



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:12 PM GMT

PDB ID : 1SJ9
Title : Crystal structure of the uridine phosphorylase from Salmonella typhimurium at 2.5Å resolution
Authors : Dontsova, M.; Gabdoulkhakov, A.; Morgunova, E.; Garber, M.; Nikonov, S.; Betzel, C.; Ealick, S.; Mikhailov, A.
Deposited on : 2004-03-03
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<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

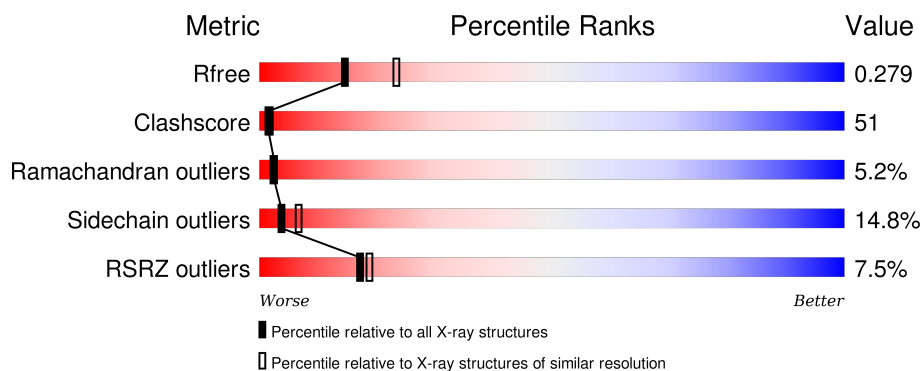
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	253	<div> <div>4%</div> <div>34%</div> <div>57%</div> <div>8%</div> </div>
1	B	253	<div> <div>7%</div> <div>34%</div> <div>55%</div> <div>9%</div> </div>
1	C	253	<div> <div>3%</div> <div>31%</div> <div>54%</div> <div>12%</div> </div>
1	D	253	<div> <div>12%</div> <div>31%</div> <div>55%</div> <div>13%</div> </div>
1	E	253	<div> <div>8%</div> <div>31%</div> <div>53%</div> <div>13%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	253	

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
2	PO4	B	9002	-	-	-	X

2 Entry composition [i](#)

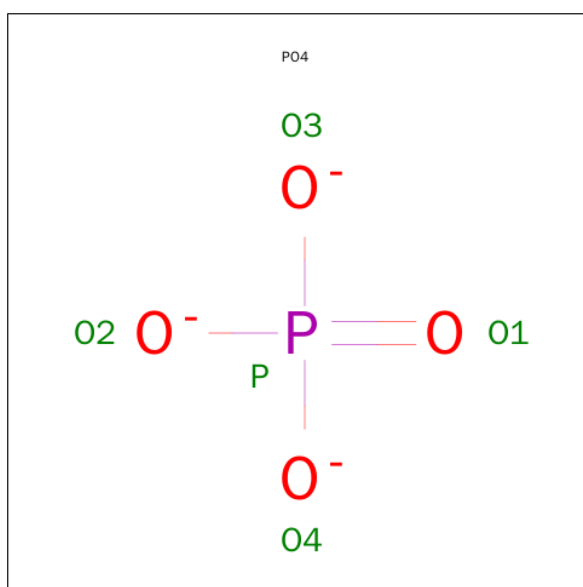
There are 3 unique types of molecules in this entry. The entry contains 11434 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Uridine phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1876	1174	330	360	12			
1	B	250	Total	C	N	O	S	0	0	0
			1876	1174	330	360	12			
1	C	250	Total	C	N	O	S	0	0	0
			1876	1174	330	360	12			
1	D	250	Total	C	N	O	S	0	0	0
			1876	1174	330	360	12			
1	E	250	Total	C	N	O	S	0	0	0
			1876	1174	330	360	12			
1	F	250	Total	C	N	O	S	0	0	0
			1876	1174	330	360	12			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	44	Total	O	0	0
			44	44		
3	B	22	Total	O	0	0
			22	22		
3	C	27	Total	O	0	0
			27	27		
3	D	22	Total	O	0	0
			22	22		
3	E	28	Total	O	0	0
			28	28		
3	F	25	Total	O	0	0
			25	25		

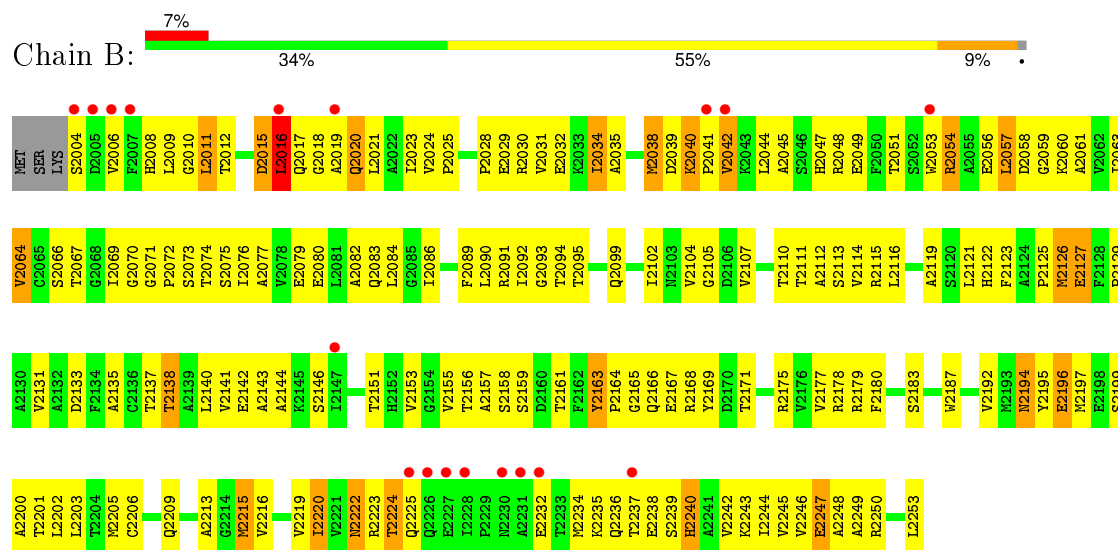
3 Residue-property plots

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: Uridine phosphorylase

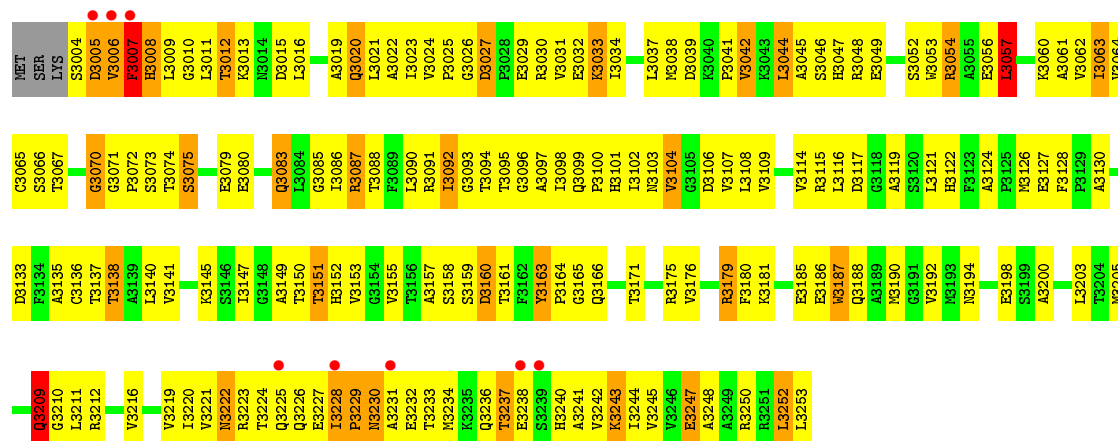


• Molecule 1: Uridine phosphorylase

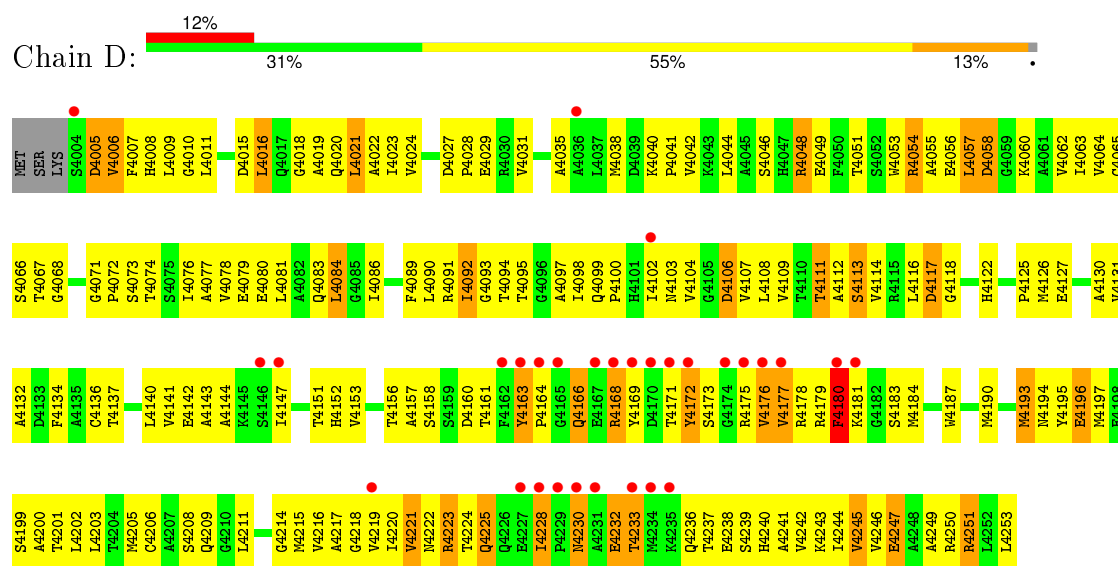


• Molecule 1: Uridine phosphorylase

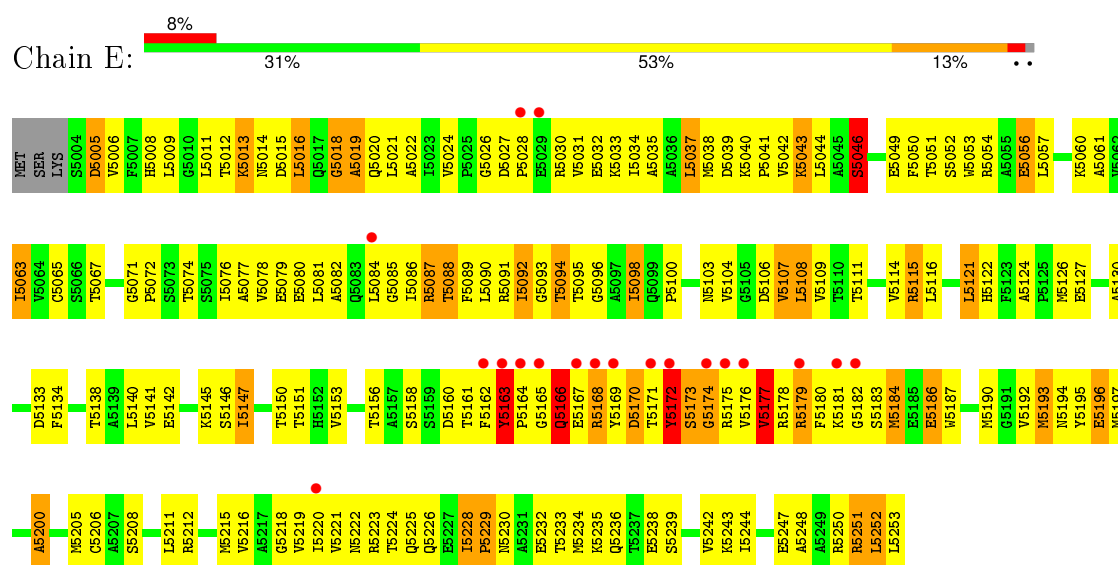




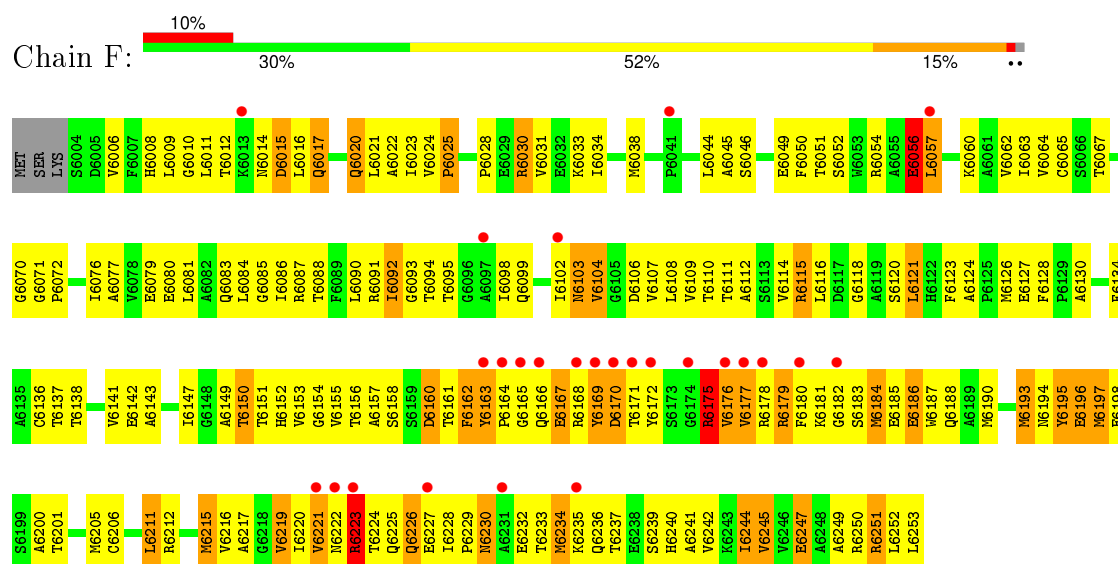
• Molecule 1: Uridine phosphorylase



• Molecule 1: Uridine phosphorylase



• Molecule 1: Uridine phosphorylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	91.37Å 91.37Å 266.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.34 – 2.50 28.34 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (28.34-2.50) 99.4 (28.34-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.47 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.221 , 0.279 0.221 , 0.279	Depositor DCC
R_{free} test set	2159 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	34.2	Xtriage
Anisotropy	1.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 75.1	EDS
Estimated twinning fraction	0.156 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Outliers	0 of 43061 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11434	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.48	0/1906	0.73	0/2584
1	B	0.47	0/1906	0.70	0/2584
1	C	0.49	0/1906	0.76	0/2584
1	D	0.47	0/1906	0.72	0/2584
1	E	0.51	0/1906	0.75	2/2584 (0.1%)
1	F	0.49	0/1906	0.74	1/2584 (0.0%)
All	All	0.49	0/11436	0.73	3/15504 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	E	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	6197	MET	N-CA-C	5.54	125.95	111.00
1	E	5173	SER	N-CA-C	5.52	125.91	111.00
1	E	5172	TYR	N-CA-C	-5.04	97.40	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	4172	TYR	Sidechain
1	E	5018	GLY	Mainchain

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	1876	0	1887	175	0
1	B	1876	0	1887	193	0
1	C	1876	0	1887	190	0
1	D	1876	0	1887	200	0
1	E	1876	0	1887	212	0
1	F	1876	0	1887	245	0
2	B	10	0	0	1	0
3	A	44	0	0	2	0
3	B	22	0	0	0	0
3	C	27	0	0	2	0
3	D	22	0	0	4	0
3	E	28	0	0	2	0
3	F	25	0	0	2	0
All	All	11434	0	11322	1156	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 51.

