Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2023 – 02:42 PM EDT

PDB ID	:	2ZIX
Title	:	Crystal structure of the Mus81-Eme1 complex
Authors	:	Chang, J.H.; Kim, J.J.; Choi, J.M.; Lee, J.H.; Cho, Y.
Deposited on	:	2008-02-25
Resolution	:	3.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

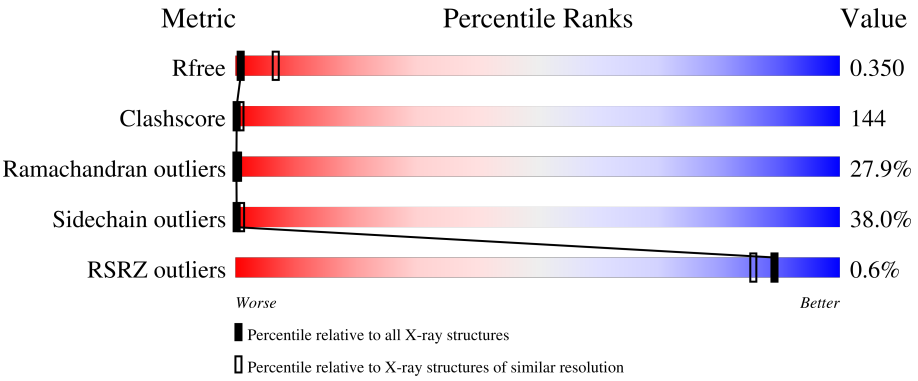
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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

Mol	Chain	Length	Quality of chain
1	A	307	5% 41% 36% 7% 12%
2	B	341	% 6% 33% 30% 7% 24%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4154 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 Crossover junction endonuclease MUS81.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	0	0
			2136	1340	397	391	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	245	MET	-	initiating methionine	UNP Q96NY9

- Molecule 2 is a protein called Crossover junction endonuclease EME1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	259	Total	C	N	O	S	0	0	0
			2018	1269	354	383	12			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	230	MET	-	expression tag	UNP Q96AY2
B	231	GLY	-	expression tag	UNP Q96AY2
B	232	SER	-	expression tag	UNP Q96AY2
B	233	SER	-	expression tag	UNP Q96AY2
B	234	HIS	-	expression tag	UNP Q96AY2
B	235	HIS	-	expression tag	UNP Q96AY2
B	236	HIS	-	expression tag	UNP Q96AY2
B	237	HIS	-	expression tag	UNP Q96AY2
B	238	HIS	-	expression tag	UNP Q96AY2
B	239	HIS	-	expression tag	UNP Q96AY2
B	240	SER	-	expression tag	UNP Q96AY2
B	241	GLN	-	expression tag	UNP Q96AY2
B	242	ASP	-	expression tag	UNP Q96AY2
B	243	PRO	-	expression tag	UNP Q96AY2
B	244	ASN	-	expression tag	UNP Q96AY2

Continued on next page...

Continued from previous page...

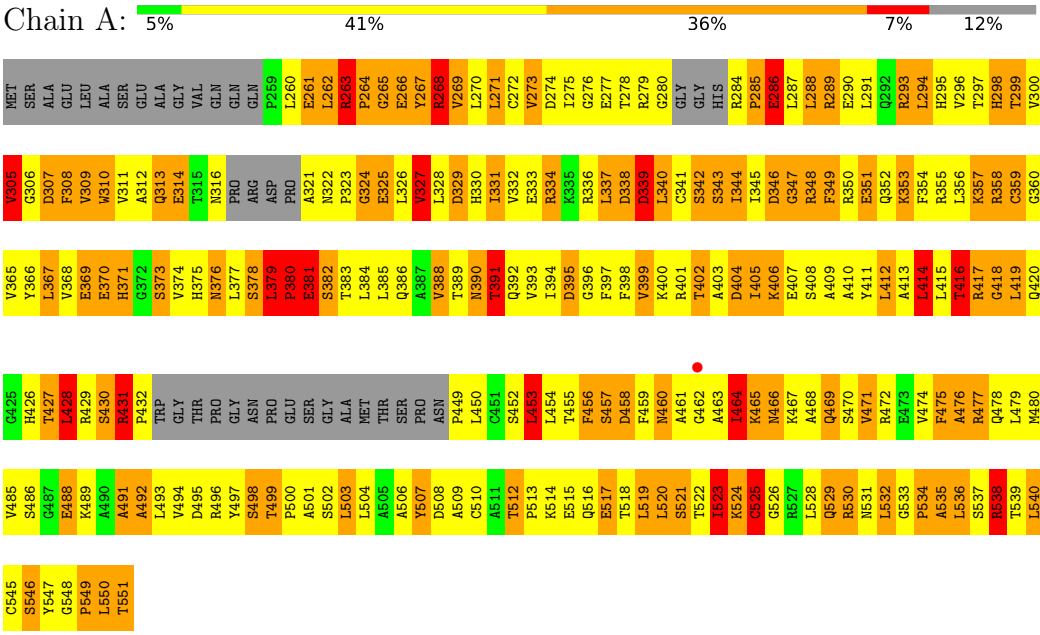
Chain	Residue	Modelled	Actual	Comment	Reference
B	245	SER	-	expression tag	UNP Q96AY2

3 Residue-property plots (i)

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

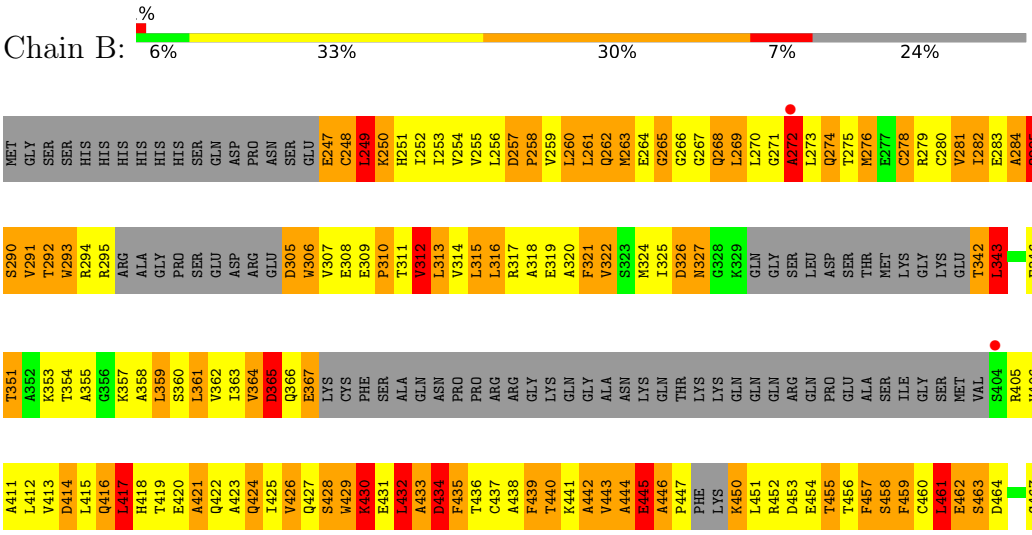
• Molecule 1: Crossover junction endonuclease MUS81

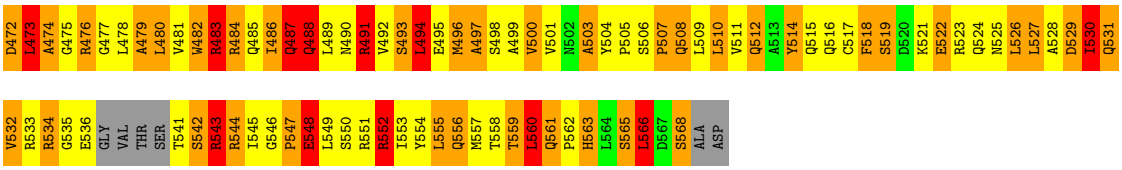
Chain A:



• Molecule 2: Crossover junction endonuclease EME1

Chain B:




D472
L473
A474
G475
R476
G477
L478
A479
L480
V481
W482
R483
R484
Q485
I486
Q487
Q488
L489
M490
R491
V492
S493
L494
E495
M496
A497
S498
A499
V500
V501
N502
A503
Y504
P505
S506
P507
Q508
L509
L510
V511
Q512
A513
Y514
Q515
Q516
C517
F518
S519
D520
K521
E522
R523
Q524
N525
L526
L527
A528
D529
I530
Q531
V532
R533
R534
G535
E536
GLY
VAL
THR
SER
T541
S542
R543
R544
I545
G546
P547
E548
L549
S550
R551
R552
I553
Y554
L555
Q556
M557
T558
T559
L560
Q561
P562
H563
L564
S565
L566
D567
S568
ALA
ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	85.81Å 85.81Å 176.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.50 19.61 – 3.50	Depositor EDS
% Data completeness (in resolution range)	92.7 (20.00-3.50) 92.7 (19.61-3.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	5.69 (at 3.52Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.285 , 0.346 0.283 , 0.350	Depositor DCC
R_{free} test set	441 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å^2)	73.1	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.10 , -28.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.32$, $< L^2 > = 0.15$	Xtriage
Estimated twinning fraction	0.188 for -h,-k,l	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	4154	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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	0.62	1/2168 (0.0%)	1.03	6/2923 (0.2%)
2	B	0.63	1/2043 (0.0%)	0.98	3/2765 (0.1%)
All	All	0.63	2/4211 (0.0%)	1.01	9/5688 (0.2%)

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	1	6
2	B	0	9
All	All	1	15

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	484	ARG	CG-CD	9.51	1.75	1.51
1	A	380	PRO	CG-CD	5.26	1.68	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	339	ASP	N-CA-C	-8.72	87.44	111.00
1	A	380	PRO	N-CA-C	6.48	128.94	112.10
2	B	365	ASP	CB-CG-OD1	6.05	123.74	118.30
1	A	538	ARG	NE-CZ-NH2	-5.44	117.58	120.30
2	B	249	LEU	CA-CB-CG	5.42	127.77	115.30
1	A	424	GLN	N-CA-C	5.20	125.03	111.00
1	A	380	PRO	CB-CA-C	5.19	124.98	112.00
1	A	367	LEU	CA-CB-CG	5.15	127.15	115.30
2	B	527	LEU	CA-CB-CG	-5.11	103.55	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	380	PRO	CA

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	268	ARG	Peptide
1	A	338	ASP	Peptide
1	A	378	SER	Peptide
1	A	379	LEU	Peptide
1	A	431	ARG	Peptide
1	A	453	LEU	Peptide
2	B	272	ALA	Peptide
2	B	276	MET	Peptide
2	B	278	CYS	Peptide
2	B	351	THR	Peptide
2	B	430	LYS	Peptide
2	B	450	LYS	Peptide
2	B	461	LEU	Peptide
2	B	463	SER	Peptide
2	B	560	LEU	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	2136	0	2188	673	1
2	B	2018	0	2033	628	1
All	All	4154	0	4221	1208	2

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 144.

