



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:27 PM UTC

PDB ID : 2Q2E / pdb_00002q2e
Title : Crystal structure of the topoisomerase VI holoenzyme from *Methanosarcina mazei*
Authors : Corbett, K.D.; Benedetti, P.; Berger, J.M.
Deposited on : 2007-05-28
Resolution : 4.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

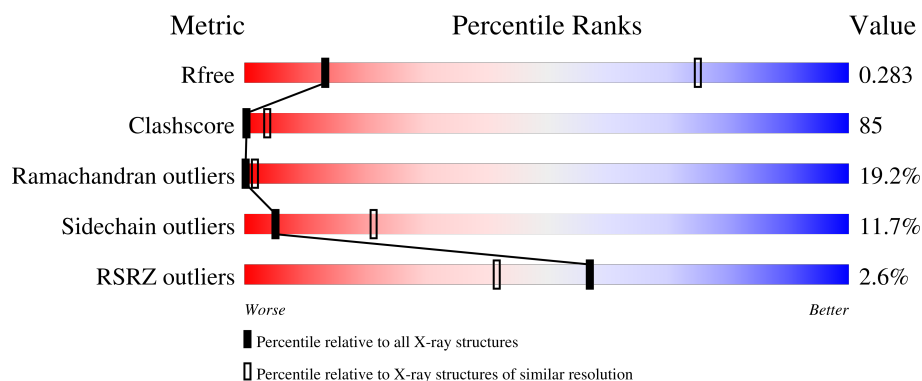
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	369	 3% 15% 46% 22% 15%
2	B	621	 2% 16% 49% 25% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7039 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 Type II DNA topoisomerase VI subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2532	1610	423	490	9			

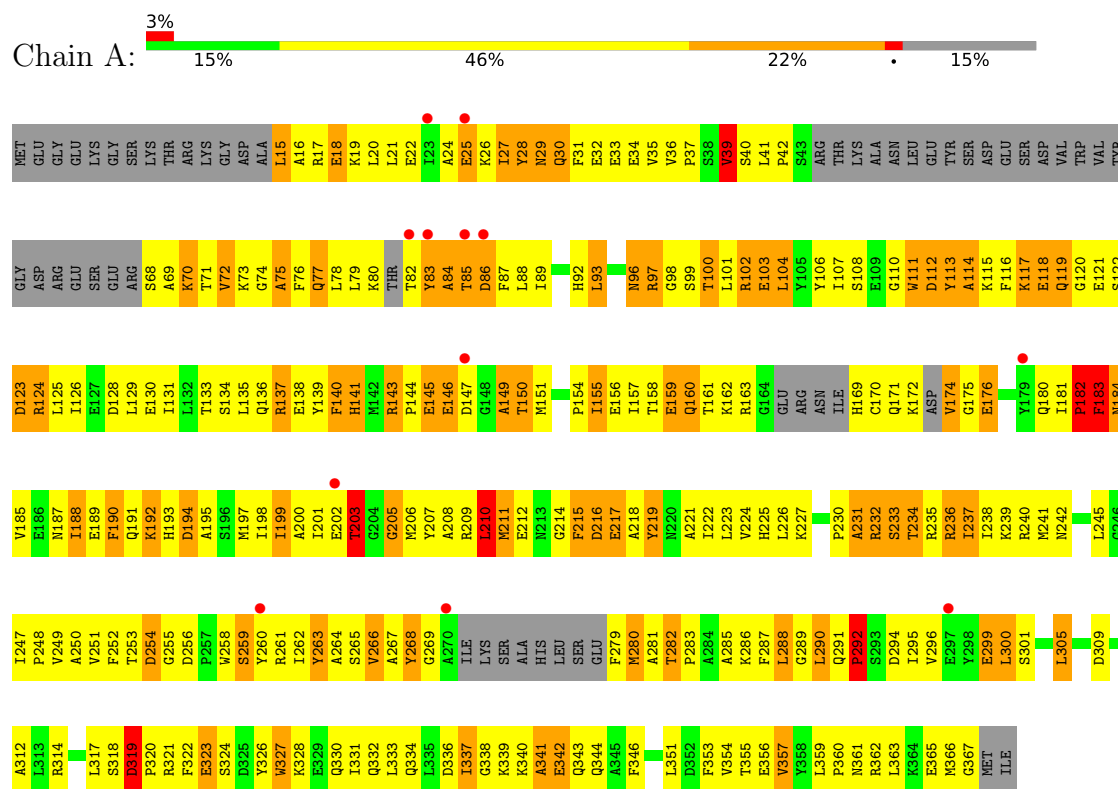
- Molecule 2 is a protein called Type 2 DNA topoisomerase 6 subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	582	Total	C	N	O	S	0	0	1
			4507	2878	768	843	18			

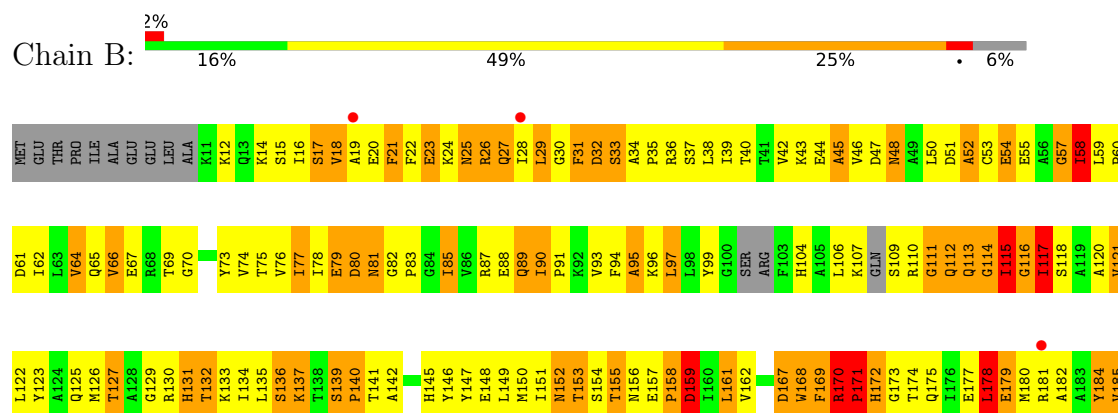
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Type II DNA topoisomerase VI subunit A



• Molecule 2: Type 2 DNA topoisomerase 6 subunit B



E558	D497	A437	A377	L317	N249	K186
P559	V498	I438	N378	S318	L250	G187
K560	D499	A439	R379	P319	R251	R188
V561	D500	D440	V380	I320	Y252	R189
V562	I501	I441	P381	G321	T253	Q190
T563	N502	P442	L382	E322	E254	S191
M564	P503	V443	L383	D323	ARG	I192
	V504	I444	Y384	L324	GLN	Y193
D567	V505	K445	Q385	I325	LYS	E194
Y568	A506	E446	Q386	Y326	LEU	Y195
D569	K507	E447	G387	R327	ALA	L196
Y570	I508	I448	G388	G328	P260	K197
V571	M509	D449	C389	L329	F261	A198
	G510	L450	V390	E330	L262	T199
S575	N511	A451	T391	K331	R263	A200
A576	L512	L452	T392	E332		I201
S577	L513	K453	H393	T333	C267	V202
	V514	E454	A394	T334	T268	N203
S580	H515	V455	V395	V335	ILE	P204
S581	H516	A456	E396	D336	GLY	H205
K582	V517	K457	D397	F337	L271	A206
L583	I518	K458	I398	I338	T272	R207
S585		L459	K399	A339	T273	I208
Y586		K460	N400	T340	A274	T209
K587		H461	K401	S341		L210
	N521	Y462	Q402	T342	I277	I211
	G522	L463	Y403	R343	C278	D212
D523	G524	S464	G404	K345		P213
E525	T525	K465	L405	P345	A281	D214
V526	V526	Q466	N406	A346	G282	G215
D527	D527	S467	Q407	Y347	L283	N216
V528	V528	M468	P408	Y348	D284	E217
A529	A529	L469	G409	S349	P285	E218
I530	I530	K470	G410	G350	V219	V219
K531	K531	K471	G411	N351	I287	F220
L596	V532	R472	I412	P352	D288	E221
Q597	K533	R473	P413	F353	P289	R222
K598	N534	E474	V414	V354	H290	A223
	PHE	K475	G415	V355	A291	T224
	GLY	E476	P416	E356	L292	D225
	THR	K477	V417	V357		K226
	SER	I477	V417	G358	A297	H227
A539	A539	I478	I418	M359		P228
Y540	Y540	T480	L419	A360		E229
S541	S541	K481	I421	Y361	L300	P230
F542	F542	V482	H422	G362	I301	A231
R543	R543	L483	V423	G363	E302	E232
V544	V544	P484	A424	N364	A303	E233
H545	H545	K485	S425	L365	F304	E234
E546	E546	L486	T426	P366	E305	I234
M547	M547	A487	M427	K367	K306	L235
L548	L548	A488	V428	E368	V307	F236
P549	P549	K489	P429	E369	K308	H237
C550	C550	V490	F430	K370	I309	P238
K551	K551	A491	T431	I371	A311	E239
V552	V552	H492	S432	S372	P312	G240
SER	SER	V493	E433	I373	P313	I241
GLY	GLY	L494	S434	M374	T314	
ALA	ALA	E495	K435	K375	D315	T245
PHE	PHE	K496	D436	F376	C316	L246
VAL	VAL					

4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	227.81Å 227.81Å 208.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 4.00 30.00 – 4.00	Depositor EDS
% Data completeness (in resolution range)	94.2 (30.00-4.00) 93.8 (30.00-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 4.01Å)	Xtriage
Refinement program	REFMAC 5.3.0026	Depositor
R, R_{free}	0.306 , 0.349 0.301 , 0.283	Depositor DCC
R_{free} test set	1298 reflections (4.03%)	wwPDB-VP
Wilson B-factor (Å ²)	153.1	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 213.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7039	wwPDB-VP
Average B, all atoms (Å ²)	192.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.50	0/2579	1.13	25/3471 (0.7%)
2	B	0.67	0/4591	1.29	68/6215 (1.1%)
All	All	0.61	0/7170	1.24	93/9686 (1.0%)

