



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:45 am GMT

PDB ID : 4BI5
Title : CRYSTAL STRUCTURE OF A DOUBLE MUTANT (C202A AND C222D) OF TRIOSEPHOSPHATE ISOMERASE FROM GIARDIA LAMBLIA.
Authors : Torres-Larios, A.; Enriquez-Flores, S.; Reyes-Vivas, H.; Oria-Hernandez, J.; Hernandez-Alcantara, G.
Deposited on : 2013-04-09
Resolution : 2.70 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:

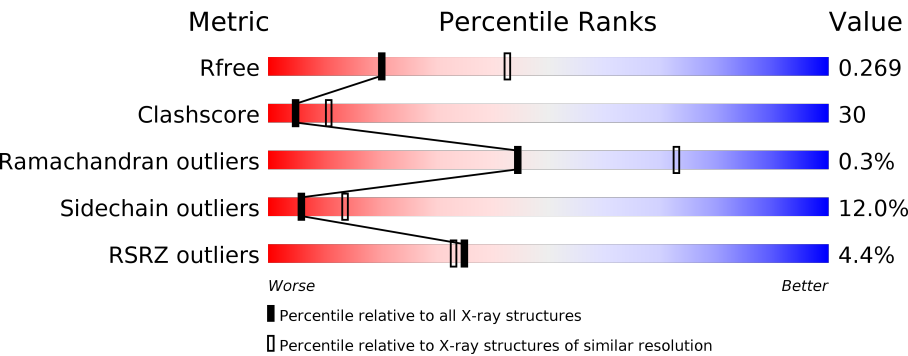
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.70 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}	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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	255	<div><div>4%</div><div><div></div><div>56%</div><div>37%</div><div>7%</div></div></div>
1	B	255	<div><div>2%</div><div><div></div><div>62%</div><div>33%</div><div>•</div></div></div>
1	C	255	<div><div>3%</div><div><div></div><div>54%</div><div>40%</div><div>5%</div></div></div>
1	D	255	<div><div>2%</div><div><div></div><div>56%</div><div>36%</div><div>8%</div></div></div>
1	E	255	<div><div>4%</div><div><div></div><div>52%</div><div>41%</div><div>6%</div></div></div>
1	F	255	<div><div>2%</div><div><div></div><div>58%</div><div>36%</div><div>5%</div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	255	
1	H	255	
1	I	255	
1	J	255	
1	K	255	
1	L	255	
1	M	255	
1	N	255	
1	O	255	
1	P	255	
1	Q	255	
1	R	255	
1	S	255	
1	T	255	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 38560 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 TRIOSEPHOSPHATE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			1928	1212	341	364	11			
1	B	254	Total	C	N	O	S	0	0	0
			1928	1212	341	364	11			
1	C	254	Total	C	N	O	S	0	0	0
			1928	1212	341	364	11			
1	D	254	Total	C	N	O	S	0	0	0
			1928	1212	341	364	11			
1	E	254	Total	C	N	O	S	0	0	0
			1928	1212	341	364	11			
1	F	254	Total	C	N	O	S	0	0	0
			1928	1212	341	364	11			
1	G	254	Total	C	N	O	S	0	0	0
			1928	1212	341	364	11			
1	H	254	Total	C	N	O	S	0	0	0
			1928	1212	341	364	11			
1	I	254	Total	C	N	O	S	0	0	0
			1928	1212	341	364	11			
1	J	254	Total	C	N	O	S	0	0	0
			1928	1212	341	364	11			
1	K	254	Total	C	N	O	S	0	0	0
			1928	1212	341	364	11			
1	L	254	Total	C	N	O	S	0	0	0
			1928	1212	341	364	11			
1	M	254	Total	C	N	O	S	0	0	0
			1928	1212	341	364	11			
1	N	254	Total	C	N	O	S	0	0	0
			1928	1212	341	364	11			
1	O	254	Total	C	N	O	S	0	0	0
			1928	1212	341	364	11			
1	P	254	Total	C	N	O	S	0	0	0
			1928	1212	341	364	11			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	254	Total 1928	C 1212	N 341	O 364	S 11	0	0	0
1	R	254	Total 1928	C 1212	N 341	O 364	S 11	0	0	0
1	S	254	Total 1928	C 1212	N 341	O 364	S 11	0	0	0
1	T	254	Total 1928	C 1212	N 341	O 364	S 11	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	ALA	CYS	ENGINEERED MUTATION	UNP P36186
A	222	ASP	CYS	ENGINEERED MUTATION	UNP P36186
B	202	ALA	CYS	ENGINEERED MUTATION	UNP P36186
B	222	ASP	CYS	ENGINEERED MUTATION	UNP P36186
C	202	ALA	CYS	ENGINEERED MUTATION	UNP P36186
C	222	ASP	CYS	ENGINEERED MUTATION	UNP P36186
D	202	ALA	CYS	ENGINEERED MUTATION	UNP P36186
D	222	ASP	CYS	ENGINEERED MUTATION	UNP P36186
E	202	ALA	CYS	ENGINEERED MUTATION	UNP P36186
E	222	ASP	CYS	ENGINEERED MUTATION	UNP P36186
F	202	ALA	CYS	ENGINEERED MUTATION	UNP P36186
F	222	ASP	CYS	ENGINEERED MUTATION	UNP P36186
G	202	ALA	CYS	ENGINEERED MUTATION	UNP P36186
G	222	ASP	CYS	ENGINEERED MUTATION	UNP P36186
H	202	ALA	CYS	ENGINEERED MUTATION	UNP P36186
H	222	ASP	CYS	ENGINEERED MUTATION	UNP P36186
I	202	ALA	CYS	ENGINEERED MUTATION	UNP P36186
I	222	ASP	CYS	ENGINEERED MUTATION	UNP P36186
J	202	ALA	CYS	ENGINEERED MUTATION	UNP P36186
J	222	ASP	CYS	ENGINEERED MUTATION	UNP P36186
K	202	ALA	CYS	ENGINEERED MUTATION	UNP P36186
K	222	ASP	CYS	ENGINEERED MUTATION	UNP P36186
L	202	ALA	CYS	ENGINEERED MUTATION	UNP P36186
L	222	ASP	CYS	ENGINEERED MUTATION	UNP P36186
M	202	ALA	CYS	ENGINEERED MUTATION	UNP P36186
M	222	ASP	CYS	ENGINEERED MUTATION	UNP P36186
N	202	ALA	CYS	ENGINEERED MUTATION	UNP P36186
N	222	ASP	CYS	ENGINEERED MUTATION	UNP P36186
O	202	ALA	CYS	ENGINEERED MUTATION	UNP P36186
O	222	ASP	CYS	ENGINEERED MUTATION	UNP P36186
P	202	ALA	CYS	ENGINEERED MUTATION	UNP P36186

Continued on next page...

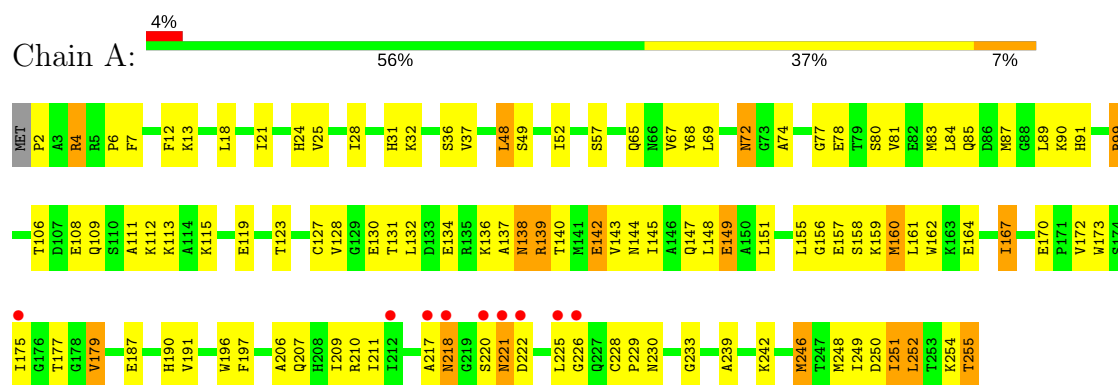
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
P	222	ASP	CYS	ENGINEERED MUTATION	UNP P36186
Q	202	ALA	CYS	ENGINEERED MUTATION	UNP P36186
Q	222	ASP	CYS	ENGINEERED MUTATION	UNP P36186
R	202	ALA	CYS	ENGINEERED MUTATION	UNP P36186
R	222	ASP	CYS	ENGINEERED MUTATION	UNP P36186
S	202	ALA	CYS	ENGINEERED MUTATION	UNP P36186
S	222	ASP	CYS	ENGINEERED MUTATION	UNP P36186
T	202	ALA	CYS	ENGINEERED MUTATION	UNP P36186
T	222	ASP	CYS	ENGINEERED MUTATION	UNP P36186

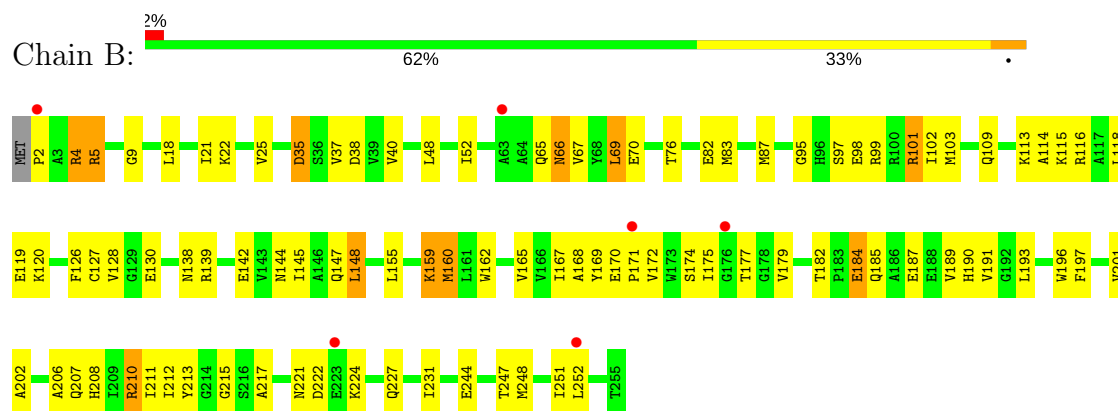
3 Residue-property plots [i](#)

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 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.

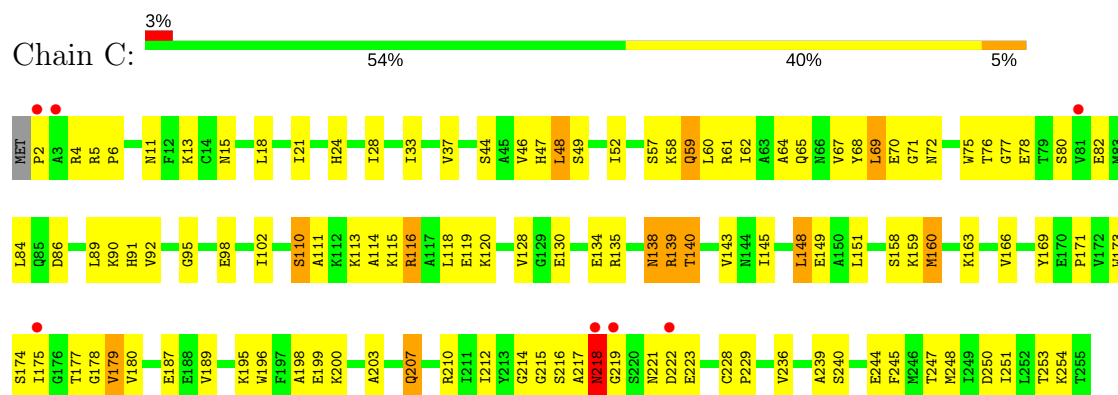
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE



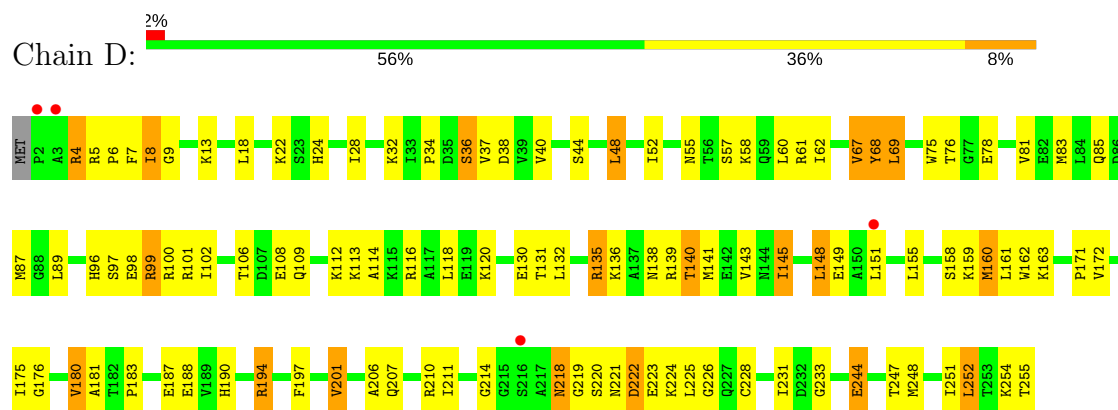
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE



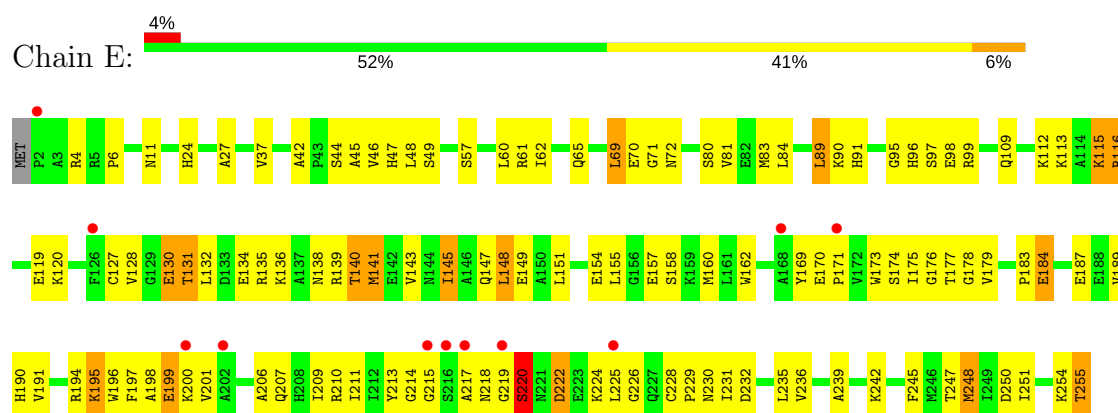
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE



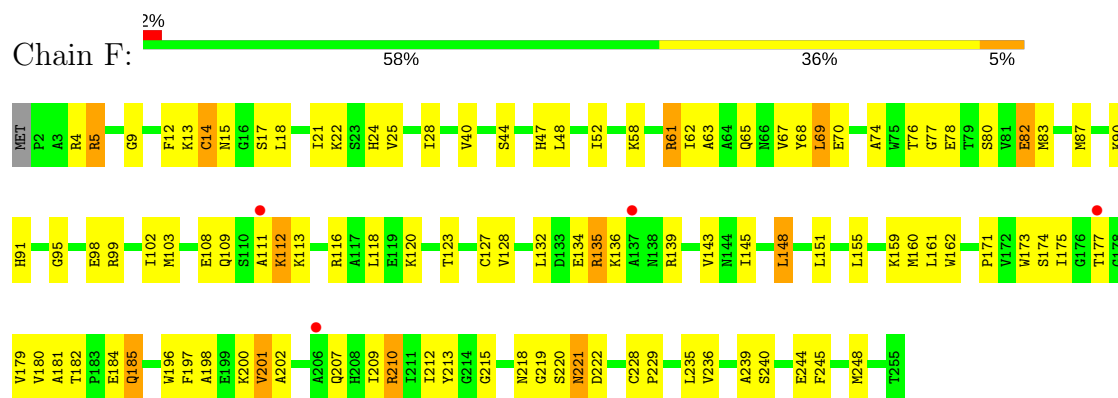
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE



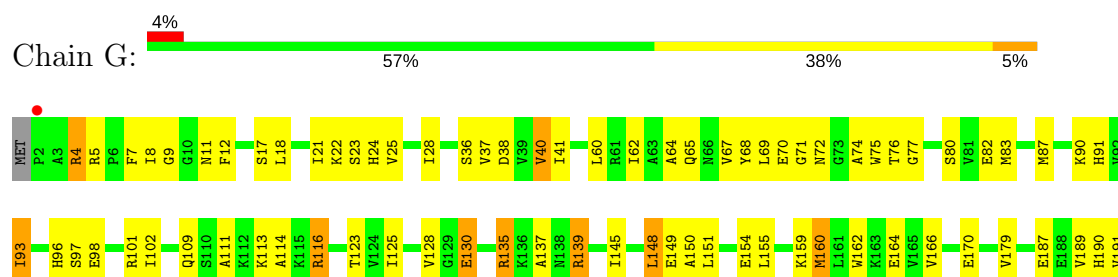
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE



• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

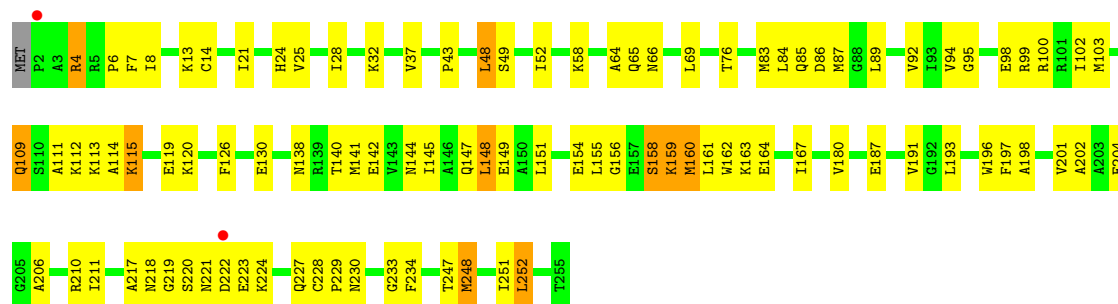


• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

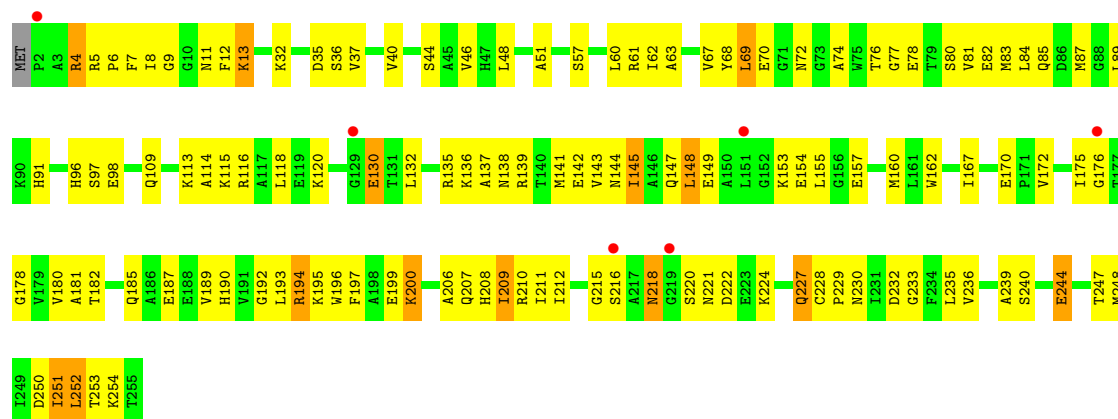




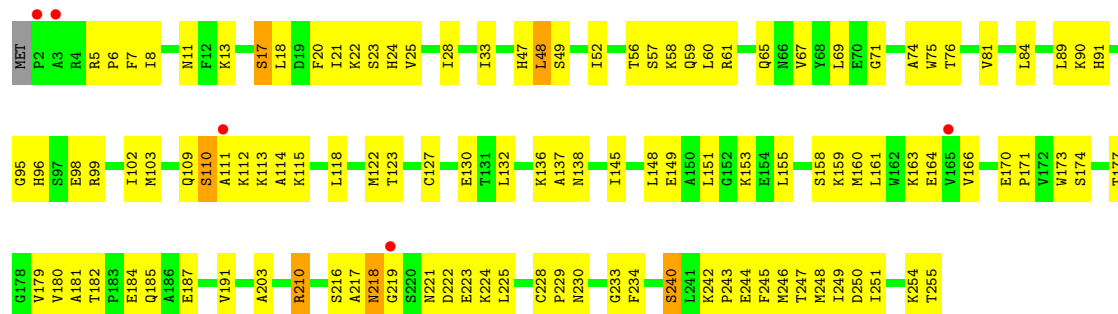
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE



• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

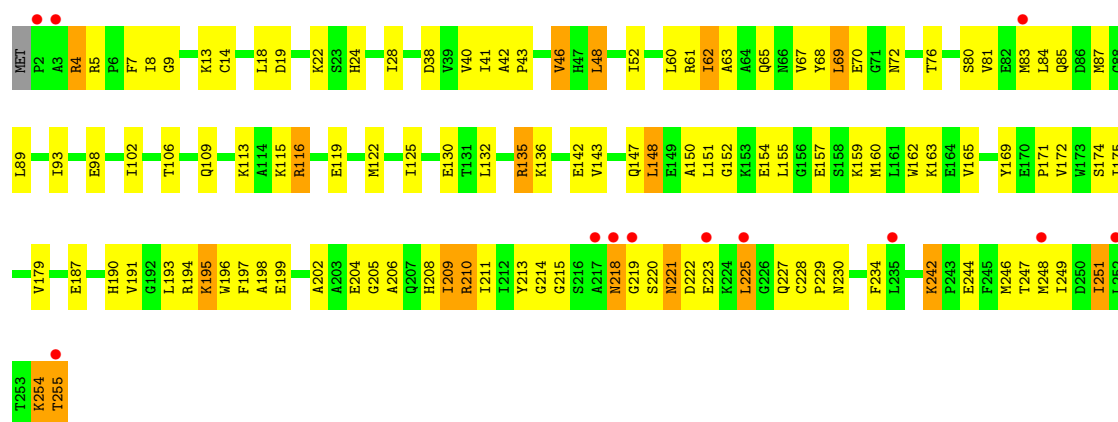


• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

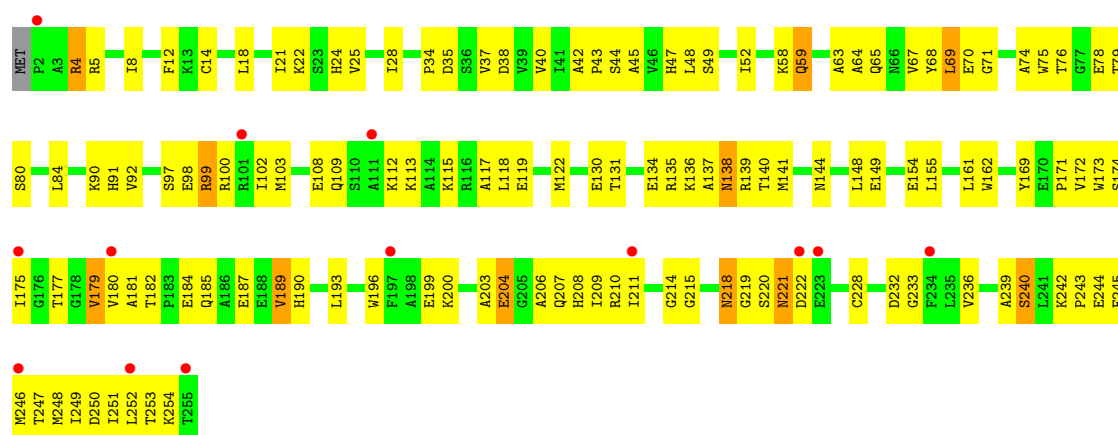


• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

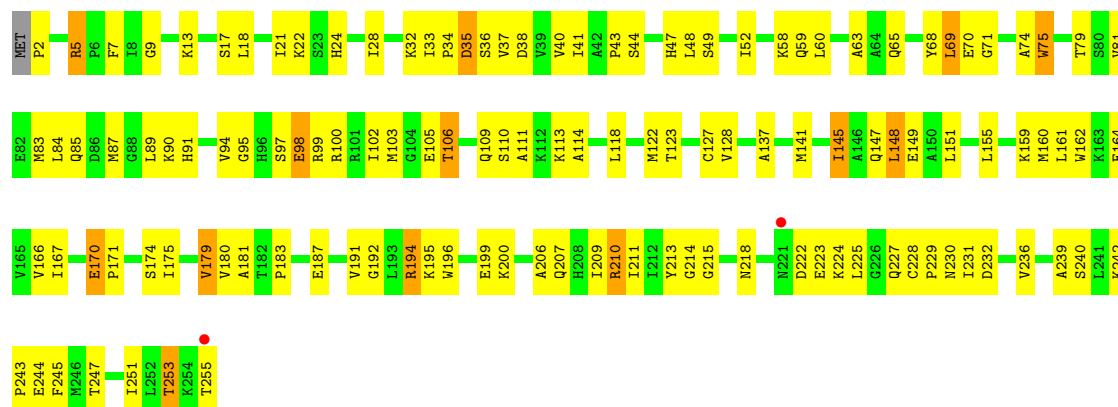




● Molecule 1: TRIOSEPHOSPHATE ISOMERASE

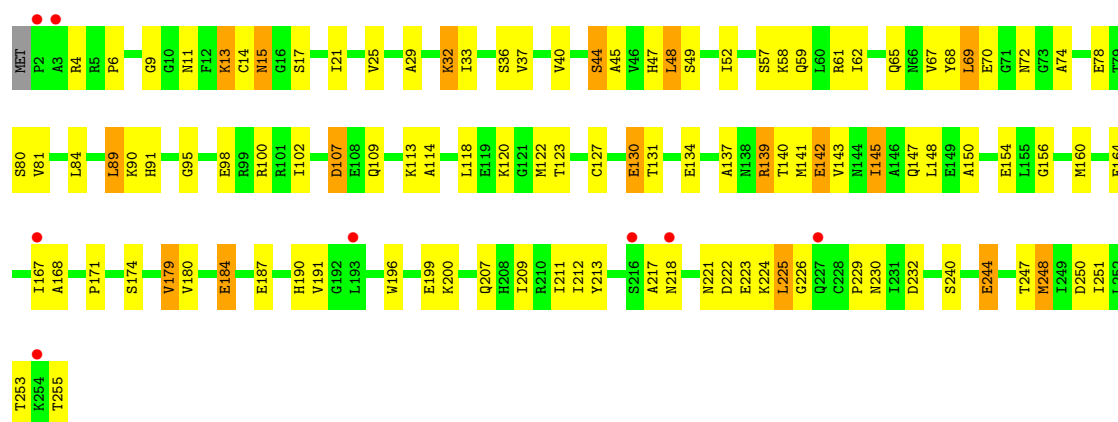


● Molecule 1: TRIOSEPHOSPHATE ISOMERASE

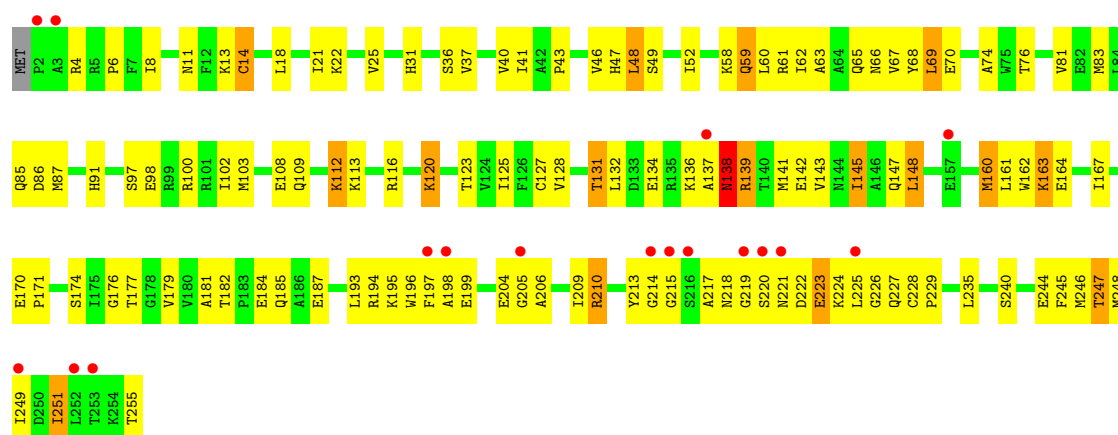


● Molecule 1: TRIOSEPHOSPHATE ISOMERASE

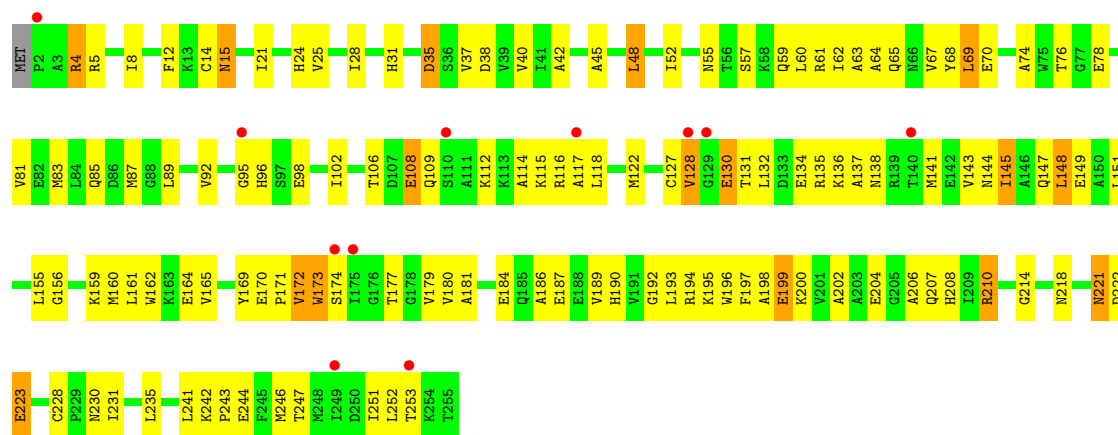




● Molecule 1: TRIOSEPHOSPHATE ISOMERASE

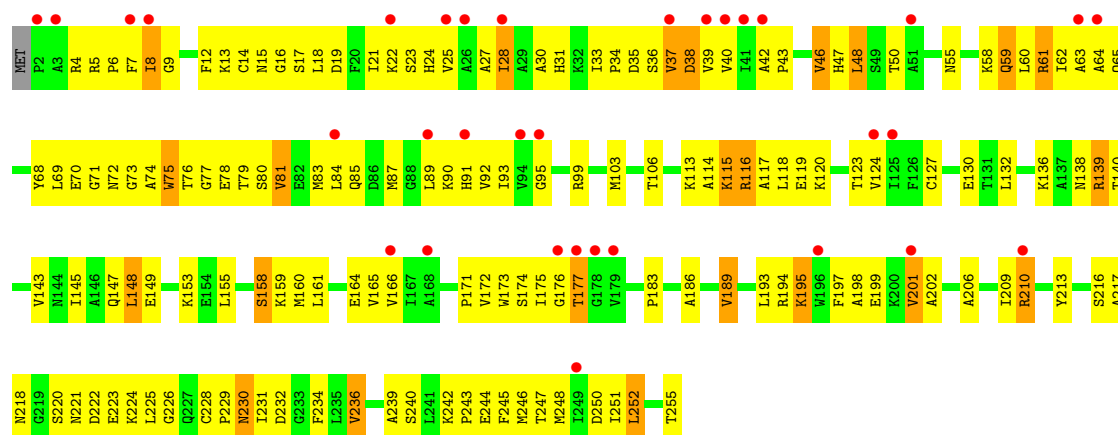


● Molecule 1: TRIOSEPHOSPHATE ISOMERASE

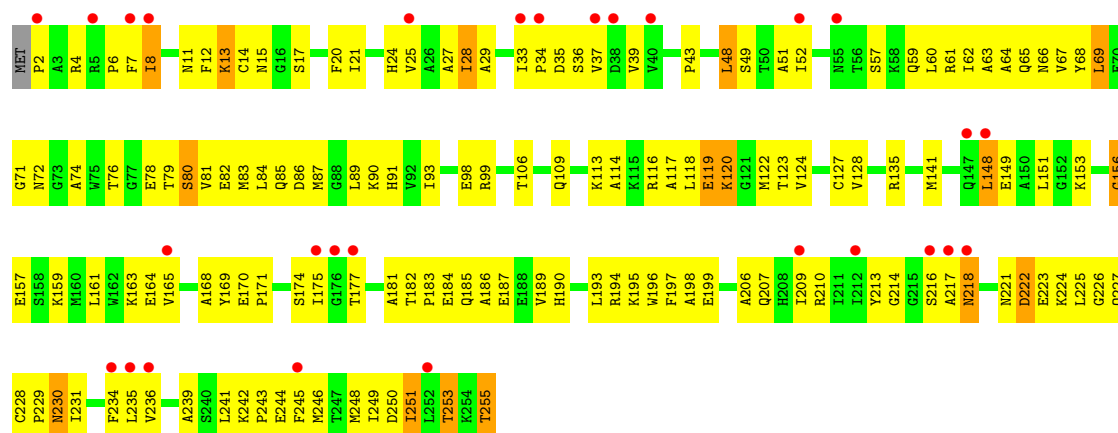
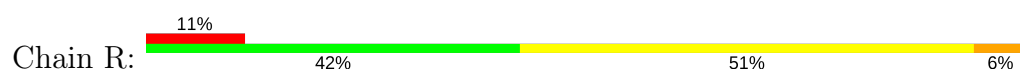


