



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:10 AM GMT

PDB ID : 3KYH
Title : Saccharomyces cerevisiae Cet1-Ceg1 capping apparatus
Authors : Lima, C.D.
Deposited on : 2009-12-06
Resolution : 3.00 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

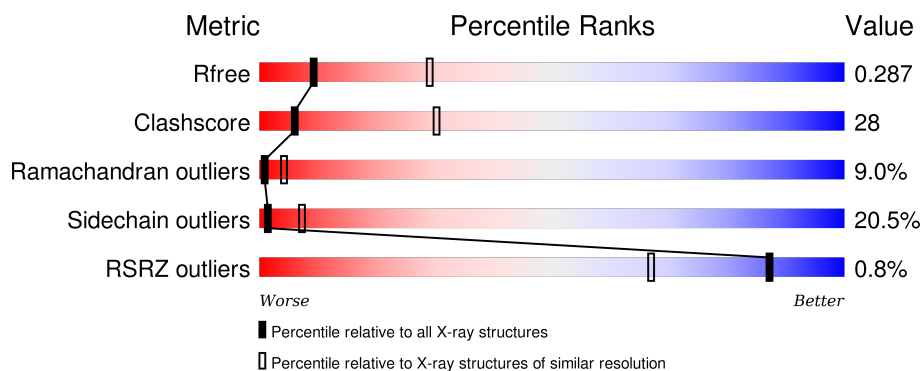
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	310	<div> <div> <div></div> <div>34%</div> <div>40%</div> <div>13%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	310	<div> <div> <div></div> <div>37%</div> <div>40%</div> <div>10%</div> <div>•</div> <div>11%</div> </div> </div>
2	C	461	<div> <div> <div></div> <div>38%</div> <div>33%</div> <div>11%</div> <div>•</div> <div>16%</div> </div> </div>
2	D	461	<div> <div> <div></div> <div>33%</div> <div>37%</div> <div>12%</div> <div>•</div> <div>16%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10696 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 mRNA-capping enzyme subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2212	1407	375	426	4			
1	B	276	Total	C	N	O	S	0	0	0
			2212	1407	375	426	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	240	MET	-	INITIATING METHIONINE	UNP O13297
B	240	MET	-	INITIATING METHIONINE	UNP O13297

- Molecule 2 is a protein called mRNA-capping enzyme subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	387	Total	C	N	O	S	0	0	0
			3136	2007	528	583	18			
2	D	387	Total	C	N	O	S	0	0	0
			3136	2007	528	583	18			

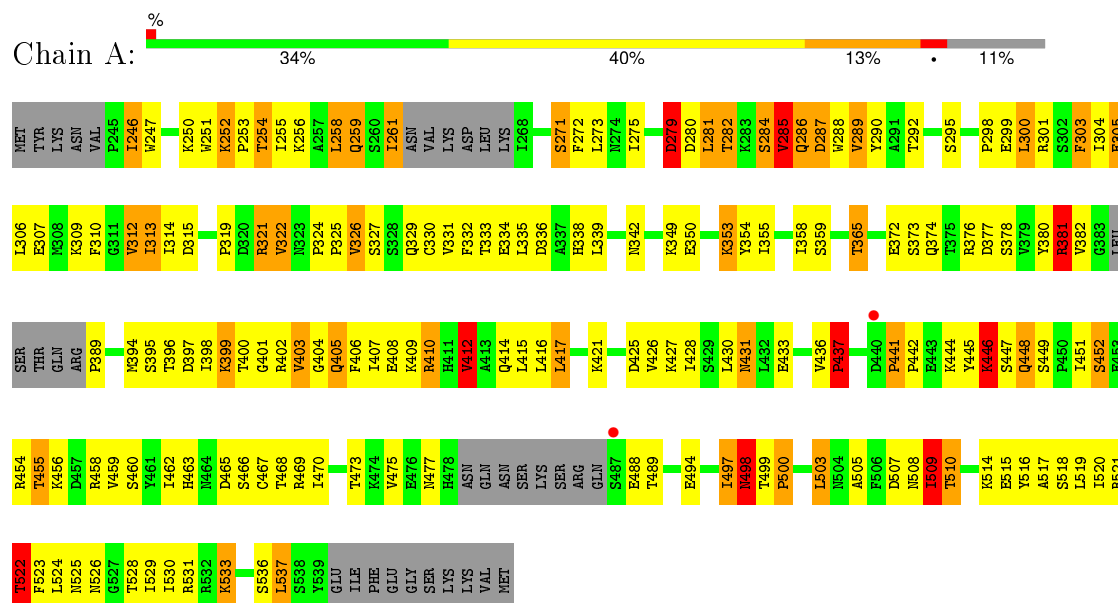
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	EXPRESSION TAG	UNP Q01159
C	0	LEU	-	EXPRESSION TAG	UNP Q01159
D	-1	SER	-	EXPRESSION TAG	UNP Q01159
D	0	LEU	-	EXPRESSION TAG	UNP Q01159

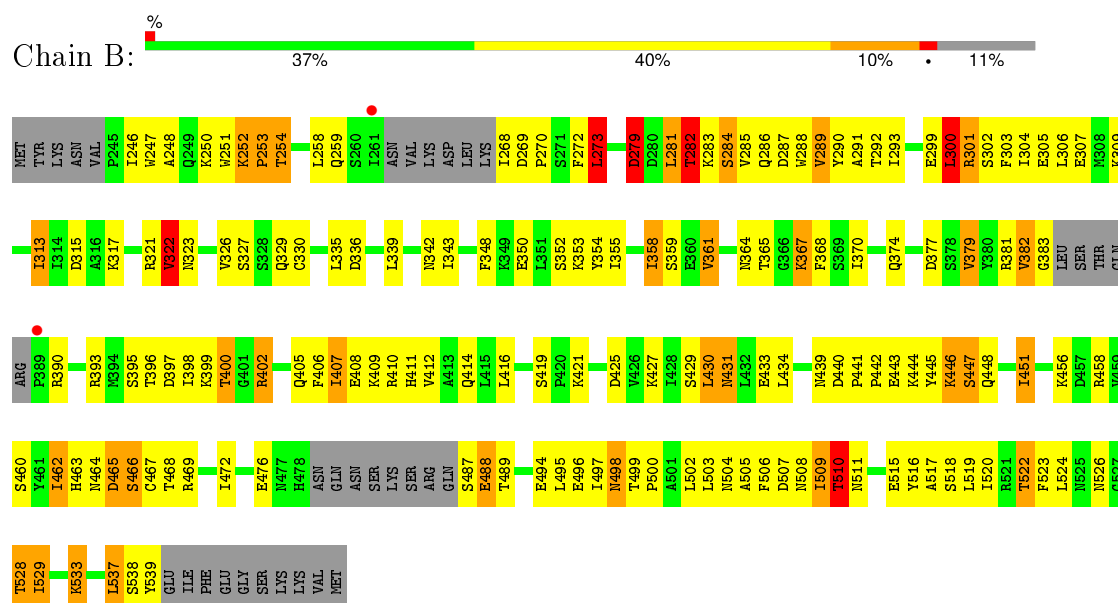
3 Residue-property plots

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

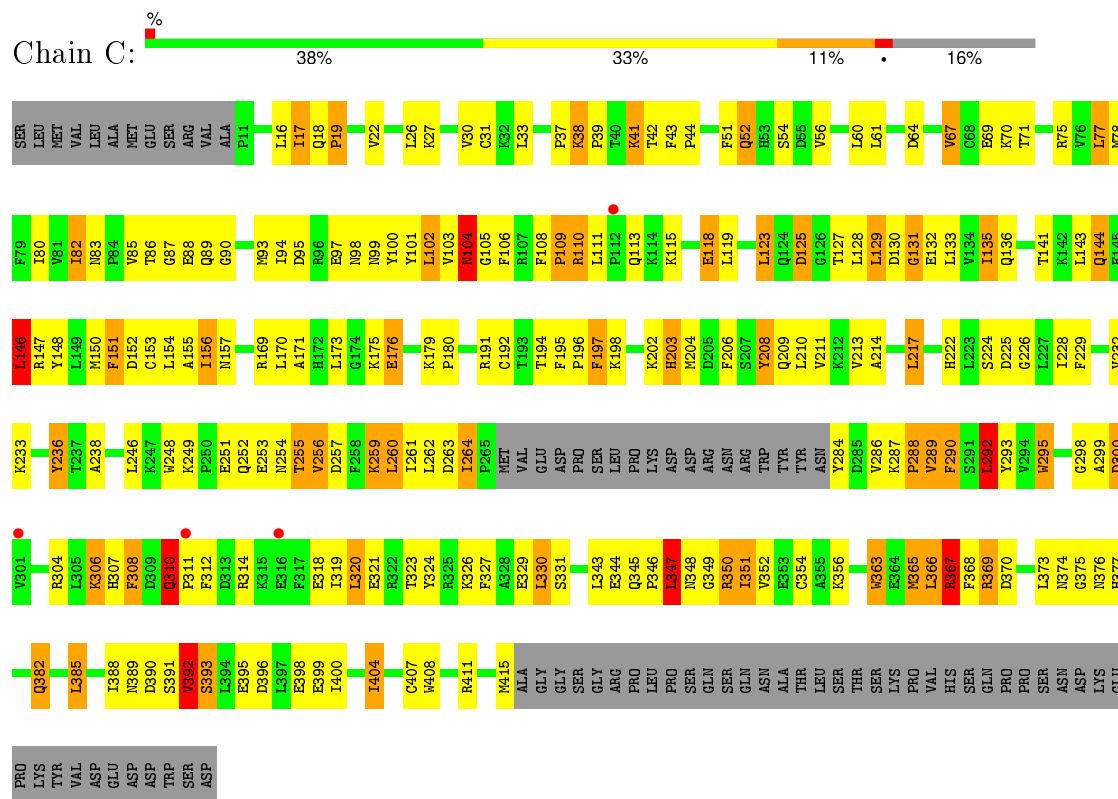
• Molecule 1: mRNA-capping enzyme subunit beta