There are no bond length outliers.

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	587	LYS	N-CA-C	11.59	123.52	108.34
2	B	223	ALA	N-CA-C	10.96	122.41	107.73
1	A	103	GLU	N-CA-C	-10.51	100.18	113.43
1	A	266	VAL	N-CA-C	-9.91	104.30	113.71
2	B	428	VAL	N-CA-C	9.86	119.34	107.61
2	B	18	VAL	N-CA-C	9.85	120.74	111.48
2	B	498	VAL	CA-C-N	9.80	132.09	119.84
2	B	498	VAL	C-N-CA	9.80	132.09	119.84
2	B	561	VAL	N-CA-C	9.59	122.25	109.21
2	B	474	GLU	N-CA-C	-9.39	101.02	111.07
1	A	237	ILE	N-CA-C	-9.30	103.81	111.81
2	B	70	GLY	CA-C-N	9.27	128.62	118.97
2	B	70	GLY	C-N-CA	9.27	128.62	118.97
2	B	488	ALA	N-CA-C	-8.90	102.55	113.41
2	B	142	ALA	CA-C-N	-8.88	111.24	120.03
2	B	142	ALA	C-N-CA	-8.88	111.24	120.03
2	B	414	VAL	N-CA-C	8.33	121.69	108.85
2	B	58	ILE	N-CA-C	8.15	126.29	109.34
1	A	327	TRP	N-CA-C	-8.07	103.45	113.38
2	B	235	LEU	N-CA-C	-8.02	100.90	110.13
2	B	398	ILE	N-CA-C	7.65	121.20	108.81
2	B	139	SER	CA-C-N	7.63	129.37	119.84
2	B	139	SER	C-N-CA	7.63	129.37	119.84
1	A	199	ILE	N-CA-C	7.46	118.81	107.77
1	A	319	ASP	CA-C-N	7.44	129.14	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	ASP	C-N-CA	7.44	129.14	119.84
2	B	25	ASN	N-CA-C	-7.17	103.85	112.59
2	B	542	PHE	N-CA-C	6.92	120.78	109.72
1	A	159	GLU	N-CA-C	6.89	122.10	112.93
2	B	95	ALA	N-CA-C	-6.79	98.74	109.07
2	B	591	ALA	N-CA-C	6.62	117.37	108.23
2	B	408	PRO	N-CA-CB	6.58	110.29	102.85
2	B	252	TYR	N-CA-C	6.57	121.13	112.72
2	B	170	ARG	CA-C-N	6.55	128.03	119.84
2	B	170	ARG	C-N-CA	6.55	128.03	119.84
2	B	544	VAL	N-CA-C	6.54	117.44	107.77
2	B	263	ARG	N-CA-C	-6.54	105.27	112.72
2	B	585	SER	N-CA-C	6.45	118.33	109.18
1	A	100	THR	N-CA-C	6.44	118.97	109.69
1	A	104	LEU	N-CA-C	-6.42	104.20	111.07
2	B	571	VAL	N-CA-C	6.36	116.54	106.88
2	B	368	GLU	N-CA-C	6.29	119.20	109.07
2	B	470	LYS	N-CA-C	-6.24	104.40	111.07
1	A	288	LEU	N-CA-C	-6.20	105.58	113.02
1	A	27	ILE	N-CA-C	-6.19	104.47	110.72
2	B	57	GLY	N-CA-C	6.16	127.79	113.18
2	B	597	GLN	N-CA-C	6.16	123.92	110.80
1	A	231	ALA	N-CA-C	6.13	113.81	108.78
1	A	210	LEU	N-CA-C	-6.11	105.69	113.02
2	B	522	GLY	N-CA-C	-6.10	98.72	113.18
2	B	33	SER	N-CA-C	6.07	119.82	110.42
2	B	184	TYR	N-CA-C	-6.06	101.64	111.04
1	A	75	ALA	N-CA-C	-6.04	104.65	112.68
2	B	18	VAL	CB-CA-C	-6.03	106.58	111.71
2	B	588	ILE	N-CA-C	6.03	121.88	109.34
2	B	288	ASP	CA-C-N	5.87	127.18	119.84
2	B	288	ASP	C-N-CA	5.87	127.18	119.84
2	B	362	GLY	N-CA-C	5.68	126.64	113.18
2	B	338	ILE	N-CA-C	5.65	117.81	108.99
2	B	549	PRO	N-CA-C	5.63	120.95	113.40
2	B	167	ASP	N-CA-C	5.59	117.42	108.41
2	B	527	ASP	N-CA-C	5.57	117.98	108.90
2	B	472	ARG	N-CA-C	-5.56	106.19	114.64
2	B	85	ILE	N-CA-C	5.54	116.71	108.46
1	A	263	TYR	N-CA-C	-5.45	104.98	111.69
1	A	25	GLU	N-CA-C	-5.45	105.76	112.90
2	B	304	PHE	N-CA-C	-5.44	105.70	112.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	509	MET	N-CA-C	-5.42	106.50	113.01
2	B	290	HIS	N-CA-C	5.41	117.31	110.33
1	A	19	LYS	N-CA-C	-5.40	106.39	112.87
2	B	562	VAL	N-CA-C	-5.36	100.13	108.81
1	A	188	ILE	N-CA-C	5.34	120.44	109.34
2	B	419	LEU	N-CA-C	5.33	117.59	108.90
1	A	131	ILE	N-CA-C	5.32	117.22	111.58
2	B	599	LEU	N-CA-C	5.31	119.04	109.44
2	B	240	GLY	N-CA-C	-5.30	107.47	114.95
2	B	473	ARG	N-CA-C	-5.29	107.48	114.31
2	B	377	ALA	N-CA-C	5.29	117.25	108.20
2	B	136	SER	N-CA-C	5.25	117.23	108.99
2	B	48	ASN	N-CA-C	-5.23	104.83	111.11
1	A	259	SER	N-CA-C	-5.23	106.96	113.55
2	B	427	ASN	CA-C-N	-5.22	118.79	123.33
2	B	427	ASN	C-N-CA	-5.22	118.79	123.33
1	A	231	ALA	CA-C-O	5.22	120.97	117.94
2	B	364	ASN	N-CA-C	-5.21	106.18	112.54
2	B	241	ILE	N-CA-C	-5.20	100.90	108.97
2	B	178	LEU	N-CA-C	5.17	117.40	109.07
1	A	357	VAL	N-CA-C	5.14	120.02	109.34
2	B	198	ALA	N-CA-C	-5.14	105.59	111.14
2	B	332	GLU	N-CA-C	5.13	118.68	112.93
2	B	316	CYS	N-CA-C	5.12	121.70	110.80
1	A	216	ASP	N-CA-C	5.07	118.93	112.34
1	A	217	GLU	N-CA-C	5.01	116.75	108.48

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	2532	0	2476	415	0
2	B	4507	0	4565	808	0
All	All	7039	0	7041	1192	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 85.

