Full wwPDB X-ray Structure Validation Report (i)

Nov 3, 2023 – 06:26 AM EDT

PDB ID	:	3W1H
Title	:	Crystal structure of the selenocysteine synthase SelA from Aquifex aeolicus
Authors	:	Itoh, Y.; Sekine, S.; Yokoyama, S.
Deposited on	:	2012-11-15
Resolution	:	3.89 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 (i) 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 (i)) were used in the production of this report:

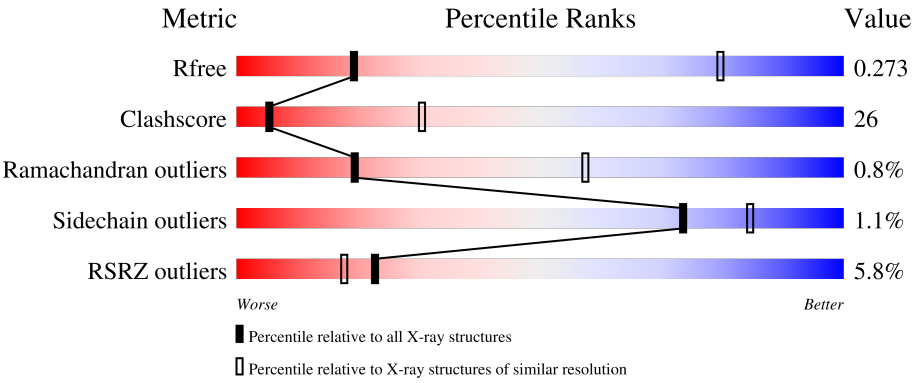
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.89 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	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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	452	6% 53% 46%
1	B	452	7% 51% 45%
1	C	452	7% 50% 49%
1	D	452	4% 45% 41% 13%
1	E	452	4% 51% 37% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	LLP	B	285	-	-	X	-

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 16913 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 L-seryl-tRNA(Sec) selenium transferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	P	S	0	0	0
			3575	2278	620	665	1	11			
1	B	443	Total	C	N	O	P	S	0	0	0
			3501	2230	606	654	1	10			
1	C	452	Total	C	N	O	P	S	0	0	0
			3575	2278	620	665	1	11			
1	D	395	Total	C	N	O	P	S	0	0	0
			3115	1980	542	582	1	10			
1	E	399	Total	C	N	O	P	S	0	0	0
			3147	2000	546	590	1	10			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ALA	LYS	engineered mutation	UNP O67140
A	21	ALA	LYS	engineered mutation	UNP O67140
A	46	ALA	LYS	engineered mutation	UNP O67140
A	48	ALA	LYS	engineered mutation	UNP O67140
B	19	ALA	LYS	engineered mutation	UNP O67140
B	21	ALA	LYS	engineered mutation	UNP O67140
B	46	ALA	LYS	engineered mutation	UNP O67140
B	48	ALA	LYS	engineered mutation	UNP O67140
C	19	ALA	LYS	engineered mutation	UNP O67140
C	21	ALA	LYS	engineered mutation	UNP O67140
C	46	ALA	LYS	engineered mutation	UNP O67140
C	48	ALA	LYS	engineered mutation	UNP O67140
D	19	ALA	LYS	engineered mutation	UNP O67140
D	21	ALA	LYS	engineered mutation	UNP O67140
D	46	ALA	LYS	engineered mutation	UNP O67140
D	48	ALA	LYS	engineered mutation	UNP O67140
E	19	ALA	LYS	engineered mutation	UNP O67140
E	21	ALA	LYS	engineered mutation	UNP O67140
E	46	ALA	LYS	engineered mutation	UNP O67140

Continued on next page...

Continued from previous page...

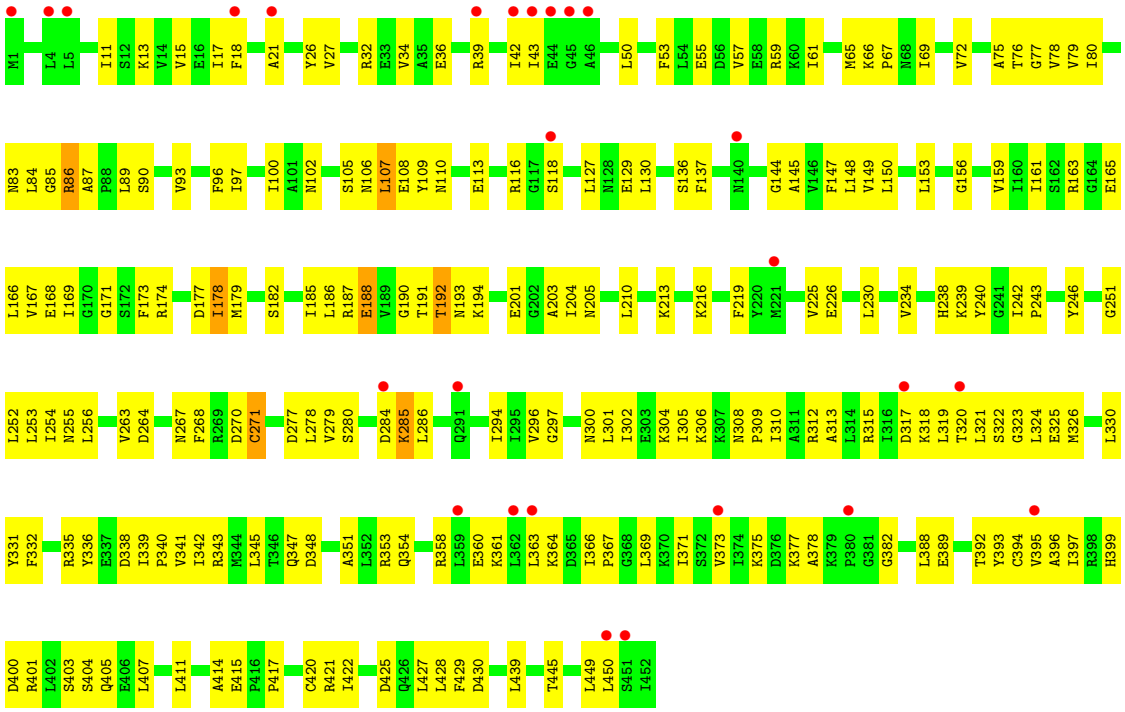
Chain	Residue	Modelled	Actual	Comment	Reference
E	48	ALA	LYS	engineered mutation	UNP O67140

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.

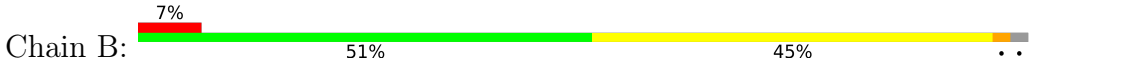
• Molecule 1: L-seryl-tRNA(Sec) selenium transferase

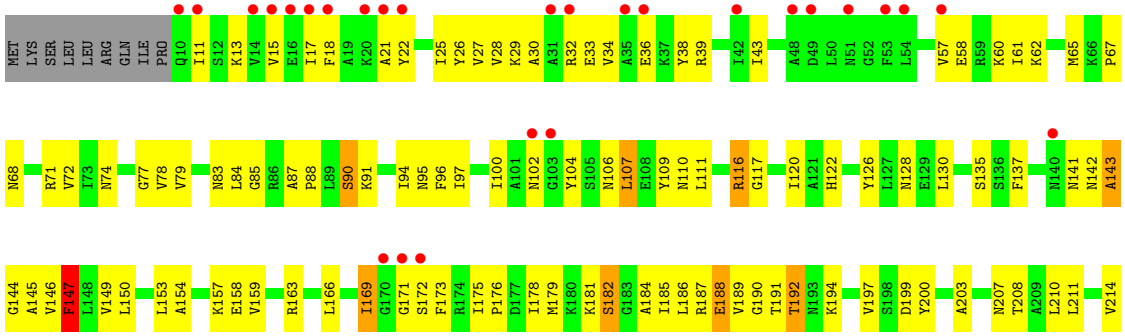
Chain A:

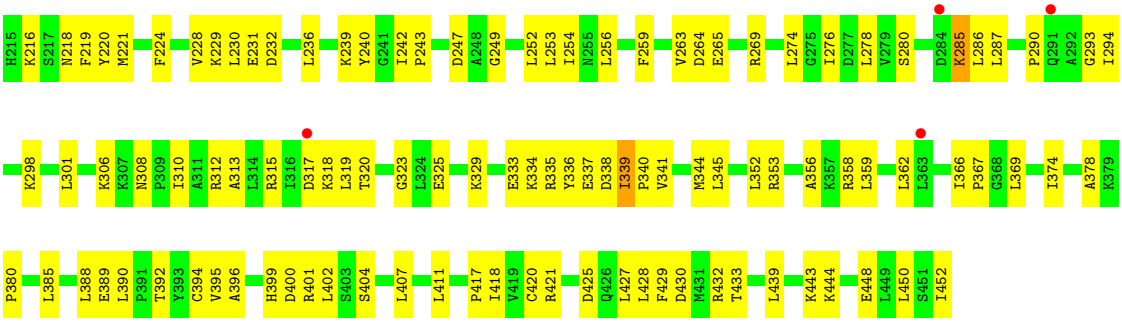


• Molecule 1: L-seryl-tRNA(Sec) selenium transferase

Chain B:

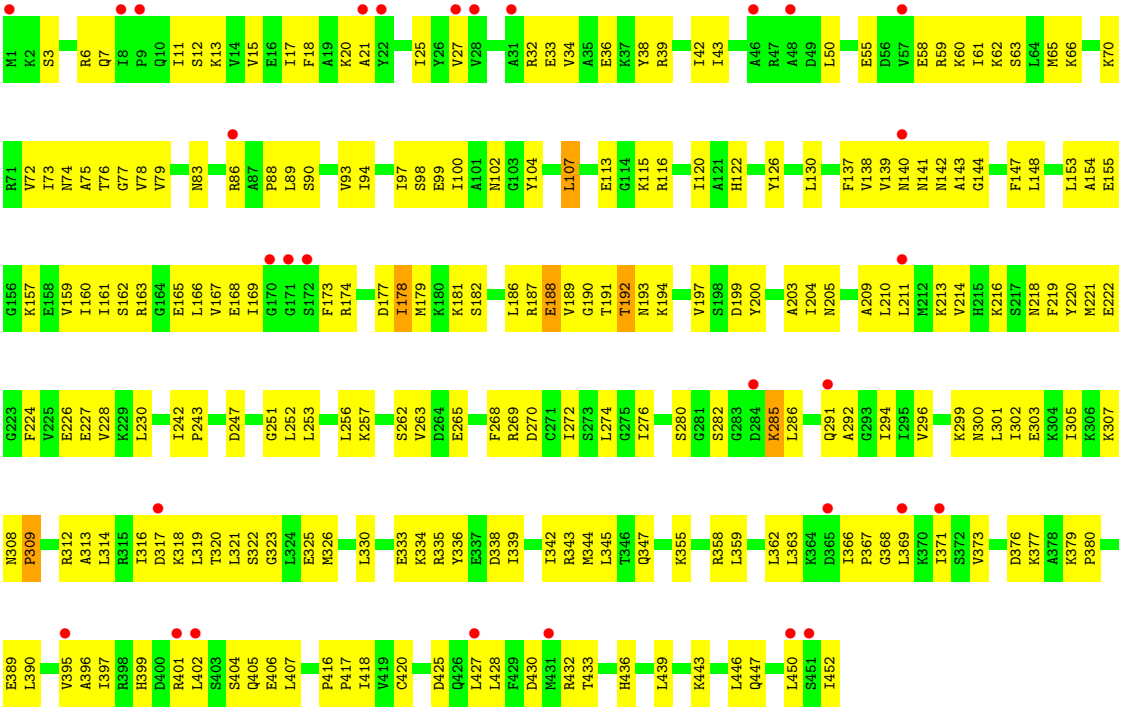






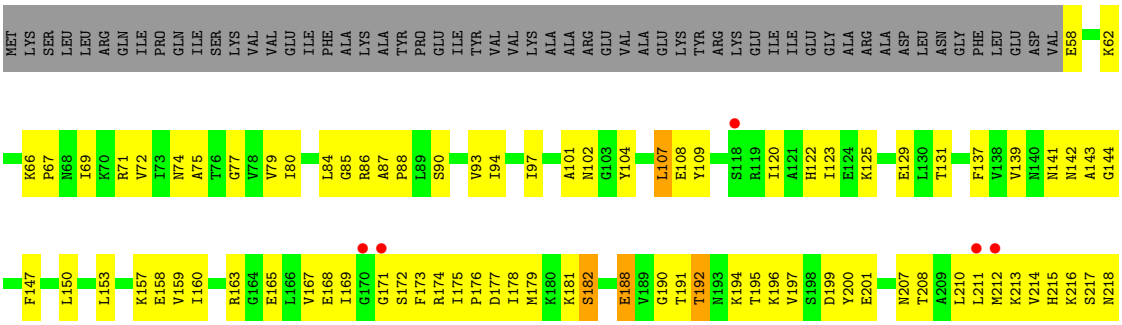
• Molecule 1: L-seryl-tRNA(Sec) selenium transferase