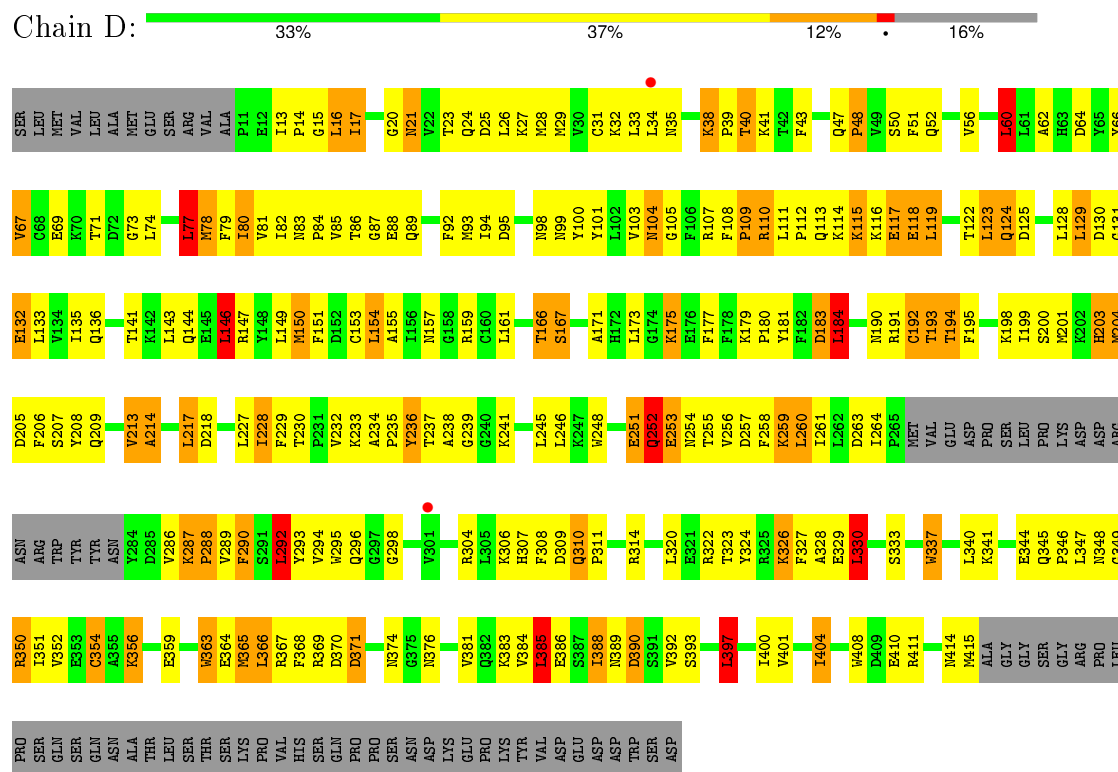
• Molecule 1: mRNA-capping enzyme subunit beta



- Molecule 2: mRNA-capping enzyme subunit alpha



- Molecule 2: mRNA-capping enzyme subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	165.99Å 165.99Å 172.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.98 – 3.00 19.98 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.2 (19.98-3.00) 95.3 (19.98-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.249 , 0.298 0.249 , 0.287	Depositor DCC
R_{free} test set	2580 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	63.7	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 22.4	EDS
Estimated twinning fraction	0.514 for H, K, L 0.486 for H+K, -K, -L 0.458 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.514 for H, K, L 0.486 for H+K, -K, -L	Depositor
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 50992 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	10696	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.92	1/2256 (0.0%)	1.24	10/3058 (0.3%)
1	B	0.99	1/2256 (0.0%)	1.29	14/3058 (0.5%)
2	C	0.67	0/3207	1.04	11/4334 (0.3%)
2	D	0.67	0/3207	1.05	7/4334 (0.2%)
All	All	0.80	2/10926 (0.0%)	1.14	42/14784 (0.3%)

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	1
1	B	0	1
2	C	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	326	VAL	CB-CG1	6.55	1.66	1.52
1	B	288	TRP	CE2-CZ2	-5.30	1.30	1.39