All (1208) 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:484:ARG:CG	2:B:484:ARG:CD	1.75	1.64
1:A:491:ALA:CB	1:A:492:ALA:HB2	1.30	1.59
1:A:414:LEU:HD21	2:B:413:VAL:CG2	1.41	1.47
1:A:414:LEU:CD2	2:B:413:VAL:HG21	1.43	1.45
1:A:491:ALA:HB3	1:A:492:ALA:CB	1.44	1.44
1:A:272:CYS:HB2	1:A:311:VAL:CG2	1.51	1.37
2:B:253:ILE:HG13	2:B:279:ARG:O	1.21	1.28
1:A:272:CYS:CB	1:A:311:VAL:HG21	1.66	1.25
1:A:497:TYR:CD1	1:A:503:LEU:HD13	1.74	1.23
1:A:308:PHE:O	1:A:309:VAL:HG23	1.39	1.23
1:A:536:LEU:O	1:A:540:LEU:HB2	1.35	1.22
1:A:312:ALA:N	1:A:325:GLU:OE1	1.69	1.21
2:B:290:SER:O	2:B:291:VAL:HG13	1.38	1.19
1:A:296:VAL:CG1	1:A:416:THR:HG21	1.73	1.18
1:A:336:ARG:CB	1:A:339:ASP:HB2	1.75	1.17
1:A:532:LEU:HD13	1:A:533:GLY:H	1.00	1.15
1:A:536:LEU:O	1:A:540:LEU:CB	1.95	1.13
1:A:499:THR:HG21	2:B:560:LEU:HG	1.23	1.12
2:B:268:GLN:HG3	2:B:432:LEU:HB3	1.29	1.12
1:A:507:TYR:HE1	1:A:541:SER:OG	1.31	1.11
2:B:544:ARG:HA	2:B:544:ARG:NE	1.59	1.11
1:A:332:VAL:HA	1:A:365:VAL:O	1.51	1.11
1:A:305:VAL:HG22	1:A:356:LEU:HB2	1.32	1.10
1:A:291:LEU:HD13	1:A:412:LEU:HD13	1.21	1.10
2:B:483:ARG:HA	2:B:486:ILE:HG13	1.32	1.10
2:B:506:SER:HB3	2:B:509:LEU:HG	1.31	1.10
1:A:291:LEU:HD22	1:A:412:LEU:CD2	1.82	1.09
1:A:359:CYS:HB2	1:A:361:LEU:HD22	1.30	1.09
2:B:492:VAL:HG13	2:B:497:ALA:CB	1.79	1.09
1:A:493:LEU:HD21	1:A:523:ILE:HG21	1.34	1.08
1:A:532:LEU:CD1	1:A:536:LEU:HD13	1.84	1.08
2:B:249:LEU:HA	2:B:445:GLU:OE1	1.53	1.08
1:A:369:GLU:O	1:A:371:HIS:CE1	2.06	1.08
1:A:492:ALA:HB3	1:A:493:LEU:HD12	1.29	1.08
1:A:336:ARG:HD2	1:A:338:ASP:HB3	1.35	1.08
1:A:369:GLU:HG3	1:A:370:GLU:N	1.51	1.08
1:A:402:THR:CB	1:A:408:SER:HA	1.83	1.08
2:B:253:ILE:CG1	2:B:279:ARG:O	2.02	1.08
1:A:291:LEU:CD2	1:A:412:LEU:HD22	1.83	1.07
1:A:334:ARG:HE	1:A:367:LEU:HD22	1.02	1.07
1:A:296:VAL:HG13	1:A:416:THR:HG21	1.25	1.06
1:A:332:VAL:CG2	1:A:365:VAL:HB	1.84	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:GLU:CG	1:A:370:GLU:H	1.66	1.06
1:A:477:ARG:HG2	1:A:477:ARG:HH11	0.99	1.06
1:A:402:THR:HB	1:A:408:SER:CA	1.84	1.06
1:A:530:ARG:HG2	1:A:530:ARG:HH21	0.95	1.05
1:A:332:VAL:HG22	1:A:365:VAL:HB	1.06	1.05
1:A:540:LEU:O	1:A:543:LEU:HD21	1.56	1.05
1:A:418:GLY:O	1:A:421:ARG:NH2	1.89	1.05
1:A:329:ASP:HB2	1:A:362:GLU:OE1	1.57	1.04
1:A:404:ASP:O	1:A:408:SER:HB3	1.57	1.04
1:A:310:TRP:O	1:A:327:VAL:HB	1.55	1.04
2:B:511:VAL:HA	2:B:514:TYR:HB2	1.37	1.03
1:A:263:ARG:NH1	1:A:264:PRO:HD2	1.73	1.03
2:B:257:ASP:CB	2:B:288:PRO:HB3	1.87	1.03
2:B:551:ARG:HH12	2:B:566:LEU:HB3	1.22	1.03
1:A:334:ARG:HG3	1:A:367:LEU:HB2	1.40	1.03
1:A:364:ARG:O	1:A:397:PHE:HA	1.57	1.03
1:A:331:ILE:HG22	1:A:361:LEU:HB3	1.38	1.03
1:A:458:ASP:O	1:A:462:GLY:CA	2.07	1.02
1:A:532:LEU:HD11	1:A:536:LEU:CD1	1.87	1.02
1:A:419:LEU:HD12	1:A:422:LEU:CD2	1.90	1.02
1:A:305:VAL:HG13	1:A:356:LEU:HD22	1.39	1.02
2:B:316:LEU:CB	2:B:363:ILE:HG22	1.90	1.02
2:B:435:PHE:CD2	2:B:435:PHE:O	2.13	1.02
2:B:531:GLN:NE2	2:B:534:ARG:HG3	1.74	1.02
1:A:332:VAL:HG22	1:A:365:VAL:CB	1.89	1.01
1:A:264:PRO:HA	1:A:427:THR:HA	1.43	1.01
1:A:383:THR:HG22	1:A:386:GLN:NE2	1.75	1.00
2:B:257:ASP:HB2	2:B:288:PRO:HB3	1.38	1.00
2:B:305:ASP:O	2:B:306:TRP:CE3	2.13	1.00
1:A:523:ILE:HG23	1:A:525:CYS:SG	2.00	1.00
1:A:532:LEU:HD13	1:A:533:GLY:N	1.73	1.00
2:B:290:SER:HA	2:B:313:LEU:O	1.60	1.00
1:A:326:LEU:CD2	1:A:428:LEU:HD11	1.90	1.00
1:A:480:MET:HA	1:A:485:VAL:CG1	1.92	1.00
2:B:316:LEU:HB2	2:B:363:ILE:HG22	1.43	0.99
2:B:271:GLY:N	2:B:274:GLN:HB3	1.75	0.99
1:A:497:TYR:CB	1:A:503:LEU:HD22	1.93	0.99
2:B:265:GLY:O	2:B:269:LEU:N	1.96	0.99
2:B:260:LEU:HD13	2:B:289:CYS:HA	1.44	0.99
1:A:336:ARG:HB3	1:A:339:ASP:CB	1.93	0.98
1:A:498:SER:O	1:A:499:THR:HB	1.58	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:493:SER:O	2:B:496:MET:N	1.95	0.98
1:A:336:ARG:HB3	1:A:339:ASP:HB2	1.00	0.98
1:A:308:PHE:O	1:A:309:VAL:CG2	2.12	0.98
2:B:524:GLN:HG2	2:B:551:ARG:HB2	1.44	0.97
1:A:287:LEU:HD13	1:A:405:ILE:HG22	1.47	0.97
2:B:280:CYS:O	2:B:281:VAL:HG23	1.65	0.97
2:B:273:LEU:HD13	2:B:437:CYS:SG	2.05	0.96
1:A:329:ASP:CB	1:A:362:GLU:OE1	2.11	0.96
1:A:541:SER:HA	1:A:544:TYR:HB2	1.46	0.96
1:A:369:GLU:HG3	1:A:370:GLU:H	0.81	0.96
2:B:247:GLU:OE1	2:B:250:LYS:NZ	1.97	0.96
2:B:287:VAL:HG21	2:B:350:ILE:HG12	1.47	0.95
1:A:341:CYS:O	1:A:343:SER:N	1.99	0.95
2:B:542:SER:O	2:B:543:ARG:HG3	1.66	0.95
2:B:492:VAL:HG13	2:B:497:ALA:HB2	1.48	0.95
1:A:262:LEU:O	1:A:263:ARG:HB3	1.65	0.94
1:A:419:LEU:HD12	1:A:422:LEU:HD22	1.48	0.94
1:A:369:GLU:HA	1:A:402:THR:O	1.67	0.94
1:A:326:LEU:HD23	1:A:428:LEU:HD11	1.49	0.94
1:A:423:TYR:HB2	1:A:449:PRO:HB3	1.47	0.94
2:B:365:ASP:OD1	2:B:366:GLN:N	2.01	0.94
1:A:369:GLU:CG	1:A:370:GLU:N	2.25	0.94
1:A:530:ARG:HG2	1:A:530:ARG:NH2	1.73	0.94
2:B:544:ARG:HA	2:B:544:ARG:CZ	1.98	0.94
1:A:463:ALA:O	1:A:465:LYS:N	1.99	0.93
2:B:416:GLN:HE21	2:B:416:GLN:N	1.67	0.93
1:A:402:THR:HB	1:A:408:SER:HA	0.94	0.93
1:A:495:ASP:O	1:A:498:SER:OG	1.85	0.93
1:A:383:THR:HG22	1:A:386:GLN:HE22	1.27	0.93
2:B:354:THR:HG23	2:B:357:LYS:HB2	1.51	0.93
1:A:421:ARG:H	1:A:421:ARG:HE	0.98	0.93
1:A:399:VAL:O	1:A:400:LYS:HG2	1.69	0.93
1:A:328:LEU:O	1:A:330:HIS:N	2.02	0.93
1:A:480:MET:HA	1:A:485:VAL:HG11	1.50	0.92
2:B:273:LEU:CD1	2:B:437:CYS:SG	2.58	0.92
2:B:314:VAL:HG22	2:B:361:LEU:HD13	1.51	0.92
2:B:435:PHE:O	2:B:435:PHE:HD2	1.51	0.92
2:B:316:LEU:O	2:B:363:ILE:HA	1.68	0.92
1:A:497:TYR:HD1	1:A:503:LEU:HD13	1.22	0.92
1:A:421:ARG:HE	1:A:421:ARG:N	1.67	0.91
1:A:293:ARG:HG2	1:A:293:ARG:HH11	1.36	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ASP:OD2	1:A:334:ARG:N	2.04	0.91
1:A:477:ARG:HG2	1:A:477:ARG:NH1	1.77	0.91
1:A:307:ASP:OD2	1:A:333:GLU:HA	1.71	0.91
1:A:395:ASP:HB2	1:A:397:PHE:CD1	2.06	0.91
2:B:255:VAL:HG13	2:B:281:VAL:O	1.71	0.91
1:A:312:ALA:O	1:A:313:GLN:HG2	1.71	0.91
1:A:331:ILE:CG2	1:A:361:LEU:HB3	2.01	0.90
1:A:551:THR:OG1	2:B:476:ARG:HG3	1.72	0.90
2:B:268:GLN:HG3	2:B:432:LEU:CB	2.02	0.90
1:A:391:THR:HA	1:A:395:ASP:OD2	1.71	0.89
1:A:395:ASP:CB	1:A:397:PHE:CE1	2.55	0.89
2:B:518:PHE:O	2:B:523:ARG:HG3	1.72	0.89
1:A:268:ARG:NH1	1:A:314:GLU:O	2.06	0.89
1:A:285:PRO:HB2	1:A:288:LEU:HB2	1.53	0.88
2:B:312:VAL:O	2:B:360:SER:N	2.05	0.88
1:A:543:LEU:HG	1:A:544:TYR:N	1.89	0.88
2:B:482:TRP:NE1	2:B:504:TYR:O	2.07	0.88
1:A:422:LEU:HD11	2:B:418:HIS:CE1	2.09	0.88
2:B:264:GLU:O	2:B:429:TRP:CZ2	2.27	0.88
2:B:416:GLN:C	2:B:418:HIS:H	1.76	0.88
2:B:433:ALA:HA	2:B:436:THR:HB	1.55	0.87
2:B:492:VAL:HG13	2:B:497:ALA:HB3	1.53	0.87
1:A:334:ARG:NE	1:A:367:LEU:HD22	1.88	0.87
1:A:420:GLN:H	1:A:421:ARG:HH21	1.21	0.87
1:A:491:ALA:CB	1:A:492:ALA:CB	2.21	0.87
2:B:491:ARG:H	2:B:491:ARG:HD2	1.38	0.87
1:A:532:LEU:HD11	1:A:536:LEU:HD13	0.92	0.87
1:A:538:ARG:HH22	2:B:473:LEU:C	1.78	0.87
2:B:264:GLU:O	2:B:429:TRP:HZ2	1.57	0.87
2:B:511:VAL:HA	2:B:514:TYR:CB	2.04	0.87
1:A:270:LEU:HD12	1:A:271:LEU:H	1.37	0.86
1:A:477:ARG:HG3	2:B:460:CYS:SG	2.15	0.86
2:B:509:LEU:O	2:B:512:GLN:N	2.08	0.86
1:A:413:ALA:HA	1:A:417:ARG:NH1	1.90	0.86
1:A:518:THR:OG1	1:A:521:SER:OG	1.92	0.86
1:A:417:ARG:O	1:A:420:GLN:HB2	1.76	0.86
2:B:433:ALA:C	2:B:435:PHE:H	1.79	0.86
1:A:353:LYS:NZ	1:A:357:LYS:NZ	2.24	0.85
1:A:456:PHE:HD1	1:A:457:SER:N	1.75	0.85
1:A:543:LEU:HG	1:A:544:TYR:H	1.40	0.85
2:B:493:SER:O	2:B:496:MET:HG3	1.75	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:LEU:HD22	1:A:428:LEU:HD21	1.59	0.85
2:B:313:LEU:HB2	2:B:360:SER:HB2	1.59	0.85
2:B:483:ARG:O	2:B:486:ILE:N	2.08	0.85
2:B:257:ASP:OD2	2:B:285:GLN:HG2	1.76	0.84
2:B:555:LEU:O	2:B:557:MET:N	2.10	0.84
2:B:255:VAL:HG13	2:B:281:VAL:C	1.98	0.84
1:A:336:ARG:HG3	1:A:369:GLU:HG2	1.59	0.84
2:B:461:LEU:O	2:B:462:GLU:HG2	1.77	0.84
2:B:305:ASP:O	2:B:306:TRP:HE3	1.59	0.84
2:B:365:ASP:O	2:B:366:GLN:HB2	1.76	0.84
2:B:250:LYS:O	2:B:251:HIS:HB2	1.78	0.84
1:A:261:GLU:OE1	1:A:428:LEU:O	1.95	0.83
1:A:360:GLY:H	1:A:459:PHE:HE2	1.23	0.83
2:B:555:LEU:C	2:B:557:MET:H	1.79	0.83
1:A:336:ARG:HD2	1:A:338:ASP:CB	2.08	0.83
1:A:476:ALA:HA	1:A:479:LEU:HB2	1.59	0.83
2:B:324:MET:SD	2:B:342:THR:HA	2.18	0.82
1:A:413:ALA:HA	1:A:417:ARG:HH12	1.42	0.82
2:B:287:VAL:HB	2:B:350:ILE:HD11	1.61	0.82
2:B:289:CYS:O	2:B:314:VAL:HA	1.79	0.82
1:A:530:ARG:HH21	1:A:530:ARG:CG	1.87	0.82
1:A:540:LEU:O	1:A:543:LEU:CD2	2.28	0.82
1:A:296:VAL:HG13	1:A:416:THR:CG2	2.08	0.82
1:A:270:LEU:CD1	1:A:271:LEU:H	1.93	0.81
1:A:337:LEU:HD22	1:A:376:ASN:ND2	1.95	0.81
1:A:514:LYS:H	1:A:514:LYS:CD	1.93	0.81
2:B:287:VAL:HG21	2:B:350:ILE:CG1	2.09	0.81
2:B:514:TYR:OH	2:B:553:ILE:HG22	1.80	0.81
1:A:284:ARG:N	1:A:286:GLU:HG2	1.94	0.81
1:A:272:CYS:CB	1:A:311:VAL:CG2	2.41	0.81
1:A:455:THR:OG1	1:A:456:PHE:N	2.13	0.81
2:B:416:GLN:NE2	2:B:416:GLN:H	1.77	0.81
1:A:263:ARG:HH11	1:A:264:PRO:HD2	1.45	0.81
1:A:264:PRO:CA	1:A:427:THR:HA	2.11	0.81
1:A:419:LEU:HD12	1:A:422:LEU:HD23	1.63	0.81
1:A:543:LEU:HD12	2:B:507:PRO:HG2	1.60	0.81
2:B:420:GLU:O	2:B:421:ALA:HB3	1.81	0.81
2:B:290:SER:O	2:B:291:VAL:CG1	2.27	0.80
1:A:390:ASN:O	1:A:392:GLN:N	2.14	0.80
2:B:544:ARG:NE	2:B:544:ARG:CA	2.38	0.80
2:B:531:GLN:NE2	2:B:534:ARG:CG	2.45	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:413:VAL:HG23	2:B:413:VAL:O	1.81	0.80
1:A:491:ALA:HB1	1:A:492:ALA:HB2	1.57	0.80
1:A:344:ILE:O	1:A:344:ILE:HG13	1.80	0.80
1:A:478:GLN:HA	1:A:481:GLN:OE1	1.82	0.80
1:A:458:ASP:O	1:A:462:GLY:N	2.15	0.80
1:A:290:GLU:OE2	1:A:291:LEU:HD23	1.82	0.80
1:A:371:HIS:HE1	1:A:403:ALA:HA	1.46	0.80
1:A:413:ALA:C	1:A:415:LEU:H	1.83	0.80
2:B:405:ARG:C	2:B:407:ASP:H	1.86	0.80
1:A:497:TYR:HB3	1:A:503:LEU:HB2	1.64	0.79
1:A:499:THR:CG2	2:B:560:LEU:HG	2.09	0.79
1:A:508:ASP:OD2	1:A:509:ALA:N	2.14	0.79
1:A:404:ASP:HB2	1:A:406:LYS:H	1.47	0.79
2:B:312:VAL:H	2:B:359:LEU:HA	1.44	0.79
2:B:483:ARG:HD2	2:B:483:ARG:C	2.03	0.79
1:A:353:LYS:HZ1	1:A:357:LYS:NZ	1.80	0.79
1:A:507:TYR:CE1	1:A:544:TYR:HB3	2.17	0.79
1:A:456:PHE:HD1	1:A:457:SER:H	1.30	0.79
1:A:523:ILE:CG2	1:A:525:CYS:SG	2.70	0.79
2:B:432:LEU:HD23	2:B:436:THR:HG21	1.65	0.79
1:A:270:LEU:HD23	1:A:311:VAL:O	1.83	0.79
2:B:467:GLY:HA2	2:B:484:ARG:NH2	1.97	0.79
1:A:366:TYR:CD1	1:A:391:THR:HG21	2.18	0.79
2:B:351:THR:HA	2:B:354:THR:O	1.83	0.78
1:A:393:VAL:HG11	2:B:443:VAL:HG22	1.63	0.78
1:A:414:LEU:HD21	2:B:413:VAL:CB	2.11	0.78
1:A:512:THR:O	1:A:515:GLU:HG2	1.83	0.78
2:B:314:VAL:CG2	2:B:361:LEU:CD1	2.61	0.78
1:A:480:MET:HA	1:A:485:VAL:HG12	1.65	0.78
2:B:316:LEU:HB3	2:B:363:ILE:HG22	1.64	0.78
1:A:341:CYS:C	1:A:343:SER:H	1.79	0.78
2:B:451:LEU:CD2	2:B:454:GLU:OE2	2.31	0.78
2:B:492:VAL:CG1	2:B:497:ALA:CB	2.61	0.78
