



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:38 pm BST

PDB ID : 1FOE  
Title : CRYSTAL STRUCTURE OF RAC1 IN COMPLEX WITH THE GUANINE NUCLEOTIDE EXCHANGE REGION OF TIAM1  
Authors : Worthylake, D.K.; Rossman, K.L.; Sondek, J.  
Deposited on : 2000-08-27  
Resolution : 2.80 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

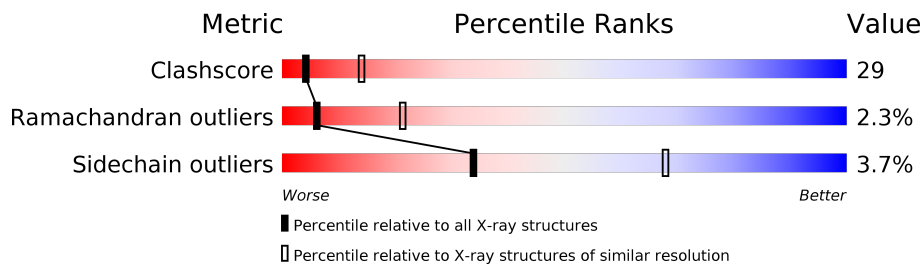
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	377	
1	C	377	
1	E	377	
1	G	377	
2	B	177	
2	D	177	
2	F	177	
2	H	177	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 17570 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 T-LYMPHOMA INVASION AND METASTASIS INDUCING PROTEIN 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	368	2989	1918	509	550	6	6	369	0	0
1	C	366	2972	1907	506	547	6	6	309	0	0
1	E	367	2980	1913	507	548	6	6	369	0	0
1	G	367	2980	1913	507	548	6	6	307	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1031	MSE	THR	MODIFIED RESIDUE	UNP Q60610
A	1032	GLY	THR	CLONING ARTIFACT	UNP Q60610
A	1063	MSE	MET	MODIFIED RESIDUE	UNP Q60610
A	1091	MSE	MET	MODIFIED RESIDUE	UNP Q60610
A	1224	MSE	MET	MODIFIED RESIDUE	UNP Q60610
A	1234	MSE	MET	MODIFIED RESIDUE	UNP Q60610
A	1264	MSE	MET	MODIFIED RESIDUE	UNP Q60610
A	1334	MSE	MET	MODIFIED RESIDUE	UNP Q60610
C	1031	MSE	THR	MODIFIED RESIDUE	UNP Q60610
C	1032	GLY	THR	CLONING ARTIFACT	UNP Q60610
C	1063	MSE	MET	MODIFIED RESIDUE	UNP Q60610
C	1091	MSE	MET	MODIFIED RESIDUE	UNP Q60610
C	1224	MSE	MET	MODIFIED RESIDUE	UNP Q60610
C	1234	MSE	MET	MODIFIED RESIDUE	UNP Q60610
C	1264	MSE	MET	MODIFIED RESIDUE	UNP Q60610
C	1334	MSE	MET	MODIFIED RESIDUE	UNP Q60610
E	1031	MSE	THR	MODIFIED RESIDUE	UNP Q60610
E	1032	GLY	THR	CLONING ARTIFACT	UNP Q60610
E	1063	MSE	MET	MODIFIED RESIDUE	UNP Q60610
E	1091	MSE	MET	MODIFIED RESIDUE	UNP Q60610

*Continued on next page...*

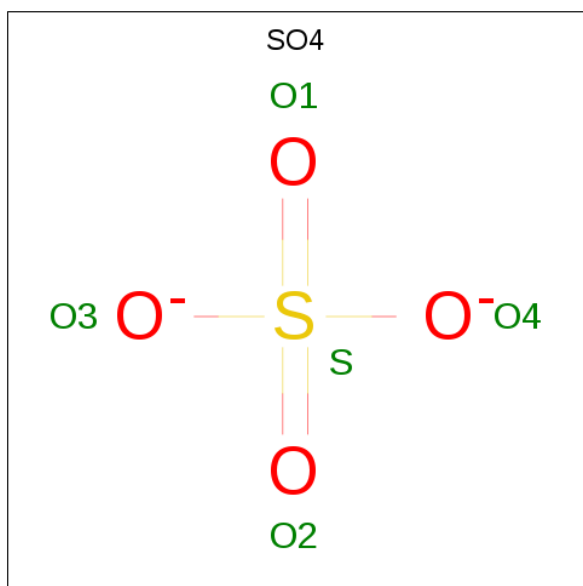
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	1224	MSE	MET	MODIFIED RESIDUE	UNP Q60610
E	1234	MSE	MET	MODIFIED RESIDUE	UNP Q60610
E	1264	MSE	MET	MODIFIED RESIDUE	UNP Q60610
E	1334	MSE	MET	MODIFIED RESIDUE	UNP Q60610
G	1031	MSE	THR	MODIFIED RESIDUE	UNP Q60610
G	1032	GLY	THR	CLONING ARTIFACT	UNP Q60610
G	1063	MSE	MET	MODIFIED RESIDUE	UNP Q60610
G	1091	MSE	MET	MODIFIED RESIDUE	UNP Q60610
G	1224	MSE	MET	MODIFIED RESIDUE	UNP Q60610
G	1234	MSE	MET	MODIFIED RESIDUE	UNP Q60610
G	1264	MSE	MET	MODIFIED RESIDUE	UNP Q60610
G	1334	MSE	MET	MODIFIED RESIDUE	UNP Q60610

- Molecule 2 is a protein called RAS-RELATED C3 BOTULINUM TOXIN SUBSTRATE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	177	Total 1384	C 889	N 228	O 259	S 8	14	0	0
2	D	177	Total 1384	C 889	N 228	O 259	S 8	14	0	0
2	F	177	Total 1384	C 889	N 228	O 259	S 8	14	0	0
2	H	177	Total 1384	C 889	N 228	O 259	S 8	14	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

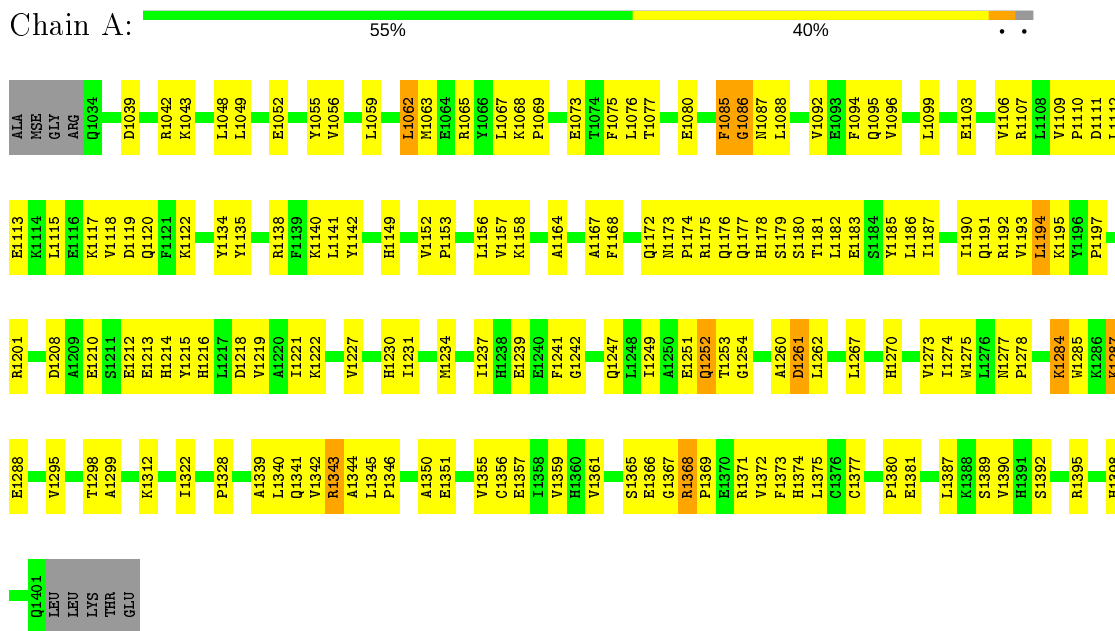
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	14	Total	O	0	0
			14	14		
4	B	6	Total	O	0	0
			6	6		
4	C	8	Total	O	0	0
			8	8		
4	D	6	Total	O	0	0
			6	6		
4	E	7	Total	O	0	0
			7	7		
4	F	7	Total	O	0	0
			7	7		
4	G	19	Total	O	0	0
			19	19		
4	H	26	Total	O	0	0
			26	26		

### 3 Residue-property plots [i](#)

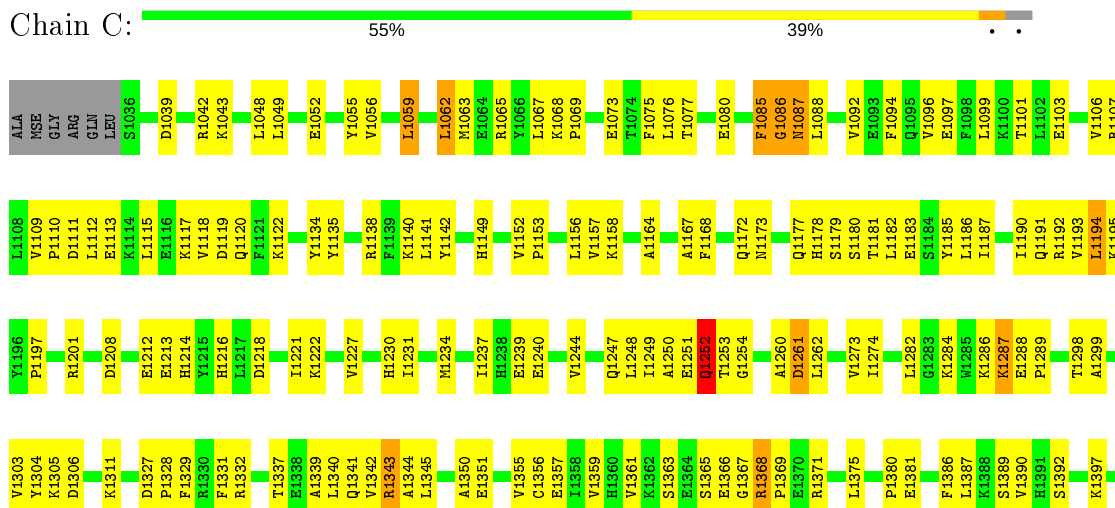
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

Note EDS was not executed.

- Molecule 1: T-LYMPHOMA INVASION AND METASTASIS INDUCING PROTEIN 1



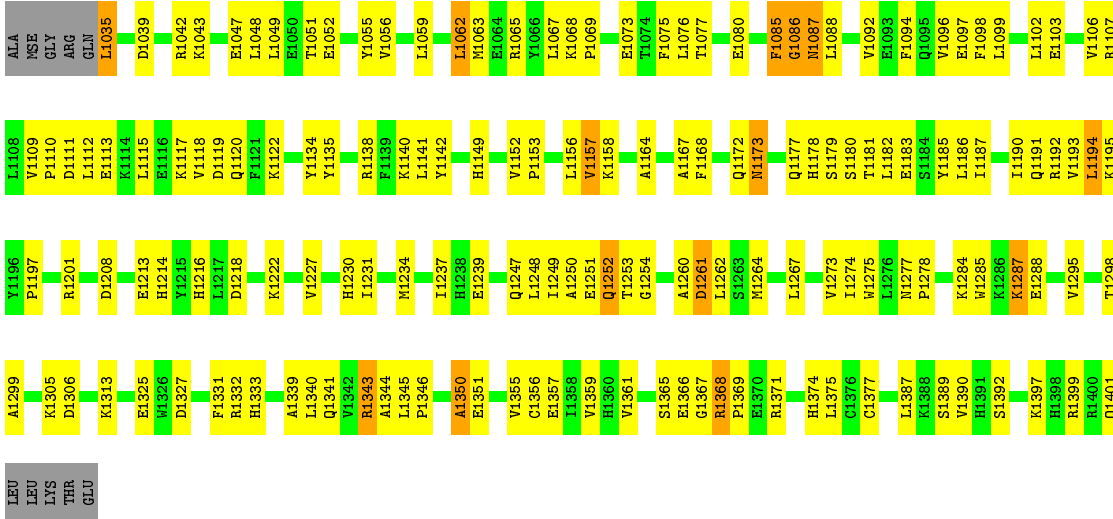
- Molecule 1: T-LYMPHOMA INVASION AND METASTASIS INDUCING PROTEIN 1