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	217	LEU	CA-CB-CG	9.07	136.16	115.30
1	A	458	ARG	NE-CZ-NH1	8.68	124.64	120.30
2	D	385	LEU	CA-CB-CG	7.84	133.32	115.30
2	C	170	LEU	CA-CB-CG	7.33	132.15	115.30
2	D	292	LEU	CA-CB-CG	6.88	131.12	115.30
2	C	125	ASP	CB-CG-OD1	6.44	124.09	118.30
2	D	385	LEU	CB-CG-CD1	6.22	121.58	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	381	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	A	415	LEU	CB-CG-CD2	6.15	121.45	111.00
1	B	458	ARG	NE-CZ-NH1	6.07	123.33	120.30
2	C	146	LEU	CA-CB-CG	5.92	128.93	115.30
1	B	273	LEU	CB-CG-CD2	-5.88	101.01	111.00
1	B	537	LEU	CB-CG-CD1	-5.85	101.06	111.00
1	A	281	LEU	CB-CG-CD2	-5.80	101.15	111.00
2	D	397	LEU	CA-CB-CG	5.77	128.57	115.30
1	B	317	LYS	CD-CE-NZ	5.67	124.73	111.70
1	B	379	VAL	CG1-CB-CG2	-5.65	101.86	110.90
1	B	300	LEU	CA-CB-CG	5.60	128.19	115.30
2	C	366	LEU	CA-CB-CG	5.60	128.17	115.30
1	B	430	LEU	CB-CG-CD2	5.55	120.43	111.00
1	A	285	VAL	CA-CB-CG2	-5.54	102.59	110.90
1	A	381	ARG	NE-CZ-NH2	-5.51	117.55	120.30
2	C	102	LEU	CB-CG-CD2	5.49	120.33	111.00
2	D	77	LEU	CA-CB-CG	5.49	127.92	115.30
2	C	169	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	B	321	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	321	ARG	NE-CZ-NH2	-5.35	117.62	120.30
2	D	146	LEU	CA-CB-CG	5.34	127.57	115.30
2	D	217	LEU	CA-CB-CG	5.30	127.50	115.30
1	B	273	LEU	CB-CG-CD1	5.29	119.99	111.00
2	C	391	SER	C-N-CA	5.28	134.90	121.70
2	C	292	LEU	CA-CB-CG	5.25	127.36	115.30
1	B	379	VAL	CB-CA-C	5.24	121.36	111.40
1	A	300	LEU	CA-CB-CG	5.24	127.35	115.30
1	B	269	ASP	CB-CG-OD1	5.24	123.02	118.30
1	B	273	LEU	CA-CB-CG	-5.24	103.25	115.30
1	B	269	ASP	CB-CG-OD2	-5.21	113.62	118.30
1	A	522	THR	N-CA-CB	5.13	120.05	110.30
1	B	279	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	305	GLU	N-CA-C	-5.03	97.43	111.00
2	C	347	LEU	N-CA-C	5.02	124.56	111.00
2	C	131	GLY	N-CA-C	5.02	125.65	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	465	ASP	Peptide
1	B	465	ASP	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	C	310	GLN	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2212	0	2218	152	0
1	B	2212	0	2218	138	0
2	C	3136	0	3126	156	0
2	D	3136	0	3126	188	0
All	All	10696	0	10688	607	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (607) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:LYS:NZ	1:B:446:LYS:HA	1.64	1.13
2:D:109:PRO:HD2	2:D:180:PRO:HB2	1.24	1.13
1:B:497:ILE:HD11	1:B:519:LEU:HD11	1.32	1.12
2:C:390:ASP:O	2:C:392:VAL:HG23	1.55	1.07
1:A:499:THR:HG22	1:A:503:LEU:HD12	1.37	1.07
1:B:518:SER:O	1:B:522:THR:HG22	1.57	1.05
2:D:93:MET:HB2	2:D:101:TYR:HB2	1.38	1.04
2:D:264:ILE:HG12	2:D:288:PRO:HB2	1.38	1.02
1:A:436:VAL:HG11	1:A:441:PRO:HG2	1.44	0.95
2:D:354:CYS:HB3	2:D:365:MET:HA	1.46	0.95
1:A:441:PRO:HD2	1:A:442:PRO:HD3	1.47	0.94
2:C:31:CYS:HB3	2:C:37:PRO:HA	1.51	0.93
2:C:43:PHE:HA	2:C:98:ASN:HD21	1.30	0.93
2:C:135:ILE:HD12	2:C:135:ILE:H	1.35	0.91
2:D:43:PHE:HA	2:D:98:ASN:HD21	1.35	0.91
1:A:255:ILE:HA	1:A:258:LEU:HB3	1.52	0.90
1:B:323:ASN:O	1:B:323:ASN:OD1	1.90	0.90
1:B:446:LYS:HZ3	1:B:446:LYS:HA	1.31	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:385:LEU:HA	2:D:388:ILE:HD11	1.53	0.89
1:B:446:LYS:HZ2	1:B:446:LYS:HA	1.40	0.86
2:C:80:ILE:CD1	2:C:127:THR:HB	2.05	0.85
2:D:109:PRO:HD2	2:D:180:PRO:CB	2.07	0.85
2:D:259:LYS:HD2	2:D:261:ILE:HG13	1.56	0.85
2:D:77:LEU:HB2	2:D:94:ILE:HD11	1.56	0.85
1:B:446:LYS:C	1:B:448:GLN:H	1.76	0.85
2:C:109:PRO:HG2	2:C:180:PRO:HB2	1.59	0.84
1:A:395:SER:O	1:A:403:VAL:HA	1.77	0.84
2:C:97:GLU:HB3	2:C:99:ASN:HD21	1.42	0.83
1:A:394:MET:HG3	1:A:406:PHE:HD2	1.40	0.83
2:C:16:LEU:O	2:C:101:TYR:HA	1.78	0.83
2:C:93:MET:HB2	2:C:101:TYR:HB2	1.61	0.82
1:B:519:LEU:HD12	1:B:519:LEU:O	1.79	0.82
2:D:251:GLU:CD	2:D:251:GLU:H	1.82	0.81
2:D:13:ILE:HG13	2:D:14:PRO:HD2	1.63	0.81
2:D:356:LYS:HA	2:D:363:TRP:HB3	1.62	0.81
2:D:109:PRO:CD	2:D:180:PRO:HB2	2.10	0.81
2:D:131:GLY:HA2	2:D:150:MET:HA	1.62	0.80
2:D:264:ILE:CG1	2:D:288:PRO:HB2	2.12	0.80
2:C:356:LYS:HA	2:C:363:TRP:HB3	1.62	0.79
2:D:136:GLN:HG3	2:D:147:ARG:HD2	1.63	0.78
2:C:77:LEU:HB2	2:C:94:ILE:CG1	2.15	0.77
2:C:77:LEU:HG	2:C:130:ASP:HA	1.65	0.77
2:C:77:LEU:HB2	2:C:94:ILE:HG12	1.67	0.77
2:C:135:ILE:N	2:C:135:ILE:HD12	1.99	0.77
2:D:78:MET:HB3	2:D:129:LEU:HG	1.65	0.77
1:B:309:LYS:HG2	1:B:494:GLU:HG2	1.65	0.76
2:C:150:MET:CE	2:C:173:LEU:HD11	2.15	0.76
1:B:497:ILE:HD11	1:B:519:LEU:CD1	2.14	0.76
2:C:259:LYS:NZ	2:C:349:GLY:O	2.19	0.76
2:D:295:TRP:HA	2:D:323:THR:O	1.85	0.76
2:C:80:ILE:HD12	2:C:127:THR:HB	1.67	0.75
1:A:305:GLU:HB3	1:A:431:ASN:ND2	2.02	0.75
1:B:292:THR:CG2	1:B:430:LEU:HD13	2.16	0.75
2:C:125:ASP:O	2:C:157:ASN:HA	1.86	0.75
1:B:246:ILE:HD12	1:B:247:TRP:H	1.51	0.74
1:B:305:GLU:HG3	1:B:496:GLU:OE1	1.87	0.74
1:A:380:TYR:CE2	1:A:445:TYR:O	2.41	0.74
1:A:498:ASN:HD21	1:A:500:PRO:HG2	1.52	0.74
2:C:43:PHE:HA	2:C:98:ASN:ND2	2.02	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:LEU:C	1:B:339:LEU:HD23	2.08	0.74
2:D:115:LYS:HG3	2:D:118:GLU:HB2	1.68	0.74
1:A:326:VAL:HG21	1:A:330:CYS:SG	2.28	0.74
2:C:150:MET:HE3	2:C:173:LEU:HD11	1.68	0.73
2:C:350:ARG:HD3	2:C:351:ILE:H	1.53	0.73
2:D:27:LYS:NZ	2:D:98:ASN:HB3	2.04	0.72
2:D:132:GLU:HB2	2:D:151:PHE:HE1	1.55	0.72
2:C:61:LEU:HD12	2:C:407:CYS:SG	2.30	0.72
1:A:499:THR:HG22	1:A:503:LEU:CD1	2.18	0.72
1:B:309:LYS:CG	1:B:494:GLU:HG2	2.19	0.72
2:C:299:ALA:HB3	2:C:323:THR:HB	1.70	0.72
2:C:259:LYS:NZ	2:C:349:GLY:C	2.44	0.71
1:A:300:LEU:O	1:A:303:PHE:HD1	1.73	0.71
1:A:441:PRO:CD	1:A:442:PRO:HD3	2.21	0.71
1:B:505:ALA:HA	1:B:515:GLU:OE1	1.91	0.70
2:C:263:ASP:OD2	2:C:289:VAL:HB	1.91	0.70
1:A:309:LYS:O	1:A:426:VAL:HG12	1.91	0.70
2:D:43:PHE:O	2:D:239:GLY:HA2	1.92	0.70
2:C:151:PHE:HB3	2:C:202:LYS:HD3	1.73	0.69
1:B:494:GLU:C	1:B:495:LEU:HD12	2.12	0.69
2:D:92:PHE:HA	2:D:101:TYR:O	1.92	0.69
2:C:56:VAL:HG11	2:C:400:ILE:HD13	1.74	0.69
1:B:509:ILE:HG23	1:B:510:THR:H	1.57	0.69
2:C:52:GLN:HB3	2:C:54:SER:OG	1.91	0.69
1:A:380:TYR:CD2	1:A:445:TYR:HB3	2.27	0.69
1:A:255:ILE:HA	1:A:258:LEU:CB	2.21	0.69
2:D:153:CYS:HB2	2:D:173:LEU:HD22	1.75	0.69
1:A:436:VAL:HG11	1:A:441:PRO:CG	2.22	0.69
1:A:445:TYR:C	1:A:447:SER:H	1.95	0.69
2:D:213:VAL:HG12	2:D:214:ALA:N	2.08	0.68
1:A:299:GLU:HG2	1:A:300:LEU:H	1.58	0.68
1:A:306:LEU:HB3	1:A:497:ILE:CG2	2.24	0.68
2:D:354:CYS:HB3	2:D:365:MET:CA	2.21	0.68
2:D:181:TYR:CE1	2:D:199:ILE:HD13	2.29	0.67
1:A:448:GLN:HA	1:A:448:GLN:HE21	1.59	0.67
1:A:298:PRO:O	1:A:301:ARG:HB2	1.95	0.67
1:A:468:THR:HG21	1:A:526:ASN:HD22	1.59	0.67
2:C:390:ASP:O	2:C:392:VAL:CG2	2.39	0.66
1:A:395:SER:HB2	1:A:404:GLY:H	1.59	0.66
1:A:498:ASN:ND2	1:A:500:PRO:HG2	2.09	0.66
1:B:313:ILE:HD13	1:B:416:LEU:HB3	1.76	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:80:ILE:HG22	2:C:90:GLY:O	1.94	0.66
2:D:128:LEU:O	2:D:154:LEU:HD12	1.95	0.66
2:D:251:GLU:CD	2:D:251:GLU:N	2.49	0.66
1:A:394:MET:HG3	1:A:406:PHE:CD2	2.29	0.66
2:D:337:TRP:CE3	2:D:337:TRP:HA	2.31	0.66
1:B:292:THR:HG22	1:B:430:LEU:HD13	1.79	0.65
2:D:304:ARG:HD2	2:D:307:HIS:HD2	1.60	0.65
2:D:27:LYS:NZ	2:D:98:ASN:CB	2.59	0.65
2:C:127:THR:HG23	2:C:156:ILE:HD12	1.78	0.65
1:B:488:GLU:OE2	1:B:488:GLU:HA	1.95	0.65
2:D:385:LEU:HA	2:D:388:ILE:CD1	2.25	0.65
1:B:300:LEU:O	1:B:302:SER:N	2.29	0.65