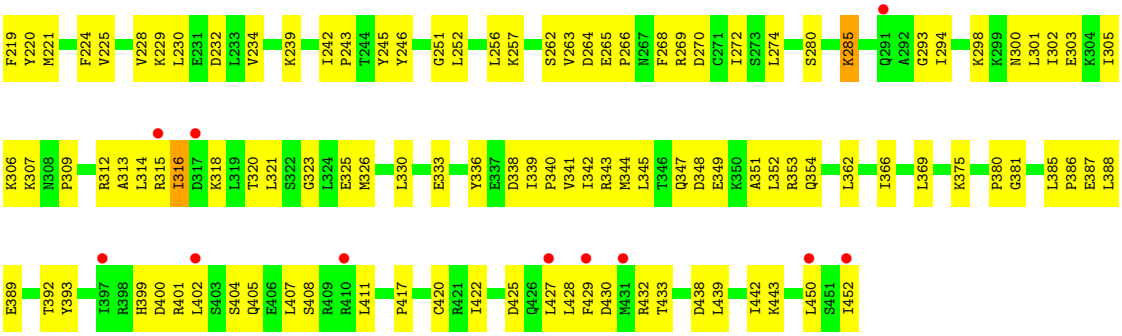
Chain C:



• Molecule 1: L-seryl-tRNA(Sec) selenium transferase

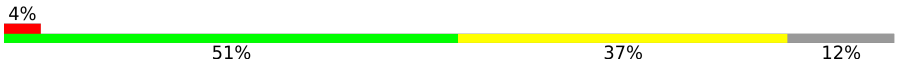
Chain D:

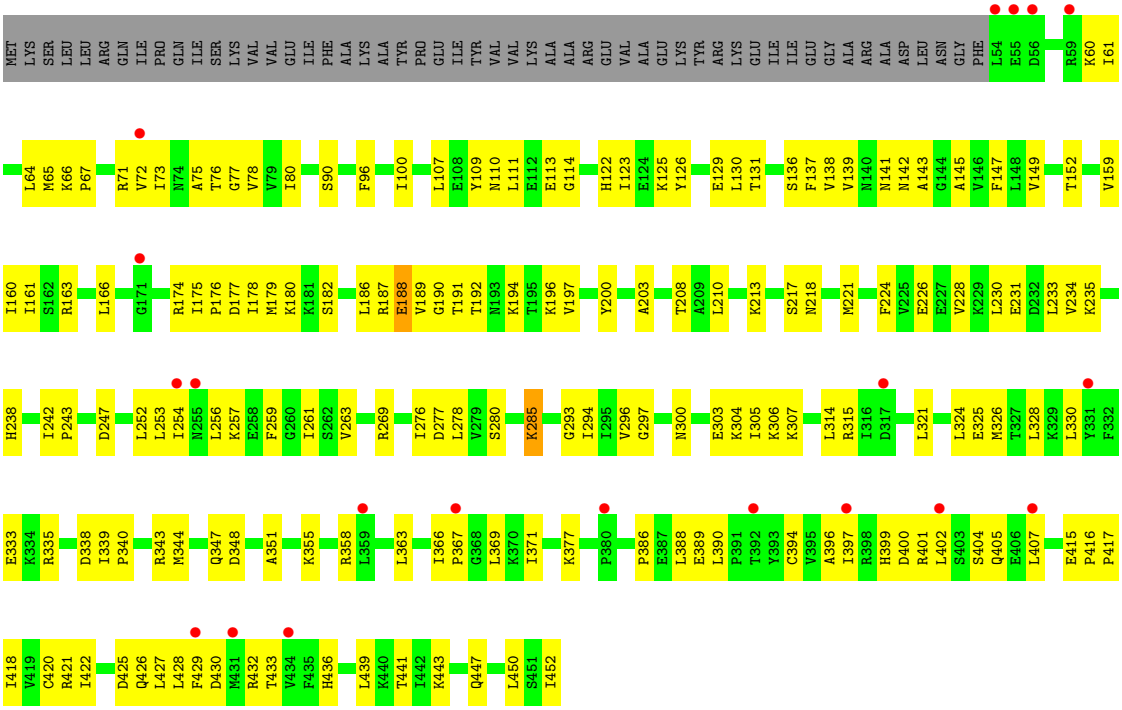




• Molecule 1: L-seryl-tRNA(Sec) selenium transferase

Chain E:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	167.03Å 167.03Å 211.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.25 – 3.89 49.25 – 3.89	Depositor EDS
% Data completeness (in resolution range)	94.1 (49.25-3.89) 94.2 (49.25-3.89)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.44 (at 3.88Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.220 , 0.282 0.203 , 0.273	Depositor DCC
R_{free} test set	1345 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	130.3	Xtriage
Anisotropy	0.692	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 135.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16913	wwPDB-VP
Average B, all atoms (Å^2)	209.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LLP

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	0.40	0/3597	0.62	0/4831
1	B	0.43	0/3522	0.64	0/4731
1	C	0.41	0/3597	0.62	0/4831
1	D	0.38	0/3130	0.60	0/4203
1	E	0.41	0/3162	0.60	0/4247
All	All	0.41	0/17008	0.62	0/22843