2:B:255:VAL:HG12	2:B:256:LEU:H	1.49	0.78
2:B:317:ARG:HG3	2:B:364:VAL:HG23	1.65	0.78
1:A:523:ILE:HG23	1:A:524:LYS:H	1.49	0.77
1:A:326:LEU:HD22	1:A:428:LEU:HD11	1.66	0.77
2:B:272:ALA:O	2:B:437:CYS:SG	2.43	0.77
1:A:535:ALA:O	1:A:538:ARG:N	2.18	0.77
2:B:256:LEU:CD1	2:B:282:ILE:HG23	2.15	0.77
2:B:486:ILE:HG22	2:B:489:LEU:HD22	1.64	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ASP:OD2	1:A:333:GLU:CA	2.33	0.77
1:A:477:ARG:HB3	2:B:488:GLN:HG3	1.64	0.77
2:B:416:GLN:HE21	2:B:416:GLN:H	1.29	0.77
1:A:260:LEU:HD22	1:A:455:THR:HG21	1.65	0.76
1:A:458:ASP:O	1:A:462:GLY:HA3	1.85	0.76
2:B:289:CYS:O	2:B:314:VAL:HB	1.84	0.76
2:B:359:LEU:CD2	2:B:421:ALA:HB2	2.16	0.76
1:A:419:LEU:CD1	1:A:422:LEU:HD23	2.15	0.76
1:A:366:TYR:HD1	1:A:391:THR:HG21	1.51	0.76
2:B:555:LEU:HD23	2:B:559:THR:HG22	1.67	0.76
1:A:336:ARG:HG3	1:A:369:GLU:CG	2.14	0.76
2:B:492:VAL:CG1	2:B:497:ALA:HB3	2.15	0.76
1:A:411:TYR:O	1:A:415:LEU:HG	1.85	0.76
2:B:256:LEU:HD12	2:B:282:ILE:HG23	1.68	0.76
1:A:395:ASP:HB2	1:A:397:PHE:CE1	2.20	0.76
2:B:480:LEU:O	2:B:483:ARG:HB3	1.84	0.76
1:A:266:GLU:HG2	1:A:268:ARG:HG2	1.67	0.76
1:A:395:ASP:HB3	1:A:397:PHE:CE1	2.20	0.76
1:A:404:ASP:HB2	1:A:406:LYS:HB3	1.68	0.76
1:A:502:SER:O	1:A:506:ALA:CB	2.34	0.76
1:A:536:LEU:O	1:A:540:LEU:HB3	1.84	0.75
2:B:267:GLY:O	2:B:268:GLN:HB2	1.84	0.75
2:B:290:SER:CA	2:B:313:LEU:O	2.35	0.75
1:A:266:GLU:HG2	1:A:268:ARG:HE	1.51	0.75
1:A:419:LEU:CG	1:A:422:LEU:HD23	2.16	0.75
2:B:326:ASP:OD1	2:B:326:ASP:N	2.19	0.75
2:B:314:VAL:CG2	2:B:361:LEU:HD13	2.16	0.75
2:B:433:ALA:CA	2:B:436:THR:HB	2.16	0.75
1:A:419:LEU:CD1	1:A:422:LEU:CD2	2.65	0.75
1:A:538:ARG:NH2	2:B:473:LEU:CA	2.50	0.75
2:B:314:VAL:HG22	2:B:361:LEU:CD1	2.16	0.75
2:B:451:LEU:HD21	2:B:454:GLU:OE2	1.85	0.75
2:B:490:ASN:O	2:B:492:VAL:N	2.20	0.75
1:A:417:ARG:H	1:A:417:ARG:HD2	1.51	0.75
2:B:489:LEU:HB2	2:B:492:VAL:HG21	1.69	0.75
1:A:507:TYR:OH	1:A:541:SER:HB2	1.87	0.74
2:B:289:CYS:O	2:B:314:VAL:CB	2.35	0.74
2:B:316:LEU:HB2	2:B:363:ILE:CG2	2.15	0.74
2:B:327:ASN:N	2:B:327:ASN:HD22	1.85	0.74
1:A:419:LEU:HD11	2:B:414:ASP:OD1	1.86	0.74
2:B:481:VAL:O	2:B:483:ARG:N	2.20	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:ARG:O	1:A:293:ARG:HB2	1.87	0.74
2:B:483:ARG:HB2	2:B:501:VAL:HG21	1.68	0.74
2:B:271:GLY:H	2:B:274:GLN:HB3	1.52	0.74
2:B:287:VAL:HG11	2:B:350:ILE:HG13	1.69	0.74
2:B:459:PHE:O	2:B:461:LEU:HD23	1.87	0.74
2:B:555:LEU:CD2	2:B:559:THR:HG22	2.17	0.74
1:A:460:ASN:CG	1:A:461:ALA:H	1.91	0.74
2:B:427:GLN:O	2:B:428:SER:HB2	1.87	0.74
1:A:272:CYS:N	1:A:311:VAL:HG22	2.03	0.73
1:A:432:PRO:O	1:A:452:SER:HA	1.88	0.73
2:B:283:GLU:HG2	2:B:284:ALA:H	1.51	0.73
1:A:497:TYR:HB2	1:A:503:LEU:HD22	1.70	0.73
1:A:502:SER:O	1:A:506:ALA:HB3	1.88	0.73
1:A:308:PHE:O	1:A:309:VAL:CB	2.35	0.73
1:A:399:VAL:HG21	2:B:435:PHE:CE1	2.24	0.73
1:A:485:VAL:HG12	1:A:485:VAL:O	1.85	0.73
2:B:526:LEU:O	2:B:527:LEU:HD23	1.89	0.73
2:B:550:SER:HA	2:B:553:ILE:HD13	1.70	0.73
1:A:296:VAL:HG11	1:A:416:THR:HG21	1.68	0.73
1:A:371:HIS:CE1	1:A:403:ALA:HA	2.23	0.73
2:B:471:VAL:HB	2:B:476:ARG:O	1.89	0.73
2:B:496:MET:O	2:B:499:ALA:N	2.18	0.73
1:A:262:LEU:O	1:A:263:ARG:CB	2.36	0.73
1:A:422:LEU:HD11	2:B:418:HIS:HE1	1.52	0.73
2:B:257:ASP:HB3	2:B:285:GLN:HB2	1.68	0.73
1:A:399:VAL:HG21	2:B:435:PHE:HE1	1.54	0.72
1:A:274:ASP:OD2	1:A:277:GLU:OE1	2.07	0.72
1:A:420:GLN:H	1:A:421:ARG:NH2	1.86	0.72
2:B:550:SER:HA	2:B:553:ILE:CD1	2.19	0.72
1:A:492:ALA:HB3	1:A:493:LEU:CD1	2.16	0.72
2:B:511:VAL:CA	2:B:514:TYR:HB2	2.17	0.72
1:A:305:VAL:HG22	1:A:356:LEU:CB	2.16	0.72
2:B:309:GLU:HB3	2:B:310:PRO:HD2	1.70	0.72
1:A:272:CYS:H	1:A:311:VAL:HG22	1.55	0.72
2:B:364:VAL:HG12	2:B:426:VAL:HG11	1.71	0.72
2:B:471:VAL:HG12	2:B:477:GLY:HA3	1.72	0.72
2:B:551:ARG:NH1	2:B:566:LEU:HB3	1.99	0.72
2:B:519:SER:O	2:B:523:ARG:HG3	1.88	0.72
1:A:284:ARG:HA	1:A:286:GLU:H	1.54	0.72
2:B:289:CYS:O	2:B:314:VAL:CA	2.37	0.72
2:B:315:LEU:HD22	2:B:316:LEU:N	2.05	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:LEU:HD12	1:A:422:LEU:O	1.89	0.72
2:B:483:ARG:CA	2:B:486:ILE:HG13	2.16	0.72
2:B:555:LEU:C	2:B:557:MET:N	2.43	0.71
1:A:329:ASP:O	1:A:362:GLU:HB3	1.89	0.71
2:B:491:ARG:H	2:B:491:ARG:CD	2.03	0.71
1:A:264:PRO:HA	1:A:427:THR:CA	2.19	0.71
1:A:381:GLU:HA	1:A:384:LEU:HD23	1.72	0.71
2:B:260:LEU:HD22	2:B:289:CYS:O	1.88	0.71
2:B:416:GLN:C	2:B:418:HIS:N	2.41	0.71
1:A:546:SER:HB2	2:B:506:SER:OG	1.90	0.71
2:B:273:LEU:HD12	2:B:437:CYS:SG	2.30	0.71
1:A:263:ARG:HG2	1:A:266:GLU:OE1	1.90	0.71
2:B:316:LEU:C	2:B:363:ILE:HA	2.10	0.71
1:A:340:LEU:O	1:A:343:SER:HB3	1.91	0.70
2:B:488:GLN:O	2:B:489:LEU:HD12	1.91	0.70
2:B:261:LEU:HD23	2:B:262:GLN:HG3	1.73	0.70
1:A:316:ASN:HD21	1:A:321:ALA:N	1.90	0.70
1:A:362:GLU:O	1:A:363:ARG:HD2	1.90	0.70
2:B:495:GLU:O	2:B:532:VAL:HG13	1.92	0.70
1:A:270:LEU:HG	1:A:271:LEU:N	2.07	0.70
1:A:497:TYR:CG	1:A:503:LEU:HD22	2.26	0.70
2:B:284:ALA:O	2:B:285:GLN:OE1	2.10	0.70
2:B:450:LYS:CB	2:B:451:LEU:HD12	2.20	0.70
2:B:551:ARG:O	2:B:554:TYR:N	2.25	0.70
1:A:369:GLU:O	1:A:371:HIS:ND1	2.24	0.70
1:A:524:LYS:O	1:A:530:ARG:O	2.09	0.70
2:B:354:THR:HG21	2:B:359:LEU:HD22	1.73	0.70
2:B:529:ASP:O	2:B:530:ILE:HG23	1.91	0.70
1:A:290:GLU:OE2	1:A:291:LEU:CD2	2.39	0.69
1:A:369:GLU:C	1:A:371:HIS:CE1	2.65	0.69
2:B:420:GLU:O	2:B:421:ALA:CB	2.39	0.69
1:A:419:LEU:HG	1:A:422:LEU:HD23	1.73	0.69
1:A:273:VAL:HA	1:A:308:PHE:HB3	1.73	0.69
1:A:293:ARG:HH11	1:A:293:ARG:CG	2.04	0.69
1:A:323:PRO:O	1:A:324:GLY:O	2.09	0.69
2:B:317:ARG:CG	2:B:364:VAL:HG23	2.22	0.69
2:B:551:ARG:C	2:B:553:ILE:H	1.96	0.69
1:A:499:THR:CB	2:B:560:LEU:O	2.40	0.69
1:A:260:LEU:HD22	1:A:455:THR:CG2	2.22	0.69
2:B:467:GLY:HA2	2:B:484:ARG:HH22	1.56	0.69
1:A:404:ASP:O	1:A:408:SER:CB	2.39	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:LEU:O	1:A:422:LEU:CD1	2.40	0.69
2:B:260:LEU:HD22	2:B:289:CYS:C	2.14	0.69
2:B:482:TRP:CD1	2:B:505:PRO:O	2.46	0.69
1:A:417:ARG:HD2	1:A:417:ARG:N	2.07	0.69
2:B:309:GLU:HB3	2:B:310:PRO:CD	2.21	0.68
2:B:416:GLN:HE21	2:B:416:GLN:CA	2.05	0.68
1:A:492:ALA:CB	1:A:493:LEU:HD12	2.15	0.68
1:A:480:MET:O	1:A:482:VAL:N	2.26	0.68
2:B:263:MET:HE1	2:B:429:TRP:CZ2	2.28	0.68
2:B:509:LEU:O	2:B:510:LEU:C	2.30	0.68
1:A:356:LEU:HD11	1:A:459:PHE:HB3	1.76	0.68
1:A:420:GLN:N	1:A:421:ARG:HH21	1.91	0.68
1:A:499:THR:HB	2:B:560:LEU:O	1.92	0.68
2:B:480:LEU:HD12	2:B:481:VAL:H	1.57	0.68
1:A:305:VAL:O	1:A:356:LEU:HB3	1.94	0.68
2:B:504:TYR:HD2	2:B:510:LEU:HD22	1.58	0.68
2:B:317:ARG:HA	2:B:364:VAL:N	2.09	0.68
1:A:413:ALA:C	1:A:415:LEU:N	2.45	0.68
1:A:497:TYR:HA	1:A:502:SER:HB2	1.75	0.68
2:B:488:GLN:H	2:B:488:GLN:NE2	1.92	0.68
1:A:304:HIS:O	1:A:305:VAL:HB	1.93	0.67
1:A:541:SER:O	1:A:543:LEU:N	2.27	0.67
2:B:317:ARG:HA	2:B:364:VAL:H	1.58	0.67
1:A:538:ARG:NH2	2:B:473:LEU:C	2.48	0.67
2:B:253:ILE:O	2:B:294:ARG:HG3	1.94	0.67
1:A:382:SER:O	1:A:385:LEU:N	2.23	0.67
2:B:481:VAL:HG12	2:B:485:GLN:HG3	1.74	0.67
1:A:337:LEU:HB3	1:A:376:ASN:ND2	2.10	0.67
1:A:523:ILE:HG23	1:A:524:LYS:N	2.10	0.67
1:A:538:ARG:NH2	2:B:473:LEU:HB3	2.10	0.67
1:A:310:TRP:O	1:A:327:VAL:CB	2.39	0.67
2:B:548:GLU:HG3	2:B:549:LEU:HD22	1.76	0.67
1:A:456:PHE:CD1	1:A:457:SER:N	2.61	0.67
2:B:506:SER:CB	2:B:509:LEU:HG	2.17	0.67
1:A:541:SER:C	1:A:543:LEU:H	1.98	0.67
2:B:255:VAL:HG12	2:B:256:LEU:N	2.10	0.66
1:A:481:GLN:NE2	2:B:485:GLN:HG2	2.10	0.66
2:B:491:ARG:O	2:B:496:MET:SD	2.53	0.66
1:A:336:ARG:CD	1:A:338:ASP:HB3	2.20	0.66
1:A:270:LEU:CG	1:A:271:LEU:H	2.08	0.66
1:A:272:CYS:SG	1:A:301:ARG:HG2	2.35	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:ASN:HD22	2:B:327:ASN:H	1.43	0.66
2:B:542:SER:O	2:B:543:ARG:CG	2.41	0.66
1:A:371:HIS:CD2	1:A:401:ARG:HG2	2.30	0.66
2:B:457:PHE:O	2:B:458:SER:HB3	1.95	0.66
1:A:285:PRO:O	1:A:287:LEU:N	2.28	0.66
1:A:296:VAL:CG1	1:A:416:THR:CG2	2.65	0.66
1:A:351:GLU:HG3	1:A:352:GLN:N	2.11	0.66
2:B:484:ARG:CG	2:B:484:ARG:NE	2.59	0.66
1:A:329:ASP:HB3	1:A:362:GLU:OE1	1.95	0.66
1:A:337:LEU:HB3	1:A:376:ASN:HD21	1.59	0.66
2:B:260:LEU:HD21	2:B:315:LEU:HB3	1.77	0.66
2:B:263:MET:HE3	2:B:429:TRP:CH2	2.31	0.66
2:B:361:LEU:HB3	2:B:422:GLN:O	1.96	0.66
2:B:469:VAL:CG2	2:B:484:ARG:HD3	2.25	0.66
2:B:524:GLN:O	2:B:550:SER:O	2.14	0.66
1:A:404:ASP:HB2	1:A:406:LYS:N	2.11	0.66
1:A:289:ARG:CG	1:A:289:ARG:HH21	2.08	0.66
1:A:360:GLY:N	1:A:459:PHE:HE2	1.94	0.66
2:B:359:LEU:O	2:B:421:ALA:HA	1.94	0.66
2:B:483:ARG:HD2	2:B:484:ARG:N	2.11	0.66
2:B:492:VAL:HA	2:B:496:MET:SD	2.35	0.65
2:B:551:ARG:NH1	2:B:568:SER:O	2.29	0.65
1:A:391:THR:HA	1:A:395:ASP:CG	2.15	0.65
1:A:486:SER:HB3	1:A:489:LYS:H	1.60	0.65
1:A:520:LEU:O	1:A:521:SER:C	2.33	0.65
2:B:528:ALA:HA	2:B:546:GLY:HA2	1.79	0.65
1:A:382:SER:O	1:A:385:LEU:HB2	1.97	0.65
1:A:353:LYS:HZ2	1:A:353:LYS:HB3	1.59	0.65
2:B:249:LEU:HG	2:B:250:LYS:H	1.62	0.65
2:B:263:MET:CE	2:B:429:TRP:CZ2	2.80	0.65
1:A:550:LEU:HD12	2:B:505:PRO:O	1.96	0.65
2:B:551:ARG:HH12	2:B:566:LEU:CB	2.04	0.65
1:A:457:SER:O	1:A:458:ASP:C	2.35	0.65
2:B:281:VAL:C	2:B:282:ILE:HD13	2.16	0.65
2:B:359:LEU:HG	2:B:421:ALA:HB2	1.79	0.65
2:B:430:LYS:O	2:B:431:GLU:HG2	1.95	0.65
1:A:497:TYR:HB3	1:A:503:LEU:HD22	1.76	0.65
2:B:314:VAL:HG23	2:B:361:LEU:CD1	2.26	0.65
1:A:521:SER:O	1:A:532:LEU:HB3	1.96	0.64
1:A:457:SER:HA	1:A:460:ASN:OD1	1.96	0.64
1:A:532:LEU:CD1	1:A:533:GLY:N	2.57	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:GLU:O	1:A:334:ARG:HB2	1.97	0.64
1:A:536:LEU:HD23	1:A:536:LEU:C	2.18	0.64
2:B:315:LEU:HD13	2:B:315:LEU:O	1.97	0.64
2:B:315:LEU:HA	2:B:362:VAL:HG13	1.79	0.64
2:B:494:LEU:HD23	2:B:494:LEU:H	1.62	0.64
1:A:341:CYS:C	1:A:343:SER:N	2.47	0.64
2:B:255:VAL:O	2:B:292:THR:O	2.16	0.64
2:B:252:ILE:CG2	2:B:253:ILE:N	2.60	0.64
2:B:473:LEU:O	2:B:474:ALA:O	2.15	0.64
1:A:337:LEU:HD22	1:A:376:ASN:HD22	1.61	0.64
1:A:471:VAL:HB	2:B:562:PRO:HA	1.80	0.64
1:A:476:ALA:O	1:A:479:LEU:N	2.31	0.64
2:B:551:ARG:C	2:B:553:ILE:N	2.51	0.64
1:A:356:LEU:O	1:A:356:LEU:HG	1.96	0.64
1:A:458:ASP:O	1:A:462:GLY:C	2.36	0.64
1:A:353:LYS:HZ3	1:A:357:LYS:NZ	1.96	0.63
1:A:272:CYS:HB2	1:A:311:VAL:HG21	0.69	0.63
1:A:272:CYS:O	1:A:308:PHE:HB3	1.98	0.63
1:A:326:LEU:HG	1:A:455:THR:CG2	2.28	0.63
1:A:382:SER:OG	1:A:383:THR:N	2.30	0.63
2:B:514:TYR:OH	2:B:553:ILE:C	2.37	0.63
1:A:357:LYS:HD2	1:A:358:ARG:N	2.14	0.63
1:A:498:SER:O	1:A:499:THR:CB	2.39	0.63
1:A:366:TYR:C	1:A:367:LEU:HD12	2.18	0.63
2:B:288:PRO:C	2:B:290:SER:H	2.02	0.63
1:A:394:ILE:O	1:A:395:ASP:C	2.37	0.63
1:A:353:LYS:NZ	1:A:357:LYS:HZ2	1.94	0.63
1:A:270:LEU:CG	1:A:271:LEU:N	2.62	0.63
1:A:414:LEU:HD11	2:B:413:VAL:HB	1.81	0.63