2:C:82:ILE:HD11	2:C:125:ASP:HB2	1.78	0.65
2:C:129:LEU:H	2:C:129:LEU:HD23	1.61	0.65
2:C:257:ASP:HB2	2:C:375:GLY:O	1.95	0.65
2:D:83:ASN:HD22	2:D:85:VAL:HB	1.62	0.64
2:C:41:LYS:HG2	2:C:42:THR:N	2.13	0.64
1:B:446:LYS:C	1:B:448:GLN:N	2.48	0.64
2:C:408:TRP:HA	2:C:411:ARG:HE	1.61	0.64
1:B:292:THR:HG21	1:B:430:LEU:HD13	1.79	0.64
1:A:520:ILE:O	1:A:523:PHE:HB3	1.98	0.64
2:C:17:ILE:HA	2:C:100:TYR:O	1.97	0.64
1:B:306:LEU:HB3	1:B:497:ILE:CG2	2.27	0.63
1:A:261:ILE:HD11	1:B:464:ASN:HB3	1.80	0.63
2:D:89:GLN:HB2	2:D:123:LEU:HD11	1.81	0.63
1:B:306:LEU:HB3	1:B:497:ILE:HG22	1.79	0.63
1:B:350:GLU:HB3	1:B:537:LEU:HD22	1.80	0.63
1:A:529:ILE:HG21	1:B:273:LEU:HD12	1.81	0.63
1:B:307:GLU:OE1	1:B:494:GLU:HB3	1.98	0.63
2:D:256:VAL:HG13	2:D:257:ASP:H	1.63	0.63
2:C:356:LYS:CA	2:C:363:TRP:HB3	2.29	0.63
2:D:78:MET:O	2:D:128:LEU:HD12	2.00	0.62
2:C:153:CYS:HB2	2:C:173:LEU:HD22	1.80	0.62
1:A:350:GLU:HB3	1:A:537:LEU:HD22	1.82	0.62
1:A:412:VAL:HG23	1:A:431:ASN:HA	1.81	0.61
2:C:31:CYS:CB	2:C:37:PRO:HA	2.28	0.61
1:B:322:VAL:O	1:B:323:ASN:HB2	1.99	0.61
1:A:397:ASP:O	1:A:401:GLY:HA2	2.00	0.61
2:D:23:THR:HG23	2:D:100:TYR:HB2	1.83	0.60
2:D:27:LYS:HD3	2:D:40:THR:O	2.00	0.60
1:A:372:GLU:HA	1:A:459:VAL:HG22	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:LYS:HG2	1:A:475:VAL:HB	1.83	0.60
2:C:264:ILE:CG1	2:C:288:PRO:HB2	2.31	0.60
2:D:337:TRP:HE3	2:D:337:TRP:HA	1.64	0.60
2:D:82:ILE:HA	2:D:88:GLU:O	2.02	0.60
1:B:286:GLN:HG2	1:B:520:ILE:HG21	1.84	0.60
2:D:15:GLY:O	2:D:16:LEU:HB3	2.02	0.60
2:C:259:LYS:HG2	2:C:324:TYR:CZ	2.37	0.60
2:C:251:GLU:OE2	2:C:393:SER:HA	2.02	0.60
1:B:445:TYR:C	1:B:446:LYS:HD2	2.22	0.59
2:C:295:TRP:HZ3	2:C:298:GLY:HA2	1.67	0.59
1:B:246:ILE:HD13	2:C:344:GLU:HG3	1.83	0.59
1:A:462:ILE:HG22	1:A:463:HIS:H	1.66	0.59
2:D:292:LEU:HG	2:D:328:ALA:HB3	1.83	0.59
1:A:451:ILE:C	1:A:451:ILE:HD12	2.23	0.59
1:A:314:ILE:O	1:A:314:ILE:HG22	2.01	0.59
1:A:436:VAL:CG1	1:A:441:PRO:HG2	2.26	0.59
2:C:307:HIS:O	2:C:310:GLN:HB3	2.03	0.59
1:B:313:ILE:CD1	1:B:416:LEU:HB3	2.32	0.59
1:B:300:LEU:HD23	1:B:434:LEU:HD21	1.83	0.59
2:D:177:PHE:O	2:D:177:PHE:CD2	2.56	0.59
2:C:80:ILE:HD11	2:C:127:THR:HB	1.85	0.59
2:D:256:VAL:CG1	2:D:257:ASP:N	2.66	0.59
2:D:229:PHE:HB2	2:D:246:LEU:HB2	1.84	0.58
2:D:259:LYS:HE3	2:D:349:GLY:HA2	1.83	0.58
1:B:396:THR:HG22	1:B:397:ASP:O	2.03	0.58
1:B:250:LYS:HD3	2:C:310:GLN:HG3	1.84	0.58
2:D:264:ILE:HG12	2:D:288:PRO:CB	2.23	0.58
2:D:78:MET:HB3	2:D:129:LEU:CG	2.34	0.58
1:B:411:HIS:CD2	1:B:431:ASN:HB3	2.38	0.58
2:D:261:ILE:HB	2:D:293:TYR:CE1	2.39	0.58
1:B:411:HIS:HD2	1:B:431:ASN:HB3	1.69	0.58
1:B:407:ILE:HD12	1:B:433:GLU:HG2	1.86	0.58
2:C:261:ILE:HB	2:C:293:TYR:CE1	2.39	0.58
1:B:382:VAL:HG12	1:B:383:GLY:N	2.19	0.58
2:C:404:ILE:O	2:C:408:TRP:HB2	2.03	0.58
1:A:381:ARG:NH1	1:A:389:PRO:HB3	2.19	0.58
1:B:339:LEU:O	1:B:339:LEU:HD23	2.04	0.57
2:C:83:ASN:ND2	2:C:86:THR:H	2.01	0.57
1:B:446:LYS:N	1:B:446:LYS:HD2	2.19	0.57
2:D:129:LEU:HD23	2:D:129:LEU:H	1.67	0.57
2:C:259:LYS:HZ1	2:C:349:GLY:C	2.01	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:350:ARG:HD3	2:C:351:ILE:N	2.20	0.57
1:B:246:ILE:CD1	2:C:344:GLU:HG3	2.35	0.57
2:C:41:LYS:HG2	2:C:42:THR:H	1.68	0.57
1:A:313:ILE:CD1	1:A:416:LEU:HB3	2.35	0.57
2:D:13:ILE:HG13	2:D:14:PRO:CD	2.33	0.57
2:D:206:PHE:HB3	2:D:408:TRP:CH2	2.39	0.57
1:A:310:PHE:CE2	1:A:426:VAL:HG11	2.39	0.57
2:D:77:LEU:HB2	2:D:94:ILE:CD1	2.31	0.56
1:A:300:LEU:O	1:A:303:PHE:CD1	2.57	0.56
2:C:27:LYS:NZ	2:C:98:ASN:HB3	2.20	0.56
1:A:310:PHE:HE2	1:A:531:ARG:HB2	1.70	0.56
2:C:399:GLU:HG3	2:C:400:ILE:HG13	1.87	0.56
1:A:454:ARG:HD3	1:A:475:VAL:HG21	1.86	0.56
1:B:393:ARG:HD2	1:B:409:LYS:HB2	1.87	0.56
1:B:285:VAL:HG11	1:B:524:LEU:HD11	1.87	0.56
1:A:250:LYS:HB2	1:A:252:LYS:HE3	1.86	0.56
2:C:44:PRO:HD3	2:C:98:ASN:HD21	1.69	0.56
1:A:462:ILE:CG1	1:A:469:ARG:HG3	2.35	0.56
1:B:289:VAL:HG11	1:B:520:ILE:HD11	1.86	0.56
2:C:260:LEU:HD12	2:C:260:LEU:C	2.25	0.56
2:D:347:LEU:CD2	2:D:350:ARG:HG2	2.36	0.56
1:B:252:LYS:N	1:B:253:PRO:HD2	2.21	0.56
2:D:350:ARG:O	2:D:351:ILE:HD13	2.06	0.56
2:C:128:LEU:H	2:C:155:ALA:HB3	1.70	0.56
2:D:351:ILE:CD1	2:D:374:ASN:HA	2.35	0.56
1:A:286:GLN:HG2	1:A:520:ILE:HG21	1.87	0.56
1:B:282:THR:HG22	1:B:283:LYS:N	2.21	0.56
2:D:80:ILE:HG21	2:D:108:PHE:CE1	2.41	0.56
1:A:519:LEU:HA	1:A:522:THR:HG23	1.86	0.56
2:D:16:LEU:CA	2:D:101:TYR:HD2	2.19	0.55
1:A:354:TYR:HD2	1:A:355:ILE:HD13	1.72	0.55
2:D:340:LEU:HD23	2:D:340:LEU:O	2.07	0.55
2:D:206:PHE:HB3	2:D:408:TRP:HH2	1.72	0.55
2:D:350:ARG:HD3	2:D:351:ILE:N	2.21	0.55
2:C:17:ILE:HG23	2:C:100:TYR:O	2.06	0.55
2:D:27:LYS:HZ3	2:D:98:ASN:HB3	1.71	0.55
2:D:261:ILE:HD13	2:D:320:LEU:HD21	1.88	0.55
2:C:60:LEU:HD11	2:C:404:ILE:HG12	1.88	0.55
1:A:272:PHE:HA	1:B:463:HIS:CE1	2.41	0.55
1:A:460:SER:HA	1:A:470:ILE:O	2.07	0.55
1:B:446:LYS:CA	1:B:446:LYS:NZ	2.55	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:80:ILE:HD13	2:D:124:GLN:HG2	1.88	0.54
2:C:89:GLN:HE22	2:C:108:PHE:H	1.53	0.54
1:B:313:ILE:HG13	1:B:425:ASP:HB3	1.90	0.54
1:A:518:SER:O	1:A:522:THR:HG22	2.07	0.54
2:C:306:LYS:HE2	2:C:319:ILE:HD13	1.88	0.54
1:A:330:CYS:HB3	1:B:330:CYS:HB3	1.89	0.54
2:D:80:ILE:HG21	2:D:108:PHE:CD1	2.42	0.54
2:C:147:ARG:HH22	2:C:198:LYS:HD3	1.72	0.54
1:B:374:GLN:O	1:B:398:ILE:HG13	2.06	0.54
2:C:382:GLN:HA	2:C:385:LEU:HD23	1.89	0.54
1:A:436:VAL:CG1	1:A:441:PRO:CG	2.85	0.54
1:B:359:SER:HA	1:B:368:PHE:CD1	2.43	0.54
1:A:445:TYR:C	1:A:447:SER:N	2.61	0.54
2:C:70:LYS:HE2	2:C:225:ASP:OD1	2.08	0.54
1:A:525:ASN:O	1:A:529:ILE:HD12	2.07	0.54
2:C:26:LEU:O	2:C:30:VAL:HG23	2.06	0.54
2:D:43:PHE:CA	2:D:98:ASN:HD21	2.14	0.54
2:C:351:ILE:HG21	2:C:374:ASN:O	2.08	0.54
2:D:260:LEU:HD23	2:D:352:VAL:HG21	1.88	0.54
2:D:257:ASP:OD1	2:D:369:ARG:HG3	2.08	0.54
1:A:247:TRP:HZ2	2:D:341:LYS:HA	1.72	0.54
2:C:395:GLU:HA	2:C:398:GLU:HB2	1.90	0.54
1:B:301:ARG:O	1:B:503:LEU:HD21	2.07	0.54
2:D:83:ASN:O	2:D:87:GLY:N	2.35	0.53
2:C:18:GLN:HB3	2:C:19:PRO:HD2	1.90	0.53
1:A:251:TRP:HA	2:D:346:PRO:HB2	1.90	0.53
1:A:455:THR:O	1:A:475:VAL:HA	2.09	0.53
1:A:246:ILE:O	2:D:346:PRO:HA	2.07	0.53
2:C:133:LEU:HD21	2:C:146:LEU:HD11	1.90	0.53
1:B:379:VAL:HG12	1:B:451:ILE:HD11	1.91	0.53
2:D:149:LEU:HA	2:D:200:SER:O	2.08	0.53
1:A:247:TRP:HH2	2:D:341:LYS:HG2	1.72	0.53
2:C:290:PHE:O	2:C:292:LEU:HD23	2.09	0.53
2:C:259:LYS:HZ2	2:C:349:GLY:C	2.12	0.53
1:A:421:LYS:NZ	1:B:284:SER:OG	2.35	0.53
2:D:179:LYS:N	2:D:180:PRO:HD2	2.24	0.53
2:C:78:MET:O	2:C:128:LEU:HD12	2.08	0.53
2:C:345:GLN:HB2	2:C:346:PRO:HD2	1.90	0.53
2:C:129:LEU:HB3	2:C:153:CYS:SG	2.49	0.53
1:A:258:LEU:HG	1:B:464:ASN:ND2	2.24	0.53
2:D:79:PHE:HB3	2:D:92:PHE:HB2	1.89	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:115:LYS:C	2:D:117:GLU:N	2.62	0.52
1:B:367:LYS:HD3	1:B:465:ASP:OD1	2.10	0.52
2:C:77:LEU:CB	2:C:94:ILE:HG12	2.38	0.52
2:D:292:LEU:HG	2:D:328:ALA:CB	2.40	0.52
1:B:355:ILE:HA	1:B:358:ILE:HG22	1.91	0.52
2:D:27:LYS:HZ3	2:D:98:ASN:CB	2.21	0.52
1:A:394:MET:CE	1:A:446:LYS:HD3	2.39	0.52
1:A:462:ILE:HG13	1:A:469:ARG:HG3	1.91	0.52
1:A:509:ILE:HG23	1:A:510:THR:H	1.75	0.52
1:A:395:SER:OG	1:A:405:GLN:HB3	2.08	0.52
2:C:129:LEU:N	2:C:129:LEU:CD2	2.73	0.52
1:A:306:LEU:HB3	1:A:497:ILE:HG21	1.90	0.52
2:C:264:ILE:HG13	2:C:288:PRO:HB2	1.90	0.52
2:D:107:ARG:O	2:D:109:PRO:HD3	2.10	0.52
2:D:27:LYS:HZ1	2:D:98:ASN:CB	2.21	0.52
