	0.41
2:E:2028:SER:C	2:E:2030:PRO:HD3	2.37	0.41
2:B:2017:THR:HG23	2:B:2062:GLU:HG3	2.03	0.41
2:E:1279:VAL:HG12	2:E:1280:SER:N	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:PHE:C	1:A:89:PHE:CD1	2.94	0.41
2:B:1405:ILE:HB	2:B:1437:ILE:HB	2.02	0.41
2:B:1150:LYS:HD2	2:B:1292:ARG:HH22	1.84	0.41
2:B:1080:ASP:O	2:B:1084:ALA:HB2	2.21	0.41
1:A:7:THR:HG21	1:A:70:GLN:OE1	2.21	0.41
2:B:2386:MET:HE1	2:B:2387:HIS:CD2	2.56	0.41
2:B:2157:ILE:C	2:B:2160:THR:OG1	2.44	0.41
2:E:2067:TYR:CD1	2:E:2067:TYR:N	2.89	0.41
2:E:1826:TYR:CA	2:E:1827:GLN:CB	2.99	0.41
2:E:1766:MET:C	2:E:1767:TYR:CD1	2.94	0.40
2:E:2230:LEU:HD23	2:E:2237:GLN:NE2	2.36	0.40
2:B:2247:LEU:HD23	2:B:2374:PHE:CB	2.51	0.40
2:E:1466:GLN:O	2:E:1469:ILE:CA	2.69	0.40
2:E:2057:ASP:O	2:E:2061:THR:HB	2.22	0.40
2:B:995:LEU:O	2:B:999:LEU:HG	2.21	0.40
1:D:16:GLY:HA3	1:D:45:HIS:CE1	2.56	0.40
2:B:2184:VAL:O	2:B:2221:ILE:CG1	2.69	0.40
2:E:1995:TRP:HZ3	2:E:2007:ARG:HG2	1.58	0.40
2:B:2191:LYS:O	2:B:2195:GLU:CG	2.44	0.40
2:B:2082:ILE:O	2:B:2083:ILE:HG13	2.21	0.40
2:E:1168:ILE:O	2:E:1168:ILE:HG13	2.21	0.40
2:B:2089:LYS:HA	2:B:2090:ALA:HA	1.74	0.40
2:B:2070:ASN:O	2:B:2071:ILE:CG2	2.69	0.40
2:E:1889:LEU:HA	2:E:1889:LEU:HD12	1.86	0.40
2:E:946:ASN:HB3	2:E:949:ASP:OD2	2.21	0.40
2:B:2207:ILE:CG1	2:B:2257:GLY:O	2.70	0.40
1:D:107:LYS:HA	1:D:108:ILE:HA	1.87	0.40
2:B:1168:ILE:O	2:B:1168:ILE:HG13	2.21	0.40
2:B:1324:GLY:HA2	2:B:1325:SER:HB3	2.03	0.40
2:E:930:ASN:ND2	2:E:933:GLU:CD	2.74	0.40
2:E:1624:LEU:HD21	2:E:1633:PHE:CD1	2.57	0.40
2:B:1107:LEU:HD23	2:B:1109:PHE:CZ	2.56	0.40
2:E:969:ILE:HG22	2:E:982:TYR:CD2	2.57	0.40
2:E:2029:ASP:OD2	2:E:2032:ILE:HD11	2.21	0.40
2:B:1153:GLU:O	2:B:1159:ARG:HD3	2.21	0.40
2:E:1477:PHE:C	2:E:1477:PHE:CD1	2.94	0.40
2:E:1894:ILE:O	2:E:1894:ILE:HG22	2.21	0.40
2:E:2203:VAL:HG22	2:E:2357:TRP:CZ3	2.57	0.40
2:B:2153:ARG:NH1	2:B:2153:ARG:HG2	2.36	0.40
2:E:1727:LEU:C	2:E:1728:ILE:CD1	2.71	0.40
2:B:1187:LEU:HA	2:B:1187:LEU:HD23	1.85	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1383:PHE:CE2	2:E:1387:VAL:HG21	2.55	0.40
1:D:141:ASP:OD1	1:D:141:ASP:C	2.60	0.40
2:B:2224:VAL:CA	2:B:2349:PHE:CE1	3.04	0.40
2:E:2177:VAL:O	2:E:2177:VAL:HG23	2.21	0.40
2:B:2162:LEU:HD23	2:B:2165:ARG:HE	1.86	0.40
2:B:2060:LEU:O	2:B:2063:TYR:CA	2.70	0.40
2:B:1893:ILE:HG23	2:B:1978:VAL:HG13	2.02	0.40
2:B:1762:ASP:OD1	2:B:1764:VAL:HG22	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1685:THR:OG1	2:E:2309:ASP:OD2[4_545]	1.96	0.24

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	319/355 (90%)	310 (97%)	9 (3%)	0	100	100