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3575	0	3759	214	0
1	B	3501	0	3668	235	0
1	C	3575	0	3759	222	0
1	D	3115	0	3271	185	0
1	E	3147	0	3301	145	0
All	All	16913	0	17758	908	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (908) 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:C:102:ASN:HB3	1:D:71:ARG:HH22	1.16	1.03
1:B:72:VAL:HG22	1:B:417:PRO:HG2	1.41	1.03
1:E:123:ILE:HD13	1:E:324:LEU:HD23	1.37	1.02
1:A:69:ILE:HG22	1:B:100:ILE:HD12	1.49	0.95
1:E:254:ILE:HD11	1:E:259:PHE:HE2	1.31	0.94
1:E:61:ILE:O	1:E:65:MET:HG3	1.66	0.94
1:B:187:ARG:HE	1:B:203:ALA:HB1	1.34	0.92
1:E:254:ILE:HD11	1:E:259:PHE:CE2	2.05	0.91
1:A:76:THR:OG1	1:A:78:VAL:HG23	1.71	0.91
1:A:145:ALA:O	1:A:149:VAL:HG23	1.71	0.90
1:B:224:PHE:CD1	1:C:218:ASN:HB2	2.08	0.88
1:C:76:THR:OG1	1:C:78:VAL:HG23	1.73	0.88
1:B:407:LEU:HD23	1:B:427:LEU:HD22	1.56	0.87
1:A:153:LEU:HD11	1:A:301:LEU:HD22	1.58	0.86
1:E:371:ILE:HG12	1:E:397:ILE:HG22	1.57	0.86
1:D:362:LEU:HB3	1:D:443:LYS:HD2	1.58	0.86
1:A:173:PHE:HE1	1:A:178:ILE:HD12	1.38	0.85
1:E:187:ARG:HE	1:E:203:ALA:HB1	1.40	0.85
1:A:193:ASN:O	1:A:225:VAL:HG13	1.78	0.84
1:A:150:LEU:HD13	1:A:179:MET:HG3	1.58	0.84
1:C:397:ILE:HD11	1:C:427:LEU:HD23	1.60	0.83
1:D:208:THR:HG22	1:D:242:ILE:HD13	1.61	0.83
1:C:355:LYS:HD3	1:C:436:HIS:CE1	2.14	0.83
1:C:100:ILE:CD1	1:D:69:ILE:HG22	2.08	0.82
1:A:159:VAL:HG13	1:A:210:LEU:HB3	1.62	0.82
1:C:163:ARG:HD2	1:C:190:GLY:O	1.80	0.82
1:C:130:LEU:HD13	1:C:253:LEU:HD21	1.60	0.82
1:A:163:ARG:HD2	1:A:190:GLY:O	1.80	0.82
1:D:399:HIS:CE1	1:D:401:ARG:HB2	2.14	0.81
1:A:130:LEU:HD13	1:A:253:LEU:HD21	1.61	0.81
1:A:373:VAL:HG22	1:A:395:VAL:HG22	1.60	0.81
1:A:27:VAL:HG22	1:A:61:ILE:HD13	1.62	0.80
1:E:355:LYS:HD3	1:E:436:HIS:CE1	2.15	0.80
1:B:32:ARG:O	1:B:36:GLU:HG2	1.82	0.80
1:A:358:ARG:HH21	1:A:439:LEU:HD12	1.46	0.79
1:D:178:ILE:CG2	1:D:179:MET:N	2.45	0.79
1:E:396:ALA:HB2	1:E:428:LEU:HD23	1.64	0.79
1:A:137:PHE:CD1	1:A:306:LYS:HG2	2.18	0.79
1:B:90:SER:HB3	1:B:338:ASP:O	1.83	0.79
1:C:216:LYS:HG2	1:C:219:PHE:CZ	2.18	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:SER:HB3	1:A:338:ASP:O	1.83	0.78
1:A:216:LYS:HG2	1:A:219:PHE:CZ	2.19	0.78
1:B:91:LYS:HE2	1:B:95:ASN:HD21	1.49	0.77
1:B:128:ASN:HD21	1:B:135:SER:HA	1.48	0.77
1:C:194:LYS:HG2	1:C:226:GLU:HB2	1.65	0.77
1:C:32:ARG:O	1:C:36:GLU:HG2	1.84	0.77
1:D:298:LYS:HB2	1:D:301:LEU:HD12	1.64	0.77
1:B:187:ARG:NE	1:B:203:ALA:HB1	2.00	0.76
1:D:167:VAL:HG12	1:D:219:PHE:HE2	1.50	0.76
1:D:407:LEU:HD23	1:D:427:LEU:HD22	1.67	0.76
1:E:73:ILE:HB	1:E:418:ILE:HG12	1.66	0.76
1:B:142:ASN:HB3	1:B:285:LLP:OP4	1.86	0.76
1:B:290:PRO:HB2	1:B:320:THR:HG22	1.67	0.76
1:B:374:ILE:HD11	1:B:428:LEU:HD21	1.67	0.76
1:E:343:ARG:O	1:E:347:GLN:HG3	1.85	0.76
1:B:58:GLU:HG2	1:B:62:LYS:HE3	1.67	0.76
1:C:100:ILE:HD12	1:D:69:ILE:HG22	1.68	0.76
1:E:77:GLY:HA3	1:E:430:ASP:CG	2.05	0.76
1:B:221:MET:HG2	1:C:221:MET:HG2	1.66	0.75
1:B:97:ILE:HD11	1:B:323:GLY:HA3	1.67	0.75
1:C:75:ALA:HB3	1:C:420:CYS:HB3	1.67	0.75
1:B:335:ARG:NH1	1:B:338:ASP:OD2	2.20	0.74
1:E:187:ARG:NE	1:E:203:ALA:HB1	2.02	0.74
1:E:217:SER:O	1:E:386:PRO:HD3	1.87	0.74
1:C:83:ASN:HB3	1:D:109:TYR:HD2	1.53	0.74
1:D:407:LEU:CD2	1:D:427:LEU:HD22	2.17	0.74
1:B:179:MET:SD	1:B:186:LEU:HB2	2.27	0.74
1:B:72:VAL:HG22	1:B:417:PRO:CG	2.16	0.73
1:B:163:ARG:NH1	1:C:188:GLU:OE1	2.21	0.73
1:B:224:PHE:HD1	1:C:218:ASN:HB2	1.48	0.73
1:C:187:ARG:HE	1:C:203:ALA:HB1	1.53	0.73
1:C:366:ILE:HG23	1:C:367:PRO:HD2	1.69	0.73
1:D:216:LYS:HG2	1:D:219:PHE:CZ	2.23	0.73
1:E:136:SER:CB	1:E:296:VAL:HG12	2.19	0.72
1:D:88:PRO:O	1:D:340:PRO:HG2	1.88	0.72
1:B:263:VAL:HG11	1:B:388:LEU:HD13	1.71	0.72
1:A:83:ASN:HB3	1:B:109:TYR:HD2	1.55	0.72
1:E:90:SER:HB3	1:E:338:ASP:O	1.89	0.72
1:B:159:VAL:HG22	1:B:210:LEU:HB3	1.71	0.72
1:D:242:ILE:HG23	1:D:243:PRO:HD2	1.71	0.71
1:A:13:LYS:O	1:A:17:ILE:HG13	1.89	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:107:LEU:HD11	1:E:321:LEU:HD23	1.71	0.71
1:A:251:GLY:HA2	1:A:268:PHE:HE2	1.54	0.71
1:B:216:LYS:HG2	1:B:219:PHE:CZ	2.26	0.70
1:D:280:SER:HA	1:D:294:ILE:O	1.91	0.70
1:E:107:LEU:O	1:E:122:HIS:HE1	1.73	0.70
1:B:178:ILE:CG2	1:B:179:MET:N	2.54	0.70
1:C:399:HIS:HE1	1:C:401:ARG:HD3	1.54	0.70
1:E:194:LYS:HZ1	1:E:224:PHE:HD2	1.37	0.70
1:A:263:VAL:HG21	1:A:388:LEU:HD13	1.73	0.70
1:E:230:LEU:HD23	1:E:233:LEU:HD12	1.72	0.70
1:A:97:ILE:HD11	1:A:323:GLY:HA3	1.74	0.70
1:E:200:TYR:CE2	1:E:228:VAL:HG21	2.27	0.70
1:B:231:GLU:HG3	1:B:274:LEU:HD11	1.74	0.70
1:A:193:ASN:HB2	1:A:225:VAL:HG22	1.73	0.69
1:A:85:GLY:O	1:A:86:ARG:O	2.11	0.69
1:D:72:VAL:HG22	1:D:417:PRO:HG2	1.73	0.69
1:D:176:PRO:HG3	1:E:191:THR:HG22	1.72	0.69
1:E:141:ASN:OD1	1:E:143:ALA:HB3	1.92	0.69
1:A:110:ASN:ND2	1:A:113:GLU:OE1	2.26	0.69
1:B:400:ASP:OD1	1:B:401:ARG:N	2.26	0.69
1:D:150:LEU:HD13	1:D:179:MET:HG3	1.75	0.69
1:A:280:SER:HA	1:A:294:ILE:O	1.93	0.68
1:C:42:ILE:HD11	1:C:50:LEU:HD21	1.74	0.68
1:A:173:PHE:CE1	1:A:178:ILE:HD12	2.26	0.68
1:C:90:SER:HB3	1:C:338:ASP:O	1.93	0.68
1:C:102:ASN:HB3	1:D:71:ARG:NH2	2.01	0.68
1:D:215:HIS:NE2	1:D:265:GLU:OE2	2.27	0.67
1:A:137:PHE:CE1	1:A:306:LYS:HG2	2.29	0.67
1:B:142:ASN:HB3	1:B:285:LLP:C5'	2.24	0.67
1:B:399:HIS:CE1	1:B:401:ARG:HB2	2.29	0.67
1:C:25:ILE:CD1	1:D:333:GLU:HA	2.24	0.67
1:A:242:ILE:HG23	1:A:243:PRO:HD2	1.76	0.67
1:E:75:ALA:HB3	1:E:420:CYS:HB3	1.75	0.67
1:B:208:THR:HG22	1:B:242:ILE:HD13	1.75	0.67
1:D:158:GLU:HG3	1:D:207:ASN:HB3	1.77	0.67
1:D:173:PHE:CZ	1:D:175:ILE:HD13	2.29	0.67
1:D:400:ASP:OD1	1:D:401:ARG:N	2.26	0.67
1:C:321:LEU:HD12	1:C:321:LEU:O	1.95	0.67
1:D:349:GLU:OE2	1:D:375:LYS:NZ	2.28	0.67
1:B:390:LEU:HB3	1:B:432:ARG:HH22	1.59	0.66
1:C:157:LYS:HE2	1:C:209:ALA:HB2	1.75	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:330:LEU:HD23	1:E:335:ARG:HD3	1.77	0.66
1:C:141:ASN:OD1	1:C:143:ALA:HB3	1.94	0.66
1:A:55:GLU:O	1:A:59:ARG:HG3	1.95	0.66
1:C:159:VAL:HG13	1:C:210:LEU:HB3	1.77	0.66
1:C:77:GLY:HA2	1:C:433:THR:HG23	1.76	0.66
1:A:331:TYR:CE2	1:A:339:ILE:HD13	2.31	0.66
1:B:452:ILE:HG23	1:B:452:ILE:OXT	1.94	0.66
1:C:72:VAL:HG22	1:C:417:PRO:HG2	1.78	0.66
1:A:251:GLY:HA2	1:A:268:PHE:CE2	2.29	0.66
1:E:161:ILE:HG21	1:E:166:LEU:HD21	1.77	0.66
1:D:439:LEU:HA	1:D:442:ILE:HD12	1.78	0.65
1:A:168:GLU:O	1:A:168:GLU:HG2	1.96	0.65
1:B:197:VAL:HG22	1:B:228:VAL:HG13	1.78	0.65
1:A:57:VAL:O	1:A:61:ILE:HG13	1.96	0.65
1:C:187:ARG:NE	1:C:203:ALA:HB1	2.11	0.65
1:E:136:SER:HB2	1:E:296:VAL:HG12	1.78	0.65
1:A:366:ILE:HG23	1:A:367:PRO:HD2	1.78	0.65
1:C:25:ILE:HD11	1:D:333:GLU:HA	1.78	0.65
1:B:200:TYR:CE2	1:B:228:VAL:HG21	2.31	0.65
1:B:337:GLU:N	1:B:337:GLU:OE1	2.28	0.65
1:A:167:VAL:HG12	1:A:219:PHE:HE2	1.61	0.65
1:B:128:ASN:ND2	1:B:135:SER:HA	2.12	0.65
1:D:163:ARG:NH1	1:E:188:GLU:OE1	2.29	0.65
1:E:405:GLN:HE22	1:E:422:ILE:HG21	1.60	0.65
1:A:72:VAL:HG13	1:A:417:PRO:HG2	1.79	0.65
1:A:399:HIS:CE1	1:A:401:ARG:HB2	2.32	0.65
1:D:93:VAL:HG22	1:D:326:MET:HG3	1.78	0.65
1:A:234:VAL:HG12	1:A:238:HIS:CD2	2.32	0.64
1:D:169:ILE:HG22	1:D:218:ASN:OD1	1.97	0.64
1:E:348:ASP:O	1:E:351:ALA:HB3	1.97	0.64
1:A:108:GLU:HB2	1:B:83:ASN:HA	1.80	0.64
1:B:344:MET:O	1:B:432:ARG:HD2	1.97	0.64
1:B:389:GLU:O	1:B:390:LEU:HD23	1.98	0.64
1:E:399:HIS:HE1	1:E:401:ARG:HD3	1.63	0.64
1:B:22:TYR:CG	1:B:61:ILE:HG21	2.33	0.64
1:C:107:LEU:O	1:C:122:HIS:HE1	1.81	0.64
1:B:254:ILE:CD1	1:B:259:PHE:HE2	2.11	0.64
1:D:208:THR:CG2	1:D:242:ILE:HD13	2.28	0.64
1:E:123:ILE:CD1	1:E:324:LEU:HD23	2.23	0.64
1:A:39:ARG:O	1:A:43:ILE:HG13	1.97	0.64
1:B:249:GLY:O	1:B:285:LLP:HD3	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:TYR:CD2	1:D:387:GLU:HG2	2.33	0.63
1:B:77:GLY:HA3	1:B:430:ASP:CG	2.19	0.63
1:A:167:VAL:HG12	1:A:219:PHE:CE2	2.32	0.63
1:B:58:GLU:O	1:B:62:LYS:HG3	1.99	0.63
1:B:120:ILE:O	1:B:120:ILE:HG22	1.97	0.63
1:B:394:CYS:HA	1:B:429:PHE:O	1.98	0.63
1:C:93:VAL:HA	1:C:326:MET:HG2	1.79	0.63
1:A:194:LYS:HG2	1:A:226:GLU:HB2	1.81	0.63
1:B:210:LEU:HD12	1:B:243:PRO:HG2	1.79	0.63
1:D:438:ASP:O	1:D:442:ILE:HG13	1.99	0.63
1:E:366:ILE:HB	1:E:369:LEU:HD12	1.81	0.63
1:B:219:PHE:CD2	1:C:193:ASN:HB3	2.34	0.63
1:B:362:LEU:O	1:B:443:LYS:HD2	1.99	0.62
1:C:73:ILE:HB	1:C:418:ILE:HG12	1.81	0.62
1:B:178:ILE:HG23	1:B:179:MET:N	2.13	0.62
1:E:394:CYS:HA	1:E:429:PHE:O	1.98	0.62
1:A:75:ALA:HB3	1:A:420:CYS:HB3	1.81	0.62
1:D:178:ILE:HG23	1:D:179:MET:N	2.14	0.62
1:E:159:VAL:HG13	1:E:210:LEU:HB3	1.80	0.62
1:C:178:ILE:CG2	1:C:179:MET:N	2.62	0.62
1:C:404:SER:OG	1:C:405:GLN:NE2	2.31	0.62
1:A:11:ILE:O	1:A:15:VAL:HG23	2.00	0.62
1:A:102:ASN:HA	1:B:94:ILE:HD11	1.81	0.62
1:A:325:GLU:OE2	1:B:68:ASN:HB2	2.00	0.62
1:A:102:ASN:OD1	1:A:102:ASN:O	2.17	0.62
1:A:178:ILE:CG2	1:A:179:MET:N	2.63	0.62
1:A:313:ALA:HB1	1:B:144:GLY:CA	2.30	0.62
1:A:32:ARG:HG2	1:A:32:ARG:HH11	1.64	0.62
1:A:161:ILE:CG2	1:A:166:LEU:HD21	2.29	0.62
1:B:145:ALA:O	1:B:149:VAL:HG23	2.00	0.62
1:C:34:VAL:O	1:C:38:TYR:HD1	1.82	0.61
1:C:130:LEU:CD1	1:C:253:LEU:HD21	2.30	0.61
1:C:144:GLY:CA	1:D:313:ALA:HB1	2.30	0.61
1:C:165:GLU:OE2	1:C:213:LYS:NZ	2.32	0.61
1:A:252:LEU:HD13	1:A:286:LEU:HB3	1.82	0.61
1:C:73:ILE:HD12	1:C:416:PRO:HG2	1.83	0.61
1:D:163:ARG:HD2	1:D:190:GLY:O	2.00	0.61
1:D:405:GLN:HE22	1:D:422:ILE:HG21	1.65	0.61
1:D:93:VAL:HA	1:D:326:MET:HG2	1.80	0.61
1:E:208:THR:HG22	1:E:242:ILE:HD13	1.83	0.61
1:D:174:ARG:HB2	1:D:177:ASP:HB2	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:389:GLU:O	1:C:390:LEU:HD23	2.01	0.61
1:D:173:PHE:CE2	1:D:175:ILE:HD13	2.35	0.61
1:B:280:SER:HA	1:B:294:ILE:O	2.00	0.60
1:C:116:ARG:HH22	1:D:171:GLY:HA3	1.66	0.60
1:C:194:LYS:NZ	1:C:224:PHE:HB3	2.16	0.60
1:C:72:VAL:HG13	1:C:417:PRO:HG2	1.83	0.60
1:C:358:ARG:HH21	1:C:439:LEU:HD12	1.66	0.60
1:D:251:GLY:HA2	1:D:268:PHE:CE2	2.36	0.60
1:A:179:MET:O	1:A:182:SER:HB3	2.02	0.60
1:C:366:ILE:HB	1:C:369:LEU:HD12	1.83	0.60
1:D:131:THR:HG22	1:D:268:PHE:HB3	1.83	0.60
1:C:97:ILE:HD11	1:C:323:GLY:HA3	1.83	0.60
1:E:136:SER:HB3	1:E:296:VAL:HG12	1.82	0.60
1:C:120:ILE:HG21	1:C:137:PHE:CD1	2.37	0.60
1:C:362:LEU:O	1:C:443:LYS:HD2	2.02	0.60
1:B:137:PHE:CE1	1:B:306:LYS:HG2	2.36	0.60
1:C:179:MET:O	1:C:182:SER:HB3	2.02	0.60
1:D:197:VAL:HG22	1:D:228:VAL:HG13	1.84	0.60
1:E:163:ARG:HD2	1:E:190:GLY:O	2.02	0.60
1:B:399:HIS:CE1	1:B:450:LEU:HD22	2.36	0.59
1:C:58:GLU:HG2	1:C:62:LYS:HE3	1.84	0.59
1:E:142:ASN:ND2	1:E:247:ASP:OD1	2.32	0.59
1:B:221:MET:CG	1:C:221:MET:HG2	2.31	0.59
1:B:242:ILE:HG23	1:B:243:PRO:HD2	1.84	0.59
1:D:251:GLY:HA2	1:D:268:PHE:HE2	1.68	0.59
1:A:366:ILE:HB	1:A:369:LEU:HD12	1.83	0.59
1:B:358:ARG:HH21	1:B:439:LEU:HD12	1.67	0.59
1:C:167:VAL:HG12	1:C:219:PHE:HE2	1.67	0.59
1:A:397:ILE:HD11	1:A:427:LEU:HD23	1.84	0.59
1:E:147:PHE:CE1	1:E:182:SER:HA	2.38	0.59
1:A:137:PHE:HD1	1:A:306:LYS:HE2	1.67	0.59
1:E:420:CYS:SG	1:E:427:LEU:HD11	2.42	0.59
1:D:178:ILE:HG22	1:D:179:MET:N	2.17	0.59
1:A:312:ARG:NH2	1:B:285:LLP:OP3	2.32	0.59
1:B:366:ILE:CG2	1:B:367:PRO:HD2	2.33	0.59
1:D:178:ILE:HG22	1:D:179:MET:H	1.68	0.59
1:E:252:LEU:HD21	1:E:256:LEU:HG	1.85	0.59
1:B:179:MET:O	1:B:182:SER:HB3	2.03	0.58
1:D:200:TYR:CD2	1:D:228:VAL:HG21	2.37	0.58
1:D:62:LYS:O	1:D:66:LYS:HG3	2.02	0.58
1:D:265:GLU:HG3	1:D:266:PRO:HD2	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:PHE:HB3	1:B:21:ALA:HB3	1.85	0.58
1:C:161:ILE:HD13	1:C:166:LEU:CD2	2.33	0.58
1:B:142:ASN:HD22	1:B:285:LLP:C5	2.16	0.58
1:C:79:VAL:HG21	1:C:345:LEU:CD2	2.34	0.58
1:D:58:GLU:HG2	1:D:62:LYS:HE3	1.85	0.58
1:D:229:LYS:O	1:D:232:ASP:HB2	2.03	0.58
1:A:72:VAL:HG22	1:A:417:PRO:HG2	1.86	0.58
1:A:210:LEU:HD12	1:A:243:PRO:HG2	1.86	0.58
1:A:351:ALA:O	1:A:354:GLN:HB3	2.04	0.58
1:A:407:LEU:O	1:A:411:LEU:HG	2.04	0.58
1:C:359:LEU:HB2	1:C:439:LEU:HD22	1.84	0.58
1:A:18:PHE:HB3	1:A:21:ALA:HB3	1.86	0.58
1:C:18:PHE:HB3	1:C:21:ALA:HB3	1.85	0.58
1:B:33:GLU:OE2	1:B:60:LYS:NZ	2.25	0.57
1:B:150:LEU:HD13	1:B:179:MET:HG3	1.85	0.57
1:E:200:TYR:CD2	1:E:228:VAL:HG21	2.39	0.57
1:C:252:LEU:HD13	1:C:286:LEU:HB3	1.86	0.57
1:A:79:VAL:HG21	1:A:345:LEU:HD23	1.86	0.57
1:D:230:LEU:O	1:D:234:VAL:HG23	2.04	0.57
1:A:96:PHE:O	1:A:100:ILE:HG12	2.03	0.57
1:C:13:LYS:O	1:C:17:ILE:HG13	2.03	0.57
1:C:230:LEU:HD22	1:C:276:ILE:HD11	1.85	0.57
1:E:242:ILE:HG23	1:E:243:PRO:HD2	1.86	0.57
1:A:267:ASN:O	1:A:271:CYS:HB2	2.05	0.57
1:A:213:LYS:HD3	1:A:230:LEU:HD21	1.86	0.57
1:A:339:ILE:O	1:A:339:ILE:HG13	2.05	0.57
1:B:116:ARG:HG3	1:B:117:GLY:N	2.20	0.57
1:C:142:ASN:HB3	1:C:285:LLP:C5'	2.34	0.57
1:E:231:GLU:CD	1:E:231:GLU:H	2.08	0.57
1:A:331:TYR:CE2	1:A:339:ILE:CD1	2.88	0.57
1:A:378:ALA:CB	1:A:421:ARG:HH12	2.18	0.57
1:B:126:TYR:HE2	1:B:325:GLU:HG3	1.70	0.57
1:A:392:THR:HG21	1:A:430:ASP:OD2	2.04	0.57
1:B:57:VAL:O	1:B:61:ILE:HG13	2.04	0.57
1:B:229:LYS:HB2	1:B:232:ASP:OD2	2.04	0.57
1:D:439:LEU:HD23	1:D:442:ILE:HD12	1.87	0.57
1:B:159:VAL:HG13	1:B:210:LEU:HB3	1.87	0.57
1:D:215:HIS:HB2	1:D:246:TYR:OH	2.04	0.57
1:B:214:VAL:HG22	1:B:247:ASP:HB3	1.87	0.56
1:C:102:ASN:OD1	1:C:102:ASN:O	2.22	0.56
1:D:256:LEU:HD23	1:D:263:VAL:CG2	2.35	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:161:ILE:CG2	1:E:166:LEU:HD21	2.35	0.56
1:E:396:ALA:HB2	1:E:428:LEU:CD2	2.33	0.56
1:C:252:LEU:CD1	1:C:286:LEU:HB3	2.35	0.56
1:E:280:SER:HA	1:E:294:ILE:O	2.03	0.56
1:E:339:ILE:HG13	1:E:339:ILE:O	2.05	0.56
1:B:173:PHE:CE2	1:B:175:ILE:HD13	2.40	0.56
1:B:254:ILE:HD11	1:B:259:PHE:HE2	1.70	0.56
1:C:120:ILE:HG21	1:C:137:PHE:HD1	1.69	0.56
1:D:188:GLU:OE1	1:E:163:ARG:NH1	2.28	0.56
1:D:300:ASN:OD1	1:D:301:LEU:HG	2.04	0.56
1:D:366:ILE:HB	1:D:369:LEU:HD12	1.87	0.56
1:A:32:ARG:O	1:A:36:GLU:HG2	2.05	0.56
1:B:200:TYR:HE2	1:B:228:VAL:HG21	1.68	0.56