All (1156) 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:2054:ARG:HB3	1:B:2054:ARG:HH11	0.98	1.11
1:D:4022:ALA:HB2	1:D:4086:ILE:HD13	1.22	1.09
1:F:6147:ILE:HD13	1:F:6244:ILE:HD11	1.39	1.04
1:B:2034:ILE:HG12	1:B:2242:VAL:HG13	1.38	1.01
1:B:2054:ARG:HH11	1:B:2054:ARG:CB	1.74	1.01
1:E:5016:LEU:HB3	1:E:5063:ILE:HD11	1.43	0.99
1:B:2099:GLN:HB2	1:B:2102:ILE:HD13	1.45	0.99
1:B:2054:ARG:HB3	1:B:2054:ARG:NH1	1.77	0.99
1:C:3004:SER:HB2	1:C:3012:THR:HA	1.44	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2094:THR:HB	1:B:2220:ILE:HD12	1.46	0.98
1:B:2019:ALA:HB2	1:B:2061:ALA:HB3	1.45	0.98
1:C:3016:LEU:HB3	1:C:3019:ALA:HB3	1.47	0.95
1:C:3126:MET:HE2	1:D:4127:GLU:HG3	1.46	0.95
1:F:6104:VAL:HA	1:F:6219:VAL:HB	1.48	0.94
1:C:3228:ILE:HD12	1:C:3229:PRO:HD2	1.48	0.94
1:F:6175:ARG:H	1:F:6175:ARG:HH11	1.17	0.93
1:F:6031:VAL:HG13	1:F:6064:VAL:HG12	1.51	0.93
1:E:5063:ILE:HD13	1:E:5086:ILE:HD11	1.52	0.92
1:B:2194:ASN:N	1:B:2194:ASN:HD22	1.68	0.92
1:D:4228:ILE:HD13	1:D:4228:ILE:H	1.35	0.92
1:F:6046:SER:HB2	1:F:6051:THR:HG23	1.51	0.91
1:B:2054:ARG:CB	1:B:2054:ARG:NH1	2.33	0.90
1:C:3071:GLY:HA2	1:C:3074:THR:HB	1.54	0.89
1:B:2107:VAL:HG13	1:B:2151:THR:HG23	1.53	0.89
1:D:4168:ARG:HB2	1:D:4168:ARG:HH11	1.37	0.89
1:F:6176:VAL:HG21	1:F:6180:PHE:HB2	1.54	0.89
1:A:1100:PRO:HG3	1:A:1224:THR:HG21	1.55	0.89
1:F:6163:TYR:HB3	1:F:6168:ARG:HB3	1.55	0.88
1:B:2137:THR:O	1:B:2141:VAL:HG23	1.73	0.87
1:B:2116:LEU:HB2	1:B:2159:SER:HA	1.55	0.87
1:A:1028:PRO:HB3	1:A:1051:THR:HB	1.57	0.87
1:C:3098:ILE:HD11	1:C:3192:VAL:HG22	1.54	0.86
1:A:1044:LEU:HD11	1:A:1054:ARG:HB2	1.56	0.86
1:D:4109:VAL:HG23	1:D:4153:VAL:HA	1.57	0.86
1:E:5232:GLU:HA	1:E:5235:LYS:HE2	1.55	0.85
1:E:5169:TYR:CE2	1:E:5176:VAL:HG21	2.12	0.85
1:E:5019:ALA:CB	1:E:5063:ILE:HD12	2.07	0.85
1:A:1044:LEU:HD21	1:A:1054:ARG:HB3	1.60	0.84
1:F:6091:ARG:HB3	1:F:6215:MET:HG2	1.58	0.84
1:C:3027:ASP:HB2	1:C:3029:GLU:HG2	1.57	0.84
1:B:2038:MET:HG2	1:B:2057:LEU:HD23	1.60	0.83
1:E:5022:ALA:HA	1:E:5063:ILE:O	1.78	0.83
1:B:2016:LEU:HD13	1:B:2063:ILE:HD13	1.60	0.83
1:B:2156:THR:HG21	1:B:2196:GLU:HG2	1.59	0.82
1:E:5013:LYS:HG2	1:E:5084:LEU:HA	1.60	0.82
1:F:6222:ASN:HB3	1:F:6225:GLN:HB3	1.61	0.82
1:F:6028:PRO:HB3	1:F:6051:THR:OG1	1.80	0.82
1:C:3187:TRP:O	1:C:3192:VAL:HG13	1.79	0.82
1:A:1144:ALA:HA	1:A:1244:ILE:HD12	1.60	0.82
1:F:6158:SER:HB2	1:F:6200:ALA:HB2	1.60	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4081:LEU:HD23	1:D:4089:PHE:HE2	1.46	0.81
1:F:6229:PRO:HB2	1:F:6234:MET:HE2	1.61	0.81
1:A:1017:GLN:HG3	1:A:1054:ARG:HE	1.46	0.81
1:B:2090:LEU:HD12	1:B:2249:ALA:HB2	1.64	0.80
1:E:5216:VAL:HG21	1:E:5244:ILE:HG21	1.62	0.80
1:B:2057:LEU:HD12	1:B:2250:ARG:HG3	1.62	0.80
1:A:1016:LEU:HA	1:A:1063:ILE:HD11	1.64	0.80
1:B:2158:SER:HA	1:B:2196:GLU:O	1.81	0.80
1:F:6141:VAL:HG12	1:F:6153:VAL:HG21	1.64	0.79
1:F:6025:PRO:HD2	1:F:6065:CYS:O	1.82	0.79
1:B:2016:LEU:HG	1:B:2084:LEU:HD23	1.64	0.79
1:C:3011:LEU:HD21	1:C:3052:SER:OG	1.82	0.79
1:E:5222:ASN:OD1	1:E:5224:THR:HG22	1.82	0.79
1:B:2044:LEU:HD21	1:B:2054:ARG:NH2	1.96	0.79
1:C:3021:LEU:HD11	1:C:3090:LEU:HD23	1.64	0.79
1:B:2243:LYS:O	1:B:2247:GLU:HG2	1.83	0.79
1:F:6009:LEU:HD11	1:F:6077:ALA:HA	1.65	0.78
1:E:5016:LEU:HB3	1:E:5063:ILE:CD1	2.14	0.78
1:C:3190:MET:HA	1:D:4208:SER:O	1.83	0.78
1:E:5016:LEU:CB	1:E:5063:ILE:HD11	2.14	0.78
1:F:6020:GLN:HG3	1:F:6085:GLY:O	1.84	0.78
1:B:2044:LEU:HD21	1:B:2054:ARG:HH22	1.49	0.77
1:F:6147:ILE:HG21	1:F:6244:ILE:HD11	1.66	0.77
1:E:5016:LEU:HD22	1:E:5063:ILE:HD11	1.65	0.77
1:D:4136:CYS:O	1:D:4140:LEU:HD23	1.82	0.77
1:B:2031:VAL:HG11	1:B:2051:THR:O	1.84	0.77
1:C:3240:HIS:O	1:C:3244:ILE:HG12	1.85	0.77
1:C:3228:ILE:CD1	1:C:3229:PRO:HD2	2.14	0.77
1:C:3005:ASP:OD1	1:C:3013:LYS:HG3	1.84	0.77
1:A:1109:VAL:HB	1:A:1153:VAL:HG22	1.67	0.77
1:E:5019:ALA:O	1:E:5020:GLN:HB2	1.84	0.77
1:C:3011:LEU:HD22	1:C:3044:LEU:HB3	1.67	0.77
1:E:5038:MET:HG2	1:E:5057:LEU:HD13	1.66	0.77
1:F:6239:SER:HA	1:F:6242:VAL:HG12	1.67	0.77
1:F:6099:GLN:HB2	1:F:6102:ILE:HG12	1.66	0.77
1:D:4077:ALA:O	1:D:4081:LEU:HB2	1.85	0.76
1:A:1025:PRO:HD2	1:A:1065:CYS:O	1.86	0.76
1:F:6033:LYS:HE3	1:F:6235:LYS:HE2	1.67	0.76
1:C:3130:ALA:O	1:C:3203:LEU:HD13	1.86	0.76
1:B:2112:ALA:O	1:B:2155:VAL:HA	1.86	0.76
1:C:3086:ILE:H	1:C:3086:ILE:HD12	1.49	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5169:TYR:CE1	1:E:5176:VAL:HG11	2.21	0.76
1:E:5024:VAL:O	1:E:5091:ARG:HD2	1.84	0.76
1:B:2179:ARG:HG3	2:B:9002:PO4:O2	1.86	0.76
1:A:1125:PRO:HD3	1:F:6177:VAL:HG21	1.68	0.75
1:D:4175:ARG:NH1	1:D:4175:ARG:HB3	2.01	0.75
1:F:6222:ASN:H	1:F:6227:GLU:HB3	1.50	0.75
1:F:6091:ARG:HG2	1:F:6215:MET:SD	2.26	0.75
1:C:3116:LEU:HB2	1:C:3159:SER:HA	1.67	0.75
1:C:3114:VAL:HB	1:C:3157:ALA:HA	1.68	0.75
1:D:4233:THR:O	1:D:4237:THR:HG22	1.87	0.74
1:E:5027:ASP:OD1	1:E:5030:ARG:HD3	1.87	0.74
1:A:1092:ILE:HD11	1:A:1241:ALA:HB3	1.68	0.74
1:B:2034:ILE:HD11	1:B:2092:ILE:HD13	1.69	0.74
1:C:3230:ASN:OD1	1:C:3232:GLU:HB2	1.87	0.74
1:E:5252:LEU:O	1:E:5253:LEU:HG	1.87	0.73
1:F:6092:ILE:HG21	1:F:6245:VAL:HG11	1.70	0.73
1:E:5024:VAL:HB	1:E:5067:THR:HG23	1.70	0.73
1:A:1015:ASP:O	1:A:1054:ARG:HD2	1.88	0.73
1:A:1147:ILE:HG13	1:A:1244:ILE:HD13	1.70	0.73
1:F:6034:ILE:HG12	1:F:6242:VAL:HG23	1.69	0.73
1:A:1138:THR:O	1:A:1142:GLU:HG2	1.86	0.73
1:D:4168:ARG:HB2	1:D:4168:ARG:NH1	2.03	0.73
1:D:4076:ILE:O	1:D:4080:GLU:HG2	1.87	0.73
1:C:3021:LEU:HD12	1:C:3022:ALA:H	1.52	0.73
1:E:5019:ALA:CB	1:E:5063:ILE:CD1	2.67	0.73
1:D:4183:SER:HB3	1:D:4187:TRP:HE1	1.53	0.73
1:C:3126:MET:CE	1:D:4127:GLU:HG3	2.17	0.73
1:A:1145:LYS:HG2	3:A:7048:HOH:O	1.88	0.73
1:E:5108:LEU:HD11	1:E:5219:VAL:HG23	1.70	0.73
1:B:2029:GLU:HG2	1:B:2029:GLU:O	1.88	0.72
1:C:3230:ASN:O	1:C:3233:THR:HG22	1.89	0.72
1:E:5107:VAL:HG22	1:E:5151:THR:HG23	1.71	0.72
1:F:6230:ASN:ND2	1:F:6233:THR:HG23	2.03	0.72
1:A:1075:SER:O	1:A:1079:GLU:HB2	1.89	0.72
1:F:6167:GLU:HB2	1:F:6180:PHE:O	1.89	0.72
1:B:2017:GLN:HB2	1:B:2054:ARG:HD3	1.72	0.71
1:C:3071:GLY:HA2	1:C:3074:THR:CB	2.20	0.71
1:F:6138:THR:O	1:F:6142:GLU:HG2	1.89	0.71
1:D:4016:LEU:HD13	1:D:4019:ALA:HB3	1.72	0.71
1:C:3115:ARG:HB2	1:C:3126:MET:HE3	1.71	0.71
1:F:6022:ALA:HB2	1:F:6086:ILE:HD13	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3016:LEU:HB3	1:C:3019:ALA:CB	2.18	0.71
1:B:2069:ILE:HD11	1:D:4048:ARG:CZ	2.20	0.71
1:D:4158:SER:OG	1:D:4200:ALA:HB2	1.91	0.71
1:F:6023:ILE:N	1:F:6023:ILE:HD12	2.06	0.71
1:A:1100:PRO:HG3	1:A:1224:THR:CG2	2.19	0.70
1:B:2008:HIS:HB3	1:B:2080:GLU:OE2	1.89	0.70
1:D:4220:ILE:HG13	1:D:4221:VAL:HG22	1.72	0.70
1:C:3088:THR:HG21	1:C:3252:LEU:CD1	2.21	0.70
1:E:5175:ARG:NH2	1:E:5177:VAL:HG23	2.06	0.70
1:A:1104:VAL:HG13	1:A:1219:VAL:O	1.90	0.70
1:B:2009:LEU:HG	1:B:2080:GLU:OE2	1.91	0.70
1:A:1032:GLU:O	1:A:1036:ALA:HB2	1.92	0.70
1:D:4161:THR:HB	1:D:4164:PRO:HD2	1.72	0.70
1:C:3057:LEU:HB3	1:C:3253:LEU:HD11	1.72	0.70
1:B:2129:PRO:HB3	3:F:7160:HOH:O	1.92	0.70
1:F:6077:ALA:O	1:F:6081:LEU:HG	1.90	0.70
1:F:6108:LEU:HD13	1:F:6193:MET:HE3	1.72	0.70
1:B:2006:VAL:O	1:B:2010:GLY:HA2	1.91	0.70
1:B:2016:LEU:HD13	1:B:2063:ILE:CD1	2.22	0.70
1:F:6092:ILE:HD11	1:F:6241:ALA:CB	2.22	0.70
1:B:2105:GLY:HA2	1:B:2237:THR:HG22	1.72	0.70
1:A:1040:LYS:HD2	1:A:1056:GLU:OE1	1.90	0.70
1:E:5133:ASP:OD2	1:E:5212:ARG:HD2	1.92	0.69
1:D:4081:LEU:HD23	1:D:4089:PHE:CE2	2.27	0.69
1:C:3021:LEU:HD13	1:C:3088:THR:CG2	2.23	0.69
1:B:2011:LEU:HD13	1:B:2084:LEU:HD22	1.74	0.69
1:A:1186:GLU:O	1:A:1190:MET:HG3	1.92	0.69
1:E:5044:LEU:HD21	1:E:5054:ARG:NH1	2.08	0.69
1:F:6147:ILE:HG21	1:F:6244:ILE:CD1	2.23	0.69
1:F:6098:ILE:HD11	1:F:6195:TYR:HB2	1.74	0.69
1:F:6158:SER:CB	1:F:6200:ALA:HB2	2.23	0.68
1:A:1081:LEU:HD12	1:A:1089:PHE:HE2	1.58	0.68
1:F:6143:ALA:HA	1:F:6251:ARG:HH12	1.58	0.68
1:D:4238:GLU:O	1:D:4242:VAL:HG23	1.93	0.68
1:C:3176:VAL:HG22	1:C:3181:LYS:HD2	1.76	0.68
1:B:2008:HIS:CE1	1:B:2076:ILE:HG21	2.28	0.68
1:C:3250:ARG:O	1:C:3253:LEU:HB2	1.94	0.68
1:F:6120:SER:OG	1:F:6121:LEU:HD12	1.94	0.68
1:B:2194:ASN:N	1:B:2194:ASN:ND2	2.41	0.68
1:F:6166:GLN:O	1:F:6167:GLU:HB3	1.94	0.68
1:B:2094:THR:HB	1:B:2220:ILE:HG21	1.74	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2159:SER:OG	1:B:2165:GLY:HA3	1.93	0.68
1:C:3057:LEU:HD11	1:C:3250:ARG:HG2	1.76	0.68
1:D:4106:ASP:O	1:D:4219:VAL:HG12	1.93	0.68
1:D:4107:VAL:HG11	1:D:4244:ILE:HD12	1.76	0.68
1:D:4060:LYS:HB2	1:D:4253:LEU:HD13	1.76	0.68
1:F:6176:VAL:HG11	1:F:6180:PHE:N	2.09	0.68
1:C:3088:THR:HG21	1:C:3252:LEU:HD13	1.75	0.67
1:F:6045:ALA:HB3	1:F:6052:SER:OG	1.94	0.67
1:F:6175:ARG:HB3	1:F:6181:LYS:HE2	1.76	0.67
1:F:6147:ILE:HD13	1:F:6244:ILE:CD1	2.21	0.67
1:D:4143:ALA:HB3	1:D:4244:ILE:HG23	1.76	0.67
1:A:1184:MET:O	1:A:1188:GLN:HG3	1.92	0.67
1:C:3041:PRO:O	1:C:3042:VAL:HG23	1.94	0.67
1:F:6175:ARG:H	1:F:6175:ARG:NH1	1.90	0.67
1:F:6175:ARG:N	1:F:6175:ARG:HH11	1.89	0.67
1:B:2175:ARG:HH22	1:D:4208:SER:HB2	1.60	0.67
1:E:5028:PRO:HA	1:E:5031:VAL:HG22	1.76	0.67
1:E:5163:TYR:HB3	1:E:5164:PRO:HD3	1.76	0.67
1:C:3247:GLU:O	1:C:3250:ARG:HB2	1.94	0.67
1:B:2115:ARG:HH21	1:B:2121:LEU:HD23	1.59	0.67
1:C:3179:ARG:O	1:C:3179:ARG:HD2	1.95	0.66
1:B:2069:ILE:HB	3:D:7066:HOH:O	1.94	0.66
1:E:5108:LEU:HD11	1:E:5219:VAL:CG2	2.26	0.66
1:C:3166:GLN:HB3	1:C:3223:ARG:HH12	1.61	0.66
1:D:4015:ASP:HB3	1:D:4044:LEU:HD13	1.78	0.66
1:A:1094:THR:HB	1:A:1220:ILE:CG2	2.26	0.66
1:F:6098:ILE:CD1	1:F:6223:ARG:HD2	2.25	0.66
1:F:6071:GLY:N	1:F:6072:PRO:HD2	2.11	0.66
1:F:6219:VAL:HG12	1:F:6221:VAL:O	1.96	0.66
1:E:5175:ARG:HH11	1:E:5175:ARG:HG3	1.60	0.66
1:E:5216:VAL:HG21	1:E:5244:ILE:CG2	2.26	0.66
1:F:6057:LEU:HD11	1:F:6250:ARG:HG3	1.78	0.66
1:F:6099:GLN:HG2	1:F:6193:MET:HA	1.77	0.66
1:E:5087:ARG:HA	1:E:5211:LEU:HD22	1.77	0.65
1:C:3024:VAL:HB	1:C:3067:THR:HG23	1.78	0.65
1:F:6161:THR:OG1	1:F:6164:PRO:HG2	1.95	0.65
1:E:5088:THR:HA	1:E:5212:ARG:O	1.96	0.65
1:E:5184:MET:HA	1:E:5187:TRP:HD1	1.61	0.65
1:C:3029:GLU:O	1:C:3033:LYS:HD3	1.96	0.65
1:C:3159:SER:OG	1:C:3165:GLY:HA3	1.95	0.65
1:E:5077:ALA:O	1:E:5081:LEU:HD13	1.95	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3019:ALA:HA	1:C:3061:ALA:O	1.95	0.65
1:B:2187:TRP:CE3	1:B:2187:TRP:HA	2.32	0.65
1:E:5024:VAL:HB	1:E:5067:THR:CG2	2.26	0.65
1:E:5008:HIS:HB3	1:E:5050:PHE:HE1	1.61	0.65
1:D:4023:ILE:HD13	1:D:4090:LEU:HB2	1.77	0.65
1:F:6090:LEU:HD21	1:F:6252:LEU:CD1	2.27	0.65
1:C:3010:GLY:HA3	1:C:3047:HIS:CE1	2.32	0.65
1:D:4233:THR:HA	1:D:4236:GLN:HB2	1.78	0.65
1:E:5238:GLU:O	1:E:5242:VAL:HG23	1.97	0.65
1:B:2019:ALA:HB1	1:B:2061:ALA:O	1.96	0.65
1:D:4100:PRO:HA	1:D:4224:THR:HG21	1.78	0.65
1:F:6229:PRO:HB2	1:F:6234:MET:CE	2.27	0.65
1:A:1129:PRO:HB3	3:E:7121:HOH:O	1.96	0.65
1:D:4027:ASP:O	1:D:4031:VAL:HG23	1.97	0.64
1:F:6223:ARG:HD3	1:F:6224:THR:HG23	1.78	0.64
1:B:2119:ALA:HA	1:B:2122:HIS:HD2	1.62	0.64
1:B:2011:LEU:HD13	1:B:2084:LEU:CD2	2.28	0.64
1:C:3007:PHE:HB3	1:C:3008:HIS:ND1	2.13	0.64
1:B:2025:PRO:O	1:B:2067:THR:HG22	1.97	0.64
1:B:2177:VAL:HG21	3:D:7061:HOH:O	1.97	0.64
1:A:1126:MET:SD	1:E:5127:GLU:HG3	2.38	0.64
1:F:6220:ILE:O	1:F:6229:PRO:HB3	1.97	0.64
1:F:6024:VAL:O	1:F:6091:ARG:HD2	1.98	0.64
1:A:1240:HIS:O	1:A:1244:ILE:HG12	1.98	0.64
1:C:3079:GLU:O	1:C:3083:GLN:HG3	1.97	0.64
1:E:5019:ALA:HB1	1:E:5063:ILE:HD12	1.80	0.64
1:B:2004:SER:HB3	1:B:2012:THR:HB	1.80	0.64
1:F:6006:VAL:HG23	1:F:6010:GLY:H	1.62	0.64
1:F:6099:GLN:HB2	1:F:6102:ILE:CG1	2.28	0.64
1:A:1071:GLY:HA2	1:A:1074:THR:HB	1.80	0.64
1:D:4251:ARG:HH11	1:D:4251:ARG:CG	2.11	0.63
1:B:2075:SER:O	1:B:2079:GLU:HB2	1.98	0.63
1:D:4094:THR:HB	1:D:4220:ILE:HG23	1.81	0.63
1:E:5012:THR:HG23	1:E:5014:ASN:H	1.62	0.63
1:F:6147:ILE:CD1	1:F:6244:ILE:HD11	2.24	0.63
1:E:5016:LEU:HD22	1:E:5063:ILE:CD1	2.29	0.63
1:C:3015:ASP:O	1:C:3054:ARG:HG3	1.97	0.63
1:A:1197:MET:HB2	3:A:7050:HOH:O	1.98	0.63
1:F:6184:MET:HB2	1:F:6195:TYR:HE2	1.62	0.63
1:F:6108:LEU:HA	1:F:6152:HIS:O	1.99	0.63
1:E:5167:GLU:HG3	1:E:5182:GLY:H	1.63	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6092:ILE:HD11	1:F:6241:ALA:HB1	1.81	0.63
1:E:5008:HIS:HB3	1:E:5050:PHE:CE1	2.33	0.62
1:E:5158:SER:HA	1:E:5196:GLU:O	1.99	0.62
1:E:5220:ILE:HG13	1:E:5221:VAL:HG12	1.79	0.62
1:B:2071:GLY:HA3	1:B:2201:THR:OG1	1.99	0.62
1:B:2023:ILE:HD11	1:B:2249:ALA:CB	2.29	0.62
1:C:3041:PRO:HA	1:C:3054:ARG:O	1.98	0.62
1:E:5049:GLU:HB2	3:E:7082:HOH:O	1.98	0.62
1:C:3237:THR:O	1:C:3242:VAL:HG23	1.98	0.62
1:F:6092:ILE:HB	1:F:6245:VAL:HG21	1.81	0.62
1:F:6092:ILE:HD13	1:F:6093:GLY:N	2.14	0.62
1:E:5091:ARG:HG3	1:E:5092:ILE:N	2.12	0.62
1:C:3116:LEU:HD13	1:C:3180:PHE:CZ	2.35	0.62
1:F:6038:MET:HE1	1:F:6062:VAL:HG11	1.82	0.62
1:D:4040:LYS:N	1:D:4041:PRO:HD3	2.14	0.62
1:A:1031:VAL:HG21	1:A:1051:THR:HG22	1.82	0.62
1:C:3190:MET:HG2	1:D:4208:SER:HB2	1.80	0.62
1:E:5228:ILE:HD13	1:E:5228:ILE:O	1.99	0.62
1:D:4166:GLN:HA	1:D:4195:TYR:CD2	2.34	0.61
1:F:6108:LEU:HD13	1:F:6193:MET:CE	2.30	0.61
1:A:1095:THR:O	1:A:1220:ILE:HG12	1.98	0.61
1:E:5016:LEU:HD13	1:E:5063:ILE:HD13	1.82	0.61
1:F:6239:SER:HA	1:F:6242:VAL:CG1	2.30	0.61
1:C:3240:HIS:C	1:C:3244:ILE:HG12	2.20	0.61
1:D:4093:GLY:O	1:D:4217:ALA:HA	2.01	0.61
1:F:6240:HIS:O	1:F:6244:ILE:HD13	2.01	0.61
1:B:2094:THR:CB	1:B:2220:ILE:HG21	2.30	0.61
1:C:3209:GLN:O	1:C:3211:LEU:HG	2.00	0.61
1:B:2099:GLN:CB	1:B:2102:ILE:HD13	2.26	0.61
1:E:5092:ILE:HA	1:E:5216:VAL:O	2.01	0.61
1:C:3041:PRO:HB2	1:C:3053:TRP:CE3	2.36	0.61
1:C:3243:LYS:HE2	1:C:3243:LYS:HA	1.80	0.61