All (1192) 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)
2:B:599:LEU:HD23	2:B:599:LEU:H	1.09	1.13
2:B:516:ARG:HH12	2:B:597:GLN:HB2	0.93	1.09
2:B:371:ILE:HG22	2:B:414:VAL:HG12	1.13	1.09
2:B:66:VAL:HG23	2:B:213:PRO:HD3	1.35	1.08
2:B:77:ILE:C	2:B:78:ILE:HD12	1.78	1.06
2:B:222:ARG:HH21	2:B:332:GLU:HB2	1.12	1.06
2:B:238:PRO:HA	2:B:241:ILE:HD12	1.35	1.05
1:A:31:PHE:HB2	2:B:489:LYS:HD3	1.39	1.05
1:A:15:LEU:HD12	1:A:96:ASN:HA	1.38	1.05
2:B:137:LYS:HG3	2:B:171:PRO:HA	1.34	1.05
2:B:374:MET:HE3	2:B:418:ILE:HD11	1.39	1.04
1:A:87:PHE:HA	2:B:492:HIS:NE2	1.73	1.03
2:B:201:ILE:HD11	2:B:329:LEU:HG	1.38	1.03
2:B:232:GLU:CD	2:B:316:CYS:HA	1.84	1.01
2:B:365:LEU:HB3	2:B:366:PRO:HD2	1.41	1.01
2:B:516:ARG:NH1	2:B:597:GLN:HB2	1.75	0.99
2:B:588:ILE:HG12	2:B:589:GLU:H	1.27	0.99
2:B:497:ASP:O	2:B:499:PRO:HD3	1.62	0.99
1:A:305:LEU:HD12	1:A:305:LEU:H	1.23	0.98
2:B:168:TRP:CE3	2:B:169:PHE:HA	1.97	0.97
2:B:190:GLN:HG2	2:B:383:LEU:HD21	1.45	0.97
2:B:222:ARG:NH2	2:B:332:GLU:HB2	1.80	0.97
1:A:83:TYR:CD1	2:B:488:ALA:HB1	2.01	0.95
2:B:246:LEU:HD23	2:B:297:ALA:HB1	1.48	0.95
2:B:307:VAL:HG22	2:B:309:ILE:HD11	1.48	0.94
2:B:335:VAL:HG22	2:B:336:ASP:H	1.33	0.94
2:B:335:VAL:HG11	2:B:338:ILE:HD11	1.50	0.93
2:B:114:GLY:O	2:B:116:GLY:N	2.01	0.93
1:A:324:SER:HB3	1:A:327:TRP:HD1	1.34	0.92
2:B:390:VAL:HG23	2:B:438:ILE:O	1.70	0.92
1:A:203:THR:OG1	1:A:206:MET:HB3	1.68	0.92
2:B:210:LEU:HD12	2:B:211:ILE:N	1.85	0.91
1:A:253:THR:HB	1:A:259:SER:HB3	1.54	0.89
1:A:20:LEU:HD12	1:A:21:LEU:N	1.88	0.89
1:A:31:PHE:HB2	2:B:489:LYS:CD	2.03	0.89
1:A:239:LYS:NZ	1:A:279:PHE:HA	1.88	0.89
2:B:490:VAL:C	2:B:492:HIS:H	1.79	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:359:MET:HE2	2:B:455:VAL:HG23	1.56	0.88
2:B:411:GLY:O	2:B:412:ILE:HG13	1.72	0.88
1:A:201:ILE:HD11	1:A:207:TYR:HD1	1.37	0.88
1:A:28:TYR:HE1	2:B:489:LYS:HG2	1.38	0.87
2:B:552:VAL:HB	2:B:587:LYS:HB2	1.56	0.87
2:B:58:ILE:HG22	2:B:59:LEU:H	1.40	0.87
1:A:156:GLU:O	1:A:157:ILE:HG13	1.73	0.87
2:B:64:VAL:HG22	2:B:78:ILE:HG13	1.55	0.87
2:B:497:ASP:CG	2:B:498:VAL:H	1.81	0.87
1:A:206:MET:H	1:A:344:GLN:HE21	1.23	0.87
2:B:546:GLU:HG3	2:B:548:LEU:HD11	1.57	0.86
2:B:61:ASP:HB2	2:B:207:ARG:HH11	1.38	0.86
2:B:367:LYS:HE2	2:B:367:LYS:HA	1.55	0.86
2:B:507:LYS:HG3	2:B:533:LYS:NZ	1.89	0.85
1:A:239:LYS:HD3	1:A:279:PHE:HD2	1.40	0.85
1:A:237:ILE:HG22	1:A:241:MET:HE2	1.58	0.85
2:B:381:PRO:O	2:B:382:LEU:HB2	1.75	0.85
2:B:65:GLN:HG3	2:B:211:ILE:HG13	1.59	0.85
2:B:125:GLN:HE22	2:B:151:ILE:HB	1.42	0.85
1:A:185:VAL:HG21	1:A:236:ARG:HB3	1.56	0.84
2:B:107:LYS:HZ2	2:B:378:ASN:CG	1.85	0.84
1:A:28:TYR:CE1	2:B:489:LYS:HG2	2.13	0.83
1:A:69:ALA:HB2	1:A:78:LEU:HD11	1.60	0.83
2:B:569:ASP:OD2	2:B:571:VAL:HG23	1.78	0.83
1:A:188:ILE:HG12	1:A:240:ARG:NH2	1.93	0.83
1:A:188:ILE:HG21	1:A:240:ARG:CZ	2.08	0.82
2:B:241:ILE:HG23	2:B:245:THR:HG21	1.60	0.82
2:B:96:LYS:HE2	2:B:114:GLY:HA3	1.60	0.82
1:A:197:MET:O	1:A:221:ALA:HA	1.79	0.82
1:A:252:PHE:HD1	1:A:289:GLY:HA2	1.41	0.81
1:A:338:GLY:O	1:A:339:LYS:HG3	1.80	0.81
2:B:371:ILE:CG2	2:B:414:VAL:HG12	2.04	0.81
2:B:127:THR:CG2	2:B:181:ARG:HB3	2.09	0.81
2:B:122:LEU:HD22	2:B:126:MET:HE2	1.63	0.81
1:A:324:SER:HB3	1:A:327:TRP:CD1	2.16	0.81
2:B:168:TRP:O	2:B:169:PHE:HB2	1.80	0.81
2:B:137:LYS:CG	2:B:172:HIS:H	1.95	0.81
1:A:31:PHE:CB	2:B:489:LYS:HD3	2.11	0.80
2:B:453:LYS:HE2	2:B:457:ARG:NH2	1.95	0.80
1:A:342:GLU:HG3	1:A:343:GLN:H	1.47	0.80
1:A:252:PHE:CD1	1:A:289:GLY:HA2	2.15	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ILE:HG21	1:A:240:ARG:NE	1.95	0.80
1:A:69:ALA:CB	1:A:78:LEU:HD11	2.11	0.80
1:A:135:LEU:HB2	1:A:140:PHE:CE1	2.16	0.80
1:A:161:THR:HG23	1:A:162:LYS:HG3	1.64	0.80
1:A:202:GLU:O	1:A:203:THR:HG23	1.82	0.80
1:A:206:MET:HE1	1:A:354:VAL:HG11	1.62	0.80
1:A:101:LEU:HD22	1:A:122:SER:HB3	1.64	0.80
1:A:198:ILE:HB	1:A:249:VAL:HG22	1.64	0.80
2:B:335:VAL:HG22	2:B:336:ASP:N	1.94	0.79