1	D	307/355 (86%)	298 (97%)	8 (3%)	1 (0%)	46	80
2	B	1384/1531 (90%)	1345 (97%)	38 (3%)	1 (0%)	56	88
2	E	1406/1531 (92%)	1360 (97%)	42 (3%)	4 (0%)	46	80
All	All	3416/3772 (91%)	3313 (97%)	97 (3%)	6 (0%)	52	84

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	2088	ILE
2	E	2286	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	2088	ILE
1	D	29	PRO
2	E	1726	GLY
2	E	2215	HIS

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	293/326 (90%)	284 (97%)	9 (3%)	47 80
1	D	289/326 (89%)	269 (93%)	20 (7%)	19 55
2	B	1256/1373 (92%)	1108 (88%)	148 (12%)	6 25
2	E	1278/1373 (93%)	1151 (90%)	127 (10%)	10 34
All	All	3116/3398 (92%)	2812 (90%)	304 (10%)	10 36

All (304) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	VAL
1	A	95	ASN
1	A	107	LYS
1	A	110	GLU
1	A	132	LYS
1	A	215	LYS
1	A	263	LYS
1	A	299	LYS
1	A	343	ASN
2	B	883	SER
2	B	885	VAL
2	B	908	ASP
2	B	929	LEU
2	B	952	ASN
2	B	953	ARG
2	B	956	LYS
2	B	960	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	969	ILE
2	B	987	LEU
2	B	1018	SER
2	B	1019	GLU
2	B	1042	SER
2	B	1074	VAL
2	B	1096	SER
2	B	1097	HIS
2	B	1105	ARG
2	B	1139	ASN
2	B	1165	LEU
2	B	1177	ASP
2	B	1213	MET
2	B	1218	GLN
2	B	1237	SER
2	B	1239	THR
2	B	1273	GLN
2	B	1282	ASP
2	B	1305	SER
2	B	1321	MET
2	B	1348	GLU
2	B	1377	SER
2	B	1406	LEU
2	B	1430	THR
2	B	1465	ARG
2	B	1466	GLN
2	B	1467	GLU
2	B	1478	GLU
2	B	1510	ILE
2	B	1512	ARG
2	B	1521	ARG
2	B	1569	SER
2	B	1571	GLU
2	B	1573	LEU
2	B	1594	GLN
2	B	1595	ARG
2	B	1598	LEU
2	B	1679	GLU
2	B	1691	SER
2	B	1703	MET
2	B	1706	VAL
2	B	1710	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1713	LYS
2	B	1727	LEU
2	B	1739	ARG
2	B	1742	ASP
2	B	1750	ARG
2	B	1802	MET
2	B	1804	THR
2	B	1805	ILE
2	B	1817	GLU
2	B	1821	LYS
2	B	1842	GLU
2	B	1845	ASN
2	B	1848	ILE
2	B	1849	LYS
2	B	1858	TYR
2	B	1859	ARG
2	B	1864	LYS
2	B	1867	GLU
2	B	1869	ASN
2	B	1882	LEU
2	B	1896	THR
2	B	1897	SER
2	B	1904	ARG
2	B	1926	LYS
2	B	1927	GLU
2	B	1932	GLN
2	B	1962	ARG
2	B	1972	ASP
2	B	1979	MET
2	B	1980	LYS
2	B	1988	LEU
2	B	1997	ASP
2	B	2001	SER
2	B	2002	TYR
2	B	2006	SER
2	B	2016	LYS
2	B	2018	ASN
2	B	2026	LEU
2	B	2032	ILE
2	B	2038	HIS
2	B	2039	LEU
2	B	2044	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	2045	ASP
2	B	2047	GLN
2	B	2048	TRP
2	B	2050	THR
2	B	2053	SER
2	B	2054	GLN
2	B	2057	ASP
2	B	2153	ARG
2	B	2155	SER
2	B	2160	THR
2	B	2163	TYR
2	B	2165	ARG
2	B	2187	LYS
2	B	2199	VAL
2	B	2202	GLN
2	B	2210	MET
2	B	2222	LYS
2	B	2237	GLN
2	B	2238	ILE
2	B	2239	SER
2	B	2243	ASP
2	B	2246	ASP
2	B	2247	LEU
2	B	2250	THR
2	B	2253	LEU
2	B	2254	GLU
2	B	2256	LEU