1:B:366:ILE:HB	1:B:369:LEU:HD12	1.88	0.56
1:E:399:HIS:CE1	1:E:401:ARG:HD3	2.40	0.56
1:B:336:TYR:O	1:B:339:ILE:HG12	2.06	0.56
1:C:100:ILE:HD11	1:D:69:ILE:HG22	1.86	0.56
1:C:339:ILE:O	1:C:339:ILE:HG13	2.04	0.56
1:A:147:PHE:CE1	1:B:310:ILE:CD1	2.88	0.56
1:C:262:SER:O	1:C:262:SER:OG	2.20	0.56
1:C:301:LEU:O	1:C:305:ILE:HG13	2.05	0.56
1:C:343:ARG:O	1:C:347:GLN:HG3	2.06	0.56
1:D:58:GLU:O	1:D:62:LYS:HG3	2.06	0.56
1:D:257:LYS:HG2	1:D:262:SER:HA	1.86	0.56
1:C:62:LYS:O	1:C:66:LYS:HG3	2.05	0.56
1:A:330:LEU:HD23	1:A:335:ARG:HD3	1.86	0.56
1:B:61:ILE:O	1:B:65:MET:HG3	2.06	0.56
1:C:376:ASP:OD1	1:C:377:LYS:N	2.38	0.56
1:A:136:SER:HB3	1:A:296:VAL:HG12	1.87	0.55
1:A:161:ILE:HG21	1:A:166:LEU:HD21	1.87	0.55
1:A:178:ILE:HG23	1:A:179:MET:N	2.21	0.55
1:A:366:ILE:CG2	1:A:367:PRO:HD2	2.35	0.55
1:A:107:LEU:HD13	1:A:318:LYS:HG3	1.89	0.55
1:C:358:ARG:NH2	1:C:439:LEU:HD12	2.22	0.55
1:E:366:ILE:HG23	1:E:367:PRO:HD2	1.88	0.55
1:B:27:VAL:HG22	1:B:61:ILE:HD13	1.88	0.55
1:A:167:VAL:CG1	1:A:219:PHE:HE2	2.19	0.55
1:E:130:LEU:HD13	1:E:253:LEU:HD21	1.89	0.55
1:B:77:GLY:HA3	1:B:430:ASP:OD2	2.07	0.55
1:A:313:ALA:HB1	1:B:144:GLY:HA2	1.89	0.55
1:B:137:PHE:CD1	1:B:306:LYS:HG2	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ARG:HG2	1:A:32:ARG:NH1	2.22	0.55
1:A:239:LYS:HD3	1:A:240:TYR:CE2	2.42	0.55
1:A:400:ASP:OD1	1:A:401:ARG:N	2.40	0.55
1:A:401:ARG:NH1	1:A:450:LEU:O	2.36	0.55
1:C:363:LEU:HD23	1:C:443:LYS:HG3	1.88	0.55
1:A:77:GLY:HA3	1:A:430:ASP:HB3	1.89	0.54
1:B:402:LEU:HD12	1:B:450:LEU:CD2	2.37	0.54
1:C:144:GLY:HA2	1:D:313:ALA:HB1	1.89	0.54
1:D:131:THR:HG22	1:D:268:PHE:CB	2.37	0.54
1:E:416:PRO:CG	1:E:441:THR:HG21	2.36	0.54
1:B:157:LYS:HB3	1:B:207:ASN:O	2.08	0.54
1:A:253:LEU:HD23	1:A:331:TYR:CD1	2.41	0.54
1:A:378:ALA:HB1	1:A:421:ARG:HH12	1.72	0.54
1:C:312:ARG:HG2	1:D:173:PHE:HB2	1.88	0.54
1:E:242:ILE:CG2	1:E:243:PRO:HD2	2.38	0.54
1:A:66:LYS:NZ	1:A:415:GLU:OE1	2.41	0.54
1:B:285:LLP:OP4	1:B:285:LLP:H4'1	2.07	0.54
1:E:197:VAL:HG22	1:E:228:VAL:HG13	1.88	0.54
1:A:129:GLU:OE2	1:B:29:LYS:HE3	2.07	0.54
1:B:220:TYR:CZ	1:C:222:GLU:HB2	2.43	0.54
1:D:75:ALA:HB3	1:D:420:CYS:HB3	1.90	0.54
1:D:221:MET:HG2	1:E:221:MET:HG2	1.90	0.54
1:D:107:LEU:O	1:D:122:HIS:HE1	1.90	0.54
1:B:126:TYR:CE2	1:B:325:GLU:HG3	2.42	0.54
1:B:146:VAL:HG12	1:B:147:PHE:N	2.22	0.54
1:C:100:ILE:HD12	1:D:69:ILE:CG2	2.37	0.54
1:A:308:ASN:C	1:A:308:ASN:OD1	2.46	0.53
1:D:452:ILE:HG23	1:D:452:ILE:OXT	2.07	0.53
1:C:11:ILE:O	1:C:15:VAL:HG23	2.07	0.53
1:C:377:LYS:HE2	1:C:389:GLU:HG2	1.89	0.53
1:B:216:LYS:HG2	1:B:219:PHE:CE1	2.44	0.53
1:E:404:SER:OG	1:E:425:ASP:HA	2.07	0.53
1:B:378:ALA:HB2	1:B:421:ARG:HH12	1.72	0.53
1:D:224:PHE:CD1	1:E:218:ASN:HB2	2.42	0.53
1:E:96:PHE:O	1:E:100:ILE:HG12	2.07	0.53
1:C:142:ASN:HB3	1:C:285:LLP:OP4	2.08	0.53
1:C:194:LYS:HZ1	1:C:224:PHE:HB3	1.73	0.53
1:A:420:CYS:SG	1:A:427:LEU:HD11	2.48	0.53
1:C:334:LYS:HD3	1:C:336:TYR:OH	2.09	0.53
1:D:90:SER:O	1:D:94:ILE:HG13	2.08	0.53
1:A:109:TYR:HD2	1:B:83:ASN:HB3	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:LEU:HD12	1:C:339:ILE:HG23	1.90	0.53
1:E:131:THR:O	1:E:269:ARG:HA	2.08	0.53
1:E:174:ARG:HB2	1:E:177:ASP:HB2	1.91	0.53
1:C:174:ARG:HB2	1:C:177:ASP:HB2	1.91	0.53
1:E:107:LEU:CD1	1:E:321:LEU:HD23	2.36	0.53
1:E:138:VAL:HG13	1:E:293:GLY:O	2.09	0.53
1:E:300:ASN:O	1:E:304:LYS:HG3	2.09	0.53
1:A:171:GLY:HA3	1:B:116:ARG:NH2	2.24	0.52
1:A:263:VAL:HG12	1:A:264:ASP:N	2.24	0.52
1:D:200:TYR:CE2	1:D:228:VAL:HG21	2.44	0.52
1:D:212:MET:HG3	1:D:245:TYR:HD1	1.74	0.52
1:E:452:ILE:HG23	1:E:452:ILE:OXT	2.09	0.52
1:A:171:GLY:HA3	1:B:116:ARG:HH22	1.74	0.52
1:A:312:ARG:CZ	1:A:315:ARG:NH2	2.72	0.52
1:B:74:ASN:OD1	1:B:74:ASN:C	2.47	0.52
1:B:166:LEU:O	1:C:191:THR:HB	2.10	0.52
1:C:333:GLU:OE1	1:C:335:ARG:HD2	2.10	0.52
1:B:236:LEU:O	1:B:239:LYS:HB3	2.10	0.52
1:B:366:ILE:HG23	1:B:367:PRO:HD2	1.91	0.52
1:D:179:MET:O	1:D:182:SER:HB3	2.10	0.52
1:A:239:LYS:HB3	1:A:240:TYR:CD2	2.45	0.52
1:B:211:LEU:HG	1:B:242:ILE:HG21	1.91	0.52
1:C:148:LEU:HG	1:C:305:ILE:HG23	1.91	0.52
1:C:404:SER:OG	1:C:425:ASP:HA	2.10	0.52
1:C:187:ARG:CD	1:C:203:ALA:HB1	2.39	0.52
1:E:179:MET:SD	1:E:186:LEU:HB2	2.49	0.52
1:A:425:ASP:CG	1:A:425:ASP:O	2.48	0.52
1:C:140:ASN:O	1:C:292:ALA:HA	2.10	0.52
1:C:302:ILE:HD13	1:C:305:ILE:HD12	1.92	0.52
1:C:407:LEU:HD23	1:C:427:LEU:HD22	1.92	0.52
1:D:348:ASP:O	1:D:351:ALA:HB3	2.10	0.51
1:C:186:LEU:HG	1:C:186:LEU:O	2.09	0.51
1:B:147:PHE:C	1:B:147:PHE:CD2	2.82	0.51
1:C:107:LEU:HD22	1:C:318:LYS:HD3	1.92	0.51
1:C:113:GLU:O	1:C:115:LYS:HG3	2.10	0.51
1:C:181:LYS:HG3	1:D:309:PRO:HG2	1.91	0.51
1:B:407:LEU:HD23	1:B:427:LEU:CD2	2.36	0.51
1:D:160:ILE:HB	1:D:211:LEU:HD23	1.92	0.51
1:E:110:ASN:ND2	1:E:113:GLU:OE1	2.42	0.51
1:B:34:VAL:O	1:B:38:TYR:HD1	1.93	0.51
1:C:366:ILE:HD11	1:C:447:GLN:HB3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:ILE:HD11	1:D:323:GLY:HA3	1.93	0.51
1:D:212:MET:HG3	1:D:245:TYR:CD1	2.46	0.51
1:D:353:ARG:HB2	1:D:393:TYR:CE2	2.45	0.51
1:A:285:LLP:OP3	1:B:312:ARG:NH2	2.31	0.51
1:B:221:MET:HA	1:C:220:TYR:O	2.11	0.51
1:B:287:LEU:C	1:B:287:LEU:HD23	2.31	0.51
1:C:420:CYS:HB2	1:C:428:LEU:O	2.10	0.51
1:E:77:GLY:HA3	1:E:430:ASP:OD2	2.10	0.51
1:B:404:SER:OG	1:B:425:ASP:HA	2.10	0.51
1:A:363:LEU:HB2	1:A:371:ILE:HD13	1.92	0.51
1:B:218:ASN:ND2	1:C:224:PHE:HB2	2.26	0.51
1:C:138:VAL:HG11	1:C:316:ILE:HD13	1.92	0.51
1:D:213:LYS:HD3	1:D:230:LEU:HD21	1.92	0.51
1:A:309:PRO:HG2	1:B:181:LYS:HG3	1.93	0.51
1:C:330:LEU:HD12	1:C:339:ILE:CG2	2.41	0.51
1:D:79:VAL:HG12	1:D:341:VAL:HG13	1.93	0.51
1:D:303:GLU:O	1:D:307:LYS:HG3	2.11	0.51
1:A:254:ILE:HD13	1:A:336:TYR:HE1	1.76	0.50
1:B:71:ARG:HG3	1:B:71:ARG:HH11	1.76	0.50
1:B:159:VAL:HG22	1:B:210:LEU:CB	2.41	0.50
1:B:208:THR:HG22	1:B:242:ILE:CD1	2.42	0.50
1:C:173:PHE:HB2	1:D:312:ARG:HG2	1.94	0.50
1:D:137:PHE:CE1	1:D:306:LYS:HG2	2.46	0.50
1:E:277:ASP:O	1:E:297:GLY:HA3	2.10	0.50
1:A:396:ALA:HB2	1:A:428:LEU:HD23	1.93	0.50
1:A:420:CYS:HB2	1:A:428:LEU:O	2.10	0.50
1:C:6:ARG:O	1:C:6:ARG:HG2	2.12	0.50
1:D:326:MET:O	1:D:330:LEU:HG	2.10	0.50
1:A:242:ILE:CG2	1:A:243:PRO:HD2	2.41	0.50
1:B:221:MET:HG2	1:C:221:MET:CG	2.39	0.50
1:D:224:PHE:HD1	1:E:218:ASN:HB2	1.76	0.50
1:B:25:ILE:HG13	1:B:26:TYR:CD2	2.46	0.50
1:C:252:LEU:HD13	1:C:286:LEU:CD1	2.42	0.50
1:C:344:MET:O	1:C:432:ARG:HD2	2.12	0.50
1:A:263:VAL:CG2	1:A:388:LEU:HD13	2.40	0.50
1:A:445:THR:O	1:A:449:LEU:HG	2.12	0.50
1:B:141:ASN:OD1	1:B:143:ALA:HB3	2.10	0.50
1:D:77:GLY:HA2	1:D:433:THR:HG23	1.94	0.50
1:E:285:LLP:NZ	1:E:285:LLP:O3	2.41	0.50
1:A:252:LEU:HD21	1:A:256:LEU:HB2	1.92	0.50
1:B:298:LYS:HB2	1:B:301:LEU:HD12	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:ASN:HB2	1:D:285:LLP:OP1	2.11	0.50
1:E:213:LYS:HD3	1:E:230:LEU:HD21	1.93	0.50
1:A:399:HIS:CE1	1:A:450:LEU:HD22	2.47	0.50
1:A:267:ASN:ND2	1:A:270:ASP:HB2	2.27	0.50
1:A:360:GLU:HG3	1:A:371:ILE:CG2	2.41	0.50
1:B:187:ARG:CD	1:B:203:ALA:HB1	2.42	0.50
1:B:425:ASP:CG	1:B:425:ASP:O	2.50	0.50
1:D:224:PHE:O	1:D:225:VAL:HG23	2.11	0.50
1:D:402:LEU:HD12	1:D:450:LEU:CD2	2.42	0.50
1:B:158:GLU:HA	1:B:185:ILE:O	2.12	0.49
1:B:220:TYR:OH	1:C:222:GLU:OE1	2.22	0.49
1:E:187:ARG:CD	1:E:203:ALA:HB1	2.42	0.49
1:E:234:VAL:HG22	1:E:276:ILE:HD13	1.93	0.49
1:E:388:LEU:HD12	1:E:389:GLU:H	1.77	0.49
1:B:189:VAL:HB	1:B:199:ASP:HB3	1.93	0.49
1:E:123:ILE:O	1:E:126:TYR:N	2.45	0.49
1:E:394:CYS:SG	1:E:421:ARG:NH2	2.86	0.49
1:E:443:LYS:O	1:E:447:GLN:HG2	2.12	0.49
1:C:3:SER:O	1:C:7:GLN:HG2	2.12	0.49
1:E:194:LYS:NZ	1:E:224:PHE:HB3	2.27	0.49
1:A:322:SER:O	1:A:325:GLU:N	2.43	0.49
1:B:308:ASN:OD1	1:B:308:ASN:C	2.51	0.49
1:C:107:LEU:HD23	1:D:85:GLY:HA2	1.94	0.49
1:D:107:LEU:CD1	1:D:321:LEU:HD23	2.42	0.49
1:D:142:ASN:HB3	1:D:285:LLP:OP4	2.12	0.49
1:D:344:MET:O	1:D:432:ARG:HD2	2.12	0.49
1:E:399:HIS:CE1	1:E:401:ARG:HB2	2.47	0.49
1:A:163:ARG:HG2	1:A:188:GLU:HB2	1.94	0.49
1:D:201:GLU:OE2	1:D:239:LYS:NZ	2.44	0.49
1:E:344:MET:SD	1:E:433:THR:HA	2.52	0.49
1:A:147:PHE:CE1	1:B:310:ILE:HD11	2.48	0.49
1:B:130:LEU:O	1:B:269:ARG:NH2	2.46	0.49
1:C:99:GLU:O	1:D:71:ARG:NH2	2.45	0.49
1:A:165:GLU:OE1	1:A:213:LYS:HG3	2.13	0.49
1:B:87:ALA:CB	1:B:341:VAL:HG21	2.43	0.49
1:B:395:VAL:O	1:B:395:VAL:HG12	2.12	0.49
1:C:420:CYS:SG	1:C:427:LEU:HD11	2.53	0.49
1:E:363:LEU:HD22	1:E:366:ILE:HD12	1.95	0.49
1:B:396:ALA:HB2	1:B:428:LEU:HD23	1.95	0.49
1:E:72:VAL:HG22	1:E:417:PRO:HG2	1.95	0.49
1:A:87:ALA:HB2	1:A:341:VAL:HG21	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ARG:O	1:B:43:ILE:HG13	2.13	0.49
1:B:147:PHE:CD2	1:B:147:PHE:O	2.66	0.49
1:B:254:ILE:HD11	1:B:259:PHE:CE2	2.47	0.49
1:E:330:LEU:CD2	1:E:335:ARG:HD3	2.42	0.49
1:A:358:ARG:NH2	1:A:439:LEU:HD12	2.21	0.49
1:D:123:ILE:HG12	1:D:321:LEU:HD11	1.95	0.49
1:D:163:ARG:HG2	1:D:188:GLU:HB2	1.95	0.49
1:B:87:ALA:HB2	1:B:341:VAL:HG21	1.94	0.48
1:E:159:VAL:HG13	1:E:210:LEU:O	2.12	0.48
1:A:102:ASN:HB3	1:B:71:ARG:HH22	1.79	0.48
1:B:428:LEU:C	1:B:429:PHE:HD1	2.17	0.48
1:D:388:LEU:HG	1:D:389:GLU:N	2.28	0.48
1:E:402:LEU:HD12	1:E:450:LEU:CD2	2.44	0.48
1:C:12:SER:O	1:C:15:VAL:HB	2.13	0.48
1:C:190:GLY:HA2	1:C:199:ASP:OD2	2.13	0.48
1:C:272:ILE:HD11	1:C:296:VAL:HG23	1.95	0.48
1:A:165:GLU:OE2	1:A:213:LYS:NZ	2.42	0.48
1:B:13:LYS:O	1:B:17:ILE:HG13	2.14	0.48
1:C:79:VAL:HG21	1:C:345:LEU:HD23	1.94	0.48
1:C:187:ARG:HD3	1:C:203:ALA:HB1	1.94	0.48
1:A:267:ASN:HD21	1:A:270:ASP:HB2	1.78	0.48
1:B:254:ILE:HD12	1:B:259:PHE:HE2	1.79	0.48
1:B:339:ILE:HA	1:B:340:PRO:HD3	1.74	0.48
1:B:411:LEU:HD22	1:B:418:ILE:HD12	1.96	0.48
1:D:298:LYS:O	1:D:302:ILE:HG12	2.13	0.48
1:B:11:ILE:HG21	1:B:28:VAL:HG13	1.96	0.48
1:B:79:VAL:HG21	1:B:345:LEU:HD23	1.95	0.48
1:C:312:ARG:HH12	1:D:285:LLP:P	2.37	0.48
1:C:363:LEU:HD21	1:C:443:LYS:HA	1.95	0.48
1:A:191:THR:O	1:A:192:THR:C	2.51	0.48
1:B:163:ARG:HD2	1:B:190:GLY:O	2.14	0.48
1:B:191:THR:O	1:B:192:THR:C	2.51	0.48
1:D:195:THR:HG22	1:D:228:VAL:HG23	1.95	0.48
1:B:102:ASN:O	1:B:102:ASN:OD1	2.32	0.48
1:C:339:ILE:HD11	1:C:342:ILE:HG13	1.94	0.48
1:D:79:VAL:CG1	1:D:341:VAL:HG13	2.43	0.48
1:A:317:ASP:OD2	1:B:317:ASP:OD2	2.31	0.48
1:B:239:LYS:HD3	1:B:240:TYR:CE2	2.49	0.48
1:B:374:ILE:HD11	1:B:428:LEU:CD2	2.42	0.48
1:B:390:LEU:CB	1:B:432:ARG:HH22	2.24	0.48
1:C:27:VAL:HG13	1:C:61:ILE:HD11	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:GLU:O	1:C:168:GLU:HG2	2.13	0.48
1:C:263:VAL:HG23	1:C:265:GLU:H	1.79	0.48
1:A:27:VAL:HG13	1:A:61:ILE:HD11	1.96	0.48
1:A:317:ASP:OD1	1:A:320:THR:HG23	2.13	0.48
1:B:219:PHE:CE2	1:C:193:ASN:HB3	2.49	0.48
1:C:42:ILE:HD11	1:C:50:LEU:CD2	2.42	0.48
1:D:408:SER:OG	1:D:422:ILE:HD11	2.14	0.48
1:B:116:ARG:HG3	1:B:117:GLY:H	1.78	0.47
1:B:218:ASN:HB2	1:C:224:PHE:CD1	2.49	0.47
1:B:25:ILE:HG13	1:B:26:TYR:HD2	1.78	0.47
1:C:74:ASN:O	1:C:433:THR:OG1	2.27	0.47
1:D:191:THR:HG22	1:E:176:PRO:HG3	1.95	0.47
1:D:351:ALA:O	1:D:354:GLN:HB3	2.15	0.47
1:A:77:GLY:CA	1:A:430:ASP:HB3	2.44	0.47
1:A:161:ILE:HG23	1:A:166:LEU:HD21	1.95	0.47
1:A:396:ALA:HB2	1:A:428:LEU:CD2	2.45	0.47
1:C:143:ALA:N	1:C:285:LLP:H5'2	2.30	0.47
1:E:175:ILE:N	1:E:176:PRO:HD2	2.29	0.47
1:E:344:MET:O	1:E:432:ARG:HD2	2.14	0.47
1:B:312:ARG:CD	1:B:315:ARG:NH1	2.78	0.47
1:B:444:LYS:NZ	1:B:448:GLU:OE1	2.46	0.47
1:C:93:VAL:HG12	1:C:94:ILE:N	2.29	0.47
1:D:102:ASN:OD1	1:D:102:ASN:O	2.33	0.47
1:E:333:GLU:HB2	1:E:335:ARG:HG3	1.97	0.47
1:C:179:MET:SD	1:C:186:LEU:HD13	2.54	0.47
1:C:301:LEU:HD23	1:C:301:LEU:HA	1.66	0.47
1:D:79:VAL:HG21	1:D:345:LEU:HG	1.97	0.47
1:D:336:TYR:HB3	1:D:342:ILE:HG21	1.96	0.47
1:A:107:LEU:HD23	1:B:85:GLY:HA2	1.97	0.47
1:A:144:GLY:HA2	1:B:313:ALA:HB1	1.97	0.47
1:B:11:ILE:O	1:B:15:VAL:HG23	2.15	0.47
1:B:106:ASN:HB2	1:B:109:TYR:O	2.15	0.47
1:B:143:ALA:N	1:B:285:LLP:H5'2	2.30	0.47
1:C:77:GLY:HA3	1:C:430:ASP:HB3	1.96	0.47
1:C:317:ASP:OD1	1:C:320:THR:HG23	2.14	0.47
1:C:319:LEU:HD12	1:D:320:THR:HG22	1.96	0.47
1:C:366:ILE:CG2	1:C:367:PRO:HD2	2.41	0.47
1:A:320:THR:HG22	1:B:319:LEU:HD12	1.97	0.47
1:B:200:TYR:HE2	1:B:228:VAL:CG2	2.28	0.47
1:C:39:ARG:O	1:C:43:ILE:HG13	2.15	0.47
1:E:396:ALA:CB	1:E:428:LEU:HD23	2.41	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:ILE:HG23	1:C:179:MET:N	2.29	0.47
1:C:189:VAL:HB	1:C:199:ASP:HB3	1.96	0.47
1:C:358:ARG:O	1:C:362:LEU:HG	2.15	0.47
1:D:427:LEU:HD23	1:D:429:PHE:HE1	1.80	0.47
1:E:160:ILE:HG23	1:E:189:VAL:CG1	2.45	0.47
1:A:169:ILE:HD11	1:A:285:LLP:H5'1	1.96	0.46
1:B:71:ARG:HG3	1:B:71:ARG:NH1	2.30	0.46
1:C:268:PHE:O	1:C:269:ARG:C	2.54	0.46
1:A:93:VAL:HA	1:A:326:MET:HG2	1.97	0.46
1:C:313:ALA:HB1	1:D:144:GLY:CA	2.46	0.46
1:A:343:ARG:O	1:A:347:GLN:HG3	2.15	0.46
1:C:194:LYS:HG2	1:C:226:GLU:CB	2.41	0.46
1:D:217:SER:O	1:D:386:PRO:HD3	2.16	0.46
1:E:76:THR:OG1	1:E:78:VAL:HG23	2.15	0.46
1:E:107:LEU:O	1:E:122:HIS:CE1	2.61	0.46
1:A:116:ARG:HH22	1:B:171:GLY:HA3	1.80	0.46
1:A:129:GLU:OE1	1:B:29:LYS:NZ	2.40	0.46
1:A:186:LEU:HD12	1:A:187:ARG:N	2.30	0.46
1:B:175:ILE:N	1:B:176:PRO:HD2	2.31	0.46
1:B:178:ILE:HG22	1:B:179:MET:H	1.79	0.46
1:C:70:LYS:O	1:C:72:VAL:HG23	2.16	0.46
1:C:77:GLY:CA	1:C:433:THR:HG23	2.44	0.46
1:C:193:ASN:HB2	1:C:224:PHE:O	2.15	0.46
1:E:161:ILE:HG21	1:E:166:LEU:CD2	2.44	0.46
1:A:147:PHE:HE1	1:B:310:ILE:HD11	1.79	0.46
1:C:362:LEU:O	1:C:443:LYS:HG3	2.14	0.46
1:D:352:LEU:HD13	1:D:392:THR:OG1	2.15	0.46
1:A:42:ILE:HD11	1:A:50:LEU:HD21	1.97	0.46
1:A:67:PRO:HG2	1:B:96:PHE:CE1	2.50	0.46
1:D:153:LEU:HD11	1:D:301:LEU:HD22	1.97	0.46
1:D:165:GLU:HB3	1:D:214:VAL:HB	1.98	0.46
1:D:312:ARG:NH1	1:D:315:ARG:NH2	2.64	0.46
1:D:318:LYS:HB3	1:D:318:LYS:HE2	1.63	0.46
1:E:366:ILE:CG2	1:E:367:PRO:HD2	2.45	0.46