1:A:169:HIS:O	1:A:174:VAL:HG13	1.82	0.79
2:B:27:GLN:HG2	2:B:32:ASP:HB2	1.62	0.79
2:B:501:ILE:O	2:B:505:VAL:HG23	1.82	0.79
2:B:557:PRO:HG3	2:B:584:LEU:HA	1.63	0.79
2:B:595:GLU:O	2:B:596:LEU:HG	1.82	0.79
2:B:599:LEU:HD23	2:B:599:LEU:N	1.94	0.78
2:B:107:LYS:HZ2	2:B:378:ASN:ND2	1.81	0.78
1:A:70:LYS:HG2	1:A:71:THR:HG23	1.64	0.78
2:B:210:LEU:HD12	2:B:210:LEU:C	2.08	0.78
2:B:375:ARG:NH1	2:B:382:LEU:HD23	1.99	0.78
1:A:88:LEU:O	1:A:92:HIS:HB2	1.83	0.78
1:A:363:LEU:O	1:A:363:LEU:HD23	1.83	0.78
2:B:551:LYS:HE3	2:B:552:VAL:C	2.09	0.78
2:B:65:GLN:O	2:B:66:VAL:HG13	1.83	0.78
2:B:365:LEU:HB3	2:B:366:PRO:CD	2.12	0.78
2:B:127:THR:HG21	2:B:181:ARG:HB3	1.64	0.77
1:A:31:PHE:CE1	1:A:32:GLU:HG3	2.20	0.77
2:B:597:GLN:O	2:B:598:LYS:HB3	1.82	0.77
2:B:411:GLY:C	2:B:412:ILE:HG13	2.08	0.77
1:A:133:THR:HG1	1:A:140:PHE:HZ	1.29	0.77
2:B:80:ASP:OD1	2:B:174:THR:HG23	1.85	0.77
2:B:202:VAL:C	2:B:204:PRO:HD3	2.09	0.77
1:A:133:THR:O	1:A:135:LEU:HG	1.84	0.77
2:B:375:ARG:HG3	2:B:375:ARG:HH11	1.49	0.77
1:A:242:ASN:OD1	1:A:282:THR:HG23	1.84	0.76
1:A:290:LEU:HD21	1:A:341:ALA:HB1	1.68	0.76
2:B:359:MET:HE2	2:B:455:VAL:CG2	2.16	0.76
1:A:200:ALA:HB3	1:A:251:VAL:HA	1.68	0.76
2:B:465:LYS:O	2:B:468:ASN:HB3	1.86	0.76
2:B:335:VAL:HG11	2:B:338:ILE:CD1	2.15	0.75
1:A:154:PRO:HG2	1:A:195:ALA:HB2	1.69	0.75
2:B:60:PRO:HA	2:B:81:ASN:ND2	2.00	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:TYR:CE1	2:B:181:ARG:HB2	2.22	0.75
2:B:114:GLY:C	2:B:116:GLY:H	1.94	0.75
2:B:145:HIS:HB3	2:B:147:TYR:CE1	2.22	0.75
1:A:20:LEU:HB2	1:A:135:LEU:HD13	1.68	0.75
2:B:551:LYS:HG2	2:B:552:VAL:N	2.01	0.75
2:B:77:ILE:N	2:B:77:ILE:HD12	2.02	0.75
2:B:353:PHE:HA	2:B:424:ALA:O	1.86	0.75
2:B:106:LEU:HB2	2:B:232:GLU:O	1.87	0.75
1:A:29:ASN:C	1:A:31:PHE:H	1.92	0.74
2:B:137:LYS:HG3	2:B:172:HIS:H	1.52	0.74
1:A:31:PHE:O	1:A:35:VAL:HG23	1.86	0.74
1:A:328:LYS:O	1:A:332:GLN:HG3	1.88	0.74
1:A:15:LEU:HD13	1:A:93:LEU:O	1.87	0.74
2:B:184:TYR:HE1	2:B:192:ILE:HG12	1.51	0.74
2:B:171:PRO:O	2:B:172:HIS:HB2	1.88	0.74
2:B:561:VAL:HG22	2:B:570:TYR:CD1	2.22	0.74
2:B:188:ARG:O	2:B:190:GLN:N	2.21	0.74
2:B:125:GLN:O	2:B:129:GLY:HA2	1.88	0.73
2:B:453:LYS:HE2	2:B:457:ARG:HH21	1.53	0.73
2:B:37:SER:HB2	2:B:182:ALA:HB1	1.70	0.73
2:B:507:LYS:HG3	2:B:533:LYS:HZ2	1.51	0.73
1:A:35:VAL:HG11	2:B:486:LEU:HD13	1.70	0.73
2:B:473:ARG:HG3	2:B:473:ARG:HH11	1.53	0.73
1:A:72:VAL:H	2:B:478:ILE:HD11	1.53	0.73
2:B:390:VAL:HG22	2:B:440:ASP:HA	1.70	0.73
1:A:225:HIS:O	1:A:226:LEU:HD23	1.89	0.73
2:B:222:ARG:HH21	2:B:332:GLU:CB	1.97	0.73
2:B:532:VAL:HG22	2:B:533:LYS:N	2.04	0.73
2:B:528:VAL:HG12	2:B:584:LEU:HD12	1.71	0.73
2:B:599:LEU:H	2:B:599:LEU:CD2	1.91	0.72
2:B:322:GLU:O	2:B:340:THR:HG21	1.89	0.72
1:A:239:LYS:HZ3	1:A:279:PHE:HA	1.53	0.72
1:A:264:ALA:HA	1:A:267:ALA:HB3	1.70	0.72
2:B:133:LYS:HB3	2:B:177:GLU:HB3	1.72	0.72
2:B:232:GLU:OE1	2:B:316:CYS:HA	1.87	0.72
2:B:74:VAL:O	2:B:179:GLU:HA	1.89	0.72
1:A:135:LEU:HB2	1:A:140:PHE:HE1	1.54	0.72
2:B:76:VAL:HG12	2:B:78:ILE:HD11	1.70	0.72
1:A:356:GLU:O	1:A:360:PRO:HG3	1.90	0.71
2:B:222:ARG:HH12	2:B:331:LYS:HB2	1.54	0.71
1:A:78:LEU:HB3	2:B:485:LYS:HZ1	1.56	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:149:LEU:HD12	2:B:150:MET:H	1.54	0.71
2:B:237:HIS:CD2	2:B:312:PRO:HG3	2.26	0.71
2:B:401:LYS:NZ	2:B:406:ASN:HD21	1.88	0.71
2:B:490:VAL:O	2:B:492:HIS:N	2.22	0.71
1:A:279:PHE:O	1:A:280:MET:HG3	1.90	0.70
2:B:561:VAL:HG22	2:B:570:TYR:HD1	1.54	0.70
2:B:335:VAL:HG21	2:B:360:ALA:HB1	1.73	0.70
1:A:78:LEU:HB3	2:B:485:LYS:NZ	2.07	0.70
2:B:184:TYR:CE1	2:B:192:ILE:HG21	2.27	0.70
1:A:234:THR:O	1:A:237:ILE:HB	1.92	0.70
2:B:78:ILE:HD12	2:B:78:ILE:N	2.06	0.70
2:B:238:PRO:HG2	2:B:239:GLU:OE1	1.90	0.69
2:B:586:TYR:C	2:B:587:LYS:HD3	2.17	0.69
2:B:96:LYS:C	2:B:97:LEU:HD23	2.17	0.69
2:B:241:ILE:HG23	2:B:245:THR:CG2	2.22	0.69
1:A:235:ARG:HD3	1:A:265:SER:O	1.92	0.69