2:C:129:LEU:N	2:C:129:LEU:HD23	2.23	0.52
2:D:95:ASP:OD2	2:D:99:ASN:HB2	2.10	0.52
2:D:67:VAL:HA	2:D:228:ILE:O	2.10	0.51
1:B:467:CYS:HB3	1:B:498:ASN:HB3	1.92	0.51
2:D:17:ILE:HG23	2:D:100:TYR:O	2.11	0.51
1:B:282:THR:O	1:B:283:LYS:C	2.49	0.51
1:B:252:LYS:C	1:B:254:THR:H	2.14	0.51
2:D:125:ASP:O	2:D:157:ASN:HA	2.10	0.51
1:B:462:ILE:HG22	1:B:463:HIS:H	1.75	0.51
2:D:17:ILE:HG13	2:D:101:TYR:CE2	2.45	0.51
1:A:258:LEU:HG	1:B:464:ASN:HD21	1.75	0.51
1:A:305:GLU:HB3	1:A:431:ASN:HD22	1.72	0.51
1:B:299:GLU:HG2	1:B:300:LEU:HD12	1.93	0.51
1:A:305:GLU:OE2	1:A:409:LYS:HE3	2.11	0.51
1:B:315:ASP:HB2	1:B:322:VAL:HG23	1.92	0.51
1:B:414:GLN:HE21	1:B:416:LEU:HD21	1.75	0.51
2:D:115:LYS:HB2	2:D:117:GLU:HB2	1.91	0.51
1:A:402:ARG:CZ	1:A:402:ARG:HB2	2.40	0.51
1:A:407:ILE:HD12	1:A:433:GLU:HG2	1.93	0.51
2:C:156:ILE:HG12	2:C:176:GLU:HB3	1.93	0.50
2:C:133:LEU:HD11	2:C:146:LEU:CD1	2.41	0.50
1:B:329:GLN:HG3	1:B:330:CYS:N	2.26	0.50
1:A:299:GLU:HG2	1:A:300:LEU:N	2.25	0.50
1:A:444:LYS:O	1:A:447:SER:HB3	2.12	0.50
2:D:256:VAL:HG13	2:D:257:ASP:N	2.26	0.50
1:A:301:ARG:O	1:A:304:ILE:HG13	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:229:PHE:HB2	2:C:246:LEU:HB2	1.93	0.50
2:C:206:PHE:H	2:C:209:GLN:HE22	1.60	0.50
1:B:283:LYS:O	1:B:286:GLN:HB2	2.10	0.50
1:A:451:ILE:HD12	1:A:452:SER:N	2.26	0.50
1:A:509:ILE:HG13	1:A:510:THR:N	2.26	0.50
2:C:323:THR:HG23	2:C:324:TYR:CD1	2.47	0.50
2:C:256:VAL:HG13	2:C:257:ASP:N	2.27	0.50
1:B:528:THR:O	1:B:529:ILE:C	2.51	0.50
1:B:390:ARG:HD2	1:B:408:GLU:OE2	2.12	0.50
2:D:286:VAL:HG12	2:D:287:LYS:H	1.77	0.50
2:C:110:ARG:HD2	2:C:123:LEU:O	2.12	0.50
1:B:463:HIS:ND1	1:B:466:SER:OG	2.44	0.49
1:A:284:SER:O	1:A:285:VAL:C	2.51	0.49
2:D:356:LYS:CA	2:D:363:TRP:HB3	2.38	0.49
2:D:177:PHE:C	2:D:177:PHE:CD2	2.86	0.49
2:D:51:PHE:HD2	2:D:248:TRP:HD1	1.60	0.49
2:D:147:ARG:NH1	2:D:200:SER:HB2	2.27	0.49
2:D:51:PHE:HE2	2:D:397:LEU:HD11	1.77	0.49
2:C:352:VAL:HG13	2:C:368:PHE:CD2	2.48	0.49
1:B:505:ALA:HB1	1:B:516:TYR:HA	1.94	0.49
2:D:294:VAL:HG21	2:D:327:PHE:HE2	1.78	0.49
1:B:409:LYS:O	1:B:410:ARG:HD3	2.12	0.49
1:B:398:ILE:HD12	1:B:399:LYS:N	2.28	0.49
1:A:285:VAL:O	1:A:289:VAL:HG23	2.13	0.49
2:C:105:GLY:HA3	2:C:194:THR:HB	1.95	0.49
2:C:115:LYS:HG3	2:C:118:GLU:HB2	1.95	0.49
2:D:347:LEU:O	2:D:349:GLY:N	2.45	0.48
1:B:526:ASN:HA	1:B:529:ILE:HD12	1.95	0.48
1:B:352:SER:HB2	1:B:472:ILE:HG21	1.95	0.48
2:D:390:ASP:O	2:D:392:VAL:HG23	2.13	0.48
1:A:394:MET:HE1	1:A:446:LYS:HD3	1.94	0.48
2:C:304:ARG:HA	2:C:307:HIS:HB2	1.93	0.48
2:D:66:TYR:CE1	2:D:232:VAL:HG22	2.49	0.48
2:C:367:ARG:HD2	2:C:369:ARG:NH1	2.28	0.48
1:A:315:ASP:OD2	1:A:334:GLU:OE2	2.30	0.48
1:A:310:PHE:CD2	1:A:426:VAL:CG1	2.97	0.48
2:D:293:TYR:CB	2:D:324:TYR:CD2	2.96	0.48
1:A:519:LEU:HB2	1:B:268:ILE:HD11	1.94	0.48
2:C:77:LEU:HB2	2:C:94:ILE:CD1	2.43	0.48
1:A:259:GLN:H	1:A:259:GLN:HE21	1.61	0.48
1:B:495:LEU:N	1:B:495:LEU:HD12	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:VAL:HG12	1:A:516:TYR:OH	2.14	0.48
1:A:307:GLU:OE2	1:A:494:GLU:HB3	2.13	0.48
2:D:105:GLY:HA3	2:D:194:THR:OG1	2.13	0.48
1:B:497:ILE:O	1:B:497:ILE:HG23	2.13	0.48
2:D:264:ILE:CD1	2:D:288:PRO:HB2	2.44	0.48
2:D:27:LYS:HB3	2:D:39:PRO:O	2.14	0.48
2:D:213:VAL:HG12	2:D:214:ALA:H	1.79	0.48
2:C:287:LYS:HA	2:C:288:PRO:HD3	1.74	0.48
2:D:327:PHE:O	2:D:328:ALA:HB2	2.13	0.48
2:C:290:PHE:CE2	2:C:330:LEU:HB3	2.49	0.48
2:D:112:PRO:HB2	2:D:113:GLN:HE21	1.79	0.48
2:D:180:PRO:O	2:D:184:LEU:HB2	2.14	0.48
1:A:462:ILE:HG22	1:A:463:HIS:N	2.28	0.48
2:C:136:GLN:HG3	2:C:147:ARG:HE	1.78	0.48
2:D:263:ASP:O	2:D:289:VAL:HB	2.14	0.48
2:D:198:LYS:HG2	2:D:199:ILE:H	1.77	0.48
1:B:354:TYR:O	1:B:358:ILE:HB	2.14	0.48
2:D:47:GLN:HB2	2:D:241:LYS:HA	1.96	0.48
2:D:83:ASN:C	2:D:85:VAL:H	2.18	0.47
2:D:28:MET:HA	2:D:31:CYS:SG	2.54	0.47
1:B:248:ALA:O	2:C:312:PHE:HD1	1.97	0.47
1:A:330:CYS:SG	1:B:326:VAL:HG11	2.54	0.47
1:A:448:GLN:HG3	1:A:449:SER:O	2.14	0.47
1:A:380:TYR:CG	1:A:445:TYR:HB3	2.50	0.47
2:C:261:ILE:HG22	2:C:262:LEU:N	2.29	0.47
1:B:462:ILE:HG23	1:B:469:ARG:HB2	1.95	0.47
2:C:197:PHE:CD1	2:C:197:PHE:C	2.87	0.47
2:D:190:ASN:C	2:D:192:CYS:H	2.18	0.47
2:C:51:PHE:CD1	2:C:246:LEU:HD13	2.50	0.47
2:D:255:THR:O	2:D:256:VAL:HG23	2.14	0.47
2:D:34:LEU:HD22	2:D:238:ALA:HB2	1.96	0.47
1:B:506:PHE:CD2	1:B:506:PHE:C	2.88	0.47
1:A:259:GLN:HA	1:B:464:ASN:OD1	2.15	0.47
1:B:416:LEU:CD2	1:B:427:LYS:HG3	2.44	0.47
1:A:408:GLU:OE1	1:A:410:ARG:HD3	2.15	0.47
2:D:62:ALA:HA	2:D:411:ARG:HH12	1.80	0.47
1:A:451:ILE:CD1	1:A:451:ILE:C	2.83	0.47
2:D:60:LEU:CD1	2:D:404:ILE:HG12	2.45	0.47
2:C:77:LEU:HB2	2:C:94:ILE:HD11	1.98	0.46
2:C:109:PRO:CG	2:C:180:PRO:HB2	2.37	0.46
2:D:153:CYS:HB2	2:D:173:LEU:HD13	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:PHE:CE2	1:A:426:VAL:CG1	2.99	0.46
1:B:300:LEU:C	1:B:302:SER:H	2.18	0.46
1:A:397:ASP:HB3	1:A:402:ARG:H	1.79	0.46
1:A:462:ILE:HG12	1:A:469:ARG:HG3	1.97	0.46
1:A:530:ILE:HD11	1:B:272:PHE:CZ	2.50	0.46
2:D:183:ASP:N	2:D:183:ASP:OD2	2.49	0.46
2:D:27:LYS:NZ	2:D:98:ASN:HB2	2.29	0.46
2:D:77:LEU:HG	2:D:130:ASP:OD1	2.16	0.46
2:C:131:GLY:HA3	2:C:148:TYR:CZ	2.50	0.46
2:D:56:VAL:HG11	2:D:400:ILE:HD13	1.96	0.46
2:D:21:ASN:HA	2:D:24:GLN:CD	2.36	0.46
2:C:44:PRO:HG2	2:C:94:ILE:HD12	1.97	0.46
2:D:293:TYR:HB3	2:D:324:TYR:CD2	2.51	0.46
2:C:78:MET:HB3	2:C:129:LEU:CD2	2.45	0.46
1:A:279:ASP:N	1:A:279:ASP:OD2	2.49	0.46
1:B:446:LYS:CA	1:B:446:LYS:HZ2	2.21	0.46
2:D:351:ILE:HD11	2:D:374:ASN:HA	1.98	0.46
1:B:282:THR:O	1:B:286:GLN:HG3	2.16	0.46
2:C:136:GLN:O	2:C:144:GLN:HA	2.16	0.46
2:D:16:LEU:HA	2:D:101:TYR:HD2	1.80	0.46
2:D:38:LYS:HB2	2:D:39:PRO:HD3	1.97	0.46
1:B:520:ILE:O	1:B:523:PHE:N	2.48	0.46
2:C:290:PHE:CD2	2:C:330:LEU:HB3	2.51	0.46
2:D:133:LEU:HD21	2:D:146:LEU:HD11	1.98	0.46
1:B:370:ILE:HA	1:B:460:SER:O	2.16	0.46
2:D:388:ILE:HG13	2:D:388:ILE:H	1.47	0.45
1:B:382:VAL:HG12	1:B:383:GLY:H	1.79	0.45
2:C:70:LYS:O	2:C:224:SER:HA	2.15	0.45
2:C:206:PHE:H	2:C:209:GLN:NE2	2.14	0.45
1:B:343:ILE:HD11	1:B:348:PHE:HB2	1.98	0.45
2:C:354:CYS:HB3	2:C:365:MET:HA	1.99	0.45
1:A:331:VAL:HG22	1:A:417:LEU:CD1	2.46	0.45
1:A:394:MET:CG	1:A:406:PHE:HD2	2.21	0.45
1:B:293:ILE:HD13	1:B:304:ILE:HD13	1.98	0.45
2:D:256:VAL:CG1	2:D:257:ASP:H	2.27	0.45
1:A:304:ILE:HD12	1:A:503:LEU:HG	1.98	0.45
2:C:95:ASP:OD2	2:C:97:GLU:O	2.34	0.45
2:D:128:LEU:HB3	2:D:154:LEU:CD1	2.46	0.45
1:A:312:VAL:HB	1:A:321:ARG:HG3	1.98	0.45
2:C:106:PHE:CZ	2:C:196:PRO:HD2	2.52	0.45
1:A:430:LEU:HD23	1:A:430:LEU:C	2.37	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:THR:HB	1:B:402:ARG:HG2	1.98	0.45
2:D:204:MET:HG3	2:D:205:ASP:H	1.80	0.45
2:D:207:SER:O	2:D:209:GLN:N	2.49	0.45
2:D:132:GLU:HB2	2:D:151:PHE:CE1	2.44	0.45
1:A:252:LYS:N	1:A:253:PRO:CD	2.79	0.45
2:C:19:PRO:HB2	2:C:22:VAL:HG23	1.98	0.45
1:A:292:THR:CG2	1:A:430:LEU:HD13	2.47	0.45
2:C:141:THR:HG22	2:C:143:LEU:HG	1.98	0.45
1:A:517:ALA:HB1	1:A:521:ARG:NH2	2.32	0.45
2:C:127:THR:CG2	2:C:156:ILE:HD12	2.46	0.45
2:D:66:TYR:O	2:D:229:PHE:HA	2.16	0.45
1:B:379:VAL:HG12	1:B:451:ILE:CD1	2.47	0.45
2:C:295:TRP:HA	2:C:323:THR:O	2.17	0.45
2:C:192:CYS:HB2	2:C:195:PHE:CD2	2.52	0.45
2:D:180:PRO:HG2	2:D:181:TYR:H	1.81	0.45
1:A:499:THR:O	1:A:503:LEU:HB2	2.17	0.45
2:D:252:GLN:O	2:D:254:ASN:O	2.35	0.45
1:B:281:LEU:O	1:B:282:THR:C	2.54	0.45
1:A:488:GLU:HG3	1:A:489:THR:H	1.82	0.45