1:A:107:LEU:CD2	1:B:85:GLY:HA2	2.46	0.46
1:B:143:ALA:O	1:B:146:VAL:HB	2.16	0.46
1:E:388:LEU:HD11	1:E:390:LEU:HG	1.96	0.46
1:A:85:GLY:O	1:A:86:ARG:C	2.54	0.46
1:A:106:ASN:O	1:A:107:LEU:C	2.54	0.46
1:A:405:GLN:HE22	1:A:422:ILE:HG21	1.80	0.46
1:C:160:ILE:HA	1:C:187:ARG:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:404:SER:OG	1:D:425:ASP:HA	2.15	0.46
1:A:26:TYR:CE2	1:B:333:GLU:OE2	2.69	0.46
1:B:452:ILE:OXT	1:B:452:ILE:CG2	2.64	0.46
1:A:69:ILE:CG2	1:B:100:ILE:HD12	2.35	0.46
1:A:79:VAL:HG21	1:A:345:LEU:CD2	2.46	0.46
1:B:142:ASN:O	1:B:143:ALA:C	2.55	0.46
1:B:252:LEU:HD12	1:B:253:LEU:H	1.81	0.46
1:C:219:PHE:O	1:C:220:TYR:HB3	2.16	0.46
1:D:159:VAL:HG13	1:D:210:LEU:HB3	1.98	0.46
1:D:216:LYS:HG2	1:D:219:PHE:CE2	2.50	0.46
1:D:251:GLY:CA	1:D:268:PHE:HE2	2.28	0.46
1:A:361:LYS:HA	1:A:364:LYS:HE3	1.98	0.45
1:B:239:LYS:HD3	1:B:240:TYR:HE2	1.81	0.45
1:B:264:ASP:O	1:B:265:GLU:C	2.53	0.45
1:B:352:LEU:HD13	1:B:392:THR:HA	1.98	0.45
1:B:378:ALA:CB	1:B:421:ARG:HH12	2.28	0.45
1:D:90:SER:HB3	1:D:338:ASP:O	2.16	0.45
1:A:332:PHE:CZ	1:B:29:LYS:HD3	2.50	0.45
1:A:353:ARG:HB2	1:A:393:TYR:CE2	2.51	0.45
1:B:90:SER:CB	1:B:338:ASP:O	2.60	0.45
1:B:220:TYR:O	1:C:221:MET:HA	2.16	0.45
1:D:159:VAL:HG22	1:D:210:LEU:HB3	1.97	0.45
1:E:194:LYS:HG2	1:E:226:GLU:HB2	1.97	0.45
1:A:194:LYS:HG2	1:A:226:GLU:CB	2.45	0.45
1:B:286:LEU:HD23	1:B:286:LEU:HA	1.73	0.45
1:C:126:TYR:CE2	1:C:325:GLU:HG3	2.51	0.45
1:C:252:LEU:HA	1:C:252:LEU:HD12	1.59	0.45
1:A:300:ASN:O	1:A:304:LYS:HG3	2.16	0.45
1:B:88:PRO:O	1:B:340:PRO:HG2	2.16	0.45
1:B:179:MET:HA	1:B:182:SER:HB3	1.99	0.45
1:C:363:LEU:HB2	1:C:371:ILE:HD13	1.99	0.45
1:D:131:THR:CG2	1:D:268:PHE:HB3	2.46	0.45
1:D:264:ASP:O	1:D:265:GLU:C	2.53	0.45
1:D:120:ILE:O	1:D:120:ILE:HG22	2.17	0.45
1:D:268:PHE:O	1:D:269:ARG:C	2.54	0.45
1:D:339:ILE:O	1:D:339:ILE:HG13	2.17	0.45
1:A:69:ILE:HG12	1:B:122:HIS:ND1	2.31	0.45
1:A:107:LEU:HD22	1:A:318:LYS:HD3	1.97	0.45
1:B:142:ASN:HD22	1:B:285:LLP:C6	2.30	0.45
1:B:154:ALA:O	1:B:184:ALA:HA	2.16	0.45
1:A:277:ASP:O	1:A:297:GLY:HA3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:LEU:HG	1:B:301:LEU:HD13	1.99	0.45
1:C:27:VAL:HG22	1:C:61:ILE:HD13	1.98	0.45
1:D:179:MET:HB2	1:D:179:MET:HE3	1.53	0.45
1:D:208:THR:HG22	1:D:242:ILE:CD1	2.37	0.45
1:D:218:ASN:ND2	1:E:224:PHE:HB2	2.32	0.45
1:C:120:ILE:HG13	1:C:137:PHE:HE1	1.82	0.45
1:E:363:LEU:HB2	1:E:371:ILE:CD1	2.46	0.45
1:A:252:LEU:HD22	1:A:286:LEU:HD13	1.99	0.45
1:C:138:VAL:CG1	1:C:316:ILE:HD13	2.46	0.45
1:A:317:ASP:OD1	1:A:319:LEU:HB2	2.17	0.44
1:C:61:ILE:O	1:C:65:MET:HG3	2.16	0.44
1:D:157:LYS:HB3	1:D:207:ASN:O	2.18	0.44
1:D:339:ILE:HA	1:D:340:PRO:HD3	1.81	0.44
1:A:77:GLY:HA3	1:A:430:ASP:CB	2.47	0.44
1:C:148:LEU:HG	1:C:305:ILE:CG2	2.47	0.44
1:D:71:ARG:HG2	1:D:72:VAL:N	2.33	0.44
1:E:109:TYR:CD1	1:E:111:LEU:HD23	2.52	0.44
1:A:147:PHE:HB2	1:A:178:ILE:HD11	2.00	0.44
1:B:194:LYS:HD3	1:C:168:GLU:OE2	2.18	0.44
1:C:251:GLY:HA2	1:C:268:PHE:CE2	2.52	0.44
1:D:80:ILE:HD11	1:D:341:VAL:HG11	2.00	0.44
1:D:343:ARG:O	1:D:347:GLN:HG3	2.17	0.44
1:E:60:LYS:O	1:E:64:LEU:HG	2.17	0.44
1:E:315:ARG:HE	1:E:315:ARG:HB3	1.48	0.44
1:C:153:LEU:HD21	1:C:301:LEU:HD22	1.99	0.44
1:D:179:MET:HA	1:D:182:SER:HB3	2.00	0.44
1:A:161:ILE:CG2	1:A:161:ILE:O	2.66	0.44
1:A:255:ASN:ND2	1:A:270:ASP:OD2	2.50	0.44
1:C:211:LEU:HG	1:C:242:ILE:HG21	2.00	0.44
1:E:363:LEU:CB	1:E:371:ILE:CD1	2.96	0.44
1:A:331:TYR:CZ	1:A:339:ILE:CD1	3.01	0.44
1:C:280:SER:HA	1:C:294:ILE:O	2.18	0.44
1:E:152:THR:HG21	1:E:305:ILE:HA	1.99	0.44
1:E:416:PRO:HG3	1:E:441:THR:HG21	2.00	0.44
1:A:252:LEU:O	1:A:268:PHE:HD2	1.99	0.44
1:A:339:ILE:HA	1:A:340:PRO:HD3	1.74	0.44
1:A:360:GLU:HG3	1:A:371:ILE:HG21	2.00	0.44
1:D:399:HIS:HE1	1:D:401:ARG:HB2	1.73	0.44
1:E:191:THR:O	1:E:192:THR:C	2.56	0.44
1:B:254:ILE:CD1	1:B:259:PHE:CE2	2.98	0.44
1:D:272:ILE:HD13	1:D:272:ILE:HA	1.86	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:187:ARG:HD3	1:E:203:ALA:HB1	1.99	0.44
1:E:326:MET:O	1:E:330:LEU:HG	2.18	0.44
1:A:201:GLU:OE2	1:A:240:TYR:OH	2.23	0.44
1:A:377:LYS:HE2	1:A:389:GLU:OE2	2.17	0.44
1:C:33:GLU:OE1	1:C:60:LYS:HD2	2.18	0.44
1:C:213:LYS:NZ	1:C:227:GLU:OE2	2.45	0.44
1:E:125:LYS:O	1:E:129:GLU:HG3	2.18	0.44
1:E:159:VAL:HG22	1:E:210:LEU:HB3	2.00	0.44
1:A:173:PHE:HB2	1:B:312:ARG:HG2	2.00	0.43
1:A:399:HIS:ND1	1:A:401:ARG:HB2	2.33	0.43
1:A:404:SER:OG	1:A:425:ASP:HA	2.18	0.43
1:B:247:ASP:OD1	1:B:247:ASP:C	2.57	0.43
1:B:252:LEU:HD21	1:B:256:LEU:HB2	1.99	0.43
1:C:256:LEU:HD12	1:C:256:LEU:O	2.17	0.43
1:C:321:LEU:HD12	1:C:321:LEU:C	2.37	0.43
1:D:380:PRO:HD2	1:D:388:LEU:HD23	2.00	0.43
1:E:324:LEU:O	1:E:328:LEU:HG	2.18	0.43
1:E:400:ASP:OD1	1:E:401:ARG:N	2.51	0.43
1:B:388:LEU:HD12	1:B:388:LEU:HA	1.81	0.43
1:B:169:ILE:O	1:B:169:ILE:HG13	2.18	0.43
1:C:309:PRO:HG2	1:D:181:LYS:HG3	2.00	0.43
1:A:194:LYS:HG2	1:A:226:GLU:N	2.33	0.43
1:A:254:ILE:HD13	1:A:336:TYR:CE1	2.53	0.43
1:A:427:LEU:HD23	1:A:429:PHE:HE1	1.83	0.43
1:C:368:GLY:C	1:C:399:HIS:CD2	2.92	0.43
1:D:66:LYS:HA	1:D:67:PRO:HD3	1.67	0.43
1:A:148:LEU:HD23	1:A:305:ILE:CG2	2.48	0.43
1:B:173:PHE:HE2	1:B:175:ILE:HD13	1.83	0.43
1:C:191:THR:O	1:C:192:THR:C	2.56	0.43
1:D:194:LYS:HE3	1:D:224:PHE:HB3	2.01	0.43
1:E:109:TYR:OH	1:E:114:GLY:O	2.36	0.43
1:B:178:ILE:CG2	1:B:179:MET:H	2.30	0.43
1:B:200:TYR:CD2	1:B:228:VAL:HG21	2.53	0.43
1:C:379:LYS:HA	1:C:380:PRO:HD3	1.72	0.43
1:D:176:PRO:HG3	1:E:191:THR:CG2	2.46	0.43
1:E:261:ILE:HG22	1:E:263:VAL:HG13	2.00	0.43
1:A:84:LEU:HB3	1:B:104:TYR:HB3	2.01	0.43
1:C:162:SER:HB2	1:C:200:TYR:OH	2.18	0.43
1:C:216:LYS:HE2	1:C:216:LYS:HB2	1.85	0.43
1:D:141:ASN:OD1	1:D:143:ALA:HB3	2.18	0.43
1:E:137:PHE:CD1	1:E:306:LYS:HG2	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:358:ARG:HH21	1:E:439:LEU:HD12	1.83	0.43
1:B:141:ASN:HB2	1:B:285:LLP:OP1	2.18	0.43
1:B:385:LEU:HA	1:B:385:LEU:HD23	1.68	0.43
1:C:291:GLN:O	1:C:291:GLN:HG2	2.18	0.43
1:A:187:ARG:CZ	1:A:203:ALA:HB1	2.49	0.43
1:A:246:TYR:O	1:A:279:VAL:HA	2.18	0.43
1:A:251:GLY:CA	1:A:268:PHE:HE2	2.28	0.43
1:B:79:VAL:HG21	1:B:345:LEU:CD2	2.49	0.43
1:B:141:ASN:O	1:B:293:GLY:HA3	2.19	0.43
1:B:399:HIS:HE1	1:B:401:ARG:HB2	1.82	0.43
1:D:123:ILE:CD1	1:D:325:GLU:HB2	2.49	0.43
1:E:145:ALA:O	1:E:149:VAL:HG23	2.19	0.43
1:E:278:LEU:HD23	1:E:278:LEU:HA	1.93	0.43
1:E:355:LYS:HD3	1:E:436:HIS:HE1	1.76	0.43
1:E:396:ALA:HB1	1:E:426:GLN:CD	2.39	0.43
1:A:80:ILE:HB	1:A:382:GLY:H	1.84	0.42
1:D:420:CYS:HB2	1:D:428:LEU:O	2.19	0.42
1:E:257:LYS:HA	1:E:261:ILE:O	2.19	0.42
1:A:161:ILE:HG23	1:A:161:ILE:O	2.18	0.42
1:B:188:GLU:H	1:B:188:GLU:HG2	1.29	0.42
1:C:83:ASN:HB3	1:D:109:TYR:CD2	2.42	0.42
1:C:107:LEU:O	1:C:122:HIS:CE1	2.65	0.42
1:C:169:ILE:HG22	1:C:218:ASN:OD1	2.19	0.42
1:C:363:LEU:O	1:C:371:ILE:HD11	2.19	0.42
1:D:216:LYS:HE2	1:D:216:LYS:HB2	1.83	0.42
1:D:339:ILE:HG13	1:D:342:ILE:HB	2.01	0.42
1:A:102:ASN:OD1	1:A:102:ASN:C	2.57	0.42
1:A:399:HIS:CD2	1:A:450:LEU:HD13	2.54	0.42
1:B:120:ILE:O	1:B:120:ILE:CG2	2.66	0.42
1:C:77:GLY:CA	1:C:430:ASP:HB3	2.49	0.42
1:D:316:ILE:H	1:D:316:ILE:HG12	1.55	0.42
1:E:231:GLU:O	1:E:235:LYS:HG3	2.19	0.42
1:A:268:PHE:HD2	1:A:268:PHE:H	1.67	0.42
1:C:247:ASP:C	1:C:247:ASP:OD1	2.56	0.42
1:C:373:VAL:HG22	1:C:395:VAL:HG22	2.01	0.42
1:D:168:GLU:OE2	1:E:196:LYS:NZ	2.50	0.42
1:D:300:ASN:OD1	1:D:301:LEU:N	2.52	0.42
1:E:303:GLU:O	1:E:307:LYS:HG3	2.19	0.42
1:A:26:TYR:OH	1:B:329:LYS:HE2	2.19	0.42
1:B:240:TYR:N	1:B:240:TYR:CD2	2.88	0.42
1:C:7:GLN:HB2	1:C:50:LEU:CD1	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:ILE:CD1	1:C:447:GLN:HB3	2.49	0.42
1:D:265:GLU:CG	1:D:266:PRO:HD2	2.50	0.42
1:E:123:ILE:CD1	1:E:321:LEU:HD12	2.49	0.42
1:A:375:LYS:HB2	1:A:393:TYR:CE1	2.55	0.42
1:A:414:ALA:HB1	1:A:445:THR:HG21	2.02	0.42
1:C:252:LEU:HD13	1:C:286:LEU:CB	2.49	0.42
1:C:363:LEU:HD22	1:C:366:ILE:HD12	2.02	0.42
1:D:191:THR:O	1:D:192:THR:C	2.58	0.42
1:C:178:ILE:HG22	1:C:179:MET:N	2.34	0.42
1:B:310:ILE:HG21	1:B:310:ILE:HD13	1.71	0.42
1:B:336:TYR:O	1:B:338:ASP:N	2.53	0.42
1:C:147:PHE:CD2	1:C:147:PHE:C	2.93	0.42
1:C:402:LEU:HD22	1:C:406:GLU:HG2	2.02	0.42
1:D:87:ALA:HB2	1:D:341:VAL:HG21	2.02	0.42
1:D:381:GLY:HA3	1:D:385:LEU:HB2	2.01	0.42
1:D:392:THR:HG21	1:D:430:ASP:OD2	2.20	0.42
1:A:26:TYR:CD2	1:A:65:MET:HG2	2.55	0.42
1:B:110:ASN:C	1:B:110:ASN:OD1	2.56	0.42
1:C:89:LEU:HD12	1:D:101:ALA:HB1	2.02	0.42
1:E:377:LYS:HE2	1:E:389:GLU:OE2	2.19	0.42
1:A:174:ARG:HB2	1:A:177:ASP:HB2	2.02	0.42
1:A:310:ILE:CD1	1:B:147:PHE:HE1	2.33	0.42
1:B:110:ASN:OD1	1:B:111:LEU:N	2.52	0.42
1:B:158:GLU:OE2	1:B:187:ARG:HD2	2.20	0.42
1:C:20:LYS:O	1:C:20:LYS:HG2	2.20	0.42
1:D:107:LEU:HD11	1:D:321:LEU:HD23	2.01	0.42
1:A:388:LEU:HD12	1:A:388:LEU:HA	1.92	0.41
1:B:116:ARG:CG	1:B:117:GLY:N	2.82	0.41
1:C:63:SER:HA	1:C:66:LYS:HD2	2.01	0.41
1:C:165:GLU:HG2	1:C:214:VAL:O	2.20	0.41
1:C:197:VAL:HG23	1:C:228:VAL:HG13	2.02	0.41
1:C:363:LEU:CD1	1:C:446:LEU:HD12	2.49	0.41
1:C:104:TYR:CE2	1:D:74:ASN:ND2	2.86	0.41
1:D:139:VAL:HB	1:D:314:LEU:HB3	2.03	0.41
1:A:210:LEU:CD1	1:A:243:PRO:HG2	2.48	0.41
1:A:348:ASP:O	1:A:351:ALA:HB3	2.20	0.41
1:B:84:LEU:HA	1:B:84:LEU:HD23	1.81	0.41
1:C:75:ALA:CB	1:C:420:CYS:HB3	2.44	0.41
1:C:270:ASP:O	1:C:274:LEU:HG	2.20	0.41
1:D:125:LYS:O	1:D:129:GLU:HG3	2.20	0.41
1:D:137:PHE:CD1	1:D:306:LYS:HG2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:ILE:CG2	1:D:243:PRO:HD2	2.44	0.41
1:E:77:GLY:HA3	1:E:430:ASP:CB	2.50	0.41
1:E:200:TYR:HE2	1:E:228:VAL:HG21	1.77	0.41
1:E:405:GLN:NE2	1:E:422:ILE:HG21	2.33	0.41
1:E:415:GLU:HA	1:E:416:PRO:HA	1.89	0.41
1:A:268:PHE:N	1:A:268:PHE:CD2	2.89	0.41
1:A:302:ILE:CG2	1:A:306:LYS:HE3	2.51	0.41
1:A:312:ARG:HB2	1:B:172:SER:OG	2.21	0.41
1:B:77:GLY:HA3	1:B:430:ASP:CB	2.50	0.41
1:D:301:LEU:O	1:D:305:ILE:HG13	2.20	0.41
1:D:353:ARG:N	1:D:393:TYR:CD2	2.88	0.41
1:E:254:ILE:HD11	1:E:259:PHE:CZ	2.52	0.41
1:E:369:LEU:HD23	1:E:369:LEU:HA	1.84	0.41
1:A:86:ARG:HB3	1:A:284:ASP:O	2.19	0.41
1:A:105:SER:O	1:B:84:LEU:HA	2.20	0.41
1:B:318:LYS:HE2	1:B:318:LYS:HB3	1.77	0.41
1:C:139:VAL:HB	1:C:314:LEU:HB3	2.02	0.41
1:C:257:LYS:HG2	1:C:262:SER:HA	2.03	0.41
1:D:270:ASP:O	1:D:274:LEU:HG	2.20	0.41
1:E:339:ILE:HA	1:E:340:PRO:HD3	1.81	0.41
1:E:407:LEU:HD23	1:E:427:LEU:HD22	2.03	0.41
1:A:107:LEU:CD1	1:A:318:LYS:HG3	2.50	0.41
1:A:342:ILE:HD13	1:A:342:ILE:HA	1.79	0.41
1:B:77:GLY:HA2	1:B:433:THR:HG23	2.02	0.41
1:B:216:LYS:HE2	1:B:216:LYS:HB2	1.88	0.41
1:C:308:ASN:HA	1:C:309:PRO:HD2	1.82	0.41
1:E:178:ILE:HG23	1:E:179:MET:N	2.36	0.41
1:A:321:LEU:O	1:A:324:LEU:HB3	2.20	0.41
1:B:107:LEU:O	1:B:122:HIS:CE1	2.74	0.41
1:C:178:ILE:O	1:C:179:MET:C	2.58	0.41
1:C:303:GLU:O	1:C:307:LYS:HG3	2.21	0.41
1:C:368:GLY:O	1:C:399:HIS:CD2	2.74	0.41
1:D:211:LEU:HD23	1:D:211:LEU:HA	1.92	0.41
1:D:411:LEU:HD23	1:D:411:LEU:HA	1.83	0.41
1:E:80:ILE:HD12	1:E:285:LLP:HA	2.02	0.41
1:A:369:LEU:HA	1:A:369:LEU:HD23	1.81	0.41
1:C:104:TYR:HB3	1:D:84:LEU:HB3	2.02	0.41
1:D:141:ASN:O	1:D:293:GLY:HA3	2.20	0.41
1:D:165:GLU:OE2	1:D:213:LYS:NZ	2.50	0.41
1:D:452:ILE:OXT	1:D:452:ILE:CG2	2.69	0.41
1:A:234:VAL:CG1	1:A:238:HIS:CD2	3.04	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:LEU:HD23	1:A:278:LEU:HA	1.95	0.41
1:B:30:ALA:O	1:B:34:VAL:HG23	2.21	0.41
1:B:78:VAL:HG13	1:B:380:PRO:O	2.21	0.41
1:B:153:LEU:HD11	1:B:301:LEU:HD22	2.01	0.41
1:B:353:ARG:O	1:B:356:ALA:N	2.54	0.41
1:C:154:ALA:O	1:C:155:GLU:C	2.58	0.41
1:C:163:ARG:HG3	1:C:189:VAL:O	2.21	0.41
1:C:204:ILE:HG22	1:C:205:ASN:N	2.36	0.41
1:C:402:LEU:HD12	1:C:450:LEU:CD2	2.50	0.41
1:D:123:ILE:HD11	1:D:325:GLU:HB2	2.03	0.41
1:D:252:LEU:O	1:D:268:PHE:HD2	2.04	0.41
1:E:71:ARG:HG2	1:E:72:VAL:N	2.36	0.41
1:E:126:TYR:HE2	1:E:325:GLU:OE2	2.04	0.41
1:E:142:ASN:O	1:E:143:ALA:C	2.59	0.41
1:E:234:VAL:HG12	1:E:238:HIS:CD2	2.56	0.41
1:A:87:ALA:CB	1:A:341:VAL:HG21	2.51	0.41
1:A:127:LEU:HA	1:A:127:LEU:HD23	1.75	0.41
1:A:309:PRO:CG	1:B:181:LYS:HG3	2.51	0.41
1:A:312:ARG:HG2	1:B:173:PHE:HB2	2.03	0.41
1:C:242:ILE:HG23	1:C:243:PRO:HD2	2.03	0.41
1:C:299:LYS:O	1:C:300:ASN:C	2.59	0.41
1:A:76:THR:HG1	1:A:78:VAL:HG23	1.81	0.40
1:A:96:PHE:CZ	1:B:67:PRO:HB3	2.56	0.40
1:A:156:GLY:C	1:A:185:ILE:HD12	2.41	0.40
1:C:452:ILE:OXT	1:C:452:ILE:HG23	2.22	0.40
1:A:204:ILE:HG22	1:A:205:ASN:N	2.36	0.40
1:C:83:ASN:HA	1:D:108:GLU:HB2	2.02	0.40
1:C:399:HIS:CD2	1:C:450:LEU:HD13	2.56	0.40
1:E:66:LYS:HA	1:E:67:PRO:HD3	1.94	0.40
1:A:34:VAL:HG12	1:A:53:PHE:CE1	2.56	0.40
1:B:396:ALA:HB2	1:B:428:LEU:CD2	2.52	0.40
1:B:420:CYS:SG	1:B:427:LEU:HD11	2.61	0.40
1:C:55:GLU:O	1:C:59:ARG:HG3	2.21	0.40
1:C:98:SER:HA	1:D:94:ILE:CG2	2.52	0.40
1:D:196:LYS:N	1:D:199:ASP:OD2	2.47	0.40
1:A:234:VAL:HG12	1:A:238:HIS:HD2	1.82	0.40
1:B:230:LEU:HD22	1:B:276:ILE:HD11	2.02	0.40
1:B:359:LEU:HB2	1:B:439:LEU:HD22	2.03	0.40
1:C:73:ILE:HD12	1:C:416:PRO:CG	2.51	0.40
1:C:88:PRO:HG3	1:D:104:TYR:CE1	2.56	0.40
1:C:282:SER:OG	1:C:285:LLP:OP4	2.40	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:139:VAL:HB	1:E:314:LEU:HB3	2.03	0.40
1:E:213:LYS:HD3	1:E:230:LEU:CD2	2.52	0.40
1:A:89:LEU:HD23	1:A:89:LEU:HA	1.88	0.40
1:A:148:LEU:CD2	1:A:305:ILE:CG2	2.99	0.40
1:C:72:VAL:HG22	1:C:417:PRO:CG	2.50	0.40
1:C:396:ALA:HB2	1:C:428:LEU:CD2	2.52	0.40
1:D:77:GLY:HA3	1:D:430:ASP:CG	2.41	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	449/452 (99%)	417 (93%)	29 (6%)	3 (1%)	22	60
1	B	440/452 (97%)	403 (92%)	31 (7%)	6 (1%)	11	46
1	C	449/452 (99%)	409 (91%)	36 (8%)	4 (1%)	17	54
1	D	392/452 (87%)	366 (93%)	22 (6%)	4 (1%)	15	52
1	E	396/452 (88%)	374 (94%)	22 (6%)	0	100	100
All	All	2126/2260 (94%)	1969 (93%)	140 (7%)	17 (1%)	19	57