2	B	2258	TRP
2	B	2265	GLU
2	B	2268	PHE
2	B	2277	HIS
2	B	2280	LEU
2	B	2283	ASP
2	B	2284	LYS
2	B	2286	ARG
2	B	2295	SER
2	B	2301	SER
2	B	2303	SER
2	B	2306	ASN
2	B	2307	LEU
2	B	2309	ASP
2	B	2318	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	2332	THR
2	B	2334	SER
2	B	2336	HIS
2	B	2339	LEU
2	B	2341	LEU
2	B	2343	ASP
2	B	2344	ARG
2	B	2345	ILE
2	B	2349	PHE
2	B	2362	MET
2	B	2367	ASN
2	B	2382	PHE
2	B	2384	ASN
2	B	2386	MET
1	D	21	SER
1	D	23	ASN
1	D	24	VAL
1	D	27	ASN
1	D	83	GLU
1	D	84	ARG
1	D	85	ASP
1	D	101	MET
1	D	102	MET
1	D	104	SER
1	D	108	ILE
1	D	109	ASP
1	D	113	THR
1	D	215	LYS
1	D	216	ASN
1	D	299	LYS
1	D	300	ASN
1	D	326	LEU
1	D	327	ILE
1	D	355	PRO
2	E	885	VAL
2	E	908	ASP
2	E	909	THR
2	E	930	ASN
2	E	942	GLU
2	E	945	ASP
2	E	953	ARG
2	E	956	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	969	ILE
2	E	987	LEU
2	E	1093	LYS
2	E	1095	MET
2	E	1096	SER
2	E	1165	LEU
2	E	1166	ASP
2	E	1189	GLU
2	E	1213	MET
2	E	1272	ARG
2	E	1273	GLN
2	E	1275	MET
2	E	1281	ASN
2	E	1282	ASP
2	E	1292	ARG
2	E	1321	MET
2	E	1348	GLU
2	E	1370	ARG
2	E	1377	SER
2	E	1382	ARG
2	E	1426	ARG
2	E	1432	GLU
2	E	1465	ARG
2	E	1477	PHE
2	E	1510	ILE
2	E	1512	ARG
2	E	1530	SER
2	E	1568	ASN
2	E	1574	PHE
2	E	1596	THR
2	E	1598	LEU
2	E	1600	GLN
2	E	1624	LEU
2	E	1679	GLU
2	E	1691	SER
2	E	1693	LYS
2	E	1694	MET
2	E	1702	THR
2	E	1704	GLU
2	E	1707	HIS
2	E	1710	GLU
2	E	1713	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	1715	SER
2	E	1722	ASP
2	E	1723	SER
2	E	1727	LEU
2	E	1729	THR
2	E	1730	ASN
2	E	1732	MET
2	E	1761	THR
2	E	1763	ASN
2	E	1765	SER
2	E	1767	TYR
2	E	1769	SER
2	E	1817	GLU
2	E	1821	LYS
2	E	1842	GLU
2	E	1859	ARG
2	E	1862	VAL
2	E	1882	LEU
2	E	1897	SER
2	E	1927	GLU
2	E	1962	ARG
2	E	1972	ASP
2	E	1985	GLN
2	E	2001	SER
2	E	2002	TYR
2	E	2007	ARG
2	E	2018	ASN
2	E	2020	GLU
2	E	2021	SER
2	E	2033	THR
2	E	2034	ILE
2	E	2035	LYS
2	E	2047	GLN
2	E	2048	TRP
2	E	2059	ILE
2	E	2061	THR
2	E	2065	ARG
2	E	2077	THR
2	E	2080	LYS
2	E	2084	LEU
2	E	2086	GLN
2	E	2087	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	2095	ARG
2	E	2163	TYR
2	E	2172	SER
2	E	2178	GLU
2	E	2179	GLU
2	E	2182	VAL
2	E	2183	TYR
2	E	2189	LEU
2	E	2197	SER
2	E	2201	ILE
2	E	2214	ASP
2	E	2215	HIS
2	E	2222	LYS
2	E	2249	ASP
2	E	2264	GLU
2	E	2266	LEU
2	E	2267	LYS
2	E	2277	HIS
2	E	2296	THR
2	E	2326	SER
2	E	2327	GLU
2	E	2332	THR
2	E	2339	LEU
2	E	2340	LEU
2	E	2360	THR
2	E	2362	MET
2	E	2367	ASN
2	E	2368	GLN
2	E	2371	ASP
2	E	2375	LYS
2	E	2380	LEU
2	E	2384	ASN
2	E	2388	ARG
2	E	2393	LEU
2	E	2396	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	GLN