Q1401  
 LEU  
 LEU  
 LYS  
 THR  
 GLU

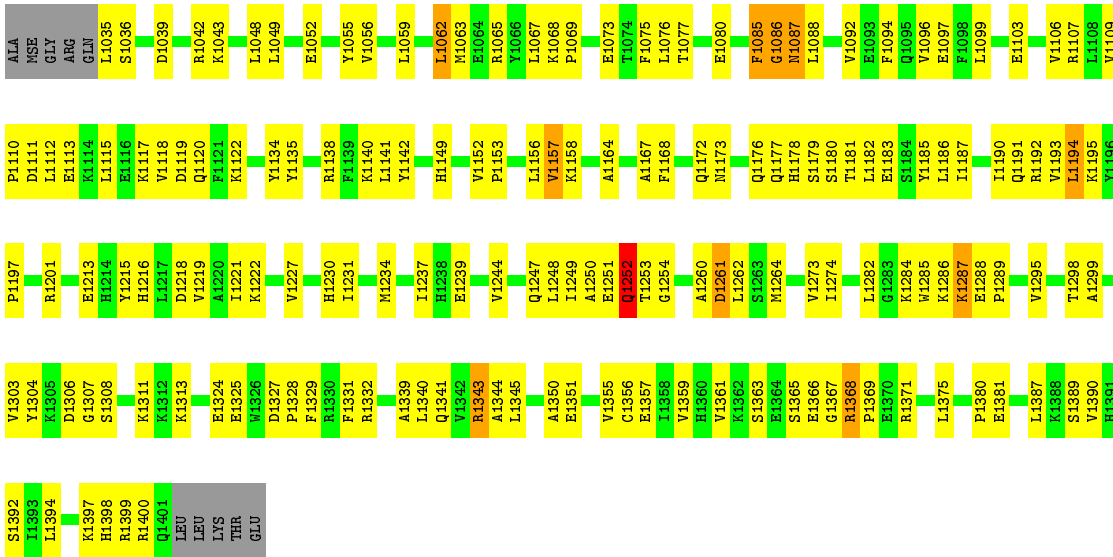
• Molecule 1: T-LYMPHOMA INVASION AND METASTASIS INDUCING PROTEIN 1

Chain E:  55% 38%



• Molecule 1: T-LYMPHOMA INVASION AND METASTASIS INDUCING PROTEIN 1

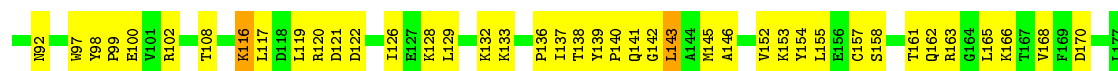
Chain G:  54% 41%



• Molecule 2: RAS-RELATED C3 BOTULINUM TOXIN SUBSTRATE

Chain B:  54% 44%





- Molecule 2: RAS-RELATED C3 BOTULINUM TOXIN SUBSTRATE

Chain D: 53% 44%



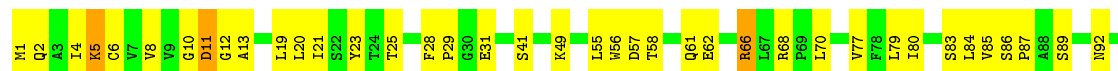
- Molecule 2: RAS-RELATED C3 BOTULINUM TOXIN SUBSTRATE

Chain F: 53% 45%



- Molecule 2: RAS-RELATED C3 BOTULINUM TOXIN SUBSTRATE

Chain H: 53% 44%





## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	186.95Å 149.27Å 149.21Å 90.00° 121.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80	Depositor
% Data completeness (in resolution range)	93.8 (15.00-2.80)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 0.3	Depositor
R, $R_{free}$	0.262 , 0.293	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	17570	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.42	0/3045	0.61	0/4095
1	C	0.41	0/3028	0.61	0/4072
1	E	0.41	0/3036	0.61	0/4083
1	G	0.45	1/3036 (0.0%)	0.62	0/4083
2	B	0.42	0/1414	0.79	3/1922 (0.2%)
2	D	0.40	0/1414	0.79	3/1922 (0.2%)
2	F	0.40	0/1414	0.79	3/1922 (0.2%)
2	H	0.51	0/1414	0.82	3/1922 (0.2%)
All	All	0.43	1/17801 (0.0%)	0.68	12/24021 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	1264	MSE	CG-SE	-5.10	1.78	1.95

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5	LYS	N-CA-CB	-13.85	85.67	110.60
2	H	5	LYS	N-CA-CB	-13.35	86.58	110.60
2	D	5	LYS	N-CA-CB	-13.34	86.59	110.60
2	F	5	LYS	N-CA-CB	-13.23	86.79	110.60
2	D	4	ILE	CB-CA-C	-8.00	95.61	111.60
2	B	4	ILE	CB-CA-C	-7.96	95.69	111.60
2	H	4	ILE	CB-CA-C	-7.86	95.89	111.60
2	F	4	ILE	CB-CA-C	-7.81	95.99	111.60
2	F	4	ILE	N-CA-C	-6.73	92.82	111.00
2	H	4	ILE	N-CA-C	-6.55	93.32	111.00
2	D	4	ILE	N-CA-C	-6.53	93.36	111.00
2	B	4	ILE	N-CA-C	-6.33	93.92	111.00

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	2989	0	3035	170	0
1	C	2972	0	3016	175	0
1	E	2980	0	3027	173	0
1	G	2980	0	3027	171	0
2	B	1384	0	1405	84	0
2	D	1384	0	1405	84	0
2	F	1384	0	1405	82	1
2	H	1384	0	1405	86	1
3	B	5	0	0	0	0
3	D	5	0	0	0	0
3	F	5	0	0	0	0
3	H	5	0	0	0	0
4	A	14	0	0	0	0
4	B	6	0	0	0	0
4	C	8	0	0	0	0
4	D	6	0	0	0	0
4	E	7	0	0	0	0
4	F	7	0	0	0	0
4	G	19	0	0	0	0
4	H	26	0	0	0	0
All	All	17570	0	17725	949	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

All (949) 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:A:1285:TRP:HH2	2:D:102:ARG:HG2	1.01	1.09
1:A:1285:TRP:CH2	2:D:102:ARG:HG2	1.88	1.08
2:B:138:THR:H	2:B:141:GLN:HE21	1.09	1.00

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1248:LEU:HD21	1:C:1332:ARG:HG3	1.46	0.97
1:E:1249:ILE:HD12	1:E:1261:ASP:H	1.29	0.96
2:H:138:THR:H	2:H:141:GLN:HE21	0.99	0.95
2:F:138:THR:H	2:F:141:GLN:HE21	1.07	0.94
2:D:138:THR:H	2:D:141:GLN:HE21	1.08	0.93
1:C:1249:ILE:HD11	1:C:1262:LEU:HG	1.52	0.91
1:A:1249:ILE:HD11	1:A:1262:LEU:HG	1.53	0.89
1:C:1056:VAL:HG21	1:C:1099:LEU:HD22	1.55	0.89
1:G:1287:LYS:HG2	1:G:1288:GLU:HG2	1.53	0.89
1:E:1343:ARG:HD3	1:E:1357:GLU:HG3	1.54	0.88
1:C:1287:LYS:HG2	1:C:1288:GLU:HG2	1.56	0.87
1:C:1193:VAL:HG23	1:C:1194:LEU:HD13	1.57	0.87
1:A:1343:ARG:HD3	1:A:1357:GLU:HG3	1.55	0.87
1:C:1343:ARG:HD3	1:C:1357:GLU:HG3	1.57	0.87
1:G:1190:ILE:HD13	2:H:70:LEU:HD13	1.55	0.86
1:E:1193:VAL:HG23	1:E:1194:LEU:HD13	1.57	0.86
1:E:1039:ASP:HA	1:E:1042:ARG:HH12	1.40	0.86
1:A:1190:ILE:HD13	2:B:70:LEU:HD13	1.55	0.86
1:E:1287:LYS:HG2	1:E:1288:GLU:HG2	1.57	0.85
1:G:1343:ARG:HD3	1:G:1357:GLU:HG3	1.56	0.85
1:A:1287:LYS:HG2	1:A:1288:GLU:HG2	1.58	0.85
1:A:1039:ASP:HA	1:A:1042:ARG:HH12	1.42	0.85
1:A:1239:GLU:OE2	2:B:66:ARG:HG3	1.77	0.84
1:G:1193:VAL:HG23	1:G:1194:LEU:HD13	1.59	0.84
2:B:138:THR:OG1	2:B:141:GLN:HG3	1.78	0.84
1:E:1190:ILE:HD13	2:F:70:LEU:HD13	1.59	0.83
1:A:1056:VAL:HG21	1:A:1099:LEU:HD22	1.58	0.83
1:E:1260:ALA:O	1:E:1261:ASP:HB2	1.75	0.83
2:H:138:THR:OG1	2:H:141:GLN:HG3	1.78	0.83
1:E:1062:LEU:HD11	1:E:1186:LEU:HD23	1.60	0.83
1:G:1035:LEU:HD12	2:H:31:GLU:HB2	1.61	0.83
1:C:1039:ASP:HA	1:C:1042:ARG:HH12	1.42	0.82
1:E:1248:LEU:HD21	1:E:1332:ARG:HG2	1.61	0.82
1:A:1039:ASP:O	1:A:1043:LYS:HG2	1.78	0.82
1:A:1284:LYS:HB3	2:D:99:PRO:HB3	1.62	0.82
1:E:1368:ARG:HG3	1:E:1368:ARG:HH11	1.44	0.82
1:E:1056:VAL:HG21	1:E:1099:LEU:HD22	1.60	0.82
1:G:1039:ASP:HA	1:G:1042:ARG:HH12	1.43	0.82
1:G:1249:ILE:HD11	1:G:1262:LEU:HG	1.61	0.82
1:E:1039:ASP:O	1:E:1043:LYS:HG2	1.80	0.81
1:G:1039:ASP:O	1:G:1043:LYS:HG2	1.79	0.81