2:B:112:GLN:HB2	2:B:435:LYS:HD3	1.74	0.69
2:B:113:GLN:O	2:B:115:ILE:HG13	1.92	0.69
2:B:137:LYS:HE3	2:B:173:GLY:H	1.55	0.69
2:B:235:LEU:HD12	2:B:267:CYS:HB3	1.74	0.69
2:B:348:TYR:O	2:B:350:GLY:N	2.25	0.69
2:B:508:ILE:CG2	2:B:509:MET:N	2.55	0.69
2:B:588:ILE:HG12	2:B:589:GLU:N	2.02	0.69
1:A:154:PRO:O	1:A:155:ILE:HG23	1.92	0.69
1:A:342:GLU:HG3	1:A:343:GLN:N	2.05	0.69
2:B:65:GLN:HG2	2:B:66:VAL:H	1.56	0.69
2:B:232:GLU:OE2	2:B:316:CYS:HA	1.91	0.69
2:B:237:HIS:CG	2:B:312:PRO:HG3	2.27	0.69
1:A:15:LEU:CD1	1:A:96:ASN:HA	2.18	0.69
1:A:20:LEU:HB2	1:A:135:LEU:CD1	2.22	0.69
2:B:90:ILE:HG22	2:B:91:PRO:N	2.08	0.69
2:B:170:ARG:HG2	2:B:170:ARG:HH11	1.57	0.69
2:B:557:PRO:HD3	2:B:585:SER:H	1.57	0.69
2:B:212:ASP:HB2	2:B:213:PRO:HD2	1.75	0.69
2:B:360:ALA:HB3	2:B:418:ILE:CG2	2.22	0.69
2:B:396:GLU:HG2	2:B:412:ILE:HG23	1.75	0.69
2:B:139:SER:HB2	2:B:140:PRO:HD2	1.74	0.68
2:B:151:ILE:O	2:B:152:ASN:C	2.35	0.68
2:B:400:TRP:HZ3	2:B:408:PRO:HA	1.58	0.68
2:B:334:THR:HB	2:B:364:ASN:HB2	1.75	0.68
1:A:253:THR:CB	1:A:259:SER:HB3	2.24	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:LYS:HG3	2:B:378:ASN:HD21	1.59	0.68
2:B:401:LYS:HZ3	2:B:406:ASN:HD21	1.39	0.68
1:A:157:ILE:HG22	1:A:158:THR:N	2.08	0.68
2:B:355:VAL:HG22	2:B:423:VAL:HG12	1.76	0.68
1:A:236:ARG:HG3	1:A:280:MET:HG3	1.74	0.68
1:A:79:LEU:O	1:A:79:LEU:HD23	1.93	0.68
1:A:214:GLY:O	1:A:215:PHE:HB2	1.92	0.68
2:B:38:LEU:HD13	2:B:184:TYR:HB2	1.76	0.68
2:B:345:PRO:HA	2:B:354:VAL:HG12	1.75	0.68
2:B:531:LYS:HE2	2:B:581:SER:HB2	1.76	0.68
2:B:324:LEU:HD12	2:B:324:LEU:H	1.60	0.67
2:B:66:VAL:O	2:B:213:PRO:HD3	1.94	0.67
1:A:203:THR:C	1:A:205:GLY:H	2.00	0.67
1:A:27:ILE:HD11	1:A:133:THR:HG21	1.76	0.67
1:A:117:LYS:HB2	1:A:117:LYS:NZ	2.10	0.67
2:B:425:SER:OG	2:B:428:VAL:HG22	1.94	0.67
1:A:239:LYS:HD3	1:A:279:PHE:CD2	2.27	0.67
2:B:137:LYS:HE3	2:B:173:GLY:CA	2.25	0.67
2:B:38:LEU:HA	2:B:180:MET:CE	2.25	0.67
2:B:516:ARG:HH12	2:B:597:GLN:CB	1.89	0.67
2:B:335:VAL:CG2	2:B:336:ASP:H	2.07	0.67
2:B:531:LYS:CD	2:B:581:SER:HB2	2.25	0.67
2:B:137:LYS:HE3	2:B:173:GLY:N	2.10	0.67
2:B:320:ILE:CD1	2:B:379:ARG:HH11	2.08	0.67
2:B:342:THR:HG23	2:B:356:GLU:HG2	1.77	0.67
2:B:343:ARG:HG3	2:B:343:ARG:HH11	1.59	0.67
2:B:518:ILE:HG22	2:B:526:VAL:HG13	1.77	0.67
1:A:39:VAL:HG12	1:A:40:SER:H	1.61	0.66
1:A:112:ASP:O	1:A:114:ALA:N	2.28	0.66
2:B:114:GLY:C	2:B:116:GLY:N	2.51	0.66
2:B:366:PRO:O	2:B:416:PRO:HG3	1.95	0.66
1:A:201:ILE:HD11	1:A:207:TYR:CD1	2.26	0.66
2:B:576:ALA:HB1	2:B:580:SER:HB3	1.78	0.66
1:A:75:ALA:HB3	2:B:481:LYS:HZ2	1.61	0.66
2:B:36:ARG:HA	2:B:39:ILE:HG22	1.77	0.66
1:A:181:ILE:HG13	1:A:181:ILE:O	1.94	0.66
2:B:48:ASN:HD21	2:B:117:ILE:HG12	1.61	0.66
2:B:66:VAL:HG12	2:B:76:VAL:HG22	1.75	0.66
1:A:230:PRO:HD3	1:A:262:ILE:HG23	1.77	0.66
2:B:27:GLN:CG	2:B:32:ASP:HB2	2.26	0.66
1:A:282:THR:O	1:A:282:THR:HG22	1.94	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:VAL:HG21	2:B:486:LEU:HD22	1.77	0.65
2:B:38:LEU:HA	2:B:180:MET:HE1	1.78	0.65
2:B:66:VAL:HA	2:B:75:THR:O	1.96	0.65
2:B:514:VAL:HG12	2:B:530:ILE:HG12	1.77	0.65
2:B:192:ILE:HG23	2:B:193:TYR:H	1.61	0.65
2:B:307:VAL:HG13	2:B:307:VAL:O	1.96	0.65
1:A:28:TYR:C	1:A:31:PHE:HD2	2.05	0.65
1:A:326:TYR:O	1:A:330:GLN:HG2	1.96	0.65
2:B:205:HIS:CD2	2:B:228:PRO:HD3	2.32	0.65
2:B:290:HIS:CG	2:B:291:ALA:N	2.64	0.65
1:A:266:VAL:O	1:A:281:ALA:HA	1.97	0.65
1:A:282:THR:HG22	1:A:285:ALA:HB2	1.79	0.65
2:B:190:GLN:CG	2:B:383:LEU:HD11	2.27	0.65
2:B:246:LEU:HD23	2:B:297:ALA:CB	2.26	0.65
1:A:233:SER:O	1:A:237:ILE:HG12	1.97	0.65
2:B:66:VAL:CG1	2:B:76:VAL:HG13	2.27	0.65
2:B:112:GLN:HA	2:B:112:GLN:OE1	1.96	0.65
2:B:284:ASP:HB2	2:B:287:ILE:HG23	1.78	0.65
1:A:83:TYR:O	1:A:85:THR:N	2.29	0.64
2:B:60:PRO:HA	2:B:81:ASN:HD22	1.60	0.64
2:B:94:PHE:CD1	2:B:134:ILE:HD11	2.32	0.64
2:B:399:LYS:HG2	2:B:403:TYR:CD1	2.33	0.64
1:A:154:PRO:CG	1:A:195:ALA:HB2	2.25	0.64
1:A:159:GLU:O	1:A:160:GLN:HB2	1.97	0.64