1:B:504:ASN:O	1:B:507:ASP:N	2.49	0.45
1:A:305:GLU:OE2	1:A:409:LYS:CE	2.64	0.45
2:D:179:LYS:HD3	2:D:183:ASP:OD1	2.16	0.44
2:C:108:PHE:HA	2:C:109:PRO:HD3	1.58	0.44
2:D:351:ILE:HD12	2:D:374:ASN:HA	1.98	0.44
2:D:257:ASP:HA	2:D:352:VAL:O	2.17	0.44
2:C:259:LYS:HZ3	2:C:351:ILE:CD1	2.30	0.44
1:A:520:ILE:HD13	1:A:520:ILE:HA	1.83	0.44
1:A:354:TYR:CD2	1:A:355:ILE:HD13	2.52	0.44
2:C:264:ILE:HD11	2:C:288:PRO:HB2	1.98	0.44
1:B:406:PHE:CZ	1:B:445:TYR:CE1	3.05	0.44
2:D:293:TYR:HB2	2:D:324:TYR:CD2	2.53	0.44
2:C:176:GLU:O	2:C:180:PRO:HG3	2.18	0.44
2:D:293:TYR:HB3	2:D:324:TYR:HD2	1.83	0.44
2:D:115:LYS:C	2:D:117:GLU:H	2.20	0.44
1:A:271:SER:C	1:A:273:LEU:H	2.21	0.44
1:A:292:THR:HG22	1:A:430:LEU:HD13	1.99	0.44
1:A:281:LEU:CD2	1:A:329:GLN:HG2	2.48	0.44
2:C:253:GLU:O	2:C:255:THR:HG22	2.17	0.44
2:D:383:LYS:O	2:D:386:GLU:HB3	2.18	0.44
2:C:347:LEU:O	2:C:349:GLY:N	2.50	0.44
2:C:104:ASN:HB3	2:C:105:GLY:H	1.59	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:PHE:CE2	1:A:334:GLU:HB2	2.52	0.44
1:A:259:GLN:NE2	1:A:259:GLN:H	2.15	0.44
2:D:154:LEU:HD23	2:D:236:TYR:CD2	2.52	0.44
2:D:109:PRO:HB2	2:D:110:ARG:H	1.56	0.44
2:D:114:LYS:O	2:D:115:LYS:C	2.57	0.44
1:A:279:ASP:CG	1:A:282:THR:HB	2.38	0.44
2:D:141:THR:HG22	2:D:143:LEU:HG	1.99	0.44
2:D:48:PRO:HB3	2:D:245:LEU:HG	1.99	0.44
1:B:406:PHE:CD2	1:B:442:PRO:HG3	2.53	0.43
2:C:295:TRP:O	2:C:377:HIS:HA	2.17	0.43
2:D:73:GLY:O	2:D:132:GLU:OE2	2.36	0.43
1:A:247:TRP:CH2	2:D:341:LYS:HG2	2.51	0.43
2:C:226:GLY:HA3	2:C:248:TRP:O	2.18	0.43
2:C:214:ALA:HA	2:C:217:LEU:HB2	1.99	0.43
1:A:394:MET:CG	1:A:406:PHE:CD2	2.99	0.43
1:B:407:ILE:HG13	1:B:409:LYS:N	2.33	0.43
2:C:135:ILE:N	2:C:135:ILE:CD1	2.70	0.43
2:C:17:ILE:HD13	2:C:99:ASN:HB3	1.98	0.43
1:B:272:PHE:O	1:B:272:PHE:CG	2.72	0.43
1:A:284:SER:O	1:A:287:ASP:N	2.52	0.43
1:B:487:SER:O	1:B:488:GLU:HB2	2.18	0.43
2:D:352:VAL:HG13	2:D:368:PHE:CD2	2.52	0.43
1:A:349:LYS:O	1:A:353:LYS:HG2	2.18	0.43
2:C:259:LYS:NZ	2:C:349:GLY:HA2	2.33	0.43
2:C:300:ASP:CG	2:C:374:ASN:HD22	2.22	0.43
1:A:462:ILE:HD11	1:B:258:LEU:HD21	2.01	0.43
2:C:319:ILE:HG13	2:C:320:LEU:H	1.83	0.43
1:A:255:ILE:CA	1:A:258:LEU:HB3	2.36	0.43
2:C:129:LEU:HA	2:C:153:CYS:HA	2.01	0.43
1:B:273:LEU:HD23	1:B:273:LEU:HA	1.41	0.43
1:A:250:LYS:HG3	2:D:310:GLN:HG3	2.00	0.43
1:A:313:ILE:HG12	1:A:339:LEU:HD12	2.01	0.43
1:B:445:TYR:HD2	1:B:445:TYR:HA	1.72	0.43
2:D:13:ILE:HD12	2:D:74:LEU:HD21	2.00	0.43
1:A:431:ASN:C	1:A:431:ASN:HD22	2.22	0.43
2:C:318:GLU:O	2:C:321:GLU:CG	2.66	0.43
2:D:366:LEU:HD23	2:D:366:LEU:N	2.33	0.43
1:A:436:VAL:HA	1:A:437:PRO:HD2	1.94	0.43
2:C:156:ILE:HG12	2:C:176:GLU:CB	2.49	0.43
2:C:67:VAL:HG21	2:C:210:LEU:HD23	2.01	0.43
1:A:395:SER:HB2	1:A:404:GLY:N	2.31	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:13:ILE:CG1	2:D:14:PRO:HD2	2.42	0.42
2:D:129:LEU:HD23	2:D:129:LEU:N	2.34	0.42
2:D:193:THR:C	2:D:195:PHE:H	2.22	0.42
2:D:20:GLY:O	2:D:23:THR:HB	2.18	0.42
2:D:347:LEU:HA	2:D:347:LEU:HD23	1.84	0.42
2:D:128:LEU:HD23	2:D:154:LEU:HD11	2.02	0.42
2:C:128:LEU:N	2:C:155:ALA:HB3	2.32	0.42
1:A:467:CYS:HB3	1:A:498:ASN:HB3	2.00	0.42
2:D:326:LYS:O	2:D:326:LYS:HD2	2.19	0.42
1:A:488:GLU:CG	1:A:489:THR:H	2.32	0.42
1:B:246:ILE:HD13	2:C:344:GLU:CG	2.49	0.42
1:B:329:GLN:CG	1:B:330:CYS:N	2.82	0.42
1:B:301:ARG:HG2	1:B:503:LEU:HD21	2.00	0.42
2:D:119:LEU:HD13	2:D:184:LEU:HG	2.00	0.42
2:D:26:LEU:HA	2:D:29:MET:HB2	2.01	0.42
1:A:307:GLU:CD	1:A:494:GLU:HB3	2.39	0.42
2:D:241:LYS:HG3	2:D:241:LYS:H	1.69	0.42
1:A:417:LEU:CD2	1:A:428:ILE:HD12	2.49	0.42
1:B:509:ILE:CG2	1:B:510:THR:H	2.26	0.42
2:D:166:THR:O	2:D:167:SER:C	2.57	0.42
2:D:290:PHE:CE2	2:D:330:LEU:HB3	2.54	0.42
1:B:502:LEU:HA	1:B:519:LEU:HD21	2.02	0.42
1:A:305:GLU:HB3	1:A:431:ASN:HD21	1.79	0.42
1:A:466:SER:HB2	1:A:522:THR:OG1	2.20	0.42
1:B:374:GLN:HA	1:B:456:LYS:O	2.19	0.42
1:A:285:VAL:HG23	1:A:285:VAL:H	1.47	0.42
1:B:251:TRP:CE3	2:C:350:ARG:HB2	2.55	0.42
1:B:393:ARG:HD2	1:B:409:LYS:CB	2.50	0.42
1:B:498:ASN:ND2	1:B:500:PRO:HD2	2.35	0.42
1:A:285:VAL:HG11	1:A:524:LEU:HD21	2.02	0.42
1:B:323:ASN:C	1:B:323:ASN:OD1	2.56	0.42
2:C:80:ILE:HG21	2:C:108:PHE:CD1	2.55	0.42
2:C:259:LYS:NZ	2:C:349:GLY:CA	2.83	0.42
1:A:376:ARG:NH2	1:A:398:ILE:HG22	2.35	0.42
2:D:26:LEU:HD21	2:D:92:PHE:CZ	2.55	0.42
1:B:313:ILE:HG12	1:B:339:LEU:HD12	2.01	0.42
2:D:234:ALA:HA	2:D:235:PRO:HD3	1.89	0.42
2:D:119:LEU:HA	2:D:122:THR:OG1	2.20	0.41
1:B:315:ASP:HB2	1:B:322:VAL:CG2	2.50	0.41
2:D:293:TYR:CD2	2:D:324:TYR:HB3	2.54	0.41
2:C:400:ILE:HG22	2:C:400:ILE:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:256:VAL:HG11	2:D:381:VAL:HG22	2.02	0.41
2:D:155:ALA:HA	2:D:161:LEU:H	1.85	0.41
2:D:287:LYS:HA	2:D:288:PRO:HD3	1.84	0.41
1:B:246:ILE:HD12	1:B:247:TRP:N	2.28	0.41
1:B:509:ILE:HG23	1:B:510:THR:N	2.31	0.41
1:A:533:LYS:HG3	1:A:537:LEU:CD1	2.50	0.41
1:A:462:ILE:CG2	1:A:463:HIS:H	2.32	0.41
2:C:85:VAL:HG12	2:C:86:THR:HG23	2.02	0.41
1:A:463:HIS:CE1	1:B:272:PHE:HA	2.55	0.41
2:D:166:THR:HB	2:D:232:VAL:O	2.20	0.41
2:D:344:GLU:HG2	2:D:345:GLN:N	2.36	0.41
1:B:252:LYS:HG2	2:C:308:PHE:CZ	2.55	0.41
1:A:313:ILE:HG13	1:A:425:ASP:HB3	2.02	0.41
1:B:538:SER:O	1:B:539:TYR:CG	2.74	0.41
2:D:384:VAL:O	2:D:388:ILE:HG13	2.20	0.41
2:D:351:ILE:CG2	2:D:374:ASN:O	2.69	0.41
1:B:251:TRP:CD2	1:B:253:PRO:HG2	2.56	0.41
1:A:397:ASP:OD1	1:A:399:LYS:HG3	2.21	0.41
2:D:258:PHE:HE2	2:D:294:VAL:HG13	1.85	0.41
2:D:252:GLN:O	2:D:253:GLU:C	2.58	0.41
2:C:208:TYR:O	2:C:208:TYR:HD1	2.03	0.41
1:A:321:ARG:NH2	1:A:425:ASP:OD1	2.54	0.41
1:A:273:LEU:HB3	1:A:275:ILE:HG12	2.02	0.41
2:D:171:ALA:O	2:D:175:LYS:HG2	2.21	0.41
2:C:259:LYS:HZ3	2:C:351:ILE:HD13	1.85	0.41
1:B:279:ASP:OD2	1:B:279:ASP:N	2.54	0.41
2:C:38:LYS:H	2:C:38:LYS:HG2	1.69	0.41
2:D:213:VAL:CG1	2:D:214:ALA:N	2.77	0.41
2:C:262:LEU:HD12	2:C:348:ASN:HA	2.02	0.41
2:D:350:ARG:HD3	2:D:351:ILE:C	2.41	0.41
1:B:292:THR:O	1:B:293:ILE:C	2.58	0.41
2:D:32:LYS:C	2:D:35:ASN:H	2.23	0.41
2:C:71:THR:HG22	2:C:222:HIS:CD2	2.56	0.41
2:C:44:PRO:HD3	2:C:98:ASN:ND2	2.36	0.41
1:B:250:LYS:O	1:B:252:LYS:HD2	2.20	0.41
2:C:152:ASP:OD2	2:C:236:TYR:CD1	2.74	0.41
2:D:410:GLU:HG2	2:D:414:ASN:ND2	2.36	0.41
1:B:476:GLU:HA	1:B:489:THR:HG22	2.01	0.41
1:A:414:GLN:NE2	1:A:427:LYS:HD2	2.36	0.41
2:D:350:ARG:HD3	2:D:351:ILE:O	2.20	0.40
1:B:252:LYS:O	1:B:254:THR:N	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ILE:HA	1:A:358:ILE:HG22	2.03	0.40
1:A:355:ILE:O	1:A:359:SER:HB3	2.21	0.40
1:B:354:TYR:CD2	1:B:533:LYS:HD2	2.56	0.40
1:A:271:SER:HB2	1:B:529:ILE:HD11	2.02	0.40
2:C:347:LEU:CD2	2:C:350:ARG:HG2	2.51	0.40
2:D:295:TRP:HZ3	2:D:298:GLY:HA2	1.87	0.40
1:A:252:LYS:C	1:A:254:THR:H	2.25	0.40
1:A:290:TYR:HB2	1:A:516:TYR:HE2	1.84	0.40
2:C:106:PHE:CE2	2:C:196:PRO:HD2	2.56	0.40
1:B:406:PHE:HZ	1:B:445:TYR:CE1	2.39	0.40
1:A:505:ALA:HB2	1:A:515:GLU:HG2	2.04	0.40
2:C:150:MET:HE1	2:C:173:LEU:HD11	2.01	0.40
2:C:256:VAL:CG1	2:C:257:ASP:N	2.85	0.40
1:B:374:GLN:O	1:B:398:ILE:CG1	2.69	0.40
2:D:60:LEU:HD11	2:D:404:ILE:HG12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	268/310 (86%)	195 (73%)	46 (17%)	27 (10%)	1	3
1	B	268/310 (86%)	192 (72%)	48 (18%)	28 (10%)	1	3
2	C	383/461 (83%)	287 (75%)	68 (18%)	28 (7%)	1	6
2	D	383/461 (83%)	280 (73%)	69 (18%)	34 (9%)	1	4
All	All	1302/1542 (84%)	954 (73%)	231 (18%)	117 (9%)	1	4