● Molecule 1: TRIOSEPHOSPHATE ISOMERASE

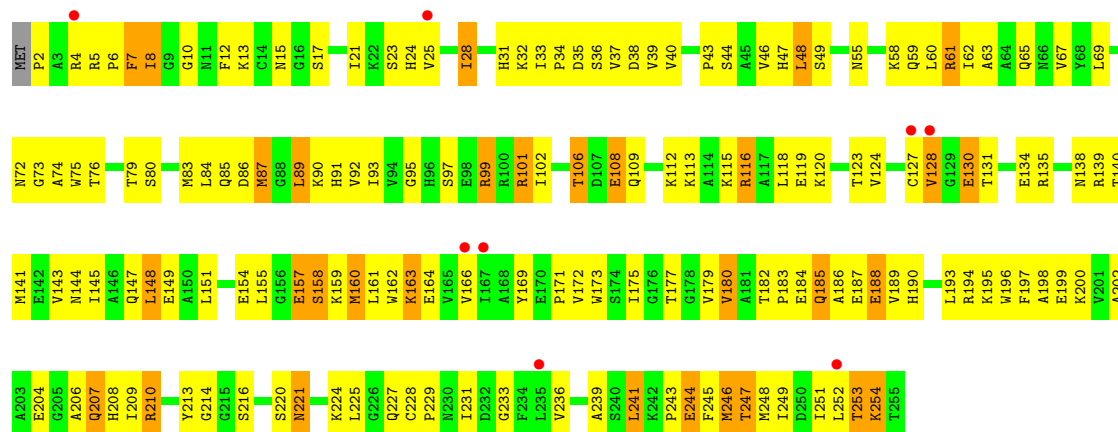




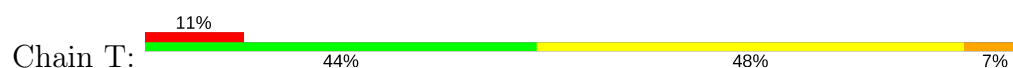
• Molecule 1: TRIOSEPHOSPHATE ISOMERASE

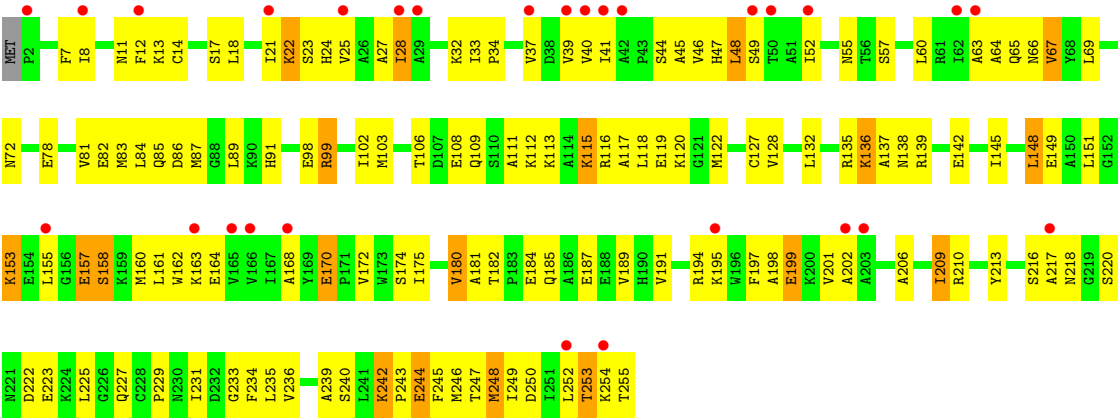


• Molecule 1: TRIOSEPHOSPHATE ISOMERASE



• Molecule 1: TRIOSEPHOSPHATE ISOMERASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	105.22Å 131.57Å 132.55Å 115.73° 89.81° 90.24°	Depositor
Resolution (Å)	78.87 – 2.70 78.88 – 2.70	Depositor EDS
% Data completeness (in resolution range)	82.0 (78.87-2.70) 65.6 (78.88-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.239 , 0.272 0.236 , 0.269	Depositor DCC
R_{free} test set	7212 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	50.3	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 21.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.418 for h,-k,-l 0.197 for -h,-l,-k 0.197 for -h,l,k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	38560	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.48	0/1960	0.49	0/2644
1	B	0.58	2/1960 (0.1%)	0.50	0/2644
1	C	0.55	0/1960	0.53	0/2644
1	D	0.40	0/1960	0.48	0/2644
1	E	0.63	0/1960	0.53	0/2644
1	F	0.49	1/1960 (0.1%)	0.52	0/2644
1	G	0.62	2/1960 (0.1%)	0.52	0/2644
1	H	0.58	0/1960	0.52	0/2644
1	I	0.37	0/1960	0.50	0/2644
1	J	0.44	0/1960	0.49	0/2644
1	K	0.34	0/1960	0.51	0/2644
1	L	0.55	0/1960	0.56	0/2644
1	M	0.34	0/1960	0.47	0/2644
1	N	0.27	0/1960	0.46	0/2644
1	O	0.30	0/1960	0.50	0/2644
1	P	0.28	0/1960	0.49	0/2644
1	Q	0.33	0/1960	0.49	0/2644
1	R	0.37	0/1960	0.50	0/2644
1	S	0.32	0/1960	0.50	0/2644
1	T	0.28	0/1960	0.50	0/2644
All	All	0.44	5/39200 (0.0%)	0.50	0/52880

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	14	CYS	CB-SG	-5.68	1.72	1.81
1	B	169	TYR	CE2-CZ	-5.38	1.31	1.38
1	G	68	TYR	CD2-CE2	-5.31	1.31	1.39
1	G	68	TYR	CE1-CZ	-5.25	1.31	1.38
1	B	169	TYR	CD2-CE2	-5.00	1.31	1.39

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1928	0	1949	111	0
1	B	1928	0	1949	82	0
1	C	1928	0	1949	95	0
1	D	1928	0	1949	103	0
1	E	1928	0	1949	136	0
1	F	1928	0	1949	93	0
1	G	1928	0	1949	98	0
1	H	1928	0	1949	80	0
1	I	1928	0	1949	137	0
1	J	1928	0	1949	104	0
1	K	1928	0	1949	113	0
1	L	1928	0	1949	141	0
1	M	1928	0	1949	104	0
1	N	1928	0	1949	110	0
1	O	1928	0	1949	141	0
1	P	1928	0	1949	127	0
1	Q	1928	0	1949	195	0
1	R	1928	0	1949	184	0
1	S	1928	0	1949	184	0
1	T	1928	0	1949	130	0
All	All	38560	0	38980	2346	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 30.

All (2346) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:THR:CG2	1:D:98:GLU:OE1	1.67	1.42
1:T:115:LYS:HG2	1:T:155:LEU:CD2	1.47	1.41
1:B:66:ASN:HD22	1:B:67:VAL:N	1.25	1.31
1:L:177:THR:HG22	1:L:179:VAL:CG2	1.60	1.30