1:A:206:MET:N	1:A:344:GLN:HE21	1.94	0.64
2:B:220:PHE:HD2	2:B:332:GLU:CD	2.05	0.64
2:B:576:ALA:HB2	2:B:582:LYS:HE3	1.80	0.64
1:A:133:THR:OG1	1:A:140:PHE:HZ	1.79	0.64
1:A:157:ILE:HG12	1:A:190:PHE:HA	1.79	0.64
2:B:137:LYS:HE3	2:B:173:GLY:C	2.21	0.64
1:A:123:ASP:O	1:A:124:ARG:C	2.40	0.64
2:B:229:GLU:HG3	2:B:230:PRO:HD2	1.79	0.64
2:B:371:ILE:HG21	2:B:413:PRO:O	1.97	0.64
2:B:523:ASP:O	2:B:588:ILE:HD12	1.97	0.64
1:A:31:PHE:CG	1:A:32:GLU:N	2.66	0.64
1:A:181:ILE:CD1	1:A:237:ILE:HG13	2.28	0.64
1:A:200:ALA:HB3	1:A:250:ALA:O	1.98	0.64
1:A:268:TYR:HB2	1:A:322:PHE:HE2	1.62	0.64
2:B:375:ARG:HD2	2:B:382:LEU:HD23	1.79	0.64
2:B:189:ARG:O	2:B:190:GLN:CB	2.46	0.64
2:B:495:GLU:O	2:B:497:ASP:N	2.31	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:309:ILE:HG22	2:B:310:MET:N	2.13	0.64
2:B:412:ILE:O	2:B:412:ILE:HD12	1.98	0.64
1:A:104:LEU:HD23	1:A:122:SER:OG	1.98	0.64
2:B:151:ILE:O	2:B:151:ILE:HG22	1.97	0.64
2:B:400:TRP:HZ2	2:B:411:GLY:N	1.96	0.64
2:B:531:LYS:CE	2:B:581:SER:HB2	2.28	0.64
2:B:497:ASP:CG	2:B:498:VAL:N	2.54	0.63
2:B:367:LYS:O	2:B:416:PRO:HG3	1.98	0.63
2:B:373:ILE:HG12	2:B:373:ILE:O	1.99	0.63
1:A:137:ARG:HD3	1:A:232:ARG:HE	1.63	0.63
2:B:50:LEU:HB3	2:B:54:GLU:OE2	1.98	0.63
2:B:325:ILE:O	2:B:329:LEU:HD12	1.98	0.63
1:A:155:ILE:O	1:A:170:CYS:HB3	1.99	0.63
2:B:34:ALA:N	2:B:35:PRO:HD2	2.14	0.63
2:B:36:ARG:HG3	2:B:384:TYR:OH	1.99	0.63
2:B:309:ILE:HG22	2:B:310:MET:H	1.61	0.63
2:B:376:PHE:O	2:B:422:HIS:HA	1.99	0.63
1:A:24:ALA:O	1:A:27:ILE:HD12	1.98	0.63
1:A:28:TYR:O	1:A:31:PHE:N	2.31	0.63
2:B:233:GLU:HG2	2:B:234:ILE:N	2.14	0.63
2:B:290:HIS:CG	2:B:291:ALA:H	2.16	0.63
2:B:601:GLN:N	2:B:601:GLN:OE1	2.31	0.63
1:A:149:ALA:CA	1:A:180:GLN:HG3	2.29	0.63
2:B:107:LYS:NZ	2:B:378:ASN:ND2	2.46	0.63
2:B:127:THR:HG22	2:B:181:ARG:HB3	1.81	0.63
2:B:135:LEU:HD23	2:B:169:PHE:CE2	2.34	0.63
2:B:527:ASP:OD2	2:B:585:SER:HB3	1.99	0.63
2:B:302:GLU:HA	2:B:305:GLU:CG	2.29	0.63
2:B:507:LYS:HE3	2:B:533:LYS:HZ3	1.64	0.63
2:B:399:LYS:O	2:B:400:TRP:CD1	2.52	0.62
1:A:346:PHE:HD1	1:A:354:VAL:HG22	1.64	0.62
2:B:168:TRP:CE3	2:B:169:PHE:CA	2.78	0.62
2:B:239:GLU:O	2:B:350:GLY:HA3	1.99	0.62
2:B:543:ARG:O	2:B:601:GLN:HB3	1.99	0.62
2:B:549:PRO:HG3	2:B:567:ASP:OD1	2.00	0.62
1:A:84:ALA:HB1	1:A:111:TRP:CE2	2.34	0.62
2:B:58:ILE:HG22	2:B:59:LEU:N	2.11	0.62
2:B:64:VAL:CG2	2:B:78:ILE:HG13	2.27	0.62
2:B:399:LYS:O	2:B:400:TRP:HB2	2.00	0.62
2:B:548:LEU:N	2:B:548:LEU:HD12	2.15	0.62
1:A:31:PHE:CD1	1:A:32:GLU:N	2.67	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:GLY:HA3	1:A:141:HIS:CE1	2.35	0.62
2:B:233:GLU:O	2:B:234:ILE:HG23	1.99	0.62
2:B:66:VAL:HG13	2:B:76:VAL:HG13	1.82	0.62
2:B:400:TRP:HH2	2:B:410:GLY:H	1.42	0.62
2:B:508:ILE:HG22	2:B:509:MET:H	1.64	0.62
1:A:118:GLU:C	1:A:120:GLY:H	2.07	0.62
1:A:198:ILE:O	1:A:199:ILE:HD13	1.99	0.62
2:B:125:GLN:NE2	2:B:151:ILE:HB	2.14	0.62
2:B:196:LEU:O	2:B:200:ALA:N	2.25	0.62
1:A:108:SER:HA	1:A:111:TRP:NE1	2.15	0.61
1:A:112:ASP:C	1:A:114:ALA:N	2.56	0.61
1:A:239:LYS:HZ2	1:A:279:PHE:HA	1.62	0.61
1:A:150:THR:CB	1:A:225:HIS:HB3	2.29	0.61
2:B:116:GLY:O	2:B:118:SER:N	2.33	0.61
2:B:150:MET:HE3	2:B:152:ASN:HB2	1.81	0.61
2:B:238:PRO:HA	2:B:241:ILE:CD1	2.20	0.61
2:B:400:TRP:CZ3	2:B:407:GLN:O	2.53	0.61
2:B:507:LYS:HG3	2:B:533:LYS:HZ3	1.63	0.61
2:B:512:LEU:HD11	2:B:542:PHE:CE2	2.35	0.61
1:A:157:ILE:HG23	1:A:189:GLU:HB3	1.82	0.61
1:A:205:GLY:HA3	1:A:344:GLN:HE22	1.66	0.61
1:A:232:ARG:O	1:A:233:SER:C	2.44	0.61
2:B:417:VAL:HG12	2:B:418:ILE:H	1.63	0.61
2:B:591:ALA:O	2:B:593:GLU:HG2	1.99	0.61
1:A:18:GLU:C	1:A:20:LEU:H	2.09	0.61
1:A:121:GLU:O	1:A:122:SER:C	2.43	0.61
1:A:208:ALA:O	1:A:211:MET:HB3	2.01	0.61
1:A:28:TYR:O	1:A:31:PHE:HB3	2.00	0.61
2:B:36:ARG:NE	2:B:384:TYR:CE2	2.68	0.61
2:B:61:ASP:HB2	2:B:207:ARG:NH1	2.12	0.61
2:B:222:ARG:HH22	2:B:332:GLU:N	1.98	0.61
1:A:80:LYS:HD2	1:A:116:PHE:HE1	1.66	0.61