1:B:2163:TYR:CD2	1:B:2171:THR:HG22	2.35	0.61
1:C:3030:ARG:HA	1:C:3033:LYS:HD3	1.81	0.61
1:F:6156:THR:HG22	1:F:6157:ALA:N	2.16	0.61
1:A:1196:GLU:OE2	1:A:1199:SER:OG	2.09	0.61
1:A:1126:MET:HG3	1:E:5126:MET:HG3	1.82	0.61
1:B:2111:THR:HG23	1:B:2153:VAL:HG12	1.82	0.61
1:E:5082:ALA:HA	1:E:5086:ILE:O	2.01	0.60
1:C:3024:VAL:HA	1:C:3065:CYS:O	2.01	0.60
1:A:1011:LEU:HD21	1:A:1044:LEU:CB	2.31	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1072:PRO:HD3	1:F:6072:PRO:HG3	1.83	0.60
1:F:6021:LEU:HD11	1:F:6252:LEU:HD12	1.82	0.60
1:B:2144:ALA:HA	1:B:2244:ILE:HD12	1.82	0.60
1:B:2168:ARG:HH11	1:B:2168:ARG:HG3	1.67	0.60
1:C:3095:THR:O	1:C:3220:ILE:HG22	2.00	0.60
1:C:3054:ARG:HH11	1:C:3054:ARG:HG3	1.66	0.60
1:A:1222:ASN:HB3	1:A:1225:GLN:HB2	1.82	0.60
1:F:6176:VAL:HG21	1:F:6180:PHE:CD1	2.35	0.60
1:F:6060:LYS:HD3	1:F:6253:LEU:HB3	1.83	0.60
1:A:1169:TYR:CE2	1:A:1176:VAL:HG23	2.36	0.60
1:E:5186:GLU:O	1:E:5190:MET:HB2	2.01	0.60
1:D:4243:LYS:O	1:D:4247:GLU:HB2	2.02	0.60
1:F:6049:GLU:OE1	1:F:6049:GLU:HA	2.01	0.60
1:A:1247:GLU:HA	1:A:1250:ARG:HH11	1.66	0.60
1:F:6176:VAL:HG21	1:F:6180:PHE:CB	2.31	0.60
1:F:6162:PHE:O	1:F:6166:GLN:HG2	2.02	0.60
1:F:6046:SER:HA	1:F:6051:THR:HA	1.82	0.60
1:A:1161:THR:HB	1:A:1164:PRO:HD2	1.82	0.60
1:D:4053:TRP:O	1:D:4054:ARG:HB2	2.02	0.60
1:D:4223:ARG:HH11	1:D:4223:ARG:HG3	1.66	0.60
1:A:1177:VAL:O	1:A:1181:LYS:HG3	2.02	0.60
1:A:1006:VAL:HG11	1:A:1083:GLN:HE22	1.67	0.60
1:B:2187:TRP:HE3	1:B:2187:TRP:HA	1.65	0.60
1:F:6239:SER:CA	1:F:6242:VAL:HG12	2.31	0.60
1:C:3075:SER:O	1:C:3079:GLU:HB2	2.00	0.60
1:F:6182:GLY:HA2	1:F:6185:GLU:OE2	2.01	0.60
1:B:2138:THR:O	1:B:2142:GLU:HB2	2.02	0.60
1:E:5019:ALA:HB2	1:E:5063:ILE:HD12	1.81	0.59
1:F:6175:ARG:H	1:F:6175:ARG:HD3	1.66	0.59
1:C:3155:VAL:HG23	1:C:3192:VAL:HB	1.84	0.59
1:A:1132:ALA:HA	1:A:1203:LEU:HD22	1.84	0.59
1:F:6112:ALA:O	1:F:6155:VAL:HA	2.01	0.59
1:A:1011:LEU:HD21	1:A:1044:LEU:HB3	1.83	0.59
1:B:2057:LEU:HB3	1:B:2253:LEU:HD21	1.83	0.59
1:F:6109:VAL:HB	1:F:6153:VAL:HG22	1.84	0.59
1:C:3021:LEU:CD1	1:C:3090:LEU:HD23	2.32	0.59
1:A:1016:LEU:CA	1:A:1063:ILE:HD11	2.32	0.59
1:B:2143:ALA:O	1:B:2146:SER:HB3	2.02	0.59
1:F:6056:GLU:HA	1:F:6060:LYS:O	2.01	0.59
1:E:5011:LEU:HD21	1:E:5044:LEU:HB3	1.83	0.59
1:D:4239:SER:O	1:D:4243:LYS:HG3	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3023:ILE:HB	1:C:3064:VAL:HG22	1.84	0.59
1:A:1009:LEU:HD13	1:A:1080:GLU:HG3	1.83	0.59
1:F:6121:LEU:HD12	1:F:6121:LEU:H	1.66	0.59
1:D:4056:GLU:HA	1:D:4060:LYS:O	2.02	0.59
1:F:6057:LEU:CD1	1:F:6250:ARG:HG3	2.32	0.59
1:D:4251:ARG:NH1	1:D:4251:ARG:HG3	2.16	0.59
1:F:6230:ASN:HD21	1:F:6233:THR:HG23	1.65	0.59
1:C:3015:ASP:HB3	1:C:3044:LEU:HD22	1.84	0.59
1:E:5028:PRO:O	1:E:5031:VAL:HG22	2.03	0.59
1:C:3122:HIS:O	1:E:5165:GLY:HA3	2.02	0.59
1:A:1022:ALA:HB2	1:A:1086:ILE:HG13	1.83	0.59
1:A:1201:THR:O	1:A:1205:MET:HG2	2.03	0.59
1:B:2246:VAL:O	1:B:2250:ARG:HB2	2.03	0.58
1:D:4163:TYR:HA	1:D:4168:ARG:HH12	1.68	0.58
1:E:5012:THR:C	1:E:5014:ASN:H	2.07	0.58
1:D:4143:ALA:O	1:D:4147:ILE:HG12	2.03	0.58
1:F:6006:VAL:HG21	1:F:6009:LEU:HB2	1.84	0.58
1:C:3221:VAL:HG22	1:C:3222:ASN:H	1.68	0.58
1:C:3108:LEU:HD22	1:C:3152:HIS:HB2	1.85	0.58
1:B:2126:MET:SD	1:F:6127:GLU:HA	2.43	0.58
1:D:4197:MET:HG3	3:D:7108:HOH:O	2.02	0.58
1:E:5016:LEU:CD2	1:E:5063:ILE:HD11	2.30	0.58
1:F:6227:GLU:HG3	1:F:6228:ILE:H	1.67	0.58
1:B:2157:ALA:HB2	1:B:2192:VAL:HG11	1.86	0.58
1:B:2089:PHE:O	1:B:2090:LEU:HD23	2.04	0.58
1:F:6006:VAL:HB	1:F:6080:GLU:HG2	1.84	0.58
1:B:2125:PRO:HB3	1:B:2127:GLU:OE1	2.04	0.58
1:D:4016:LEU:HG	1:D:4084:LEU:HB3	1.85	0.58
1:A:1044:LEU:HD21	1:A:1054:ARG:CB	2.33	0.58
1:A:1094:THR:HB	1:A:1220:ILE:HG21	1.86	0.58
1:A:1096:GLY:HA2	1:A:1221:VAL:O	2.03	0.58
1:D:4022:ALA:HA	1:D:4063:ILE:O	2.04	0.58
1:C:3164:PRO:HG2	1:E:5122:HIS:HB3	1.86	0.58
1:D:4114:VAL:HG11	1:D:4187:TRP:CZ3	2.39	0.58
1:E:5161:THR:HB	1:E:5166:GLN:OE1	2.03	0.58
1:F:6038:MET:CE	1:F:6062:VAL:HG11	2.34	0.58
1:A:1048:ARG:HG2	1:A:1049:GLU:H	1.67	0.58
1:B:2194:ASN:H	1:B:2194:ASN:HD22	1.51	0.58
1:B:2140:LEU:HD23	1:B:2248:ALA:CB	2.34	0.58
1:E:5092:ILE:HG12	1:E:5093:GLY:N	2.19	0.58
1:C:3229:PRO:O	1:C:3230:ASN:HB3	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1022:ALA:CB	1:A:1086:ILE:HG21	2.33	0.58
1:E:5009:LEU:HD21	1:E:5077:ALA:HA	1.85	0.58
1:C:3116:LEU:HD13	1:C:3180:PHE:CE2	2.39	0.57
1:A:1049:GLU:HB2	1:F:6049:GLU:CD	2.25	0.57
1:F:6021:LEU:HD23	1:F:6022:ALA:N	2.20	0.57
1:D:4144:ALA:HB2	1:D:4244:ILE:HD13	1.86	0.57
1:D:4251:ARG:HH11	1:D:4251:ARG:HG3	1.69	0.57
1:B:2054:ARG:HB2	1:B:2054:ARG:NH1	2.15	0.57
1:F:6161:THR:CB	1:F:6164:PRO:HG2	2.33	0.57
1:A:1159:SER:OG	1:A:1165:GLY:HA3	2.04	0.57
1:C:3022:ALA:HA	1:C:3063:ILE:O	2.03	0.57
1:C:3023:ILE:HG23	1:C:3245:VAL:HG21	1.85	0.57
1:F:6167:GLU:O	1:F:6167:GLU:HG3	1.99	0.57
1:D:4175:ARG:HH11	1:D:4175:ARG:HB3	1.68	0.57
1:E:5104:VAL:HG23	1:E:5219:VAL:O	2.05	0.57
1:D:4058:ASP:OD1	1:D:4250:ARG:HG3	2.05	0.57
1:F:6044:LEU:HD11	1:F:6054:ARG:HB2	1.86	0.57
1:F:6158:SER:HA	1:F:6196:GLU:O	2.05	0.57
1:A:1072:PRO:HB3	1:F:6160:ASP:O	2.04	0.57
1:C:3030:ARG:O	1:C:3033:LYS:HG2	2.05	0.57
1:F:6092:ILE:HG12	1:F:6216:VAL:HG13	1.87	0.57
1:C:3041:PRO:HB2	1:C:3053:TRP:HE3	1.70	0.57
1:B:2031:VAL:HG12	1:B:2053:TRP:HB2	1.87	0.57
1:E:5008:HIS:HB2	1:E:5080:GLU:OE1	2.04	0.57
1:C:3158:SER:HB3	1:C:3200:ALA:HB2	1.84	0.57
1:A:1092:ILE:HD11	1:A:1241:ALA:CB	2.35	0.56
1:F:6247:GLU:HA	1:F:6247:GLU:OE1	2.03	0.56
1:F:6090:LEU:HD21	1:F:6252:LEU:HD11	1.86	0.56
1:D:4183:SER:HB3	1:D:4187:TRP:NE1	2.20	0.56
1:C:3039:ASP:OD2	1:C:3056:GLU:HB2	2.05	0.56
1:A:1241:ALA:O	1:A:1245:VAL:HG12	2.05	0.56
1:F:6021:LEU:HG	1:F:6088:THR:HB	1.87	0.56
1:D:4158:SER:CB	1:D:4200:ALA:HB2	2.35	0.56
1:D:4240:HIS:O	1:D:4244:ILE:HG13	2.04	0.56
1:B:2038:MET:HG2	1:B:2057:LEU:CD2	2.35	0.56
1:F:6098:ILE:HD13	1:F:6223:ARG:HD2	1.87	0.56
1:B:2072:PRO:HB3	1:D:4160:ASP:HB3	1.86	0.56
1:D:4184:MET:HA	1:D:4195:TYR:OH	2.06	0.56
1:D:4067:THR:HB	1:D:4074:THR:HG23	1.86	0.56
1:F:6095:THR:O	1:F:6219:VAL:HA	2.06	0.56
1:B:2187:TRP:HD1	1:B:2195:TYR:HH	1.54	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2069:ILE:HD11	1:D:4048:ARG:NH2	2.20	0.56
1:D:4031:VAL:HG21	1:D:4066:SER:HB3	1.88	0.56
1:F:6227:GLU:HG3	1:F:6228:ILE:N	2.20	0.56
1:F:6008:HIS:HB3	1:F:6050:PHE:HE1	1.71	0.56
1:D:4057:LEU:HB3	1:D:4253:LEU:HD12	1.88	0.56
1:A:1116:LEU:HB2	1:A:1158:SER:O	2.06	0.56
1:A:1183:SER:O	1:A:1186:GLU:HB3	2.06	0.56
1:A:1190:MET:HE1	1:E:5208:SER:HB2	1.88	0.56
1:F:6092:ILE:HD11	1:F:6241:ALA:HB3	1.87	0.56
1:B:2110:THR:HB	1:B:2215:MET:HB3	1.87	0.56
1:B:2102:ILE:CG2	1:B:2219:VAL:HG21	2.36	0.55
1:E:5012:THR:HG22	1:E:5015:ASP:OD2	2.06	0.55
1:E:5046:SER:HB2	1:E:5051:THR:HG23	1.88	0.55
1:B:2059:GLY:C	1:B:2060:LYS:HD2	2.26	0.55
1:C:3228:ILE:CG1	1:C:3229:PRO:HD2	2.36	0.55
1:B:2116:LEU:HB2	1:B:2158:SER:O	2.06	0.55
1:F:6017:GLN:HG3	1:F:6054:ARG:CD	2.36	0.55
1:B:2057:LEU:CD1	1:B:2250:ARG:HG3	2.36	0.55
1:B:2021:LEU:H	1:B:2086:ILE:CD1	2.19	0.55
1:F:6163:TYR:HB3	1:F:6168:ARG:CB	2.34	0.55
1:C:3029:GLU:HG3	1:C:3030:ARG:HD2	1.89	0.55
1:D:4060:LYS:CB	1:D:4253:LEU:HD13	2.35	0.55
1:F:6006:VAL:HG11	1:F:6084:LEU:HD11	1.88	0.55
1:E:5054:ARG:HH11	1:E:5054:ARG:CB	2.19	0.55
1:A:1167:GLU:HG2	1:A:1169:TYR:CE1	2.41	0.55
1:D:4130:ALA:O	1:D:4203:LEU:HD13	2.05	0.55
1:D:4161:THR:HG1	1:D:4180:PHE:HE2	1.55	0.55
1:F:6156:THR:HG23	1:F:6194:ASN:CG	2.26	0.55
1:D:4024:VAL:O	1:D:4091:ARG:HG3	2.06	0.55
1:D:4108:LEU:HD12	1:D:4152:HIS:HB2	1.88	0.55
1:B:2247:GLU:O	1:B:2250:ARG:HB3	2.07	0.55
1:E:5175:ARG:HD2	1:E:5177:VAL:H	1.71	0.55
1:F:6099:GLN:CG	1:F:6193:MET:HA	2.36	0.55
1:B:2243:LYS:C	1:B:2247:GLU:HG2	2.27	0.55
1:C:3079:GLU:OE1	1:E:5164:PRO:HB3	2.07	0.55
1:A:1161:THR:OG1	1:A:1164:PRO:HG2	2.07	0.55
1:A:1247:GLU:OE1	1:A:1250:ARG:HD2	2.07	0.55
1:B:2199:SER:O	1:B:2203:LEU:HG	2.07	0.55
1:C:3004:SER:CB	1:C:3012:THR:HA	2.27	0.55
1:E:5176:VAL:HG12	1:E:5176:VAL:O	2.07	0.55
1:E:5163:TYR:N	1:E:5166:GLN:OE1	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2171:THR:HB	1:D:4079:GLU:OE2	2.07	0.55
1:F:6222:ASN:O	1:F:6225:GLN:N	2.40	0.54
1:F:6221:VAL:HB	1:F:6229:PRO:HD3	1.88	0.54
1:C:3137:THR:O	1:C:3141:VAL:HG23	2.07	0.54
1:B:2049:GLU:OE1	1:D:4048:ARG:HB3	2.07	0.54
1:D:4117:ASP:OD1	1:D:4200:ALA:HB1	2.06	0.54
1:D:4222:ASN:OD1	1:D:4224:THR:HB	2.06	0.54
1:B:2222:ASN:ND2	1:B:2224:THR:OG1	2.39	0.54
1:C:3021:LEU:HD22	1:C:3252:LEU:CD1	2.37	0.54
1:F:6247:GLU:OE1	1:F:6250:ARG:HD2	2.06	0.54
1:F:6239:SER:O	1:F:6242:VAL:HG12	2.07	0.54
1:C:3222:ASN:OD1	1:C:3225:GLN:HG3	2.07	0.54
1:C:3021:LEU:HD13	1:C:3088:THR:HG22	1.89	0.54
1:E:5234:MET:O	1:E:5238:GLU:HB2	2.08	0.54
1:A:1136:CYS:O	1:A:1140:LEU:HG	2.06	0.54
1:F:6176:VAL:CG2	1:F:6180:PHE:HB2	2.33	0.54
1:C:3092:ILE:HD11	1:C:3241:ALA:HB1	1.89	0.54
1:A:1021:LEU:C	1:A:1086:ILE:HD12	2.28	0.54
1:D:4028:PRO:HA	1:D:4031:VAL:CG2	2.37	0.54
1:B:2111:THR:CG2	1:B:2153:VAL:HG12	2.37	0.54
1:B:2175:ARG:HH22	1:D:4208:SER:CB	2.19	0.54
1:C:3179:ARG:HG3	1:C:3179:ARG:HH11	1.72	0.54
1:E:5085:GLY:O	1:E:5087:ARG:HG2	2.07	0.54
1:A:1159:SER:O	1:A:1197:MET:HG2	2.06	0.54
1:A:1158:SER:HB2	1:A:1199:SER:OG	2.06	0.54
1:A:1162:PHE:O	1:A:1168:ARG:HD2	2.07	0.54
1:C:3096:GLY:HA2	1:C:3221:VAL:O	2.08	0.54
1:E:5109:VAL:HG11	1:E:5141:VAL:HG23	1.89	0.54
1:D:4078:VAL:O	1:D:4078:VAL:HG12	2.08	0.54
1:C:3020:GLN:O	1:C:3086:ILE:HG23	2.08	0.53
1:A:1025:PRO:HB3	1:A:1092:ILE:HG22	1.89	0.53
1:D:4214:GLY:HA2	3:D:7107:HOH:O	2.08	0.53
1:B:2242:VAL:O	1:B:2245:VAL:HG12	2.08	0.53
1:F:6176:VAL:HG22	1:F:6177:VAL:H	1.71	0.53
1:A:1006:VAL:HG11	1:A:1080:GLU:OE2	2.08	0.53
1:C:3140:LEU:HD23	1:C:3248:ALA:CB	2.37	0.53
1:C:3008:HIS:ND1	1:C:3080:GLU:OE1	2.40	0.53
1:D:4177:VAL:HG22	1:D:4178:ARG:H	1.74	0.53
1:B:2156:THR:HA	1:B:2194:ASN:ND2	2.24	0.53
1:E:5107:VAL:HG13	1:E:5151:THR:HA	1.88	0.53
1:A:1020:GLN:OE1	1:A:1021:LEU:HB2	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2006:VAL:CG1	1:B:2009:LEU:H	2.21	0.53
1:D:4098:ILE:HG12	1:D:4193:MET:O	2.09	0.53
1:D:4206:CYS:HB3	1:D:4211:LEU:HB2	1.89	0.53
1:E:5183:SER:OG	1:F:6178:ARG:NH2	2.41	0.53
1:C:3034:ILE:O	1:C:3037:LEU:HB2	2.07	0.53
1:E:5020:GLN:HA	1:E:5086:ILE:HA	1.89	0.53
1:C:3023:ILE:O	1:C:3064:VAL:HG13	2.08	0.53
1:F:6230:ASN:O	1:F:6234:MET:HB2	2.08	0.53
1:F:6156:THR:HG22	1:F:6157:ALA:H	1.73	0.53
1:A:1009:LEU:HD13	1:A:1080:GLU:CB	2.38	0.53
1:A:1109:VAL:O	1:A:1193:MET:HE1	2.09	0.53
1:E:5030:ARG:O	1:E:5034:ILE:HG12	2.07	0.53
1:B:2240:HIS:O	1:B:2243:LYS:HB2	2.08	0.53
1:D:4109:VAL:CG2	1:D:4153:VAL:HA	2.36	0.53
1:A:1005:ASP:OD2	1:A:1006:VAL:HG22	2.08	0.53
1:A:1104:VAL:HA	1:A:1219:VAL:CG1	2.39	0.53
1:A:1094:THR:HB	1:A:1220:ILE:HG23	1.89	0.53
1:A:1072:PRO:O	1:A:1076:ILE:HG12	2.09	0.53
1:F:6006:VAL:CG1	1:F:6084:LEU:HD11	2.39	0.53
1:D:4242:VAL:O	1:D:4246:VAL:HG23	2.08	0.53
1:D:4179:ARG:O	1:D:4181:LYS:N	2.42	0.53
1:E:5115:ARG:HH21	1:E:5121:LEU:HD13	1.72	0.53
1:B:2020:GLN:HA	1:B:2086:ILE:HA	1.91	0.53
1:C:3029:GLU:OE2	1:C:3030:ARG:NH1	2.42	0.53
1:B:2023:ILE:HD11	1:B:2249:ALA:HB2	1.90	0.53
1:E:5091:ARG:O	1:E:5215:MET:HA	2.08	0.53
1:B:2006:VAL:HG12	1:B:2010:GLY:H	1.73	0.53
1:C:3008:HIS:HD1	1:C:3008:HIS:H	1.56	0.53
1:F:6250:ARG:O	1:F:6253:LEU:HD12	2.09	0.53
1:D:4024:VAL:HB	1:D:4067:THR:CG2	2.39	0.53
1:B:2107:VAL:CG1	1:B:2151:THR:HG23	2.31	0.52
1:A:1024:VAL:HA	1:A:1065:CYS:O	2.09	0.52
1:F:6088:THR:HG21	1:F:6252:LEU:HD13	1.91	0.52
1:C:3127:GLU:HG2	1:D:4116:LEU:HD23	1.90	0.52
1:A:1249:ALA:O	1:A:1253:LEU:HG	2.09	0.52
1:A:1024:VAL:O	1:A:1091:ARG:HD2	2.09	0.52
1:F:6102:ILE:HG23	1:F:6152:HIS:CD2	2.44	0.52
1:A:1243:LYS:O	1:A:1247:GLU:HB2	2.09	0.52
1:D:4018:GLY:O	1:D:4020:GLN:NE2	2.43	0.52
1:D:4016:LEU:HD22	1:D:4063:ILE:CD1	2.39	0.52
1:F:6222:ASN:HB3	1:F:6225:GLN:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5011:LEU:HD22	1:E:5015:ASP:HB2	1.90	0.52
1:A:1131:VAL:HG22	1:A:1132:ALA:O	2.09	0.52
1:E:5021:LEU:HD23	1:E:5022:ALA:N	2.24	0.52
1:E:5086:ILE:N	1:E:5086:ILE:HD12	2.24	0.52
1:C:3086:ILE:N	1:C:3086:ILE:HD12	2.23	0.52
1:E:5038:MET:HG2	1:E:5057:LEU:CD1	2.36	0.52
1:E:5168:ARG:HG3	1:E:5168:ARG:HH11	1.74	0.52
1:B:2094:THR:CG2	1:B:2220:ILE:HG21	2.38	0.52
1:F:6158:SER:HB3	1:F:6197:MET:O	2.09	0.52
1:D:4009:LEU:CD1	1:D:4080:GLU:HB2	2.39	0.52
1:C:3007:PHE:HB3	1:C:3008:HIS:HD1	1.75	0.52
1:F:6099:GLN:CB	1:F:6102:ILE:HG12	2.37	0.52
1:B:2161:THR:O	1:B:2166:GLN:HG3	2.09	0.52
1:B:2012:THR:HG23	1:B:2015:ASP:H	1.74	0.52
1:A:1164:PRO:HG2	1:A:1165:GLY:H	1.74	0.52
1:E:5074:THR:O	1:E:5078:VAL:HG23	2.10	0.52
1:E:5011:LEU:HD21	1:E:5044:LEU:CB	2.40	0.52
1:F:6031:VAL:HG13	1:F:6064:VAL:CG1	2.34	0.52
1:A:1082:ALA:HA	1:A:1086:ILE:O	2.10	0.52
1:B:2028:PRO:HG3	1:B:2049:GLU:HG3	1.92	0.52
1:A:1098:ILE:HD12	1:A:1188:GLN:HG2	1.91	0.52
1:E:5006:VAL:HB	1:E:5080:GLU:HG2	1.91	0.52
1:C:3220:ILE:HG13	1:C:3234:MET:HG3	1.92	0.52
1:F:6123:PHE:HA	3:F:7002:HOH:O	2.10	0.52
1:C:3231:ALA:HA	1:C:3234:MET:HB2	1.91	0.52
1:D:4223:ARG:HG3	1:D:4223:ARG:NH1	2.24	0.52
1:A:1022:ALA:HB3	1:A:1086:ILE:HG21	1.92	0.51
1:B:2114:VAL:HG12	1:B:2116:LEU:HD21	1.91	0.51
1:B:2016:LEU:CG	1:B:2084:LEU:HD23	2.39	0.51
1:F:6006:VAL:HG11	1:F:6084:LEU:CD1	2.40	0.51
1:B:2163:TYR:HB2	1:B:2164:PRO:CD	2.40	0.51
1:E:5247:GLU:O	1:E:5251:ARG:HD2	2.10	0.51
1:E:5016:LEU:CG	1:E:5063:ILE:HD11	2.40	0.51
1:C:3187:TRP:HE3	1:C:3187:TRP:HA	1.75	0.51
1:B:2045:ALA:O	1:B:2051:THR:HG23	2.09	0.51
1:E:5094:THR:OG1	1:E:5220:ILE:HD13	2.10	0.51
1:C:3141:VAL:O	1:C:3145:LYS:HG3	2.10	0.51