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:ASN:ND2	1:B:67:VAL:H	1.30	1.27
1:L:200:LYS:O	1:L:200:LYS:HD2	1.39	1.19
1:Q:183:PRO:HB3	1:Q:225:LEU:HD23	1.25	1.17
1:P:210:ARG:HG3	1:P:210:ARG:HH11	1.03	1.15
1:N:14:CYS:C	1:N:15:ASN:HD22	1.51	1.14
1:O:58:LYS:HG3	1:O:59:GLN:NE2	1.65	1.12
1:P:14:CYS:C	1:P:15:ASN:HD22	1.52	1.12
1:C:217:ALA:O	1:C:218:ASN:HB3	1.46	1.12
1:L:177:THR:HG22	1:L:179:VAL:HG23	1.13	1.12
1:T:115:LYS:CG	1:T:155:LEU:CD2	2.28	1.11
1:C:178:GLY:HA2	1:R:175:ILE:HD13	1.30	1.10
1:T:115:LYS:HG2	1:T:155:LEU:HD23	1.27	1.10
1:O:58:LYS:HE2	1:O:59:GLN:OE1	1.52	1.10
1:T:115:LYS:CG	1:T:155:LEU:HD23	1.79	1.09
1:E:251:ILE:HA	1:E:254:LYS:HE3	1.32	1.09
1:E:171:PRO:HG2	1:E:215:GLY:HA3	1.16	1.08
1:S:210:ARG:HG2	1:S:210:ARG:HH11	0.92	1.08
1:L:177:THR:CG2	1:L:179:VAL:HG23	1.82	1.08
1:B:66:ASN:ND2	1:B:67:VAL:N	1.91	1.07
1:Q:183:PRO:CB	1:Q:225:LEU:HD23	1.83	1.07
1:G:213:TYR:HB3	1:G:234:PHE:CD1	1.89	1.07
1:E:171:PRO:CG	1:E:215:GLY:HA3	1.85	1.07
1:I:84:LEU:HD22	1:I:89:LEU:HD12	1.31	1.07
1:F:171:PRO:O	1:F:175:ILE:HD13	1.53	1.06
1:E:175:ILE:HA	1:I:176:GLY:HA3	1.33	1.06
1:E:217:ALA:HB3	1:I:178:GLY:CA	1.86	1.06
1:E:217:ALA:HB3	1:I:178:GLY:HA2	1.36	1.06
1:O:226:GLY:HA3	1:O:255:THR:HG21	1.36	1.06
1:Q:61:ARG:HH22	1:Q:90:LYS:HG2	1.19	1.06
1:O:58:LYS:HG3	1:O:59:GLN:CD	1.77	1.05
1:Q:210:ARG:H	1:Q:210:ARG:HD3	1.20	1.05
1:R:225:LEU:HB3	1:R:234:PHE:CE1	1.93	1.04
1:H:218:ASN:O	1:H:222:ASP:HB2	1.58	1.02
1:L:171:PRO:HG2	1:L:174:SER:OG	1.60	1.02
1:Q:197:PHE:O	1:Q:201:VAL:HB	1.58	1.02
1:C:175:ILE:O	1:R:175:ILE:HG21	1.60	1.01
1:T:115:LYS:HG2	1:T:155:LEU:HD21	1.39	1.01
1:O:218:ASN:HD22	1:O:220:SER:H	1.08	1.01
1:Q:75:TRP:CD1	1:R:14:CYS:SG	2.52	1.01
1:L:218:ASN:N	1:L:221:ASN:HD21	1.57	1.01
1:S:158:SER:HB2	1:S:161:LEU:HD23	1.42	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:59:GLN:NE2	1:O:59:GLN:H	1.56	1.01
1:R:225:LEU:HB3	1:R:234:PHE:HE1	1.23	1.00
1:R:195:LYS:O	1:R:199:GLU:HB2	1.62	1.00
1:S:221:ASN:CB	1:S:224:LYS:HE2	1.92	1.00
1:L:177:THR:CG2	1:L:179:VAL:CG2	2.39	0.99
1:C:76:THR:HG23	1:D:98:GLU:CD	1.83	0.98
1:M:2:PRO:HG2	1:M:207:GLN:HB3	1.45	0.98
1:S:6:PRO:HG2	1:S:37:VAL:HA	1.46	0.98
1:P:173:TRP:O	1:P:177:THR:HG21	1.62	0.98
1:B:102:ILE:HG12	1:O:179:VAL:HG22	1.46	0.98
1:L:218:ASN:H	1:L:221:ASN:ND2	1.62	0.98
1:M:191:VAL:HG22	1:M:230:ASN:OD1	1.64	0.97
1:N:226:GLY:C	1:N:255:THR:HG21	1.83	0.97
1:A:172:VAL:HA	1:A:175:ILE:CD1	1.95	0.97
1:O:171:PRO:HD2	1:O:214:GLY:O	1.63	0.96
1:S:210:ARG:HG2	1:S:210:ARG:NH1	1.72	0.96
1:R:251:ILE:O	1:R:255:THR:HB	1.66	0.96
1:K:159:LYS:O	1:K:160:MET:HG2	1.64	0.95
1:S:7:PHE:HE2	1:S:166:VAL:HG21	1.31	0.95
1:C:76:THR:HG23	1:D:98:GLU:OE1	0.77	0.95
1:H:160:MET:O	1:H:163:LYS:HG3	1.65	0.95
1:O:58:LYS:CG	1:O:59:GLN:NE2	2.30	0.94
1:E:190:HIS:HE2	1:E:213:TYR:HB2	1.28	0.94
1:G:97:SER:HB3	1:G:170:GLU:OE1	1.66	0.94
1:Q:61:ARG:NH2	1:Q:90:LYS:HG2	1.83	0.94
1:M:94:VAL:HG11	1:M:114:ALA:HB2	1.49	0.94
1:O:58:LYS:CG	1:O:59:GLN:HE22	1.80	0.94
1:G:236:VAL:CG1	1:G:239:ALA:HB3	1.98	0.93
1:G:69:LEU:HD12	1:G:70:GLU:HG2	1.50	0.93
1:R:228:CYS:CB	1:R:231:ILE:HG13	1.99	0.92
1:G:195:LYS:O	1:G:199:GLU:HG3	1.69	0.92
1:E:169:TYR:CE1	1:E:189:VAL:HG11	2.04	0.92
1:Q:7:PHE:HD1	1:Q:38:ASP:HB2	1.34	0.91
1:Q:89:LEU:HD12	1:Q:90:LYS:H	1.35	0.91
1:S:61:ARG:HG3	1:S:61:ARG:HH11	1.33	0.91
1:T:109:GLN:O	1:T:113:LYS:HG3	1.71	0.91
1:E:171:PRO:HD2	1:E:215:GLY:CA	1.99	0.91
1:E:190:HIS:NE2	1:E:213:TYR:HB2	1.85	0.90
1:H:126:PHE:CZ	1:H:151:LEU:HD11	2.06	0.90
1:E:171:PRO:HD2	1:E:215:GLY:HA2	1.52	0.90
1:L:221:ASN:HD22	1:L:222:ASP:N	1.69	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:210:ARG:NH1	1:P:210:ARG:HG3	1.82	0.89
1:D:4:ARG:HD3	1:D:207:GLN:O	1.72	0.89
1:E:4:ARG:HD3	1:E:207:GLN:O	1.72	0.89
1:K:172:VAL:HA	1:K:175:ILE:HD12	1.55	0.89
1:I:194:ARG:CG	1:I:194:ARG:HH11	1.86	0.89
1:S:210:ARG:HH11	1:S:210:ARG:CG	1.84	0.88
1:J:11:ASN:ND2	1:J:13:LYS:HG3	1.88	0.88
1:Q:89:LEU:HD12	1:Q:90:LYS:N	1.89	0.87
1:T:115:LYS:CD	1:T:155:LEU:HD23	2.04	0.87
1:M:99:ARG:HA	1:M:103:MET:HB2	1.54	0.87
1:Q:7:PHE:CD1	1:Q:38:ASP:HB2	2.09	0.87
1:E:135:ARG:HA	1:E:140:THR:HG22	1.54	0.87
1:R:66:ASN:OD1	1:R:67:VAL:N	2.07	0.87
1:O:218:ASN:ND2	1:O:220:SER:H	1.73	0.86
1:B:224:LYS:O	1:B:227:GLN:HG3	1.74	0.86
1:B:69:LEU:HD23	1:B:70:GLU:HG2	1.58	0.86
1:O:58:LYS:HG2	1:O:59:GLN:HE22	1.39	0.86
1:I:4:ARG:HG2	1:I:4:ARG:HH11	1.41	0.85
1:B:97:SER:HB3	1:B:170:GLU:OE1	1.76	0.85
1:O:59:GLN:HE21	1:O:59:GLN:H	1.19	0.85
1:Q:79:THR:HG21	1:Q:84:LEU:HD21	1.59	0.85
1:H:217:ALA:HB1	1:H:248:MET:HE1	1.58	0.85
1:P:131:THR:HA	1:P:172:VAL:CG1	2.06	0.85
1:G:236:VAL:HG11	1:G:239:ALA:HB3	1.57	0.85
1:R:183:PRO:HG2	1:R:224:LYS:HD3	1.59	0.85
1:K:165:VAL:O	1:K:209:ILE:HD11	1.76	0.85
1:E:130:GLU:OE2	1:E:135:ARG:HB2	1.76	0.84
1:O:171:PRO:HG3	1:O:215:GLY:HA3	1.57	0.84
1:P:131:THR:HA	1:P:172:VAL:HG11	1.59	0.84
1:R:228:CYS:HB2	1:R:231:ILE:HG13	1.58	0.84
1:H:84:LEU:HD22	1:H:89:LEU:HD12	1.59	0.83
1:O:213:TYR:CZ	1:O:215:GLY:HA3	2.13	0.83
1:S:130:GLU:OE2	1:S:140:THR:HG23	1.77	0.83
1:C:69:LEU:HD23	1:C:70:GLU:HG2	1.58	0.83
1:T:155:LEU:HD22	1:T:161:LEU:HD12	1.59	0.83
1:Q:195:LYS:O	1:Q:199:GLU:HB2	1.78	0.83
1:Q:61:ARG:HH22	1:Q:90:LYS:CG	1.92	0.83
1:T:115:LYS:HD3	1:T:155:LEU:CD2	2.09	0.83
1:L:69:LEU:HD23	1:L:70:GLU:HG2	1.61	0.83
1:A:218:ASN:C	1:A:218:ASN:HD22	1.81	0.83
1:G:213:TYR:HB3	1:G:234:PHE:CE1	2.11	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:17:SER:O	1:T:21:ILE:HG12	1.78	0.83
1:F:218:ASN:HB2	1:F:220:SER:OG	1.78	0.83
1:C:175:ILE:O	1:R:175:ILE:CG2	2.26	0.82
1:O:171:PRO:HG3	1:O:215:GLY:CA	2.08	0.82
1:S:157:GLU:OE1	1:S:157:GLU:HA	1.78	0.82
1:F:171:PRO:HB3	1:F:173:TRP:NE1	1.93	0.82
1:N:14:CYS:C	1:N:15:ASN:ND2	2.30	0.82
1:Q:234:PHE:CD2	1:Q:248:MET:CE	2.61	0.82
1:A:172:VAL:HG13	1:A:175:ILE:HD12	1.59	0.82
1:E:218:ASN:OD1	1:E:219:GLY:N	2.13	0.82
1:D:218:ASN:HD22	1:D:219:GLY:N	1.77	0.82
1:S:8:ILE:HD11	1:S:245:PHE:CE1	2.15	0.82
1:Q:197:PHE:CD2	1:Q:206:ALA:HA	2.14	0.82
1:R:4:ARG:HD3	1:R:207:GLN:O	1.79	0.82
1:R:246:MET:HA	1:R:249:ILE:HD12	1.60	0.82
1:E:219:GLY:O	1:E:220:SER:HB3	1.79	0.81
1:S:183:PRO:HD2	1:S:184:GLU:OE1	1.81	0.81
1:I:194:ARG:HG2	1:I:194:ARG:HH11	1.45	0.81
1:K:218:ASN:HD22	1:K:219:GLY:N	1.78	0.81
1:P:173:TRP:O	1:P:177:THR:CG2	2.29	0.81
1:R:2:PRO:HB3	1:R:207:GLN:HG2	1.62	0.81
1:R:63:ALA:HB2	1:R:91:HIS:HB2	1.60	0.81
1:S:7:PHE:CE2	1:S:166:VAL:HG21	2.15	0.81
1:J:242:LYS:HB3	1:J:244:GLU:OE1	1.80	0.80
1:N:15:ASN:N	1:N:15:ASN:HD22	1.78	0.80
1:A:217:ALA:HB1	1:A:248:MET:HE3	1.62	0.80
1:I:13:LYS:HG3	1:J:76:THR:CG2	2.11	0.80
1:K:223:GLU:HG3	1:K:254:LYS:HZ1	1.45	0.80
1:Q:183:PRO:CB	1:Q:225:LEU:CD2	2.58	0.80
1:H:187:GLU:O	1:H:191:VAL:HG23	1.81	0.80
1:J:222:ASP:HA	1:J:225:LEU:HB2	1.63	0.80
1:N:226:GLY:CA	1:N:255:THR:HG21	2.12	0.80
1:E:247:THR:O	1:E:251:ILE:HD13	1.81	0.80
1:T:115:LYS:HG2	1:T:155:LEU:CG	2.11	0.80
1:P:108:GLU:O	1:P:112:LYS:HG3	1.82	0.80
1:T:83:MET:O	1:T:86:ASP:HB3	1.82	0.80
1:O:226:GLY:CA	1:O:255:THR:HG21	2.12	0.79
1:T:115:LYS:CD	1:T:155:LEU:CD2	2.59	0.79
1:R:69:LEU:H	1:R:69:LEU:HD23	1.45	0.79
1:O:59:GLN:N	1:O:59:GLN:NE2	2.30	0.79
1:N:191:VAL:HG22	1:N:230:ASN:HD22	1.46	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:132:LEU:O	1:P:136:LYS:HG3	1.83	0.79
1:N:6:PRO:HB2	1:N:37:VAL:HG13	1.64	0.79
1:M:228:CYS:HB2	1:M:231:ILE:HD12	1.63	0.78
1:I:109:GLN:O	1:I:113:LYS:HG3	1.82	0.78
1:I:11:ASN:HD21	1:J:76:THR:HG21	1.47	0.78
1:K:159:LYS:O	1:K:160:MET:CG	2.30	0.78
1:S:221:ASN:HB2	1:S:224:LYS:HE2	1.65	0.78
1:H:160:MET:O	1:H:163:LYS:CG	2.31	0.78
1:J:240:SER:HA	1:J:245:PHE:HB2	1.65	0.78
1:L:108:GLU:O	1:L:112:LYS:HG3	1.83	0.78
1:P:5:ARG:O	1:P:210:ARG:HD3	1.82	0.78
1:Q:5:ARG:HH12	1:Q:36:SER:HA	1.48	0.78
1:R:225:LEU:HA	1:R:228:CYS:SG	2.23	0.78
1:G:69:LEU:CD1	1:G:70:GLU:HG2	2.13	0.78
1:G:225:LEU:HB3	1:G:234:PHE:HZ	1.48	0.78
1:L:204:GLU:CD	1:L:204:GLU:H	1.86	0.78
1:M:225:LEU:O	1:M:231:ILE:HD12	1.83	0.78
1:S:177:THR:HG22	1:S:179:VAL:HG22	1.65	0.78
1:R:217:ALA:O	1:R:218:ASN:C	2.22	0.78
1:S:61:ARG:HG3	1:S:61:ARG:NH1	1.96	0.78
1:O:61:ARG:HE	1:O:62:ILE:H	1.32	0.77
1:P:96:HIS:HD2	1:P:98:GLU:H	1.32	0.77
1:A:48:LEU:O	1:A:52:ILE:HG13	1.85	0.77
1:H:160:MET:O	1:H:163:LYS:CD	2.32	0.77
1:O:58:LYS:CE	1:O:59:GLN:OE1	2.30	0.77
1:K:171:PRO:HG3	1:K:213:TYR:CE1	2.19	0.77
1:R:14:CYS:O	1:R:14:CYS:SG	2.43	0.77
1:L:171:PRO:HD2	1:L:214:GLY:O	1.85	0.77
1:R:225:LEU:CB	1:R:234:PHE:CE1	2.65	0.77
1:F:4:ARG:HD3	1:F:207:GLN:O	1.83	0.77
1:B:48:LEU:O	1:B:52:ILE:HG13	1.85	0.77
1:E:45:ALA:HA	1:E:48:LEU:CD2	2.15	0.77
1:H:160:MET:O	1:H:163:LYS:HD3	1.84	0.77
1:E:217:ALA:HB3	1:I:178:GLY:HA3	1.66	0.77
1:K:195:LYS:HG2	1:K:196:TRP:N	1.99	0.77
1:E:210:ARG:HA	1:E:232:ASP:OD2	1.85	0.77
1:K:171:PRO:HG3	1:K:213:TYR:HE1	1.50	0.77
1:A:172:VAL:HA	1:A:175:ILE:HD11	1.66	0.76
1:H:126:PHE:CD1	1:H:151:LEU:HD21	2.20	0.76
1:Q:7:PHE:CE2	1:Q:210:ARG:HG3	2.20	0.76
1:I:4:ARG:CG	1:I:4:ARG:HH11	1.97	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:ILE:HD11	1:D:89:LEU:HD21	1.67	0.76
1:N:223:GLU:HA	1:N:223:GLU:OE1	1.84	0.76
1:Q:248:MET:O	1:Q:251:ILE:HG22	1.86	0.76
1:I:11:ASN:HD21	1:J:76:THR:CG2	1.98	0.76
1:O:171:PRO:CG	1:O:215:GLY:HA2	2.15	0.76
1:Q:85:GLN:HE22	1:Q:120:LYS:HB3	1.48	0.76
1:N:45:ALA:HA	1:N:48:LEU:HD22	1.68	0.76
1:E:132:LEU:O	1:E:136:LYS:HG3	1.86	0.76
1:J:98:GLU:O	1:J:102:ILE:HB	1.86	0.76
1:Q:201:VAL:HG12	1:Q:202:ALA:N	2.01	0.76
1:N:226:GLY:O	1:N:255:THR:HG21	1.86	0.76
1:I:247:THR:O	1:I:251:ILE:HD13	1.86	0.75
1:J:182:THR:HG22	1:J:184:GLU:OE1	1.85	0.75
1:L:171:PRO:CG	1:L:174:SER:OG	2.33	0.75
1:O:76:THR:HG23	1:P:65:GLN:HB3	1.67	0.75
1:N:191:VAL:HG22	1:N:230:ASN:ND2	2.02	0.75
1:R:225:LEU:C	1:R:234:PHE:HZ	1.89	0.75
1:G:224:LYS:O	1:G:227:GLN:HG3	1.85	0.75
1:J:177:THR:HG22	1:J:179:VAL:H	1.52	0.75
1:R:250:ASP:HA	1:R:253:THR:CG2	2.16	0.75
1:I:13:LYS:HG3	1:J:76:THR:HG22	1.68	0.75
1:K:218:ASN:O	1:K:222:ASP:HB2	1.87	0.75
1:L:109:GLN:O	1:L:113:LYS:HG3	1.86	0.75
1:M:2:PRO:HG2	1:M:207:GLN:CB	2.16	0.75
1:R:52:ILE:HD13	1:R:62:ILE:HD12	1.67	0.75
1:A:67:VAL:O	1:A:113:LYS:HD3	1.87	0.74
1:C:217:ALA:O	1:C:218:ASN:CB	2.31	0.74
1:T:236:VAL:HG13	1:T:239:ALA:HB3	1.69	0.74
1:B:189:VAL:O	1:B:193:LEU:HG	1.86	0.74
1:L:219:GLY:H	1:L:222:ASP:CG	1.91	0.74
1:S:7:PHE:HD1	1:S:8:ILE:N	1.85	0.74
1:B:213:TYR:CZ	1:B:215:GLY:HA3	2.22	0.74
1:M:187:GLU:O	1:M:191:VAL:HG23	1.87	0.74
1:R:106:THR:OG1	1:R:109:GLN:HG3	1.87	0.74
1:P:15:ASN:HD22	1:P:15:ASN:N	1.85	0.74
1:C:21:ILE:HG13	1:C:47:HIS:HB3	1.70	0.74
1:F:98:GLU:O	1:F:102:ILE:HB	1.86	0.74
1:J:69:LEU:HD23	1:J:69:LEU:H	1.51	0.74
1:L:98:GLU:HA	1:L:102:ILE:HD12	1.69	0.74
1:A:206:ALA:O	1:A:209:ILE:HG22	1.86	0.74
1:H:198:ALA:HA	1:H:202:ALA:O	1.88	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:24:HIS:O	1:J:28:ILE:HG13	1.87	0.74
1:N:69:LEU:HB3	1:N:113:LYS:HG2	1.70	0.74
1:P:177:THR:CG2	1:P:179:VAL:HG22	2.18	0.74
1:O:69:LEU:HD23	1:O:70:GLU:HG2	1.70	0.73
1:N:139:ARG:HB3	1:N:139:ARG:HH11	1.52	0.73
1:Q:123:THR:HA	1:Q:164:GLU:HG3	1.68	0.73
1:C:76:THR:HG22	1:D:13:LYS:HD3	1.69	0.73
1:F:175:ILE:HD12	1:F:175:ILE:N	2.02	0.73
1:N:217:ALA:HB1	1:N:248:MET:HE1	1.70	0.73
1:Q:210:ARG:H	1:Q:210:ARG:CD	2.00	0.73
1:R:15:ASN:HD21	1:R:241:LEU:HD11	1.50	0.73
1:I:11:ASN:ND2	1:J:76:THR:HG21	2.03	0.73
1:N:248:MET:O	1:N:251:ILE:HG22	1.89	0.73
1:N:226:GLY:O	1:N:255:THR:CG2	2.36	0.73
1:O:58:LYS:HG3	1:O:59:GLN:OE1	1.88	0.73
1:R:190:HIS:CE1	1:R:231:ILE:HD13	2.24	0.73
1:S:130:GLU:OE2	1:S:135:ARG:NH2	2.21	0.73
1:N:90:LYS:HE3	1:N:91:HIS:CE1	2.24	0.73
1:D:158:SER:OG	1:D:160:MET:HE2	1.89	0.73
1:J:217:ALA:O	1:J:248:MET:HE1	1.89	0.73
1:M:95:GLY:O	1:M:127:CYS:HB2	1.87	0.73
1:O:220:SER:O	1:O:221:ASN:HB3	1.88	0.73
1:Q:4:ARG:HD2	1:Q:232:ASP:OD2	1.87	0.73
1:Q:62:ILE:O	1:Q:89:LEU:CD1	2.37	0.73
1:D:218:ASN:ND2	1:D:220:SER:H	1.86	0.73
1:H:115:LYS:HE2	1:H:119:GLU:OE2	1.88	0.73
1:M:98:GLU:O	1:M:102:ILE:HB	1.88	0.73
1:L:141:MET:HE3	1:L:141:MET:HA	1.71	0.72
1:P:170:GLU:OE2	1:P:235:LEU:HD23	1.89	0.72
1:I:194:ARG:CG	1:I:194:ARG:NH1	2.47	0.72
1:O:143:VAL:O	1:O:147:GLN:HG3	1.88	0.72
1:R:228:CYS:HB2	1:R:231:ILE:CG1	2.19	0.72
1:I:69:LEU:HD23	1:I:70:GLU:HG2	1.71	0.72
1:S:221:ASN:HB3	1:S:224:LYS:HE2	1.69	0.72
1:C:67:VAL:O	1:C:113:LYS:HD3	1.89	0.72
1:E:251:ILE:HA	1:E:254:LYS:CE	2.16	0.72
1:H:126:PHE:CE1	1:H:151:LEU:HD21	2.24	0.72
1:P:40:VAL:CG1	1:P:63:ALA:HB2	2.19	0.72
1:D:247:THR:O	1:D:251:ILE:HD13	1.88	0.72
1:M:2:PRO:CG	1:M:207:GLN:HB3	2.17	0.72
1:R:175:ILE:O	1:R:175:ILE:HG13	1.88	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:171:PRO:HB3	1:F:173:TRP:HE1	1.54	0.72
1:I:195:LYS:NZ	1:I:199:GLU:OE2	2.23	0.72
1:R:175:ILE:HG23	1:R:177:THR:OG1	1.90	0.72
1:S:130:GLU:O	1:S:172:VAL:HB	1.90	0.72
1:T:98:GLU:HA	1:T:102:ILE:HD12	1.69	0.72
1:Q:210:ARG:N	1:Q:210:ARG:HD3	2.01	0.72
1:O:145:ILE:HG23	1:O:196:TRP:CD1	2.25	0.72
1:P:195:LYS:HG3	1:P:199:GLU:OE1	1.89	0.72
1:B:69:LEU:CD2	1:B:70:GLU:HG2	2.20	0.72
1:Q:61:ARG:HH11	1:Q:61:ARG:HG3	1.52	0.72
1:E:171:PRO:CD	1:E:215:GLY:CA	2.67	0.71
1:T:85:GLN:HE22	1:T:120:LYS:HB3	1.55	0.71
1:T:63:ALA:HB2	1:T:91:HIS:HB2	1.70	0.71
1:O:48:LEU:O	1:O:52:ILE:HG13	1.90	0.71
1:S:97:SER:O	1:S:101:ARG:HB2	1.90	0.71
1:T:195:LYS:O	1:T:199:GLU:HB2	1.90	0.71
1:T:242:LYS:HB2	1:T:243:PRO:HD2	1.72	0.71
1:T:46:VAL:HG23	1:T:47:HIS:CD2	2.25	0.71
1:G:213:TYR:HD2	1:G:234:PHE:CD1	2.09	0.71
1:J:24:HIS:NE2	1:J:240:SER:O	2.21	0.71
1:Q:183:PRO:HG3	1:Q:225:LEU:CD2	2.21	0.71
1:R:217:ALA:O	1:R:218:ASN:O	2.08	0.71
1:F:24:HIS:O	1:F:28:ILE:HG13	1.91	0.71
1:N:68:TYR:HB2	1:N:78:GLU:HB3	1.73	0.71
1:S:160:MET:HE3	1:S:160:MET:H	1.56	0.71
1:B:213:TYR:CE2	1:B:215:GLY:HA3	2.25	0.71
1:Q:230:ASN:N	1:Q:230:ASN:HD22	1.88	0.71
1:A:137:ALA:O	1:A:138:ASN:HB3	1.90	0.71
1:B:217:ALA:HB1	1:B:222:ASP:OD1	1.90	0.71
1:C:90:LYS:HD3	1:C:91:HIS:CE1	2.26	0.70
1:D:244:GLU:O	1:D:248:MET:HG3	1.91	0.70
1:G:213:TYR:CD2	1:G:234:PHE:CE1	2.79	0.70
1:L:242:LYS:HB3	1:L:243:PRO:HD2	1.72	0.70
1:P:177:THR:HG23	1:P:179:VAL:HG22	1.72	0.70
1:S:130:GLU:HG2	1:S:144:ASN:HD21	1.55	0.70
1:A:172:VAL:HA	1:A:175:ILE:CG1	2.20	0.70
1:S:155:LEU:HG	1:S:161:LEU:HD11	1.71	0.70
1:T:115:LYS:CG	1:T:155:LEU:HD21	2.07	0.70
1:L:200:LYS:CD	1:L:200:LYS:O	2.30	0.70
1:C:98:GLU:O	1:C:102:ILE:HB	1.91	0.70
1:I:145:ILE:HG12	1:I:196:TRP:CD1	2.26	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:228:CYS:HB3	1:Q:231:ILE:HG13	1.73	0.70
1:C:115:LYS:O	1:C:119:GLU:HG3	1.90	0.70
1:C:69:LEU:HD22	1:C:69:LEU:H	1.54	0.70
1:R:206:ALA:O	1:R:209:ILE:HG22	1.92	0.70
1:L:218:ASN:H	1:L:221:ASN:HD21	0.80	0.70
1:I:194:ARG:NH2	1:I:232:ASP:OD2	2.24	0.70
1:R:69:LEU:H	1:R:69:LEU:CD2	2.05	0.70
1:C:218:ASN:OD1	1:C:219:GLY:N	2.23	0.70
1:P:170:GLU:HG2	1:P:214:GLY:HA3	1.73	0.70
1:Q:234:PHE:CE2	1:Q:248:MET:CE	2.75	0.70
1:A:132:LEU:O	1:A:136:LYS:HG3	1.92	0.70
1:F:13:LYS:H	1:F:65:GLN:NE2	1.90	0.70
1:Q:46:VAL:HG23	1:Q:47:HIS:CD2	2.26	0.70
1:S:92:VAL:CG1	1:S:124:VAL:HG22	2.22	0.70
1:M:5:ARG:HH11	1:M:5:ARG:HG2	1.54	0.69
1:O:182:THR:H	1:O:185:GLN:HE21	1.37	0.69
1:Q:171:PRO:HB2	1:Q:174:SER:OG	1.92	0.69
1:M:5:ARG:HH11	1:M:5:ARG:CG	2.05	0.69
1:O:197:PHE:CD2	1:O:206:ALA:HA	2.27	0.69
1:Q:183:PRO:HA	1:Q:225:LEU:CD2	2.22	0.69
1:A:217:ALA:CB	1:A:248:MET:HE3	2.23	0.69
1:D:130:GLU:OE2	1:D:135:ARG:HB2	1.92	0.69
1:E:171:PRO:CG	1:E:215:GLY:CA	2.68	0.69
1:I:187:GLU:OE1	1:I:228:CYS:HB3	1.91	0.69
1:I:72:ASN:ND2	1:I:80:SER:OG	2.25	0.69
1:Q:197:PHE:HD2	1:Q:206:ALA:HA	1.54	0.69
1:Q:234:PHE:CE2	1:Q:248:MET:HE3	2.26	0.69
1:Q:7:PHE:CE2	1:Q:210:ARG:NH1	2.61	0.69
1:F:171:PRO:O	1:F:175:ILE:CD1	2.34	0.69
1:G:225:LEU:HB3	1:G:234:PHE:CZ	2.26	0.69
1:H:100:ARG:NH2	1:H:126:PHE:CZ	2.60	0.69
1:I:37:VAL:HG21	1:I:253:THR:OG1	1.93	0.69
1:Q:115:LYS:HE2	1:Q:119:GLU:OE2	1.92	0.69
1:Q:17:SER:O	1:Q:21:ILE:HG12	1.92	0.69
1:G:18:LEU:O	1:G:22:LYS:HG3	1.92	0.69
1:I:194:ARG:HG3	1:I:194:ARG:NH1	2.07	0.69
1:Q:183:PRO:CG	1:Q:225:LEU:HD23	2.22	0.69
1:B:222:ASP:OD2	1:B:248:MET:HE3	1.93	0.69
1:H:220:SER:O	1:H:221:ASN:HB3	1.90	0.69
1:A:158:SER:HB3	1:A:161:LEU:HG	1.73	0.69
1:F:182:THR:OG1	1:F:185:GLN:HB2	1.93	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:143:VAL:O	1:K:147:GLN:HG3	1.93	0.69
1:M:187:GLU:OE1	1:M:228:CYS:HB3	1.92	0.69
1:P:98:GLU:HA	1:P:102:ILE:HD12	1.74	0.69
1:Q:62:ILE:O	1:Q:89:LEU:HD13	1.92	0.69
1:Q:63:ALA:HA	1:Q:89:LEU:HD21	1.75	0.69
1:T:115:LYS:HD3	1:T:155:LEU:HD23	1.71	0.69
1:A:187:GLU:O	1:A:191:VAL:HG23	1.92	0.69
1:C:218:ASN:OD1	1:C:218:ASN:C	2.29	0.69
1:R:48:LEU:O	1:R:52:ILE:HG12	1.92	0.69
1:I:4:ARG:HD2	1:I:208:HIS:C	2.14	0.68
1:N:134:GLU:O	1:N:139:ARG:HB2	1.92	0.68
1:S:172:VAL:HA	1:S:175:ILE:HG12	1.75	0.68
1:S:197:PHE:CE2	1:S:209:ILE:HD13	2.27	0.68
1:J:216:SER:O	1:J:221:ASN:ND2	2.26	0.68
1:Q:61:ARG:NH1	1:Q:61:ARG:HG3	2.08	0.68
1:A:130:GLU:OE2	1:A:140:THR:HG23	1.94	0.68
1:C:77:GLY:HA3	1:D:99:ARG:HH11	1.59	0.68
1:E:195:LYS:O	1:E:199:GLU:HG2	1.93	0.68
1:E:98:GLU:OE2	1:F:74:ALA:HB1	1.93	0.68
1:F:69:LEU:HD23	1:F:70:GLU:HG2	1.74	0.68
1:G:69:LEU:HD12	1:G:69:LEU:C	2.13	0.68
1:S:63:ALA:HB2	1:S:91:HIS:HB2	1.75	0.68
1:A:145:ILE:O	1:A:149:GLU:HB2	1.93	0.68
1:L:43:PRO:HD2	1:L:48:LEU:CD1	2.23	0.68
1:S:118:LEU:HD13	1:S:161:LEU:HD12	1.74	0.68
1:H:48:LEU:O	1:H:52:ILE:HG13	1.92	0.68
1:K:187:GLU:OE1	1:K:228:CYS:HB3	1.93	0.68
1:I:83:MET:O	1:I:87:MET:HG3	1.94	0.68
1:O:198:ALA:HB2	1:O:206:ALA:CB	2.24	0.68
1:R:17:SER:O	1:R:21:ILE:HG12	1.93	0.68
1:K:106:THR:OG1	1:K:109:GLN:HG3	1.94	0.68
1:K:171:PRO:CG	1:K:213:TYR:CE1	2.77	0.68
1:L:177:THR:HG22	1:L:179:VAL:HG21	1.72	0.68
1:M:109:GLN:O	1:M:113:LYS:HG3	1.94	0.68
1:S:109:GLN:O	1:S:113:LYS:HG3	1.94	0.68
1:J:111:ALA:HB1	1:J:151:LEU:HA	1.76	0.68
1:K:247:THR:O	1:K:251:ILE:HD13	1.94	0.68
1:A:134:GLU:HG2	1:A:143:VAL:HG21	1.76	0.68
1:K:41:ILE:HG23	1:K:60:LEU:HD11	1.76	0.68
1:R:29:ALA:HA	1:R:57:SER:OG	1.93	0.68
1:S:177:THR:CG2	1:S:179:VAL:HG22	2.24	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ASN:ND2	1:A:218:ASN:C	2.48	0.67
1:C:130:GLU:OE2	1:C:140:THR:HB	1.94	0.67
1:F:177:THR:O	1:F:177:THR:HG22	1.93	0.67
1:I:218:ASN:O	1:I:222:ASP:HB2	1.93	0.67
1:I:84:LEU:HD22	1:I:89:LEU:CD1	2.15	0.67
1:R:156:GLY:O	1:R:159:LYS:HG3	1.94	0.67
1:R:230:ASN:N	1:R:230:ASN:HD22	1.92	0.67
1:A:172:VAL:HA	1:A:175:ILE:HG13	1.74	0.67
1:I:4:ARG:HB2	1:I:4:ARG:CZ	2.25	0.67
1:K:159:LYS:O	1:K:160:MET:CB	2.41	0.67
1:O:221:ASN:HA	1:O:224:LYS:NZ	2.09	0.67
1:Q:197:PHE:O	1:Q:201:VAL:CB	2.39	0.67
1:R:194:ARG:HH11	1:R:209:ILE:HG23	1.60	0.67
1:T:69:LEU:HB3	1:T:113:LYS:HG2	1.76	0.67
1:A:24:HIS:O	1:A:28:ILE:HG13	1.95	0.67
1:D:109:GLN:O	1:D:113:LYS:HG3	1.95	0.67
1:K:227:GLN:O	1:K:228:CYS:C	2.33	0.67
1:K:81:VAL:HG13	1:K:122:MET:SD	2.33	0.67
1:O:171:PRO:CG	1:O:215:GLY:CA	2.73	0.67
1:R:194:ARG:HH11	1:R:209:ILE:CG2	2.06	0.67
1:S:65:GLN:O	1:S:93:ILE:HB	1.95	0.67
1:A:218:ASN:HD21	1:A:221:ASN:H	1.43	0.67
1:G:130:GLU:OE2	1:G:135:ARG:HB2	1.95	0.67
1:M:195:LYS:O	1:M:199:GLU:HG3	1.95	0.67
1:R:8:ILE:HG22	1:R:39:VAL:HA	1.75	0.67
1:S:171:PRO:HA	1:S:173:TRP:HE1	1.59	0.67
1:C:11:ASN:ND2	1:C:13:LYS:HG2	2.09	0.67
1:P:210:ARG:CG	1:P:210:ARG:HH11	1.95	0.67
1:O:18:LEU:O	1:O:22:LYS:HG3	1.94	0.67
1:R:34:PRO:HB2	1:R:36:SER:OG	1.94	0.67
1:R:71:GLY:CA	1:R:116:ARG:NH2	2.58	0.67
1:R:226:GLY:N	1:R:234:PHE:HZ	1.92	0.67
1:G:69:LEU:HD12	1:G:70:GLU:CG	2.25	0.67
1:I:218:ASN:HD21	1:I:220:SER:HB3	1.59	0.67
1:N:190:HIS:CE1	1:N:211:ILE:HG22	2.29	0.67
1:N:187:GLU:OE2	1:N:229:PRO:HG2	1.95	0.67
1:B:182:THR:OG1	1:B:185:GLN:HG3	1.96	0.66
1:E:115:LYS:HG2	1:E:155:LEU:HD23	1.75	0.66
1:Q:172:VAL:O	1:Q:175:ILE:HG22	1.95	0.66
1:Q:183:PRO:CA	1:Q:225:LEU:CD2	2.73	0.66
1:R:12:PHE:O	1:R:13:LYS:HB2	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:72:ASN:HA	1:H:14:CYS:O	1.95	0.66
1:H:21:ILE:O	1:H:25:VAL:HG23	1.94	0.66
1:Q:177:THR:CG2	1:Q:177:THR:O	2.43	0.66
1:Q:7:PHE:CD2	1:Q:210:ARG:HG3	2.30	0.66
1:R:114:ALA:O	1:R:118:LEU:HD13	1.95	0.66
1:R:118:LEU:HD23	1:R:161:LEU:HB3	1.76	0.66
1:H:218:ASN:OD1	1:H:219:GLY:N	2.29	0.66
1:S:67:VAL:O	1:S:113:LYS:HD3	1.94	0.66
1:T:213:TYR:HB2	1:T:231:ILE:HD13	1.76	0.66
1:H:155:LEU:HD12	1:H:162:TRP:NE1	2.10	0.66
1:L:97:SER:OG	1:L:175:ILE:CD1	2.43	0.66
1:R:227:GLN:HA	1:R:227:GLN:HE21	1.59	0.66
1:N:145:ILE:HG23	1:N:196:TRP:CD1	2.30	0.66
1:L:118:LEU:HD13	1:L:161:LEU:O	1.96	0.66
1:N:4:ARG:HD3	1:N:207:GLN:O	1.95	0.66
1:Q:13:LYS:HD3	1:R:74:ALA:HA	1.78	0.66
1:H:126:PHE:CG	1:H:151:LEU:HD21	2.30	0.66
1:K:4:ARG:HG2	1:K:208:HIS:HA	1.78	0.66
1:L:90:LYS:HE3	1:L:91:HIS:CE1	2.31	0.66
1:O:223:GLU:O	1:O:227:GLN:HG3	1.95	0.66
1:A:138:ASN:O	1:A:138:ASN:ND2	2.29	0.66
1:D:108:GLU:O	1:D:112:LYS:HG3	1.95	0.66
1:P:128:VAL:HG12	1:P:147:GLN:HB2	1.76	0.66
1:Q:225:LEU:O	1:Q:228:CYS:HB2	1.95	0.66
1:R:109:GLN:O	1:R:113:LYS:HG3	1.96	0.66
1:A:137:ALA:O	1:A:138:ASN:CB	2.41	0.66
1:M:170:GLU:HB2	1:M:175:ILE:HD11	1.78	0.66
1:B:18:LEU:O	1:B:22:LYS:HG3	1.96	0.66
1:I:244:GLU:O	1:I:248:MET:HG3	1.94	0.66
1:K:218:ASN:ND2	1:K:219:GLY:N	2.43	0.66
1:P:98:GLU:O	1:P:102:ILE:HB	1.95	0.66
1:F:116:ARG:O	1:F:120:LYS:HG3	1.96	0.65
1:G:64:ALA:O	1:G:93:ILE:HG23	1.96	0.65
1:G:9:GLY:HA2	1:G:40:VAL:O	1.96	0.65
1:I:74:ALA:HB1	1:J:98:GLU:OE2	1.96	0.65
1:K:132:LEU:O	1:K:136:LYS:HG3	1.97	0.65
1:L:220:SER:OG	1:L:221:ASN:N	2.28	0.65
1:Q:165:VAL:O	1:Q:210:ARG:NE	2.28	0.65
1:A:160:MET:H	1:A:160:MET:HE3	1.61	0.65
1:T:236:VAL:CG1	1:T:239:ALA:HB3	2.26	0.65
1:K:109:GLN:O	1:K:113:LYS:HG3	1.97	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:177:THR:CG2	1:L:179:VAL:HG21	2.24	0.65
1:N:67:VAL:O	1:N:113:LYS:HD3	1.97	0.65
1:R:68:TYR:CD1	1:R:78:GLU:HG3	2.31	0.65
1:R:71:GLY:HA2	1:R:116:ARG:NH2	2.12	0.65
1:T:69:LEU:H	1:T:69:LEU:HD23	1.62	0.65
1:A:84:LEU:HD22	1:A:89:LEU:HD12	1.76	0.65
1:H:221:ASN:ND2	1:H:221:ASN:O	2.30	0.65
1:L:130:GLU:O	1:L:172:VAL:HB	1.97	0.65
1:S:115:LYS:O	1:S:119:GLU:HG3	1.97	0.65
1:G:17:SER:O	1:G:21:ILE:HG12	1.97	0.65
1:L:40:VAL:CG1	1:L:63:ALA:HB2	2.27	0.65
1:D:171:PRO:HD2	1:D:214:GLY:O	1.97	0.65
1:I:4:ARG:HD2	1:I:208:HIS:CA	2.27	0.65
1:I:83:MET:HG2	1:J:47:HIS:CE1	2.32	0.65
1:L:138:ASN:O	1:L:138:ASN:ND2	2.30	0.65
1:L:155:LEU:HD12	1:L:162:TRP:CE2	2.32	0.65
1:N:209:ILE:HG23	1:N:211:ILE:HD11	1.79	0.65
1:P:14:CYS:O	1:P:15:ASN:ND2	2.30	0.65
1:P:48:LEU:O	1:P:52:ILE:HG13	1.96	0.65
1:O:137:ALA:O	1:O:138:ASN:HB2	1.96	0.65
1:T:206:ALA:O	1:T:209:ILE:HG22	1.97	0.65
1:A:139:ARG:NH1	1:A:142:GLU:OE2	2.30	0.64
1:T:25:VAL:HA	1:T:28:ILE:HG13	1.78	0.64
1:E:155:LEU:HD12	1:E:162:TRP:CE2	2.32	0.64
1:L:134:GLU:O	1:L:139:ARG:N	2.30	0.64
1:A:217:ALA:HB1	1:A:248:MET:CE	2.27	0.64
1:H:99:ARG:HA	1:H:103:MET:HB2	1.80	0.64
1:Q:158:SER:HB2	1:Q:161:LEU:HD12	1.79	0.64
1:S:239:ALA:O	1:S:245:PHE:HB2	1.97	0.64
1:Q:143:VAL:O	1:Q:147:GLN:HG3	1.98	0.64
1:M:242:LYS:HB3	1:M:243:PRO:HD2	1.79	0.64
1:N:14:CYS:O	1:N:15:ASN:ND2	2.30	0.64
1:P:148:LEU:HB3	1:P:196:TRP:CH2	2.33	0.64
1:I:233:GLY:HA2	1:I:252:LEU:CD1	2.28	0.64
1:J:137:ALA:O	1:J:138:ASN:CB	2.43	0.64
1:L:4:ARG:HD2	1:L:207:GLN:O	1.98	0.64
1:M:13:LYS:H	1:M:65:GLN:NE2	1.96	0.64
1:Q:132:LEU:HG	1:Q:136:LYS:HE2	1.80	0.64
1:Q:198:ALA:HB2	1:Q:206:ALA:CB	2.27	0.64
1:F:145:ILE:HG23	1:F:196:TRP:NE1	2.14	0.63
1:H:6:PRO:HB2	1:H:37:VAL:HG13	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:251:ILE:HD13	1:L:254:LYS:NZ	2.13	0.63
1:Q:239:ALA:O	1:Q:245:PHE:HB2	1.98	0.63
1:L:137:ALA:O	1:L:138:ASN:HB3	1.98	0.63
1:L:222:ASP:OD2	1:L:248:MET:HE3	1.98	0.63
1:Q:244:GLU:O	1:Q:247:THR:HB	1.98	0.63
1:S:39:VAL:HG12	1:S:60:LEU:HD12	1.79	0.63
1:G:65:GLN:O	1:G:93:ILE:HG12	1.98	0.63
1:P:148:LEU:HB3	1:P:196:TRP:CZ3	2.34	0.63
1:D:155:LEU:HD12	1:D:162:TRP:NE1	2.14	0.63
1:S:131:THR:OG1	1:S:134:GLU:HG3	1.98	0.63
1:S:43:PRO:HG2	1:S:48:LEU:HD12	1.81	0.63
1:B:244:GLU:O	1:B:248:MET:HG3	1.99	0.63
1:K:194:ARG:HD3	1:K:206:ALA:O	1.98	0.63
1:S:8:ILE:HD11	1:S:245:PHE:CZ	2.33	0.63
1:L:48:LEU:O	1:L:52:ILE:HG13	1.98	0.63
1:P:69:LEU:HD23	1:P:70:GLU:HG2	1.80	0.63
1:H:220:SER:O	1:H:221:ASN:CB	2.46	0.63
1:J:127:CYS:HB3	1:J:170:GLU:OE2	1.98	0.63
1:M:171:PRO:HG2	1:M:174:SER:HB2	1.80	0.63
1:N:137:ALA:HB3	1:N:139:ARG:HG3	1.80	0.63
1:S:173:TRP:CD1	1:S:173:TRP:N	2.56	0.63
1:T:98:GLU:O	1:T:102:ILE:HB	1.99	0.63
1:T:34:PRO:HG2	1:T:253:THR:OG1	1.98	0.63
1:B:175:ILE:O	1:O:176:GLY:N	2.32	0.63
1:D:18:LEU:O	1:D:22:LYS:HG3	1.98	0.63
1:G:67:VAL:O	1:G:113:LYS:HD3	1.99	0.63
1:L:182:THR:OG1	1:L:185:GLN:HG3	1.99	0.63
1:D:57:SER:HB3	1:D:60:LEU:HB3	1.81	0.62
1:L:222:ASP:OD2	1:L:248:MET:CE	2.46	0.62
1:E:97:SER:HB3	1:E:170:GLU:OE1	1.99	0.62
1:L:67:VAL:O	1:L:113:LYS:HD3	1.99	0.62
1:M:106:THR:OG1	1:M:109:GLN:HG3	1.99	0.62
1:N:171:PRO:HB2	1:N:174:SER:OG	1.98	0.62
1:O:109:GLN:O	1:O:113:LYS:HG3	1.99	0.62
1:P:149:GLU:OE1	1:P:200:LYS:HE3	1.98	0.62
1:E:190:HIS:CE1	1:E:213:TYR:HB2	2.32	0.62
1:F:175:ILE:H	1:F:175:ILE:HD12	1.61	0.62
1:I:141:MET:O	1:I:145:ILE:HB	1.99	0.62
1:K:204:GLU:HG2	1:K:205:GLY:N	2.14	0.62
1:Q:183:PRO:CG	1:Q:225:LEU:CD2	2.77	0.62
1:E:197:PHE:O	1:E:201:VAL:N	2.33	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:109:GLN:O	1:F:113:LYS:HG3	1.99	0.62
1:N:139:ARG:HH12	1:N:143:VAL:HG22	1.63	0.62
1:O:213:TYR:CE1	1:O:215:GLY:HA3	2.35	0.62
1:Q:222:ASP:OD1	1:Q:223:GLU:N	2.33	0.62
1:Q:8:ILE:CG2	1:Q:39:VAL:HG22	2.30	0.62
1:R:174:SER:O	1:R:175:ILE:CG2	2.48	0.62
1:D:159:LYS:C	1:D:161:LEU:H	2.03	0.62
1:N:48:LEU:O	1:N:52:ILE:HG13	1.98	0.62
1:Q:15:ASN:OD1	1:R:72:ASN:HB3	1.99	0.62
1:T:172:VAL:HA	1:T:175:ILE:HD12	1.80	0.62
1:E:222:ASP:O	1:E:226:GLY:N	2.27	0.62
1:G:213:TYR:HD2	1:G:234:PHE:CE1	2.18	0.62
1:G:9:GLY:O	1:G:235:LEU:HA	2.00	0.62
1:L:218:ASN:HB2	1:L:221:ASN:OD1	1.99	0.62
1:A:139:ARG:NH1	1:A:142:GLU:OE1	2.33	0.62
1:A:144:ASN:O	1:A:148:LEU:HB2	2.00	0.62
1:O:197:PHE:HD2	1:O:206:ALA:HA	1.64	0.62
1:O:83:MET:O	1:O:87:MET:HG3	1.99	0.62
1:R:228:CYS:CB	1:R:231:ILE:CG1	2.77	0.62
1:E:174:SER:O	1:I:176:GLY:HA3	2.00	0.62
1:G:69:LEU:O	1:G:116:ARG:HD2	2.00	0.61
1:M:118:LEU:HB3	1:M:161:LEU:HD22	1.82	0.61
1:M:40:VAL:CG1	1:M:63:ALA:HB2	2.29	0.61
1:S:6:PRO:CD	1:S:36:SER:O	2.48	0.61
1:G:109:GLN:O	1:G:113:LYS:HG3	2.00	0.61
1:G:218:ASN:O	1:G:220:SER:N	2.33	0.61
1:I:5:ARG:NH2	1:I:35:ASP:O	2.33	0.61
1:L:64:ALA:HB3	1:L:92:VAL:HG23	1.80	0.61
1:R:71:GLY:HA2	1:R:116:ARG:HH21	1.65	0.61
1:S:79:THR:HG21	1:S:84:LEU:HD21	1.82	0.61
1:E:175:ILE:HA	1:I:176:GLY:CA	2.20	0.61
1:E:171:PRO:CD	1:E:215:GLY:HA3	2.30	0.61
1:G:21:ILE:O	1:G:25:VAL:HG23	2.01	0.61
1:J:95:GLY:HA2	1:J:110:SER:OG	2.00	0.61
1:K:98:GLU:O	1:K:102:ILE:HB	2.00	0.61
1:O:171:PRO:CD	1:O:214:GLY:O	2.46	0.61
1:C:178:GLY:CA	1:R:175:ILE:HD13	2.21	0.61
1:S:246:MET:O	1:S:249:ILE:HB	2.00	0.61
1:A:145:ILE:HG23	1:A:196:TRP:CD1	2.35	0.61
1:G:213:TYR:CD2	1:G:234:PHE:CD1	2.88	0.61
1:M:228:CYS:HB2	1:M:231:ILE:CD1	2.30	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:95:GLY:O	1:P:127:CYS:HB2	2.00	0.61
1:A:31:HIS:NE2	1:A:250:ASP:OD1	2.31	0.61
1:M:111:ALA:HB1	1:M:151:LEU:HA	1.81	0.61
1:N:109:GLN:O	1:N:113:LYS:HG3	2.00	0.61
1:Q:9:GLY:HA2	1:Q:40:VAL:HG13	1.83	0.61
1:A:177:THR:OG1	1:A:179:VAL:HG13	2.00	0.61
1:C:240:SER:HA	1:C:245:PHE:HB2	1.82	0.61
1:O:98:GLU:OE2	1:P:74:ALA:HB1	2.01	0.61
1:R:225:LEU:CB	1:R:234:PHE:HE1	2.03	0.61
1:R:251:ILE:HD13	1:R:251:ILE:N	2.15	0.61
1:C:72:ASN:ND2	1:C:80:SER:OG	2.33	0.61
1:H:197:PHE:O	1:H:201:VAL:HB	2.00	0.61
1:J:132:LEU:HD22	1:J:177:THR:HG21	1.83	0.61
1:Q:197:PHE:CE1	1:Q:209:ILE:HD13	2.35	0.61
1:Q:89:LEU:CD1	1:Q:91:HIS:H	2.13	0.61
1:R:15:ASN:OD1	1:R:15:ASN:N	2.34	0.61
1:R:60:LEU:O	1:R:61:ARG:HD2	2.00	0.61
1:R:61:ARG:HH22	1:R:90:LYS:HD3	1.64	0.61
1:P:14:CYS:C	1:P:15:ASN:ND2	2.38	0.61
1:S:95:GLY:O	1:S:127:CYS:HB2	1.99	0.61
1:Q:243:PRO:HA	1:Q:246:MET:CE	2.31	0.61
1:R:174:SER:C	1:R:175:ILE:HG22	2.21	0.61
1:A:123:THR:HA	1:A:164:GLU:HG3	1.81	0.61
1:A:21:ILE:O	1:A:25:VAL:HG23	2.01	0.61
1:E:195:LYS:O	1:E:199:GLU:CG	2.49	0.61
1:J:48:LEU:O	1:J:52:ILE:HG13	2.01	0.61
1:R:156:GLY:O	1:R:159:LYS:CG	2.49	0.61
1:C:195:LYS:O	1:C:199:GLU:HG3	2.01	0.60
1:C:6:PRO:HB2	1:C:37:VAL:HG13	1.83	0.60
1:E:191:VAL:HG22	1:E:230:ASN:ND2	2.16	0.60
1:F:175:ILE:H	1:F:175:ILE:CD1	2.14	0.60
1:N:143:VAL:O	1:N:147:GLN:HG3	2.01	0.60
1:Q:166:VAL:HG22	1:Q:210:ARG:CZ	2.31	0.60
1:S:83:MET:O	1:S:87:MET:HG3	2.01	0.60
1:B:4:ARG:HG2	1:B:208:HIS:O	2.02	0.60
1:D:194:ARG:HD3	1:D:206:ALA:O	2.01	0.60
1:H:109:GLN:O	1:H:113:LYS:HG3	2.01	0.60
1:B:98:GLU:O	1:B:102:ILE:HB	2.00	0.60
1:E:98:GLU:HB2	1:F:76:THR:HG22	1.83	0.60
1:G:213:TYR:CD2	1:G:234:PHE:HE1	2.18	0.60
1:I:4:ARG:NH1	1:I:232:ASP:OD1	2.34	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:155:LEU:HD12	1:K:162:TRP:CE2	2.37	0.60
1:K:251:ILE:O	1:K:255:THR:HB	2.02	0.60
1:P:148:LEU:HG	1:P:196:TRP:CZ3	2.36	0.60
1:S:92:VAL:HG12	1:S:124:VAL:HG22	1.84	0.60
1:T:185:GLN:O	1:T:189:VAL:HG23	2.01	0.60
1:D:81:VAL:O	1:D:85:GLN:HG3	2.02	0.60
1:D:8:ILE:HB	1:D:252:LEU:HD22	1.83	0.60
1:O:160:MET:O	1:O:163:LYS:HB2	2.00	0.60
1:P:195:LYS:O	1:P:199:GLU:HB2	2.02	0.60
1:R:157:GLU:OE1	1:R:157:GLU:HA	2.01	0.60
1:C:76:THR:N	1:D:98:GLU:OE1	2.33	0.60
1:I:4:ARG:HD2	1:I:208:HIS:HA	1.83	0.60
1:I:4:ARG:CB	1:I:4:ARG:NH1	2.64	0.60
1:A:218:ASN:ND2	1:A:220:SER:N	2.50	0.60
1:J:130:GLU:OE2	1:J:173:TRP:CD1	2.54	0.60
1:Q:201:VAL:HG12	1:Q:202:ALA:H	1.65	0.60
1:D:218:ASN:C	1:D:218:ASN:HD22	2.05	0.60
1:N:4:ARG:HE	1:N:232:ASP:CG	2.05	0.60
1:O:164:GLU:HA	1:O:164:GLU:OE1	2.02	0.60
1:R:183:PRO:HB2	1:R:224:LYS:HE2	1.84	0.60
1:R:225:LEU:HB3	1:R:234:PHE:CZ	2.35	0.60
1:S:7:PHE:O	1:S:233:GLY:HA3	2.00	0.60
1:T:243:PRO:HA	1:T:246:MET:CE	2.32	0.60
1:B:155:LEU:HD12	1:B:162:TRP:NE1	2.16	0.60
1:J:123:THR:HG23	1:J:164:GLU:O	2.02	0.60
1:L:236:VAL:HG11	1:L:239:ALA:HB3	1.82	0.60
1:Q:92:VAL:HG12	1:Q:124:VAL:HG22	1.84	0.60
1:T:11:ASN:ND2	1:T:13:LYS:HG3	2.16	0.60
1:T:157:GLU:OE1	1:T:157:GLU:HA	2.00	0.60
1:A:83:MET:O	1:A:87:MET:HG3	2.02	0.60
1:J:244:GLU:N	1:J:244:GLU:OE1	2.28	0.60
1:K:151:LEU:O	1:K:155:LEU:HG	2.01	0.60
1:R:227:GLN:HA	1:R:227:GLN:NE2	2.15	0.60
1:T:250:ASP:O	1:T:253:THR:HB	2.02	0.60
1:F:174:SER:HB2	1:F:179:VAL:HG12	1.82	0.59
1:G:97:SER:CB	1:G:170:GLU:OE1	2.45	0.59
1:K:197:PHE:CD1	1:K:206:ALA:HA	2.37	0.59
1:C:111:ALA:HB1	1:C:151:LEU:HA	1.84	0.59
1:I:98:GLU:OE1	1:J:76:THR:HG23	2.02	0.59
1:N:199:GLU:C	1:N:200:LYS:HD2	2.22	0.59
1:S:21:ILE:O	1:S:25:VAL:HG23	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:203:ALA:HB3	1:L:204:GLU:OE2	2.03	0.59
1:O:137:ALA:O	1:O:138:ASN:CB	2.49	0.59
1:I:11:ASN:ND2	1:J:76:THR:CG2	2.63	0.59
1:O:162:TRP:CH2	1:O:196:TRP:HH2	2.21	0.59
1:Q:7:PHE:CE1	1:Q:38:ASP:CG	2.76	0.59
1:R:82:GLU:H	1:R:82:GLU:CD	2.06	0.59
1:E:171:PRO:HB2	1:E:174:SER:OG	2.01	0.59
1:E:219:GLY:O	1:E:220:SER:CB	2.50	0.59
1:H:162:TRP:CE3	1:H:197:PHE:HE2	2.20	0.59
1:J:21:ILE:O	1:J:25:VAL:HG23	2.01	0.59
1:Q:69:LEU:O	1:Q:116:ARG:HD2	2.02	0.59
1:F:155:LEU:HD12	1:F:162:TRP:NE1	2.16	0.59
1:H:141:MET:O	1:H:145:ILE:HG12	2.02	0.59
1:I:78:GLU:OE1	1:I:78:GLU:HA	2.02	0.59
1:L:204:GLU:N	1:L:204:GLU:CD	2.55	0.59
1:Q:39:VAL:HG12	1:Q:60:LEU:HD12	1.84	0.59
1:C:171:PRO:HD2	1:C:214:GLY:O	2.02	0.59
1:R:149:GLU:HG2	1:R:196:TRP:HZ2	1.68	0.59
1:S:151:LEU:O	1:S:155:LEU:HD13	2.03	0.59
1:B:97:SER:O	1:B:101:ARG:HB2	2.03	0.59
1:F:13:LYS:N	1:F:65:GLN:HE22	2.01	0.59
1:F:218:ASN:O	1:F:221:ASN:OD1	2.20	0.59
1:I:250:ASP:O	1:I:254:LYS:HD3	2.03	0.59
1:L:236:VAL:CG1	1:L:239:ALA:HB3	2.33	0.59
1:M:244:GLU:O	1:M:247:THR:HB	2.03	0.59
1:A:143:VAL:O	1:A:147:GLN:HG3	2.03	0.59
1:C:187:GLU:OE1	1:C:228:CYS:HB3	2.02	0.59
1:K:222:ASP:OD1	1:K:234:PHE:CZ	2.55	0.59
1:M:7:PHE:HB2	1:M:210:ARG:HH11	1.68	0.59
1:O:222:ASP:OD1	1:O:225:LEU:HD12	2.03	0.59
1:R:239:ALA:O	1:R:245:PHE:HB2	2.03	0.59
1:R:250:ASP:HA	1:R:253:THR:HG22	1.85	0.59
1:O:218:ASN:HD22	1:O:220:SER:N	1.90	0.59
1:E:171:PRO:HG2	1:E:215:GLY:CA	2.10	0.58
1:K:218:ASN:ND2	1:K:219:GLY:H	2.00	0.58
1:L:177:THR:CB	1:L:179:VAL:HG23	2.33	0.58
1:M:81:VAL:HG13	1:M:122:MET:SD	2.43	0.58
1:O:14:CYS:SG	1:P:78:GLU:O	2.53	0.58
1:Q:173:TRP:CZ3	1:Q:174:SER:HB3	2.37	0.58
1:E:254:LYS:C	1:E:255:THR:OG1	2.36	0.58
1:K:165:VAL:O	1:K:209:ILE:CD1	2.49	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:195:LYS:O	1:K:199:GLU:HG3	2.03	0.58
1:N:21:ILE:O	1:N:25:VAL:HG23	2.02	0.58
1:E:171:PRO:HD2	1:E:214:GLY:O	2.03	0.58
1:P:221:ASN:OD1	1:P:222:ASP:N	2.36	0.58
1:F:196:TRP:O	1:F:200:LYS:HB2	2.03	0.58
1:M:13:LYS:N	1:M:65:GLN:HE22	2.01	0.58
1:P:159:LYS:O	1:P:162:TRP:HD1	1.85	0.58
1:Q:173:TRP:CE3	1:Q:174:SER:HB3	2.38	0.58
1:R:228:CYS:SG	1:R:231:ILE:HG13	2.43	0.58
1:B:97:SER:CB	1:B:170:GLU:OE1	2.51	0.58
1:B:171:PRO:HG3	1:B:215:GLY:HA2	1.83	0.58
1:C:76:THR:CG2	1:D:98:GLU:CD	2.57	0.58
1:D:37:VAL:CG1	1:D:252:LEU:HD21	2.33	0.58
1:F:108:GLU:O	1:F:112:LYS:HG3	2.04	0.58
1:L:8:ILE:HB	1:L:252:LEU:HD22	1.85	0.58
1:M:13:LYS:N	1:M:65:GLN:NE2	2.51	0.58
1:R:174:SER:O	1:R:175:ILE:HG22	2.04	0.58
1:G:187:GLU:O	1:G:191:VAL:HG23	2.03	0.58
1:I:130:GLU:OE2	1:I:135:ARG:NE	2.31	0.58
1:K:69:LEU:HD23	1:K:70:GLU:HG2	1.86	0.58
1:S:221:ASN:O	1:S:224:LYS:HG3	2.02	0.58
1:D:218:ASN:C	1:D:218:ASN:ND2	2.57	0.58
1:E:141:MET:HA	1:E:141:MET:CE	2.34	0.58
1:F:18:LEU:O	1:F:22:LYS:HG3	2.04	0.58
1:K:221:ASN:H	1:K:221:ASN:ND2	2.01	0.58
1:A:74:ALA:HB1	1:B:98:GLU:OE2	2.04	0.58
1:E:171:PRO:O	1:E:175:ILE:HG13	2.03	0.58
1:K:130:GLU:OE1	1:K:169:TYR:HE1	1.85	0.58
1:Q:7:PHE:HE2	1:Q:210:ARG:HG3	1.67	0.58
1:L:18:LEU:O	1:L:22:LYS:HG3	2.04	0.58
1:M:225:LEU:O	1:M:231:ILE:CD1	2.52	0.58
1:Q:183:PRO:HG3	1:Q:225:LEU:HD21	1.86	0.58
1:Q:218:ASN:N	1:Q:221:ASN:OD1	2.36	0.58
1:Q:91:HIS:CD2	1:Q:123:THR:HG21	2.39	0.58
1:C:187:GLU:OE2	1:C:229:PRO:HG2	2.04	0.58
1:E:190:HIS:ND1	1:E:211:ILE:HG22	2.17	0.58
1:F:13:LYS:N	1:F:65:GLN:NE2	2.52	0.58
1:J:11:ASN:HD22	1:J:13:LYS:HG3	1.68	0.58
1:M:194:ARG:HD3	1:M:206:ALA:O	2.03	0.58
1:R:225:LEU:CB	1:R:234:PHE:CZ	2.85	0.58
1:S:34:PRO:HG2	1:S:253:THR:OG1	2.02	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:83:MET:O	1:M:87:MET:HG3	2.04	0.57
1:O:247:THR:O	1:O:251:ILE:HD13	2.04	0.57
1:R:66:ASN:ND2	1:R:99:ARG:NE	2.51	0.57
1:E:128:VAL:HG11	1:E:148:LEU:HD13	1.85	0.57
1:I:81:VAL:O	1:I:85:GLN:HG3	2.04	0.57
1:O:100:ARG:NH1	1:O:128:VAL:HA	2.19	0.57
1:P:64:ALA:HB3	1:P:92:VAL:HG23	1.84	0.57