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1193:VAL:HG23	1:A:1194:LEU:HD13	1.59	0.81
1:C:1039:ASP:O	1:C:1043:LYS:HG2	1.81	0.81
1:E:1234:MSE:HE2	1:E:1234:MSE:HA	1.62	0.81
1:G:1234:MSE:HA	1:G:1234:MSE:HE2	1.64	0.80
1:C:1368:ARG:HH11	1:C:1368:ARG:HG3	1.47	0.79
1:E:1249:ILE:HD11	1:E:1262:LEU:HG	1.62	0.79
1:A:1249:ILE:HD12	1:A:1261:ASP:H	1.47	0.79
1:G:1056:VAL:HG21	1:G:1099:LEU:HD22	1.65	0.79
1:A:1062:LEU:HD11	1:A:1186:LEU:HD23	1.63	0.78
1:G:1368:ARG:HG3	1:G:1368:ARG:HH11	1.47	0.78
2:D:138:THR:OG1	2:D:141:GLN:HG3	1.83	0.78
1:C:1234:MSE:HE2	1:C:1234:MSE:HA	1.64	0.78
1:G:1248:LEU:HD21	1:G:1332:ARG:HG3	1.67	0.77
1:A:1368:ARG:HH11	1:A:1368:ARG:HG3	1.50	0.77
1:C:1249:ILE:HD12	1:C:1261:ASP:H	1.49	0.77
1:G:1062:LEU:HD11	1:G:1186:LEU:HD23	1.67	0.76
2:F:138:THR:OG1	2:F:141:GLN:HG3	1.85	0.76
1:C:1062:LEU:HD11	1:C:1186:LEU:HD23	1.65	0.76
1:A:1234:MSE:HE2	1:A:1234:MSE:HA	1.66	0.76
1:G:1304:TYR:HB3	1:G:1331:PHE:HB3	1.68	0.76
1:E:1285:TRP:HZ2	2:H:98:TYR:CE2	2.05	0.74
1:C:1190:ILE:HD13	2:D:70:LEU:HD13	1.70	0.74
1:G:1249:ILE:HG23	1:G:1260:ALA:HA	1.70	0.73
1:C:1287:LYS:HD2	1:G:1306:ASP:OD2	1.89	0.73
1:E:1287:LYS:HD3	1:E:1287:LYS:N	2.03	0.73
1:C:1075:PHE:HE1	1:C:1168:PHE:HB2	1.53	0.73
1:E:1039:ASP:HA	1:E:1042:ARG:NH1	2.04	0.72
2:D:66:ARG:HH11	2:D:66:ARG:HG3	1.54	0.72
1:A:1287:LYS:N	1:A:1287:LYS:HD3	2.04	0.72
2:F:21:ILE:O	2:F:25:THR:HG22	1.90	0.71
1:A:1039:ASP:HA	1:A:1042:ARG:NH1	2.05	0.71
1:C:1039:ASP:HA	1:C:1042:ARG:NH1	2.05	0.71
1:C:1287:LYS:N	1:C:1287:LYS:HD3	2.06	0.71
1:A:1075:PHE:HE1	1:A:1168:PHE:HB2	1.55	0.70
1:E:1251:GLU:HG2	1:E:1251:GLU:O	1.90	0.70
1:A:1092:VAL:O	1:A:1096:VAL:HG23	1.91	0.70
1:E:1075:PHE:HE1	1:E:1168:PHE:HB2	1.55	0.70
1:G:1092:VAL:O	1:G:1096:VAL:HG23	1.91	0.70
1:C:1240:GLU:OE2	1:C:1305:LYS:NZ	2.24	0.70
1:G:1039:ASP:HA	1:G:1042:ARG:NH1	2.05	0.69
2:H:21:ILE:O	2:H:25:THR:HG22	1.91	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1249:ILE:HD12	1:G:1261:ASP:H	1.57	0.69
1:A:1251:GLU:HG2	1:A:1251:GLU:O	1.91	0.69
2:F:66:ARG:HG3	2:F:66:ARG:HH11	1.56	0.69
1:G:1273:VAL:HG21	1:G:1375:LEU:HB3	1.73	0.69
1:A:1249:ILE:HG23	1:A:1260:ALA:HA	1.73	0.69
1:A:1157:VAL:HG12	1:A:1157:VAL:O	1.92	0.69
2:H:122:ASP:O	2:H:126:ILE:HG13	1.93	0.69
1:E:1249:ILE:HG23	1:E:1260:ALA:HA	1.74	0.69
1:E:1092:VAL:O	1:E:1096:VAL:HG23	1.92	0.68
1:G:1062:LEU:HD13	1:G:1088:LEU:HD11	1.74	0.68
1:C:1249:ILE:HG23	1:C:1260:ALA:HA	1.74	0.68
1:E:1157:VAL:HG12	1:E:1157:VAL:O	1.93	0.68
1:A:1062:LEU:HD13	1:A:1088:LEU:HD11	1.74	0.68
1:A:1260:ALA:O	1:A:1261:ASP:HB2	1.93	0.68
1:G:1251:GLU:O	1:G:1251:GLU:HG2	1.93	0.68
1:G:1287:LYS:N	1:G:1287:LYS:HD3	2.08	0.67
1:C:1157:VAL:O	1:C:1157:VAL:HG12	1.94	0.67
1:G:1157:VAL:HG12	1:G:1157:VAL:O	1.94	0.67
1:E:1194:LEU:HD23	2:F:61:GLN:HB3	1.76	0.67
2:D:21:ILE:O	2:D:25:THR:HG22	1.95	0.67
1:C:1092:VAL:O	1:C:1096:VAL:HG23	1.95	0.67
1:G:1075:PHE:HE1	1:G:1168:PHE:HB2	1.59	0.67
2:H:66:ARG:HG3	2:H:66:ARG:HH11	1.59	0.66
1:A:1239:GLU:OE1	2:B:66:ARG:NH1	2.28	0.66
2:B:66:ARG:HH11	2:B:66:ARG:HG3	1.58	0.66
1:C:1156:LEU:HD13	1:C:1183:GLU:HG3	1.76	0.66
1:C:1251:GLU:O	1:C:1251:GLU:HG2	1.96	0.66
1:E:1156:LEU:HD13	1:E:1183:GLU:HG3	1.78	0.66
2:F:139:TYR:HE2	2:F:143:LEU:HD12	1.61	0.66
2:F:161:THR:HG21	2:F:163:ARG:HD2	1.78	0.66
1:A:1218:ASP:O	1:A:1222:LYS:HD3	1.96	0.66
2:B:21:ILE:O	2:B:25:THR:HG22	1.96	0.66
1:E:1234:MSE:HE1	1:E:1267:LEU:HD23	1.77	0.66
2:D:116:LYS:HG3	2:D:119:LEU:HD23	1.77	0.66
2:B:116:LYS:HG3	2:B:119:LEU:HD23	1.77	0.65
2:B:128:LYS:HE2	2:B:132:LYS:HZ1	1.61	0.65
2:F:138:THR:H	2:F:141:GLN:NE2	1.89	0.65
2:F:102:ARG:NH2	2:F:108:THR:O	2.28	0.65
2:F:6:CYS:HB3	2:F:55:LEU:HD23	1.78	0.65
2:D:102:ARG:NH2	2:D:108:THR:O	2.29	0.65
2:H:102:ARG:NH2	2:H:108:THR:O	2.28	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1260:ALA:O	1:C:1261:ASP:HB2	1.95	0.65
1:C:1156:LEU:CD1	1:C:1183:GLU:HG3	2.26	0.65
2:F:128:LYS:HE2	2:F:132:LYS:HZ1	1.62	0.65
2:D:120:ARG:NH2	2:D:139:TYR:N	2.45	0.64
2:F:116:LYS:HG3	2:F:119:LEU:HD23	1.78	0.64
2:B:120:ARG:NH2	2:B:139:TYR:N	2.45	0.64
1:C:1062:LEU:HD13	1:C:1088:LEU:HD11	1.77	0.64
2:B:122:ASP:O	2:B:126:ILE:HG13	1.97	0.64
1:E:1239:GLU:OE2	2:F:66:ARG:HG3	1.97	0.64
1:A:1346:PRO:HG3	1:E:1374:HIS:ND1	2.12	0.64
2:F:120:ARG:NH2	2:F:139:TYR:N	2.45	0.64
1:G:1156:LEU:HD13	1:G:1183:GLU:HG3	1.79	0.64
2:D:161:THR:HG21	2:D:163:ARG:HD2	1.79	0.64
1:G:1176:GLN:NE2	2:H:1:MET:N	2.45	0.64
1:C:1140:LYS:HD2	1:C:1230:HIS:CD2	2.33	0.64
2:B:157:CYS:HB2	2:B:165:LEU:HD12	1.80	0.64
1:E:1179:SER:H	2:F:41:SER:HB2	1.63	0.63
2:B:102:ARG:NH2	2:B:108:THR:O	2.31	0.63
1:C:1273:VAL:HG21	1:C:1375:LEU:HB3	1.81	0.63
2:D:138:THR:H	2:D:141:GLN:NE2	1.90	0.63
1:E:1218:ASP:O	1:E:1222:LYS:HD3	1.98	0.63
1:E:1248:LEU:HD21	1:E:1332:ARG:CG	2.28	0.63
1:C:1056:VAL:HG21	1:C:1099:LEU:CD2	2.27	0.63
1:E:1062:LEU:HD13	1:E:1088:LEU:HD11	1.79	0.63
1:G:1086:GLY:O	1:G:1088:LEU:N	2.32	0.63
2:F:84:LEU:HD12	2:F:117:LEU:HA	1.81	0.63
1:E:1331:PHE:CZ	1:E:1333:HIS:HB2	2.34	0.63
2:B:84:LEU:HD12	2:B:117:LEU:HA	1.81	0.63
2:B:161:THR:HG21	2:B:163:ARG:HD2	1.81	0.63
2:H:128:LYS:HE2	2:H:132:LYS:HZ1	1.63	0.63
1:E:1156:LEU:CD1	1:E:1183:GLU:HG3	2.28	0.62
1:E:1260:ALA:O	1:E:1261:ASP:CB	2.45	0.62
1:G:1218:ASP:O	1:G:1222:LYS:HD3	1.99	0.62
1:E:1088:LEU:O	1:E:1092:VAL:HG23	2.00	0.62
1:C:1287:LYS:HG2	1:C:1288:GLU:N	2.15	0.62
2:D:84:LEU:HD12	2:D:117:LEU:HA	1.82	0.62
2:F:139:TYR:CE2	2:F:143:LEU:HD12	2.34	0.62
1:G:1178:HIS:HA	1:G:1181:THR:HG23	1.82	0.62
1:G:1287:LYS:HG2	1:G:1288:GLU:N	2.14	0.62
2:H:116:LYS:HG3	2:H:119:LEU:HD23	1.80	0.62
1:A:1086:GLY:O	1:A:1088:LEU:N	2.33	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1178:HIS:HA	1:C:1181:THR:HG23	1.82	0.61
2:D:122:ASP:O	2:D:126:ILE:HG13	1.99	0.61
1:G:1156:LEU:CD1	1:G:1183:GLU:HG3	2.29	0.61
1:C:1088:LEU:O	1:C:1092:VAL:HG23	1.99	0.61
1:C:1218:ASP:O	1:C:1222:LYS:HD3	2.00	0.61
2:D:139:TYR:HE2	2:D:143:LEU:HD12	1.65	0.61
1:G:1365:SER:O	1:G:1366:GLU:HB3	2.01	0.61
1:A:1178:HIS:HA	1:A:1181:THR:HG23	1.83	0.61
1:E:1140:LYS:HD2	1:E:1230:HIS:CD2	2.36	0.61
1:C:1112:LEU:HA	1:C:1115:LEU:HD13	1.83	0.61
1:G:1112:LEU:HA	1:G:1115:LEU:HD13	1.83	0.61
1:C:1304:TYR:HB3	1:C:1331:PHE:HB3	1.81	0.60
2:F:122:ASP:O	2:F:126:ILE:HG13	2.00	0.60
1:G:1140:LYS:HD2	1:G:1230:HIS:CD2	2.36	0.60
2:H:161:THR:HG21	2:H:163:ARG:HD2	1.82	0.60
1:C:1247:GLN:HB3	1:C:1332:ARG:NH1	2.16	0.60
2:D:157:CYS:HB2	2:D:165:LEU:HD12	1.83	0.60
2:H:6:CYS:HB3	2:H:55:LEU:HD23	1.83	0.60
2:B:138:THR:H	2:B:141:GLN:NE2	1.89	0.60
2:H:120:ARG:NH2	2:H:139:TYR:N	2.49	0.60
1:E:1365:SER:O	1:E:1366:GLU:HB3	2.02	0.60
2:B:6:CYS:HB3	2:B:55:LEU:HD23	1.83	0.60
1:E:1076:LEU:HB3	1:E:1080:GLU:HB2	1.84	0.60
1:G:1088:LEU:O	1:G:1092:VAL:HG23	2.02	0.60
1:A:1076:LEU:HB3	1:A:1080:GLU:HB2	1.82	0.60
1:C:1075:PHE:HE1	1:C:1168:PHE:CB	2.15	0.60
1:C:1365:SER:O	1:C:1366:GLU:HB3	2.02	0.60
2:F:157:CYS:HB2	2:F:165:LEU:HD12	1.82	0.60
2:H:138:THR:H	2:H:141:GLN:NE2	1.84	0.60
1:C:1179:SER:H	2:D:41:SER:HB2	1.67	0.60
2:F:154:TYR:C	2:F:155:LEU:HD12	2.23	0.60
1:E:1086:GLY:O	1:E:1088:LEU:N	2.35	0.59
1:E:1365:SER:C	1:E:1367:GLY:H	2.05	0.59
1:A:1140:LYS:HD2	1:A:1230:HIS:CD2	2.37	0.59
1:A:1194:LEU:HD23	2:B:61:GLN:HB3	1.84	0.59
1:C:1076:LEU:HB3	1:C:1080:GLU:HB2	1.83	0.59
1:G:1343:ARG:N	1:G:1343:ARG:HD2	2.17	0.59
2:D:154:TYR:C	2:D:155:LEU:HD12	2.23	0.59
1:E:1343:ARG:HD3	1:E:1357:GLU:CG	2.29	0.59
1:C:1103:GLU:O	1:C:1106:VAL:HG12	2.02	0.59
1:E:1042:ARG:HE	1:E:1113:GLU:HA	1.67	0.59