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	ARG
1	B	107	LEU
1	C	192	THR
1	A	107	LEU
1	A	192	THR
1	C	86	ARG
1	C	107	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	147	PHE
1	B	192	THR
1	D	147	PHE
1	D	86	ARG
1	B	116	ARG
1	B	334	LYS
1	D	107	LEU
1	D	192	THR
1	B	143	ALA
1	C	309	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	390/390 (100%)	384 (98%)	6 (2%)	65	80
1	B	381/390 (98%)	375 (98%)	6 (2%)	62	79
1	C	390/390 (100%)	387 (99%)	3 (1%)	81	89
1	D	342/390 (88%)	338 (99%)	4 (1%)	71	83
1	E	346/390 (89%)	344 (99%)	2 (1%)	86	91
All	All	1849/1950 (95%)	1828 (99%)	21 (1%)	73	84

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	SER
1	A	178	ILE
1	A	188	GLU
1	A	271	CYS
1	A	394	CYS
1	A	403	SER
1	B	90	SER
1	B	147	PHE
1	B	169	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	182	SER
1	B	188	GLU
1	B	339	ILE
1	C	178	ILE
1	C	188	GLU
1	C	322	SER
1	D	172	SER
1	D	182	SER
1	D	188	GLU
1	D	316	ILE
1	E	180	LYS
1	E	188	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	347	GLN
1	A	399	HIS
1	A	405	GLN
1	B	95	ASN
1	B	122	HIS
1	B	142	ASN
1	B	206	GLN
1	C	122	HIS
1	C	291	GLN
1	C	347	GLN
1	C	405	GLN
1	C	436	HIS
1	D	122	HIS
1	D	238	HIS
1	D	347	GLN
1	D	405	GLN
1	E	106	ASN
1	E	122	HIS
1	E	140	ASN
1	E	238	HIS
1	E	300	ASN
1	E	399	HIS
1	E	405	GLN
1	E	436	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	LLP	C	285	1	23,24,25	1.59	4 (17%)	25,32,34	1.49	2 (8%)
1	LLP	B	285	1	23,24,25	1.54	5 (21%)	25,32,34	1.42	3 (12%)
1	LLP	D	285	1	23,24,25	1.65	6 (26%)	25,32,34	1.44	2 (8%)
1	LLP	A	285	1	23,24,25	1.61	6 (26%)	25,32,34	1.50	2 (8%)
1	LLP	E	285	1	23,24,25	1.71	4 (17%)	25,32,34	1.41	3 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	C	285	1	-	5/16/17/19	0/1/1/1
1	LLP	B	285	1	-	6/16/17/19	0/1/1/1
1	LLP	D	285	1	-	5/16/17/19	0/1/1/1
1	LLP	A	285	1	-	5/16/17/19	0/1/1/1
1	LLP	E	285	1	-	4/16/17/19	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	285	LLP	C4-C4'	4.14	1.54	1.46
1	D	285	LLP	C4-C4'	3.76	1.53	1.46
1	A	285	LLP	C4-C4'	3.67	1.53	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	285	LLP	C4-C4'	3.64	1.53	1.46
1	B	285	LLP	C2'-C2	3.53	1.56	1.50
1	C	285	LLP	C2'-C2	3.28	1.55	1.50
1	D	285	LLP	C2'-C2	3.22	1.55	1.50
1	E	285	LLP	CE-NZ	-3.22	1.39	1.46
1	E	285	LLP	C4'-NZ	3.21	1.38	1.27
1	E	285	LLP	C2'-C2	3.19	1.55	1.50
1	D	285	LLP	C4'-NZ	2.95	1.37	1.27
1	A	285	LLP	C2'-C2	2.91	1.55	1.50
1	A	285	LLP	C4'-NZ	2.84	1.36	1.27
1	B	285	LLP	C4-C4'	2.80	1.52	1.46
1	C	285	LLP	C4'-NZ	2.80	1.36	1.27
1	A	285	LLP	CE-NZ	-2.37	1.41	1.46
1	D	285	LLP	C6-C5	2.36	1.42	1.37
1	A	285	LLP	C5'-C5	2.36	1.57	1.50
1	A	285	LLP	C3-C2	-2.35	1.38	1.40
1	D	285	LLP	C5'-C5	2.26	1.57	1.50
1	D	285	LLP	CE-NZ	-2.20	1.42	1.46
1	C	285	LLP	C5'-C5	2.16	1.56	1.50
1	B	285	LLP	C4'-NZ	2.10	1.34	1.27
1	B	285	LLP	OP4-C5'	-2.09	1.37	1.45
1	B	285	LLP	C6-C5	2.03	1.42	1.37