All (117) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	279	ASP
1	A	286	GLN
1	A	336	ASP
1	A	342	ASN
1	B	279	ASP
1	B	289	VAL
1	B	291	ALA
1	B	301	ARG
1	B	342	ASN
1	B	440	ASP
1	B	447	SER
1	B	509	ILE
1	B	510	THR
2	C	109	PRO
2	C	118	GLU
2	C	203	HIS
2	C	232	VAL
2	C	233	LYS
2	C	238	ALA
2	C	376	ASN
2	C	392	VAL
2	D	16	LEU
2	D	104	ASN
2	D	109	PRO
2	D	118	GLU
2	D	194	THR
2	D	217	LEU
2	D	348	ASN
2	D	401	VAL
1	A	271	SER
1	A	285	VAL
1	A	289	VAL
1	A	322	VAL
1	A	325	PRO
1	A	446	LYS
1	A	509	ILE
1	B	254	THR
1	B	290	TYR
1	B	336	ASP
2	C	19	PRO
2	C	87	GLY
2	C	88	GLU
2	C	176	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	288	PRO
2	C	311	PRO
2	C	320	LEU
2	C	330	LEU
2	C	331	SER
2	D	86	THR
2	D	167	SER
2	D	208	TYR
2	D	214	ALA
2	D	311	PRO
1	A	288	TRP
1	A	498	ASN
1	B	253	PRO
1	B	273	LEU
1	B	313	ILE
1	B	498	ASN
1	B	511	ASN
2	C	39	PRO
2	C	104	ASN
2	C	208	TYR
2	C	236	TYR
2	C	373	LEU
2	C	396	ASP
2	D	116	LYS
2	D	166	THR
2	D	252	GLN
2	D	288	PRO
2	D	314	ARG
2	D	330	LEU
2	D	356	LYS
2	D	359	GLU
2	D	393	SER
1	A	324	PRO
1	A	333	THR
1	A	405	GLN
1	A	441	PRO
1	A	528	THR
1	B	281	LEU
1	B	282	THR
1	B	421	LYS
1	B	517	ALA
1	B	528	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	113	GLN
2	C	171	ALA
2	C	314	ARG
2	D	184	LEU
2	D	192	CYS
2	D	203	HIS
2	D	253	GLU
2	D	371	ASP
1	A	284	SER
1	A	319	PRO
1	A	365	THR
1	A	437	PRO
1	A	510	THR
1	B	382	VAL
2	C	213	VAL
2	C	367	ARG
2	D	309	ASP
2	D	322	ARG
1	A	382	VAL
1	B	270	PRO
2	D	60	LEU
2	D	115	LYS
2	D	213	VAL
2	D	236	TYR
1	A	412	VAL
1	B	529	ILE
1	A	403	VAL
1	B	361	VAL
1	B	412	VAL
2	D	48	PRO
1	B	322	VAL
1	A	500	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	254/290 (88%)	203 (80%)	51 (20%)	1	8
1	B	254/290 (88%)	211 (83%)	43 (17%)	2	13
2	C	352/421 (84%)	279 (79%)	73 (21%)	1	7
2	D	352/421 (84%)	270 (77%)	82 (23%)	1	4
All	All	1212/1422 (85%)	963 (80%)	249 (20%)	1	7