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1112:LEU:HA	1:E:1115:LEU:HD13	1.84	0.59
2:H:84:LEU:HD12	2:H:117:LEU:HA	1.83	0.59
2:F:83:SER:HB3	2:F:86:SER:HB3	1.84	0.59
1:G:1343:ARG:HD3	1:G:1357:GLU:CG	2.32	0.59
1:C:1042:ARG:HE	1:C:1113:GLU:HA	1.68	0.59
1:C:1343:ARG:HD2	1:C:1343:ARG:N	2.17	0.59
1:E:1274:ILE:HG21	1:E:1288:GLU:HB2	1.85	0.59
1:G:1076:LEU:HB3	1:G:1080:GLU:HB2	1.85	0.59
1:A:1365:SER:O	1:A:1366:GLU:HB3	2.03	0.58
1:C:1149:HIS:HA	1:C:1152:VAL:HG23	1.85	0.58
1:E:1117:LYS:HB2	1:E:1120:GLN:HG3	1.84	0.58
2:H:157:CYS:HB2	2:H:165:LEU:HD12	1.85	0.58
1:A:1274:ILE:HG21	1:A:1288:GLU:HB2	1.85	0.58
1:A:1212:GLU:CD	1:G:1097:GLU:HG2	2.23	0.58
2:D:139:TYR:CE2	2:D:143:LEU:HD12	2.39	0.58
1:E:1063:MSE:CE	1:E:1088:LEU:HD22	2.34	0.58
1:E:1178:HIS:HA	1:E:1181:THR:HG23	1.83	0.58
1:A:1042:ARG:HE	1:A:1113:GLU:HA	1.68	0.58
2:H:128:LYS:HE2	2:H:132:LYS:NZ	2.18	0.58
1:A:1343:ARG:CD	1:A:1357:GLU:HG3	2.32	0.58
1:C:1365:SER:C	1:C:1367:GLY:H	2.06	0.58
2:D:6:CYS:HB3	2:D:55:LEU:HD23	1.85	0.58
1:A:1365:SER:C	1:A:1367:GLY:H	2.06	0.58
1:C:1075:PHE:CE1	1:C:1168:PHE:HB2	2.36	0.58
1:G:1365:SER:C	1:G:1367:GLY:H	2.07	0.58
2:H:83:SER:HB3	2:H:86:SER:HB3	1.86	0.58
1:A:1149:HIS:HA	1:A:1152:VAL:HG23	1.84	0.57
1:E:1343:ARG:HD2	1:E:1343:ARG:N	2.19	0.57
2:F:128:LYS:HE2	2:F:132:LYS:NZ	2.18	0.57
1:A:1112:LEU:HA	1:A:1115:LEU:HD13	1.86	0.57
1:A:1287:LYS:HG2	1:A:1288:GLU:N	2.19	0.57
1:G:1176:GLN:HE22	2:H:1:MET:N	2.02	0.57
1:A:1117:LYS:HB2	1:A:1120:GLN:HG3	1.87	0.57
2:D:138:THR:N	2:D:141:GLN:HE21	1.91	0.57
1:E:1075:PHE:HE1	1:E:1168:PHE:CB	2.17	0.57
1:A:1103:GLU:O	1:A:1106:VAL:HG12	2.04	0.57
1:E:1149:HIS:HA	1:E:1152:VAL:HG23	1.86	0.57
1:E:1287:LYS:HG2	1:E:1288:GLU:N	2.19	0.57
1:C:1086:GLY:O	1:C:1088:LEU:N	2.38	0.57
1:C:1117:LYS:HB2	1:C:1120:GLN:HG3	1.87	0.57
1:C:1274:ILE:CG2	1:C:1288:GLU:HB2	2.35	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1274:ILE:CG2	1:E:1288:GLU:HB2	2.34	0.57
1:A:1067:LEU:HB3	1:A:1085:PHE:CZ	2.40	0.57
1:A:1075:PHE:HE1	1:A:1168:PHE:CB	2.17	0.57
1:A:1274:ILE:CG2	1:A:1288:GLU:HB2	2.35	0.57
1:A:1343:ARG:N	1:A:1343:ARG:HD2	2.20	0.57
1:C:1274:ILE:HG21	1:C:1288:GLU:HB2	1.86	0.57
1:E:1287:LYS:HZ2	1:E:1288:GLU:H	1.53	0.57
1:A:1056:VAL:HG21	1:A:1099:LEU:CD2	2.32	0.57
2:B:154:TYR:C	2:B:155:LEU:HD12	2.25	0.57
1:E:1343:ARG:CD	1:E:1357:GLU:HG3	2.31	0.57
1:G:1260:ALA:O	1:G:1261:ASP:HB2	2.05	0.57
1:C:1343:ARG:HD3	1:C:1357:GLU:CG	2.32	0.57
1:E:1177:GLN:HG3	2:F:41:SER:HB3	1.86	0.57
2:D:83:SER:HB3	2:D:86:SER:HB3	1.86	0.56
1:A:1088:LEU:O	1:A:1092:VAL:HG23	2.05	0.56
1:A:1287:LYS:HZ2	1:A:1288:GLU:H	1.53	0.56
1:C:1056:VAL:CG2	1:C:1099:LEU:HD22	2.32	0.56
2:H:87:PRO:HA	2:H:137:ILE:HD11	1.88	0.56
1:G:1042:ARG:HE	1:G:1113:GLU:HA	1.69	0.56
2:H:139:TYR:HE2	2:H:143:LEU:HD12	1.70	0.56
2:D:128:LYS:HE2	2:D:132:LYS:HZ1	1.70	0.56
2:D:128:LYS:HE2	2:D:132:LYS:NZ	2.20	0.56
2:D:87:PRO:HA	2:D:137:ILE:HD11	1.87	0.56
2:B:139:TYR:HE2	2:B:143:LEU:HD12	1.70	0.56
1:C:1287:LYS:CD	1:G:1306:ASP:OD2	2.54	0.56
1:G:1063:MSE:CE	1:G:1088:LEU:HD22	2.35	0.56
2:H:138:THR:N	2:H:141:GLN:HE21	1.84	0.56
1:C:1343:ARG:HD2	1:C:1343:ARG:H	1.71	0.56
1:E:1067:LEU:HB3	1:E:1085:PHE:CZ	2.41	0.56
1:G:1103:GLU:O	1:G:1106:VAL:HG12	2.06	0.56
1:A:1343:ARG:HD3	1:A:1357:GLU:CG	2.30	0.56
2:B:128:LYS:HE2	2:B:132:LYS:NZ	2.19	0.56
1:C:1247:GLN:O	1:C:1251:GLU:HB3	2.05	0.56
1:G:1345:LEU:HD12	1:G:1355:VAL:HG12	1.88	0.56
1:E:1075:PHE:CE1	1:E:1168:PHE:HB2	2.39	0.55
1:A:1190:ILE:HD13	2:B:70:LEU:CD1	2.35	0.55
2:B:139:TYR:CE2	2:B:143:LEU:HD12	2.41	0.55
2:B:87:PRO:HA	2:B:137:ILE:HD11	1.87	0.55
1:G:1343:ARG:H	1:G:1343:ARG:HD2	1.70	0.55
1:A:1295:VAL:HG11	1:A:1389:SER:OG	2.06	0.55
2:B:83:SER:HB3	2:B:86:SER:HB3	1.87	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1248:LEU:HD21	1:C:1332:ARG:CG	2.31	0.55
1:G:1111:ASP:OD2	1:G:1113:GLU:HB2	2.06	0.55
2:F:139:TYR:HB3	2:F:140:PRO:HD3	1.88	0.55
1:A:1173:ASN:HD21	1:A:1180:SER:HB2	1.72	0.55
1:C:1287:LYS:HD2	1:G:1306:ASP:CG	2.27	0.55
1:E:1109:VAL:HG13	1:E:1110:PRO:HD2	1.89	0.55
2:H:98:TYR:HB3	2:H:99:PRO:HD3	1.89	0.55
1:A:1215:TYR:OH	1:G:1138:ARG:HG3	2.07	0.55
2:B:98:TYR:OH	2:B:102:ARG:HD2	2.07	0.55
1:C:1063:MSE:CE	1:C:1088:LEU:HD22	2.37	0.55
1:C:1288:GLU:OE1	1:G:1308:SER:HB2	2.07	0.55
2:F:87:PRO:HA	2:F:137:ILE:HD11	1.88	0.55
1:G:1067:LEU:HB3	1:G:1085:PHE:CZ	2.42	0.55
1:A:1119:ASP:O	1:A:1122:LYS:HG3	2.07	0.55
1:C:1218:ASP:OD1	1:C:1222:LYS:HE3	2.06	0.55
1:C:1306:ASP:OD2	1:G:1287:LYS:N	2.31	0.55
1:A:1345:LEU:HD12	1:A:1355:VAL:HG12	1.89	0.54
1:C:1173:ASN:HD21	1:C:1180:SER:HB2	1.71	0.54
1:C:1227:VAL:O	1:C:1231:ILE:HG12	2.06	0.54
1:E:1035:LEU:HB2	1:E:1039:ASP:HB2	1.88	0.54
1:E:1343:ARG:HD2	1:E:1343:ARG:H	1.72	0.54
2:H:139:TYR:CE2	2:H:143:LEU:HD12	2.42	0.54
1:G:1179:SER:H	2:H:41:SER:HB2	1.71	0.54
2:B:138:THR:N	2:B:141:GLN:HE21	1.92	0.54
1:C:1216:HIS:HB3	1:E:1134:TYR:CE2	2.42	0.54
1:E:1247:GLN:O	1:E:1251:GLU:HB3	2.06	0.54
2:H:154:TYR:C	2:H:155:LEU:HD12	2.27	0.54
1:E:1103:GLU:O	1:E:1106:VAL:HG12	2.07	0.54
1:G:1176:GLN:NE2	2:H:1:MET:H3	2.03	0.54
2:B:139:TYR:HB3	2:B:140:PRO:HD3	1.89	0.54
1:C:1067:LEU:HB3	1:C:1085:PHE:CZ	2.41	0.54
1:E:1094:PHE:HE1	1:E:1135:TYR:HD2	1.55	0.54
1:G:1035:LEU:HD12	2:H:31:GLU:CB	2.35	0.54
1:G:1075:PHE:CE1	1:G:1168:PHE:HB2	2.43	0.54
1:G:1274:ILE:HG21	1:G:1288:GLU:HB2	1.88	0.54
1:A:1234:MSE:HE1	1:A:1267:LEU:HD23	1.90	0.54
1:A:1343:ARG:HD2	1:A:1343:ARG:H	1.72	0.54
1:C:1287:LYS:HZ2	1:C:1288:GLU:H	1.56	0.54
1:A:1247:GLN:O	1:A:1251:GLU:HB3	2.08	0.54
2:F:98:TYR:HB3	2:F:99:PRO:HD3	1.90	0.54
1:A:1075:PHE:CE1	1:A:1168:PHE:HB2	2.38	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1115:LEU:HD12	1:E:1115:LEU:N	2.23	0.54
1:A:1063:MSE:CE	1:A:1088:LEU:HD22	2.37	0.53
1:A:1218:ASP:OD1	1:A:1222:LYS:HE3	2.09	0.53
1:G:1117:LYS:HB2	1:G:1120:GLN:HG3	1.89	0.53
1:A:1135:TYR:CE2	1:A:1138:ARG:NH2	2.75	0.53
1:G:1094:PHE:HE1	1:G:1135:TYR:HD2	1.56	0.53
1:G:1343:ARG:CD	1:G:1357:GLU:HG3	2.33	0.53
1:A:1135:TYR:HE2	1:A:1138:ARG:NH2	2.05	0.53
1:A:1395:ARG:O	1:A:1398:HIS:HB3	2.07	0.53
2:F:8:VAL:HG22	2:F:79:LEU:HD12	1.90	0.53
2:H:138:THR:HG1	2:H:141:GLN:HG3	1.70	0.53
1:A:1111:ASP:OD2	1:A:1113:GLU:HB2	2.09	0.53
1:A:1260:ALA:O	1:A:1261:ASP:CB	2.55	0.53
1:C:1156:LEU:HD21	1:C:1182:LEU:HD23	1.91	0.53
1:G:1274:ILE:CG2	1:G:1288:GLU:HB2	2.38	0.53
1:A:1056:VAL:CG2	1:A:1099:LEU:HD22	2.36	0.53
1:E:1285:TRP:HH2	2:H:102:ARG:HG2	1.74	0.53
1:C:1368:ARG:CG	1:C:1368:ARG:HH11	2.19	0.53
1:E:1187:ILE:O	1:E:1191:GLN:HG3	2.09	0.53
1:A:1109:VAL:HG13	1:A:1110:PRO:HD2	1.89	0.53
1:E:1135:TYR:CE2	1:E:1138:ARG:NH2	2.77	0.53
1:G:1247:GLN:O	1:G:1251:GLU:HB3	2.09	0.53
1:C:1345:LEU:HD12	1:C:1355:VAL:HG12	1.90	0.53
1:C:1140:LYS:HD2	1:C:1230:HIS:HD2	1.74	0.53
1:C:1179:SER:H	2:D:41:SER:CB	2.22	0.53
1:G:1075:PHE:HE1	1:G:1168:PHE:CB	2.20	0.53
1:G:1140:LYS:HE2	1:G:1227:VAL:HA	1.89	0.53
1:A:1115:LEU:N	1:A:1115:LEU:HD12	2.24	0.52
1:A:1094:PHE:HE1	1:A:1135:TYR:HD2	1.58	0.52
1:A:1239:GLU:CD	2:B:66:ARG:NH1	2.63	0.52
2:B:57:ASP:OD1	2:B:58:THR:N	2.41	0.52
1:C:1115:LEU:HD12	1:C:1115:LEU:N	2.23	0.52
2:D:139:TYR:HB3	2:D:140:PRO:HD3	1.90	0.52
1:E:1035:LEU:HB2	1:E:1039:ASP:CB	2.39	0.52
1:G:1115:LEU:N	1:G:1115:LEU:HD12	2.23	0.52
1:C:1282:LEU:HG	1:C:1289:PRO:HG2	1.91	0.52
2:H:155:LEU:CD2	2:H:168:VAL:HA	2.39	0.52
1:E:1298:THR:O	1:E:1299:ALA:HB2	2.08	0.52
1:A:1346:PRO:HG3	1:E:1374:HIS:CG	2.44	0.52
2:F:12:GLY:O	2:F:13:ALA:HB3	2.10	0.52
1:E:1249:ILE:HD12	1:E:1261:ASP:N	2.12	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1306:ASP:OD2	1:G:1286:LYS:HA	2.10	0.52
1:G:1287:LYS:HG2	1:G:1288:GLU:H	1.72	0.52
1:C:1287:LYS:HG2	1:C:1288:GLU:H	1.74	0.52
1:C:1345:LEU:HD12	1:C:1355:VAL:CG1	2.40	0.52
1:G:1149:HIS:HA	1:G:1152:VAL:HG23	1.92	0.52
2:B:68:ARG:NH1	2:B:100:GLU:OE1	2.43	0.52
1:A:1177:GLN:HG3	2:B:41:SER:HB3	1.90	0.52
1:G:1287:LYS:HZ2	1:G:1288:GLU:H	1.55	0.52
1:C:1140:LYS:HE2	1:C:1227:VAL:HA	1.92	0.52
1:C:1343:ARG:CD	1:C:1357:GLU:HG3	2.33	0.52
1:C:1109:VAL:HG13	1:C:1110:PRO:HD2	1.92	0.52
1:C:1062:LEU:HG	1:C:1185:TYR:HB3	1.92	0.52
1:C:1234:MSE:HE2	1:C:1237:ILE:HD12	1.91	0.52
1:E:1056:VAL:HG21	1:E:1099:LEU:CD2	2.35	0.52
1:E:1285:TRP:CZ2	2:H:98:TYR:CE2	2.92	0.52
1:A:1346:PRO:HG3	1:E:1374:HIS:CE1	2.45	0.52
1:C:1094:PHE:HE1	1:C:1135:TYR:HD2	1.58	0.51
1:E:1273:VAL:HG21	1:E:1375:LEU:HB3	1.92	0.51
2:F:5:LYS:HE3	2:F:56:TRP:CE3	2.46	0.51
2:H:139:TYR:HB3	2:H:140:PRO:HD3	1.91	0.51