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	285	LLP	OP4-C5'-C5	6.10	120.98	109.35
1	D	285	LLP	OP4-C5'-C5	5.39	119.63	109.35
1	A	285	LLP	OP4-C5'-C5	5.20	119.26	109.35
1	E	285	LLP	OP4-C5'-C5	4.68	118.27	109.35
1	B	285	LLP	OP4-C5'-C5	4.08	117.13	109.35
1	A	285	LLP	OP3-P-OP4	3.72	116.62	106.73
1	B	285	LLP	C5-C6-N1	-2.84	119.08	123.82
1	C	285	LLP	OP3-P-OP4	2.35	113.00	106.73
1	B	285	LLP	OP3-P-OP4	2.31	112.88	106.73
1	E	285	LLP	C5-C4-C4'	2.13	125.06	121.56
1	E	285	LLP	C3-C4-C4'	-2.03	116.64	120.41
1	D	285	LLP	C5-C6-N1	-2.01	120.47	123.82

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	285	LLP	C4-C5-C5'-OP4
1	A	285	LLP	C6-C5-C5'-OP4
1	A	285	LLP	C-CA-CB-CG
1	A	285	LLP	O-C-CA-CB
1	B	285	LLP	C4-C5-C5'-OP4
1	B	285	LLP	C6-C5-C5'-OP4
1	B	285	LLP	C-CA-CB-CG
1	B	285	LLP	O-C-CA-CB
1	C	285	LLP	C4-C5-C5'-OP4
1	C	285	LLP	C6-C5-C5'-OP4
1	C	285	LLP	O-C-CA-CB
1	D	285	LLP	C-CA-CB-CG
1	D	285	LLP	O-C-CA-CB
1	E	285	LLP	C4-C5-C5'-OP4
1	E	285	LLP	C6-C5-C5'-OP4
1	E	285	LLP	C-CA-CB-CG
1	E	285	LLP	O-C-CA-CB
1	B	285	LLP	CE-CD-CG-CB
1	C	285	LLP	CE-CD-CG-CB
1	D	285	LLP	CE-CD-CG-CB
1	A	285	LLP	CE-CD-CG-CB
1	D	285	LLP	C6-C5-C5'-OP4
1	D	285	LLP	C4-C5-C5'-OP4
1	C	285	LLP	C-CA-CB-CG
1	B	285	LLP	N-CA-CB-CG