All (249) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	246	ILE
1	A	252	LYS
1	A	254	THR
1	A	256	LYS
1	A	258	LEU
1	A	259	GLN
1	A	261	ILE
1	A	279	ASP
1	A	280	ASP
1	A	282	THR
1	A	287	ASP
1	A	295	SER
1	A	303	PHE
1	A	312	VAL
1	A	313	ILE
1	A	322	VAL
1	A	327	SER
1	A	335	LEU
1	A	338	HIS
1	A	353	LYS
1	A	365	THR
1	A	373	SER
1	A	374	GLN
1	A	377	ASP
1	A	378	SER
1	A	381	ARG
1	A	396	THR
1	A	399	LYS
1	A	400	THR
1	A	410	ARG
1	A	412	VAL
1	A	417	LEU
1	A	431	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	437	PRO
1	A	446	LYS
1	A	448	GLN
1	A	452	SER
1	A	455	THR
1	A	473	THR
1	A	477	ASN
1	A	497	ILE
1	A	498	ASN
1	A	503	LEU
1	A	507	ASP
1	A	508	ASN
1	A	509	ILE
1	A	514	LYS
1	A	522	THR
1	A	533	LYS
1	A	536	SER
1	A	537	LEU
1	B	252	LYS
1	B	259	GLN
1	B	279	ASP
1	B	282	THR
1	B	284	SER
1	B	287	ASP
1	B	300	LEU
1	B	303	PHE
1	B	322	VAL
1	B	327	SER
1	B	335	LEU
1	B	353	LYS
1	B	358	ILE
1	B	361	VAL
1	B	364	ASN
1	B	365	THR
1	B	367	LYS
1	B	377	ASP
1	B	381	ARG
1	B	395	SER
1	B	400	THR
1	B	402	ARG
1	B	405	GLN
1	B	407	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	419	SER
1	B	429	SER
1	B	431	ASN
1	B	439	ASN
1	B	441	PRO
1	B	443	GLU
1	B	444	LYS
1	B	446	LYS
1	B	447	SER
1	B	451	ILE
1	B	462	ILE
1	B	466	SER
1	B	468	THR
1	B	488	GLU
1	B	499	THR
1	B	508	ASN
1	B	510	THR
1	B	522	THR
1	B	533	LYS
2	C	17	ILE
2	C	33	LEU
2	C	38	LYS
2	C	41	LYS
2	C	52	GLN
2	C	64	ASP
2	C	67	VAL
2	C	69	GLU
2	C	75	ARG
2	C	77	LEU
2	C	82	ILE
2	C	102	LEU
2	C	103	VAL
2	C	104	ASN
2	C	110	ARG
2	C	111	LEU
2	C	119	LEU
2	C	123	LEU
2	C	129	LEU
2	C	132	GLU
2	C	135	ILE
2	C	144	GLN
2	C	146	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	151	PHE
2	C	154	LEU
2	C	156	ILE
2	C	175	LYS
2	C	179	LYS
2	C	191	ARG
2	C	197	PHE
2	C	203	HIS
2	C	204	MET
2	C	211	VAL
2	C	228	ILE
2	C	249	LYS
2	C	252	GLN
2	C	254	ASN
2	C	255	THR
2	C	256	VAL
2	C	259	LYS
2	C	260	LEU
2	C	264	ILE
2	C	284	TYR
2	C	286	VAL
2	C	289	VAL
2	C	290	PHE
2	C	292	LEU
2	C	295	TRP
2	C	300	ASP
2	C	306	LYS
2	C	308	PHE
2	C	310	GLN
2	C	326	LYS
2	C	327	PHE
2	C	329	GLU
2	C	343	LEU
2	C	347	LEU
2	C	350	ARG
2	C	351	ILE
2	C	363	TRP
2	C	365	MET
2	C	366	LEU
2	C	367	ARG
2	C	369	ARG
2	C	370	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	382	GLN
2	C	385	LEU
2	C	388	ILE
2	C	389	ASN
2	C	392	VAL
2	C	393	SER
2	C	404	ILE
2	C	415	MET
2	D	17	ILE
2	D	21	ASN
2	D	25	ASP
2	D	33	LEU
2	D	38	LYS
2	D	40	THR
2	D	41	LYS
2	D	50	SER
2	D	52	GLN
2	D	60	LEU
2	D	64	ASP
2	D	67	VAL
2	D	69	GLU
2	D	71	THR
2	D	77	LEU
2	D	78	MET
2	D	80	ILE
2	D	81	VAL
2	D	84	PRO
2	D	103	VAL
2	D	104	ASN
2	D	110	ARG
2	D	111	LEU
2	D	117	GLU
2	D	119	LEU
2	D	123	LEU
2	D	124	GLN
2	D	129	LEU
2	D	132	GLU
2	D	135	ILE
2	D	144	GLN
2	D	146	LEU
2	D	150	MET
2	D	154	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	159	ARG
2	D	175	LYS
2	D	183	ASP
2	D	184	LEU
2	D	191	ARG
2	D	193	THR
2	D	201	MET
2	D	203	HIS
2	D	204	MET
2	D	218	ASP
2	D	227	LEU
2	D	228	ILE
2	D	230	THR
2	D	233	LYS
2	D	237	THR
2	D	251	GLU
2	D	252	GLN
2	D	259	LYS
2	D	260	LEU
2	D	287	LYS
2	D	290	PHE
2	D	292	LEU
2	D	296	GLN
2	D	306	LYS
2	D	308	PHE
2	D	310	GLN
2	D	326	LYS
2	D	329	GLU
2	D	330	LEU
2	D	333	SER
2	D	337	TRP
2	D	350	ARG
2	D	354	CYS
2	D	363	TRP
2	D	364	GLU
2	D	365	MET
2	D	366	LEU
2	D	367	ARG
2	D	370	ASP
2	D	371	ASP
2	D	376	ASN
2	D	385	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	388	ILE
2	D	389	ASN
2	D	390	ASP
2	D	397	LEU
2	D	404	ILE
2	D	415	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	259	GLN
1	A	274	ASN
1	A	286	GLN
1	A	342	ASN
1	A	405	GLN
1	A	411	HIS
1	A	414	GLN
1	A	431	ASN
1	A	448	GLN
1	A	498	ASN
1	B	259	GLN
1	B	323	ASN
1	B	411	HIS
1	B	414	GLN
1	B	431	ASN
1	B	464	ASN
1	B	498	ASN
2	C	47	GLN
2	C	83	ASN
2	C	89	GLN
2	C	98	ASN
2	C	99	ASN
2	C	144	GLN
2	C	209	GLN
2	C	339	ASN
2	C	357	ASN
2	C	374	ASN
2	C	382	GLN
2	D	35	ASN
2	D	47	GLN
2	D	83	ASN
2	D	98	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	104	ASN
2	D	113	GLN
2	D	144	GLN
2	D	203	HIS
2	D	209	GLN
2	D	252	GLN
2	D	307	HIS
2	D	339	ASN
2	D	357	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	276/310 (89%)	-0.24	2 (0%) 89 70	24, 55, 112, 145	0
1	B	276/310 (89%)	-0.25	2 (0%) 89 70	19, 53, 100, 156	0
2	C	387/461 (83%)	-0.09	4 (1%) 84 60	46, 92, 123, 154	0
2	D	387/461 (83%)	-0.15	2 (0%) 91 76	50, 91, 124, 155	0
All	All	1326/1542 (85%)	-0.17	10 (0%) 87 67	19, 80, 121, 156	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	261	ILE	8.6
1	A	487	SER	6.2
1	A	440	ASP	4.4
2	C	311	PRO	2.7
2	D	301	VAL	2.4
2	C	112	PRO	2.2
2	C	316	GLU	2.2
2	C	301	VAL	2.2
1	B	389	PRO	2.1
2	D	34	LEU	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.