2:B:152:VAL:HG12	2:B:153:LYS:HG2	1.91	0.51
2:D:96:LYS:O	2:D:99:PRO:HD2	2.10	0.51
1:A:1187:ILE:O	1:A:1191:GLN:HG3	2.09	0.51
1:C:1191:GLN:O	1:C:1195:LYS:HG2	2.11	0.51
1:C:1260:ALA:O	1:C:1261:ASP:CB	2.57	0.51
1:C:1194:LEU:HD23	2:D:61:GLN:HB3	1.93	0.51
2:D:68:ARG:NH1	2:D:100:GLU:OE1	2.44	0.51
1:A:1183:GLU:CD	2:B:74:GLN:NE2	2.64	0.51
1:G:1109:VAL:HG13	1:G:1110:PRO:HD2	1.91	0.51
1:G:1398:HIS:C	1:G:1400:ARG:H	2.14	0.51
1:A:1345:LEU:HD12	1:A:1355:VAL:CG1	2.40	0.51
1:C:1111:ASP:OD2	1:C:1113:GLU:HB2	2.10	0.51
1:E:1140:LYS:HE2	1:E:1227:VAL:HA	1.91	0.51
1:G:1339:ALA:HB1	1:G:1361:VAL:HG22	1.92	0.51
1:A:1339:ALA:HB1	1:A:1361:VAL:HG22	1.92	0.51
1:E:1339:ALA:HB1	1:E:1361:VAL:HG22	1.93	0.51
2:B:58:THR:O	2:B:61:GLN:HG2	2.11	0.51
2:B:8:VAL:HG22	2:B:79:LEU:HD12	1.93	0.51
1:C:1119:ASP:O	1:C:1122:LYS:HG3	2.11	0.51
1:E:1218:ASP:OD1	1:E:1222:LYS:HE3	2.10	0.51
1:G:1194:LEU:HD23	2:H:61:GLN:HB3	1.93	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1368:ARG:HG3	1:E:1368:ARG:NH1	2.20	0.51
1:A:1173:ASN:ND2	1:A:1180:SER:HB2	2.26	0.50
2:B:142:GLY:HA3	2:B:154:TYR:CZ	2.46	0.50
2:F:138:THR:OG1	2:F:140:PRO:HD2	2.12	0.50
1:G:1282:LEU:HG	1:G:1289:PRO:HG2	1.93	0.50
1:A:1234:MSE:SE	1:A:1267:LEU:HD23	2.61	0.50
2:F:145:MET:HA	2:F:145:MET:CE	2.41	0.50
1:C:1339:ALA:HB1	1:C:1361:VAL:HG22	1.93	0.50
1:C:1341:GLN:HB3	1:C:1359:VAL:HB	1.93	0.50
1:E:1345:LEU:HD12	1:E:1355:VAL:HG12	1.93	0.50
1:G:1119:ASP:O	1:G:1122:LYS:HG3	2.11	0.50
1:C:1328:PRO:HG2	1:C:1329:PHE:CD1	2.46	0.50
1:G:1282:LEU:HD21	1:G:1289:PRO:HB3	1.94	0.50
2:B:138:THR:HG23	2:B:141:GLN:HE21	1.76	0.50
1:A:1239:GLU:CD	2:B:66:ARG:HH11	2.15	0.50
1:C:1282:LEU:HB2	1:G:1285:TRP:CE2	2.47	0.50
1:E:1135:TYR:HE2	1:E:1138:ARG:NH2	2.10	0.50
1:E:1142:TYR:CE2	1:E:1193:VAL:HG13	2.46	0.50
1:G:1187:ILE:O	1:G:1191:GLN:HG3	2.11	0.50
1:A:1140:LYS:HE2	1:A:1227:VAL:HA	1.94	0.50
2:D:66:ARG:CG	2:D:66:ARG:HH11	2.23	0.50
2:B:145:MET:HA	2:B:145:MET:CE	2.42	0.50
1:C:1177:GLN:HG3	2:D:41:SER:HB3	1.94	0.50
2:F:142:GLY:HA3	2:F:154:TYR:CZ	2.47	0.50
2:F:153:LYS:HB3	2:F:155:LEU:CD1	2.41	0.50
2:H:19:LEU:C	2:H:19:LEU:HD23	2.32	0.50
1:E:1062:LEU:HG	1:E:1185:TYR:HB3	1.94	0.50
1:E:1179:SER:H	2:F:41:SER:CB	2.24	0.50
1:E:1397:LYS:O	1:E:1401:GLN:HB2	2.12	0.50
1:G:1345:LEU:HD12	1:G:1355:VAL:CG1	2.40	0.50
2:H:10:GLY:HA2	2:H:97:TRP:CE2	2.47	0.50
2:D:138:THR:OG1	2:D:140:PRO:HD2	2.11	0.50
1:E:1368:ARG:CG	1:E:1368:ARG:HH11	2.17	0.50
1:G:1135:TYR:CE2	1:G:1138:ARG:NH2	2.79	0.50
2:H:152:VAL:HG12	2:H:153:LYS:HG2	1.94	0.50
2:H:28:PHE:CD1	2:H:29:PRO:HD2	2.46	0.50
1:C:1173:ASN:ND2	1:C:1180:SER:HB2	2.26	0.49
1:A:1273:VAL:HG21	1:A:1375:LEU:HB3	1.94	0.49
1:C:1287:LYS:CG	1:C:1288:GLU:N	2.75	0.49
2:D:155:LEU:CD2	2:D:168:VAL:HA	2.41	0.49
2:F:153:LYS:HB3	2:F:155:LEU:HD11	1.94	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:19:LEU:HD23	2:F:19:LEU:C	2.33	0.49
1:C:1306:ASP:OD2	1:G:1287:LYS:HD2	2.13	0.49
1:A:1212:GLU:OE1	1:G:1138:ARG:NH2	2.45	0.49
2:H:146:ALA:CB	2:H:154:TYR:HB2	2.42	0.49
1:C:1049:LEU:HD11	1:C:1106:VAL:HB	1.94	0.49
1:C:1350:ALA:O	1:C:1351:GLU:HB3	2.12	0.49
2:D:28:PHE:CD1	2:D:29:PRO:HD2	2.47	0.49
1:E:1049:LEU:HD11	1:E:1106:VAL:HB	1.94	0.49
2:F:155:LEU:N	2:F:155:LEU:HD12	2.27	0.49
2:B:28:PHE:CD1	2:B:29:PRO:HD2	2.47	0.49
2:D:153:LYS:HB3	2:D:155:LEU:CD1	2.43	0.49
2:D:153:LYS:HB3	2:D:155:LEU:HD11	1.94	0.49
1:E:1153:PRO:O	1:E:1157:VAL:HG23	2.13	0.49
1:A:1134:TYR:CE2	1:G:1216:HIS:HB3	2.47	0.49
2:H:12:GLY:O	2:H:13:ALA:HB3	2.13	0.49
2:B:145:MET:HA	2:B:145:MET:HE3	1.94	0.49
2:B:98:TYR:HB3	2:B:99:PRO:HD3	1.94	0.49
1:E:1111:ASP:OD2	1:E:1113:GLU:HB2	2.11	0.49
2:F:138:THR:N	2:F:141:GLN:HE21	1.91	0.49
2:H:153:LYS:HB3	2:H:155:LEU:CD1	2.42	0.49
1:A:1062:LEU:HG	1:A:1185:TYR:HB3	1.95	0.49
1:A:1340:LEU:HD11	1:A:1390:VAL:CG1	2.42	0.49
2:D:145:MET:CE	2:D:145:MET:HA	2.43	0.49
2:F:155:LEU:CD2	2:F:168:VAL:HA	2.42	0.49
1:E:1195:LYS:NZ	2:F:59:ALA:HB3	2.28	0.49
1:C:1282:LEU:HD21	1:C:1289:PRO:HB3	1.94	0.49
1:C:1340:LEU:HD11	1:C:1390:VAL:CG1	2.43	0.49
1:E:1227:VAL:O	1:E:1231:ILE:HG12	2.12	0.49
2:F:133:LYS:N	2:F:133:LYS:HD3	2.28	0.49
1:G:1173:ASN:ND2	1:G:1180:SER:HB2	2.28	0.49
1:A:1368:ARG:HH11	1:A:1368:ARG:CG	2.21	0.49
1:E:1273:VAL:HG23	1:E:1377:CYS:HA	1.95	0.49
2:F:146:ALA:CB	2:F:154:TYR:HB2	2.42	0.49
1:G:1173:ASN:HD21	1:G:1180:SER:HB2	1.77	0.49
1:G:1287:LYS:CG	1:G:1288:GLU:N	2.76	0.49
1:G:1350:ALA:O	1:G:1351:GLU:HB3	2.13	0.49
1:G:1341:GLN:HB3	1:G:1359:VAL:HB	1.94	0.49
1:C:1149:HIS:CE1	1:C:1186:LEU:O	2.66	0.49
1:C:1298:THR:O	1:C:1299:ALA:HB2	2.13	0.49
1:G:1049:LEU:HD11	1:G:1106:VAL:HB	1.93	0.49
1:G:1298:THR:O	1:G:1299:ALA:HB2	2.12	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:145:MET:CE	2:H:145:MET:HA	2.43	0.49
1:E:1156:LEU:HD21	1:E:1182:LEU:HD23	1.94	0.48
1:E:1191:GLN:O	1:E:1195:LYS:HG2	2.13	0.48
1:A:1368:ARG:NH1	1:A:1368:ARG:HG3	2.25	0.48
1:C:1248:LEU:CD2	1:C:1332:ARG:HG3	2.32	0.48
2:F:66:ARG:HH11	2:F:66:ARG:CG	2.25	0.48
2:D:8:VAL:HG22	2:D:79:LEU:HD12	1.94	0.48
2:D:142:GLY:HA3	2:D:154:TYR:CZ	2.47	0.48
1:G:1328:PRO:HG2	1:G:1329:PHE:CD1	2.49	0.48
2:B:155:LEU:CD2	2:B:168:VAL:HA	2.43	0.48
2:D:161:THR:HB	2:D:163:ARG:HG2	1.94	0.48
1:G:1156:LEU:C	1:G:1158:LYS:H	2.16	0.48
2:B:12:GLY:O	2:B:13:ALA:HB3	2.13	0.48
1:C:1156:LEU:CD2	1:C:1182:LEU:HD23	2.44	0.48
1:G:1135:TYR:HE2	1:G:1138:ARG:NH2	2.11	0.48
1:G:1218:ASP:OD1	1:G:1222:LYS:HE3	2.13	0.48
1:C:1287:LYS:CG	1:C:1288:GLU:H	2.27	0.48
1:E:1035:LEU:HG	2:F:31:GLU:OE1	2.14	0.48
1:E:1340:LEU:HD11	1:E:1390:VAL:CG1	2.44	0.48
2:F:68:ARG:NH1	2:F:100:GLU:OE1	2.46	0.48
2:F:28:PHE:CD1	2:F:29:PRO:HD2	2.49	0.48
2:H:153:LYS:HB3	2:H:155:LEU:HD11	1.96	0.48
2:H:142:GLY:HA3	2:H:154:TYR:CZ	2.48	0.48
1:A:1052:GLU:OE2	1:A:1095:GLN:NE2	2.43	0.48
2:B:153:LYS:HB3	2:B:155:LEU:HD11	1.96	0.48
1:C:1135:TYR:CE2	1:C:1138:ARG:NH2	2.81	0.48
2:D:152:VAL:HG12	2:D:153:LYS:HG2	1.94	0.48
1:E:1341:GLN:HB3	1:E:1359:VAL:HB	1.96	0.48
1:G:1056:VAL:HG21	1:G:1099:LEU:CD2	2.40	0.48
1:C:1134:TYR:CE2	1:E:1216:HIS:HB3	2.48	0.48
2:D:146:ALA:CB	2:D:154:TYR:HB2	2.43	0.48
2:D:19:LEU:C	2:D:19:LEU:HD23	2.34	0.48
1:E:1119:ASP:O	1:E:1122:LYS:HG3	2.13	0.48
1:E:1350:ALA:O	1:E:1351:GLU:HB3	2.13	0.48
1:G:1164:ALA:O	1:G:1167:ALA:HB3	2.14	0.48
1:G:1176:GLN:HE22	2:H:1:MET:H3	1.61	0.48
2:B:10:GLY:HA2	2:B:97:TRP:CE2	2.49	0.48
1:A:1191:GLN:O	1:A:1195:LYS:HG2	2.14	0.47
1:A:1227:VAL:O	1:A:1231:ILE:HG12	2.14	0.47
1:A:1298:THR:O	1:A:1299:ALA:HB2	2.12	0.47
2:B:146:ALA:CB	2:B:154:TYR:HB2	2.44	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1368:ARG:NH1	1:C:1368:ARG:HG3	2.23	0.47
1:G:1179:SER:HB3	2:H:41:SER:HB2	1.96	0.47
2:H:5:LYS:HE3	2:H:56:TRP:CE3	2.49	0.47
2:H:96:LYS:O	2:H:99:PRO:HD2	2.14	0.47
1:A:1077:THR:OG1	1:A:1080:GLU:HG3	2.14	0.47
1:A:1350:ALA:O	1:A:1351:GLU:HB3	2.14	0.47
2:B:138:THR:HG23	2:B:141:GLN:NE2	2.29	0.47
2:B:153:LYS:HB3	2:B:155:LEU:CD1	2.43	0.47
1:E:1055:TYR:CD2	1:E:1192:ARG:HG2	2.49	0.47
2:B:161:THR:HB	2:B:163:ARG:HG2	1.96	0.47
2:D:58:THR:O	2:D:61:GLN:HG2	2.14	0.47
2:H:6:CYS:HB3	2:H:55:LEU:CD2	2.45	0.47
1:A:1142:TYR:CE2	1:A:1193:VAL:HG13	2.49	0.47
1:A:1216:HIS:HB3	1:G:1134:TYR:CE2	2.49	0.47
1:G:1153:PRO:O	1:G:1157:VAL:HG23	2.14	0.47
1:G:1227:VAL:O	1:G:1231:ILE:HG12	2.14	0.47
2:H:133:LYS:HD3	2:H:133:LYS:N	2.30	0.47
2:H:68:ARG:HD2	2:H:100:GLU:OE2	2.14	0.47
1:A:1055:TYR:CD2	1:A:1192:ARG:HG2	2.50	0.47
2:B:138:THR:OG1	2:B:140:PRO:HD2	2.14	0.47
1:C:1152:VAL:HB	1:C:1153:PRO:HD3	1.95	0.47
2:D:98:TYR:HB3	2:D:99:PRO:HD3	1.97	0.47
1:E:1052:GLU:O	1:E:1056:VAL:HG23	2.15	0.47
1:E:1287:LYS:CD	1:E:1287:LYS:N	2.76	0.47
1:A:1389:SER:O	1:A:1392:SER:HB3	2.14	0.47
2:B:133:LYS:N	2:B:133:LYS:HD3	2.30	0.47
2:B:66:ARG:HH11	2:B:66:ARG:CG	2.27	0.47
2:D:10:GLY:HA2	2:D:97:TRP:CE2	2.49	0.47
2:F:152:VAL:HG12	2:F:153:LYS:HG2	1.96	0.47
1:A:1049:LEU:HD11	1:A:1106:VAL:HB	1.96	0.47
2:B:19:LEU:HD23	2:B:19:LEU:C	2.35	0.47
2:D:155:LEU:N	2:D:155:LEU:HD12	2.30	0.47
1:E:1164:ALA:O	1:E:1167:ALA:HB3	2.15	0.47
2:H:8:VAL:HG22	2:H:79:LEU:HD12	1.97	0.47
2:B:6:CYS:HB3	2:B:55:LEU:CD2	2.45	0.47
1:C:1077:THR:OG1	1:C:1080:GLU:HG3	2.14	0.47
2:D:133:LYS:HD3	2:D:133:LYS:N	2.30	0.47
1:E:1067:LEU:CD1	1:E:1088:LEU:HD13	2.45	0.47
1:E:1287:LYS:HG2	1:E:1288:GLU:H	1.79	0.47
1:E:1345:LEU:HD12	1:E:1355:VAL:CG1	2.45	0.47
2:F:161:THR:HB	2:F:163:ARG:HG2	1.97	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1287:LYS:CG	1:G:1288:GLU:H	2.27	0.47