1:A:534:PRO:O	1:A:537:SER:OG	2.16	0.63
2:B:252:ILE:HG23	2:B:294:ARG:O	1.98	0.63
2:B:531:GLN:NE2	2:B:533:ARG:O	2.32	0.62
1:A:481:GLN:NE2	2:B:484:ARG:HG2	2.13	0.62
2:B:409:GLU:O	2:B:413:VAL:HG13	1.99	0.62
2:B:433:ALA:HB1	2:B:437:CYS:HB2	1.80	0.62
1:A:460:ASN:CG	1:A:461:ALA:N	2.52	0.62
1:A:260:LEU:HD13	1:A:455:THR:HG23	1.80	0.62
1:A:291:LEU:HD22	1:A:412:LEU:HD22	0.87	0.62
1:A:322:ASN:N	1:A:323:PRO:HD3	2.14	0.62
2:B:495:GLU:O	2:B:532:VAL:CG1	2.48	0.62
2:B:354:THR:HG21	2:B:359:LEU:HD13	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:PRO:C	1:A:287:LEU:H	2.03	0.62
1:A:366:TYR:HB2	1:A:397:PHE:HD2	1.63	0.62
1:A:478:GLN:HB2	2:B:485:GLN:HB3	1.82	0.62
2:B:313:LEU:HD12	2:B:361:LEU:H	1.64	0.62
2:B:317:ARG:HB2	2:B:319:GLU:HG2	1.82	0.62
2:B:511:VAL:O	2:B:515:GLN:HG2	1.99	0.61
2:B:481:VAL:CG1	2:B:485:GLN:HE21	2.13	0.61
2:B:551:ARG:O	2:B:553:ILE:N	2.33	0.61
1:A:514:LYS:H	1:A:514:LYS:HD2	1.64	0.61
2:B:487:GLN:O	2:B:489:LEU:N	2.33	0.61
2:B:316:LEU:N	2:B:362:VAL:O	2.31	0.61
1:A:266:GLU:HG2	1:A:268:ARG:NE	2.15	0.61
1:A:333:GLU:HB3	1:A:366:TYR:CD2	2.36	0.61
1:A:353:LYS:HZ1	1:A:357:LYS:HZ1	1.46	0.61
1:A:493:LEU:HD21	1:A:523:ILE:CG2	2.23	0.61
1:A:550:LEU:CD1	2:B:505:PRO:O	2.49	0.61
2:B:257:ASP:OD2	2:B:285:GLN:CG	2.48	0.61
1:A:266:GLU:OE2	1:A:268:ARG:NH2	2.32	0.61
1:A:330:HIS:HB3	1:A:363:ARG:O	2.01	0.61
1:A:520:LEU:CD1	1:A:536:LEU:HD22	2.31	0.61
2:B:501:VAL:HG12	2:B:501:VAL:O	2.01	0.60
1:A:337:LEU:CD2	1:A:376:ASN:ND2	2.64	0.60
1:A:465:LYS:H	1:A:465:LYS:HD2	1.65	0.60
2:B:254:VAL:HG22	2:B:293:TRP:CD1	2.36	0.60
1:A:499:THR:HG21	2:B:560:LEU:HA	1.83	0.60
1:A:332:VAL:CA	1:A:365:VAL:O	2.38	0.60
2:B:291:VAL:O	2:B:312:VAL:HG12	2.02	0.60
2:B:471:VAL:CG1	2:B:477:GLY:O	2.49	0.60
1:A:471:VAL:O	1:A:471:VAL:HG12	2.01	0.60
1:A:522:THR:HA	1:A:532:LEU:CB	2.31	0.60
1:A:354:PHE:HA	1:A:357:LYS:HB2	1.83	0.60
1:A:359:CYS:HB2	1:A:361:LEU:CD2	2.21	0.60
1:A:538:ARG:HH22	2:B:473:LEU:CA	2.14	0.60
2:B:283:GLU:HG2	2:B:284:ALA:N	2.17	0.60
2:B:503:ALA:C	2:B:504:TYR:HD1	2.05	0.60
2:B:504:TYR:N	2:B:505:PRO:HD3	2.16	0.60
1:A:312:ALA:C	1:A:313:GLN:HG2	2.20	0.60
2:B:551:ARG:CZ	2:B:568:SER:O	2.49	0.60
2:B:256:LEU:HD12	2:B:282:ILE:CG2	2.32	0.60
1:A:456:PHE:O	1:A:458:ASP:N	2.25	0.59
2:B:347:VAL:HG22	2:B:351:THR:OG1	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:451:LEU:HD23	2:B:454:GLU:OE2	2.02	0.59
1:A:551:THR:OG1	2:B:476:ARG:CG	2.47	0.59
2:B:293:TRP:HZ2	2:B:439:PHE:HZ	1.50	0.59
1:A:328:LEU:C	1:A:330:HIS:H	2.04	0.59
1:A:550:LEU:HD12	2:B:506:SER:HA	1.84	0.59
1:A:336:ARG:CG	1:A:370:GLU:HB3	2.32	0.59
1:A:499:THR:HG23	1:A:501:ALA:N	2.18	0.59
2:B:459:PHE:O	2:B:461:LEU:CD2	2.51	0.59
2:B:496:MET:C	2:B:498:SER:H	2.05	0.59
1:A:354:PHE:HD1	1:A:357:LYS:HE2	1.67	0.59
1:A:406:LYS:HG2	1:A:407:GLU:N	2.17	0.59
1:A:423:TYR:HD2	1:A:426:HIS:HD2	1.51	0.59
1:A:474:VAL:HB	2:B:556:GLN:OE1	2.01	0.59
1:A:404:ASP:CB	1:A:406:LYS:HB3	2.32	0.59
2:B:255:VAL:O	2:B:292:THR:HG22	2.03	0.59
2:B:255:VAL:CG1	2:B:256:LEU:H	2.15	0.59
2:B:405:ARG:C	2:B:407:ASP:N	2.56	0.59
2:B:542:SER:C	2:B:543:ARG:HG3	2.22	0.59
2:B:254:VAL:HG12	2:B:254:VAL:O	2.03	0.59
2:B:429:TRP:HA	2:B:429:TRP:CE3	2.36	0.59
1:A:405:ILE:HA	1:A:408:SER:OG	2.03	0.59
2:B:432:LEU:CD2	2:B:436:THR:HG21	2.33	0.59
1:A:399:VAL:O	1:A:400:LYS:CG	2.47	0.58
1:A:523:ILE:O	1:A:524:LYS:HB2	2.03	0.58
2:B:507:PRO:O	2:B:509:LEU:N	2.36	0.58
2:B:544:ARG:HA	2:B:544:ARG:HE	1.61	0.58
2:B:252:ILE:HG22	2:B:253:ILE:N	2.17	0.58
2:B:503:ALA:C	2:B:505:PRO:HD3	2.24	0.58
1:A:275:ILE:HG22	1:A:275:ILE:O	2.02	0.58
2:B:531:GLN:HE21	2:B:534:ARG:HG3	1.63	0.58
1:A:331:ILE:CG2	1:A:361:LEU:HG	2.33	0.58
1:A:395:ASP:N	1:A:395:ASP:OD1	2.35	0.58
1:A:398:PHE:HB2	2:B:422:GLN:HE21	1.67	0.58
1:A:543:LEU:HA	1:A:546:SER:OG	2.03	0.58
2:B:324:MET:SD	2:B:342:THR:CA	2.91	0.58
2:B:257:ASP:CG	2:B:288:PRO:HB3	2.23	0.58
2:B:293:TRP:HZ2	2:B:439:PHE:CZ	2.21	0.58
1:A:491:ALA:HB3	1:A:492:ALA:HB2	0.60	0.58
1:A:518:THR:OG1	1:A:518:THR:O	2.20	0.58
1:A:538:ARG:HH21	2:B:473:LEU:HA	1.68	0.58
2:B:324:MET:SD	2:B:342:THR:HB	2.44	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:ASN:ND2	1:A:321:ALA:N	2.51	0.58
1:A:423:TYR:CD2	1:A:426:HIS:HD2	2.22	0.58
1:A:502:SER:O	1:A:506:ALA:HB2	2.03	0.58
2:B:258:PRO:HB3	2:B:282:ILE:HB	1.84	0.58
2:B:506:SER:HB3	2:B:509:LEU:CG	2.22	0.58
1:A:266:GLU:CG	1:A:268:ARG:HG2	2.34	0.58
1:A:289:ARG:HG2	1:A:289:ARG:NH2	2.19	0.58
1:A:503:LEU:HD12	1:A:507:TYR:HD2	1.69	0.58
2:B:281:VAL:CG1	2:B:282:ILE:N	2.67	0.58
2:B:480:LEU:CD1	2:B:481:VAL:H	2.17	0.58
1:A:542:GLN:O	1:A:546:SER:OG	2.22	0.58
2:B:354:THR:CG2	2:B:357:LYS:HB2	2.31	0.58
2:B:421:ALA:O	2:B:422:GLN:OE1	2.21	0.57
2:B:433:ALA:HA	2:B:437:CYS:N	2.19	0.57
2:B:271:GLY:C	2:B:273:LEU:H	2.07	0.57
2:B:527:LEU:HD12	2:B:553:ILE:HD13	1.86	0.57
2:B:257:ASP:HB2	2:B:288:PRO:CB	2.23	0.57
2:B:481:VAL:HA	2:B:484:ARG:HB3	1.86	0.57
1:A:349:PHE:O	1:A:353:LYS:N	2.28	0.57
2:B:416:GLN:O	2:B:418:HIS:N	2.38	0.57
1:A:337:LEU:CD2	1:A:376:ASN:HD21	2.18	0.57
1:A:396:GLY:N	1:A:397:PHE:HD1	2.03	0.57
1:A:520:LEU:HD11	1:A:536:LEU:CD2	2.35	0.57
2:B:364:VAL:CG1	2:B:426:VAL:HG21	2.35	0.57
2:B:412:LEU:HA	2:B:415:LEU:HD21	1.87	0.57
1:A:334:ARG:HG3	1:A:367:LEU:CB	2.25	0.57
1:A:464:ILE:HA	1:A:467:LYS:HB3	1.87	0.57
1:A:480:MET:CE	2:B:460:CYS:O	2.53	0.57
2:B:254:VAL:HG22	2:B:293:TRP:HD1	1.69	0.57
2:B:526:LEU:N	2:B:550:SER:OG	2.38	0.57
1:A:305:VAL:CG2	1:A:356:LEU:HB2	2.20	0.57
2:B:316:LEU:O	2:B:364:VAL:N	2.36	0.57
1:A:275:ILE:C	1:A:277:GLU:H	2.08	0.57
1:A:497:TYR:CD1	1:A:503:LEU:CD1	2.68	0.57
1:A:514:LYS:H	1:A:514:LYS:HD3	1.67	0.57
1:A:539:THR:HA	1:A:542:GLN:NE2	2.20	0.57
1:A:477:ARG:CB	2:B:488:GLN:HG3	2.34	0.56
2:B:254:VAL:O	2:B:280:CYS:HA	2.05	0.56
2:B:359:LEU:CG	2:B:421:ALA:HB2	2.35	0.56
2:B:426:VAL:HG12	2:B:428:SER:H	1.70	0.56
2:B:484:ARG:CD	2:B:484:ARG:CB	2.75	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ILE:HG13	1:A:332:VAL:N	2.20	0.56
2:B:365:ASP:CG	2:B:367:GLU:H	2.08	0.56
2:B:429:TRP:O	2:B:431:GLU:N	2.37	0.56
1:A:486:SER:HB3	1:A:489:LYS:HB2	1.88	0.56
1:A:512:THR:HG23	1:A:515:GLU:OE2	2.05	0.56
1:A:538:ARG:NH2	2:B:473:LEU:CB	2.69	0.56
1:A:336:ARG:CG	1:A:369:GLU:HG2	2.34	0.56
1:A:361:LEU:O	1:A:364:ARG:HG3	2.05	0.56
1:A:400:LYS:HA	2:B:424:GLN:NE2	2.21	0.56
1:A:470:SER:HB2	2:B:563:HIS:HA	1.88	0.56
1:A:481:GLN:HE22	2:B:485:GLN:HG2	1.70	0.56
2:B:433:ALA:N	2:B:436:THR:HB	2.20	0.56
2:B:483:ARG:NH1	2:B:484:ARG:HA	2.20	0.56
2:B:493:SER:O	2:B:495:GLU:N	2.39	0.56
1:A:264:PRO:HG3	1:A:427:THR:OG1	2.05	0.56
1:A:347:GLY:HA3	2:B:464:ASP:OD2	2.05	0.56
1:A:366:TYR:HB2	1:A:397:PHE:CD2	2.40	0.56
1:A:423:TYR:O	1:A:424:GLN:O	2.23	0.56
1:A:469:GLN:O	2:B:565:SER:HA	2.06	0.56
1:A:499:THR:CG2	1:A:502:SER:H	2.18	0.56
2:B:283:GLU:O	2:B:284:ALA:O	2.23	0.56
2:B:357:LYS:O	2:B:358:ALA:HB3	2.06	0.56
2:B:543:ARG:C	2:B:544:ARG:HE	2.08	0.56
1:A:336:ARG:CD	1:A:338:ASP:CB	2.82	0.56
2:B:251:HIS:ND1	2:B:295:ARG:NH2	2.53	0.56
1:A:331:ILE:HG21	1:A:361:LEU:HG	1.87	0.56
1:A:545:CYS:C	2:B:508:GLN:HG3	2.26	0.56
2:B:261:LEU:HD23	2:B:261:LEU:N	2.21	0.56
2:B:444:ALA:HB3	2:B:445:GLU:OE2	2.06	0.56
2:B:494:LEU:HD23	2:B:494:LEU:N	2.18	0.56
1:A:491:ALA:CA	1:A:492:ALA:CB	2.83	0.55
1:A:538:ARG:NH2	2:B:473:LEU:HA	2.21	0.55
2:B:284:ALA:O	2:B:285:GLN:CD	2.44	0.55
2:B:313:LEU:HD12	2:B:361:LEU:N	2.21	0.55
2:B:261:LEU:N	2:B:261:LEU:CD2	2.69	0.55
1:A:359:CYS:CB	1:A:361:LEU:HD22	2.20	0.55
2:B:416:GLN:HE21	2:B:417:LEU:H	1.55	0.55
2:B:507:PRO:O	2:B:508:GLN:C	2.43	0.55
1:A:398:PHE:CG	2:B:422:GLN:NE2	2.75	0.55
1:A:407:GLU:HA	1:A:410:ALA:HB2	1.88	0.55
1:A:550:LEU:CD2	2:B:478:LEU:HB2	2.36	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:GLY:O	2:B:275:THR:N	2.30	0.55
1:A:409:ALA:O	1:A:412:LEU:HB3	2.06	0.55
1:A:522:THR:OG1	1:A:523:ILE:N	2.40	0.55
1:A:401:ARG:O	1:A:403:ALA:N	2.39	0.55
1:A:467:LYS:HG3	1:A:468:ALA:N	2.22	0.55
2:B:269:LEU:C	2:B:269:LEU:HD13	2.26	0.55
2:B:482:TRP:O	2:B:483:ARG:HB2	2.07	0.55
1:A:347:GLY:HA3	2:B:464:ASP:CG	2.27	0.55
1:A:367:LEU:CD2	1:A:400:LYS:HB2	2.37	0.55
1:A:453:LEU:HD12	1:A:454:LEU:HB2	1.89	0.55
1:A:496:ARG:HB3	1:A:497:TYR:CD2	2.41	0.55
2:B:271:GLY:C	2:B:273:LEU:N	2.59	0.55
2:B:507:PRO:HB2	2:B:508:GLN:HE21	1.70	0.55
1:A:307:ASP:OD2	1:A:333:GLU:C	2.44	0.55
1:A:311:VAL:C	1:A:325:GLU:OE1	2.40	0.55
1:A:523:ILE:CG2	1:A:524:LYS:H	2.18	0.55
2:B:527:LEU:HD12	2:B:553:ILE:CD1	2.37	0.55
1:A:336:ARG:HA	1:A:369:GLU:HG2	1.89	0.55
1:A:413:ALA:CA	1:A:417:ARG:NH1	2.68	0.55
1:A:476:ALA:C	1:A:479:LEU:H	2.11	0.54
2:B:518:PHE:CD2	2:B:519:SER:N	2.75	0.54
1:A:284:ARG:CA	1:A:286:GLU:HG2	2.37	0.54
1:A:298:HIS:ND1	1:A:298:HIS:O	2.40	0.54
1:A:499:THR:OG1	2:B:560:LEU:O	2.24	0.54
1:A:548:GLY:N	2:B:509:LEU:HD21	2.22	0.54
2:B:313:LEU:HG	2:B:314:VAL:N	2.22	0.54
2:B:261:LEU:HD23	2:B:261:LEU:H	1.71	0.54
2:B:351:THR:HG22	2:B:351:THR:O	2.07	0.54
2:B:483:ARG:C	2:B:485:GLN:N	2.61	0.54
1:A:421:ARG:N	1:A:421:ARG:NE	2.49	0.54
2:B:264:GLU:HB3	2:B:429:TRP:CE2	2.42	0.54
2:B:276:MET:SD	2:B:437:CYS:HB3	2.48	0.54
2:B:342:THR:O	2:B:342:THR:OG1	2.23	0.54
2:B:517:CYS:O	2:B:518:PHE:O	2.26	0.54
1:A:270:LEU:HG	1:A:271:LEU:H	1.69	0.54
2:B:248:CYS:O	2:B:249:LEU:O	2.26	0.54
1:A:261:GLU:HA	1:A:428:LEU:HG	1.89	0.54
2:B:271:GLY:O	2:B:274:GLN:N	2.40	0.54
2:B:315:LEU:HD22	2:B:315:LEU:C	2.28	0.54
2:B:508:GLN:HE21	2:B:508:GLN:H	1.53	0.54
1:A:530:ARG:NH2	1:A:530:ARG:CG	2.54	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:405:ARG:O	2:B:407:ASP:N	2.41	0.54
2:B:514:TYR:CZ	2:B:553:ILE:HG22	2.41	0.54
2:B:518:PHE:O	2:B:519:SER:O	2.25	0.54
2:B:543:ARG:HB3	2:B:543:ARG:CZ	2.36	0.54
1:A:390:ASN:C	1:A:392:GLN:H	2.11	0.54
2:B:314:VAL:O	2:B:362:VAL:N	2.33	0.54
1:A:354:PHE:O	1:A:354:PHE:CG	2.61	0.54
2:B:364:VAL:HG12	2:B:426:VAL:HG21	1.90	0.54
2:B:416:GLN:HE21	2:B:417:LEU:N	2.05	0.54
2:B:471:VAL:HG12	2:B:477:GLY:O	2.08	0.54
1:A:289:ARG:HH21	1:A:289:ARG:HG2	1.71	0.54
2:B:427:GLN:O	2:B:428:SER:CB	2.56	0.54
2:B:436:THR:O	2:B:436:THR:HG22	2.07	0.54
2:B:527:LEU:HD12	2:B:553:ILE:HG12	1.90	0.54
2:B:531:GLN:HE22	2:B:534:ARG:CG	2.20	0.54
2:B:548:GLU:OE2	2:B:549:LEU:HD21	2.07	0.54
1:A:369:GLU:O	1:A:371:HIS:NE2	2.41	0.53
2:B:314:VAL:HG23	2:B:361:LEU:HD12	1.90	0.53
1:A:514:LYS:CD	1:A:514:LYS:N	2.67	0.53
1:A:550:LEU:HD21	2:B:478:LEU:HB2	1.89	0.53
1:A:371:HIS:ND1	1:A:371:HIS:N	2.56	0.53
2:B:527:LEU:HD12	2:B:553:ILE:CG1	2.39	0.53
1:A:551:THR:OG1	2:B:475:GLY:O	2.25	0.53
2:B:249:LEU:HA	2:B:445:GLU:CD	2.27	0.53
2:B:314:VAL:CG2	2:B:361:LEU:HD12	2.38	0.53