1:Q:248:MET:HA	1:Q:251:ILE:HG22	1.85	0.57
1:R:28:ILE:HG12	1:R:246:MET:HE3	1.85	0.57
1:S:130:GLU:CD	1:S:140:THR:HG23	2.25	0.57
1:T:246:MET:HA	1:T:249:ILE:CD1	2.34	0.57
1:I:57:SER:HB3	1:I:60:LEU:HB3	1.86	0.57
1:O:139:ARG:HD2	1:O:142:GLU:OE2	2.03	0.57
1:R:12:PHE:O	1:R:15:ASN:OD1	2.23	0.57
1:R:186:ALA:O	1:R:189:VAL:HG22	2.04	0.57
1:R:66:ASN:ND2	1:R:99:ARG:CD	2.67	0.57
1:S:75:TRP:HD1	1:T:14:CYS:SG	2.28	0.57
1:A:7:PHE:O	1:A:233:GLY:HA3	2.05	0.57
1:H:95:GLY:O	1:H:100:ARG:HG3	2.04	0.57
1:K:195:LYS:CG	1:K:196:TRP:N	2.68	0.57
1:L:251:ILE:HA	1:L:254:LYS:HD2	1.86	0.57
1:O:195:LYS:O	1:O:199:GLU:HG3	2.04	0.57
1:R:15:ASN:ND2	1:R:241:LEU:HD11	2.19	0.57
1:S:46:VAL:HG23	1:S:47:HIS:CD2	2.38	0.57
1:C:135:ARG:HA	1:C:140:THR:HG22	1.87	0.57
1:I:155:LEU:HD12	1:I:162:TRP:CE2	2.39	0.57
1:I:4:ARG:CG	1:I:4:ARG:NH1	2.63	0.57
1:J:222:ASP:N	1:J:222:ASP:OD1	2.36	0.57
1:K:251:ILE:HA	1:K:254:LYS:HE3	1.85	0.57
1:P:68:TYR:CE2	1:P:70:GLU:HB2	2.39	0.57
1:S:186:ALA:HB2	1:S:213:TYR:CE1	2.40	0.57
1:A:222:ASP:HA	1:A:225:LEU:HB2	1.87	0.57
1:B:5:ARG:NH1	1:B:35:ASP:O	2.32	0.57
1:J:182:THR:CG2	1:J:184:GLU:OE1	2.53	0.57
1:N:130:GLU:O	1:N:130:GLU:HG2	2.04	0.57
1:T:137:ALA:O	1:T:138:ASN:HB3	2.04	0.57
1:I:48:LEU:HD23	1:I:89:LEU:HD11	1.86	0.57
1:Q:177:THR:HG23	1:Q:177:THR:O	2.05	0.57
1:I:4:ARG:CD	1:I:208:HIS:HA	2.34	0.57
1:Q:61:ARG:CG	1:Q:61:ARG:HH11	2.18	0.57
1:Q:62:ILE:O	1:Q:89:LEU:HD11	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:169:TYR:CE2	1:R:189:VAL:HG21	2.40	0.57
1:S:6:PRO:HG2	1:S:37:VAL:CA	2.29	0.57
1:G:9:GLY:O	1:G:235:LEU:HD12	2.05	0.57
1:K:160:MET:HA	1:K:163:LYS:HG2	1.87	0.57
1:R:51:ALA:HB1	1:R:62:ILE:HD13	1.86	0.57
1:R:69:LEU:N	1:R:69:LEU:HD23	2.18	0.57
1:I:76:THR:HG23	1:J:65:GLN:HB3	1.87	0.56
1:P:130:GLU:HG3	1:P:144:ASN:HD21	1.68	0.56
1:Q:7:PHE:HE1	1:Q:38:ASP:CG	2.07	0.56
1:S:151:LEU:HD23	1:S:162:TRP:CH2	2.40	0.56
1:S:25:VAL:HA	1:S:28:ILE:HG13	1.87	0.56
1:B:5:ARG:O	1:B:210:ARG:HD2	2.05	0.56
1:E:72:ASN:ND2	1:E:80:SER:OG	2.38	0.56
1:H:126:PHE:CZ	1:H:151:LEU:HD21	2.40	0.56
1:I:236:VAL:CG1	1:I:239:ALA:HB3	2.35	0.56
1:M:105:GLU:HG2	1:M:110:SER:OG	2.04	0.56
1:T:239:ALA:O	1:T:245:PHE:HB2	2.05	0.56
1:C:57:SER:HB3	1:C:60:LEU:HB3	1.88	0.56
1:E:143:VAL:O	1:E:147:GLN:HG3	2.05	0.56
1:I:194:ARG:HD2	1:I:230:ASN:OD1	2.05	0.56
1:J:223:GLU:OE2	1:J:254:LYS:HE3	2.05	0.56
1:M:210:ARG:HG3	1:M:232:ASP:CB	2.36	0.56
1:M:98:GLU:HG2	1:N:74:ALA:O	2.05	0.56
1:P:145:ILE:O	1:P:149:GLU:HG2	2.05	0.56
1:R:66:ASN:ND2	1:R:99:ARG:HD2	2.20	0.56
1:D:221:ASN:O	1:D:224:LYS:HG2	2.04	0.56
1:F:174:SER:OG	1:F:175:ILE:HD12	2.06	0.56
1:F:90:LYS:HD3	1:F:91:HIS:CE1	2.39	0.56
1:Q:114:ALA:O	1:Q:118:LEU:HG	2.05	0.56
1:Q:18:LEU:O	1:Q:22:LYS:HG3	2.05	0.56
1:R:116:ARG:O	1:R:119:GLU:OE1	2.22	0.56
1:C:64:ALA:HB3	1:C:92:VAL:HG23	1.88	0.56
1:E:90:LYS:HG3	1:E:90:LYS:O	2.05	0.56
1:G:217:ALA:HB1	1:G:248:MET:HE1	1.87	0.56
1:I:155:LEU:HD12	1:I:162:TRP:NE1	2.20	0.56
1:J:180:VAL:HG22	1:J:181:ALA:N	2.19	0.56
1:P:198:ALA:HA	1:P:202:ALA:O	2.06	0.56
1:S:31:HIS:CB	1:S:246:MET:HG2	2.36	0.56
1:C:95:GLY:HA2	1:C:110:SER:OG	2.05	0.56
1:G:189:VAL:O	1:G:193:LEU:HG	2.05	0.56
1:M:222:ASP:OD1	1:M:223:GLU:N	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:131:THR:OG1	1:N:134:GLU:HG3	2.06	0.56
1:O:220:SER:O	1:O:221:ASN:CB	2.52	0.56
1:P:145:ILE:HG13	1:P:196:TRP:CD1	2.41	0.56
1:R:63:ALA:CB	1:R:91:HIS:HB2	2.31	0.56
1:S:172:VAL:HA	1:S:175:ILE:CG1	2.34	0.56
1:E:95:GLY:C	1:E:127:CYS:HB2	2.26	0.56
1:J:114:ALA:O	1:J:118:LEU:HG	2.05	0.56
1:Q:183:PRO:HG3	1:Q:225:LEU:HD23	1.87	0.56
1:R:81:VAL:HG13	1:R:122:MET:SD	2.46	0.56
1:N:139:ARG:HD2	1:N:142:GLU:OE1	2.03	0.56
1:O:69:LEU:HD22	1:O:69:LEU:H	1.69	0.56
1:Q:248:MET:O	1:Q:251:ILE:CG2	2.54	0.56
1:C:215:GLY:O	1:C:216:SER:C	2.41	0.56
1:D:221:ASN:O	1:D:224:LYS:CG	2.54	0.56
1:I:4:ARG:NH1	1:I:194:ARG:NH2	2.53	0.56
1:J:191:VAL:HG22	1:J:230:ASN:ND2	2.21	0.56
1:O:108:GLU:O	1:O:112:LYS:HB2	2.06	0.56
1:O:148:LEU:HD23	1:O:193:LEU:HD22	1.88	0.56
1:D:67:VAL:O	1:D:113:LYS:HD3	2.06	0.56
1:K:213:TYR:HD2	1:K:234:PHE:HE1	1.53	0.56
1:N:15:ASN:N	1:N:15:ASN:ND2	2.50	0.56
1:P:135:ARG:HE	1:P:173:TRP:HZ2	1.52	0.56
1:R:216:SER:O	1:R:217:ALA:HB3	2.06	0.56
1:C:128:VAL:HG11	1:C:148:LEU:HD13	1.86	0.56
1:D:24:HIS:O	1:D:28:ILE:HG13	2.06	0.56
1:K:42:ALA:HB1	1:K:65:GLN:HG3	1.88	0.56
1:Q:21:ILE:O	1:Q:25:VAL:HG23	2.05	0.56
1:T:222:ASP:HA	1:T:225:LEU:HD12	1.88	0.56
1:A:218:ASN:ND2	1:A:221:ASN:H	2.05	0.55
1:C:215:GLY:O	1:C:217:ALA:N	2.39	0.55
1:F:17:SER:O	1:F:21:ILE:HG12	2.06	0.55
1:K:41:ILE:HG12	1:K:62:ILE:HD12	1.87	0.55
1:L:169:TYR:CE2	1:L:189:VAL:HG21	2.41	0.55
1:P:62:ILE:N	1:P:62:ILE:HD12	2.21	0.55
1:R:127:CYS:HB3	1:R:170:GLU:OE2	2.07	0.55
1:T:99:ARG:HA	1:T:103:MET:HB2	1.88	0.55
1:T:242:LYS:CB	1:T:243:PRO:HD2	2.35	0.55
1:D:158:SER:OG	1:D:160:MET:CE	2.54	0.55
1:D:40:VAL:HG22	1:D:61:ARG:HB2	1.88	0.55
1:J:155:LEU:HD22	1:J:161:LEU:HB2	1.88	0.55
1:J:90:LYS:HG2	1:J:90:LYS:O	2.04	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:197:PHE:HD1	1:P:206:ALA:HB2	1.71	0.55
1:Q:166:VAL:HG22	1:Q:210:ARG:NE	2.21	0.55
1:S:91:HIS:HA	1:S:123:THR:O	2.06	0.55
1:D:37:VAL:HG11	1:D:252:LEU:CD2	2.37	0.55
1:F:240:SER:HA	1:F:245:PHE:CD1	2.41	0.55
1:J:81:VAL:HG13	1:J:122:MET:SD	2.46	0.55
1:J:187:GLU:OE1	1:J:228:CYS:HB3	2.05	0.55
1:M:218:ASN:O	1:M:222:ASP:HB3	2.07	0.55
1:M:74:ALA:HB1	1:N:98:GLU:OE2	2.05	0.55
1:O:160:MET:HG2	1:O:161:LEU:N	2.21	0.55
1:O:65:GLN:HB3	1:P:76:THR:CG2	2.36	0.55
1:R:66:ASN:HD22	1:R:99:ARG:CZ	2.19	0.55
1:S:253:THR:HG22	1:S:254:LYS:N	2.20	0.55
1:S:74:ALA:HB1	1:T:98:GLU:OE2	2.06	0.55
1:C:4:ARG:CG	1:C:207:GLN:O	2.53	0.55
1:G:225:LEU:O	1:G:228:CYS:HB2	2.05	0.55
1:G:77:GLY:HA3	1:H:99:ARG:HH11	1.70	0.55
1:P:184:GLU:H	1:P:184:GLU:CD	2.10	0.55
1:S:145:ILE:HG23	1:S:196:TRP:CD1	2.42	0.55
1:A:218:ASN:HD22	1:A:220:SER:N	2.05	0.55
1:L:251:ILE:HD13	1:L:254:LYS:HD2	1.89	0.55
1:R:251:ILE:CD1	1:R:251:ILE:N	2.69	0.55
1:A:218:ASN:ND2	1:A:220:SER:H	2.05	0.55
1:F:174:SER:O	1:F:179:VAL:HB	2.06	0.55
1:G:236:VAL:HG21	1:G:248:MET:SD	2.46	0.55
1:E:175:ILE:HG12	1:I:176:GLY:O	2.07	0.55
1:I:215:GLY:O	1:I:216:SER:C	2.45	0.55
1:K:213:TYR:CE2	1:K:215:GLY:HA2	2.41	0.55
1:L:244:GLU:O	1:L:245:PHE:C	2.43	0.55
1:P:247:THR:O	1:P:251:ILE:HD13	2.07	0.55
1:S:204:GLU:OE1	1:S:208:HIS:HE1	1.89	0.55
1:Q:234:PHE:CD2	1:Q:248:MET:HE2	2.40	0.55
1:Q:248:MET:C	1:Q:251:ILE:HG22	2.27	0.55
1:S:197:PHE:CD1	1:S:206:ALA:HA	2.42	0.55
1:T:81:VAL:O	1:T:85:GLN:HG3	2.05	0.55
1:F:9:GLY:HA2	1:F:40:VAL:O	2.07	0.55
1:G:229:PRO:HB2	1:G:230:ASN:HD22	1.71	0.55
1:M:141:MET:O	1:M:145:ILE:HB	2.07	0.55
1:N:226:GLY:C	1:N:255:THR:CG2	2.66	0.55
1:C:2:PRO:HD2	1:C:207:GLN:HG2	1.87	0.55
1:C:98:GLU:OE1	1:D:76:THR:N	2.34	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:198:ALA:HB2	1:E:206:ALA:CB	2.37	0.55
1:I:132:LEU:O	1:I:136:LYS:HG3	2.06	0.55
1:I:37:VAL:HG11	1:I:252:LEU:HD23	1.88	0.55
1:R:141:MET:HE1	1:R:193:LEU:HD23	1.89	0.55
1:S:55:ASN:OD1	1:S:60:LEU:HD23	2.07	0.55
1:C:173:TRP:O	1:C:177:THR:HG21	2.07	0.55
1:C:244:GLU:O	1:C:247:THR:HB	2.07	0.55
1:H:158:SER:HB2	1:H:161:LEU:HG	1.88	0.55
1:P:114:ALA:O	1:P:118:LEU:HG	2.07	0.55
1:R:85:GLN:HE22	1:R:120:LYS:HB3	1.71	0.55
1:R:228:CYS:HB2	1:R:231:ILE:HB	1.89	0.55
1:C:33:ILE:HB	1:C:59:GLN:HE21	1.72	0.54
1:I:236:VAL:HG11	1:I:239:ALA:HB3	1.89	0.54
1:Q:236:VAL:HG12	1:Q:240:SER:HB3	1.89	0.54
1:T:24:HIS:O	1:T:27:ALA:HB3	2.07	0.54
1:B:95:GLY:C	1:B:127:CYS:HB2	2.28	0.54
1:C:215:GLY:C	1:C:217:ALA:N	2.56	0.54
1:H:197:PHE:CZ	1:H:201:VAL:HG11	2.42	0.54
1:L:37:VAL:CG1	1:L:252:LEU:HD23	2.38	0.54
1:M:5:ARG:HH12	1:M:36:SER:C	2.11	0.54
1:O:58:LYS:CG	1:O:59:GLN:OE1	2.55	0.54
1:P:31:HIS:CE1	1:P:246:MET:HB3	2.42	0.54
1:Q:27:ALA:O	1:Q:30:ALA:HB3	2.07	0.54
1:A:137:ALA:HB3	1:A:139:ARG:HG3	1.90	0.54
1:I:67:VAL:O	1:I:113:LYS:HD3	2.07	0.54
1:Q:139:ARG:O	1:Q:143:VAL:HG23	2.07	0.54
1:R:15:ASN:ND2	1:R:241:LEU:CD1	2.70	0.54
1:S:72:ASN:ND2	1:S:80:SER:OG	2.40	0.54
1:A:99:ARG:HD2	1:B:76:THR:O	2.08	0.54
1:E:187:GLU:O	1:E:191:VAL:HG23	2.06	0.54
1:L:244:GLU:O	1:L:247:THR:N	2.40	0.54
1:O:98:GLU:O	1:O:102:ILE:HB	2.07	0.54
1:A:4:ARG:HH22	1:A:230:ASN:HA	1.73	0.54
1:D:159:LYS:C	1:D:161:LEU:N	2.61	0.54
1:E:4:ARG:NH2	1:E:229:PRO:O	2.41	0.54
1:F:40:VAL:HG22	1:F:61:ARG:HB2	1.90	0.54
1:G:137:ALA:HB3	1:G:139:ARG:HG3	1.90	0.54
1:B:217:ALA:HB1	1:B:222:ASP:CG	2.28	0.54
1:I:12:PHE:O	1:I:13:LYS:HB2	2.07	0.54
1:L:90:LYS:HE3	1:L:91:HIS:HE1	1.73	0.54
1:N:141:MET:O	1:N:145:ILE:CG1	2.56	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:79:THR:CG2	1:Q:84:LEU:HD21	2.36	0.54
1:S:115:LYS:HD2	1:S:154:GLU:O	2.08	0.54
1:S:197:PHE:HE2	1:S:209:ILE:HD13	1.72	0.54
1:S:5:ARG:HG2	1:S:6:PRO:HD2	1.88	0.54
1:T:64:ALA:CB	1:T:84:LEU:HD11	2.38	0.54
1:A:131:THR:HG22	1:A:132:LEU:N	2.22	0.54
1:C:47:HIS:CE1	1:D:83:MET:HG2	2.42	0.54
1:E:169:TYR:CZ	1:E:189:VAL:HG11	2.42	0.54
1:L:200:LYS:C	1:L:200:LYS:HD2	2.11	0.54
1:D:102:ILE:HD11	1:N:179:VAL:HA	1.88	0.54
1:P:24:HIS:O	1:P:28:ILE:HG13	2.07	0.54
1:Q:83:MET:O	1:Q:87:MET:HG2	2.07	0.54
1:A:108:GLU:OE2	1:A:112:LYS:NZ	2.40	0.54
1:D:218:ASN:HD21	1:D:220:SER:H	1.53	0.54
1:G:93:ILE:HD11	1:G:96:HIS:HB2	1.89	0.54
1:H:144:ASN:HB3	1:H:193:LEU:HD21	1.90	0.54
1:N:226:GLY:HA3	1:N:255:THR:HG21	1.87	0.54
1:O:132:LEU:HD22	1:O:177:THR:HB	1.90	0.54
1:P:162:TRP:HA	1:P:165:VAL:CG2	2.38	0.54
1:Q:175:ILE:O	1:Q:177:THR:HB	2.06	0.54
1:Q:7:PHE:CD1	1:Q:38:ASP:CB	2.87	0.54
1:T:44:SER:O	1:T:48:LEU:HD13	2.08	0.54
1:O:6:PRO:HB2	1:O:37:VAL:HG13	1.90	0.54
1:P:180:VAL:HG22	1:P:181:ALA:N	2.22	0.54
1:P:21:ILE:O	1:P:25:VAL:HG23	2.08	0.54
1:Q:73:GLY:N	1:R:14:CYS:SG	2.81	0.54
1:A:162:TRP:CE3	1:A:197:PHE:HE2	2.26	0.54
1:C:253:THR:HG22	1:C:254:LYS:N	2.23	0.54
1:F:219:GLY:HA2	1:F:222:ASP:OD2	2.08	0.54
1:G:145:ILE:O	1:G:149:GLU:HG2	2.08	0.54
1:M:170:GLU:CB	1:M:175:ILE:HD11	2.38	0.54
1:M:5:ARG:NH2	1:M:35:ASP:O	2.40	0.54
1:M:18:LEU:HD23	1:M:47:HIS:HD2	1.72	0.54
1:N:223:GLU:OE1	1:N:251:ILE:HD11	2.08	0.54
1:O:103:MET:CE	1:P:78:GLU:HG3	2.38	0.54
1:P:162:TRP:HA	1:P:165:VAL:HG23	1.90	0.54
1:Q:218:ASN:O	1:Q:221:ASN:OD1	2.26	0.54
1:Q:234:PHE:CD2	1:Q:248:MET:HE3	2.41	0.54
1:A:111:ALA:HB1	1:A:151:LEU:HA	1.89	0.53
1:D:218:ASN:O	1:D:222:ASP:HB3	2.07	0.53
1:D:6:PRO:HB3	1:D:252:LEU:HD11	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:123:THR:HA	1:G:164:GLU:HB3	1.89	0.53
1:S:243:PRO:O	1:S:246:MET:HE3	2.07	0.53
1:S:5:ARG:CG	1:S:6:PRO:HD2	2.37	0.53
1:A:4:ARG:HD2	1:A:207:GLN:O	2.08	0.53
1:H:98:GLU:O	1:H:102:ILE:HB	2.08	0.53
1:L:233:GLY:HA2	1:L:252:LEU:HD11	1.91	0.53
1:Q:55:ASN:HD22	1:Q:62:ILE:HD13	1.73	0.53
1:T:48:LEU:O	1:T:52:ILE:HD12	2.09	0.53
1:E:83:MET:HE1	1:F:14:CYS:HA	1.90	0.53
1:H:24:HIS:O	1:H:28:ILE:HG13	2.09	0.53
1:K:115:LYS:HG3	1:K:155:LEU:HD23	1.90	0.53
1:O:66:ASN:ND2	1:O:67:VAL:H	2.07	0.53
1:Q:63:ALA:HB2	1:Q:91:HIS:HB2	1.90	0.53
1:S:6:PRO:CG	1:S:37:VAL:HG12	2.38	0.53
1:T:245:PHE:HA	1:T:248:MET:HG3	1.91	0.53
1:A:72:ASN:HD22	1:A:72:ASN:N	2.06	0.53
1:F:145:ILE:HG23	1:F:196:TRP:CD1	2.44	0.53
1:G:213:TYR:CB	1:G:234:PHE:CE1	2.88	0.53
1:J:203:ALA:HB3	1:M:200:LYS:HE3	1.91	0.53
1:O:46:VAL:HB	1:P:87:MET:SD	2.48	0.53
1:R:83:MET:O	1:R:86:ASP:HB3	2.07	0.53
1:S:224:LYS:HG3	1:S:225:LEU:H	1.73	0.53
1:B:144:ASN:HD22	1:B:193:LEU:CD2	2.21	0.53
1:E:171:PRO:HG3	1:E:213:TYR:CE1	2.44	0.53
1:H:85:GLN:HE22	1:H:120:LYS:HB3	1.74	0.53
1:L:69:LEU:CD2	1:L:70:GLU:HG2	2.35	0.53
1:N:84:LEU:O	1:N:89:LEU:HB2	2.09	0.53
1:Q:31:HIS:O	1:Q:33:ILE:HG13	2.09	0.53
1:Q:92:VAL:CG1	1:Q:124:VAL:HG22	2.38	0.53
1:S:151:LEU:HD23	1:S:162:TRP:CZ3	2.43	0.53
1:S:38:ASP:OD2	1:S:210:ARG:NH2	2.40	0.53
1:S:83:MET:HG2	1:T:46:VAL:HG21	1.91	0.53
1:T:82:GLU:CD	1:T:116:ARG:HH12	2.12	0.53
1:C:4:ARG:HG2	1:C:207:GLN:O	2.07	0.53
1:E:187:GLU:OE1	1:E:228:CYS:HB3	2.09	0.53
1:F:67:VAL:O	1:F:113:LYS:HD3	2.09	0.53
1:E:96:HIS:HB3	1:F:76:THR:HG21	1.89	0.53
1:J:251:ILE:HD12	1:J:254:LYS:NZ	2.23	0.53
1:J:84:LEU:HD22	1:J:89:LEU:HD12	1.90	0.53
1:L:24:HIS:O	1:L:28:ILE:HG13	2.09	0.53
1:O:182:THR:H	1:O:185:GLN:NE2	2.05	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:158:SER:HB2	1:S:161:LEU:CD2	2.29	0.53
1:F:95:GLY:O	1:F:127:CYS:HB2	2.09	0.53
1:G:96:HIS:CE1	1:G:98:GLU:HG3	2.44	0.53
1:J:217:ALA:O	1:J:248:MET:CE	2.57	0.53
1:K:116:ARG:O	1:K:119:GLU:HB2	2.08	0.53
1:M:41:ILE:HG12	1:M:60:LEU:HD11	1.91	0.53
1:O:197:PHE:HE2	1:O:205:GLY:C	2.12	0.53
1:P:37:VAL:HG21	1:P:253:THR:OG1	2.09	0.53
1:Q:81:VAL:HG23	1:Q:116:ARG:HH11	1.74	0.53
1:C:4:ARG:HD3	1:C:207:GLN:O	2.09	0.53
1:E:194:ARG:NH1	1:E:211:ILE:HD12	2.24	0.53
1:I:148:LEU:HG	1:I:196:TRP:CZ3	2.43	0.53
1:L:155:LEU:HD22	1:L:161:LEU:HB2	1.91	0.53
1:M:18:LEU:O	1:M:22:LYS:HG3	2.07	0.53
1:O:66:ASN:ND2	1:O:67:VAL:N	2.56	0.53
1:P:8:ILE:HB	1:P:252:LEU:HD22	1.91	0.53
1:Q:12:PHE:HB2	1:Q:42:ALA:O	2.09	0.53
1:S:2:PRO:HD2	1:S:207:GLN:HB2	1.91	0.53
1:L:34:PRO:HG3	1:L:253:THR:OG1	2.08	0.53
1:O:139:ARG:CB	1:O:142:GLU:HB3	2.39	0.53
1:Q:242:LYS:O	1:Q:245:PHE:HB3	2.09	0.53
1:A:160:MET:H	1:A:160:MET:CE	2.22	0.53
1:E:130:GLU:OE2	1:E:140:THR:HB	2.09	0.53
1:F:236:VAL:CG1	1:F:239:ALA:HB3	2.39	0.53
1:G:5:ARG:HG3	1:G:36:SER:O	2.09	0.53
1:H:187:GLU:OE1	1:H:228:CYS:HB3	2.08	0.53
1:J:69:LEU:HB3	1:J:113:LYS:HG2	1.91	0.53
1:K:69:LEU:CD2	1:K:70:GLU:HG2	2.39	0.53
1:L:174:SER:O	1:L:215:GLY:HA3	2.09	0.53
1:N:255:THR:O	1:N:255:THR:HG22	2.09	0.53
1:Q:221:ASN:O	1:Q:225:LEU:HG	2.09	0.53
1:S:139:ARG:O	1:S:143:VAL:HG23	2.09	0.53
1:S:243:PRO:HA	1:S:246:MET:HE1	1.91	0.53
1:S:99:ARG:NH2	1:T:78:GLU:OE2	2.42	0.53
1:A:109:GLN:O	1:A:113:LYS:HG3	2.08	0.52
1:K:187:GLU:O	1:K:191:VAL:HG23	2.09	0.52
1:L:155:LEU:HD12	1:L:162:TRP:NE1	2.23	0.52
1:O:21:ILE:O	1:O:25:VAL:HG23	2.08	0.52
1:P:131:THR:HG22	1:P:172:VAL:HG11	1.91	0.52
1:R:242:LYS:HB3	1:R:243:PRO:HD2	1.91	0.52
1:Q:99:ARG:HD3	1:R:76:THR:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:127:CYS:HA	1:T:168:ALA:O	2.09	0.52
1:A:115:LYS:CE	1:A:119:GLU:OE2	2.57	0.52
1:L:221:ASN:HD22	1:L:221:ASN:C	2.11	0.52
1:D:176:GLY:HA3	1:N:174:SER:O	2.09	0.52
1:S:241:LEU:HD23	1:S:241:LEU:N	2.24	0.52
1:T:115:LYS:HG2	1:T:155:LEU:HG	1.90	0.52
1:B:213:TYR:HB2	1:B:231:ILE:HD13	1.91	0.52
1:C:76:THR:CG2	1:D:13:LYS:HD3	2.36	0.52
1:E:206:ALA:O	1:E:209:ILE:HG22	2.09	0.52
1:S:17:SER:O	1:S:21:ILE:HG12	2.09	0.52
1:T:217:ALA:HB1	1:T:248:MET:HE1	1.91	0.52
1:T:37:VAL:HG11	1:T:252:LEU:HD23	1.91	0.52
1:D:180:VAL:HG13	1:D:181:ALA:N	2.24	0.52
1:E:69:LEU:HD23	1:E:70:GLU:HG2	1.91	0.52
1:E:178:GLY:HA3	1:I:172:VAL:CG1	2.39	0.52
1:I:13:LYS:HA	1:J:76:THR:HG22	1.90	0.52
1:O:217:ALA:HB1	1:O:222:ASP:OD1	2.09	0.52
1:E:236:VAL:CG1	1:E:239:ALA:HB3	2.39	0.52
1:J:56:THR:HG22	1:K:19:ASP:OD1	2.10	0.52
1:Q:183:PRO:HA	1:Q:225:LEU:HD22	1.91	0.52
1:R:11:ASN:OD1	1:R:13:LYS:N	2.42	0.52
1:S:185:GLN:HA	1:S:188:GLU:OE1	2.10	0.52
1:S:6:PRO:CG	1:S:37:VAL:HA	2.31	0.52
1:A:115:LYS:HE3	1:A:119:GLU:OE2	2.10	0.52
1:A:90:LYS:HE2	1:A:123:THR:OG1	2.09	0.52
1:A:131:THR:HG22	1:A:132:LEU:H	1.74	0.52
1:F:244:GLU:O	1:F:248:MET:HG3	2.09	0.52
1:P:171:PRO:HB2	1:P:174:SER:OG	2.09	0.52
1:R:81:VAL:HG21	1:R:116:ARG:HG2	1.92	0.52
1:A:68:TYR:HD1	1:A:78:GLU:OE1	1.93	0.52
1:F:236:VAL:HG11	1:F:239:ALA:HB3	1.91	0.52
1:J:7:PHE:O	1:J:233:GLY:HA3	2.10	0.52
1:S:182:THR:OG1	1:S:185:GLN:HB2	2.10	0.52
1:S:55:ASN:HB2	1:S:62:ILE:HD11	1.89	0.52
1:T:213:TYR:CD2	1:T:225:LEU:HD13	2.45	0.52
1:B:4:ARG:HD3	1:B:207:GLN:O	2.10	0.52
1:C:84:LEU:HD22	1:C:89:LEU:HD12	1.90	0.52
1:G:69:LEU:CD1	1:G:69:LEU:C	2.77	0.52
1:E:217:ALA:CB	1:I:178:GLY:HA3	2.38	0.52
1:I:37:VAL:HG11	1:I:252:LEU:CD2	2.40	0.52
1:L:12:PHE:HB2	1:L:42:ALA:O	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:194:ARG:HE	1:P:230:ASN:HD22	1.58	0.52
1:R:230:ASN:ND2	1:R:230:ASN:N	2.58	0.52
1:S:118:LEU:HD13	1:S:161:LEU:CD1	2.39	0.52
1:E:222:ASP:HB2	1:E:251:ILE:HG21	1.91	0.52
1:F:179:VAL:HG12	1:F:180:VAL:N	2.24	0.52
1:Q:7:PHE:HD1	1:Q:38:ASP:CB	2.13	0.52
1:C:68:TYR:HB2	1:C:78:GLU:HB3	1.92	0.52
1:G:69:LEU:HD12	1:G:70:GLU:N	2.24	0.52
1:I:69:LEU:HB3	1:I:113:LYS:HG2	1.91	0.52
1:I:13:LYS:HG2	1:J:74:ALA:HA	1.93	0.52
1:S:171:PRO:HA	1:S:173:TRP:NE1	2.23	0.52
1:T:243:PRO:HA	1:T:246:MET:HE2	1.92	0.52
1:A:13:LYS:N	1:A:65:GLN:NE2	2.58	0.51
1:F:155:LEU:HD12	1:F:162:TRP:CE2	2.45	0.51
1:G:244:GLU:O	1:G:247:THR:HB	2.10	0.51
1:J:11:ASN:HD21	1:J:13:LYS:HG3	1.72	0.51
1:M:41:ILE:O	1:M:43:PRO:HD3	2.09	0.51
1:O:61:ARG:NE	1:O:62:ILE:H	2.03	0.51
1:B:139:ARG:HD2	1:B:142:GLU:OE1	2.10	0.51
1:C:134:GLU:O	1:C:139:ARG:HG3	2.09	0.51
1:F:69:LEU:HB3	1:F:113:LYS:HG2	1.91	0.51
1:G:83:MET:O	1:G:87:MET:HG3	2.10	0.51
1:H:130:GLU:OE2	1:H:140:THR:HG23	2.10	0.51
1:I:4:ARG:HB2	1:I:4:ARG:NH1	2.24	0.51
1:J:21:ILE:HG13	1:J:47:HIS:HB3	1.92	0.51
1:N:141:MET:O	1:N:145:ILE:HG13	2.10	0.51
1:R:175:ILE:O	1:R:177:THR:HG23	2.10	0.51
1:T:13:LYS:H	1:T:65:GLN:NE2	2.08	0.51
1:A:139:ARG:NH1	1:A:142:GLU:CD	2.63	0.51
1:A:6:PRO:HB2	1:A:37:VAL:HG22	1.92	0.51
1:E:46:VAL:HB	1:F:87:MET:SD	2.51	0.51
1:G:41:ILE:HG23	1:G:60:LEU:HD11	1.91	0.51
1:R:128:VAL:HG11	1:R:148:LEU:HD13	1.92	0.51
1:R:175:ILE:CG2	1:R:177:THR:OG1	2.57	0.51
1:S:61:ARG:HH22	1:S:90:LYS:HB2	1.75	0.51
1:A:246:MET:HA	1:A:249:ILE:HD12	1.92	0.51
1:C:134:GLU:HG2	1:C:143:VAL:HG21	1.92	0.51
1:G:71:GLY:O	1:G:75:TRP:NE1	2.44	0.51
1:I:194:ARG:HH12	1:I:211:ILE:HG13	1.74	0.51
1:I:4:ARG:CB	1:I:4:ARG:HH11	2.22	0.51
1:N:141:MET:HE3	1:N:145:ILE:HD11	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:15:ASN:HD21	1:R:241:LEU:CD1	2.21	0.51
1:S:210:ARG:CG	1:S:210:ARG:NH1	2.55	0.51
1:A:239:ALA:HA	1:A:242:LYS:HG2	1.91	0.51
1:A:77:GLY:H	1:B:65:GLN:HE21	1.59	0.51
1:C:24:HIS:NE2	1:C:240:SER:O	2.42	0.51
1:F:134:GLU:OE1	1:F:143:VAL:HG11	2.10	0.51
1:F:181:ALA:HB3	1:F:213:TYR:OH	2.11	0.51
1:M:174:SER:HA	1:M:179:VAL:O	2.10	0.51
1:M:228:CYS:CB	1:M:231:ILE:HD12	2.38	0.51
1:M:37:VAL:HG12	1:M:38:ASP:N	2.25	0.51
1:N:199:GLU:O	1:N:200:LYS:HD2	2.11	0.51
1:O:58:LYS:CG	1:O:59:GLN:CD	2.66	0.51
1:R:194:ARG:NH1	1:R:209:ILE:HG23	2.23	0.51
1:S:160:MET:O	1:S:163:LYS:HB3	2.10	0.51
1:B:37:VAL:CG1	1:B:252:LEU:HD23	2.41	0.51
1:G:213:TYR:CB	1:G:234:PHE:CD1	2.80	0.51
1:H:145:ILE:HG23	1:H:196:TRP:CD1	2.45	0.51
1:J:221:ASN:OD1	1:J:222:ASP:N	2.43	0.51
1:O:139:ARG:HD2	1:O:142:GLU:CD	2.31	0.51
1:P:81:VAL:O	1:P:85:GLN:HG3	2.11	0.51
1:S:112:LYS:O	1:S:116:ARG:HB2	2.11	0.51
1:S:202:ALA:O	1:S:206:ALA:HB2	2.11	0.51
1:T:106:THR:OG1	1:T:109:GLN:HG3	2.11	0.51
1:B:187:GLU:O	1:B:191:VAL:HG23	2.11	0.51
1:C:24:HIS:O	1:C:28:ILE:HG13	2.10	0.51
1:R:68:TYR:CG	1:R:78:GLU:HG3	2.46	0.51
1:S:108:GLU:O	1:S:112:LYS:HG3	2.10	0.51
1:A:159:LYS:O	1:A:162:TRP:HB2	2.11	0.51
1:P:135:ARG:NE	1:P:173:TRP:CZ2	2.78	0.51
1:Q:7:PHE:HE2	1:Q:210:ARG:HH11	1.59	0.51
1:A:155:LEU:HD12	1:A:162:TRP:NE1	2.26	0.51
1:B:171:PRO:HB2	1:B:174:SER:OG	2.10	0.51
1:D:139:ARG:O	1:D:143:VAL:HG23	2.10	0.51
1:E:4:ARG:CD	1:E:207:GLN:O	2.54	0.51
1:J:67:VAL:O	1:J:113:LYS:HD3	2.10	0.51
1:K:209:ILE:HD12	1:K:210:ARG:H	1.75	0.51
1:K:187:GLU:HB2	1:K:228:CYS:SG	2.51	0.51
1:L:135:ARG:O	1:L:138:ASN:HA	2.11	0.51
1:S:5:ARG:HH22	1:S:35:ASP:C	2.14	0.51
1:T:158:SER:HB3	1:T:161:LEU:HG	1.93	0.51
1:C:58:LYS:HB2	1:C:59:GLN:OE1	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:213:TYR:CE2	1:M:214:GLY:O	2.64	0.51
1:O:184:GLU:CD	1:O:184:GLU:H	2.14	0.51
1:O:76:THR:CG2	1:P:65:GLN:HB3	2.39	0.51
1:Q:175:ILE:O	1:Q:176:GLY:C	2.49	0.51
1:Q:197:PHE:HD2	1:Q:206:ALA:CA	2.22	0.51
1:S:31:HIS:HB2	1:S:246:MET:HG2	1.93	0.51
1:A:172:VAL:CA	1:A:175:ILE:HG13	2.41	0.50
1:E:190:HIS:CE1	1:E:211:ILE:HG22	2.46	0.50
1:F:128:VAL:HG11	1:F:148:LEU:HD13	1.92	0.50
1:G:150:ALA:O	1:G:154:GLU:HG2	2.11	0.50
1:G:37:VAL:HG12	1:G:38:ASP:N	2.26	0.50
1:Q:89:LEU:HD12	1:Q:91:HIS:H	1.74	0.50
1:R:187:GLU:OE2	1:R:230:ASN:N	2.44	0.50
1:T:187:GLU:OE2	1:T:229:PRO:HG2	2.10	0.50
1:A:172:VAL:CG1	1:A:175:ILE:HD12	2.37	0.50
1:D:69:LEU:O	1:D:116:ARG:HD2	2.10	0.50
1:L:218:ASN:HB2	1:L:221:ASN:CG	2.31	0.50
1:Q:230:ASN:ND2	1:Q:230:ASN:N	2.58	0.50
1:B:2:PRO:HB3	1:B:207:GLN:HG2	1.93	0.50
1:B:244:GLU:O	1:B:247:THR:HB	2.11	0.50
1:G:82:GLU:N	1:G:82:GLU:OE1	2.44	0.50
1:L:137:ALA:O	1:L:138:ASN:CB	2.59	0.50
1:L:141:MET:CE	1:L:141:MET:HA	2.41	0.50
1:T:108:GLU:OE2	1:T:112:LYS:HE3	2.10	0.50
1:E:176:GLY:HA3	1:I:132:LEU:HB2	1.93	0.50
1:E:6:PRO:HB2	1:E:37:VAL:HG13	1.92	0.50
1:I:13:LYS:HG3	1:J:76:THR:HG23	1.92	0.50
1:N:222:ASP:O	1:N:223:GLU:C	2.48	0.50
1:N:70:GLU:OE1	1:N:70:GLU:HA	2.12	0.50
1:O:139:ARG:NH1	1:O:142:GLU:OE2	2.44	0.50
1:S:173:TRP:HD1	1:S:173:TRP:H	1.49	0.50
1:T:7:PHE:C	1:T:7:PHE:CD1	2.85	0.50
1:E:141:MET:HE2	1:E:145:ILE:HD12	1.94	0.50
1:E:190:HIS:HE2	1:E:213:TYR:CB	2.14	0.50
1:L:180:VAL:HG22	1:L:181:ALA:N	2.26	0.50
1:L:206:ALA:O	1:L:209:ILE:HG22	2.12	0.50
1:N:196:TRP:O	1:N:200:LYS:HB2	2.11	0.50
1:R:24:HIS:O	1:R:27:ALA:HB3	2.11	0.50
1:A:138:ASN:HD22	1:A:138:ASN:C	2.11	0.50
1:D:37:VAL:HG13	1:D:252:LEU:HD21	1.94	0.50
1:E:254:LYS:C	1:E:255:THR:HG1	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:251:ILE:HD12	1:J:254:LYS:HZ1	1.76	0.50
1:O:224:LYS:O	1:O:227:GLN:HB2	2.11	0.50
1:Q:243:PRO:HA	1:Q:246:MET:HE2	1.94	0.50
1:I:141:MET:CE	1:I:192:GLY:HA3	2.42	0.50
1:I:4:ARG:NE	1:I:207:GLN:O	2.43	0.50
1:I:51:ALA:HB1	1:I:62:ILE:HD12	1.94	0.50
1:K:152:GLY:HA2	1:K:162:TRP:HZ2	1.77	0.50
1:K:174:SER:HA	1:K:179:VAL:O	2.11	0.50
1:K:223:GLU:CG	1:K:254:LYS:HZ1	2.18	0.50
1:M:18:LEU:HD23	1:M:47:HIS:CD2	2.47	0.50
1:P:137:ALA:O	1:P:138:ASN:HB3	2.11	0.50
1:Q:39:VAL:HG12	1:Q:60:LEU:CD1	2.41	0.50
1:R:91:HIS:CD2	1:R:123:THR:CG2	2.94	0.50
1:R:227:GLN:CA	1:R:227:GLN:HE21	2.21	0.50
1:T:64:ALA:HB2	1:T:84:LEU:HD11	1.94	0.50
1:T:7:PHE:CD1	1:T:8:ILE:N	2.80	0.50
1:E:194:ARG:CZ	1:E:211:ILE:HD12	2.42	0.50
1:F:21:ILE:HG13	1:F:47:HIS:HB3	1.93	0.50
1:T:84:LEU:HB3	1:T:122:MET:HE1	1.93	0.50
1:D:158:SER:HA	1:D:160:MET:HE1	1.94	0.50
1:H:147:GLN:O	1:H:151:LEU:HD13	2.12	0.50
1:K:218:ASN:H	1:K:221:ASN:HD21	1.59	0.50
1:M:17:SER:O	1:M:21:ILE:HG12	2.12	0.50
1:M:9:GLY:HA2	1:M:40:VAL:O	2.12	0.50
1:E:134:GLU:HB3	1:E:143:VAL:HG21	1.94	0.49
1:E:198:ALA:HB2	1:E:206:ALA:HB2	1.93	0.49
1:F:99:ARG:HA	1:F:103:MET:HB2	1.93	0.49
1:K:42:ALA:O	1:K:65:GLN:NE2	2.44	0.49
1:Q:166:VAL:HG23	1:Q:210:ARG:NH2	2.27	0.49
1:C:46:VAL:HB	1:D:87:MET:SD	2.53	0.49
1:H:100:ARG:NH2	1:H:126:PHE:CE2	2.80	0.49
1:H:156:GLY:O	1:H:159:LYS:HG2	2.12	0.49
1:I:40:VAL:HG22	1:I:61:ARG:HB2	1.94	0.49
1:J:250:ASP:O	1:J:254:LYS:HG2	2.12	0.49
1:K:209:ILE:HD12	1:K:210:ARG:N	2.27	0.49
1:L:251:ILE:HA	1:L:254:LYS:CD	2.42	0.49
1:O:58:LYS:CD	1:O:59:GLN:OE1	2.60	0.49
1:P:106:THR:OG1	1:P:109:GLN:HG3	2.12	0.49
1:D:197:PHE:HD1	1:D:206:ALA:HB2	1.78	0.49
1:H:167:ILE:HB	1:H:211:ILE:HG23	1.94	0.49
1:I:149:GLU:O	1:I:153:LYS:N	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:213:TYR:O	1:K:215:GLY:N	2.36	0.49
1:K:40:VAL:CG1	1:K:63:ALA:HB2	2.42	0.49
1:M:5:ARG:O	1:M:210:ARG:NH1	2.45	0.49
1:N:190:HIS:ND1	1:N:211:ILE:HG22	2.28	0.49
1:O:67:VAL:HG22	1:O:68:TYR:H	1.77	0.49
1:P:42:ALA:HB1	1:P:65:GLN:HG2	1.93	0.49
1:Q:33:ILE:HB	1:Q:59:GLN:HE21	1.76	0.49
1:A:251:ILE:O	1:A:255:THR:HB	2.12	0.49
1:H:126:PHE:CD2	1:H:151:LEU:HD21	2.47	0.49
1:K:150:ALA:O	1:K:154:GLU:HG2	2.12	0.49
1:K:83:MET:CE	1:L:44:SER:OG	2.61	0.49
1:L:169:TYR:CZ	1:L:189:VAL:HG21	2.47	0.49
1:N:218:ASN:HD22	1:N:221:ASN:HD22	1.61	0.49
1:P:141:MET:O	1:P:145:ILE:HB	2.12	0.49
1:Q:248:MET:CA	1:Q:251:ILE:HG22	2.41	0.49
1:Q:68:TYR:HB2	1:Q:78:GLU:HB3	1.94	0.49
1:S:75:TRP:HD1	1:T:14:CYS:CB	2.25	0.49
1:N:139:ARG:NH1	1:N:143:VAL:CG2	2.76	0.49
1:P:155:LEU:HD22	1:P:161:LEU:HB2	1.94	0.49
1:P:172:VAL:HG12	1:P:173:TRP:N	2.27	0.49
1:R:24:HIS:O	1:R:28:ILE:HG13	2.12	0.49
1:S:195:LYS:HD3	1:S:199:GLU:OE2	2.13	0.49
1:H:64:ALA:HB3	1:H:92:VAL:HG23	1.93	0.49
1:J:109:GLN:O	1:J:113:LYS:HG3	2.13	0.49
1:J:180:VAL:CG2	1:J:181:ALA:N	2.75	0.49
1:L:99:ARG:HA	1:L:103:MET:SD	2.53	0.49
1:L:149:GLU:HA	1:L:149:GLU:OE1	2.12	0.49
1:O:218:ASN:HB3	1:O:220:SER:O	2.12	0.49
1:R:246:MET:HA	1:R:249:ILE:CD1	2.35	0.49
1:R:36:SER:OG	1:R:37:VAL:HG23	2.12	0.49
1:S:7:PHE:CE1	1:S:40:VAL:CG2	2.95	0.49
1:S:6:PRO:CG	1:S:36:SER:O	2.60	0.49
1:T:118:LEU:HD13	1:T:155:LEU:HD11	1.94	0.49
1:B:128:VAL:HG11	1:B:148:LEU:HD13	1.95	0.49
1:B:66:ASN:HD22	1:B:67:VAL:H	0.58	0.49
1:F:171:PRO:HG2	1:F:213:TYR:OH	2.11	0.49
1:J:132:LEU:HD22	1:J:177:THR:CG2	2.41	0.49
1:N:98:GLU:O	1:N:102:ILE:HB	2.12	0.49
1:P:180:VAL:HG22	1:P:181:ALA:H	1.78	0.49
1:Q:236:VAL:CG1	1:Q:240:SER:N	2.76	0.49
1:S:2:PRO:HD2	1:S:207:GLN:CB	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:ASN:ND2	1:D:220:SER:N	2.56	0.49
1:D:222:ASP:HA	1:D:225:LEU:HD12	1.94	0.49
1:I:141:MET:HE1	1:I:192:GLY:HA3	1.94	0.49
1:O:221:ASN:O	1:O:221:ASN:OD1	2.31	0.49
1:T:182:THR:OG1	1:T:185:GLN:HG3	2.12	0.49
1:T:227:GLN:NE2	1:T:255:THR:HG22	2.28	0.49
1:A:132:LEU:HG	1:A:136:LYS:HE3	1.95	0.49
1:B:167:ILE:O	1:B:211:ILE:HA	2.13	0.49
1:M:164:GLU:OE1	1:M:164:GLU:HA	2.13	0.49
1:M:79:THR:HG21	1:M:84:LEU:HD21	1.95	0.49
1:P:55:ASN:HD22	1:P:62:ILE:CD1	2.25	0.49
1:Q:186:ALA:HB2	1:Q:213:TYR:CE1	2.48	0.49
1:Q:31:HIS:HE2	1:Q:250:ASP:CG	2.16	0.49
1:S:221:ASN:CA	1:S:224:LYS:HE2	2.43	0.49
1:T:235:LEU:C	1:T:235:LEU:HD23	2.33	0.49
1:E:214:GLY:HA3	1:E:235:LEU:O	2.13	0.49
1:F:132:LEU:O	1:F:136:LYS:HB2	2.13	0.49
1:J:219:GLY:O	1:J:222:ASP:OD1	2.30	0.49
1:L:137:ALA:HB3	1:L:139:ARG:HG3	1.95	0.49
1:L:218:ASN:CB	1:L:221:ASN:ND2	2.76	0.49
1:M:240:SER:HA	1:M:245:PHE:HB2	1.95	0.49
1:Q:198:ALA:HB2	1:Q:206:ALA:HB2	1.95	0.49
1:R:228:CYS:HB2	1:R:231:ILE:CB	2.43	0.49
1:S:228:CYS:CB	1:S:231:ILE:HG13	2.43	0.49
1:E:115:LYS:HE3	1:E:119:GLU:OE2	2.12	0.48
1:E:179:VAL:HG13	1:E:179:VAL:O	2.12	0.48
1:L:21:ILE:O	1:L:25:VAL:HG23	2.12	0.48
1:M:5:ARG:CG	1:M:5:ARG:NH1	2.69	0.48
1:O:59:GLN:N	1:O:59:GLN:HE21	1.98	0.48
1:P:190:HIS:CE1	1:P:231:ILE:HG12	2.48	0.48
1:Q:85:GLN:NE2	1:Q:120:LYS:HB3	2.20	0.48
1:Q:5:ARG:NH2	1:Q:35:ASP:O	2.44	0.48
1:E:81:VAL:HG11	1:E:120:LYS:HB2	1.94	0.48
1:E:116:ARG:NH2	1:E:120:LYS:HZ1	2.12	0.48
1:E:99:ARG:HG3	1:F:76:THR:HG23	1.93	0.48
1:E:176:GLY:N	1:I:175:ILE:O	2.43	0.48
1:K:130:GLU:OE1	1:K:169:TYR:CE1	2.66	0.48
1:N:209:ILE:HG23	1:N:211:ILE:CD1	2.43	0.48
1:F:68:TYR:HB2	1:F:78:GLU:HB3	1.96	0.48
1:I:194:ARG:HH12	1:I:209:ILE:HG23	1.78	0.48
1:N:130:GLU:OE1	1:N:140:THR:HG23	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:123:THR:HG23	1:O:164:GLU:O	2.13	0.48
1:P:40:VAL:HG11	1:P:63:ALA:HB2	1.95	0.48
1:Q:31:HIS:NE2	1:Q:250:ASP:OD1	2.39	0.48
1:Q:80:SER:O	1:Q:83:MET:HB2	2.14	0.48
1:R:114:ALA:HB3	1:R:151:LEU:HD13	1.94	0.48
1:S:145:ILE:O	1:S:149:GLU:HG2	2.13	0.48
1:E:139:ARG:O	1:E:143:VAL:HG23	2.13	0.48
1:E:141:MET:CE	1:E:145:ILE:HD12	2.43	0.48
1:H:229:PRO:HG2	1:H:230:ASN:HD22	1.78	0.48
1:K:81:VAL:O	1:K:85:GLN:HG3	2.13	0.48
1:M:187:GLU:OE2	1:M:230:ASN:OD1	2.31	0.48
1:N:139:ARG:HH12	1:N:143:VAL:CG2	2.26	0.48
1:R:236:VAL:CG1	1:R:239:ALA:HB3	2.44	0.48
1:T:198:ALA:HA	1:T:202:ALA:O	2.13	0.48
1:A:72:ASN:ND2	1:A:80:SER:OG	2.47	0.48
1:D:52:ILE:HA	1:D:62:ILE:HD13	1.95	0.48
1:M:145:ILE:HG13	1:M:196:TRP:CD1	2.48	0.48
1:P:151:LEU:HD12	1:P:151:LEU:O	2.13	0.48
1:Q:145:ILE:O	1:Q:149:GLU:HG3	2.12	0.48
1:S:243:PRO:HA	1:S:246:MET:CE	2.42	0.48
1:L:5:ARG:NH1	1:L:35:ASP:O	2.46	0.48
1:L:79:THR:HG21	1:L:84:LEU:HD21	1.93	0.48
1:N:90:LYS:HE3	1:N:91:HIS:HE1	1.76	0.48
1:R:20:PHE:CE1	1:R:24:HIS:HB2	2.49	0.48
1:T:244:GLU:O	1:T:247:THR:HB	2.14	0.48
1:A:250:ASP:O	1:A:254:LYS:HE2	2.12	0.48
1:D:187:GLU:OE1	1:D:228:CYS:HB3	2.14	0.48
1:G:236:VAL:HG13	1:G:239:ALA:HB3	1.91	0.48
1:J:57:SER:HB3	1:J:60:LEU:HB3	1.95	0.48
1:K:9:GLY:HA2	1:K:40:VAL:O	2.14	0.48
1:Q:248:MET:HA	1:Q:251:ILE:CG2	2.44	0.48
1:R:226:GLY:N	1:R:234:PHE:CZ	2.78	0.48
1:G:24:HIS:O	1:G:28:ILE:HG13	2.14	0.48
1:K:246:MET:O	1:K:249:ILE:HB	2.14	0.48
1:K:48:LEU:O	1:K:52:ILE:HG13	2.14	0.48
1:K:14:CYS:SG	1:L:80:SER:HB3	2.54	0.48
1:O:103:MET:HE2	1:P:78:GLU:HG3	1.95	0.48
1:O:132:LEU:O	1:O:136:LYS:HG3	2.14	0.48
1:S:196:TRP:CE3	1:S:197:PHE:HA	2.48	0.48
1:S:221:ASN:ND2	1:S:221:ASN:N	2.62	0.48
1:S:244:GLU:HG3	1:S:245:PHE:N	2.29	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:145:ILE:O	1:T:149:GLU:HG3	2.14	0.48
1:A:4:ARG:NH2	1:A:229:PRO:O	2.46	0.48
1:B:168:ALA:HA	1:B:212:ILE:O	2.14	0.48
1:B:37:VAL:HG12	1:B:38:ASP:N	2.29	0.48
1:D:219:GLY:O	1:D:222:ASP:OD1	2.31	0.48
1:E:171:PRO:CD	1:E:215:GLY:HA2	2.34	0.48
1:E:251:ILE:HD12	1:E:254:LYS:HE3	1.96	0.48
1:K:18:LEU:O	1:K:22:LYS:HG3	2.13	0.48
1:L:118:LEU:HD23	1:L:122:MET:O	2.14	0.48
1:L:251:ILE:HD13	1:L:254:LYS:HZ2	1.76	0.48
1:N:32:LYS:HG3	1:N:32:LYS:O	2.14	0.48
1:O:184:GLU:N	1:O:184:GLU:CD	2.67	0.48
1:R:171:PRO:HD2	1:R:214:GLY:O	2.13	0.48
1:R:64:ALA:CB	1:R:84:LEU:HD11	2.44	0.48
1:S:43:PRO:HG2	1:S:48:LEU:CD1	2.43	0.48
1:B:116:ARG:O	1:B:120:LYS:HG3	2.14	0.48
1:D:226:GLY:O	1:D:255:THR:HG21	2.14	0.48
1:F:179:VAL:CG1	1:F:180:VAL:N	2.76	0.48
1:I:72:ASN:HD21	1:I:82:GLU:HB2	1.79	0.48
1:K:171:PRO:HG2	1:K:213:TYR:CE1	2.48	0.48
1:K:24:HIS:O	1:K:28:ILE:HG13	2.14	0.48
1:M:2:PRO:HG2	1:M:207:GLN:CG	2.43	0.48
1:N:139:ARG:HD2	1:N:142:GLU:CD	2.35	0.48
1:O:131:THR:HG23	1:O:134:GLU:OE1	2.13	0.48
1:Q:197:PHE:CD2	1:Q:206:ALA:CA	2.94	0.48
1:R:39:VAL:O	1:R:60:LEU:HD12	2.14	0.48
1:S:247:THR:O	1:S:251:ILE:HG12	2.14	0.48
1:S:7:PHE:CD1	1:S:7:PHE:C	2.87	0.48
1:S:7:PHE:CE1	1:S:40:VAL:HG21	2.49	0.48
1:T:55:ASN:OD1	1:T:60:LEU:HD23	2.13	0.48
1:B:144:ASN:ND2	1:B:193:LEU:HD21	2.29	0.47
1:D:114:ALA:O	1:D:118:LEU:HG	2.14	0.47
1:I:4:ARG:HH12	1:I:194:ARG:NH2	2.12	0.47
1:M:2:PRO:CB	1:M:207:GLN:HB3	2.43	0.47
1:M:69:LEU:HD12	1:M:70:GLU:HG2	1.96	0.47
1:N:123:THR:HA	1:N:164:GLU:HB3	1.96	0.47
1:O:100:ARG:HH12	1:O:128:VAL:HA	1.78	0.47
1:S:188:GLU:HG2	1:S:189:VAL:N	2.28	0.47
1:S:12:PHE:HB2	1:S:43:PRO:HA	1.96	0.47
1:S:76:THR:O	1:T:99:ARG:HD2	2.14	0.47
1:A:68:TYR:CD1	1:A:78:GLU:HG3	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:TYR:HE2	1:C:70:GLU:HG3	1.79	0.47
1:E:190:HIS:CD2	1:E:231:ILE:HG12	2.49	0.47
1:F:40:VAL:CG1	1:F:63:ALA:HB2	2.44	0.47
1:G:97:SER:O	1:G:101:ARG:HG2	2.14	0.47
1:H:7:PHE:O	1:H:233:GLY:HA3	2.14	0.47
1:J:254:LYS:HG3	1:J:255:THR:H	1.79	0.47
1:L:187:GLU:OE1	1:L:228:CYS:HB3	2.13	0.47
1:M:99:ARG:CA	1:M:103:MET:HB2	2.37	0.47
1:O:66:ASN:HD22	1:O:67:VAL:H	1.60	0.47
1:B:99:ARG:HA	1:B:103:MET:HB2	1.97	0.47
1:D:190:HIS:CE1	1:D:211:ILE:O	2.67	0.47
1:E:196:TRP:O	1:E:200:LYS:N	2.38	0.47
1:R:250:ASP:HA	1:R:253:THR:HG23	1.96	0.47
1:E:183:PRO:HG2	1:E:224:LYS:CD	2.45	0.47
1:E:251:ILE:CA	1:E:254:LYS:HE3	2.24	0.47
1:F:218:ASN:C	1:F:220:SER:N	2.65	0.47
1:G:98:GLU:O	1:G:102:ILE:HB	2.14	0.47
1:G:164:GLU:OE1	1:G:164:GLU:HA	2.12	0.47
1:G:80:SER:OG	1:G:83:MET:HG3	2.14	0.47
1:H:151:LEU:O	1:H:155:LEU:HG	2.15	0.47
1:L:43:PRO:HB2	1:L:47:HIS:HB2	1.97	0.47
1:M:236:VAL:CG1	1:M:239:ALA:HB3	2.45	0.47
1:O:41:ILE:HG23	1:O:60:LEU:HD11	1.96	0.47
1:Q:183:PRO:HB3	1:Q:225:LEU:CD2	2.15	0.47
1:Q:85:GLN:HE22	1:Q:120:LYS:CB	2.24	0.47
1:S:4:ARG:HD3	1:S:207:GLN:O	2.14	0.47
1:D:254:LYS:HG3	1:D:255:THR:N	2.29	0.47
1:I:4:ARG:HH12	1:I:232:ASP:CG	2.17	0.47
1:I:7:PHE:O	1:I:233:GLY:HA3	2.14	0.47
1:I:37:VAL:CG1	1:I:252:LEU:CD2	2.92	0.47
1:I:83:MET:HG2	1:J:47:HIS:HE1	1.79	0.47
1:J:158:SER:HG	1:J:161:LEU:HG	1.80	0.47
1:M:90:LYS:HE3	1:M:123:THR:OG1	2.15	0.47
1:P:221:ASN:C	1:P:221:ASN:OD1	2.53	0.47
1:P:222:ASP:OD1	1:P:223:GLU:N	2.48	0.47
1:Q:73:GLY:O	1:R:14:CYS:SG	2.73	0.47
1:R:123:THR:HA	1:R:164:GLU:HB3	1.96	0.47
1:R:225:LEU:C	1:R:234:PHE:CZ	2.80	0.47
1:S:6:PRO:HD2	1:S:36:SER:O	2.14	0.47
1:A:128:VAL:HG11	1:A:148:LEU:HD13	1.97	0.47
1:K:67:VAL:O	1:K:113:LYS:HD3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:81:VAL:O	1:M:85:GLN:HG3	2.14	0.47
1:O:174:SER:HA	1:O:179:VAL:O	2.13	0.47
1:O:74:ALA:O	1:P:98:GLU:HG2	2.13	0.47
1:R:71:GLY:HA3	1:R:116:ARG:NH2	2.29	0.47
1:A:239:ALA:O	1:A:242:LYS:HG3	2.14	0.47
1:C:145:ILE:O	1:C:149:GLU:HG2	2.15	0.47
1:E:109:GLN:O	1:E:113:LYS:HG3	2.14	0.47
1:P:145:ILE:O	1:P:149:GLU:N	2.42	0.47
1:R:85:GLN:HE22	1:R:120:LYS:CB	2.28	0.47
1:R:117:ALA:HB3	1:R:124:VAL:HG21	1.96	0.47
1:T:132:LEU:O	1:T:136:LYS:HG3	2.15	0.47
1:D:132:LEU:O	1:D:136:LYS:HG3	2.15	0.47
1:K:197:PHE:HD1	1:K:206:ALA:HB2	1.80	0.47
1:K:218:ASN:OD1	1:K:244:GLU:OE1	2.32	0.47
1:L:98:GLU:O	1:L:102:ILE:HB	2.15	0.47
1:N:190:HIS:NE2	1:N:213:TYR:HB2	2.30	0.47
1:O:100:ARG:CZ	1:O:127:CYS:O	2.62	0.47
1:Q:216:SER:O	1:Q:221:ASN:ND2	2.46	0.47
1:R:174:SER:C	1:R:175:ILE:CG2	2.83	0.47
1:R:57:SER:HB2	1:R:60:LEU:HB3	1.97	0.47
1:T:84:LEU:HD22	1:T:89:LEU:HD12	1.97	0.47
1:F:175:ILE:CD1	1:F:175:ILE:N	2.68	0.47
1:I:197:PHE:HD2	1:I:206:ALA:HB2	1.80	0.47
1:L:141:MET:HB3	1:L:141:MET:HE2	1.56	0.47
1:N:100:ARG:NH2	1:N:127:CYS:O	2.45	0.47
1:N:4:ARG:NE	1:N:232:ASP:OD1	2.45	0.47
1:O:198:ALA:CA	1:O:206:ALA:HB2	2.45	0.47
1:Q:115:LYS:HG3	1:Q:155:LEU:HD23	1.96	0.47
1:R:213:TYR:O	1:R:234:PHE:HA	2.14	0.47
1:A:222:ASP:O	1:A:226:GLY:N	2.44	0.47
1:C:48:LEU:O	1:C:52:ILE:HG13	2.14	0.47
1:C:76:THR:O	1:D:99:ARG:HD2	2.15	0.47
1:E:116:ARG:CZ	1:E:120:LYS:NZ	2.78	0.47
1:E:173:TRP:O	1:E:177:THR:OG1	2.26	0.47
1:F:134:GLU:OE1	1:F:143:VAL:HG21	2.14	0.47
1:O:11:ASN:OD1	1:O:65:GLN:HG2	2.15	0.47
1:P:169:TYR:CE2	1:P:189:VAL:HG21	2.49	0.47
1:P:37:VAL:HG11	1:P:252:LEU:HD23	1.97	0.47
1:R:236:VAL:HG21	1:R:248:MET:SD	2.55	0.47
1:S:186:ALA:CB	1:S:213:TYR:CE1	2.98	0.47
1:G:69:LEU:CD1	1:G:70:GLU:CG	2.88	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:126:PHE:CE2	1:H:151:LEU:HD21	2.50	0.47
1:J:17:SER:H	1:J:20:PHE:HB3	1.79	0.47
1:K:148:LEU:CD2	1:K:193:LEU:HD22	2.45	0.47
1:N:167:ILE:O	1:N:212:ILE:N	2.41	0.47
1:N:191:VAL:CG2	1:N:230:ASN:HD22	2.22	0.47
1:N:29:ALA:HB1	1:N:57:SER:HB2	1.97	0.47
1:O:187:GLU:OE1	1:O:228:CYS:HB3	2.15	0.47
1:Q:165:VAL:C	1:Q:210:ARG:HE	2.18	0.47
1:A:2:PRO:HG2	1:A:207:GLN:HB3	1.96	0.46
1:C:15:ASN:N	1:D:83:MET:HE1	2.31	0.46
1:D:148:LEU:O	1:D:151:LEU:HB3	2.15	0.46
1:D:151:LEU:O	1:D:155:LEU:HG	2.15	0.46
1:D:222:ASP:OD1	1:D:223:GLU:N	2.48	0.46
1:G:4:ARG:HD3	1:G:207:GLN:O	2.15	0.46
1:I:196:TRP:CD1	1:I:200:LYS:HG3	2.50	0.46
1:J:254:LYS:HG3	1:J:255:THR:N	2.31	0.46
1:K:80:SER:HB3	1:L:14:CYS:SG	2.55	0.46
1:L:240:SER:HA	1:L:245:PHE:HB2	1.97	0.46
1:N:222:ASP:O	1:N:225:LEU:N	2.48	0.46