1:A:1190:MET:CE	1:E:5208:SER:HB2	2.41	0.51
1:C:3009:LEU:HD13	1:C:3080:GLU:OE2	2.11	0.51
1:D:4009:LEU:HD22	1:D:4065:CYS:SG	2.51	0.51
1:F:6103:ASN:O	1:F:6106:ASP:OD2	2.28	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6236:GLN:HG2	1:F:6240:HIS:CE1	2.46	0.51
1:A:1042:VAL:HG21	1:A:1054:ARG:HH12	1.74	0.51
1:C:3165:GLY:CA	1:E:5122:HIS:HD2	2.22	0.51
1:D:4023:ILE:CD1	1:D:4090:LEU:HB2	2.41	0.51
1:B:2205:MET:O	1:B:2209:GLN:HG2	2.10	0.51
1:E:5171:THR:HB	1:E:5172:TYR:HD1	1.76	0.51
1:E:5009:LEU:HD11	1:E:5081:LEU:HD12	1.92	0.51
1:D:4251:ARG:NH1	1:D:4251:ARG:CG	2.72	0.51
1:C:3136:CYS:SG	1:C:3212:ARG:HD2	2.50	0.51
1:C:3063:ILE:HD11	1:C:3065:CYS:HB2	1.93	0.51
1:C:3095:THR:OG1	1:C:3096:GLY:N	2.44	0.51
1:D:4201:THR:O	1:D:4205:MET:HG2	2.11	0.51
1:B:2044:LEU:HD21	1:B:2054:ARG:CZ	2.41	0.51
1:E:5006:VAL:HG21	1:E:5009:LEU:HB2	1.93	0.51
1:F:6156:THR:CG2	1:F:6196:GLU:OE2	2.58	0.50
1:D:4049:GLU:HA	1:D:4049:GLU:OE2	2.10	0.50
1:A:1104:VAL:HA	1:A:1219:VAL:HB	1.93	0.50
1:D:4028:PRO:HB3	1:D:4051:THR:HB	1.93	0.50
1:A:1167:GLU:HG2	1:A:1169:TYR:HE1	1.75	0.50
1:E:5016:LEU:HD13	1:E:5063:ILE:CD1	2.41	0.50
1:D:4163:TYR:H	1:D:4164:PRO:HD2	1.76	0.50
1:D:4007:PHE:HD2	1:D:4008:HIS:CE1	2.30	0.50
1:B:2009:LEU:CD1	1:B:2080:GLU:HB2	2.41	0.50
1:F:6183:SER:O	1:F:6186:GLU:HB3	2.11	0.50
1:E:5009:LEU:CD1	1:E:5080:GLU:HB3	2.41	0.50
1:E:5230:ASN:HB3	1:E:5233:THR:OG1	2.11	0.50
1:E:5103:ASN:O	1:E:5106:ASP:OD2	2.28	0.50
1:A:1031:VAL:HG13	1:A:1064:VAL:HG12	1.94	0.50
1:E:5054:ARG:HB3	1:E:5054:ARG:NH1	2.27	0.50
1:F:6056:GLU:O	1:F:6056:GLU:HG2	2.11	0.50
1:E:5040:LYS:N	1:E:5041:PRO:HD3	2.26	0.50
1:B:2095:THR:O	1:B:2220:ILE:HD13	2.11	0.50
1:C:3115:ARG:NH1	1:C:3128:PHE:O	2.44	0.50
1:E:5177:VAL:HG13	1:E:5178:ARG:N	2.27	0.50
1:C:3186:GLU:HG3	1:C:3190:MET:HE3	1.94	0.50
1:D:4232:GLU:HG3	1:D:4233:THR:H	1.76	0.50
1:E:5098:ILE:CG2	1:E:5223:ARG:HH21	2.24	0.50
1:A:1127:GLU:HG2	1:E:5116:LEU:HD23	1.92	0.50
1:A:1154:GLY:N	1:A:1193:MET:HE1	2.27	0.50
1:A:1145:LYS:O	1:A:1148:GLY:N	2.44	0.50
1:A:1126:MET:CG	1:E:5126:MET:HG3	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5016:LEU:HB3	1:E:5019:ALA:CB	2.42	0.50
1:E:5175:ARG:NH1	1:E:5175:ARG:HG3	2.27	0.50
1:A:1120:SER:HB2	1:A:1204:THR:HG21	1.94	0.50
1:C:3187:TRP:CE3	1:C:3187:TRP:HA	2.46	0.50
1:D:4060:LYS:HG3	1:D:4253:LEU:HB3	1.94	0.50
1:B:2091:ARG:O	1:B:2215:MET:HE2	2.12	0.50
1:C:3021:LEU:HD12	1:C:3022:ALA:N	2.24	0.49
1:A:1104:VAL:HG22	1:A:1219:VAL:HG12	1.93	0.49
1:A:1202:LEU:HD12	1:A:1206:CYS:SG	2.52	0.49
1:B:2006:VAL:HG12	1:B:2009:LEU:H	1.76	0.49
1:F:6115:ARG:NH2	1:F:6121:LEU:HA	2.27	0.49
1:C:3179:ARG:NH1	1:C:3179:ARG:HG3	2.26	0.49
1:E:5158:SER:OG	1:E:5200:ALA:HB2	2.11	0.49
1:D:4108:LEU:CD1	1:D:4152:HIS:HB2	2.42	0.49
1:A:1138:THR:HA	1:E:5134:PHE:HZ	1.77	0.49
1:E:5168:ARG:HD3	1:E:5223:ARG:HH12	1.77	0.49
1:E:5096:GLY:HA2	1:E:5221:VAL:O	2.13	0.49
1:C:3152:HIS:CE1	3:C:7096:HOH:O	2.65	0.49
1:B:2058:ASP:HB2	1:B:2253:LEU:HD11	1.94	0.49
1:E:5090:LEU:HD11	1:E:5252:LEU:HD13	1.94	0.49
1:D:4107:VAL:HG21	1:D:4244:ILE:HD11	1.95	0.49
1:B:2163:TYR:HB2	1:B:2164:PRO:HD3	1.94	0.49
1:A:1136:CYS:SG	1:A:1212:ARG:HB3	2.52	0.49
1:C:3115:ARG:HB2	1:C:3126:MET:CE	2.41	0.49
1:F:6092:ILE:C	1:F:6092:ILE:HD13	2.33	0.49
1:D:4216:VAL:HG11	1:D:4245:VAL:HG13	1.94	0.49
1:C:3021:LEU:HD22	1:C:3252:LEU:HD11	1.94	0.49
1:B:2122:HIS:HB3	1:D:4161:THR:HG21	1.95	0.49
1:A:1081:LEU:HD12	1:A:1089:PHE:CE2	2.43	0.49
1:A:1081:LEU:O	1:A:1084:LEU:N	2.45	0.49
1:B:2032:GLU:HG3	1:B:2053:TRP:CZ2	2.46	0.49
1:D:4009:LEU:HG	1:D:4080:GLU:HB2	1.95	0.49
1:A:1023:ILE:HD12	1:A:1023:ILE:N	2.26	0.49
1:A:1239:SER:O	1:A:1242:VAL:HB	2.12	0.49
1:B:2042:VAL:HG13	1:B:2054:ARG:NH1	2.28	0.49
1:D:4097:ALA:HB3	1:D:4222:ASN:ND2	2.27	0.49
1:A:1116:LEU:HD21	1:A:1187:TRP:CZ2	2.48	0.49
1:D:4178:ARG:NE	1:D:4178:ARG:HA	2.27	0.49
1:D:4225:GLN:OE1	1:D:4225:GLN:HA	2.11	0.49
1:A:1125:PRO:CD	1:F:6177:VAL:HG21	2.38	0.49
1:B:2019:ALA:CB	1:B:2061:ALA:HB3	2.32	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3236:GLN:O	1:C:3240:HIS:HB2	2.13	0.49
1:F:6030:ARG:NH1	1:F:6033:LYS:HG3	2.28	0.49
1:E:5160:ASP:O	1:E:5161:THR:HG23	2.12	0.49
1:E:5078:VAL:HB	1:E:5205:MET:SD	2.53	0.49
1:F:6175:ARG:CB	1:F:6181:LYS:HE2	2.42	0.49
1:D:4104:VAL:O	1:D:4219:VAL:O	2.31	0.49
1:E:5033:LYS:O	1:E:5037:LEU:HD22	2.12	0.49
1:F:6198:GLU:H	1:F:6198:GLU:CD	2.16	0.49
1:B:2094:THR:HG22	1:B:2220:ILE:HG21	1.94	0.48
1:B:2141:VAL:O	1:B:2144:ALA:HB3	2.13	0.48
1:E:5252:LEU:C	1:E:5253:LEU:HG	2.33	0.48
1:F:6112:ALA:HA	1:F:6130:ALA:O	2.13	0.48
1:C:3171:THR:HB	1:E:5079:GLU:OE1	2.12	0.48
1:C:3023:ILE:O	1:C:3025:PRO:HD3	2.13	0.48
1:D:4220:ILE:HG13	1:D:4221:VAL:CG2	2.40	0.48
1:C:3031:VAL:CG2	1:C:3066:SER:HB2	2.43	0.48
1:D:4063:ILE:HB	1:D:4086:ILE:HD11	1.95	0.48
1:F:6176:VAL:HG12	1:F:6181:LYS:HE3	1.94	0.48
1:B:2156:THR:CG2	1:B:2196:GLU:HG2	2.35	0.48
1:C:3127:GLU:OE2	1:C:3127:GLU:N	2.44	0.48
1:D:4106:ASP:N	1:D:4106:ASP:OD1	2.46	0.48
1:C:3126:MET:CE	1:D:4127:GLU:HA	2.44	0.48
1:D:4175:ARG:CZ	1:D:4175:ARG:HB3	2.44	0.48
1:A:1200:ALA:O	1:A:1204:THR:HB	2.13	0.48
1:F:6220:ILE:O	1:F:6221:VAL:HB	2.14	0.48
1:F:6175:ARG:N	1:F:6175:ARG:NH1	2.55	0.48
1:F:6092:ILE:CD1	1:F:6241:ALA:HB1	2.44	0.48
1:E:5072:PRO:O	1:E:5076:ILE:HG12	2.13	0.48
1:C:3094:THR:O	1:C:3095:THR:HB	2.13	0.48
1:D:4102:ILE:HG12	1:D:4152:HIS:CE1	2.49	0.48
1:B:2232:GLU:HG2	1:B:2235:LYS:HG2	1.94	0.48
1:A:1156:THR:HG23	1:A:1194:ASN:ND2	2.28	0.48
1:C:3126:MET:HE3	1:D:4127:GLU:HA	1.96	0.48
1:C:3032:GLU:HG3	1:C:3033:LYS:N	2.28	0.48
1:D:4238:GLU:O	1:D:4241:ALA:N	2.46	0.48
1:B:2070:GLY:O	1:B:2073:SER:HB3	2.14	0.48
1:D:4168:ARG:NH1	1:D:4168:ARG:CB	2.77	0.48
1:E:5174:GLY:O	1:E:5176:VAL:HG23	2.13	0.48
1:B:2012:THR:HA	1:B:2084:LEU:HD11	1.95	0.48
1:F:6088:THR:HA	1:F:6212:ARG:O	2.13	0.48
1:F:6085:GLY:HA2	1:F:6087:ARG:NH2	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4038:MET:HE1	1:D:4057:LEU:HD23	1.95	0.48
1:D:4196:GLU:OE1	1:D:4199:SER:N	2.47	0.48
1:F:6177:VAL:HG13	1:F:6177:VAL:O	2.14	0.48
1:D:4109:VAL:O	1:D:4109:VAL:HG23	2.13	0.48
1:A:1145:LYS:NZ	1:A:1145:LYS:HB3	2.29	0.48
1:E:5012:THR:HG23	1:E:5014:ASN:N	2.29	0.48
1:A:1095:THR:OG1	1:A:1096:GLY:N	2.47	0.48
1:E:5236:GLN:O	1:E:5239:SER:HB2	2.13	0.48
1:A:1154:GLY:H	1:A:1193:MET:HE1	1.78	0.48
1:C:3057:LEU:CD1	1:C:3250:ARG:HG2	2.43	0.48
1:F:6121:LEU:CD1	1:F:6121:LEU:H	2.27	0.48
1:D:4015:ASP:CB	1:D:4044:LEU:HD13	2.43	0.48
1:E:5184:MET:HA	1:E:5187:TRP:CD1	2.45	0.48
1:F:6237:THR:HA	1:F:6240:HIS:CD2	2.49	0.47
1:F:6023:ILE:N	1:F:6023:ILE:CD1	2.76	0.47
1:E:5206:CYS:HB3	1:E:5211:LEU:O	2.14	0.47
1:E:5040:LYS:O	1:E:5042:VAL:HG23	2.14	0.47
1:F:6060:LYS:HB2	1:F:6253:LEU:HD22	1.96	0.47
1:F:6114:VAL:O	1:F:6116:LEU:HG	2.13	0.47
1:D:4015:ASP:HB3	1:D:4044:LEU:HD22	1.96	0.47
1:D:4031:VAL:HG13	1:D:4064:VAL:HG12	1.95	0.47
1:A:1247:GLU:O	1:A:1250:ARG:HB2	2.14	0.47
1:A:1016:LEU:HD22	1:A:1063:ILE:HG13	1.96	0.47
1:F:6012:THR:O	1:F:6015:ASP:HB2	2.15	0.47
1:E:5156:THR:HG23	1:E:5194:ASN:OD1	2.14	0.47
1:F:6016:LEU:HG	1:F:6063:ILE:HG13	1.96	0.47
1:C:3147:ILE:CD1	1:C:3244:ILE:HD11	2.44	0.47
1:E:5035:ALA:HA	1:E:5038:MET:HE3	1.97	0.47
1:E:5104:VAL:HA	1:E:5219:VAL:HG12	1.96	0.47
1:F:6179:ARG:HH11	1:F:6179:ARG:HB2	1.78	0.47
1:A:1149:ALA:HB2	1:A:1240:HIS:NE2	2.30	0.47
1:A:1138:THR:HA	1:E:5134:PHE:CZ	2.49	0.47
1:B:2049:GLU:OE2	1:D:4049:GLU:HB2	2.14	0.47
1:E:5009:LEU:CD1	1:E:5081:LEU:HD12	2.44	0.47
1:B:2161:THR:OG1	1:B:2164:PRO:HG2	2.14	0.47
1:B:2163:TYR:HB3	1:B:2171:THR:HG21	1.95	0.47
1:C:3133:ASP:OD2	1:C:3135:ALA:HB3	2.15	0.47
1:B:2021:LEU:H	1:B:2086:ILE:HD12	1.79	0.47
1:B:2021:LEU:C	1:B:2086:ILE:HD12	2.35	0.47
1:C:3022:ALA:HB2	1:C:3086:ILE:HG12	1.95	0.47
1:C:3229:PRO:HB2	1:C:3230:ASN:H	1.37	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1038:MET:HB3	1:A:1056:GLU:O	2.14	0.47
1:A:1187:TRP:HD1	1:A:1195:TYR:HH	1.62	0.47
1:D:4177:VAL:HG22	1:D:4178:ARG:N	2.29	0.47
1:E:5019:ALA:O	1:E:5020:GLN:CB	2.49	0.47
1:A:1016:LEU:HA	1:A:1063:ILE:CD1	2.41	0.47
1:A:1076:ILE:O	1:A:1080:GLU:HG2	2.14	0.47
1:F:6108:LEU:HB2	1:F:6193:MET:HE1	1.97	0.47
1:B:2113:SER:HA	1:B:2155:VAL:HG13	1.97	0.47
1:E:5196:GLU:HG3	1:E:5197:MET:N	2.30	0.47
1:E:5115:ARG:HG2	1:E:5130:ALA:HB2	1.97	0.47
1:C:3031:VAL:HG23	1:C:3066:SER:HB2	1.96	0.47
1:C:3106:ASP:O	1:C:3219:VAL:HG23	2.14	0.47
1:B:2238:GLU:O	1:B:2242:VAL:HG23	2.15	0.47
1:B:2092:ILE:HA	1:B:2216:VAL:O	2.14	0.47
1:C:3057:LEU:O	1:C:3060:LYS:HB2	2.15	0.47
1:A:1252:LEU:O	1:A:1253:LEU:C	2.54	0.47
1:A:1155:VAL:HG12	1:A:1192:VAL:HG22	1.97	0.47
1:F:6230:ASN:OD1	1:F:6232:GLU:HG3	2.15	0.47
1:C:3027:ASP:N	1:C:3027:ASP:OD1	2.48	0.47
1:B:2016:LEU:C	1:B:2018:GLY:H	2.19	0.47
1:A:1016:LEU:HD12	1:A:1084:LEU:O	2.15	0.47
1:D:4183:SER:O	1:D:4187:TRP:CD1	2.68	0.47
1:C:3124:ALA:HB1	1:D:4190:MET:HE3	1.97	0.47
1:B:2019:ALA:HB2	1:B:2061:ALA:CB	2.31	0.46
1:D:4028:PRO:HA	1:D:4031:VAL:HB	1.97	0.46
1:E:5016:LEU:HD13	1:E:5086:ILE:CD1	2.45	0.46
1:F:6163:TYR:CD2	1:F:6168:ARG:HD2	2.49	0.46
1:E:5169:TYR:CZ	1:E:5176:VAL:HG21	2.50	0.46
1:A:1009:LEU:HD13	1:A:1080:GLU:CG	2.45	0.46
1:E:5008:HIS:N	1:E:5080:GLU:OE2	2.42	0.46
1:A:1178:ARG:HA	1:A:1181:LYS:HE2	1.97	0.46
1:C:3138:THR:HA	1:D:4134:PHE:CZ	2.50	0.46
1:D:4230:ASN:N	1:D:4230:ASN:HD22	2.13	0.46
1:F:6150:THR:HG22	1:F:6152:HIS:NE2	2.30	0.46
1:D:4094:THR:HB	1:D:4220:ILE:CG2	2.45	0.46
1:B:2121:LEU:C	1:B:2123:PHE:H	2.17	0.46
1:D:4142:GLU:HB2	1:D:4251:ARG:HE	1.80	0.46
1:C:3039:ASP:C	1:C:3039:ASP:OD2	2.54	0.46
1:F:6165:GLY:HA2	1:F:6180:PHE:CD2	2.50	0.46
1:B:2028:PRO:HD3	1:B:2049:GLU:OE1	2.14	0.46
1:E:5005:ASP:HB2	1:E:5012:THR:HA	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4040:LYS:O	1:D:4042:VAL:HG23	2.16	0.46
1:D:4157:ALA:HB3	1:D:4195:TYR:CD1	2.50	0.46
1:E:5016:LEU:HB3	1:E:5019:ALA:HB2	1.97	0.46
1:F:6184:MET:O	1:F:6184:MET:HE2	2.16	0.46
1:F:6176:VAL:HG11	1:F:6180:PHE:C	2.35	0.46
1:A:1072:PRO:CD	1:F:6072:PRO:HG3	2.46	0.46
1:F:6179:ARG:NH1	1:F:6179:ARG:HB2	2.30	0.46
1:C:3091:ARG:HH11	1:C:3091:ARG:HG3	1.81	0.46
1:A:1175:ARG:CG	1:A:1175:ARG:HH11	2.29	0.46
1:B:2159:SER:HG	1:B:2165:GLY:HA3	1.80	0.46
1:C:3073:SER:OG	1:C:3074:THR:N	2.45	0.46
1:A:1024:VAL:HB	1:A:1067:THR:HG23	1.98	0.46
1:F:6079:GLU:O	1:F:6083:GLN:HG3	2.15	0.46
1:C:3108:LEU:O	1:C:3216:VAL:HA	2.15	0.46
1:A:1042:VAL:HG21	1:A:1054:ARG:NH1	2.31	0.46
1:B:2051:THR:H	1:B:2066:SER:HB3	1.80	0.46
1:E:5038:MET:HB3	1:E:5056:GLU:O	2.15	0.46
1:E:5044:LEU:HD11	1:E:5054:ARG:HB2	1.98	0.46
1:C:3008:HIS:ND1	1:C:3008:HIS:N	2.63	0.46
1:D:4247:GLU:HA	1:D:4250:ARG:HH12	1.80	0.46
1:B:2239:SER:OG	1:B:2240:HIS:N	2.48	0.46
1:C:3155:VAL:HG22	1:C:3192:VAL:HA	1.96	0.46
1:E:5147:ILE:HD12	1:E:5244:ILE:HG13	1.97	0.46
1:F:6109:VAL:CB	1:F:6153:VAL:HG22	2.44	0.46
1:E:5179:ARG:HE	1:E:5179:ARG:C	2.17	0.46
1:C:3186:GLU:HG3	1:C:3190:MET:CE	2.46	0.46
1:B:2071:GLY:O	1:B:2201:THR:HG21	2.16	0.46
1:D:4006:VAL:HG12	1:D:4010:GLY:H	1.81	0.46
1:E:5016:LEU:HD13	1:E:5086:ILE:HD11	1.98	0.46
1:C:3233:THR:HG23	1:C:3233:THR:O	2.15	0.46
1:F:6249:ALA:O	1:F:6253:LEU:CD1	2.64	0.46
1:E:5167:GLU:HB2	1:E:5180:PHE:O	2.16	0.46
1:D:4016:LEU:HD22	1:D:4063:ILE:HD11	1.98	0.45
1:B:2175:ARG:NH2	1:D:4208:SER:O	2.47	0.45
1:C:3060:LYS:HG3	1:C:3253:LEU:HD22	1.97	0.45
1:B:2159:SER:O	1:B:2197:MET:HG2	2.16	0.45
1:A:1113:SER:CB	1:A:1156:THR:O	2.64	0.45
1:C:3242:VAL:O	1:C:3245:VAL:HG12	2.16	0.45
1:F:6176:VAL:HG11	1:F:6180:PHE:H	1.80	0.45
1:E:5179:ARG:HG3	1:E:5180:PHE:N	2.31	0.45
1:E:5094:THR:O	1:E:5095:THR:HB	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1222:ASN:HB3	1:A:1225:GLN:NE2	2.32	0.45
1:F:6025:PRO:HG3	1:F:6031:VAL:HG22	1.99	0.45
1:B:2187:TRP:HD1	1:B:2195:TYR:OH	1.99	0.45
1:F:6183:SER:O	1:F:6186:GLU:N	2.48	0.45
1:E:5167:GLU:OE1	1:E:5184:MET:HG3	2.16	0.45
1:C:3243:LYS:HE2	1:C:3243:LYS:CA	2.47	0.45
1:E:5033:LYS:HD2	1:E:5033:LYS:HA	1.70	0.45
1:B:2206:CYS:SG	1:B:2213:ALA:HB2	2.57	0.45
1:D:4113:SER:HB3	1:D:4156:THR:O	2.17	0.45
1:A:1238:GLU:HG3	1:A:1238:GLU:H	1.60	0.45
1:F:6236:GLN:HG2	1:F:6240:HIS:NE2	2.32	0.45
1:B:2104:VAL:HA	1:B:2219:VAL:CG1	2.46	0.45
1:A:1011:LEU:CD2	1:A:1044:LEU:HB3	2.47	0.45
1:E:5187:TRP:O	1:E:5192:VAL:HG23	2.16	0.45
1:E:5095:THR:HG23	1:E:5096:GLY:N	2.31	0.45
1:D:4205:MET:O	1:D:4209:GLN:HG3	2.16	0.45
1:B:2131:VAL:O	1:B:2131:VAL:HG13	2.17	0.45
1:E:5018:GLY:O	1:E:5019:ALA:C	2.54	0.45
1:C:3063:ILE:C	1:C:3063:ILE:HD13	2.37	0.45
1:F:6030:ARG:HH12	1:F:6033:LYS:HG3	1.81	0.45
1:F:6092:ILE:CG1	1:F:6241:ALA:HB1	2.46	0.45
1:B:2067:THR:OG1	1:B:2074:THR:HA	2.17	0.45
1:D:4247:GLU:OE1	1:D:4250:ARG:NH1	2.48	0.45
1:C:3097:ALA:HA	1:C:3194:ASN:CB	2.47	0.45
1:C:3063:ILE:O	1:C:3063:ILE:HD13	2.16	0.45
1:F:6108:LEU:HD12	1:F:6108:LEU:O	2.16	0.45
1:D:4103:ASN:HB2	1:D:4106:ASP:OD1	2.16	0.45
1:B:2199:SER:HB3	1:B:2215:MET:HG3	1.98	0.45
1:F:6201:THR:O	1:F:6205:MET:HG2	2.16	0.45
1:F:6147:ILE:CG2	1:F:6244:ILE:HD11	2.42	0.45
1:F:6176:VAL:HG22	1:F:6177:VAL:N	2.31	0.45
1:B:2107:VAL:O	1:B:2151:THR:HA	2.17	0.45
1:D:4176:VAL:HG12	1:D:4180:PHE:HB3	1.99	0.45
1:F:6092:ILE:HB	1:F:6245:VAL:CG2	2.45	0.45
1:B:2028:PRO:CG	1:B:2049:GLU:HG3	2.47	0.45
1:E:5167:GLU:OE1	1:E:5184:MET:CG	2.65	0.45
1:B:2071:GLY:N	1:B:2072:PRO:HD2	2.31	0.45
1:D:4108:LEU:HD23	1:D:4193:MET:HB2	1.97	0.45
1:D:4095:THR:N	1:D:4218:GLY:O	2.47	0.45
1:D:4029:GLU:O	1:D:4029:GLU:CD	2.56	0.45
1:B:2161:THR:OG1	1:D:4122:HIS:ND1	2.44	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6014:ASN:O	1:F:6017:GLN:HG2	2.17	0.45