There are no ring outliers.

5 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	285	LLP	4	0
1	B	285	LLP	9	0
1	D	285	LLP	3	0
1	A	285	LLP	2	0
1	E	285	LLP	2	0

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	451/452 (99%)	0.32	26 (5%)	23	18	127, 198, 298, 335	0
1	B	442/452 (97%)	0.24	31 (7%)	16	12	120, 186, 310, 350	0
1	C	451/452 (99%)	0.29	30 (6%)	17	13	122, 198, 299, 337	0
1	D	394/452 (87%)	0.19	16 (4%)	37	29	134, 192, 274, 309	0
1	E	398/452 (88%)	0.12	20 (5%)	28	24	156, 222, 312, 372	0
All	All	2136/2260 (94%)	0.23	123 (5%)	23	18	120, 199, 301, 372	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	9.3
1	C	451	SER	6.4
1	C	9	PRO	6.1
1	B	17	ILE	5.5
1	C	1	MET	5.3
1	A	45	GLY	4.9
1	A	291	GLN	4.8
1	A	43	ILE	4.5
1	E	55	GLU	4.4
1	C	369	LEU	4.3
1	C	22	TYR	4.3
1	C	8	ILE	4.3
1	B	317	ASP	4.2
1	B	170	GLY	4.1
1	B	18	PHE	4.0
1	E	331	TYR	4.0
1	B	20	LYS	3.9
1	A	42	ILE	3.9
1	B	49	ASP	3.9
1	D	317	ASP	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	11	ILE	3.8
1	A	284	ASP	3.7
1	C	172	SER	3.7
1	B	171	GLY	3.7
1	A	317	ASP	3.7
1	B	10	GLN	3.7
1	A	451	SER	3.6
1	B	48	ALA	3.5
1	E	392	THR	3.4
1	E	402	LEU	3.4
1	D	450	LEU	3.4
1	C	48	ALA	3.4
1	D	170	GLY	3.3
1	A	362	LEU	3.3
1	A	18	PHE	3.3
1	E	254	ILE	3.3
1	B	22	TYR	3.2
1	C	450	LEU	3.2
1	A	39	ARG	3.1
1	C	291	GLN	3.1
1	B	291	GLN	3.1
1	C	27	VAL	3.0
1	A	118	SER	3.0
1	A	140	ASN	3.0
1	A	373	VAL	3.0
1	D	315	ARG	3.0
1	C	31	ALA	2.9
1	A	4	LEU	2.9
1	A	450	LEU	2.9
1	C	371	ILE	2.9
1	E	407	LEU	2.8
1	B	51	ASN	2.8
1	D	397	ILE	2.8
1	B	172	SER	2.8
1	C	431	MET	2.8
1	B	15	VAL	2.8
1	C	21	ALA	2.8
1	C	170	GLY	2.7
1	C	284	ASP	2.7
1	E	380	PRO	2.7
1	C	317	ASP	2.7
1	D	410	ARG	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	320	THR	2.7
1	A	5	LEU	2.6
1	A	359	LEU	2.6
1	C	365	ASP	2.6
1	C	427	LEU	2.6
1	C	57	VAL	2.6
1	B	16	GLU	2.6
1	D	118	SER	2.6
1	E	431	MET	2.5
1	B	21	ALA	2.5
1	D	429	PHE	2.5
1	D	211	LEU	2.5
1	A	46	ALA	2.5
1	C	140	ASN	2.5
1	A	395	VAL	2.5
1	B	284	ASP	2.5
1	E	171	GLY	2.5
1	D	171	GLY	2.4
1	A	44	GLU	2.4
1	C	171	GLY	2.4
1	C	86	ARG	2.4
1	E	367	PRO	2.4
1	D	291	GLN	2.4
1	E	397	ILE	2.3
1	E	56	ASP	2.3
1	E	434	VAL	2.3
1	E	59	ARG	2.3
1	B	32	ARG	2.3
1	A	363	LEU	2.3
1	E	429	PHE	2.3
1	A	221	MET	2.3
1	B	14	VAL	2.3
1	E	255	ASN	2.3
1	D	212	MET	2.3
1	C	395	VAL	2.2
1	D	402	LEU	2.2
1	C	401	ARG	2.2
1	D	427	LEU	2.2
1	A	21	ALA	2.2
1	B	140	ASN	2.2
1	C	402	LEU	2.2
1	E	72	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	363	LEU	2.1
1	D	452	ILE	2.1
1	B	42	ILE	2.1
1	B	54	LEU	2.1
1	B	36	GLU	2.1
1	C	28	VAL	2.1
1	B	53	PHE	2.1
1	B	31	ALA	2.1
1	B	35	ALA	2.1
1	C	46	ALA	2.1
1	A	380	PRO	2.1
1	B	102	ASN	2.1
1	C	211	LEU	2.1
1	E	54	LEU	2.1
1	D	431	MET	2.0
1	E	317	ASP	2.0
1	E	359	LEU	2.0
1	B	103	GLY	2.0
1	B	57	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	LLP	E	285	24/25	0.86	0.36	176,200,215,225	0
1	LLP	B	285	24/25	0.92	0.34	123,153,174,176	0
1	LLP	C	285	24/25	0.92	0.33	113,163,182,192	0
1	LLP	A	285	24/25	0.92	0.38	136,182,191,202	0
1	LLP	D	285	24/25	0.93	0.30	146,165,183,193	0

6.3 Carbohydrates (i)

There are no monosaccharides 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.