2:H:68:ARG:NH1	2:H:100:GLU:OE1	2.47	0.47
1:C:1287:LYS:CD	1:C:1287:LYS:N	2.77	0.47
1:C:1337:THR:HG21	1:C:1397:LYS:HB2	1.97	0.47
2:F:10:GLY:HA2	2:F:97:TRP:CE2	2.49	0.47
1:G:1239:GLU:OE2	2:H:66:ARG:HG3	2.15	0.47
2:B:11:ASP:OD1	2:B:89:SER:HA	2.15	0.47
1:C:1055:TYR:CD2	1:C:1192:ARG:HG2	2.50	0.47
1:G:1138:ARG:O	1:G:1141:LEU:HG	2.15	0.47
1:C:1156:LEU:C	1:C:1158:LYS:H	2.18	0.47
1:E:1197:PRO:HB2	1:E:1201:ARG:HH12	1.80	0.47
1:A:1273:VAL:HG23	1:A:1377:CYS:HA	1.97	0.46
1:C:1234:MSE:CE	1:C:1237:ILE:HD12	2.45	0.46
1:C:1368:ARG:NH1	1:C:1368:ARG:CG	2.78	0.46
1:A:1157:VAL:CG1	1:A:1157:VAL:O	2.63	0.46
2:B:128:LYS:HD3	2:B:128:LYS:C	2.36	0.46
2:B:155:LEU:HD12	2:B:155:LEU:N	2.30	0.46
2:D:158:SER:O	2:D:162:GLN:N	2.47	0.46
1:E:1149:HIS:CE1	1:E:1186:LEU:O	2.68	0.46
2:D:137:ILE:HD12	2:D:137:ILE:N	2.31	0.46
2:F:58:THR:O	2:F:61:GLN:HG2	2.15	0.46
1:A:1179:SER:H	2:B:41:SER:HB2	1.80	0.46
1:A:1368:ARG:HD2	1:A:1369:PRO:O	2.15	0.46
1:G:1303:VAL:HG11	1:G:1329:PHE:HD2	1.81	0.46
1:G:1340:LEU:HD11	1:G:1390:VAL:CG1	2.45	0.46
2:D:57:ASP:OD1	2:D:58:THR:N	2.48	0.46
1:E:1234:MSE:HE2	1:E:1237:ILE:HD12	1.97	0.46
2:H:11:ASP:OD1	2:H:89:SER:HA	2.16	0.46
2:B:158:SER:O	2:B:162:GLN:N	2.49	0.46
1:C:1067:LEU:CD1	1:C:1088:LEU:HD13	2.44	0.46
2:D:129:LEU:HD12	2:D:136:PRO:HG3	1.97	0.46
2:D:155:LEU:N	2:D:155:LEU:CD1	2.79	0.46
2:F:128:LYS:C	2:F:128:LYS:HD3	2.36	0.46
2:F:137:ILE:N	2:F:137:ILE:HD12	2.31	0.46
1:A:1042:ARG:NE	1:A:1113:GLU:HA	2.31	0.46
1:A:1164:ALA:O	1:A:1167:ALA:HB3	2.15	0.46
1:A:1341:GLN:HB3	1:A:1359:VAL:HB	1.96	0.46
1:C:1115:LEU:HA	1:C:1120:GLN:NE2	2.30	0.46
1:C:1135:TYR:HE2	1:C:1138:ARG:NH2	2.13	0.46
2:D:128:LYS:C	2:D:128:LYS:HD3	2.36	0.46
1:E:1173:ASN:HD21	1:E:1180:SER:HB2	1.79	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1179:SER:H	2:H:41:SER:CB	2.28	0.46
1:A:1067:LEU:CD1	1:A:1088:LEU:HD13	2.45	0.46
1:E:1168:PHE:O	1:E:1172:GLN:HG2	2.16	0.46
1:E:1063:MSE:HE2	1:E:1088:LEU:HD22	1.98	0.46
1:E:1287:LYS:CG	1:E:1288:GLU:N	2.79	0.46
1:A:1287:LYS:CG	1:A:1288:GLU:N	2.79	0.46
1:C:1063:MSE:HE2	1:C:1088:LEU:HD22	1.97	0.46
1:C:1052:GLU:HG3	1:C:1099:LEU:HD13	1.97	0.46
1:E:1056:VAL:CG2	1:E:1099:LEU:HD22	2.38	0.46
1:E:1138:ARG:O	1:E:1141:LEU:HG	2.16	0.46
1:G:1152:VAL:HB	1:G:1153:PRO:HD3	1.97	0.46
1:A:1287:LYS:HG2	1:A:1288:GLU:H	1.81	0.45
1:C:1306:ASP:OD2	1:G:1287:LYS:CD	2.64	0.45
2:D:120:ARG:HH21	2:D:139:TYR:N	2.13	0.45
1:E:1077:THR:OG1	1:E:1080:GLU:HG3	2.16	0.45
2:B:121:ASP:HA	2:B:126:ILE:HD11	1.98	0.45
1:C:1164:ALA:O	1:C:1167:ALA:HB3	2.15	0.45
1:G:1062:LEU:HG	1:G:1185:TYR:HB3	1.98	0.45
1:A:1052:GLU:O	1:A:1056:VAL:HG23	2.16	0.45
2:F:121:ASP:HA	2:F:126:ILE:HD11	1.98	0.45
1:G:1248:LEU:HD21	1:G:1332:ARG:CG	2.42	0.45
2:D:23:TYR:HE1	2:D:166:LYS:HD3	1.81	0.45
1:G:1191:GLN:O	1:G:1195:LYS:HG2	2.16	0.45
2:B:155:LEU:CD1	2:B:155:LEU:N	2.80	0.45
1:C:1138:ARG:O	1:C:1141:LEU:HG	2.16	0.45
1:E:1156:LEU:CD2	1:E:1182:LEU:HD23	2.47	0.45
1:G:1190:ILE:HD13	2:H:70:LEU:CD1	2.38	0.45
1:A:1340:LEU:HD11	1:A:1390:VAL:HG13	1.99	0.45
2:H:80:ILE:HD12	2:H:110:ILE:HG21	1.98	0.45
2:H:137:ILE:N	2:H:137:ILE:HD12	2.31	0.45
1:A:1063:MSE:HE2	1:A:1088:LEU:HD22	1.98	0.45
1:A:1153:PRO:O	1:A:1157:VAL:HG23	2.17	0.45
2:B:23:TYR:HE1	2:B:166:LYS:HD3	1.81	0.45
1:A:1190:ILE:CD1	2:B:70:LEU:HD13	2.38	0.45
1:C:1086:GLY:O	1:C:1087:ASN:OD1	2.35	0.45
1:G:1067:LEU:CD1	1:G:1088:LEU:HD13	2.46	0.45
1:A:1212:GLU:HG3	1:G:1097:GLU:HG3	1.99	0.45
1:A:1156:LEU:C	1:A:1158:LYS:H	2.19	0.45
1:A:1183:GLU:CD	2:B:74:GLN:HE21	2.21	0.45
1:C:1355:VAL:HG12	1:C:1356:CYS:N	2.32	0.45
2:D:66:ARG:NH1	2:D:66:ARG:HG3	2.29	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1035:LEU:HD12	1:E:1035:LEU:O	2.17	0.45
1:E:1173:ASN:ND2	1:E:1180:SER:HB2	2.32	0.45
1:E:1365:SER:O	1:E:1367:GLY:N	2.50	0.45
2:F:11:ASP:OD1	2:F:92:ASN:ND2	2.45	0.45
2:F:155:LEU:N	2:F:155:LEU:CD1	2.79	0.45
1:G:1157:VAL:CG1	1:G:1157:VAL:O	2.64	0.45
1:C:1340:LEU:HD11	1:C:1390:VAL:HG13	1.99	0.45
2:D:121:ASP:HA	2:D:126:ILE:HD11	1.99	0.45
1:E:1115:LEU:HA	1:E:1120:GLN:NE2	2.31	0.45
2:F:138:THR:HG23	2:F:141:GLN:NE2	2.31	0.45
2:F:120:ARG:HH21	2:F:139:TYR:N	2.13	0.45
2:F:6:CYS:HB3	2:F:55:LEU:CD2	2.43	0.45
2:H:58:THR:O	2:H:61:GLN:HG2	2.16	0.45
1:A:1213:GLU:H	1:A:1213:GLU:CD	2.20	0.45
2:B:137:ILE:HD12	2:B:137:ILE:N	2.32	0.45
1:C:1073:GLU:HG2	1:C:1075:PHE:CD1	2.52	0.45
1:C:1142:TYR:CE2	1:C:1193:VAL:HG13	2.51	0.45
1:G:1063:MSE:HE2	1:G:1088:LEU:HD22	1.98	0.45
1:G:1142:TYR:CE2	1:G:1193:VAL:HG13	2.52	0.45
1:G:1368:ARG:NH1	1:G:1368:ARG:HG3	2.23	0.45
1:G:1177:GLN:HG3	2:H:41:SER:HB3	1.98	0.45
2:D:138:THR:HG23	2:D:141:GLN:NE2	2.32	0.44
2:D:5:LYS:HE3	2:D:56:TRP:CE3	2.52	0.44
2:D:6:CYS:HB3	2:D:55:LEU:CD2	2.46	0.44
1:E:1156:LEU:C	1:E:1158:LYS:H	2.19	0.44
2:F:158:SER:O	2:F:162:GLN:N	2.50	0.44
1:A:1344:ALA:HB2	1:A:1387:LEU:CD1	2.47	0.44
1:C:1103:GLU:O	1:C:1107:ARG:HG3	2.17	0.44
1:C:1212:GLU:CD	1:E:1097:GLU:HG2	2.37	0.44
2:D:138:THR:HG23	2:D:141:GLN:HE21	1.82	0.44
1:G:1042:ARG:NE	1:G:1113:GLU:HA	2.32	0.44
1:E:1068:LYS:N	1:E:1069:PRO:HD2	2.33	0.44
1:E:1152:VAL:HB	1:E:1153:PRO:HD3	2.00	0.44
1:E:1340:LEU:HD11	1:E:1390:VAL:HG13	1.99	0.44
2:F:23:TYR:HE1	2:F:166:LYS:HD3	1.82	0.44
1:C:1287:LYS:HE2	1:G:1307:GLY:O	2.17	0.44
2:H:138:THR:OG1	2:H:140:PRO:HD2	2.18	0.44
1:A:1052:GLU:HG3	1:A:1099:LEU:HD13	2.00	0.44
2:D:68:ARG:HD2	2:D:100:GLU:OE2	2.18	0.44
1:A:1285:TRP:HZ2	2:D:98:TYR:CE2	2.36	0.44
1:A:1374:HIS:ND1	1:E:1346:PRO:HG3	2.32	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1368:ARG:HD2	1:E:1369:PRO:O	2.17	0.44
2:H:162:GLN:HG3	2:H:165:LEU:HD22	1.99	0.44
1:A:1115:LEU:HA	1:A:1120:GLN:NE2	2.33	0.44
1:A:1138:ARG:O	1:A:1141:LEU:HG	2.17	0.44
1:A:1215:TYR:O	1:A:1219:VAL:HG23	2.18	0.44
1:A:1368:ARG:NH1	1:A:1368:ARG:CG	2.80	0.44
1:E:1073:GLU:HG2	1:E:1075:PHE:CD1	2.52	0.44
2:H:155:LEU:HD12	2:H:155:LEU:N	2.32	0.44
2:H:1:MET:HG2	2:H:2:GLN:N	2.33	0.44
1:E:1140:LYS:HD2	1:E:1230:HIS:HD2	1.82	0.44
1:E:1234:MSE:CE	1:E:1237:ILE:HD12	2.47	0.44
1:E:1389:SER:O	1:E:1392:SER:HB3	2.17	0.44
1:G:1368:ARG:NH1	1:G:1368:ARG:CG	2.78	0.44
1:A:1073:GLU:HG2	1:A:1075:PHE:CD1	2.52	0.44
2:D:66:ARG:CG	2:D:66:ARG:NH1	2.80	0.44
1:G:1149:HIS:CE1	1:G:1186:LEU:O	2.71	0.44
2:H:158:SER:O	2:H:162:GLN:N	2.50	0.44
1:E:1344:ALA:HB2	1:E:1387:LEU:CD1	2.48	0.44
2:H:23:TYR:HE1	2:H:166:LYS:HD3	1.83	0.44
2:H:66:ARG:NH1	2:H:66:ARG:HG3	2.31	0.44
1:A:1208:ASP:O	1:A:1214:HIS:HB2	2.17	0.44
1:A:1277:ASN:OD1	1:A:1374:HIS:HB2	2.18	0.44
1:C:1153:PRO:O	1:C:1157:VAL:HG23	2.18	0.44
1:C:1168:PHE:O	1:C:1172:GLN:HG2	2.18	0.44
1:E:1052:GLU:HG3	1:E:1099:LEU:HD13	2.00	0.44
2:F:96:LYS:O	2:F:99:PRO:HD2	2.17	0.44
2:H:129:LEU:HD12	2:H:136:PRO:HG3	2.00	0.44
1:A:1068:LYS:N	1:A:1069:PRO:HD2	2.33	0.43
1:A:1149:HIS:CE1	1:A:1186:LEU:O	2.71	0.43
1:A:1201:ARG:HG2	1:A:1221:ILE:HD13	2.00	0.43
1:C:1247:GLN:HB3	1:C:1332:ARG:HH11	1.83	0.43
1:A:1042:ARG:HH11	1:A:1042:ARG:HB3	1.83	0.43
1:E:1365:SER:C	1:E:1367:GLY:N	2.70	0.43
1:C:1042:ARG:NE	1:C:1113:GLU:HA	2.31	0.43
1:C:1327:ASP:HA	1:C:1328:PRO:HD2	1.85	0.43
1:C:1368:ARG:HD2	1:C:1369:PRO:O	2.18	0.43
2:H:161:THR:HB	2:H:163:ARG:HG2	2.00	0.43
1:A:1287:LYS:CD	1:A:1287:LYS:N	2.76	0.43
2:F:17:THR:O	2:F:21:ILE:HG13	2.18	0.43
1:G:1201:ARG:HG2	1:G:1221:ILE:HD13	2.00	0.43
2:H:128:LYS:HD3	2:H:128:LYS:C	2.38	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1187:ILE:O	1:C:1191:GLN:HG3	2.19	0.43
1:C:1239:GLU:OE2	2:D:66:ARG:HG3	2.18	0.43
2:D:162:GLN:HG3	2:D:165:LEU:HD22	1.99	0.43
1:E:1042:ARG:HH11	1:E:1042:ARG:HB3	1.82	0.43
1:E:1234:MSE:CE	1:E:1267:LEU:HD23	2.47	0.43
1:E:1344:ALA:HB2	1:E:1387:LEU:HD13	2.00	0.43
1:G:1368:ARG:HD2	1:G:1369:PRO:O	2.18	0.43
2:H:155:LEU:CD1	2:H:155:LEU:N	2.82	0.43
1:A:1152:VAL:HB	1:A:1153:PRO:HD3	1.99	0.43
2:B:11:ASP:OD1	2:B:92:ASN:ND2	2.47	0.43
1:C:1213:GLU:H	1:C:1213:GLU:CD	2.22	0.43
2:F:85:VAL:HG11	2:F:125:THR:HG21	2.00	0.43
1:G:1156:LEU:HD21	1:G:1182:LEU:HD23	2.00	0.43
1:A:1197:PRO:HB2	1:A:1201:ARG:HH12	1.84	0.43
1:A:1344:ALA:HB2	1:A:1387:LEU:HD13	1.99	0.43
1:C:1052:GLU:O	1:C:1056:VAL:HG23	2.19	0.43
1:C:1363:SER:N	1:C:1368:ARG:O	2.49	0.43
1:E:1157:VAL:O	1:E:1157:VAL:CG1	2.64	0.43
1:E:1213:GLU:CD	1:E:1213:GLU:H	2.22	0.43
2:F:161:THR:HG22	2:F:163:ARG:HB3	2.00	0.43
1:G:1073:GLU:HG2	1:G:1075:PHE:CD1	2.54	0.43
1:G:1077:THR:OG1	1:G:1080:GLU:HG3	2.19	0.43
1:G:1086:GLY:O	1:G:1087:ASN:OD1	2.37	0.43
1:G:1365:SER:C	1:G:1367:GLY:N	2.72	0.43