1:C:3016:LEU:HD23	1:C:3063:ILE:HG21	1.98	0.45
1:C:3147:ILE:HD13	1:C:3244:ILE:HD11	1.99	0.45
1:A:1030:ARG:HE	1:A:1030:ARG:HA	1.82	0.45
1:C:3185:GLU:HA	1:C:3188:GLN:HE21	1.82	0.45
1:B:2158:SER:HB2	1:B:2200:ALA:HB2	1.98	0.44
1:F:6080:GLU:HA	1:F:6083:GLN:HE21	1.82	0.44
1:F:6116:LEU:HD11	1:F:6187:TRP:CZ2	2.53	0.44
1:E:5192:VAL:HG12	1:E:5193:MET:N	2.32	0.44
1:B:2168:ARG:NH1	1:B:2168:ARG:HG3	2.30	0.44
1:C:3138:THR:HA	1:D:4134:PHE:HZ	1.82	0.44
1:A:1137:THR:O	1:A:1141:VAL:HG23	2.17	0.44
1:E:5016:LEU:HD22	1:E:5063:ILE:CG1	2.47	0.44
1:B:2019:ALA:CB	1:B:2061:ALA:O	2.65	0.44
1:F:6006:VAL:HG22	1:F:6011:LEU:H	1.80	0.44
1:F:6090:LEU:HD12	1:F:6249:ALA:HB2	1.98	0.44
1:F:6085:GLY:HA2	1:F:6087:ARG:HH22	1.82	0.44
1:E:5223:ARG:HH11	1:E:5223:ARG:HG3	1.82	0.44
1:A:1232:GLU:O	1:A:1232:GLU:HG3	2.17	0.44
1:E:5147:ILE:CD1	1:E:5244:ILE:HG13	2.47	0.44
1:F:6121:LEU:HD12	1:F:6121:LEU:N	2.31	0.44
1:E:5043:LYS:HB2	1:E:5053:TRP:CE2	2.52	0.44
1:E:5016:LEU:O	1:E:5061:ALA:HB1	2.17	0.44
1:F:6163:TYR:N	1:F:6164:PRO:HD2	2.31	0.44
1:E:5175:ARG:CZ	1:E:5177:VAL:HA	2.47	0.44
1:B:2138:THR:HA	1:F:6134:PHE:HZ	1.82	0.44
1:C:3124:ALA:CB	1:D:4190:MET:HE3	2.47	0.44
1:D:4071:GLY:N	1:D:4072:PRO:CD	2.81	0.44
1:A:1190:MET:HE1	1:E:5124:ALA:HB2	2.00	0.44
1:D:4038:MET:HB2	1:D:4055:ALA:CB	2.46	0.44
1:A:1127:GLU:HA	1:E:5126:MET:SD	2.57	0.44
1:D:4166:GLN:HA	1:D:4195:TYR:CE2	2.52	0.44
1:C:3119:ALA:O	1:C:3122:HIS:HB2	2.18	0.44
1:B:2030:ARG:NH1	1:B:2093:GLY:HA2	2.32	0.44
1:F:6046:SER:CB	1:F:6051:THR:HG23	2.35	0.44
1:C:3140:LEU:HD23	1:C:3248:ALA:HB2	1.99	0.44
1:A:1151:THR:HG22	1:A:1152:HIS:N	2.32	0.44
1:D:4005:ASP:OD2	1:D:4011:LEU:O	2.36	0.44
1:C:3116:LEU:HD13	1:C:3180:PHE:HZ	1.81	0.44
1:A:1108:LEU:HA	1:A:1152:HIS:O	2.17	0.44
1:E:5107:VAL:HG23	1:E:5216:VAL:HG23	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2180:PHE:HA	1:B:2183:SER:OG	2.17	0.44
1:A:1083:GLN:HB3	1:A:1083:GLN:HE21	1.59	0.44
1:D:4099:GLN:HA	1:D:4099:GLN:OE1	2.18	0.44
1:C:3102:ILE:O	1:C:3225:GLN:OE1	2.35	0.44
1:C:3107:VAL:O	1:C:3108:LEU:HD23	2.17	0.44
1:D:4230:ASN:N	1:D:4230:ASN:ND2	2.65	0.44
1:C:3070:GLY:N	1:C:3198:GLU:OE2	2.49	0.44
1:D:4068:GLY:HA3	1:D:4073:SER:OG	2.18	0.44
1:B:2242:VAL:O	1:B:2246:VAL:HG23	2.18	0.43
1:E:5086:ILE:CD1	1:E:5086:ILE:H	2.31	0.43
1:B:2019:ALA:O	1:B:2086:ILE:HD13	2.18	0.43
1:E:5176:VAL:O	1:E:5177:VAL:HG12	2.18	0.43
1:C:3161:THR:HG21	1:E:5122:HIS:HB2	2.00	0.43
1:B:2028:PRO:HD3	1:B:2049:GLU:CG	2.48	0.43
1:B:2129:PRO:HD3	1:F:6114:VAL:HA	2.00	0.43
1:E:5071:GLY:N	1:E:5072:PRO:CD	2.81	0.43
1:E:5114:VAL:O	1:E:5116:LEU:N	2.51	0.43
1:B:2163:TYR:HA	1:B:2168:ARG:HB2	1.98	0.43
1:D:4137:THR:O	1:D:4141:VAL:HG23	2.18	0.43
1:E:5086:ILE:HG22	1:E:5089:PHE:CE1	2.52	0.43
1:F:6024:VAL:HG23	1:F:6024:VAL:O	2.17	0.43
1:B:2082:ALA:C	1:B:2084:LEU:H	2.20	0.43
1:D:4233:THR:HA	1:D:4236:GLN:OE1	2.18	0.43
1:C:3099:GLN:HA	1:C:3100:PRO:HD3	1.80	0.43
1:F:6081:LEU:HD22	1:F:6086:ILE:HD12	1.99	0.43
1:C:3038:MET:HB3	1:C:3057:LEU:HD23	2.00	0.43
1:E:5011:LEU:HD22	1:E:5015:ASP:CB	2.48	0.43
1:E:5044:LEU:HD21	1:E:5054:ARG:HH12	1.82	0.43
1:D:4249:ALA:O	1:D:4253:LEU:HG	2.17	0.43
1:C:3101:HIS:CE1	1:C:3102:ILE:HG13	2.53	0.43
1:F:6149:ALA:O	1:F:6151:THR:N	2.51	0.43
1:E:5138:THR:O	1:E:5142:GLU:HG2	2.18	0.43
1:B:2143:ALA:HB1	1:B:2247:GLU:HB2	1.99	0.43
1:D:4164:PRO:HA	1:D:4169:TYR:CE2	2.53	0.43
1:E:5145:LYS:C	1:E:5147:ILE:H	2.22	0.43
1:E:5091:ARG:HG2	1:E:5215:MET:HG3	2.00	0.43
1:F:6141:VAL:CG1	1:F:6153:VAL:HG21	2.41	0.43
1:C:3092:ILE:HD13	1:C:3093:GLY:N	2.32	0.43
1:F:6206:CYS:HB3	1:F:6211:LEU:O	2.18	0.43
1:C:3025:PRO:HD2	1:C:3065:CYS:O	2.18	0.43
1:F:6167:GLU:CG	1:F:6167:GLU:O	2.65	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6176:VAL:HG11	1:F:6180:PHE:CA	2.48	0.43
1:A:1017:GLN:HG3	1:A:1054:ARG:NE	2.25	0.43
1:F:6092:ILE:HA	1:F:6216:VAL:O	2.19	0.43
1:F:6216:VAL:HG22	1:F:6217:ALA:N	2.34	0.43
1:C:3092:ILE:O	1:C:3092:ILE:HG23	2.19	0.43
1:D:4112:ALA:HB2	1:D:4131:VAL:HA	2.00	0.43
1:A:1228:ILE:O	1:A:1228:ILE:HG13	2.18	0.43
1:F:6102:ILE:HD12	1:F:6152:HIS:CE1	2.54	0.43
1:D:4116:LEU:HD11	1:D:4187:TRP:CZ2	2.53	0.43
1:F:6143:ALA:CA	1:F:6251:ARG:HH12	2.30	0.43
1:E:5233:THR:O	1:E:5236:GLN:HB3	2.18	0.43
1:B:2070:GLY:C	1:B:2072:PRO:HD2	2.38	0.43
1:B:2167:GLU:HG2	1:B:2169:TYR:CE1	2.54	0.43
1:E:5022:ALA:CA	1:E:5063:ILE:O	2.60	0.43
1:B:2156:THR:HG22	1:B:2157:ALA:N	2.34	0.43
1:D:4007:PHE:CD2	1:D:4008:HIS:CE1	3.06	0.43
1:D:4107:VAL:HG11	1:D:4244:ILE:CD1	2.47	0.43
1:C:3122:HIS:O	1:E:5165:GLY:CA	2.66	0.43
1:F:6017:GLN:HG3	1:F:6054:ARG:HD2	2.01	0.43
1:C:3149:ALA:O	1:C:3151:THR:HG22	2.19	0.43
1:E:5089:PHE:N	1:E:5089:PHE:CD1	2.86	0.43
1:E:5147:ILE:HD12	1:E:5244:ILE:CG1	2.49	0.43
1:A:1072:PRO:HG2	1:F:6070:GLY:HA3	2.01	0.43
1:F:6109:VAL:HB	1:F:6153:VAL:HG13	1.99	0.43
1:B:2127:GLU:HA	1:F:6126:MET:SD	2.59	0.43
1:A:1163:TYR:HA	1:A:1168:ARG:HB2	2.01	0.43
1:D:4178:ARG:NE	1:D:4178:ARG:CA	2.80	0.43
1:D:4216:VAL:CG1	1:D:4245:VAL:HG13	2.49	0.43
1:F:6156:THR:HG21	1:F:6196:GLU:OE2	2.19	0.43
1:A:1033:LYS:O	1:A:1036:ALA:HB3	2.19	0.43
1:A:1035:ALA:HA	1:A:1038:MET:HE2	2.01	0.43
1:E:5054:ARG:NH1	1:E:5054:ARG:CB	2.82	0.43
1:D:4038:MET:HE1	1:D:4062:VAL:HG21	1.99	0.43
1:E:5085:GLY:HA2	1:E:5087:ARG:HH21	1.84	0.43
1:D:4099:GLN:HA	1:D:4100:PRO:HD3	1.82	0.43
1:D:4125:PRO:C	1:D:4127:GLU:H	2.23	0.43
1:F:6104:VAL:HG12	1:F:6222:ASN:ND2	2.33	0.43
1:A:1022:ALA:O	1:A:1089:PHE:HA	2.18	0.43
1:E:5163:TYR:HB3	1:E:5164:PRO:CD	2.46	0.43
1:E:5243:LYS:O	1:E:5247:GLU:HB2	2.18	0.43
1:A:1242:VAL:O	1:A:1246:VAL:HG23	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1155:VAL:CG1	1:A:1192:VAL:HG22	2.49	0.43
1:F:6169:TYR:O	1:F:6170:ASP:OD2	2.37	0.43
1:B:2220:ILE:HB	1:B:2234:MET:SD	2.59	0.42
1:A:1052:SER:HB3	1:A:1065:CYS:SG	2.59	0.42
1:F:6156:THR:HG23	1:F:6194:ASN:OD1	2.19	0.42
1:F:6136:CYS:SG	1:F:6212:ARG:HB3	2.59	0.42
1:B:2024:VAL:O	1:B:2091:ARG:HG3	2.18	0.42
1:D:4199:SER:O	1:D:4203:LEU:HG	2.18	0.42
1:A:1143:ALA:CB	1:A:1248:ALA:HB2	2.49	0.42
1:C:3071:GLY:N	1:C:3072:PRO:CD	2.82	0.42
1:A:1017:GLN:CD	1:A:1054:ARG:HH21	2.23	0.42
1:A:1144:ALA:O	1:A:1149:ALA:HB3	2.20	0.42
1:E:5039:ASP:O	1:E:5056:GLU:N	2.48	0.42
1:C:3163:TYR:HB2	1:C:3164:PRO:CD	2.50	0.42
1:C:3165:GLY:HA3	1:E:5122:HIS:HD2	1.83	0.42
1:F:6114:VAL:O	1:F:6116:LEU:N	2.52	0.42
1:F:6186:GLU:O	1:F:6190:MET:HG2	2.19	0.42
1:D:4035:ALA:O	1:D:4038:MET:N	2.42	0.42
1:E:5109:VAL:O	1:E:5153:VAL:HA	2.19	0.42
1:E:5140:LEU:HD23	1:E:5248:ALA:CB	2.49	0.42
1:D:4194:ASN:OD1	1:D:4194:ASN:N	2.52	0.42
1:B:2040:LYS:N	1:B:2041:PRO:CD	2.82	0.42
1:F:6233:THR:OG1	1:F:6234:MET:N	2.53	0.42
1:E:5057:LEU:O	1:E:5060:LYS:HG2	2.19	0.42
1:E:5052:SER:HB3	1:E:5065:CYS:SG	2.59	0.42
1:B:2179:ARG:HG2	1:B:2180:PHE:CD1	2.54	0.42
1:C:3179:ARG:HG3	3:C:7125:HOH:O	2.18	0.42
1:A:1187:TRP:HD1	1:A:1195:TYR:OH	2.02	0.42
1:F:6044:LEU:HD21	1:F:6054:ARG:CB	2.49	0.42
1:D:4111:THR:O	1:D:4132:ALA:N	2.40	0.42
1:B:2223:ARG:HH11	1:B:2223:ARG:HG2	1.84	0.42
1:B:2083:GLN:HE22	1:D:4171:THR:HG22	1.84	0.42
1:D:4161:THR:OG1	1:D:4180:PHE:HE2	2.03	0.42
1:A:1052:SER:HA	1:A:1064:VAL:O	2.20	0.42
1:E:5012:THR:C	1:E:5014:ASN:N	2.73	0.42
1:C:3109:VAL:O	1:C:3153:VAL:HA	2.20	0.42
1:B:2104:VAL:HA	1:B:2219:VAL:HG12	2.01	0.42
1:D:4161:THR:HB	1:D:4164:PRO:CD	2.45	0.42
1:B:2244:ILE:O	1:B:2248:ALA:CB	2.67	0.42
1:A:1011:LEU:HD21	1:A:1044:LEU:HB2	1.99	0.42
1:D:4079:GLU:O	1:D:4083:GLN:HG3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1140:LEU:HD22	1:A:1216:VAL:CG1	2.49	0.42
1:F:6230:ASN:N	1:F:6234:MET:HE2	2.35	0.42
1:A:1009:LEU:HD22	1:A:1080:GLU:HB3	2.01	0.42
1:F:6109:VAL:HB	1:F:6153:VAL:CG2	2.50	0.42
1:F:6006:VAL:CG2	1:F:6010:GLY:H	2.29	0.42
1:F:6249:ALA:O	1:F:6253:LEU:HD12	2.20	0.42
1:E:5038:MET:CG	1:E:5057:LEU:HD13	2.43	0.42
1:E:5077:ALA:O	1:E:5081:LEU:CD1	2.66	0.42
1:F:6044:LEU:HD21	1:F:6054:ARG:HB3	2.02	0.42
1:C:3124:ALA:HB1	1:D:4190:MET:CE	2.48	0.42
1:F:6124:ALA:HB1	1:F:6128:PHE:CB	2.50	0.42
1:D:4021:LEU:HD21	1:D:4090:LEU:HG	2.01	0.42
1:A:1127:GLU:CD	1:A:1127:GLU:H	2.23	0.42
1:C:3205:MET:O	1:C:3209:GLN:CG	2.67	0.42
1:A:1087:ARG:HD3	1:A:1087:ARG:HA	1.88	0.42
1:A:1010:GLY:O	1:A:1045:ALA:HB2	2.20	0.42
1:D:4011:LEU:HB2	1:D:4084:LEU:HD21	2.01	0.42
1:E:5086:ILE:H	1:E:5086:ILE:HD12	1.85	0.42
1:F:6239:SER:C	1:F:6242:VAL:HG12	2.40	0.42
1:D:4158:SER:HB3	1:D:4200:ALA:HB2	2.00	0.42
1:A:1187:TRP:HA	1:A:1187:TRP:HE3	1.85	0.42
1:B:2039:ASP:HB2	1:B:2056:GLU:O	2.19	0.42
1:F:6110:THR:HA	1:F:6154:GLY:O	2.20	0.42
1:E:5015:ASP:HB3	1:E:5044:LEU:HD13	2.01	0.41
1:F:6118:GLY:HA2	1:F:6121:LEU:HD13	2.02	0.41
1:D:4166:GLN:OE1	1:D:4166:GLN:N	2.53	0.41
1:F:6198:GLU:N	1:F:6198:GLU:CD	2.74	0.41
1:C:3163:TYR:HB2	1:C:3164:PRO:HD3	2.02	0.41
1:E:5027:ASP:HB2	1:E:5028:PRO:HD2	2.02	0.41
1:B:2127:GLU:HB2	1:F:6116:LEU:HD23	2.01	0.41
1:D:4028:PRO:HA	1:D:4031:VAL:HG23	2.02	0.41
1:B:2091:ARG:NE	1:B:2215:MET:HE3	2.36	0.41
1:C:3085:GLY:O	1:C:3087:ARG:HG3	2.20	0.41
1:B:2023:ILE:HB	1:B:2064:VAL:HG13	2.02	0.41
1:C:3176:VAL:O	1:C:3181:LYS:HD3	2.19	0.41
1:D:4038:MET:CE	1:D:4057:LEU:HD23	2.51	0.41
1:D:4040:LYS:N	1:D:4041:PRO:CD	2.83	0.41
1:A:1014:ASN:ND2	1:A:1014:ASN:O	2.53	0.41
1:D:4125:PRO:HB2	1:D:4127:GLU:OE1	2.20	0.41
1:B:2114:VAL:HG11	1:B:2187:TRP:CH2	2.55	0.41
1:C:3011:LEU:HD23	1:C:3045:ALA:CB	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6021:LEU:HD23	1:F:6021:LEU:C	2.41	0.41
1:A:1048:ARG:HG2	1:F:6049:GLU:OE2	2.19	0.41
1:A:1163:TYR:O	1:A:1168:ARG:HB2	2.19	0.41
1:F:6098:ILE:CG2	1:F:6184:MET:HG2	2.51	0.41
1:B:2023:ILE:O	1:B:2064:VAL:HA	2.20	0.41
1:E:5166:GLN:NE2	1:E:5168:ARG:HH12	2.18	0.41
1:E:5076:ILE:O	1:E:5080:GLU:HB2	2.21	0.41
1:C:3222:ASN:ND2	1:C:3224:THR:OG1	2.53	0.41
1:D:4247:GLU:OE1	1:D:4250:ARG:NH2	2.52	0.41
1:B:2083:GLN:HE22	1:D:4171:THR:CG2	2.33	0.41
1:A:1234:MET:O	1:A:1237:THR:HB	2.20	0.41
1:F:6221:VAL:HG23	1:F:6227:GLU:O	2.20	0.41
1:A:1009:LEU:HD21	1:A:1081:LEU:HD23	2.03	0.41
1:D:4057:LEU:HB3	1:D:4253:LEU:CD1	2.50	0.41
1:D:4046:SER:HA	1:D:4051:THR:HA	2.03	0.41
1:A:1196:GLU:OE2	1:A:1199:SER:N	2.53	0.41
1:B:2054:ARG:CB	1:B:2054:ARG:CZ	2.95	0.41
1:F:6088:THR:HG23	1:F:6136:CYS:SG	2.61	0.41
1:B:2175:ARG:NH2	1:D:4208:SER:HB2	2.30	0.41
1:D:4103:ASN:O	1:D:4219:VAL:HG11	2.21	0.41
1:E:5162:PHE:O	1:E:5163:TYR:HB2	2.21	0.41
1:A:1187:TRP:HA	1:A:1187:TRP:CE3	2.56	0.41
1:B:2133:ASP:OD1	1:B:2135:ALA:HB3	2.21	0.41
1:C:3103:ASN:N	1:C:3106:ASP:OD2	2.54	0.41
1:C:3117:ASP:HA	1:C:3160:ASP:OD2	2.21	0.41
1:E:5100:PRO:O	1:E:5225:GLN:NE2	2.46	0.41
1:B:2156:THR:HA	1:B:2194:ASN:HD21	1.86	0.41
1:F:6008:HIS:HB3	1:F:6050:PHE:CE1	2.54	0.41
1:F:6076:ILE:O	1:F:6080:GLU:HB2	2.20	0.41
1:E:5230:ASN:O	1:E:5234:MET:HG3	2.21	0.41
1:A:1250:ARG:HA	1:A:1253:LEU:HD12	2.02	0.41
1:D:4067:THR:CG2	1:D:4074:THR:HG23	2.51	0.41
1:C:3141:VAL:HG12	1:C:3145:LYS:HE2	2.02	0.41
1:E:5086:ILE:CD1	1:E:5086:ILE:N	2.83	0.41
1:B:2021:LEU:HD23	1:B:2021:LEU:C	2.41	0.41
1:C:3088:THR:HG21	1:C:3252:LEU:HD11	1.99	0.41
1:F:6156:THR:HG22	1:F:6196:GLU:OE2	2.20	0.41
1:F:6109:VAL:O	1:F:6153:VAL:HA	2.20	0.41
1:F:6008:HIS:CG	1:F:6076:ILE:HG21	2.55	0.41
1:F:6187:TRP:CE3	1:F:6190:MET:HG3	2.56	0.41
1:F:6115:ARG:HH22	1:F:6121:LEU:HA	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5008:HIS:CD2	1:E:5076:ILE:HG21	2.56	0.41
1:E:5095:THR:N	1:E:5218:GLY:O	2.53	0.41
1:E:5049:GLU:OE2	1:E:5049:GLU:O	2.39	0.41
1:D:4081:LEU:HG	1:D:4086:ILE:HD12	2.03	0.41
1:F:6175:ARG:CD	1:F:6175:ARG:H	2.31	0.41
1:E:5006:VAL:HB	1:E:5080:GLU:OE2	2.20	0.41
1:C:3092:ILE:C	1:C:3092:ILE:HD13	2.41	0.41
1:C:3103:ASN:ND2	1:C:3103:ASN:N	2.69	0.41
1:B:2234:MET:O	1:B:2238:GLU:HG3	2.20	0.40
1:A:1092:ILE:HD13	1:A:1093:GLY:N	2.36	0.40
1:D:4008:HIS:HB2	1:D:4080:GLU:OE1	2.21	0.40
1:F:6012:THR:CG2	1:F:6014:ASN:OD1	2.69	0.40
1:B:2035:ALA:HA	1:B:2038:MET:SD	2.62	0.40
1:F:6222:ASN:O	1:F:6223:ARG:C	2.59	0.40
1:F:6024:VAL:HB	1:F:6067:THR:HG21	2.03	0.40
1:E:5015:ASP:HB3	1:E:5044:LEU:HD22	2.03	0.40
1:D:4142:GLU:CB	1:D:4251:ARG:HE	2.34	0.40
1:D:4053:TRP:HB3	1:D:4054:ARG:H	1.61	0.40
1:B:2135:ALA:HA	1:B:2138:THR:OG1	2.21	0.40
1:A:1226:GLN:HE21	1:A:1226:GLN:HB2	1.65	0.40
1:C:3086:ILE:H	1:C:3086:ILE:CD1	2.26	0.40
1:B:2195:TYR:O	1:B:2196:GLU:HB3	2.22	0.40
1:F:6046:SER:HB2	1:F:6051:THR:CG2	2.37	0.40
1:A:1009:LEU:HD13	1:A:1080:GLU:HB2	2.03	0.40
1:E:5162:PHE:N	1:E:5166:GLN:OE1	2.54	0.40
1:C:3049:GLU:CD	1:E:5049:GLU:HG2	2.41	0.40
1:C:3097:ALA:HA	1:C:3194:ASN:HB3	2.04	0.40
1:D:4161:THR:OG1	1:D:4164:PRO:HG2	2.21	0.40
1:E:5146:SER:O	1:E:5147:ILE:HG13	2.22	0.40
1:E:5076:ILE:HG22	1:E:5080:GLU:OE1	2.22	0.40
1:E:5228:ILE:HA	1:E:5229:PRO:HD2	1.91	0.40
1:C:3107:VAL:C	1:C:3108:LEU:HD23	2.42	0.40
1:D:4067:THR:CB	1:D:4074:THR:HG23	2.50	0.40
1:A:1163:TYR:CD2	1:A:1171:THR:HG22	2.57	0.40
1:A:1200:ALA:O	1:A:1204:THR:CB	2.70	0.40
1:D:4092:ILE:HB	1:D:4245:VAL:HG11	2.02	0.40
1:F:6176:VAL:HG21	1:F:6180:PHE:HD1	1.82	0.40
1:D:4117:ASP:N	1:D:4158:SER:O	2.54	0.40
1:C:3060:LYS:CB	1:C:3253:LEU:HD22	2.52	0.40
1:C:3136:CYS:O	1:C:3140:LEU:HG	2.21	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	248/253 (98%)	208 (84%)	33 (13%)	7 (3%)	6	9
1	B	248/253 (98%)	203 (82%)	38 (15%)	7 (3%)	6	9
1	C	248/253 (98%)	190 (77%)	38 (15%)	20 (8%)	1	1
1	D	248/253 (98%)	198 (80%)	40 (16%)	10 (4%)	4	4
1	E	248/253 (98%)	193 (78%)	38 (15%)	17 (7%)	1	1
1	F	248/253 (98%)	200 (81%)	31 (12%)	17 (7%)	1	1
All	All	1488/1518 (98%)	1192 (80%)	218 (15%)	78 (5%)	2	2