1:S:61:ARG:CG	1:S:61:ARG:HH11	2.11	0.46
1:B:184:GLU:N	1:B:184:GLU:OE1	2.48	0.46
1:C:198:ALA:HA	1:C:203:ALA:HA	1.97	0.46
1:I:4:ARG:HH12	1:I:194:ARG:HH21	1.63	0.46
1:J:251:ILE:HA	1:J:254:LYS:NZ	2.30	0.46
1:P:192:GLY:O	1:P:195:LYS:HB3	2.16	0.46
1:Q:223:GLU:HB2	1:Q:251:ILE:HD11	1.97	0.46
1:Q:95:GLY:C	1:Q:127:CYS:HB2	2.36	0.46
1:A:197:PHE:HD1	1:A:206:ALA:HB2	1.81	0.46
1:D:37:VAL:HG11	1:D:252:LEU:HD21	1.96	0.46
1:E:183:PRO:HG2	1:E:224:LYS:CE	2.45	0.46
1:Q:186:ALA:HB1	1:Q:213:TYR:CD1	2.51	0.46
1:Q:4:ARG:NH2	1:Q:229:PRO:O	2.47	0.46
1:Q:69:LEU:HD12	1:Q:113:LYS:HG3	1.98	0.46
1:S:130:GLU:OE2	1:S:169:TYR:OH	2.30	0.46
1:S:196:TRP:O	1:S:200:LYS:HG2	2.15	0.46
1:T:218:ASN:N	1:T:218:ASN:HD22	2.13	0.46
1:B:128:VAL:HG21	1:B:144:ASN:ND2	2.31	0.46
1:C:171:PRO:CD	1:C:214:GLY:O	2.63	0.46
1:C:18:LEU:HA	1:C:18:LEU:HD23	1.77	0.46
1:F:197:PHE:CZ	1:F:201:VAL:HG11	2.50	0.46
1:K:41:ILE:O	1:K:43:PRO:HD3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:155:LEU:HD23	1:L:155:LEU:HA	1.75	0.46
1:N:9:GLY:HA2	1:N:40:VAL:O	2.15	0.46
1:O:221:ASN:HA	1:O:224:LYS:HZ1	1.80	0.46
1:Q:71:GLY:O	1:Q:75:TRP:NE1	2.35	0.46
1:A:145:ILE:O	1:A:149:GLU:N	2.42	0.46
1:C:177:THR:OG1	1:C:179:VAL:HG13	2.16	0.46
1:H:111:ALA:HB2	1:H:151:LEU:HD12	1.97	0.46
1:I:4:ARG:NH1	1:I:232:ASP:CG	2.69	0.46
1:J:99:ARG:HA	1:J:103:MET:HB2	1.96	0.46
1:N:81:VAL:HG13	1:N:122:MET:SD	2.56	0.46
1:Q:201:VAL:CG1	1:Q:202:ALA:H	2.26	0.46
1:C:69:LEU:H	1:C:69:LEU:CD2	2.26	0.46
1:D:48:LEU:O	1:D:52:ILE:HG13	2.15	0.46
1:E:11:ASN:OD1	1:E:65:GLN:HG2	2.15	0.46
1:F:135:ARG:HE	1:F:135:ARG:HB2	1.58	0.46
1:F:171:PRO:HB2	1:F:174:SER:OG	2.14	0.46
1:G:114:ALA:HB3	1:G:151:LEU:HD13	1.97	0.46
1:G:135:ARG:HB2	1:G:135:ARG:HE	1.55	0.46
1:I:224:LYS:O	1:I:227:GLN:HB2	2.16	0.46
1:K:72:ASN:HA	1:L:14:CYS:O	2.16	0.46
1:L:184:GLU:CD	1:L:184:GLU:H	2.19	0.46
1:M:98:GLU:HG3	1:M:102:ILE:HD12	1.97	0.46
1:O:222:ASP:HA	1:O:225:LEU:HB2	1.96	0.46
1:Q:186:ALA:CB	1:Q:213:TYR:CE1	2.99	0.46
1:R:2:PRO:HB3	1:R:207:GLN:CG	2.41	0.46
1:S:158:SER:CB	1:S:161:LEU:HD23	2.30	0.46
1:S:84:LEU:O	1:S:89:LEU:HB2	2.15	0.46
1:T:243:PRO:HA	1:T:246:MET:HE1	1.98	0.46
1:D:161:LEU:C	1:D:163:LYS:H	2.19	0.46
1:I:218:ASN:O	1:I:222:ASP:CB	2.61	0.46
1:L:251:ILE:O	1:L:254:LYS:HG2	2.16	0.46
1:K:76:THR:HG22	1:L:98:GLU:HB2	1.98	0.46
1:N:29:ALA:CB	1:N:57:SER:HB2	2.46	0.46
1:Q:148:LEU:HA	1:Q:148:LEU:HD13	1.73	0.46
1:R:127:CYS:HA	1:R:168:ALA:O	2.16	0.46
1:T:180:VAL:CG2	1:T:181:ALA:N	2.78	0.46
1:A:72:ASN:H	1:A:72:ASN:HD22	1.63	0.46
1:E:90:LYS:HE2	1:E:91:HIS:CE1	2.51	0.46
1:L:141:MET:CE	1:L:141:MET:CA	2.94	0.46
1:O:213:TYR:CE2	1:O:215:GLY:O	2.69	0.46
1:O:40:VAL:HG11	1:O:63:ALA:HB2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:137:ALA:HA	1:P:137:ALA:HA	1.97	0.46
1:Q:210:ARG:N	1:Q:210:ARG:CD	2.67	0.46
1:R:182:THR:OG1	1:R:185:GLN:HG3	2.15	0.46
1:S:164:GLU:OE1	1:S:164:GLU:HA	2.15	0.46
1:T:155:LEU:HD13	1:T:161:LEU:HB2	1.96	0.46
1:T:213:TYR:O	1:T:234:PHE:HA	2.16	0.46
1:T:39:VAL:HG12	1:T:60:LEU:HD13	1.97	0.46
1:T:63:ALA:CB	1:T:91:HIS:HB2	2.41	0.46
1:E:236:VAL:HG11	1:E:239:ALA:HB3	1.97	0.46
1:F:111:ALA:HB1	1:F:151:LEU:HA	1.96	0.46
1:H:111:ALA:HA	1:H:151:LEU:HG	1.97	0.46
1:N:244:GLU:O	1:N:248:MET:CG	2.64	0.46
1:O:198:ALA:HA	1:O:206:ALA:HB2	1.97	0.46
1:O:21:ILE:HG13	1:O:47:HIS:HB3	1.98	0.46
1:P:187:GLU:OE1	1:P:228:CYS:HB3	2.15	0.46
1:Q:75:TRP:NE1	1:R:14:CYS:SG	2.82	0.46
1:R:161:LEU:C	1:R:163:LYS:N	2.68	0.46
1:S:61:ARG:NH2	1:S:90:LYS:HB2	2.31	0.46
1:C:196:TRP:NE1	1:C:200:LYS:HG3	2.30	0.46
1:C:244:GLU:O	1:C:248:MET:HG3	2.16	0.46
1:G:224:LYS:HB3	1:G:224:LYS:HE3	1.33	0.46
1:J:218:ASN:N	1:J:218:ASN:OD1	2.49	0.46
1:L:244:GLU:HA	1:L:244:GLU:OE1	2.16	0.46
1:M:181:ALA:HB3	1:M:213:TYR:OH	2.16	0.46
1:N:140:THR:HG22	1:N:141:MET:N	2.29	0.46
1:P:134:GLU:CD	1:P:143:VAL:HG21	2.37	0.46
1:R:250:ASP:O	1:R:253:THR:HG23	2.16	0.46
1:S:198:ALA:HB2	1:S:206:ALA:CB	2.46	0.46
1:S:213:TYR:HB2	1:S:231:ILE:HD13	1.98	0.46
1:T:187:GLU:OE2	1:T:191:VAL:HG23	2.16	0.46
1:A:218:ASN:H	1:A:222:ASP:CG	2.18	0.45
1:B:109:GLN:O	1:B:113:LYS:HG3	2.16	0.45
1:B:9:GLY:HA2	1:B:40:VAL:O	2.16	0.45
1:D:158:SER:CB	1:D:160:MET:HE1	2.46	0.45
1:E:136:LYS:HE2	1:E:136:LYS:HB3	1.79	0.45
1:G:128:VAL:HG11	1:G:148:LEU:HD13	1.98	0.45
1:G:76:THR:HG22	1:H:65:GLN:HB3	1.96	0.45
1:H:197:PHE:HB3	1:H:206:ALA:HB2	1.99	0.45
1:N:114:ALA:O	1:N:118:LEU:HG	2.17	0.45
1:O:196:TRP:CE3	1:O:197:PHE:N	2.84	0.45
1:P:204:GLU:O	1:P:208:HIS:CE1	2.69	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:15:ASN:OD1	1:T:72:ASN:HB3	2.15	0.45
1:T:197:PHE:CD1	1:T:201:VAL:HG21	2.50	0.45
1:A:81:VAL:O	1:A:85:GLN:HG3	2.16	0.45
1:B:114:ALA:HB2	1:B:126:PHE:CE1	2.51	0.45
1:G:221:ASN:O	1:G:224:LYS:HB2	2.17	0.45
1:J:137:ALA:O	1:J:138:ASN:HB2	2.17	0.45
1:K:159:LYS:O	1:K:160:MET:HB3	2.14	0.45
1:K:198:ALA:HB2	1:K:206:ALA:CB	2.46	0.45
1:M:34:PRO:HG3	1:M:253:THR:HG21	1.99	0.45
1:M:34:PRO:HB2	1:M:36:SER:OG	2.16	0.45
1:N:72:ASN:ND2	1:N:80:SER:OG	2.50	0.45
1:O:240:SER:HA	1:O:245:PHE:CD1	2.51	0.45
1:O:81:VAL:O	1:O:85:GLN:HG3	2.15	0.45
1:Q:251:ILE:HG23	1:Q:252:LEU:N	2.31	0.45
1:T:118:LEU:CD1	1:T:155:LEU:HD11	2.46	0.45
1:A:13:LYS:HG2	1:B:76:THR:OG1	2.16	0.45
1:E:171:PRO:HG3	1:E:213:TYR:HE1	1.80	0.45
1:F:228:CYS:HA	1:F:229:PRO:HD3	1.83	0.45
1:G:190:HIS:ND1	1:G:231:ILE:HG12	2.31	0.45
1:J:158:SER:OG	1:J:161:LEU:HG	2.16	0.45
1:L:196:TRP:O	1:L:200:LYS:N	2.45	0.45
1:M:24:HIS:O	1:M:28:ILE:HG13	2.15	0.45
1:N:17:SER:O	1:N:21:ILE:HG12	2.17	0.45
1:O:210:ARG:HB2	1:O:210:ARG:HE	1.68	0.45
1:P:159:LYS:O	1:P:162:TRP:CD1	2.69	0.45
1:P:164:GLU:OE1	1:P:164:GLU:HA	2.15	0.45
1:P:4:ARG:HD2	1:P:207:GLN:O	2.15	0.45
1:P:5:ARG:NH1	1:P:35:ASP:O	2.43	0.45
1:Q:5:ARG:HA	1:Q:6:PRO:HD2	1.61	0.45
1:T:18:LEU:O	1:T:22:LYS:HG3	2.17	0.45
1:C:71:GLY:O	1:C:75:TRP:NE1	2.49	0.45
1:E:151:LEU:O	1:E:155:LEU:HG	2.17	0.45
1:E:228:CYS:HB2	1:E:231:ILE:HD12	1.99	0.45
1:I:233:GLY:HA2	1:I:252:LEU:HD11	1.95	0.45
1:K:221:ASN:C	1:K:221:ASN:HD22	2.20	0.45
1:L:37:VAL:HG11	1:L:252:LEU:HD23	1.98	0.45
1:Q:218:ASN:N	1:Q:218:ASN:HD22	2.14	0.45
1:F:12:PHE:CD1	1:F:12:PHE:N	2.85	0.45
1:G:155:LEU:HD12	1:G:162:TRP:NE1	2.31	0.45
1:I:139:ARG:NH1	1:I:142:GLU:OE1	2.49	0.45
1:I:68:TYR:CE2	1:I:70:GLU:HG3	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:171:PRO:HB2	1:J:174:SER:OG	2.17	0.45
1:K:83:MET:O	1:K:87:MET:HG3	2.17	0.45
1:L:131:THR:HA	1:L:172:VAL:HB	1.99	0.45
1:R:190:HIS:NE2	1:R:231:ILE:HD13	2.31	0.45
1:S:141:MET:HE1	1:S:193:LEU:HD23	1.99	0.45
1:S:171:PRO:HD3	1:S:214:GLY:O	2.17	0.45
1:T:45:ALA:HA	1:T:48:LEU:HD22	1.98	0.45
1:C:196:TRP:CD1	1:C:200:LYS:HG3	2.52	0.45
1:J:18:LEU:O	1:J:22:LYS:HG3	2.16	0.45
1:K:13:LYS:HD3	1:L:74:ALA:HA	1.99	0.45
1:M:228:CYS:HB2	1:M:231:ILE:CG1	2.46	0.45
1:P:194:ARG:NE	1:P:230:ASN:HD22	2.14	0.45
1:P:45:ALA:HA	1:P:48:LEU:HD22	1.98	0.45
1:Q:217:ALA:HA	1:Q:221:ASN:HD21	1.80	0.45
1:Q:12:PHE:HB2	1:Q:43:PRO:HA	1.99	0.45
1:R:221:ASN:N	1:R:221:ASN:OD1	2.50	0.45
1:S:194:ARG:HD3	1:S:206:ALA:O	2.16	0.45
1:S:2:PRO:CD	1:S:207:GLN:HB2	2.47	0.45
1:S:7:PHE:HD1	1:S:7:PHE:C	2.19	0.45
1:B:5:ARG:NH2	1:B:38:ASP:OD1	2.48	0.45
1:D:96:HIS:CE1	1:D:98:GLU:CD	2.90	0.45
1:E:97:SER:CB	1:E:170:GLU:OE1	2.64	0.45
1:M:155:LEU:HD12	1:M:162:TRP:NE1	2.31	0.45
1:Q:46:VAL:CG2	1:Q:47:HIS:CD2	2.98	0.45
1:Q:74:ALA:HB1	1:R:98:GLU:OE2	2.17	0.45
1:Q:91:HIS:HA	1:Q:123:THR:O	2.16	0.45
1:S:171:PRO:CD	1:S:214:GLY:O	2.64	0.45
1:T:184:GLU:OE1	1:T:184:GLU:N	2.49	0.45
1:A:36:SER:HB3	1:G:160:MET:CE	2.47	0.45
1:D:251:ILE:HA	1:D:254:LYS:HG2	1.98	0.45
1:F:177:THR:CG2	1:F:177:THR:O	2.63	0.45
1:F:184:GLU:CD	1:F:184:GLU:H	2.20	0.45
1:G:77:GLY:HA3	1:H:99:ARG:NH1	2.31	0.45
1:H:83:MET:O	1:H:87:MET:HG3	2.17	0.45
1:L:136:LYS:C	1:L:138:ASN:N	2.69	0.45
1:L:193:LEU:O	1:L:196:TRP:HB3	2.16	0.45
1:M:228:CYS:HA	1:M:229:PRO:HD3	1.82	0.45
1:O:97:SER:CB	1:O:170:GLU:OE1	2.64	0.45
1:Q:72:ASN:ND2	1:Q:80:SER:OG	2.50	0.45
1:Q:75:TRP:HD1	1:R:14:CYS:SG	2.29	0.45
1:T:128:VAL:HG11	1:T:148:LEU:HD13	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:HIS:CD2	1:A:123:THR:HB	2.52	0.45
1:A:160:MET:N	1:A:160:MET:HE3	2.32	0.45
1:B:217:ALA:HB1	1:B:222:ASP:OD2	2.17	0.45
1:G:166:VAL:HG13	1:G:210:ARG:HB3	1.98	0.45
1:R:68:TYR:CZ	1:R:69:LEU:HD21	2.52	0.45
1:S:101:ARG:N	1:S:101:ARG:HD3	2.31	0.45
1:S:106:THR:HG23	1:S:109:GLN:CD	2.37	0.45
1:S:95:GLY:C	1:S:127:CYS:HB2	2.37	0.45
1:S:163:LYS:HG2	1:S:164:GLU:HG2	1.98	0.45
1:S:8:ILE:HG22	1:S:252:LEU:CD2	2.47	0.45
1:C:68:TYR:CE2	1:C:70:GLU:HG3	2.52	0.45
1:F:175:ILE:HG12	1:F:215:GLY:HA2	1.98	0.45
1:G:90:LYS:HB3	1:G:91:HIS:CE1	2.52	0.45
1:I:180:VAL:HG23	1:I:181:ALA:N	2.30	0.45
1:I:6:PRO:HB2	1:I:37:VAL:HG13	1.98	0.45
1:I:9:GLY:HA2	1:I:40:VAL:O	2.16	0.45
1:J:243:PRO:HA	1:J:246:MET:CE	2.46	0.45
1:M:210:ARG:HG3	1:M:232:ASP:OD2	2.16	0.45
1:N:244:GLU:O	1:N:248:MET:HG3	2.17	0.45
1:P:67:VAL:HB	1:P:92:VAL:HG21	1.99	0.45
1:S:190:HIS:CE1	1:S:213:TYR:HB2	2.52	0.45
1:D:145:ILE:HG23	1:D:149:GLU:OE2	2.17	0.44
1:H:145:ILE:O	1:H:149:GLU:HG2	2.17	0.44
1:P:200:LYS:HG2	1:P:200:LYS:O	2.17	0.44
1:Q:171:PRO:HB2	1:Q:174:SER:HG	1.83	0.44
1:Q:4:ARG:HD2	1:Q:232:ASP:CG	2.37	0.44
1:S:187:GLU:OE2	1:S:229:PRO:HG2	2.17	0.44
1:B:190:HIS:ND1	1:B:231:ILE:HG12	2.32	0.44
1:H:111:ALA:HB1	1:H:151:LEU:HA	1.98	0.44
1:H:163:LYS:HG3	1:H:163:LYS:H	1.44	0.44
1:I:68:TYR:HB2	1:I:78:GLU:HB3	2.00	0.44
1:L:58:LYS:HD2	1:L:58:LYS:O	2.16	0.44
1:N:139:ARG:HB3	1:N:139:ARG:NH1	2.24	0.44
1:N:33:ILE:O	1:N:59:GLN:HG2	2.17	0.44
1:R:183:PRO:HG2	1:R:224:LYS:CD	2.40	0.44
1:T:227:GLN:N	1:T:227:GLN:OE1	2.50	0.44
1:A:187:GLU:HB2	1:A:228:CYS:SG	2.57	0.44
1:B:201:VAL:O	1:B:202:ALA:HB2	2.17	0.44
1:C:82:GLU:OE1	1:C:116:ARG:NH1	2.51	0.44
1:D:197:PHE:O	1:D:201:VAL:HB	2.17	0.44
1:G:11:ASN:OD1	1:G:65:GLN:HG2	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:9:GLY:C	1:G:235:LEU:HD12	2.37	0.44
1:H:247:THR:O	1:H:251:ILE:HG13	2.16	0.44
1:I:200:LYS:HE2	1:I:200:LYS:HB3	1.55	0.44
1:I:96:HIS:CE1	1:I:98:GLU:OE1	2.70	0.44
1:K:84:LEU:HD22	1:K:89:LEU:HD12	2.00	0.44
1:N:184:GLU:CD	1:N:184:GLU:H	2.21	0.44
1:N:58:LYS:O	1:N:58:LYS:HG2	2.17	0.44
1:O:81:VAL:HG11	1:O:120:LYS:HD3	1.99	0.44
1:O:139:ARG:HB3	1:O:142:GLU:HB3	1.99	0.44
1:P:218:ASN:O	1:P:222:ASP:HB3	2.18	0.44
1:R:187:GLU:OE1	1:R:187:GLU:HA	2.17	0.44
1:S:245:PHE:HA	1:S:248:MET:HG3	1.99	0.44
1:T:8:ILE:HB	1:T:252:LEU:HD22	1.98	0.44
1:G:4:ARG:HB2	1:G:4:ARG:HE	1.40	0.44
1:L:218:ASN:N	1:L:221:ASN:ND2	2.39	0.44
1:O:67:VAL:O	1:O:113:LYS:HD3	2.17	0.44
1:R:195:LYS:HB3	1:R:195:LYS:HE3	1.82	0.44
1:T:194:ARG:NH1	1:T:206:ALA:O	2.49	0.44
1:T:57:SER:HB3	1:T:60:LEU:HB3	1.99	0.44
1:D:140:THR:HG22	1:D:141:MET:N	2.32	0.44
1:D:226:GLY:C	1:D:255:THR:HG21	2.38	0.44
1:E:69:LEU:HD12	1:E:112:LYS:CB	2.47	0.44
1:I:194:ARG:NH1	1:I:211:ILE:HG13	2.33	0.44
1:M:145:ILE:CG1	1:M:196:TRP:CD1	3.01	0.44
1:M:166:VAL:HG22	1:M:210:ARG:HB3	2.00	0.44
1:O:65:GLN:HB3	1:P:76:THR:HG23	1.99	0.44
1:P:130:GLU:O	1:P:172:VAL:HB	2.17	0.44
1:A:140:THR:O	1:A:144:ASN:ND2	2.50	0.44
1:D:5:ARG:HA	1:D:6:PRO:HD3	1.86	0.44
1:G:145:ILE:HG23	1:G:196:TRP:NE1	2.32	0.44
1:G:160:MET:H	1:G:160:MET:HG3	1.33	0.44
1:L:140:THR:O	1:L:144:ASN:ND2	2.50	0.44
1:P:149:GLU:OE1	1:P:200:LYS:CE	2.65	0.44
1:P:171:PRO:HD2	1:P:214:GLY:O	2.18	0.44
1:R:222:ASP:OD1	1:R:223:GLU:N	2.50	0.44
1:A:91:HIS:HA	1:A:123:THR:O	2.17	0.44
1:D:106:THR:OG1	1:D:109:GLN:HG3	2.18	0.44
1:E:24:HIS:O	1:E:27:ALA:HB3	2.17	0.44
1:E:174:SER:O	1:I:176:GLY:CA	2.65	0.44
1:I:190:HIS:CE1	1:I:211:ILE:HG22	2.52	0.44
1:J:173:TRP:HH2	1:J:185:GLN:OE1	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:242:LYS:HE2	1:K:242:LYS:HB3	1.68	0.44
1:O:41:ILE:O	1:O:43:PRO:HD3	2.18	0.44
1:P:251:ILE:HD12	1:P:251:ILE:N	2.33	0.44
1:D:172:VAL:HA	1:D:175:ILE:HG12	2.00	0.44
1:E:116:ARG:NH1	1:E:120:LYS:HZ3	2.16	0.44
1:E:44:SER:O	1:E:48:LEU:HD22	2.18	0.44
1:G:28:ILE:HD13	1:G:245:PHE:CD2	2.52	0.44
1:G:74:ALA:HB1	1:H:98:GLU:OE2	2.17	0.44
1:J:91:HIS:CD2	1:J:123:THR:HB	2.53	0.44
1:J:246:MET:HA	1:J:249:ILE:HD12	1.99	0.44
1:K:160:MET:HA	1:K:163:LYS:HZ2	1.83	0.44
1:L:5:ARG:HE	1:L:38:ASP:CG	2.21	0.44
1:M:83:MET:HE2	1:N:44:SER:HB2	2.00	0.44
1:P:177:THR:HG21	1:P:179:VAL:HG22	1.98	0.44
1:A:13:LYS:H	1:A:65:GLN:NE2	2.16	0.44
1:A:167:ILE:HB	1:A:211:ILE:HG23	1.99	0.44
1:B:144:ASN:HD22	1:B:193:LEU:HD21	1.83	0.44
1:C:174:SER:HA	1:C:177:THR:HG1	1.83	0.44
1:D:9:GLY:HA2	1:D:40:VAL:O	2.18	0.44
1:E:184:GLU:N	1:E:184:GLU:OE1	2.51	0.44
1:E:45:ALA:HA	1:E:48:LEU:HD21	1.95	0.44
1:H:94:VAL:HG11	1:H:114:ALA:HB2	2.00	0.44
1:H:148:LEU:HA	1:H:148:LEU:HD12	1.80	0.44
1:J:96:HIS:HA	1:J:127:CYS:HB2	2.00	0.44
1:L:37:VAL:HG13	1:L:252:LEU:HD23	2.00	0.44
1:O:63:ALA:HB2	1:O:91:HIS:HB2	1.99	0.44
1:P:5:ARG:HE	1:P:38:ASP:CG	2.21	0.44
1:B:82:GLU:OE2	1:B:116:ARG:NH2	2.45	0.43
1:C:221:ASN:HD22	1:C:221:ASN:N	2.14	0.43
1:C:222:ASP:OD1	1:C:223:GLU:N	2.51	0.43
1:F:197:PHE:O	1:F:201:VAL:N	2.50	0.43
1:F:212:ILE:CD1	1:F:235:LEU:HB2	2.48	0.43
1:F:52:ILE:HA	1:F:62:ILE:HD13	2.00	0.43
1:L:180:VAL:CG2	1:L:181:ALA:N	2.81	0.43
1:M:98:GLU:HA	1:M:102:ILE:HD12	2.00	0.43
1:N:218:ASN:ND2	1:N:221:ASN:ND2	2.65	0.43
1:N:45:ALA:HA	1:N:48:LEU:CD2	2.45	0.43
1:P:190:HIS:ND1	1:P:231:ILE:HG12	2.33	0.43
1:Q:229:PRO:HB2	1:Q:230:ASN:HD22	1.82	0.43
1:Q:70:GLU:HB2	1:Q:75:TRP:CE2	2.53	0.43
1:T:66:ASN:HD21	1:T:113:LYS:NZ	2.16	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:CYS:HB3	1:A:170:GLU:OE2	2.18	0.43
1:D:221:ASN:O	1:D:224:LYS:HG3	2.18	0.43
1:D:7:PHE:O	1:D:233:GLY:HA3	2.18	0.43
1:E:46:VAL:HG23	1:E:47:HIS:CD2	2.53	0.43
1:E:80:SER:HG	1:E:83:MET:H	1.66	0.43
1:I:5:ARG:HA	1:I:6:PRO:HD3	1.86	0.43
1:M:21:ILE:HG13	1:M:47:HIS:HB3	2.00	0.43
1:N:218:ASN:HD22	1:N:221:ASN:ND2	2.16	0.43
1:P:81:VAL:HG21	1:P:117:ALA:HA	1.99	0.43
1:Q:31:HIS:CE1	1:Q:246:MET:HB3	2.52	0.43
1:Q:4:ARG:NH1	1:Q:194:ARG:CZ	2.81	0.43
1:Q:72:ASN:HA	1:R:14:CYS:O	2.17	0.43
1:T:39:VAL:HG12	1:T:60:LEU:CD1	2.48	0.43
1:E:130:GLU:CD	1:E:140:THR:HB	2.39	0.43
1:E:239:ALA:HA	1:E:242:LYS:HE3	2.01	0.43
1:I:77:GLY:HA3	1:J:99:ARG:HH11	1.83	0.43
1:M:128:VAL:HG12	1:M:147:GLN:HB2	1.99	0.43
1:N:222:ASP:OD2	1:N:248:MET:HE3	2.19	0.43
1:B:172:VAL:O	1:O:176:GLY:HA2	2.18	0.43
1:O:40:VAL:CG1	1:O:63:ALA:HB2	2.47	0.43
1:O:97:SER:HB3	1:O:170:GLU:OE1	2.18	0.43
1:P:81:VAL:HG13	1:P:122:MET:SD	2.58	0.43
1:Q:183:PRO:HG2	1:Q:224:LYS:HD3	2.00	0.43
1:Q:64:ALA:N	1:Q:89:LEU:HD21	2.33	0.43
1:S:67:VAL:HG23	1:S:79:THR:HG22	2.01	0.43
1:A:252:LEU:HA	1:A:252:LEU:HD12	1.78	0.43
1:D:151:LEU:HD23	1:D:162:TRP:CH2	2.53	0.43
1:I:228:CYS:HA	1:I:229:PRO:HD2	1.91	0.43
1:I:48:LEU:CD2	1:I:89:LEU:HD11	2.48	0.43
1:K:13:LYS:HG2	1:L:76:THR:OG1	2.18	0.43
1:L:40:VAL:HG11	1:L:63:ALA:HB2	1.99	0.43
1:O:100:ARG:NH1	1:O:147:GLN:CD	2.72	0.43
1:O:182:THR:HG23	1:O:185:GLN:NE2	2.33	0.43
1:O:197:PHE:HE2	1:O:205:GLY:O	2.00	0.43
1:S:143:VAL:O	1:S:147:GLN:HG3	2.18	0.43
1:A:151:LEU:O	1:A:155:LEU:HG	2.19	0.43
1:E:183:PRO:HG2	1:E:224:LYS:HE2	2.01	0.43
1:F:118:LEU:HB3	1:F:161:LEU:HD22	2.00	0.43
1:F:80:SER:OG	1:F:83:MET:HG3	2.19	0.43
1:I:182:THR:OG1	1:I:185:GLN:HG3	2.19	0.43
1:I:197:PHE:CD2	1:I:206:ALA:HA	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:69:LEU:HD22	1:J:113:LYS:HE2	2.00	0.43
1:J:166:VAL:HG13	1:J:210:ARG:HB3	1.99	0.43
1:K:40:VAL:HA	1:K:61:ARG:O	2.18	0.43
1:M:167:ILE:O	1:M:211:ILE:HA	2.18	0.43
1:M:63:ALA:HB2	1:M:91:HIS:HB2	2.00	0.43
1:O:181:ALA:HB3	1:O:213:TYR:OH	2.18	0.43
1:Q:166:VAL:CG2	1:Q:210:ARG:NH2	2.81	0.43
1:Q:7:PHE:HE1	1:Q:38:ASP:OD1	2.02	0.43
1:R:214:GLY:HA2	1:R:235:LEU:HB3	2.00	0.43
1:T:111:ALA:HB1	1:T:151:LEU:HA	2.01	0.43
1:T:180:VAL:HG22	1:T:181:ALA:N	2.34	0.43
1:B:144:ASN:HD22	1:B:193:LEU:HD22	1.83	0.43
1:B:21:ILE:O	1:B:25:VAL:HG23	2.19	0.43
1:E:155:LEU:HD12	1:E:162:TRP:NE1	2.33	0.43
1:E:251:ILE:O	1:E:254:LYS:HG2	2.18	0.43
1:H:94:VAL:HG12	1:H:126:PHE:CD1	2.54	0.43
1:L:117:ALA:O	1:L:122:MET:HB2	2.18	0.43
1:L:246:MET:HA	1:L:249:ILE:HD12	1.99	0.43
1:M:223:GLU:O	1:M:227:GLN:HG3	2.19	0.43
1:O:100:ARG:HH11	1:O:147:GLN:NE2	2.17	0.43
1:P:151:LEU:HD12	1:P:155:LEU:HG	2.01	0.43
1:Q:189:VAL:O	1:Q:193:LEU:HG	2.19	0.43
1:Q:81:VAL:HG11	1:Q:117:ALA:HA	2.01	0.43
1:R:184:GLU:OE1	1:R:224:LYS:NZ	2.48	0.43
1:S:24:HIS:NE2	1:S:241:LEU:HA	2.34	0.43
1:B:197:PHE:HD2	1:B:206:ALA:HB2	1.83	0.43
1:F:82:GLU:H	1:F:82:GLU:HG2	1.41	0.43
1:G:221:ASN:HA	1:G:224:LYS:HG3	2.00	0.43
1:I:115:LYS:HD2	1:I:154:GLU:O	2.18	0.43
1:J:69:LEU:H	1:J:69:LEU:CD2	2.27	0.43
1:L:189:VAL:O	1:L:193:LEU:HG	2.19	0.43
1:N:134:GLU:OE1	1:N:143:VAL:HG11	2.19	0.43
1:P:83:MET:O	1:P:87:MET:HG3	2.18	0.43
1:Q:85:GLN:NE2	1:Q:120:LYS:O	2.52	0.43
1:S:39:VAL:HG12	1:S:60:LEU:CD1	2.47	0.43
1:A:172:VAL:HA	1:A:175:ILE:HD12	1.95	0.43
1:C:160:MET:O	1:C:163:LYS:HB2	2.19	0.43
1:C:78:GLU:HA	1:C:78:GLU:OE1	2.19	0.43
1:K:135:ARG:HB2	1:K:135:ARG:HE	1.58	0.43
1:L:250:ASP:O	1:L:254:LYS:HE3	2.19	0.43
1:M:210:ARG:HE	1:M:210:ARG:HB2	1.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:14:CYS:SG	1:R:80:SER:HB3	2.59	0.43
1:Q:16:GLY:O	1:Q:47:HIS:HE1	2.01	0.43
1:Q:77:GLY:H	1:R:65:GLN:NE2	2.17	0.43
1:T:127:CYS:HB3	1:T:170:GLU:OE2	2.19	0.43
1:T:99:ARG:HE	1:T:99:ARG:HB3	1.52	0.43
1:B:130:GLU:O	1:B:172:VAL:HB	2.19	0.43
1:C:195:LYS:HB2	1:C:195:LYS:HE3	1.76	0.43
1:F:151:LEU:HD23	1:F:162:TRP:CH2	2.54	0.43
1:J:132:LEU:HA	1:J:173:TRP:HB3	2.01	0.43
1:M:71:GLY:O	1:M:75:TRP:NE1	2.52	0.43
1:N:13:LYS:O	1:N:15:ASN:N	2.51	0.43
1:N:250:ASP:O	1:N:253:THR:HB	2.19	0.43
1:O:4:ARG:HD2	1:O:209:ILE:O	2.18	0.43
1:P:12:PHE:N	1:P:12:PHE:CD1	2.87	0.43
1:Q:33:ILE:HB	1:Q:59:GLN:NE2	2.34	0.43
1:R:187:GLU:OE2	1:R:229:PRO:HB2	2.18	0.43
1:S:10:GLY:HA2	1:S:236:VAL:HB	2.00	0.43
1:S:2:PRO:HG2	1:S:207:GLN:HB2	2.01	0.43
1:T:157:GLU:OE1	1:T:157:GLU:CA	2.67	0.43
1:D:37:VAL:HG11	1:D:252:LEU:HD23	2.00	0.43
1:D:55:ASN:HD22	1:D:62:ILE:HD12	1.84	0.43
1:E:42:ALA:O	1:E:65:GLN:NE2	2.45	0.43
1:F:90:LYS:HE2	1:F:123:THR:OG1	2.19	0.43
1:F:198:ALA:HA	1:F:202:ALA:O	2.18	0.43
1:G:4:ARG:HD2	1:G:194:ARG:HH12	1.82	0.43
1:J:71:GLY:O	1:J:75:TRP:NE1	2.49	0.43
1:K:154:GLU:HA	1:K:154:GLU:OE1	2.19	0.43
1:K:93:ILE:HG12	1:K:125:ILE:HD12	2.01	0.43
1:O:83:MET:HE1	1:P:14:CYS:C	2.40	0.43
1:Q:69:LEU:HD12	1:Q:113:LYS:HE2	2.01	0.43
1:R:91:HIS:HA	1:R:123:THR:O	2.18	0.43
1:S:155:LEU:CG	1:S:161:LEU:HD11	2.46	0.43
1:S:246:MET:H	1:S:246:MET:HE3	1.83	0.43
1:T:118:LEU:HD13	1:T:155:LEU:CD1	2.49	0.43
1:T:115:LYS:CD	1:T:155:LEU:HD21	2.39	0.43
1:B:162:TRP:HA	1:B:165:VAL:HG23	2.00	0.42
1:B:37:VAL:HG13	1:B:252:LEU:HD23	2.01	0.42
1:B:37:VAL:HG11	1:B:252:LEU:HD23	2.01	0.42
1:D:148:LEU:HA	1:D:148:LEU:HD12	1.72	0.42
1:E:115:LYS:NZ	1:E:154:GLU:O	2.49	0.42
1:F:12:PHE:O	1:F:15:ASN:ND2	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:148:LEU:CD2	1:H:193:LEU:HD22	2.49	0.42
1:H:204:GLU:HG3	1:H:204:GLU:O	2.18	0.42
1:I:4:ARG:NH1	1:I:4:ARG:HG2	2.22	0.42
1:K:7:PHE:CD1	1:K:7:PHE:C	2.93	0.42
1:L:115:LYS:O	1:L:119:GLU:HG3	2.19	0.42
1:L:71:GLY:O	1:L:75:TRP:NE1	2.52	0.42
1:N:142:GLU:HG3	1:N:143:VAL:N	2.32	0.42
1:N:221:ASN:O	1:N:223:GLU:N	2.52	0.42
1:P:118:LEU:HD13	1:P:161:LEU:O	2.19	0.42
1:P:15:ASN:ND2	1:P:15:ASN:N	2.56	0.42
1:R:66:ASN:ND2	1:R:99:ARG:CZ	2.82	0.42
1:S:13:LYS:O	1:S:65:GLN:NE2	2.50	0.42
1:S:141:MET:CE	1:S:193:LEU:HD23	2.49	0.42
1:A:246:MET:O	1:A:249:ILE:HB	2.19	0.42
1:D:97:SER:O	1:D:101:ARG:HB2	2.18	0.42
1:E:84:LEU:HD22	1:E:89:LEU:HD12	2.00	0.42
1:I:114:ALA:O	1:I:118:LEU:HG	2.19	0.42
1:N:221:ASN:OD1	1:N:222:ASP:OD1	2.36	0.42
1:O:246:MET:O	1:O:249:ILE:HB	2.18	0.42
1:P:177:THR:O	1:P:179:VAL:N	2.46	0.42
1:Q:91:HIS:CD2	1:Q:123:THR:CG2	3.02	0.42
1:R:181:ALA:HA	1:R:185:GLN:OE1	2.19	0.42
1:R:197:PHE:CD2	1:R:206:ALA:HA	2.54	0.42
1:S:92:VAL:HG13	1:S:124:VAL:HG22	1.97	0.42
1:S:128:VAL:HG12	1:S:147:GLN:HB2	1.99	0.42
1:S:8:ILE:HG23	1:S:39:VAL:HG22	2.01	0.42
1:T:115:LYS:O	1:T:119:GLU:HG3	2.19	0.42
1:T:11:ASN:HD21	1:T:13:LYS:HG3	1.84	0.42
1:T:149:GLU:O	1:T:153:LYS:HB3	2.19	0.42
1:T:8:ILE:HG22	1:T:39:VAL:HG22	2.01	0.42
1:E:71:GLY:O	1:E:72:ASN:C	2.54	0.42
1:I:116:ARG:O	1:I:120:LYS:HG3	2.20	0.42
1:K:76:THR:OG1	1:L:65:GLN:HB3	2.18	0.42
1:L:177:THR:C	1:L:179:VAL:H	2.20	0.42
1:L:196:TRP:O	1:L:200:LYS:HB3	2.19	0.42
1:L:5:ARG:O	1:L:210:ARG:CD	2.67	0.42
1:O:227:GLN:O	1:O:228:CYS:C	2.56	0.42
1:R:198:ALA:HB2	1:R:206:ALA:CB	2.50	0.42
1:R:236:VAL:HG11	1:R:239:ALA:HB3	2.00	0.42
1:R:6:PRO:HD2	1:R:36:SER:O	2.18	0.42
1:S:58:LYS:N	1:S:58:LYS:HD2	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:73:GLY:O	1:T:14:CYS:HB3	2.19	0.42
1:T:148:LEU:HD12	1:T:148:LEU:HA	1.87	0.42
1:T:162:TRP:CD2	1:T:197:PHE:HE1	2.37	0.42
1:T:40:VAL:HG12	1:T:41:ILE:N	2.34	0.42
1:A:139:ARG:HH11	1:A:142:GLU:CD	2.22	0.42
1:D:190:HIS:CE1	1:D:231:ILE:HG12	2.55	0.42
1:E:141:MET:HA	1:E:141:MET:HE3	2.00	0.42
1:E:57:SER:HB3	1:E:60:LEU:HB3	2.02	0.42
1:F:219:GLY:HA2	1:F:222:ASP:CG	2.39	0.42
1:H:115:LYS:CE	1:H:119:GLU:OE2	2.64	0.42
1:H:4:ARG:HH22	1:H:230:ASN:HA	1.84	0.42
1:K:251:ILE:CD1	1:K:251:ILE:N	2.83	0.42
1:L:171:PRO:CG	1:L:174:SER:HG	2.28	0.42
1:O:141:MET:O	1:O:145:ILE:HG13	2.20	0.42
1:Q:183:PRO:CG	1:Q:225:LEU:HD21	2.48	0.42
1:R:28:ILE:HG12	1:R:246:MET:CE	2.49	0.42
1:S:85:GLN:NE2	1:S:120:LYS:O	2.52	0.42
1:C:138:ASN:HD22	1:C:138:ASN:HA	1.68	0.42
1:C:5:ARG:HA	1:C:6:PRO:HD3	1.79	0.42
1:F:139:ARG:O	1:F:143:VAL:HG23	2.19	0.42
1:E:99:ARG:HH11	1:F:77:GLY:HA3	1.85	0.42
1:I:218:ASN:OD1	1:I:221:ASN:N	2.48	0.42
1:J:118:LEU:HD13	1:J:161:LEU:O	2.20	0.42
1:J:242:LYS:CB	1:J:244:GLU:OE1	2.59	0.42
1:J:5:ARG:HA	1:J:6:PRO:HD3	1.80	0.42
1:K:221:ASN:O	1:K:225:LEU:HD12	2.19	0.42
1:L:69:LEU:HB3	1:L:113:LYS:HG2	2.02	0.42
1:L:218:ASN:HB3	1:L:220:SER:H	1.85	0.42
1:L:78:GLU:HA	1:L:78:GLU:OE1	2.20	0.42
1:N:142:GLU:CG	1:N:143:VAL:N	2.82	0.42
1:P:156:GLY:O	1:P:159:LYS:HG3	2.19	0.42
1:P:131:THR:CA	1:P:172:VAL:HG11	2.41	0.42
1:Q:132:LEU:O	1:Q:136:LYS:HG3	2.20	0.42
1:R:218:ASN:N	1:R:218:ASN:HD22	2.16	0.42
1:A:187:GLU:CD	1:A:229:PRO:HD2	2.40	0.42
1:D:116:ARG:O	1:D:120:LYS:HG3	2.20	0.42
1:D:161:LEU:HD23	1:D:161:LEU:HA	1.83	0.42
1:D:221:ASN:HA	1:D:224:LYS:HG2	2.00	0.42
1:J:251:ILE:HA	1:J:254:LYS:HZ3	1.83	0.42
1:L:21:ILE:HG13	1:L:47:HIS:HB3	2.01	0.42
1:N:4:ARG:NH2	1:N:232:ASP:OD1	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:255:THR:O	1:O:255:THR:HG22	2.19	0.42
1:Q:76:THR:N	1:R:98:GLU:OE1	2.47	0.42
1:S:7:PHE:CE1	1:S:40:VAL:HG23	2.55	0.42
1:T:253:THR:HG22	1:T:254:LYS:N	2.33	0.42
1:A:106:THR:OG1	1:A:109:GLN:HG3	2.19	0.42
1:B:215:GLY:O	1:B:217:ALA:N	2.53	0.42
1:B:67:VAL:O	1:B:113:LYS:HD3	2.19	0.42
1:D:183:PRO:CG	1:D:224:LYS:HD3	2.50	0.42
1:D:171:PRO:CD	1:D:214:GLY:O	2.66	0.42
1:J:173:TRP:CH2	1:J:185:GLN:OE1	2.73	0.42
1:J:244:GLU:O	1:J:248:MET:HG3	2.19	0.42
1:P:62:ILE:CD1	1:P:62:ILE:N	2.82	0.42
1:Q:48:LEU:HD12	1:Q:48:LEU:HA	1.70	0.42
1:R:43:PRO:HG2	1:R:51:ALA:CB	2.50	0.42
1:S:5:ARG:O	1:S:210:ARG:NH1	2.52	0.42
1:T:139:ARG:HG2	1:T:142:GLU:OE1	2.20	0.42
1:T:197:PHE:CE1	1:T:201:VAL:HG21	2.55	0.42
1:C:90:LYS:HG2	1:C:90:LYS:O	2.18	0.42
1:E:245:PHE:HA	1:E:248:MET:HG3	2.02	0.42
1:F:212:ILE:HD11	1:F:235:LEU:HB2	2.01	0.42
1:G:80:SER:HG	1:G:83:MET:HG3	1.84	0.42
1:H:43:PRO:HG2	1:H:48:LEU:CD1	2.49	0.42
1:H:8:ILE:HB	1:H:252:LEU:HD23	2.01	0.42
1:N:95:GLY:O	1:N:127:CYS:HB2	2.18	0.42
1:O:116:ARG:O	1:O:120:LYS:HG3	2.19	0.42
1:R:12:PHE:CD1	1:R:12:PHE:N	2.88	0.42
1:R:25:VAL:HA	1:R:28:ILE:HG13	2.01	0.42
1:S:145:ILE:O	1:S:149:GLU:CG	2.68	0.42
1:B:4:ARG:HB2	1:B:4:ARG:HE	1.43	0.42
1:D:221:ASN:HA	1:D:224:LYS:HE3	2.02	0.42
1:D:218:ASN:OD1	1:D:221:ASN:OD1	2.38	0.42
1:I:144:ASN:O	1:I:148:LEU:HB2	2.19	0.42
1:I:212:ILE:CD1	1:I:235:LEU:HB2	2.50	0.42
1:L:97:SER:OG	1:L:175:ILE:HD11	2.18	0.42
1:P:134:GLU:HG2	1:P:143:VAL:HG21	2.00	0.42
1:Q:34:PRO:HG2	1:Q:37:VAL:HG23	2.02	0.42
1:I:87:MET:HE2	1:I:87:MET:HB3	1.92	0.42
1:K:5:ARG:HE	1:K:38:ASP:CG	2.21	0.42
1:M:141:MET:HE3	1:M:141:MET:HB3	1.93	0.42
1:Q:236:VAL:HG11	1:Q:240:SER:N	2.35	0.42
1:D:68:TYR:HB2	1:D:78:GLU:HB3	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:196:TRP:O	1:G:200:LYS:HB2	2.20	0.41
1:G:37:VAL:CG1	1:G:38:ASP:N	2.83	0.41
1:K:197:PHE:CD1	1:K:206:ALA:CA	3.02	0.41
1:L:177:THR:HG21	1:L:179:VAL:HG21	2.00	0.41
1:M:151:LEU:HD23	1:M:162:TRP:CH2	2.55	0.41
1:N:32:LYS:O	1:N:32:LYS:CG	2.67	0.41
1:R:116:ARG:NH1	1:R:116:ARG:HG3	2.35	0.41
1:T:242:LYS:HB2	1:T:243:PRO:CD	2.43	0.41
1:T:66:ASN:ND2	1:T:67:VAL:H	2.18	0.41
1:B:83:MET:O	1:B:87:MET:HG3	2.20	0.41
1:D:101:ARG:CZ	1:D:131:THR:HG23	2.50	0.41
1:F:145:ILE:HD13	1:F:196:TRP:CD1	2.55	0.41
1:F:148:LEU:HB3	1:F:196:TRP:CH2	2.54	0.41
1:F:21:ILE:O	1:F:25:VAL:HG23	2.20	0.41
1:I:76:THR:CG2	1:J:65:GLN:HB3	2.49	0.41
1:L:219:GLY:HA2	1:L:222:ASP:HB2	2.02	0.41
1:M:145:ILE:O	1:M:149:GLU:HG2	2.20	0.41
1:M:148:LEU:HD12	1:M:148:LEU:HA	1.82	0.41
1:N:141:MET:O	1:N:145:ILE:HG12	2.20	0.41
1:Q:138:ASN:ND2	1:Q:138:ASN:O	2.53	0.41
1:Q:65:GLN:O	1:Q:93:ILE:HG22	2.20	0.41
1:R:33:ILE:O	1:R:59:GLN:NE2	2.53	0.41
1:R:34:PRO:C	1:R:36:SER:N	2.73	0.41
1:S:5:ARG:HE	1:S:38:ASP:CG	2.23	0.41
1:J:164:GLU:HA	1:J:164:GLU:OE1	2.20	0.41
1:J:228:CYS:HA	1:J:229:PRO:HD2	1.80	0.41
1:N:61:ARG:HD2	1:N:61:ARG:HA	1.87	0.41
1:N:11:ASN:OD1	1:N:65:GLN:HG2	2.20	0.41
1:O:116:ARG:HH11	1:O:116:ARG:HG2	1.84	0.41
1:O:218:ASN:CG	1:O:219:GLY:N	2.74	0.41
1:R:151:LEU:HD12	1:R:151:LEU:O	2.21	0.41
1:R:34:PRO:C	1:R:36:SER:H	2.22	0.41
1:S:6:PRO:HG3	1:S:37:VAL:HG12	2.02	0.41
1:S:74:ALA:HA	1:T:13:LYS:HD3	2.02	0.41
1:T:7:PHE:O	1:T:233:GLY:HA3	2.20	0.41
1:T:242:LYS:CB	1:T:243:PRO:CD	2.98	0.41
1:A:12:PHE:N	1:A:12:PHE:CD1	2.88	0.41
1:B:115:LYS:O	1:B:119:GLU:HB2	2.20	0.41
1:B:128:VAL:CG2	1:B:144:ASN:HD21	2.33	0.41
1:B:145:ILE:HG12	1:B:196:TRP:CD1	2.55	0.41
1:E:131:THR:OG1	1:E:134:GLU:HG3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:12:PHE:CD1	1:G:12:PHE:N	2.88	0.41
1:J:5:ARG:O	1:J:210:ARG:HD2	2.21	0.41
1:K:193:LEU:HA	1:K:193:LEU:HD23	1.89	0.41
1:M:69:LEU:HG	1:M:69:LEU:H	1.71	0.41
1:N:107:ASP:OD1	1:N:107:ASP:N	2.53	0.41
1:S:180:VAL:HG23	1:S:216:SER:HB3	2.01	0.41
1:S:7:PHE:HE1	1:S:40:VAL:CG2	2.32	0.41
1:A:167:ILE:HG13	1:A:211:ILE:HG12	2.02	0.41
1:A:190:HIS:HB3	1:A:230:ASN:O	2.20	0.41
1:A:218:ASN:O	1:A:222:ASP:CG	2.59	0.41
1:B:95:GLY:O	1:B:127:CYS:HB2	2.21	0.41
1:B:247:THR:O	1:B:251:ILE:HD13	2.21	0.41
1:D:34:PRO:HB2	1:D:36:SER:OG	2.21	0.41
1:H:221:ASN:HD22	1:H:224:LYS:HB2	1.85	0.41
1:J:217:ALA:HB1	1:J:234:PHE:CD1	2.56	0.41
1:J:243:PRO:HD2	1:J:244:GLU:OE1	2.21	0.41
1:K:197:PHE:HE1	1:K:206:ALA:N	2.18	0.41
1:L:218:ASN:HB3	1:L:220:SER:OG	2.21	0.41
1:R:229:PRO:HB2	1:R:230:ASN:HD22	1.85	0.41
1:S:182:THR:HB	1:S:184:GLU:OE1	2.21	0.41
1:S:33:ILE:HA	1:S:34:PRO:HD3	1.91	0.41
1:A:137:ALA:HB3	1:A:139:ARG:CG	2.49	0.41
1:C:174:SER:HB2	1:C:180:VAL:HA	2.02	0.41
1:C:228:CYS:HA	1:C:229:PRO:HD2	1.90	0.41
1:C:72:ASN:N	1:C:72:ASN:HD22	2.17	0.41
1:K:142:GLU:HG2	1:K:143:VAL:N	2.36	0.41
1:K:202:ALA:HB1	1:K:204:GLU:CD	2.41	0.41
1:K:229:PRO:HB2	1:K:230:ASN:HD22	1.86	0.41
1:K:43:PRO:C	1:K:65:GLN:NE2	2.74	0.41
1:K:67:VAL:HG22	1:K:68:TYR:H	1.85	0.41
1:K:8:ILE:HG13	1:K:9:GLY:N	2.36	0.41
1:O:67:VAL:HG22	1:O:68:TYR:N	2.36	0.41
1:Q:130:GLU:CD	1:Q:140:THR:HG23	2.41	0.41
1:R:161:LEU:C	1:R:163:LYS:H	2.22	0.41
1:T:217:ALA:O	1:T:248:MET:HE1	2.21	0.41
1:A:218:ASN:HD22	1:A:220:SER:H	1.64	0.41
1:B:128:VAL:HB	1:B:147:GLN:OE1	2.20	0.41
1:B:159:LYS:HG2	1:B:160:MET:N	2.35	0.41
1:C:169:TYR:CE1	1:C:189:VAL:HG11	2.56	0.41
1:D:161:LEU:C	1:D:163:LYS:N	2.72	0.41
1:G:213:TYR:CD2	1:G:234:PHE:HD1	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:7:PHE:CZ	1:G:40:VAL:HG11	2.56	0.41
1:I:143:VAL:O	1:I:147:GLN:HG3	2.20	0.41
1:I:189:VAL:O	1:I:193:LEU:HG	2.21	0.41
1:I:253:THR:HG22	1:I:254:LYS:HD2	2.02	0.41
1:J:145:ILE:HG22	1:J:149:GLU:HG2	2.01	0.41
1:J:8:ILE:HD13	1:J:245:PHE:CE1	2.55	0.41
1:K:190:HIS:CE1	1:K:211:ILE:HG22	2.56	0.41
1:K:195:LYS:HE3	1:K:195:LYS:HB2	1.70	0.41
1:L:221:ASN:HD22	1:L:222:ASP:H	1.61	0.41
1:R:4:ARG:NH2	1:R:194:ARG:NH2	2.68	0.41
1:R:7:PHE:CD1	1:R:7:PHE:C	2.93	0.41
1:F:171:PRO:HG2	1:F:213:TYR:CZ	2.54	0.41
1:K:204:GLU:HG2	1:K:205:GLY:H	1.83	0.41
1:N:134:GLU:HB3	1:N:143:VAL:HG21	2.01	0.41
1:O:221:ASN:O	1:O:225:LEU:HG	2.21	0.41
1:P:189:VAL:O	1:P:193:LEU:HG	2.20	0.41
1:Q:166:VAL:CG2	1:Q:210:ARG:CZ	2.99	0.41
1:T:197:PHE:O	1:T:201:VAL:HB	2.21	0.41
1:A:218:ASN:ND2	1:A:218:ASN:O	2.53	0.41
1:C:166:VAL:CG1	1:C:212:ILE:HD13	2.51	0.41
1:C:169:TYR:CZ	1:C:189:VAL:HG11	2.56	0.41
1:C:236:VAL:CG1	1:C:239:ALA:HB3	2.51	0.41
1:H:163:LYS:HE2	1:H:163:LYS:HB2	1.89	0.41
1:I:194:ARG:NH1	1:I:209:ILE:HG23	2.36	0.41
1:I:218:ASN:OD1	1:I:221:ASN:ND2	2.53	0.41
1:K:130:GLU:OE2	1:K:169:TYR:OH	2.34	0.41
1:O:31:HIS:HB2	1:O:246:MET:HG2	2.03	0.41
1:P:128:VAL:HG12	1:P:147:GLN:OE1	2.20	0.41
1:R:116:ARG:HG3	1:R:116:ARG:HH11	1.86	0.41
1:R:118:LEU:HD21	1:R:165:VAL:HG23	2.02	0.41
1:S:195:LYS:O	1:S:199:GLU:HG3	2.21	0.41
1:B:128:VAL:HG21	1:B:144:ASN:HD21	1.86	0.41
1:C:250:ASP:O	1:C:253:THR:HB	2.21	0.41
1:E:178:GLY:HA3	1:I:172:VAL:HG13	2.03	0.41
1:E:250:ASP:O	1:E:254:LYS:HG2	2.20	0.41
1:E:96:HIS:CG	1:F:76:THR:HG21	2.56	0.41
1:G:74:ALA:HA	1:H:13:LYS:HD3	2.03	0.41
1:H:223:GLU:O	1:H:227:GLN:HG3	2.21	0.41
1:I:137:ALA:HB3	1:I:139:ARG:HG3	2.02	0.41
1:I:72:ASN:HD22	1:I:72:ASN:N	2.18	0.41
1:M:180:VAL:HG23	1:M:215:GLY:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:95:GLY:O	1:M:100:ARG:NE	2.50	0.41
1:Q:222:ASP:O	1:Q:226:GLY:N	2.49	0.41
1:R:48:LEU:HA	1:R:48:LEU:HD12	1.75	0.41
1:R:67:VAL:HG23	1:R:79:THR:HG22	2.02	0.41
1:A:130:GLU:O	1:A:173:TRP:HD1	2.04	0.41
1:C:13:LYS:HA	1:C:65:GLN:OE1	2.21	0.41
1:D:160:MET:O	1:D:163:LYS:HB2	2.21	0.41
1:D:224:LYS:HG3	1:D:225:LEU:N	2.36	0.41
1:G:96:HIS:ND1	1:G:98:GLU:HG3	2.36	0.41
1:H:66:ASN:HD21	1:H:113:LYS:NZ	2.19	0.41
1:H:155:LEU:HD12	1:H:162:TRP:CE2	2.55	0.41
1:I:63:ALA:HB2	1:I:91:HIS:HB2	2.03	0.41
1:J:247:THR:O	1:J:251:ILE:HD13	2.21	0.41
1:K:202:ALA:HB1	1:K:204:GLU:OE1	2.20	0.41
1:M:183:PRO:HA	1:M:225:LEU:HD23	2.03	0.41
1:P:57:SER:HB3	1:P:60:LEU:HB3	2.03	0.41
1:Q:61:ARG:HD2	1:Q:61:ARG:HA	1.50	0.41
1:S:224:LYS:O	1:S:227:GLN:HB2	2.21	0.41
1:S:246:MET:CE	1:S:246:MET:H	2.34	0.41
1:S:5:ARG:NH1	1:S:35:ASP:O	2.47	0.41
1:B:118:LEU:HD12	1:B:155:LEU:HD21	2.03	0.40
1:B:66:ASN:ND2	1:B:67:VAL:O	2.53	0.40
1:C:116:ARG:O	1:C:120:LYS:HG3	2.20	0.40
1:D:68:TYR:CE2	1:D:75:TRP:HB3	2.55	0.40
1:E:184:GLU:CD	1:E:184:GLU:H	2.24	0.40
1:G:111:ALA:HB1	1:G:154:GLU:CG	2.51	0.40
1:G:65:GLN:HB3	1:H:76:THR:HG23	2.03	0.40
1:E:175:ILE:HG23	1:I:176:GLY:O	2.21	0.40
1:L:204:GLU:O	1:L:207:GLN:HB2	2.22	0.40
1:L:59:GLN:HB2	1:L:59:GLN:HE21	1.71	0.40
1:M:141:MET:HE2	1:M:192:GLY:HA3	2.03	0.40
1:N:187:GLU:O	1:N:191:VAL:HG23	2.21	0.40
1:O:194:ARG:CG	1:O:206:ALA:O	2.69	0.40
1:O:125:ILE:HG21	1:O:235:LEU:HD13	2.02	0.40
1:P:69:LEU:CD2	1:P:70:GLU:HG2	2.50	0.40
1:A:251:ILE:HA	1:A:251:ILE:HD12	1.80	0.40
1:F:68:TYR:CE1	1:F:69:LEU:HD22	2.57	0.40
1:I:130:GLU:O	1:I:130:GLU:HG2	2.18	0.40
1:M:83:MET:HG2	1:N:47:HIS:HE1	1.86	0.40
1:P:186:ALA:HB1	1:P:231:ILE:HD11	2.03	0.40
1:P:242:LYS:C	1:P:244:GLU:N	2.74	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:195:LYS:O	1:Q:199:GLU:CB	2.60	0.40
1:R:68:TYR:CE1	1:R:69:LEU:CD2	3.04	0.40
1:E:61:ARG:HD2	1:E:61:ARG:HA	1.85	0.40
1:F:5:ARG:O	1:F:210:ARG:HD2	2.21	0.40
1:F:90:LYS:O	1:F:90:LYS:HG2	2.21	0.40
1:H:222:ASP:OD1	1:H:234:PHE:CZ	2.74	0.40
1:L:112:LYS:HE3	1:L:154:GLU:OE2	2.22	0.40
1:L:190:HIS:CE1	1:L:211:ILE:HG22	2.57	0.40
1:L:218:ASN:N	1:L:222:ASP:OD1	2.55	0.40
1:M:240:SER:HA	1:M:245:PHE:CD1	2.57	0.40
1:M:5:ARG:HH12	1:M:37:VAL:N	2.19	0.40
1:M:33:ILE:O	1:M:59:GLN:HG2	2.20	0.40
1:M:52:ILE:HD11	1:M:89:LEU:HD21	2.04	0.40
1:N:150:ALA:O	1:N:154:GLU:HG2	2.22	0.40
1:N:168:ALA:HA	1:N:212:ILE:O	2.21	0.40
1:O:218:ASN:ND2	1:O:219:GLY:N	2.70	0.40
1:O:226:GLY:C	1:O:255:THR:HG21	2.40	0.40
1:Q:24:HIS:NE2	1:Q:28:ILE:HD11	2.36	0.40
1:T:117:ALA:O	1:T:122:MET:HB2	2.21	0.40
1:T:12:PHE:O	1:T:13:LYS:HB2	2.20	0.40
1:D:37:VAL:HG12	1:D:38:ASP:N	2.36	0.40
1:E:187:GLU:HG3	1:E:187:GLU:O	2.21	0.40
1:G:75:TRP:HD1	1:H:14:CYS:HB3	1.86	0.40
1:I:97:SER:N	1:I:170:GLU:OE1	2.54	0.40
1:K:196:TRP:CE3	1:K:197:PHE:N	2.89	0.40
1:L:68:TYR:CE2	1:L:70:GLU:HB2	2.56	0.40
1:P:12:PHE:HA	1:P:241:LEU:HD21	2.02	0.40
1:P:149:GLU:OE1	1:P:149:GLU:HA	2.21	0.40
1:R:65:GLN:O	1:R:93:ILE:O	2.40	0.40
1:S:158:SER:O	1:S:161:LEU:HD23	2.22	0.40
1:S:185:GLN:O	1:S:188:GLU:CD	2.60	0.40
1:S:21:ILE:HD13	1:S:21:ILE:N	2.37	0.40
1:S:225:LEU:O	1:S:228:CYS:HB2	2.21	0.40
1:T:249:ILE:O	1:T:252:LEU:HB3	2.21	0.40
1:C:114:ALA:O	1:C:118:LEU:HG	2.21	0.40
1:G:93:ILE:HA	1:G:125:ILE:HB	2.04	0.40
1:J:132:LEU:O	1:J:136:LYS:HB2	2.22	0.40
1:J:33:ILE:HB	1:J:59:GLN:HE21	1.86	0.40
1:K:46:VAL:HG13	1:L:45:ALA:HB1	2.04	0.40
1:K:72:ASN:ND2	1:K:80:SER:OG	2.55	0.40
1:L:12:PHE:N	1:L:12:PHE:CD1	2.90	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:228:CYS:HA	1:O:229:PRO:HD3	1.79	0.40
1:S:128:VAL:HG11	1:S:148:LEU:HD13	2.03	0.40
1:S:186:ALA:HB1	1:S:213:TYR:CD1	2.57	0.40
1:S:8:ILE:CG2	1:S:39:VAL:HG22	2.52	0.40
1:T:84:LEU:HD23	1:T:84:LEU:HA	1.67	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	252/255 (99%)	241 (96%)	10 (4%)	1 (0%)	38	66
1	B	252/255 (99%)	247 (98%)	5 (2%)	0	100	100
1	C	252/255 (99%)	240 (95%)	11 (4%)	1 (0%)	38	66
1	D	252/255 (99%)	244 (97%)	7 (3%)	1 (0%)	38	66
1	E	252/255 (99%)	240 (95%)	11 (4%)	1 (0%)	38	66
1	F	252/255 (99%)	244 (97%)	7 (3%)	1 (0%)	38	66
1	G	252/255 (99%)	243 (96%)	8 (3%)	1 (0%)	38	66
1	H	252/255 (99%)	240 (95%)	12 (5%)	0	100	100
1	I	252/255 (99%)	243 (96%)	9 (4%)	0	100	100
1	J	252/255 (99%)	244 (97%)	8 (3%)	0	100	100
1	K	252/255 (99%)	240 (95%)	11 (4%)	1 (0%)	38	66
1	L	252/255 (99%)	239 (95%)	13 (5%)	0	100	100
1	M	252/255 (99%)	244 (97%)	8 (3%)	0	100	100
1	N	252/255 (99%)	239 (95%)	11 (4%)	2 (1%)	22	49
1	O	252/255 (99%)	237 (94%)	14 (6%)	1 (0%)	38	66
1	P	252/255 (99%)	233 (92%)	18 (7%)	1 (0%)	38	66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	252/255 (99%)	237 (94%)	14 (6%)	1 (0%)	38	66
1	R	252/255 (99%)	242 (96%)	7 (3%)	3 (1%)	15	37
1	S	252/255 (99%)	238 (94%)	14 (6%)	0	100	100
1	T	252/255 (99%)	246 (98%)	6 (2%)	0	100	100
All	All	5040/5100 (99%)	4821 (96%)	204 (4%)	15 (0%)	44	73