2:B:312:VAL:O	2:B:359:LEU:HB2	2.08	0.53
2:B:271:GLY:HA2	2:B:275:THR:HG23	1.89	0.53
2:B:316:LEU:O	2:B:363:ILE:CA	2.51	0.53
1:A:278:THR:O	1:A:280:GLY:N	2.41	0.53
1:A:347:GLY:O	1:A:349:PHE:N	2.42	0.53
1:A:394:ILE:HG23	1:A:395:ASP:N	2.23	0.53
1:A:513:PRO:HD2	1:A:514:LYS:NZ	2.24	0.53
2:B:318:ALA:HA	2:B:321:PHE:HB3	1.91	0.53
1:A:476:ALA:HA	1:A:479:LEU:CB	2.35	0.53
1:A:538:ARG:NH2	1:A:539:THR:HG22	2.23	0.53
2:B:287:VAL:CB	2:B:350:ILE:HD11	2.35	0.53
2:B:293:TRP:HE1	2:B:440:THR:HG22	1.74	0.53
2:B:413:VAL:CG2	2:B:413:VAL:O	2.54	0.53
1:A:470:SER:C	1:A:472:ARG:H	2.12	0.53
1:A:497:TYR:HA	1:A:502:SER:CB	2.39	0.53
1:A:341:CYS:O	1:A:344:ILE:N	2.35	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:GLU:O	1:A:382:SER:O	2.27	0.52
1:A:480:MET:HG2	1:A:486:SER:O	2.08	0.52
2:B:254:VAL:CG2	2:B:293:TRP:HD1	2.22	0.52
2:B:270:LEU:HD11	2:B:274:GLN:NE2	2.24	0.52
2:B:547:PRO:C	2:B:549:LEU:H	2.13	0.52
2:B:551:ARG:NH1	2:B:566:LEU:HD23	2.24	0.52
2:B:325:ILE:HD13	2:B:411:ALA:HB1	1.91	0.52
2:B:468:GLY:H	2:B:484:ARG:NH2	2.06	0.52
2:B:524:GLN:CG	2:B:551:ARG:HB2	2.29	0.52
1:A:337:LEU:HB2	1:A:368:VAL:HG11	1.91	0.52
1:A:477:ARG:HH11	1:A:477:ARG:CG	1.91	0.52
1:A:541:SER:C	1:A:543:LEU:N	2.63	0.52
2:B:514:TYR:OH	2:B:554:TYR:N	2.42	0.52
2:B:533:ARG:HD3	2:B:541:THR:N	2.25	0.52
1:A:338:ASP:O	1:A:341:CYS:N	2.37	0.52
1:A:398:PHE:CB	2:B:422:GLN:HE21	2.20	0.52
2:B:268:GLN:CD	2:B:430:LYS:HA	2.30	0.52
2:B:351:THR:HG23	2:B:354:THR:O	2.10	0.52
1:A:332:VAL:HG22	1:A:365:VAL:CA	2.38	0.52
2:B:327:ASN:N	2:B:327:ASN:ND2	2.51	0.52
2:B:416:GLN:N	2:B:416:GLN:NE2	2.39	0.52
2:B:442:ALA:C	2:B:444:ALA:H	2.13	0.52
1:A:356:LEU:O	1:A:356:LEU:CG	2.57	0.52
1:A:395:ASP:CB	1:A:397:PHE:HE1	2.22	0.52
1:A:507:TYR:CE1	1:A:541:SER:OG	2.22	0.52
2:B:254:VAL:HA	2:B:293:TRP:HA	1.91	0.52
2:B:422:GLN:OE1	2:B:422:GLN:HA	2.10	0.52
2:B:426:VAL:HG12	2:B:427:GLN:N	2.24	0.52
1:A:291:LEU:HD13	1:A:412:LEU:CD1	2.15	0.52
1:A:393:VAL:HG11	2:B:443:VAL:CG2	2.37	0.52
1:A:548:GLY:HA2	2:B:509:LEU:HD11	1.92	0.52
2:B:457:PHE:O	2:B:458:SER:CB	2.57	0.52
2:B:554:TYR:O	2:B:558:THR:N	2.43	0.52
2:B:252:ILE:CG2	2:B:253:ILE:H	2.22	0.52
2:B:271:GLY:C	2:B:274:GLN:H	2.12	0.52
2:B:548:GLU:O	2:B:552:ARG:HD2	2.10	0.52
2:B:519:SER:O	2:B:523:ARG:CG	2.58	0.52
2:B:553:ILE:O	2:B:554:TYR:C	2.47	0.52
1:A:325:GLU:OE2	1:A:327:VAL:HG12	2.10	0.51
1:A:356:LEU:C	1:A:359:CYS:SG	2.88	0.51
2:B:445:GLU:HG3	2:B:447:PRO:HD2	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ILE:HG13	1:A:332:VAL:H	1.74	0.51
1:A:367:LEU:HD23	1:A:402:THR:HG23	1.91	0.51
1:A:457:SER:O	1:A:460:ASN:OD1	2.28	0.51
2:B:311:THR:O	2:B:312:VAL:HG13	2.09	0.51
2:B:351:THR:HG23	2:B:355:ALA:HA	1.92	0.51
1:A:367:LEU:HG	1:A:400:LYS:HB2	1.91	0.51
1:A:485:VAL:CG1	1:A:485:VAL:O	2.57	0.51
1:A:536:LEU:HD23	1:A:537:SER:N	2.24	0.51
1:A:544:TYR:HA	2:B:508:GLN:NE2	2.26	0.51
2:B:482:TRP:HA	2:B:482:TRP:CE3	2.45	0.51
2:B:566:LEU:C	2:B:568:SER:N	2.64	0.51
1:A:334:ARG:CG	1:A:367:LEU:HB2	2.29	0.51
2:B:322:VAL:HA	2:B:325:ILE:HD12	1.91	0.51
2:B:268:GLN:O	2:B:432:LEU:O	2.28	0.51
2:B:310:PRO:O	2:B:357:LYS:CG	2.59	0.51
2:B:446:ALA:H	2:B:447:PRO:CD	2.23	0.51
2:B:491:ARG:O	2:B:496:MET:CE	2.59	0.51
1:A:366:TYR:O	1:A:367:LEU:HD12	2.11	0.51
2:B:260:LEU:HD13	2:B:289:CYS:CA	2.28	0.51
2:B:433:ALA:O	2:B:435:PHE:N	2.44	0.51
1:A:385:LEU:O	1:A:389:THR:HG23	2.10	0.51
2:B:347:VAL:HG23	2:B:350:ILE:HG22	1.93	0.51
1:A:381:GLU:O	1:A:382:SER:C	2.49	0.51
1:A:538:ARG:HH22	2:B:473:LEU:HB3	1.76	0.51
2:B:270:LEU:HG	2:B:274:GLN:OE1	2.11	0.51
2:B:509:LEU:N	2:B:509:LEU:HD23	2.26	0.51
1:A:461:ALA:O	1:A:464:ILE:HB	2.11	0.50
2:B:504:TYR:HD2	2:B:510:LEU:CD2	2.23	0.50
1:A:342:SER:O	1:A:346:ASP:OD2	2.29	0.50
1:A:347:GLY:CA	2:B:464:ASP:OD2	2.59	0.50
1:A:463:ALA:O	1:A:464:ILE:C	2.49	0.50
1:A:470:SER:O	1:A:474:VAL:HG23	2.11	0.50
1:A:307:ASP:C	1:A:308:PHE:CD1	2.85	0.50
1:A:503:LEU:O	1:A:504:LEU:HD23	2.12	0.50
1:A:546:SER:HB2	2:B:506:SER:CB	2.40	0.50
2:B:260:LEU:CD2	2:B:289:CYS:O	2.59	0.50
1:A:414:LEU:O	1:A:418:GLY:HA3	2.12	0.50
1:A:480:MET:HE1	2:B:460:CYS:O	2.12	0.50
1:A:362:GLU:C	1:A:363:ARG:HD2	2.32	0.50
1:A:293:ARG:CG	1:A:293:ARG:NH1	2.69	0.50
1:A:414:LEU:CD2	2:B:413:VAL:HG11	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:263:MET:CE	2:B:429:TRP:CH2	2.94	0.50
2:B:265:GLY:C	2:B:267:GLY:N	2.63	0.50
1:A:333:GLU:O	1:A:366:TYR:HA	2.12	0.50
1:A:336:ARG:HG3	1:A:370:GLU:HB3	1.94	0.50
1:A:482:VAL:HA	2:B:469:VAL:O	2.12	0.50
2:B:347:VAL:O	2:B:349:ASP:N	2.44	0.50
1:A:520:LEU:O	1:A:522:THR:O	2.30	0.50
2:B:496:MET:C	2:B:498:SER:N	2.65	0.50
1:A:414:LEU:HD21	2:B:413:VAL:HG21	0.58	0.50
2:B:282:ILE:HD13	2:B:282:ILE:N	2.27	0.50
2:B:269:LEU:C	2:B:269:LEU:CD1	2.80	0.49
2:B:293:TRP:CH2	2:B:311:THR:OG1	2.65	0.49
2:B:486:ILE:HG22	2:B:489:LEU:CD2	2.39	0.49
2:B:488:GLN:C	2:B:489:LEU:HD12	2.32	0.49
1:A:405:ILE:O	1:A:408:SER:OG	2.27	0.49
1:A:418:GLY:O	1:A:420:GLN:N	2.43	0.49
1:A:474:VAL:CG1	2:B:556:GLN:OE1	2.59	0.49
1:A:517:GLU:HB3	1:A:538:ARG:HG3	1.94	0.49
2:B:455:THR:OG1	2:B:456:THR:N	2.46	0.49
1:A:326:LEU:HG	1:A:455:THR:HG22	1.93	0.49
1:A:338:ASP:C	1:A:341:CYS:H	2.16	0.49
1:A:514:LYS:HD2	1:A:514:LYS:N	2.27	0.49
2:B:259:VAL:O	2:B:260:LEU:HB2	2.12	0.49
1:A:348:ARG:O	1:A:349:PHE:O	2.29	0.49
1:A:422:LEU:CD1	2:B:418:HIS:HE1	2.23	0.49
2:B:365:ASP:OD1	2:B:367:GLU:N	2.43	0.49
2:B:525:ASN:O	2:B:525:ASN:OD1	2.30	0.49
1:A:497:TYR:CD2	1:A:497:TYR:N	2.80	0.49
1:A:546:SER:C	1:A:548:GLY:H	2.15	0.49
2:B:293:TRP:NE1	2:B:440:THR:HG22	2.28	0.49
2:B:364:VAL:HG21	2:B:429:TRP:HZ3	1.77	0.49
2:B:486:ILE:HB	2:B:497:ALA:HB1	1.94	0.49
1:A:285:PRO:CB	1:A:288:LEU:HB2	2.36	0.49
1:A:430:SER:O	1:A:453:LEU:O	2.31	0.49
1:A:543:LEU:HB2	2:B:507:PRO:HD2	1.95	0.49
2:B:315:LEU:HA	2:B:362:VAL:CG1	2.41	0.49
1:A:285:PRO:C	1:A:287:LEU:N	2.66	0.49
1:A:395:ASP:C	1:A:397:PHE:CE1	2.86	0.49
1:A:520:LEU:O	1:A:522:THR:N	2.46	0.49
2:B:354:THR:HG21	2:B:359:LEU:CD2	2.42	0.49
2:B:472:ASP:O	2:B:473:LEU:C	2.50	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:VAL:HG12	1:A:367:LEU:CD1	2.43	0.49
2:B:248:CYS:SG	2:B:249:LEU:N	2.86	0.49
2:B:259:VAL:O	2:B:288:PRO:O	2.31	0.49
2:B:295:ARG:HB3	2:B:307:VAL:HB	1.95	0.49
2:B:506:SER:H	2:B:509:LEU:HD12	1.78	0.49
1:A:273:VAL:HA	1:A:308:PHE:CD1	2.48	0.48
2:B:471:VAL:HG11	2:B:478:LEU:HD23	1.95	0.48
1:A:304:HIS:ND1	1:A:304:HIS:N	2.61	0.48
1:A:309:VAL:HG13	1:A:310:TRP:H	1.79	0.48
1:A:413:ALA:HB1	1:A:417:ARG:NH2	2.28	0.48
1:A:306:GLY:O	1:A:307:ASP:C	2.50	0.48
1:A:539:THR:OG1	1:A:540:LEU:N	2.46	0.48
2:B:313:LEU:HG	2:B:361:LEU:HA	1.96	0.48
1:A:272:CYS:N	1:A:311:VAL:CG2	2.76	0.48
1:A:393:VAL:CG1	2:B:443:VAL:CG2	2.91	0.48
2:B:433:ALA:HB1	2:B:437:CYS:SG	2.53	0.48
2:B:443:VAL:HG23	2:B:443:VAL:O	2.13	0.48
2:B:472:ASP:O	2:B:474:ALA:O	2.31	0.48
1:A:338:ASP:O	1:A:341:CYS:HB2	2.14	0.48
2:B:486:ILE:CG2	2:B:489:LEU:HD22	2.41	0.48
1:A:270:LEU:HD12	1:A:271:LEU:N	2.18	0.48
1:A:534:PRO:O	1:A:535:ALA:C	2.51	0.48
2:B:483:ARG:CB	2:B:501:VAL:HG21	2.40	0.48
1:A:284:ARG:HA	1:A:286:GLU:N	2.24	0.48
1:A:393:VAL:CG1	2:B:443:VAL:HG22	2.40	0.48
1:A:534:PRO:HG2	1:A:535:ALA:H	1.79	0.48
1:A:389:THR:O	1:A:390:ASN:C	2.50	0.48
1:A:390:ASN:C	1:A:392:GLN:N	2.66	0.48
1:A:391:THR:O	1:A:395:ASP:HB2	2.14	0.48
1:A:518:THR:O	1:A:519:LEU:C	2.52	0.48
2:B:411:ALA:O	2:B:415:LEU:HD21	2.14	0.48
1:A:453:LEU:HB2	1:A:454:LEU:HD23	1.95	0.48
2:B:321:PHE:CD1	2:B:321:PHE:C	2.87	0.48
2:B:362:VAL:HG22	2:B:363:ILE:N	2.29	0.48
1:A:453:LEU:HG	1:A:454:LEU:N	2.29	0.47
2:B:439:PHE:CG	2:B:440:THR:N	2.82	0.47
2:B:482:TRP:O	2:B:501:VAL:HG21	2.14	0.47
1:A:300:VAL:HG13	1:A:300:VAL:O	2.13	0.47
1:A:364:ARG:O	1:A:397:PHE:CA	2.46	0.47
2:B:483:ARG:C	2:B:486:ILE:H	2.16	0.47
2:B:310:PRO:O	2:B:357:LYS:HG2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:495:GLU:O	2:B:499:ALA:HB2	2.14	0.47
1:A:478:GLN:O	2:B:485:GLN:CD	2.52	0.47
2:B:313:LEU:HD12	2:B:361:LEU:C	2.34	0.47
2:B:525:ASN:HA	2:B:550:SER:HB3	1.94	0.47
2:B:550:SER:HA	2:B:553:ILE:HD12	1.96	0.47
2:B:482:TRP:CH2	2:B:510:LEU:HG	2.50	0.47
2:B:259:VAL:O	2:B:260:LEU:CB	2.62	0.47
2:B:471:VAL:HG12	2:B:477:GLY:CA	2.43	0.47
2:B:482:TRP:O	2:B:501:VAL:HG11	2.14	0.47
1:A:275:ILE:HA	1:A:278:THR:OG1	2.14	0.47
1:A:331:ILE:HB	1:A:361:LEU:HG	1.95	0.47
1:A:365:VAL:HG13	1:A:398:PHE:HB3	1.97	0.47
1:A:463:ALA:C	1:A:465:LYS:N	2.63	0.47
1:A:494:VAL:O	1:A:498:SER:CA	2.63	0.47
1:A:548:GLY:HA2	2:B:509:LEU:HD21	1.94	0.47
2:B:507:PRO:O	2:B:510:LEU:N	2.47	0.47
2:B:556:GLN:O	2:B:556:GLN:HG3	2.15	0.47
1:A:284:ARG:HA	1:A:286:GLU:HG2	1.97	0.47
1:A:404:ASP:HB2	1:A:406:LYS:CB	2.40	0.47
2:B:261:LEU:HD23	2:B:262:GLN:H	1.80	0.47
2:B:264:GLU:O	2:B:429:TRP:CE2	2.67	0.47
2:B:542:SER:O	2:B:543:ARG:CB	2.61	0.47
1:A:351:GLU:HA	2:B:459:PHE:HE2	1.79	0.47
1:A:486:SER:CB	1:A:489:LYS:HB2	2.45	0.47
2:B:415:LEU:O	2:B:418:HIS:HB2	2.14	0.47
1:A:307:ASP:HB2	1:A:333:GLU:HA	1.97	0.47
1:A:349:PHE:CE1	1:A:353:LYS:HG3	2.50	0.47
1:A:353:LYS:NZ	1:A:353:LYS:C	2.68	0.47
1:A:471:VAL:O	1:A:471:VAL:CG1	2.63	0.47
1:A:546:SER:O	2:B:508:GLN:HB2	2.15	0.47
1:A:331:ILE:CG2	1:A:361:LEU:CB	2.83	0.46
1:A:432:PRO:HA	1:A:453:LEU:HA	1.97	0.46
1:A:458:ASP:O	1:A:463:ALA:N	2.48	0.46
1:A:522:THR:HA	1:A:532:LEU:HB3	1.97	0.46
2:B:281:VAL:HG12	2:B:282:ILE:N	2.30	0.46
2:B:347:VAL:HG13	2:B:348:THR:N	2.30	0.46
2:B:471:VAL:CG1	2:B:477:GLY:HA3	2.43	0.46
2:B:559:THR:CG2	2:B:561:GLN:NE2	2.78	0.46
1:A:457:SER:CA	1:A:460:ASN:OD1	2.64	0.46
1:A:326:LEU:HD22	1:A:428:LEU:CD1	2.41	0.46
1:A:354:PHE:HA	1:A:357:LYS:HZ3	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:GLU:CA	1:A:402:THR:O	2.54	0.46
1:A:477:ARG:NH1	1:A:477:ARG:CG	2.59	0.46
2:B:255:VAL:CG1	2:B:256:LEU:N	2.75	0.46
2:B:280:CYS:O	2:B:281:VAL:CG2	2.51	0.46
2:B:287:VAL:O	2:B:289:CYS:N	2.48	0.46
2:B:508:GLN:H	2:B:508:GLN:NE2	2.13	0.46
1:A:369:GLU:O	1:A:371:HIS:CG	2.68	0.46
2:B:305:ASP:C	2:B:306:TRP:CE3	2.85	0.46
2:B:409:GLU:O	2:B:412:LEU:HG	2.15	0.46
2:B:471:VAL:HG11	2:B:477:GLY:O	2.15	0.46
2:B:483:ARG:HG2	2:B:497:ALA:O	2.16	0.46
2:B:543:ARG:O	2:B:544:ARG:NE	2.42	0.46
2:B:554:TYR:CD1	2:B:558:THR:HB	2.50	0.46
1:A:477:ARG:HG3	2:B:460:CYS:CB	2.45	0.46
1:A:264:PRO:HB3	1:A:427:THR:CB	2.46	0.46
1:A:270:LEU:HD11	1:A:299:THR:OG1	2.14	0.46
1:A:337:LEU:N	1:A:368:VAL:HG13	2.30	0.46
1:A:516:GLN:O	1:A:519:LEU:HB2	2.15	0.46
1:A:326:LEU:HD22	1:A:428:LEU:CD2	2.37	0.46
2:B:482:TRP:HA	2:B:482:TRP:HE3	1.81	0.46
2:B:493:SER:C	2:B:495:GLU:N	2.69	0.46
2:B:555:LEU:HD21	2:B:559:THR:HG22	1.94	0.46
2:B:433:ALA:HB1	2:B:437:CYS:CB	2.44	0.46