All (78) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1007	PHE
1	A	1230	ASN
1	A	1231	ALA
1	B	2048	ARG
1	C	3006	VAL
1	C	3007	PHE
1	C	3229	PRO
1	D	4172	TYR
1	D	4173	SER
1	D	4180	PHE
1	E	5019	ALA
1	E	5046	SER
1	E	5115	ARG
1	E	5163	TYR
1	E	5177	VAL
1	E	5229	PRO
1	F	6115	ARG
1	F	6150	THR
1	F	6223	ARG
1	F	6226	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1234	MET
1	A	1251	ARG
1	B	2077	ALA
1	B	2240	HIS
1	C	3005	ASP
1	C	3046	SER
1	C	3070	GLY
1	C	3104	VAL
1	C	3209	GLN
1	C	3238	GLU
1	D	4006	VAL
1	D	4054	ARG
1	E	5170	ASP
1	E	5226	GLN
1	F	6162	PHE
1	F	6169	TYR
1	F	6170	ASP
1	F	6175	ARG
1	F	6179	ARG
1	F	6221	VAL
1	C	3012	THR
1	C	3044	LEU
1	C	3226	GLN
1	C	3230	ASN
1	D	4118	GLY
1	E	5147	ILE
1	E	5200	ALA
1	B	2038	MET
1	B	2047	HIS
1	C	3057	LEU
1	C	3163	TYR
1	D	4117	ASP
1	D	4126	MET
1	D	4163	TYR
1	E	5150	THR
1	E	5166	GLN
1	F	6056	GLU
1	F	6176	VAL
1	F	6177	VAL
1	A	1163	TYR
1	C	3252	LEU
1	D	4177	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	5013	LYS
1	E	5026	GLY
1	E	5168	ARG
1	F	6121	LEU
1	F	6234	MET
1	B	2016	LEU
1	C	3042	VAL
1	C	3150	THR
1	E	5252	LEU
1	F	6025	PRO
1	F	6171	THR
1	B	2163	TYR
1	E	5174	GLY
1	A	1118	GLY
1	C	3026	GLY
1	C	3210	GLY