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	218	ASN
1	E	220	SER
1	G	219	GLY
1	R	218	ASN
1	Q	201	VAL
1	R	13	LYS
1	K	214	GLY
1	N	13	LYS
1	O	138	ASN
1	R	156	GLY
1	A	156	GLY
1	P	243	PRO
1	D	201	VAL
1	N	156	GLY
1	F	201	VAL

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	202/203 (100%)	178 (88%)	24 (12%)	6	14
1	B	202/203 (100%)	187 (93%)	15 (7%)	16	37
1	C	202/203 (100%)	180 (89%)	22 (11%)	7	17
1	D	202/203 (100%)	176 (87%)	26 (13%)	5	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	202/203 (100%)	177 (88%)	25 (12%)	5	13
1	F	202/203 (100%)	186 (92%)	16 (8%)	14	33
1	G	202/203 (100%)	181 (90%)	21 (10%)	8	18
1	H	202/203 (100%)	180 (89%)	22 (11%)	7	17
1	I	202/203 (100%)	177 (88%)	25 (12%)	5	13
1	J	202/203 (100%)	184 (91%)	18 (9%)	11	26
1	K	202/203 (100%)	181 (90%)	21 (10%)	8	18
1	L	202/203 (100%)	184 (91%)	18 (9%)	11	26
1	M	202/203 (100%)	176 (87%)	26 (13%)	5	12
1	N	202/203 (100%)	176 (87%)	26 (13%)	5	12
1	O	202/203 (100%)	176 (87%)	26 (13%)	5	12
1	P	202/203 (100%)	180 (89%)	22 (11%)	7	17
1	Q	202/203 (100%)	169 (84%)	33 (16%)	3	7
1	R	202/203 (100%)	181 (90%)	21 (10%)	8	18
1	S	202/203 (100%)	160 (79%)	42 (21%)	1	3
1	T	202/203 (100%)	168 (83%)	34 (17%)	2	6
All	All	4040/4060 (100%)	3557 (88%)	483 (12%)	6	14