1:A:285:PRO:HG3	1:A:288:LEU:HD12	1.98	0.46
1:A:362:GLU:HG2	1:A:363:ARG:HG2	1.97	0.46
1:A:474:VAL:HG12	1:A:478:GLN:OE1	2.15	0.46
2:B:410:GLU:HA	2:B:413:VAL:HG22	1.97	0.46
1:A:266:GLU:HG2	1:A:268:ARG:CG	2.43	0.46
1:A:394:ILE:HG23	1:A:395:ASP:H	1.81	0.46
1:A:497:TYR:HB3	1:A:503:LEU:CB	2.40	0.46
2:B:527:LEU:HB2	2:B:550:SER:HB2	1.98	0.46
2:B:547:PRO:O	2:B:549:LEU:N	2.49	0.46
1:A:326:LEU:HG	1:A:455:THR:HG21	1.97	0.45
1:A:328:LEU:HD21	1:A:330:HIS:ND1	2.31	0.45
1:A:471:VAL:HA	1:A:474:VAL:HG23	1.97	0.45
1:A:475:PHE:HD1	1:A:475:PHE:O	1.98	0.45
1:A:261:GLU:O	1:A:262:LEU:HB2	2.17	0.45
1:A:348:ARG:O	1:A:349:PHE:C	2.53	0.45
1:A:353:LYS:HZ3	1:A:357:LYS:HZ2	1.60	0.45
1:A:457:SER:O	1:A:459:PHE:N	2.48	0.45
2:B:268:GLN:CG	2:B:432:LEU:HB3	2.22	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:317:ARG:CB	2:B:319:GLU:HG2	2.45	0.45
2:B:433:ALA:HA	2:B:436:THR:CB	2.36	0.45
1:A:299:THR:HG21	1:A:301:ARG:NH2	2.31	0.45
1:A:480:MET:HB2	1:A:480:MET:HE2	1.77	0.45
2:B:268:GLN:OE1	2:B:430:LYS:HA	2.16	0.45
2:B:269:LEU:CD1	2:B:270:LEU:N	2.79	0.45
2:B:491:ARG:HD2	2:B:491:ARG:N	2.20	0.45
2:B:526:LEU:C	2:B:527:LEU:HG	2.35	0.45
1:A:287:LEU:HD21	1:A:409:ALA:HB2	1.98	0.45
1:A:389:THR:HG21	2:B:438:ALA:CB	2.46	0.45
2:B:252:ILE:HG23	2:B:253:ILE:H	1.81	0.45
2:B:264:GLU:HB3	2:B:429:TRP:CZ2	2.52	0.45
2:B:316:LEU:O	2:B:364:VAL:HG22	2.15	0.45
2:B:321:PHE:CE1	2:B:325:ILE:HD11	2.51	0.45
1:A:542:GLN:HA	1:A:545:CYS:HG	1.81	0.45
2:B:293:TRP:HZ3	2:B:311:THR:O	2.00	0.45
2:B:527:LEU:HD23	2:B:527:LEU:HA	1.73	0.45
1:A:268:ARG:NH1	1:A:314:GLU:HA	2.31	0.45
1:A:423:TYR:HD2	1:A:426:HIS:CD2	2.34	0.45
1:A:550:LEU:HD23	1:A:551:THR:N	2.32	0.45
2:B:309:GLU:HA	2:B:309:GLU:OE2	2.17	0.45
2:B:314:VAL:O	2:B:361:LEU:HD12	2.17	0.45
1:A:469:GLN:HE21	1:A:469:GLN:HB3	1.50	0.45
1:A:493:LEU:CD2	1:A:523:ILE:HD13	2.46	0.45
2:B:359:LEU:HD23	2:B:359:LEU:N	2.32	0.45
2:B:527:LEU:CD1	2:B:553:ILE:HG12	2.47	0.45
2:B:559:THR:HG23	2:B:561:GLN:H	1.82	0.45
1:A:263:ARG:C	1:A:265:GLY:H	2.19	0.45
1:A:294:LEU:CD2	1:A:413:ALA:HB2	2.46	0.45
1:A:370:GLU:C	1:A:371:HIS:ND1	2.70	0.45
1:A:431:ARG:HB2	1:A:432:PRO:C	2.37	0.45
2:B:257:ASP:HA	2:B:258:PRO:HD2	1.64	0.45
2:B:359:LEU:HD23	2:B:421:ALA:HB2	1.93	0.45
1:A:349:PHE:CE2	1:A:350:ARG:HG2	2.52	0.45
1:A:394:ILE:O	1:A:396:GLY:N	2.50	0.45
1:A:524:LYS:O	1:A:525:CYS:O	2.35	0.45
2:B:516:GLN:OE1	2:B:516:GLN:N	2.50	0.45
1:A:288:LEU:HB3	1:A:289:ARG:H	1.65	0.44
1:A:371:HIS:NE2	1:A:401:ARG:HG2	2.31	0.44
1:A:522:THR:O	1:A:523:ILE:HB	2.17	0.44
2:B:288:PRO:C	2:B:290:SER:N	2.68	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:290:SER:HB2	2:B:291:VAL:H	1.59	0.44
2:B:414:ASP:C	2:B:415:LEU:HD23	2.37	0.44
1:A:294:LEU:HD23	1:A:417:ARG:HH22	1.83	0.44
1:A:353:LYS:HD3	1:A:395:ASP:OD2	2.18	0.44
1:A:354:PHE:CE2	1:A:466:ASN:ND2	2.85	0.44
2:B:261:LEU:HD11	2:B:282:ILE:HG21	1.99	0.44
1:A:354:PHE:HE2	1:A:466:ASN:HD21	1.63	0.44
1:A:385:LEU:HD13	2:B:434:ASP:O	2.16	0.44
1:A:548:GLY:HA3	1:A:549:PRO:HD2	1.64	0.44
2:B:482:TRP:O	2:B:483:ARG:CB	2.65	0.44
2:B:543:ARG:O	2:B:544:ARG:NH2	2.50	0.44
1:A:331:ILE:CB	1:A:361:LEU:HG	2.47	0.44
1:A:414:LEU:HD21	2:B:413:VAL:CG1	2.47	0.44
2:B:270:LEU:HD12	2:B:274:GLN:HB2	2.00	0.44
2:B:453:ASP:O	2:B:454:GLU:HG2	2.18	0.44
2:B:480:LEU:CD1	2:B:481:VAL:N	2.81	0.44
1:A:411:TYR:O	1:A:412:LEU:C	2.56	0.44
1:A:422:LEU:O	1:A:422:LEU:HD13	2.17	0.44
2:B:441:LYS:O	2:B:442:ALA:HB3	2.17	0.44
2:B:542:SER:C	2:B:543:ARG:CG	2.83	0.44
1:A:260:LEU:CB	1:A:430:SER:HB2	2.48	0.44
1:A:267:TYR:CD1	1:A:267:TYR:N	2.86	0.44
1:A:543:LEU:C	1:A:545:CYS:H	2.21	0.44
2:B:305:ASP:O	2:B:306:TRP:CD2	2.65	0.44
2:B:253:ILE:O	2:B:294:ARG:N	2.51	0.43
2:B:256:LEU:CD1	2:B:282:ILE:CG2	2.90	0.43
2:B:257:ASP:N	2:B:285:GLN:OE1	2.49	0.43
2:B:431:GLU:O	2:B:433:ALA:N	2.42	0.43
1:A:333:GLU:C	1:A:366:TYR:HD2	2.21	0.43
1:A:337:LEU:CB	1:A:368:VAL:HG11	2.48	0.43
1:A:342:SER:HA	1:A:345:ILE:HG22	1.99	0.43
1:A:367:LEU:CG	1:A:400:LYS:HB2	2.48	0.43
1:A:528:LEU:HD23	1:A:528:LEU:O	2.18	0.43
2:B:285:GLN:CB	2:B:288:PRO:HG3	2.48	0.43
1:A:351:GLU:O	1:A:354:PHE:N	2.51	0.43
1:A:352:GLN:HA	1:A:355:ARG:HB3	1.99	0.43
2:B:322:VAL:HA	2:B:325:ILE:CD1	2.47	0.43
1:A:477:ARG:HB3	2:B:488:GLN:CG	2.42	0.43
1:A:486:SER:OG	1:A:488:GLU:HG3	2.19	0.43
2:B:350:ILE:O	2:B:350:ILE:HG23	2.18	0.43
1:A:270:LEU:CD2	1:A:311:VAL:O	2.62	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:ASP:OD2	1:A:508:ASP:C	2.57	0.43
1:A:532:LEU:HA	1:A:532:LEU:HD22	1.61	0.43
2:B:260:LEU:HD21	2:B:315:LEU:H	1.83	0.43
1:A:338:ASP:O	1:A:341:CYS:CB	2.66	0.43
1:A:499:THR:HG22	1:A:502:SER:H	1.83	0.43
1:A:548:GLY:CA	2:B:509:LEU:HD21	2.48	0.43
1:A:260:LEU:HB2	1:A:430:SER:HB2	2.00	0.43
1:A:331:ILE:HG21	1:A:361:LEU:HB3	1.95	0.43
1:A:481:GLN:O	1:A:482:VAL:HG22	2.19	0.43
1:A:269:VAL:CG1	1:A:270:LEU:N	2.82	0.43
1:A:414:LEU:CD2	2:B:413:VAL:CG2	2.35	0.43
1:A:414:LEU:HB3	1:A:415:LEU:HD23	2.01	0.43
1:A:524:LYS:C	1:A:525:CYS:SG	2.97	0.43
2:B:260:LEU:CD1	2:B:315:LEU:HD12	2.48	0.43
2:B:310:PRO:C	2:B:357:LYS:HE2	2.39	0.43
2:B:309:GLU:CB	2:B:310:PRO:CD	2.92	0.43
2:B:432:LEU:O	2:B:433:ALA:CB	2.67	0.43
2:B:455:THR:OG1	2:B:457:PHE:N	2.42	0.43
2:B:517:CYS:HB2	2:B:523:ARG:HG2	1.99	0.43
2:B:526:LEU:O	2:B:527:LEU:CD2	2.64	0.43
1:A:260:LEU:HA	1:A:260:LEU:HD23	1.74	0.43
1:A:267:TYR:CE2	1:A:423:TYR:CZ	3.07	0.43
1:A:274:ASP:OD2	1:A:277:GLU:CD	2.57	0.43
1:A:337:LEU:N	1:A:368:VAL:CG1	2.82	0.43
2:B:261:LEU:CD2	2:B:262:GLN:HG3	2.46	0.43
2:B:293:TRP:CZ3	2:B:311:THR:O	2.72	0.43
2:B:295:ARG:C	2:B:307:VAL:HG23	2.39	0.43
2:B:483:ARG:HH11	2:B:484:ARG:HA	1.83	0.43
1:A:354:PHE:C	1:A:357:LYS:HB2	2.40	0.42
1:A:498:SER:N	1:A:502:SER:OG	2.52	0.42
1:A:523:ILE:C	1:A:524:LYS:HD2	2.40	0.42
2:B:357:LYS:O	2:B:358:ALA:CB	2.67	0.42
1:A:300:VAL:O	1:A:300:VAL:CG1	2.67	0.42
1:A:513:PRO:HD2	1:A:514:LYS:HZ2	1.84	0.42
2:B:317:ARG:HG3	2:B:364:VAL:CG2	2.45	0.42
2:B:482:TRP:HH2	2:B:510:LEU:HG	1.84	0.42
1:A:309:VAL:HG13	1:A:310:TRP:N	2.34	0.42
1:A:365:VAL:HG12	1:A:367:LEU:HD11	2.00	0.42
1:A:480:MET:CA	1:A:485:VAL:HG12	2.44	0.42
2:B:253:ILE:HD12	2:B:279:ARG:HB2	2.01	0.42
2:B:254:VAL:O	2:B:280:CYS:HB3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:416:GLN:NE2	2:B:416:GLN:CA	2.76	0.42
1:A:309:VAL:CG1	1:A:310:TRP:N	2.83	0.42
1:A:354:PHE:HB3	2:B:459:PHE:HZ	1.84	0.42
2:B:412:LEU:O	2:B:415:LEU:HG	2.20	0.42
2:B:471:VAL:HG11	2:B:478:LEU:CD2	2.49	0.42
1:A:350:ARG:HA	1:A:353:LYS:HB2	2.02	0.42
1:A:385:LEU:HA	1:A:388:VAL:HG23	2.01	0.42
1:A:453:LEU:HG	1:A:454:LEU:H	1.84	0.42
2:B:365:ASP:O	2:B:366:GLN:CB	2.56	0.42
2:B:473:LEU:C	2:B:474:ALA:O	2.57	0.42
1:A:260:LEU:HD12	1:A:430:SER:O	2.19	0.42
1:A:354:PHE:HB3	2:B:459:PHE:CZ	2.54	0.42
1:A:405:ILE:CA	1:A:408:SER:OG	2.68	0.42
1:A:501:ALA:HB3	2:B:560:LEU:HD12	2.01	0.42
2:B:490:ASN:HB2	2:B:552:ARG:HH22	1.84	0.42
1:A:476:ALA:O	1:A:477:ARG:C	2.58	0.42
2:B:252:ILE:HA	2:B:295:ARG:HA	2.01	0.42
2:B:289:CYS:C	2:B:314:VAL:HG12	2.40	0.42
2:B:464:ASP:HB2	2:B:467:GLY:N	2.35	0.42
1:A:426:HIS:HB2	1:A:427:THR:H	1.53	0.42
1:A:497:TYR:C	1:A:502:SER:OG	2.58	0.42
1:A:501:ALA:CB	2:B:560:LEU:HD12	2.50	0.42
1:A:345:ILE:HD12	1:A:345:ILE:HA	1.88	0.42
1:A:472:ARG:HG2	2:B:457:PHE:HE1	1.85	0.42
1:A:551:THR:OG1	2:B:476:ARG:HA	2.20	0.42
2:B:343:LEU:CD1	2:B:348:THR:O	2.68	0.42
2:B:354:THR:HG21	2:B:359:LEU:CD1	2.46	0.42
1:A:413:ALA:O	1:A:415:LEU:N	2.53	0.42
1:A:522:THR:HA	1:A:532:LEU:HB2	2.01	0.42
2:B:416:GLN:NE2	2:B:417:LEU:H	2.15	0.42
1:A:308:PHE:O	1:A:309:VAL:HB	2.17	0.41
1:A:474:VAL:CB	2:B:556:GLN:OE1	2.66	0.41
1:A:497:TYR:HB3	1:A:503:LEU:CD2	2.49	0.41
1:A:522:THR:C	1:A:523:ILE:HG22	2.41	0.41
1:A:424:GLN:HE21	1:A:424:GLN:HB3	1.61	0.41
1:A:543:LEU:HB2	2:B:507:PRO:CD	2.50	0.41
2:B:252:ILE:HD11	2:B:295:ARG:HG3	2.01	0.41
2:B:265:GLY:O	2:B:269:LEU:HB3	2.19	0.41
2:B:359:LEU:CD2	2:B:359:LEU:N	2.83	0.41
1:A:275:ILE:O	1:A:275:ILE:CG2	2.67	0.41
1:A:522:THR:O	1:A:523:ILE:CB	2.67	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:255:VAL:HG22	2:B:281:VAL:N	2.35	0.41
2:B:268:GLN:NE2	2:B:430:LYS:HA	2.36	0.41
1:A:290:GLU:OE2	1:A:291:LEU:HD21	2.19	0.41
2:B:271:GLY:O	2:B:273:LEU:N	2.54	0.41
2:B:305:ASP:C	2:B:306:TRP:CD2	2.94	0.41
2:B:309:GLU:OE2	2:B:310:PRO:HD3	2.20	0.41
2:B:313:LEU:HD12	2:B:361:LEU:CA	2.50	0.41
2:B:319:GLU:HB2	2:B:320:ALA:H	1.77	0.41
1:A:275:ILE:C	1:A:277:GLU:N	2.69	0.41
1:A:299:THR:HG21	1:A:301:ARG:CZ	2.51	0.41
1:A:396:GLY:N	1:A:397:PHE:CD1	2.87	0.41
1:A:486:SER:HB3	1:A:489:LYS:N	2.30	0.41
1:A:539:THR:HA	1:A:542:GLN:CD	2.41	0.41
2:B:494:LEU:H	2:B:494:LEU:CD2	2.21	0.41
2:B:501:VAL:O	2:B:501:VAL:CG1	2.67	0.41
2:B:555:LEU:HD23	2:B:555:LEU:HA	1.83	0.41
1:A:369:GLU:O	1:A:370:GLU:C	2.59	0.41
1:A:398:PHE:CG	1:A:399:VAL:N	2.88	0.41
1:A:465:LYS:O	1:A:466:ASN:HB2	2.21	0.41
2:B:483:ARG:C	2:B:485:GLN:H	2.21	0.41
2:B:493:SER:N	2:B:496:MET:SD	2.94	0.41
2:B:496:MET:O	2:B:500:VAL:HG22	2.21	0.41
1:A:274:ASP:OD1	1:A:276:GLY:N	2.54	0.41
1:A:288:LEU:C	1:A:290:GLU:N	2.73	0.41
1:A:333:GLU:HB3	1:A:366:TYR:CE2	2.55	0.41
1:A:538:ARG:CZ	1:A:542:GLN:HE22	2.33	0.41
2:B:258:PRO:CA	2:B:282:ILE:HG22	2.51	0.41
2:B:264:GLU:HB3	2:B:429:TRP:NE1	2.36	0.41
2:B:269:LEU:HD12	2:B:270:LEU:N	2.36	0.41
2:B:290:SER:CA	2:B:314:VAL:HG12	2.51	0.41
2:B:413:VAL:O	2:B:414:ASP:HB2	2.20	0.41
2:B:478:LEU:O	2:B:479:ALA:C	2.59	0.41
2:B:496:MET:O	2:B:498:SER:N	2.53	0.41
1:A:347:GLY:CA	2:B:464:ASP:CG	2.90	0.41
1:A:395:ASP:C	1:A:397:PHE:CD1	2.95	0.41
1:A:478:GLN:HB2	2:B:485:GLN:OE1	2.21	0.41
2:B:315:LEU:HD22	2:B:316:LEU:CA	2.50	0.41
2:B:435:PHE:CD2	2:B:435:PHE:C	2.85	0.41
2:B:458:SER:O	2:B:461:LEU:HG	2.21	0.41
1:A:499:THR:HG1	2:B:560:LEU:C	2.25	0.40
2:B:468:GLY:H	2:B:484:ARG:HH22	1.68	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:487:GLN:HA	2:B:492:VAL:HG11	2.03	0.40
1:A:357:LYS:N	1:A:359:CYS:SG	2.95	0.40
1:A:388:VAL:O	1:A:391:THR:N	2.53	0.40
1:A:389:THR:HG21	2:B:438:ALA:HB3	2.03	0.40
1:A:478:GLN:O	2:B:485:GLN:NE2	2.54	0.40
1:A:524:LYS:HA	1:A:530:ARG:O	2.21	0.40
2:B:263:MET:HB2	2:B:263:MET:HE2	1.36	0.40
1:A:272:CYS:O	1:A:308:PHE:CB	2.67	0.40
1:A:296:VAL:HG11	1:A:416:THR:CG2	2.44	0.40
2:B:507:PRO:C	2:B:509:LEU:N	2.74	0.40
1:A:328:LEU:HD21	1:A:330:HIS:CE1	2.56	0.40
1:A:328:LEU:HD12	1:A:329:ASP:N	2.37	0.40
1:A:337:LEU:CB	1:A:376:ASN:HD21	2.31	0.40
1:A:389:THR:OG1	1:A:390:ASN:N	2.54	0.40
1:A:479:LEU:O	1:A:481:GLN:N	2.53	0.40
1:A:491:ALA:CB	1:A:492:ALA:CA	2.96	0.40
1:A:535:ALA:O	1:A:536:LEU:C	2.60	0.40
2:B:318:ALA:HB1	2:B:321:PHE:HD2	1.87	0.40