1	A	343	ASN
2	B	1030	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1087	ASN
2	B	1139	ASN
2	B	1470	GLN
2	B	1471	GLN
2	B	1863	HIS
2	B	1869	ASN
2	B	1895	HIS
2	B	1985	GLN
2	B	2038	HIS
2	B	2054	GLN
2	B	2087	ASN
2	B	2202	GLN
2	B	2237	GLN
2	B	2318	ASN
2	B	2338	GLN
2	B	2368	GLN
2	B	2373	ASN
2	B	2384	ASN
2	B	2387	HIS
1	D	48	HIS
1	D	219	ASN
1	D	244	HIS
2	E	930	ASN
2	E	1087	ASN
2	E	1091	ASN
2	E	1097	HIS
2	E	1140	ASN
2	E	1218	GLN
2	E	1281	ASN
2	E	1470	GLN
2	E	1540	ASN
2	E	1600	GLN
2	E	1655	GLN
2	E	1763	ASN
2	E	1863	HIS
2	E	1985	GLN
2	E	2018	ASN
2	E	2054	GLN
2	E	2087	ASN
2	E	2159	ASN
2	E	2202	GLN
2	E	2232	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	2237	GLN
2	E	2260	HIS
2	E	2358	ASN
2	E	2373	ASN
2	E	2384	ASN

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	327/355 (92%)	-0.30	4 (1%)	81	64	40, 75, 133, 168	1 (0%)
1	D	317/355 (89%)	-0.35	1 (0%)	94	88	38, 73, 131, 170	0
2	B	1398/1531 (91%)	-0.08	39 (2%)	56	32	38, 103, 176, 253	0
2	E	1420/1531 (92%)	-0.13	29 (2%)	68	46	37, 90, 160, 245	0
All	All	3462/3772 (91%)	-0.15	73 (2%)	67	44	37, 92, 165, 253	1 (0%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	2096	GLN	16.1
2	E	2093	VAL	7.1
2	E	2323	ASN	6.6
2	B	2385	GLU	6.0
2	E	2321	ILE	5.6
2	B	2268	PHE	5.4
2	E	2326	SER	5.4
2	B	2174	ASP	5.3
2	E	2325	LEU	5.3
2	B	2059	ILE	5.2
2	B	2361	PHE	5.0
2	E	2322	MET	4.8
2	B	2221	ILE	4.0
2	B	2322	MET	3.9
2	B	2060	LEU	3.7
2	B	2251	GLU	3.7
2	E	2095	ARG	3.7
2	E	2361	PHE	3.6
2	E	2059	ILE	3.6
2	B	1433	ASP	3.6
2	B	1324	GLY	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	329	GLY	3.4
2	E	2081	ASP	3.3
2	B	2320	ASP	3.3
2	E	1680	SER	3.2
2	E	2082	ILE	3.2
2	E	2057	ASP	3.2
2	B	2052	GLU	3.1
2	E	2214	ASP	3.0
2	E	2094	LYS	3.0
2	E	2324	VAL	3.0
2	E	2072	SER	3.0
2	B	2072	SER	3.0
2	B	1292	ARG	2.9
2	E	2385	GLU	2.8
2	B	1899	TRP	2.8
2	E	2071	ILE	2.8
2	E	2092	SER	2.7
2	B	2275	ALA	2.7
2	B	2262	GLN	2.6
2	B	2091	PRO	2.5
2	B	1238	LEU	2.5
2	B	2288	CYS	2.5
2	B	2384	ASN	2.5
2	E	1323	SER	2.4
1	A	110	GLU	2.4
2	B	2179	GLU	2.4
2	E	2320	ASP	2.4
2	E	2382	PHE	2.3
2	E	1681	VAL	2.3
1	A	40	HIS	2.3
2	B	2183	TYR	2.3
2	B	2214	ASP	2.3
2	B	2289	ILE	2.3
2	B	1894	ILE	2.3
2	B	1674	ASP	2.2
2	B	2087	ASN	2.2
2	B	2264	GLU	2.2
1	A	169	GLU	2.2
2	B	2286	ARG	2.2
2	B	2317	GLU	2.2
2	B	2333	PHE	2.1
2	E	2060	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	2070	ASN	2.1
2	B	2311	GLY	2.1
2	B	1867	GLU	2.1
2	E	2153	ARG	2.1
2	B	2210	MET	2.1
2	E	2178	GLU	2.0
2	B	1676	LEU	2.0
1	D	40	HIS	2.0
2	B	2269	MET	2.0
2	B	2382	PHE	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.