All (483) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	18	LEU
1	A	32	LYS
1	A	48	LEU
1	A	49	SER
1	A	57	SER
1	A	69	LEU
1	A	72	ASN
1	A	99	ARG
1	A	138	ASN
1	A	139	ARG
1	A	142	GLU
1	A	149	GLU
1	A	157	GLU
1	A	160	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	167	ILE
1	A	179	VAL
1	A	210	ARG
1	A	218	ASN
1	A	221	ASN
1	A	246	MET
1	A	251	ILE
1	A	252	LEU
1	A	255	THR
1	B	4	ARG
1	B	5	ARG
1	B	35	ASP
1	B	66	ASN
1	B	69	LEU
1	B	101	ARG
1	B	138	ASN
1	B	148	LEU
1	B	159	LYS
1	B	160	MET
1	B	177	THR
1	B	179	VAL
1	B	184	GLU
1	B	210	ARG
1	B	221	ASN
1	C	44	SER
1	C	48	LEU
1	C	49	SER
1	C	59	GLN
1	C	61	ARG
1	C	62	ILE
1	C	69	LEU
1	C	86	ASP
1	C	110	SER
1	C	116	ARG
1	C	138	ASN
1	C	139	ARG
1	C	140	THR
1	C	148	LEU
1	C	158	SER
1	C	159	LYS
1	C	160	MET
1	C	179	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	207	GLN
1	C	210	ARG
1	C	218	ASN
1	C	251	ILE
1	D	4	ARG
1	D	8	ILE
1	D	32	LYS
1	D	36	SER
1	D	44	SER
1	D	48	LEU
1	D	58	LYS
1	D	67	VAL
1	D	68	TYR
1	D	69	LEU
1	D	99	ARG
1	D	100	ARG
1	D	135	ARG
1	D	138	ASN
1	D	140	THR
1	D	145	ILE
1	D	148	LEU
1	D	160	MET
1	D	180	VAL
1	D	188	GLU
1	D	194	ARG
1	D	210	ARG
1	D	218	ASN
1	D	222	ASP
1	D	244	GLU
1	D	252	LEU
1	E	49	SER
1	E	62	ILE
1	E	69	LEU
1	E	89	LEU
1	E	115	LYS
1	E	116	ARG
1	E	130	GLU
1	E	131	THR
1	E	138	ASN
1	E	140	THR
1	E	141	MET
1	E	145	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	148	LEU
1	E	149	GLU
1	E	157	GLU
1	E	158	SER
1	E	160	MET
1	E	184	GLU
1	E	195	LYS
1	E	199	GLU
1	E	220	SER
1	E	222	ASP
1	E	225	LEU
1	E	248	MET
1	E	255	THR
1	F	5	ARG
1	F	44	SER
1	F	48	LEU
1	F	58	LYS
1	F	61	ARG
1	F	69	LEU
1	F	82	GLU
1	F	112	LYS
1	F	135	ARG
1	F	148	LEU
1	F	159	LYS
1	F	160	MET
1	F	185	GLN
1	F	209	ILE
1	F	210	ARG
1	F	221	ASN
1	G	4	ARG
1	G	8	ILE
1	G	23	SER
1	G	40	VAL
1	G	62	ILE
1	G	93	ILE
1	G	116	ARG
1	G	130	GLU
1	G	135	ARG
1	G	139	ARG
1	G	148	LEU
1	G	159	LYS
1	G	160	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	179	VAL
1	G	210	ARG
1	G	211	ILE
1	G	224	LYS
1	G	225	LEU
1	G	242	LYS
1	G	252	LEU
1	G	254	LYS
1	H	4	ARG
1	H	32	LYS
1	H	48	LEU
1	H	49	SER
1	H	58	LYS
1	H	69	LEU
1	H	86	ASP
1	H	109	GLN
1	H	112	LYS
1	H	115	LYS
1	H	138	ASN
1	H	142	GLU
1	H	148	LEU
1	H	154	GLU
1	H	158	SER
1	H	159	LYS
1	H	160	MET
1	H	164	GLU
1	H	180	VAL
1	H	210	ARG
1	H	248	MET
1	H	252	LEU
1	I	4	ARG
1	I	8	ILE
1	I	13	LYS
1	I	32	LYS
1	I	36	SER
1	I	44	SER
1	I	46	VAL
1	I	69	LEU
1	I	130	GLU
1	I	138	ASN
1	I	145	ILE
1	I	148	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	157	GLU
1	I	160	MET
1	I	167	ILE
1	I	194	ARG
1	I	200	LYS
1	I	209	ILE
1	I	210	ARG
1	I	218	ASN
1	I	227	GLN
1	I	240	SER
1	I	244	GLU
1	I	251	ILE
1	I	252	LEU
1	J	17	SER
1	J	23	SER
1	J	48	LEU
1	J	49	SER
1	J	58	LYS
1	J	61	ARG
1	J	110	SER
1	J	112	LYS
1	J	115	LYS
1	J	148	LEU
1	J	153	LYS
1	J	159	LYS
1	J	160	MET
1	J	163	LYS
1	J	210	ARG
1	J	218	ASN
1	J	224	LYS
1	J	240	SER
1	K	4	ARG
1	K	46	VAL
1	K	48	LEU
1	K	62	ILE
1	K	69	LEU
1	K	116	ARG
1	K	135	ARG
1	K	148	LEU
1	K	157	GLU
1	K	195	LYS
1	K	209	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	210	ARG
1	K	218	ASN
1	K	220	SER
1	K	221	ASN
1	K	225	LEU
1	K	242	LYS
1	K	248	MET
1	K	251	ILE
1	K	254	LYS
1	K	255	THR
1	L	4	ARG
1	L	49	SER
1	L	59	GLN
1	L	69	LEU
1	L	99	ARG
1	L	100	ARG
1	L	138	ASN
1	L	148	LEU
1	L	173	TRP
1	L	179	VAL
1	L	189	VAL
1	L	199	GLU
1	L	204	GLU
1	L	208	HIS
1	L	218	ASN
1	L	221	ASN
1	L	232	ASP
1	L	240	SER
1	M	5	ARG
1	M	32	LYS
1	M	35	ASP
1	M	44	SER
1	M	48	LEU
1	M	49	SER
1	M	58	LYS
1	M	68	TYR
1	M	69	LEU
1	M	75	TRP
1	M	97	SER
1	M	98	GLU
1	M	106	THR
1	M	145	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	148	LEU
1	M	159	LYS
1	M	160	MET
1	M	170	GLU
1	M	179	VAL
1	M	194	ARG
1	M	209	ILE
1	M	210	ARG
1	M	224	LYS
1	M	251	ILE
1	M	253	THR
1	M	255	THR
1	N	15	ASN
1	N	32	LYS
1	N	36	SER
1	N	44	SER
1	N	48	LEU
1	N	49	SER
1	N	62	ILE
1	N	69	LEU
1	N	89	LEU
1	N	107	ASP
1	N	120	LYS
1	N	130	GLU
1	N	139	ARG
1	N	142	GLU
1	N	145	ILE
1	N	148	LEU
1	N	160	MET
1	N	179	VAL
1	N	180	VAL
1	N	184	GLU
1	N	224	LYS
1	N	225	LEU
1	N	240	SER
1	N	244	GLU
1	N	247	THR
1	N	248	MET
1	O	8	ILE
1	O	13	LYS
1	O	14	CYS
1	O	36	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	48	LEU
1	O	49	SER
1	O	59	GLN
1	O	69	LEU
1	O	86	ASP
1	O	112	LYS
1	O	120	LYS
1	O	131	THR
1	O	138	ASN
1	O	139	ARG
1	O	145	ILE
1	O	148	LEU
1	O	160	MET
1	O	163	LYS
1	O	167	ILE
1	O	204	GLU
1	O	210	ARG
1	O	223	GLU
1	O	244	GLU
1	O	247	THR
1	O	248	MET
1	O	251	ILE
1	P	4	ARG
1	P	15	ASN
1	P	35	ASP
1	P	48	LEU
1	P	59	GLN
1	P	61	ARG
1	P	69	LEU
1	P	89	LEU
1	P	108	GLU
1	P	115	LYS
1	P	116	ARG
1	P	128	VAL
1	P	130	GLU
1	P	145	ILE
1	P	148	LEU
1	P	160	MET
1	P	172	VAL
1	P	173	TRP
1	P	199	GLU
1	P	210	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	221	ASN
1	P	223	GLU
1	Q	8	ILE
1	Q	19	ASP
1	Q	23	SER
1	Q	28	ILE
1	Q	37	VAL
1	Q	38	ASP
1	Q	46	VAL
1	Q	48	LEU
1	Q	50	THR
1	Q	58	LYS
1	Q	59	GLN
1	Q	61	ARG
1	Q	75	TRP
1	Q	81	VAL
1	Q	103	MET
1	Q	106	THR
1	Q	115	LYS
1	Q	116	ARG
1	Q	139	ARG
1	Q	148	LEU
1	Q	153	LYS
1	Q	158	SER
1	Q	159	LYS
1	Q	160	MET
1	Q	177	THR
1	Q	189	VAL
1	Q	195	LYS
1	Q	210	ARG
1	Q	220	SER
1	Q	230	ASN
1	Q	236	VAL
1	Q	252	LEU
1	Q	255	THR
1	R	8	ILE
1	R	28	ILE
1	R	35	ASP
1	R	48	LEU
1	R	49	SER
1	R	69	LEU
1	R	80	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	R	87	MET
1	R	89	LEU
1	R	119	GLU
1	R	120	LYS
1	R	135	ARG
1	R	148	LEU
1	R	153	LYS
1	R	210	ARG
1	R	222	ASP
1	R	230	ASN
1	R	244	GLU
1	R	251	ILE
1	R	253	THR
1	R	255	THR
1	S	7	PHE
1	S	8	ILE
1	S	23	SER
1	S	28	ILE
1	S	32	LYS
1	S	44	SER
1	S	48	LEU
1	S	49	SER
1	S	59	GLN
1	S	61	ARG
1	S	69	LEU
1	S	86	ASP
1	S	87	MET
1	S	89	LEU
1	S	99	ARG
1	S	101	ARG
1	S	102	ILE
1	S	106	THR
1	S	108	GLU
1	S	116	ARG
1	S	128	VAL
1	S	130	GLU
1	S	138	ASN
1	S	148	LEU
1	S	157	GLU
1	S	158	SER
1	S	159	LYS
1	S	160	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S	163	LYS
1	S	180	VAL
1	S	185	GLN
1	S	188	GLU
1	S	207	GLN
1	S	210	ARG
1	S	220	SER
1	S	221	ASN
1	S	241	LEU
1	S	244	GLU
1	S	246	MET
1	S	247	THR
1	S	253	THR
1	S	254	LYS
1	T	22	LYS
1	T	23	SER
1	T	28	ILE
1	T	32	LYS
1	T	33	ILE
1	T	48	LEU
1	T	49	SER
1	T	67	VAL
1	T	87	MET
1	T	99	ARG
1	T	115	LYS
1	T	135	ARG
1	T	136	LYS
1	T	148	LEU
1	T	153	LYS
1	T	157	GLU
1	T	158	SER
1	T	160	MET
1	T	163	LYS
1	T	164	GLU
1	T	170	GLU
1	T	174	SER
1	T	180	VAL
1	T	199	GLU
1	T	209	ILE
1	T	210	ARG
1	T	216	SER
1	T	220	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	T	223	GLU
1	T	240	SER
1	T	242	LYS
1	T	244	GLU
1	T	248	MET
1	T	253	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (112) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	72	ASN
1	A	91	HIS
1	A	138	ASN
1	A	208	HIS
1	A	218	ASN
1	B	65	GLN
1	B	66	ASN
1	B	72	ASN
1	B	144	ASN
1	C	47	HIS
1	C	72	ASN
1	C	91	HIS
1	C	138	ASN
1	C	221	ASN
1	D	47	HIS
1	D	72	ASN
1	D	144	ASN
1	D	207	GLN
1	D	218	ASN
1	E	66	ASN
1	E	72	ASN
1	E	91	HIS
1	F	47	HIS
1	F	65	GLN
1	F	91	HIS
1	G	66	ASN
1	G	72	ASN
1	G	230	ASN
1	H	47	HIS
1	H	66	ASN
1	H	85	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	221	ASN
1	H	230	ASN
1	I	11	ASN
1	I	72	ASN
1	I	91	HIS
1	I	138	ASN
1	I	221	ASN
1	J	11	ASN
1	J	47	HIS
1	J	72	ASN
1	J	91	HIS
1	J	207	GLN
1	K	59	GLN
1	K	66	ASN
1	K	72	ASN
1	K	218	ASN
1	K	221	ASN
1	K	230	ASN
1	L	47	HIS
1	L	59	GLN
1	L	72	ASN
1	L	91	HIS
1	L	138	ASN
1	L	144	ASN
1	L	221	ASN
1	M	47	HIS
1	M	59	GLN
1	M	65	GLN
1	M	66	ASN
1	M	72	ASN
1	N	15	ASN
1	N	47	HIS
1	N	66	ASN
1	N	72	ASN
1	N	91	HIS
1	N	218	ASN
1	O	59	GLN
1	O	66	ASN
1	O	72	ASN
1	O	185	GLN
1	O	190	HIS
1	O	208	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	218	ASN
1	P	15	ASN
1	P	59	GLN
1	P	66	ASN
1	P	72	ASN
1	P	91	HIS
1	P	96	HIS
1	P	138	ASN
1	P	144	ASN
1	P	230	ASN
1	Q	47	HIS
1	Q	59	GLN
1	Q	66	ASN
1	Q	72	ASN
1	Q	85	GLN
1	Q	91	HIS
1	Q	190	HIS
1	Q	218	ASN
1	Q	230	ASN
1	R	47	HIS
1	R	72	ASN
1	R	85	GLN
1	R	190	HIS
1	R	218	ASN
1	R	230	ASN
1	S	47	HIS
1	S	72	ASN
1	S	144	ASN
1	S	190	HIS
1	S	221	ASN
1	S	230	ASN
1	T	47	HIS
1	T	65	GLN
1	T	66	ASN
1	T	72	ASN
1	T	85	GLN
1	T	190	HIS
1	T	218	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	254/255 (99%)	0.06	9 (3%) 44 44	26, 40, 72, 88	0
1	B	254/255 (99%)	0.08	6 (2%) 59 60	21, 37, 70, 89	0
1	C	254/255 (99%)	0.08	7 (2%) 53 54	22, 39, 72, 93	0
1	D	254/255 (99%)	0.04	4 (1%) 72 73	25, 40, 71, 84	0
1	E	254/255 (99%)	0.14	11 (4%) 36 34	24, 44, 75, 90	0
1	F	254/255 (99%)	0.06	4 (1%) 72 73	23, 39, 71, 88	0
1	G	254/255 (99%)	0.14	9 (3%) 44 44	24, 38, 70, 92	0
1	H	254/255 (99%)	0.04	2 (0%) 86 86	24, 39, 73, 91	0
1	I	254/255 (99%)	0.10	6 (2%) 59 60	25, 40, 70, 85	0
1	J	254/255 (99%)	0.02	5 (1%) 65 66	24, 38, 72, 93	0
1	K	254/255 (99%)	0.22	12 (4%) 32 30	25, 48, 76, 93	0
1	L	254/255 (99%)	0.32	13 (5%) 29 27	27, 52, 79, 90	0
1	M	254/255 (99%)	0.08	2 (0%) 86 86	24, 42, 75, 87	0
1	N	254/255 (99%)	0.12	8 (3%) 49 49	23, 43, 76, 92	0
1	O	254/255 (99%)	0.31	17 (6%) 19 16	24, 45, 77, 93	0
1	P	254/255 (99%)	0.27	11 (4%) 36 34	27, 51, 80, 95	0
1	Q	254/255 (99%)	0.61	33 (12%) 4 3	40, 65, 86, 96	0
1	R	254/255 (99%)	0.53	28 (11%) 6 5	35, 64, 87, 95	0
1	S	254/255 (99%)	0.30	8 (3%) 49 49	41, 64, 85, 96	0
1	T	254/255 (99%)	0.47	28 (11%) 6 5	36, 62, 87, 96	0
All	All	5080/5100 (99%)	0.20	223 (4%) 35 33	21, 46, 79, 96	0