All (2) 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:266:GLY:O	2:B:266:GLY:O[6_555]	1.90	0.30
1:A:380:PRO:CD	1:A:538:ARG:NH1[4_555]	2.18	0.02

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	262/307 (85%)	127 (48%)	59 (22%)	76 (29%)	0 0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	247/341 (72%)	100 (40%)	81 (33%)	66 (27%)	0 0
All	All	509/648 (78%)	227 (45%)	140 (28%)	142 (28%)	0 0

All (142) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	262	LEU
1	A	263	ARG
1	A	279	ARG
1	A	285	PRO
1	A	305	VAL
1	A	324	GLY
1	A	329	ASP
1	A	334	ARG
1	A	349	PHE
1	A	359	CYS
1	A	362	GLU
1	A	370	GLU
1	A	373	SER
1	A	380	PRO
1	A	382	SER
1	A	388	VAL
1	A	418	GLY
1	A	424	GLN
1	A	464	ILE
1	A	481	GLN
1	A	499	THR
1	A	510	CYS
1	A	523	ILE
1	A	531	ASN
1	A	535	ALA
1	A	536	LEU
1	A	542	GLN
2	B	249	LEU
2	B	260	LEU
2	B	268	GLN
2	B	284	ALA
2	B	291	VAL
2	B	306	TRP
2	B	349	ASP
2	B	406	VAL
2	B	414	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	417	LEU
2	B	426	VAL
2	B	428	SER
2	B	430	LYS
2	B	432	LEU
2	B	440	THR
2	B	442	ALA
2	B	445	GLU
2	B	474	ALA
2	B	482	TRP
2	B	483	ARG
2	B	491	ARG
2	B	494	LEU
2	B	518	PHE
2	B	519	SER
2	B	532	VAL
2	B	543	ARG
2	B	552	ARG
2	B	556	GLN
2	B	563	HIS
1	A	286	GLU
1	A	295	HIS
1	A	307	ASP
1	A	309	VAL
1	A	310	TRP
1	A	327	VAL
1	A	342	SER
1	A	348	ARG
1	A	378	SER
1	A	381	GLU
1	A	391	THR
1	A	402	THR
1	A	406	LYS
1	A	428	LEU
1	A	457	SER
1	A	466	ASN
1	A	491	ALA
1	A	492	ALA
1	A	524	LYS
1	A	525	CYS
1	A	526	GLY
1	A	529	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	549	PRO
2	B	285	GLN
2	B	308	GLU
2	B	310	PRO
2	B	312	VAL
2	B	361	LEU
2	B	433	ALA
2	B	435	PHE
2	B	473	LEU
2	B	488	GLN
2	B	497	ALA
2	B	503	ALA
2	B	548	GLU
2	B	566	LEU
1	A	265	GLY
1	A	273	VAL
1	A	288	LEU
1	A	414	LEU
1	A	416	THR
1	A	458	ASP
1	A	475	PHE
1	A	476	ALA
1	A	519	LEU
1	A	534	PRO
1	A	538	ARG
2	B	272	ALA
2	B	421	ALA
2	B	423	ALA
2	B	446	ALA
2	B	458	SER
2	B	479	ALA
2	B	487	GLN
2	B	547	PRO
1	A	264	PRO
1	A	325	GLU
1	A	427	THR
1	A	453	LEU
1	A	521	SER
1	A	546	SER
2	B	250	LYS
2	B	258	PRO
2	B	348	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	462	GLU
2	B	507	PRO
2	B	508	GLN
2	B	522	GLU
1	A	347	GLY
1	A	390	ASN
1	A	419	LEU
1	A	460	ASN
1	A	471	VAL
1	A	547	TYR
2	B	265	GLY
2	B	343	LEU
2	B	434	ASP
2	B	468	GLY
2	B	248	CYS
2	B	281	VAL
2	B	444	ALA
2	B	530	ILE
2	B	535	GLY
1	A	431	ARG
1	A	379	LEU
1	A	500	PRO