1:A:1380:PRO:HG2	1:A:1381:GLU:OE2	2.19	0.43
2:F:68:ARG:HD2	2:F:100:GLU:OE2	2.19	0.43
1:C:1286:LYS:HB3	1:C:1289:PRO:HG3	2.01	0.43
1:A:1176:GLN:NE2	2:B:1:MET:N	2.67	0.43
2:B:8:VAL:HG21	2:B:20:LEU:HD21	2.01	0.43
1:C:1118:VAL:HG23	1:C:1119:ASP:N	2.34	0.43
2:D:137:ILE:HG23	2:D:141:GLN:HB2	2.00	0.43
1:E:1103:GLU:O	1:E:1107:ARG:HG3	2.18	0.43
1:G:1118:VAL:HG23	1:G:1119:ASP:N	2.33	0.43
1:G:1115:LEU:HA	1:G:1120:GLN:NE2	2.34	0.43
1:G:1260:ALA:O	1:G:1261:ASP:CB	2.66	0.43
1:G:1368:ARG:HA	1:G:1369:PRO:HD3	1.75	0.43
1:C:1365:SER:C	1:C:1367:GLY:N	2.71	0.42
1:E:1118:VAL:HG23	1:E:1119:ASP:N	2.34	0.42
2:F:66:ARG:HG3	2:F:66:ARG:NH1	2.30	0.42
1:A:1365:SER:O	1:A:1367:GLY:N	2.52	0.42
1:C:1282:LEU:HD21	1:C:1289:PRO:CB	2.48	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:129:LEU:HD12	2:F:136:PRO:HG3	2.01	0.42
1:G:1055:TYR:CD2	1:G:1192:ARG:HG2	2.54	0.42
2:H:66:ARG:CG	2:H:66:ARG:HH11	2.28	0.42
1:A:1275:TRP:O	1:A:1278:PRO:HD3	2.19	0.42
2:B:120:ARG:HH21	2:B:139:TYR:N	2.15	0.42
1:G:1168:PHE:O	1:G:1172:GLN:HG2	2.19	0.42
1:G:1234:MSE:HE2	1:G:1237:ILE:HD12	2.00	0.42
1:G:1389:SER:O	1:G:1392:SER:HB3	2.20	0.42
2:H:85:VAL:HG11	2:H:125:THR:HG21	2.01	0.42
2:H:49:LYS:HD3	2:H:177:LEU:HD13	2.01	0.42
1:A:1241:PHE:O	1:A:1242:GLY:C	2.57	0.42
1:A:1342:VAL:O	1:A:1342:VAL:HG13	2.20	0.42
1:C:1344:ALA:HB2	1:C:1387:LEU:CD1	2.49	0.42
1:C:1365:SER:O	1:C:1367:GLY:N	2.50	0.42
1:C:1389:SER:O	1:C:1392:SER:HB3	2.19	0.42
1:E:1065:ARG:HH11	1:E:1065:ARG:HG2	1.84	0.42
1:E:1042:ARG:NE	1:E:1113:GLU:HA	2.30	0.42
1:E:1094:PHE:CE1	1:E:1135:TYR:HD2	2.36	0.42
1:G:1380:PRO:HG2	1:G:1381:GLU:OE2	2.19	0.42
2:H:137:ILE:HG23	2:H:141:GLN:HB2	2.00	0.42
1:A:1118:VAL:HG23	1:A:1119:ASP:N	2.33	0.42
2:B:17:THR:O	2:B:21:ILE:HG13	2.20	0.42
2:D:120:ARG:NH2	2:D:139:TYR:H	2.16	0.42
1:E:1368:ARG:NH1	1:E:1368:ARG:CG	2.76	0.42
1:G:1036:SER:O	1:G:1039:ASP:N	2.53	0.42
1:A:1355:VAL:HG12	1:A:1356:CYS:N	2.34	0.42
2:B:5:LYS:HE3	2:B:56:TRP:CE3	2.53	0.42
1:C:1244:VAL:HG21	1:C:1329:PHE:CD2	2.55	0.42
2:D:160:LEU:HD13	2:D:160:LEU:C	2.40	0.42
1:E:1178:HIS:C	1:E:1180:SER:H	2.23	0.42
1:E:1234:MSE:O	1:E:1264:MSE:HE2	2.19	0.42
2:F:138:THR:HG23	2:F:141:GLN:HE21	1.84	0.42
1:E:1086:GLY:O	1:E:1087:ASN:OD1	2.38	0.42
1:G:1215:TYR:O	1:G:1219:VAL:HG23	2.20	0.42
1:A:1107:ARG:C	1:A:1109:VAL:H	2.23	0.42
1:C:1097:GLU:O	1:C:1101:THR:HG23	2.19	0.42
1:E:1107:ARG:C	1:E:1109:VAL:H	2.23	0.42
1:E:1239:GLU:OE1	2:F:66:ARG:NH1	2.53	0.42
2:F:146:ALA:HB2	2:F:154:TYR:HB2	2.02	0.42
1:G:1115:LEU:N	1:G:1115:LEU:CD1	2.83	0.42
1:G:1244:VAL:HG21	1:G:1329:PHE:CD2	2.54	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:57:ASP:OD1	2:H:58:THR:N	2.53	0.42
1:A:1178:HIS:HA	1:A:1181:THR:CG2	2.50	0.42
2:B:5:LYS:HG3	2:B:75:THR:HA	2.00	0.42
1:C:1282:LEU:HD22	1:G:1285:TRP:CZ3	2.55	0.42
2:D:108:THR:HA	2:D:109:PRO:HD2	1.90	0.42
2:D:5:LYS:HG3	2:D:75:THR:HA	2.00	0.42
2:D:68:ARG:N	2:D:69:PRO:HD2	2.34	0.42
1:E:1287:LYS:CG	1:E:1288:GLU:H	2.32	0.42
2:F:108:THR:HA	2:F:109:PRO:HD2	1.92	0.42
1:G:1042:ARG:HB3	1:G:1042:ARG:HH11	1.85	0.42
1:G:1065:ARG:HH11	1:G:1065:ARG:HG2	1.84	0.42
1:G:1363:SER:N	1:G:1368:ARG:O	2.48	0.42
1:G:1295:VAL:HG11	1:G:1389:SER:OG	2.20	0.42
1:A:1115:LEU:N	1:A:1115:LEU:CD1	2.83	0.42
1:A:1168:PHE:O	1:A:1172:GLN:HG2	2.20	0.42
2:B:24:THR:HG22	2:B:40:TYR:CE2	2.55	0.42
1:C:1042:ARG:HB3	1:C:1042:ARG:HH11	1.85	0.42
1:C:1065:ARG:HH11	1:C:1065:ARG:HG2	1.85	0.42
1:C:1178:HIS:C	1:C:1180:SER:H	2.22	0.42
1:C:1201:ARG:HG2	1:C:1221:ILE:HD13	2.02	0.42
2:D:161:THR:HG22	2:D:161:THR:O	2.20	0.42
2:D:87:PRO:O	2:D:90:PHE:HB3	2.20	0.42
1:E:1275:TRP:O	1:E:1278:PRO:HD3	2.20	0.42
1:E:1295:VAL:HG11	1:E:1389:SER:OG	2.19	0.42
2:H:120:ARG:HH21	2:H:139:TYR:N	2.17	0.42
2:H:8:VAL:HG21	2:H:20:LEU:HD21	2.02	0.42
1:A:1373:PHE:HB3	1:A:1375:LEU:HD21	2.02	0.41
2:B:129:LEU:HD12	2:B:136:PRO:HG3	2.01	0.41
1:C:1197:PRO:HB2	1:C:1201:ARG:HH12	1.85	0.41
1:E:1115:LEU:H	1:E:1115:LEU:CD1	2.34	0.41
1:E:1115:LEU:CD1	1:E:1115:LEU:N	2.83	0.41
1:E:1277:ASN:OD1	1:E:1374:HIS:HB2	2.20	0.41
2:F:57:ASP:OD1	2:F:58:THR:N	2.51	0.41
1:G:1107:ARG:C	1:G:1109:VAL:H	2.23	0.41
2:H:146:ALA:HB2	2:H:154:TYR:HB2	2.02	0.41
1:A:1365:SER:C	1:A:1367:GLY:N	2.72	0.41
2:D:68:ARG:HB3	2:D:69:PRO:HD3	2.02	0.41
1:E:1063:MSE:HG3	1:E:1068:LYS:HE3	2.03	0.41
2:F:5:LYS:HG3	2:F:75:THR:HA	2.03	0.41
2:F:66:ARG:CG	2:F:66:ARG:NH1	2.82	0.41
2:B:146:ALA:HB2	2:B:154:TYR:HB2	2.02	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1240:GLU:CG	1:C:1305:LYS:NZ	2.82	0.41
2:D:17:THR:O	2:D:21:ILE:HG13	2.20	0.41
1:E:1094:PHE:HE1	1:E:1135:TYR:CD2	2.37	0.41
1:E:1399:ARG:C	1:E:1401:GLN:H	2.22	0.41
1:G:1197:PRO:HB2	1:G:1201:ARG:HH12	1.84	0.41
1:G:1304:TYR:CB	1:G:1331:PHE:HB3	2.43	0.41
1:A:1287:LYS:CG	1:A:1288:GLU:H	2.33	0.41
1:A:1359:VAL:HG22	1:A:1372:VAL:HG22	2.03	0.41
1:C:1059:LEU:HA	1:C:1059:LEU:HD12	1.94	0.41
2:D:85:VAL:HG11	2:D:125:THR:HG21	2.03	0.41
2:D:12:GLY:O	2:D:13:ALA:HB3	2.21	0.41
1:E:1368:ARG:HA	1:E:1369:PRO:HD3	1.76	0.41
1:G:1052:GLU:O	1:G:1056:VAL:HG23	2.21	0.41
1:G:1252:GLN:HE21	1:G:1252:GLN:HB2	1.66	0.41
2:B:162:GLN:HE21	2:B:162:GLN:HB2	1.66	0.41
2:B:161:THR:HG22	2:B:161:THR:O	2.20	0.41
2:F:158:SER:HB3	2:F:161:THR:HB	2.03	0.41
1:G:1327:ASP:HA	1:G:1328:PRO:HD2	1.86	0.41
1:A:1076:LEU:HA	1:A:1080:GLU:OE1	2.21	0.41
1:A:1174:PRO:HG2	1:A:1175:ARG:H	1.86	0.41
1:A:1177:GLN:HG3	2:B:41:SER:CB	2.50	0.41
1:A:1234:MSE:HE2	1:A:1237:ILE:HD12	2.02	0.41
1:C:1068:LYS:N	1:C:1069:PRO:HD2	2.35	0.41
2:D:11:ASP:OD1	2:D:92:ASN:ND2	2.51	0.41
2:F:87:PRO:O	2:F:90:PHE:HB3	2.20	0.41
1:G:1052:GLU:HG3	1:G:1099:LEU:HD13	2.03	0.41
1:G:1250:ALA:C	1:G:1252:GLN:N	2.73	0.41
1:A:1115:LEU:H	1:A:1115:LEU:CD1	2.34	0.41
2:F:137:ILE:HG23	2:F:141:GLN:HB2	2.02	0.41
2:F:37:PHE:HD2	2:F:57:ASP:HB2	1.86	0.41
1:G:1250:ALA:C	1:G:1252:GLN:H	2.22	0.41
2:H:161:THR:HG22	2:H:161:THR:O	2.21	0.41
2:H:66:ARG:NH1	2:H:66:ARG:CG	2.84	0.41
1:A:1065:ARG:HG2	1:A:1065:ARG:HH11	1.85	0.41
1:A:1178:HIS:C	1:A:1180:SER:H	2.24	0.41
2:B:68:ARG:HB3	2:B:69:PRO:HD3	2.03	0.41
1:C:1115:LEU:CD1	1:C:1115:LEU:H	2.33	0.41
1:C:1208:ASP:O	1:C:1214:HIS:HB2	2.21	0.41
1:C:1380:PRO:HG2	1:C:1381:GLU:OE2	2.20	0.41
1:E:1047:GLU:O	1:E:1051:THR:HG23	2.21	0.41
1:G:1213:GLU:H	1:G:1213:GLU:CD	2.23	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1355:VAL:HG12	1:G:1356:CYS:N	2.36	0.41
2:B:66:ARG:CG	2:B:66:ARG:NH1	2.84	0.41
1:C:1115:LEU:CD1	1:C:1115:LEU:N	2.84	0.41
1:C:1250:ALA:C	1:C:1252:GLN:H	2.23	0.41
2:D:146:ALA:HB2	2:D:154:TYR:HB2	2.03	0.41
1:E:1106:VAL:CG2	1:E:1112:LEU:HD11	2.51	0.41
2:F:160:LEU:HD13	2:F:160:LEU:C	2.41	0.41
2:F:161:THR:HG22	2:F:161:THR:O	2.20	0.41
1:A:1103:GLU:O	1:A:1107:ARG:HG3	2.21	0.41
1:A:1210:GLU:OE1	1:A:1210:GLU:HA	2.21	0.41
1:C:1252:GLN:HE21	1:C:1252:GLN:HB2	1.64	0.41
1:C:1345:LEU:H	1:C:1356:CYS:HA	1.86	0.41
1:E:1250:ALA:O	1:E:1251:GLU:HB3	2.20	0.41
1:E:1355:VAL:HG12	1:E:1356:CYS:N	2.36	0.41
1:G:1178:HIS:C	1:G:1180:SER:H	2.24	0.41
1:G:1340:LEU:HD12	1:G:1394:LEU:HD21	2.03	0.41
2:H:11:ASP:OD1	2:H:92:ASN:ND2	2.47	0.41
1:C:1344:ALA:HB2	1:C:1387:LEU:HD13	2.01	0.40
2:D:37:PHE:HD2	2:D:57:ASP:HB2	1.87	0.40
1:E:1086:GLY:C	1:E:1088:LEU:N	2.74	0.40
1:E:1098:PHE:CE2	1:E:1102:LEU:HD11	2.56	0.40
1:E:1208:ASP:O	1:E:1214:HIS:HB2	2.21	0.40
1:G:1086:GLY:C	1:G:1088:LEU:N	2.74	0.40
1:G:1287:LYS:N	1:G:1287:LYS:CD	2.80	0.40
1:G:1365:SER:O	1:G:1367:GLY:N	2.55	0.40
1:A:1346:PRO:HG2	1:E:1345:LEU:CD1	2.52	0.40
1:C:1303:VAL:CG1	1:C:1329:PHE:HD2	2.35	0.40
1:C:1342:VAL:O	1:C:1342:VAL:HG13	2.21	0.40
2:B:137:ILE:HG23	2:B:141:GLN:HB2	2.03	0.40
1:C:1106:VAL:CG2	1:C:1112:LEU:HD11	2.51	0.40
1:E:1249:ILE:CD1	1:E:1261:ASP:H	2.14	0.40
1:G:1344:ALA:HB2	1:G:1387:LEU:CD1	2.51	0.40
1:A:1237:ILE:HD11	1:A:1270:HIS:CD2	2.56	0.40
1:C:1273:VAL:CG2	1:C:1375:LEU:HB3	2.51	0.40
1:E:1085:PHE:O	1:E:1088:LEU:HB2	2.20	0.40
2:F:40:TYR:HB3	2:F:55:LEU:HB2	2.04	0.40
1:G:1340:LEU:HD11	1:G:1390:VAL:HG13	2.03	0.40
2:H:98:TYR:OH	2:H:102:ARG:HD2	2.21	0.40
1:A:1179:SER:HB3	2:B:41:SER:HB2	2.03	0.40
1:A:1156:LEU:HD21	1:A:1182:LEU:HD23	2.03	0.40
1:C:1234:MSE:CE	1:C:1234:MSE:HA	2.44	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1250:ALA:C	1:C:1252:GLN:N	2.75	0.40
1:C:1386:PHE:O	1:C:1390:VAL:HG23	2.21	0.40
1:G:1068:LYS:N	1:G:1069:PRO:HD2	2.35	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:139:TYR:OH	2:H:107:ASN:OD1[2_657]	2.06	0.14