All (223) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	2	PRO	11.8
1	R	217	ALA	10.8
1	K	219	GLY	9.0
1	Q	40	VAL	7.8
1	O	2	PRO	7.8
1	A	217	ALA	7.7
1	R	176	GLY	7.7
1	P	175	ILE	7.6
1	C	2	PRO	7.2
1	T	2	PRO	6.6
1	E	216	SER	6.5
1	O	219	GLY	6.4
1	L	2	PRO	6.3
1	Q	210	ARG	6.3
1	A	222	ASP	6.2
1	T	40	VAL	5.9
1	G	2	PRO	5.8
1	J	2	PRO	5.8
1	R	234	PHE	5.5
1	E	217	ALA	5.5
1	G	219	GLY	5.4
1	L	180	VAL	5.3
1	Q	166	VAL	5.3
1	K	218	ASN	5.3
1	Q	25	VAL	5.2
1	Q	176	GLY	5.1
1	C	3	ALA	5.1
1	O	252	LEU	5.0
1	K	235	LEU	4.9
1	R	33	ILE	4.8
1	H	222	ASP	4.8
1	S	166	VAL	4.8
1	E	215	GLY	4.7
1	K	2	PRO	4.7
1	Q	42	ALA	4.6
1	O	225	LEU	4.5
1	Q	124	VAL	4.4
1	I	219	GLY	4.4
1	T	41	ILE	4.4
1	Q	63	ALA	4.3
1	R	40	VAL	4.2
1	I	176	GLY	4.1
1	T	42	ALA	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	219	GLY	4.1
1	R	2	PRO	4.1
1	P	253	THR	4.0
1	I	2	PRO	4.0
1	T	12	PHE	4.0
1	T	217	ALA	4.0
1	Q	196	TRP	3.9
1	Q	168	ALA	3.9
1	T	52	ILE	3.9
1	I	216	SER	3.9
1	D	216	SER	3.9
1	Q	125	ILE	3.7
1	A	175	ILE	3.7
1	C	219	GLY	3.7
1	S	252	LEU	3.7
1	L	111	ALA	3.6
1	C	81	VAL	3.6
1	M	255	THR	3.6
1	P	128	VAL	3.6
1	R	216	SER	3.6
1	H	2	PRO	3.6
1	Q	37	VAL	3.5
1	Q	249	ILE	3.5
1	K	248	MET	3.5
1	R	55	ASN	3.5
1	T	29	ALA	3.5
1	J	219	GLY	3.5
1	L	175	ILE	3.5
1	A	225	LEU	3.5
1	N	227	GLN	3.4
1	P	95	GLY	3.4
1	O	3	ALA	3.4
1	T	166	VAL	3.3
1	Q	8	ILE	3.3
1	T	63	ALA	3.3
1	R	209	ILE	3.3
1	K	3	ALA	3.3
1	C	175	ILE	3.2
1	G	217	ALA	3.1
1	R	25	VAL	3.1
1	E	2	PRO	3.1
1	G	220	SER	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	252	LEU	3.1
1	T	37	VAL	3.1
1	R	38	ASP	3.1
1	R	148	LEU	3.1
1	L	255	THR	3.0
1	O	198	ALA	3.0
1	Q	179	VAL	3.0
1	T	155	LEU	3.0
1	N	3	ALA	3.0
1	A	226	GLY	3.0
1	P	110	SER	2.9
1	D	2	PRO	2.9
1	G	234	PHE	2.9
1	R	7	PHE	2.9
1	R	245	PHE	2.9
1	A	220	SER	2.9
1	Q	89	LEU	2.9
1	B	63	ALA	2.9
1	R	236	VAL	2.9
1	Q	94	VAL	2.8
1	B	176	GLY	2.8
1	D	3	ALA	2.8
1	P	2	PRO	2.8
1	K	225	LEU	2.8
1	R	37	VAL	2.8
1	T	252	LEU	2.8
1	N	218	ASN	2.7
1	R	235	LEU	2.7
1	E	202	ALA	2.7
1	E	225	LEU	2.7
1	Q	51	ALA	2.7
1	K	83	MET	2.7
1	Q	41	ILE	2.7
1	R	177	THR	2.7
1	P	249	ILE	2.7
1	N	216	SER	2.7
1	R	52	ILE	2.7
1	F	177	THR	2.7
1	T	39	VAL	2.6
1	Q	7	PHE	2.6
1	L	222	ASP	2.6
1	L	101	ARG	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	Q	84	LEU	2.6
1	T	49	SER	2.6
1	S	128	VAL	2.6
1	I	129	GLY	2.6
1	T	25	VAL	2.6
1	L	234	PHE	2.6
1	Q	26	ALA	2.5
1	S	25	VAL	2.5
1	R	218	ASN	2.5
1	G	255	THR	2.5
1	O	215	GLY	2.5
1	O	221	ASN	2.5
1	K	217	ALA	2.5
1	P	174	SER	2.5
1	F	206	ALA	2.5
1	Q	39	VAL	2.4
1	L	197	PHE	2.4
1	Q	178	GLY	2.4
1	F	137	ALA	2.4
1	Q	22	LYS	2.4
1	Q	177	THR	2.4
1	T	168	ALA	2.4
1	T	8	ILE	2.4
1	O	220	SER	2.4
1	J	111	ALA	2.4
1	G	236	VAL	2.4
1	I	151	LEU	2.4
1	T	203	ALA	2.4
1	A	221	ASN	2.3
1	B	171	PRO	2.3
1	S	4	ARG	2.3
1	E	168	ALA	2.3
1	N	254	LYS	2.3
1	R	34	PRO	2.3
1	B	252	LEU	2.3
1	S	127	CYS	2.3
1	R	8	ILE	2.3
1	T	28	ILE	2.3
1	Q	2	PRO	2.3
1	M	221	ASN	2.3
1	T	21	ILE	2.3
1	R	165	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	255	THR	2.3
1	T	195	LYS	2.2
1	O	214	GLY	2.2
1	T	165	VAL	2.2
1	O	197	PHE	2.2
1	A	212	ILE	2.2
1	J	165	VAL	2.2
1	N	167	ILE	2.2
1	K	252	LEU	2.2
1	L	223	GLU	2.2
1	S	235	LEU	2.2
1	B	223	GLU	2.2
1	K	223	GLU	2.2
1	E	171	PRO	2.2
1	T	163	LYS	2.2
1	T	254	LYS	2.2
1	J	3	ALA	2.2
1	O	205	GLY	2.2
1	Q	64	ALA	2.2
1	T	202	ALA	2.2
1	O	249	ILE	2.2
1	B	2	PRO	2.2
1	R	252	LEU	2.2
1	T	50	THR	2.2
1	R	175	ILE	2.1
1	Q	3	ALA	2.1
1	A	218	ASN	2.1
1	C	218	ASN	2.1
1	E	126	PHE	2.1
1	O	216	SER	2.1
1	F	111	ALA	2.1
1	O	137	ALA	2.1
1	O	253	THR	2.1
1	L	252	LEU	2.1
1	R	5	ARG	2.1
1	R	147	GLN	2.1
1	D	151	LEU	2.1
1	Q	28	ILE	2.1
1	S	167	ILE	2.1
1	P	129	GLY	2.1
1	N	193	LEU	2.1
1	Q	91	HIS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	Q	201	VAL	2.1
1	R	212	ILE	2.1
1	P	117	ALA	2.1
1	L	246	MET	2.1
1	O	157	GLU	2.1
1	L	211	ILE	2.1
1	G	216	SER	2.1
1	Q	95	GLY	2.1
1	T	62	ILE	2.0
1	C	222	ASP	2.0
1	P	140	THR	2.0
1	E	200	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.