1:A:124:ARG:O	1:A:128:ASP:N	2.33	0.61
1:A:183:PHE:O	1:A:184:ASN:HB2	2.01	0.61
2:B:307:VAL:HG22	2:B:309:ILE:CD1	2.28	0.61
2:B:598:LYS:HE2	2:B:613:THR:CB	2.31	0.61
2:B:107:LYS:HZ3	2:B:424:ALA:HB1	1.64	0.61
1:A:157:ILE:CG2	1:A:158:THR:N	2.64	0.61
2:B:66:VAL:HG23	2:B:213:PRO:CD	2.21	0.61
2:B:96:LYS:O	2:B:97:LEU:HD23	2.00	0.61
2:B:360:ALA:O	2:B:418:ILE:HG22	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:LYS:HG2	2:B:172:HIS:H	1.66	0.61
2:B:482:VAL:HG11	2:B:505:VAL:HG22	1.82	0.61
2:B:545:HIS:CG	2:B:571:VAL:HG22	2.35	0.61
2:B:73:TYR:HA	2:B:181:ARG:HA	1.83	0.60
2:B:169:PHE:HD1	2:B:169:PHE:O	1.84	0.60
2:B:399:LYS:HG2	2:B:403:TYR:CG	2.36	0.60
2:B:478:ILE:O	2:B:478:ILE:HG22	2.01	0.60
1:A:28:TYR:O	1:A:30:GLN:N	2.34	0.60
2:B:430:PHE:CD1	2:B:435:LYS:HA	2.36	0.60
2:B:485:LYS:C	2:B:487:ALA:H	2.09	0.60
1:A:287:PHE:CE1	1:A:289:GLY:HA3	2.36	0.60
1:A:351:LEU:HD12	1:A:351:LEU:N	2.15	0.60
2:B:250:LEU:O	2:B:252:TYR:N	2.33	0.60
2:B:241:ILE:HG23	2:B:245:THR:CB	2.31	0.60
1:A:242:ASN:CG	1:A:282:THR:HG23	2.26	0.60
2:B:399:LYS:O	2:B:400:TRP:CB	2.49	0.60
2:B:532:VAL:HG22	2:B:533:LYS:H	1.65	0.60
1:A:17:ARG:HH12	1:A:141:HIS:CB	2.14	0.60
1:A:176:GLU:CD	1:A:176:GLU:H	2.09	0.60
2:B:125:GLN:HE22	2:B:151:ILE:CB	2.13	0.60
2:B:464:SER:O	2:B:468:ASN:HB2	2.00	0.60
1:A:79:LEU:CD2	1:A:114:ALA:HB2	2.31	0.60
2:B:514:VAL:HG23	2:B:514:VAL:O	1.99	0.60
2:B:550:CYS:O	2:B:551:LYS:HB3	2.00	0.60
1:A:17:ARG:HD2	1:A:139:TYR:O	2.02	0.60
1:A:263:TYR:O	1:A:267:ALA:N	2.35	0.60
2:B:320:ILE:HD13	2:B:379:ARG:HH11	1.64	0.60
2:B:106:LEU:HD23	2:B:106:LEU:H	1.67	0.59
2:B:135:LEU:HD12	2:B:145:HIS:O	2.01	0.59
2:B:125:GLN:OE1	2:B:150:MET:HA	2.01	0.59
2:B:430:PHE:CZ	2:B:435:LYS:HG2	2.37	0.59
2:B:75:THR:HG23	2:B:179:GLU:OE1	2.02	0.59
2:B:375:ARG:NH1	2:B:375:ARG:HG3	2.17	0.59
1:A:360:PRO:HG2	1:A:361:ASN:H	1.67	0.59
2:B:500:ASP:O	2:B:503:PRO:HD2	2.02	0.59
1:A:102:ARG:HD3	1:A:119:GLN:NE2	2.17	0.59
2:B:33:SER:HB3	2:B:35:PRO:HD2	1.84	0.59
2:B:507:LYS:HE3	2:B:533:LYS:NZ	2.18	0.59
1:A:150:THR:OG1	1:A:225:HIS:HB3	2.03	0.59
2:B:448:ILE:O	2:B:451:ALA:HB3	2.02	0.59
1:A:206:MET:HG2	1:A:343:GLN:HE21	1.68	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ALA:HA	1:A:235:ARG:NH2	2.18	0.59
2:B:192:ILE:HG23	2:B:193:TYR:N	2.17	0.59
2:B:263:ARG:HD2	2:B:271:LEU:HG	1.84	0.59
1:A:69:ALA:HA	1:A:74:GLY:O	2.02	0.59
2:B:53:CYS:O	2:B:55:GLU:N	2.35	0.59
2:B:73:TYR:CD1	2:B:181:ARG:HB2	2.38	0.59
2:B:197:LYS:HA	2:B:220:PHE:CE2	2.37	0.59
2:B:470:LYS:C	2:B:472:ARG:H	2.10	0.59
2:B:25:ASN:C	2:B:27:GLN:H	2.10	0.58
2:B:110:ARG:HG3	2:B:380:VAL:HG22	1.84	0.58
1:A:20:LEU:HD22	1:A:139:TYR:HB3	1.85	0.58
2:B:531:LYS:HG2	2:B:581:SER:HA	1.86	0.58
1:A:156:GLU:C	1:A:157:ILE:HG13	2.28	0.58
1:A:201:ILE:HD12	1:A:207:TYR:HA	1.86	0.58
1:A:288:LEU:C	1:A:288:LEU:HD12	2.27	0.58
1:A:21:LEU:O	1:A:25:GLU:HG3	2.02	0.58
2:B:115:ILE:N	2:B:115:ILE:HD12	2.18	0.58
2:B:601:GLN:OE1	2:B:613:THR:O	2.21	0.58
2:B:189:ARG:O	2:B:190:GLN:HB3	2.02	0.58
2:B:205:HIS:NE2	2:B:228:PRO:HD3	2.18	0.58
2:B:263:ARG:NH1	2:B:271:LEU:HD11	2.18	0.58
2:B:455:VAL:O	2:B:457:ARG:N	2.37	0.58
1:A:31:PHE:O	1:A:35:VAL:N	2.36	0.58
2:B:90:ILE:HG12	2:B:147:TYR:CD2	2.39	0.58
2:B:64:VAL:HG12	2:B:64:VAL:O	2.03	0.58
2:B:588:ILE:CG1	2:B:589:GLU:H	2.10	0.58
1:A:29:ASN:C	1:A:31:PHE:N	2.61	0.58
1:A:31:PHE:HB2	2:B:489:LYS:NZ	2.19	0.58
1:A:230:PRO:CD	1:A:262:ILE:HG23	2.34	0.58
2:B:407:GLN:CB	2:B:414:VAL:H	2.17	0.58
1:A:156:GLU:HG2	1:A:157:ILE:N	2.18	0.57
2:B:239:GLU:OE1	2:B:239:GLU:N	2.35	0.57
2:B:357:VAL:HG11	2:B:452:ILE:HA	1.85	0.57
1:A:17:ARG:HH12	1:A:141:HIS:CG	2.22	0.57
1:A:69:ALA:O	1:A:70:LYS:HB3	2.02	0.57
1:A:87:PHE:HD1	2:B:492:HIS:CD2	2.22	0.57
1:A:326:TYR:O	1:A:330:GLN:NE2	2.30	0.57
1:A:35:VAL:CG1	2:B:486:LEU:HD13	2.34	0.57
1:A:83:TYR:C	1:A:85:THR:N	2.61	0.57
2:B:69:THR:HG21	2:B:75:THR:HG23	1.87	0.57