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	199/202 (98%)	173 (87%)	26 (13%)	5	9
1	B	199/202 (98%)	175 (88%)	24 (12%)	6	11
1	C	199/202 (98%)	169 (85%)	30 (15%)	3	6
1	D	199/202 (98%)	169 (85%)	30 (15%)	3	6
1	E	199/202 (98%)	166 (83%)	33 (17%)	3	5
1	F	199/202 (98%)	165 (83%)	34 (17%)	2	4
All	All	1194/1212 (98%)	1017 (85%)	177 (15%)	4	7

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1006	VAL
1	A	1009	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1013	LYS
1	A	1014	ASN
1	A	1020	GLN
1	A	1030	ARG
1	A	1039	ASP
1	A	1051	THR
1	A	1075	SER
1	A	1083	GLN
1	A	1090	LEU
1	A	1092	ILE
1	A	1113	SER
1	A	1160	ASP
1	A	1175	ARG
1	A	1179	ARG
1	A	1184	MET
1	A	1187	TRP
1	A	1216	VAL
1	A	1222	ASN
1	A	1226	GLN
1	A	1227	GLU
1	A	1228	ILE
1	A	1236	GLN
1	A	1238	GLU
1	A	1247	GLU
1	B	2011	LEU
1	B	2015	ASP
1	B	2016	LEU
1	B	2020	GLN
1	B	2034	ILE
1	B	2040	LYS
1	B	2042	VAL
1	B	2054	ARG
1	B	2057	LEU
1	B	2064	VAL
1	B	2126	MET
1	B	2127	GLU
1	B	2138	THR
1	B	2178	ARG
1	B	2194	ASN
1	B	2196	GLU
1	B	2202	LEU
1	B	2215	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	2220	ILE
1	B	2222	ASN
1	B	2224	THR
1	B	2225	GLN
1	B	2236	GLN
1	B	2247	GLU
1	C	3006	VAL
1	C	3007	PHE
1	C	3008	HIS
1	C	3020	GLN
1	C	3027	ASP
1	C	3033	LYS
1	C	3048	ARG
1	C	3054	ARG
1	C	3057	LEU
1	C	3062	VAL
1	C	3063	ILE
1	C	3075	SER
1	C	3083	GLN
1	C	3087	ARG
1	C	3092	ILE
1	C	3104	VAL
1	C	3121	LEU
1	C	3138	THR
1	C	3151	THR
1	C	3160	ASP
1	C	3175	ARG
1	C	3179	ARG
1	C	3187	TRP
1	C	3209	GLN
1	C	3222	ASN
1	C	3227	GLU
1	C	3228	ILE
1	C	3237	THR
1	C	3243	LYS
1	C	3247	GLU
1	D	4005	ASP
1	D	4016	LEU
1	D	4021	LEU
1	D	4048	ARG
1	D	4057	LEU
1	D	4058	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	4084	LEU
1	D	4092	ILE
1	D	4106	ASP
1	D	4111	THR
1	D	4113	SER
1	D	4151	THR
1	D	4166	GLN
1	D	4168	ARG
1	D	4176	VAL
1	D	4180	PHE
1	D	4193	MET
1	D	4196	GLU
1	D	4202	LEU
1	D	4215	MET
1	D	4221	VAL
1	D	4223	ARG
1	D	4225	GLN
1	D	4228	ILE
1	D	4230	ASN
1	D	4232	GLU
1	D	4233	THR
1	D	4245	VAL
1	D	4247	GLU
1	D	4251	ARG
1	E	5005	ASP
1	E	5016	LEU
1	E	5032	GLU
1	E	5037	LEU
1	E	5043	LYS
1	E	5046	SER
1	E	5056	GLU
1	E	5063	ILE
1	E	5087	ARG
1	E	5088	THR
1	E	5092	ILE
1	E	5094	THR
1	E	5098	ILE
1	E	5107	VAL
1	E	5108	LEU
1	E	5111	THR
1	E	5121	LEU
1	E	5163	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	5166	GLN
1	E	5170	ASP
1	E	5172	TYR
1	E	5173	SER
1	E	5177	VAL
1	E	5179	ARG
1	E	5181	LYS
1	E	5184	MET
1	E	5186	GLU
1	E	5193	MET
1	E	5195	TYR
1	E	5196	GLU
1	E	5228	ILE
1	E	5250	ARG
1	E	5251	ARG
1	F	6015	ASP
1	F	6017	GLN
1	F	6020	GLN
1	F	6030	ARG
1	F	6056	GLU
1	F	6057	LEU
1	F	6092	ILE
1	F	6094	THR
1	F	6103	ASN
1	F	6104	VAL
1	F	6107	VAL
1	F	6111	THR
1	F	6137	THR
1	F	6160	ASP
1	F	6163	TYR
1	F	6167	GLU
1	F	6172	TYR
1	F	6175	ARG
1	F	6184	MET
1	F	6186	GLU
1	F	6188	GLN
1	F	6193	MET
1	F	6195	TYR
1	F	6196	GLU
1	F	6211	LEU
1	F	6215	MET
1	F	6219	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	6223	ARG
1	F	6226	GLN
1	F	6230	ASN
1	F	6244	ILE
1	F	6245	VAL
1	F	6247	GLU
1	F	6251	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1014	ASN
1	A	1047	HIS
1	A	1083	GLN
1	A	1101	HIS
1	A	1152	HIS
1	A	1188	GLN
1	A	1225	GLN
1	A	1226	GLN
1	B	2008	HIS
1	B	2122	HIS
1	B	2194	ASN
1	B	2222	ASN
1	B	2236	GLN
1	C	3014	ASN
1	C	3017	GLN
1	C	3047	HIS
1	C	3103	ASN
1	C	3152	HIS
1	C	3188	GLN
1	C	3209	GLN
1	D	4014	ASN
1	D	4226	GLN
1	D	4230	ASN
1	D	4240	HIS
1	E	5101	HIS
1	E	5122	HIS
1	F	6083	GLN
1	F	6101	HIS
1	F	6188	GLN
1	F	6226	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 ligands 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	$\# Z > 2$
2	PO4	B	9001	-	4,4,4	1.29	0	6,6,6	0.27	0
2	PO4	B	9002	-	4,4,4	0.71	0	6,6,6	0.27	0