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	233/260 (90%)	150 (64%)	83 (36%)	0 1
2	B	220/290 (76%)	131 (60%)	89 (40%)	0 1
All	All	453/550 (82%)	281 (62%)	172 (38%)	0 1

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	261	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	263	ARG
1	A	266	GLU
1	A	267	TYR
1	A	268	ARG
1	A	269	VAL
1	A	271	LEU
1	A	286	GLU
1	A	289	ARG
1	A	293	ARG
1	A	294	LEU
1	A	297	THR
1	A	298	HIS
1	A	299	THR
1	A	303	LEU
1	A	304	HIS
1	A	305	VAL
1	A	308	PHE
1	A	313	GLN
1	A	314	GLU
1	A	327	VAL
1	A	331	ILE
1	A	337	LEU
1	A	339	ASP
1	A	340	LEU
1	A	343	SER
1	A	344	ILE
1	A	346	ASP
1	A	351	GLU
1	A	353	LYS
1	A	357	LYS
1	A	358	ARG
1	A	361	LEU
1	A	364	ARG
1	A	369	GLU
1	A	371	HIS
1	A	373	SER
1	A	374	VAL
1	A	375	HIS
1	A	376	ASN
1	A	377	LEU
1	A	379	LEU
1	A	380	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	381	GLU
1	A	391	THR
1	A	395	ASP
1	A	399	VAL
1	A	404	ASP
1	A	405	ILE
1	A	412	LEU
1	A	414	LEU
1	A	416	THR
1	A	417	ARG
1	A	421	ARG
1	A	422	LEU
1	A	423	TYR
1	A	428	LEU
1	A	429	ARG
1	A	430	SER
1	A	431	ARG
1	A	450	LEU
1	A	456	PHE
1	A	464	ILE
1	A	465	LYS
1	A	469	GLN
1	A	477	ARG
1	A	483	ARG
1	A	488	GLU
1	A	498	SER
1	A	503	LEU
1	A	507	TYR
1	A	512	THR
1	A	517	GLU
1	A	520	LEU
1	A	523	ILE
1	A	525	CYS
1	A	529	GLN
1	A	530	ARG
1	A	532	LEU
1	A	540	LEU
1	A	543	LEU
1	A	550	LEU
1	A	551	THR
2	B	247	GLU
2	B	257	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	261	LEU
2	B	262	GLN
2	B	263	MET
2	B	269	LEU
2	B	274	GLN
2	B	278	CYS
2	B	282	ILE
2	B	285	GLN
2	B	287	VAL
2	B	289	CYS
2	B	290	SER
2	B	292	THR
2	B	293	TRP
2	B	305	ASP
2	B	312	VAL
2	B	313	LEU
2	B	315	LEU
2	B	316	LEU
2	B	321	PHE
2	B	322	VAL
2	B	326	ASP
2	B	327	ASN
2	B	342	THR
2	B	343	LEU
2	B	346	PHE
2	B	348	THR
2	B	353	LYS
2	B	359	LEU
2	B	364	VAL
2	B	365	ASP
2	B	367	GLU
2	B	409	GLU
2	B	410	GLU
2	B	416	GLN
2	B	417	LEU
2	B	419	THR
2	B	424	GLN
2	B	425	ILE
2	B	429	TRP
2	B	432	LEU
2	B	434	ASP
2	B	439	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	443	VAL
2	B	445	GLU
2	B	452	ARG
2	B	455	THR
2	B	457	PHE
2	B	459	PHE
2	B	461	LEU
2	B	463	SER
2	B	472	ASP
2	B	473	LEU
2	B	476	ARG
2	B	480	LEU
2	B	483	ARG
2	B	486	ILE
2	B	487	GLN
2	B	488	GLN
2	B	491	ARG
2	B	493	SER
2	B	494	LEU
2	B	496	MET
2	B	500	VAL
2	B	510	LEU
2	B	512	GLN
2	B	514	TYR
2	B	521	LYS
2	B	522	GLU
2	B	526	LEU
2	B	529	ASP
2	B	530	ILE
2	B	531	GLN
2	B	534	ARG
2	B	536	GLU
2	B	542	SER
2	B	543	ARG
2	B	544	ARG
2	B	545	ILE
2	B	548	GLU
2	B	552	ARG
2	B	555	LEU
2	B	559	THR
2	B	560	LEU
2	B	561	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	565	SER
2	B	566	LEU
2	B	568	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	313	GLN
1	A	371	HIS
1	A	376	ASN
1	A	386	GLN
1	A	424	GLN
1	A	426	HIS
1	A	469	GLN
1	A	481	GLN
1	A	531	ASN
1	A	542	GLN
2	B	327	ASN
2	B	366	GLN
2	B	416	GLN
2	B	422	GLN
2	B	485	GLN
2	B	487	GLN
2	B	490	ASN
2	B	508	GLN
2	B	525	ASN
2	B	531	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	270/307 (87%)	-0.73	1 (0%)	92	90	8, 34, 44, 53	0
2	B	259/341 (75%)	-0.67	2 (0%)	86	81	15, 35, 45, 52	0
All	All	529/648 (81%)	-0.70	3 (0%)	89	86	8, 34, 44, 53	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	404	SER	3.4
1	A	462	GLY	2.9
2	B	272	ALA	2.4

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.