## 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	366/377 (97%)	313 (86%)	43 (12%)	10 (3%)	5	17
1	C	364/377 (97%)	315 (86%)	41 (11%)	8 (2%)	6	22
1	E	365/377 (97%)	322 (88%)	30 (8%)	13 (4%)	3	11
1	G	365/377 (97%)	322 (88%)	31 (8%)	12 (3%)	4	13
2	B	175/177 (99%)	164 (94%)	9 (5%)	2 (1%)	14	41
2	D	175/177 (99%)	164 (94%)	9 (5%)	2 (1%)	14	41
2	F	175/177 (99%)	162 (93%)	12 (7%)	1 (1%)	25	56
2	H	175/177 (99%)	163 (93%)	11 (6%)	1 (1%)	25	56
All	All	2160/2216 (98%)	1925 (89%)	186 (9%)	49 (2%)	6	21

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1087	ASN
1	A	1253	THR

Continued on next page...

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1261	ASP
1	C	1087	ASN
1	C	1253	THR
1	C	1261	ASP
1	E	1087	ASN
1	E	1253	THR
1	E	1261	ASP
1	G	1087	ASN
1	G	1253	THR
1	G	1261	ASP
1	A	1086	GLY
1	A	1252	GLN
2	B	11	ASP
1	C	1086	GLY
1	C	1252	GLN
2	D	11	ASP
1	E	1086	GLY
1	E	1305	LYS
1	E	1306	ASP
2	F	11	ASP
1	G	1086	GLY
1	G	1252	GLN
1	G	1325	GLU
1	A	1085	PHE
1	A	1312	LYS
1	A	1322	ILE
1	C	1085	PHE
1	E	1085	PHE
1	E	1252	GLN
1	G	1085	PHE
2	H	11	ASP
1	C	1311	LYS
1	E	1325	GLU
1	A	1254	GLY
1	A	1328	PRO
1	C	1254	GLY
2	D	65	ASP
1	E	1254	GLY
1	G	1254	GLY
1	G	1324	GLU
1	G	1399	ARG
2	B	65	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	1350	ALA
1	G	1311	LYS
1	E	1327	ASP
1	G	1157	VAL
1	E	1157	VAL

### 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	332/332 (100%)	322 (97%)	10 (3%)	41	75
1	C	330/332 (99%)	320 (97%)	10 (3%)	41	75
1	E	331/332 (100%)	318 (96%)	13 (4%)	32	66
1	G	331/332 (100%)	319 (96%)	12 (4%)	35	69
2	B	153/153 (100%)	146 (95%)	7 (5%)	27	60
2	D	153/153 (100%)	146 (95%)	7 (5%)	27	60
2	F	153/153 (100%)	147 (96%)	6 (4%)	32	66
2	H	153/153 (100%)	147 (96%)	6 (4%)	32	66
All	All	1936/1940 (100%)	1865 (96%)	71 (4%)	34	68

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1048	LEU
1	A	1059	LEU
1	A	1062	LEU
1	A	1194	LEU
1	A	1252	GLN
1	A	1284	LYS
1	A	1287	LYS
1	A	1343	ARG
1	A	1368	ARG
1	A	1371	ARG

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	50	PRO
2	B	62	GLU
2	B	66	ARG
2	B	77	VAL
2	B	116	LYS
2	B	143	LEU
2	B	170	ASP
1	C	1048	LEU
1	C	1059	LEU
1	C	1062	LEU
1	C	1194	LEU
1	C	1252	GLN
1	C	1284	LYS
1	C	1287	LYS
1	C	1343	ARG
1	C	1368	ARG
1	C	1371	ARG
2	D	50	PRO
2	D	62	GLU
2	D	66	ARG
2	D	77	VAL
2	D	116	LYS
2	D	143	LEU
2	D	170	ASP
1	E	1035	LEU
1	E	1048	LEU
1	E	1059	LEU
1	E	1062	LEU
1	E	1173	ASN
1	E	1194	LEU
1	E	1252	GLN
1	E	1284	LYS
1	E	1287	LYS
1	E	1313	LYS
1	E	1343	ARG
1	E	1368	ARG
1	E	1371	ARG
2	F	50	PRO
2	F	62	GLU
2	F	66	ARG
2	F	77	VAL
2	F	116	LYS

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	F	170	ASP
1	G	1048	LEU
1	G	1059	LEU
1	G	1062	LEU
1	G	1194	LEU
1	G	1252	GLN
1	G	1284	LYS
1	G	1287	LYS
1	G	1313	LYS
1	G	1343	ARG
1	G	1368	ARG
1	G	1371	ARG
1	G	1397	LYS
2	H	62	GLU
2	H	66	ARG
2	H	77	VAL
2	H	116	LYS
2	H	143	LEU
2	H	170	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1120	GLN
1	A	1149	HIS
1	A	1173	ASN
1	A	1176	GLN
1	A	1230	HIS
1	A	1235	GLN
1	A	1374	HIS
2	B	2	GLN
2	B	74	GLN
2	B	141	GLN
1	C	1120	GLN
1	C	1149	HIS
1	C	1173	ASN
1	C	1230	HIS
1	C	1235	GLN
1	C	1374	HIS
2	D	2	GLN
2	D	74	GLN
2	D	141	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	1120	GLN
1	E	1149	HIS
1	E	1173	ASN
1	E	1176	GLN
1	E	1230	HIS
1	E	1235	GLN
1	E	1374	HIS
2	F	2	GLN
2	F	74	GLN
2	F	141	GLN
1	G	1120	GLN
1	G	1149	HIS
1	G	1173	ASN
1	G	1176	GLN
1	G	1230	HIS
1	G	1235	GLN
1	G	1374	HIS
2	H	2	GLN
2	H	74	GLN
2	H	141	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

4 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	$\# Z  > 2$
3	SO4	B	4001	-	4,4,4	0.30	0	6,6,6	0.13	0
3	SO4	F	4003	-	4,4,4	0.23	0	6,6,6	0.14	0
3	SO4	H	4004	-	4,4,4	0.32	0	6,6,6	0.34	0
3	SO4	D	4002	-	4,4,4	0.28	0	6,6,6	0.22	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.

No monomer is involved in short contacts.

## 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.