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
2	PO4	B	9001	-	-	0/0/0/0	0/0/0/0
2	PO4	B	9002	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	9002	PO4	1	0

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 ⓘ

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, 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	250/253 (98%)	0.02	11 (4%) 38 43	9, 39, 88, 99	0
1	B	250/253 (98%)	0.30	18 (7%) 18 20	8, 42, 86, 99	0
1	C	250/253 (98%)	0.08	8 (3%) 51 56	12, 42, 77, 99	0
1	D	250/253 (98%)	0.50	30 (12%) 6 6	14, 44, 99, 99	0
1	E	250/253 (98%)	0.27	19 (7%) 17 18	8, 42, 94, 99	0
1	F	250/253 (98%)	0.30	26 (10%) 8 8	11, 43, 98, 99	0
All	All	1500/1518 (98%)	0.24	112 (7%) 17 19	8, 42, 94, 99	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2227	GLU	12.5
1	B	2230	ASN	10.8
1	D	4175	ARG	8.5
1	C	3239	SER	8.4
1	F	6177	VAL	8.3
1	B	2226	GLN	7.7
1	B	2004	SER	7.5
1	D	4170	ASP	6.8
1	F	6171	THR	6.7
1	D	4163	TYR	6.6
1	E	5176	VAL	6.5
1	D	4169	TYR	6.3
1	D	4174	GLY	6.1
1	B	2006	VAL	6.0
1	A	1226	GLN	5.8
1	B	2231	ALA	5.7
1	F	6178	ARG	5.6
1	C	3006	VAL	5.6
1	E	5163	TYR	5.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	3231	ALA	5.5
1	D	4167	GLU	5.4
1	A	1233	THR	5.4
1	D	4228	ILE	5.3
1	E	5164	PRO	5.2
1	B	2005	ASP	5.2
1	D	4164	PRO	5.1
1	D	4231	ALA	5.0
1	D	4180	PHE	4.9
1	D	4176	VAL	4.9
1	E	5172	TYR	4.9
1	D	4234	MET	4.9
1	A	1006	VAL	4.9
1	E	5162	PHE	4.7
1	D	4181	LYS	4.7
1	F	6163	TYR	4.7
1	E	5165	GLY	4.6
1	A	1234	MET	4.3
1	D	4227	GLU	4.3
1	F	6102	ILE	4.2
1	F	6176	VAL	4.2
1	B	2007	PHE	4.2
1	A	1231	ALA	4.2
1	D	4177	VAL	4.2
1	F	6165	GLY	4.2
1	E	5167	GLU	4.2
1	D	4162	PHE	4.1
1	D	4171	THR	4.1
1	F	6169	TYR	4.1
1	B	2225	GLN	4.0
1	F	6172	TYR	4.0
1	D	4146	SER	3.9
1	F	6168	ARG	3.8
1	E	5168	ARG	3.7
1	D	4229	PRO	3.7
1	F	6174	GLY	3.7
1	E	5169	TYR	3.6
1	D	4230	ASN	3.6
1	D	4235	LYS	3.6
1	D	4168	ARG	3.6
1	D	4102	ILE	3.5
1	B	2041	PRO	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	2228	ILE	3.5
1	F	6231	ALA	3.4
1	D	4172	TYR	3.4
1	F	6164	PRO	3.4
1	F	6170	ASP	3.2
1	F	6227	GLU	3.1
1	B	2053	TRP	3.1
1	D	4036	ALA	3.1
1	F	6235	LYS	3.0
1	C	3228	ILE	3.0
1	E	5181	LYS	3.0
1	A	1229	PRO	3.0
1	D	4165	GLY	3.0
1	A	1007	PHE	2.9
1	F	6182	GLY	2.8
1	E	5175	ARG	2.8
1	C	3005	ASP	2.8
1	F	6013	LYS	2.7
1	C	3007	PHE	2.7
1	E	5182	GLY	2.7
1	B	2237	THR	2.6
1	A	1230	ASN	2.6
1	E	5029	GLU	2.6
1	B	2147	ILE	2.5
1	F	6223	ARG	2.5
1	B	2232	GLU	2.5
1	E	5028	PRO	2.4
1	F	6041	PRO	2.4
1	B	2016	LEU	2.4
1	D	4233	THR	2.4
1	E	5174	GLY	2.4
1	F	6180	PHE	2.4
1	D	4004	SER	2.4
1	E	5171	THR	2.4
1	F	6057	LEU	2.3
1	D	4147	ILE	2.3
1	F	6222	ASN	2.3
1	F	6097	ALA	2.3
1	C	3225	GLN	2.2
1	E	5220	ILE	2.2
1	F	6221	VAL	2.2
1	B	2042	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1236	GLN	2.1
1	C	3238	GLU	2.1
1	F	6166	GLN	2.1
1	B	2019	ALA	2.1
1	E	5179	ARG	2.1
1	D	4219	VAL	2.1
1	A	1232	GLU	2.0
1	A	1030	ARG	2.0
1	E	5084	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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å ²)	Q<0.9
2	PO4	B	9002	5/5	0.95	0.47	13.19	20,20,20,20	0
2	PO4	B	9001	5/5	0.98	0.13	-0.99	11,12,55,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.