2:B:237:HIS:CG	2:B:238:PRO:HD2	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:TYR:CZ	2:B:489:LYS:HA	2.39	0.57
1:A:112:ASP:C	1:A:114:ALA:H	2.11	0.57
1:A:201:ILE:HG22	1:A:252:PHE:HB3	1.87	0.57
2:B:430:PHE:CE2	2:B:435:LYS:HG2	2.39	0.57
2:B:345:PRO:CA	2:B:354:VAL:HG12	2.35	0.57
2:B:455:VAL:C	2:B:457:ARG:N	2.58	0.57
2:B:514:VAL:HG12	2:B:530:ILE:CG1	2.34	0.57
2:B:549:PRO:HB2	2:B:589:GLU:OE2	2.05	0.57
1:A:21:LEU:O	1:A:21:LEU:HD23	2.05	0.57
1:A:237:ILE:HG22	1:A:241:MET:CE	2.32	0.57
1:A:18:GLU:C	1:A:20:LEU:N	2.61	0.57
1:A:191:GLN:O	1:A:192:LYS:HB2	2.03	0.57
2:B:213:PRO:O	2:B:214:ASP:OD1	2.23	0.57
1:A:79:LEU:HD22	1:A:114:ALA:HB2	1.87	0.57
1:A:102:ARG:HD3	1:A:119:GLN:HE22	1.68	0.57
1:A:108:SER:C	1:A:110:GLY:H	2.12	0.57
1:A:149:ALA:HB2	1:A:180:GLN:CD	2.30	0.57
2:B:156:ASN:O	2:B:157:GLU:C	2.47	0.57
2:B:211:ILE:HG13	2:B:211:ILE:O	2.05	0.57
2:B:384:TYR:HB2	2:B:436:ASP:OD1	2.05	0.57
2:B:448:ILE:HG22	2:B:452:ILE:HD11	1.87	0.56
1:A:159:GLU:O	1:A:160:GLN:CB	2.54	0.56
1:A:282:THR:N	1:A:283:PRO:CD	2.69	0.56
2:B:80:ASP:O	2:B:81:ASN:CB	2.52	0.56
2:B:149:LEU:HD12	2:B:150:MET:N	2.19	0.56
2:B:253:THR:HG22	2:B:254:GLU:N	2.21	0.56
2:B:135:LEU:HD23	2:B:169:PHE:HE2	1.70	0.56
2:B:278:CYS:HB2	2:B:285:PRO:HG3	1.87	0.56
2:B:401:LYS:NZ	2:B:406:ASN:ND2	2.53	0.56
2:B:473:ARG:HG3	2:B:473:ARG:NH1	2.20	0.56
2:B:557:PRO:CD	2:B:585:SER:H	2.19	0.56
2:B:597:GLN:O	2:B:598:LYS:CB	2.50	0.56
2:B:188:ARG:HG3	2:B:189:ARG:H	1.70	0.56
2:B:320:ILE:HD13	2:B:379:ARG:NH1	2.21	0.56
1:A:282:THR:H	1:A:283:PRO:CD	2.18	0.56
2:B:26:ARG:HG2	2:B:26:ARG:HH11	1.70	0.56
2:B:400:TRP:CZ2	2:B:411:GLY:N	2.74	0.56
1:A:79:LEU:HD23	1:A:79:LEU:C	2.29	0.56
1:A:83:TYR:O	1:A:84:ALA:C	2.48	0.56
1:A:206:MET:CE	1:A:354:VAL:HG11	2.35	0.56
1:A:235:ARG:C	1:A:237:ILE:H	2.13	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:LEU:HD11	1:A:346:PHE:CE2	2.40	0.56
1:A:203:THR:N	1:A:225:HIS:NE2	2.44	0.56
2:B:399:LYS:HA	2:B:399:LYS:HE3	1.88	0.56
1:A:162:LYS:NZ	1:A:182:PRO:HG2	2.20	0.56
1:A:249:VAL:O	1:A:285:ALA:HB1	2.06	0.56
2:B:21:PHE:HD1	2:B:21:PHE:O	1.88	0.56
2:B:394:ALA:HA	2:B:445:LYS:HE3	1.86	0.56
2:B:477:ILE:C	2:B:479:ILE:H	2.14	0.56
1:A:290:LEU:HD21	1:A:341:ALA:CB	2.35	0.56
2:B:148:GLU:HB2	2:B:162:VAL:HG23	1.85	0.56
1:A:32:GLU:C	1:A:34:GLU:N	2.61	0.56
2:B:375:ARG:CD	2:B:382:LEU:HD23	2.36	0.56
2:B:300:LEU:O	2:B:303:ALA:HB3	2.07	0.55
2:B:371:ILE:HB	2:B:414:VAL:HA	1.88	0.55
2:B:372:SER:O	2:B:418:ILE:HA	2.06	0.55
1:A:205:GLY:HA3	1:A:344:GLN:NE2	2.21	0.55
1:A:346:PHE:CD1	1:A:354:VAL:HG22	2.41	0.55
2:B:334:THR:CB	2:B:364:ASN:HB2	2.36	0.55
1:A:149:ALA:HA	1:A:180:GLN:HA	1.87	0.55
2:B:27:GLN:C	2:B:29:LEU:N	2.61	0.55
2:B:168:TRP:CE3	2:B:169:PHE:N	2.75	0.55
2:B:245:THR:O	2:B:249:MET:HG2	2.06	0.55
2:B:359:MET:CE	2:B:455:VAL:HG23	2.32	0.55
2:B:212:ASP:OD1	2:B:216:ASN:OD1	2.25	0.55
2:B:375:ARG:CZ	2:B:382:LEU:HD23	2.37	0.55
2:B:382:LEU:HD11	2:B:436:ASP:HA	1.87	0.55
1:A:100:THR:N	1:A:103:GLU:OE1	2.31	0.55
2:B:137:LYS:HG3	2:B:172:HIS:N	2.20	0.55
1:A:209:ARG:O	1:A:209:ARG:HG2	2.05	0.55
2:B:16:ILE:HG22	2:B:16:ILE:O	2.05	0.55
2:B:534:ASN:CG	2:B:534:ASN:O	2.47	0.55
1:A:41:LEU:HA	1:A:69:ALA:HB3	1.87	0.55
1:A:181:ILE:HD12	1:A:237:ILE:HG13	1.89	0.55
1:A:203:THR:H	1:A:225:HIS:CD2	2.25	0.54
2:B:66:VAL:O	2:B:213:PRO:HB3	2.06	0.54
2:B:343:ARG:HG3	2:B:343:ARG:NH1	2.22	0.54
2:B:383:LEU:C	2:B:384:TYR:HD1	2.15	0.54
1:A:31:PHE:CG	2:B:489:LYS:HD3	2.41	0.54
1:A:314:ARG:O	1:A:318:SER:HB2	2.08	0.54
2:B:90:ILE:CD1	2:B:147:TYR:HE2	2.20	0.54
2:B:283:LEU:HD22	2:B:287:ILE:HD11	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:401:LYS:HZ2	2:B:406:ASN:CG	2.15	0.54
2:B:547:MET:C	2:B:548:LEU:HD12	2.32	0.54
1:A:80:LYS:HD2	1:A:116:PHE:CE1	2.43	0.54
1:A:106:TYR:C	1:A:108:SER:H	2.15	0.54
2:B:112:GLN:O	2:B:115:ILE:HD11	2.07	0.54
2:B:112:GLN:C	2:B:115:ILE:HD11	2.32	0.54
1:A:82:THR:N	1:A:85:THR:HG1	2.06	0.54
1:A:200:ALA:O	1:A:252:PHE:N	2.37	0.54
1:A:225:HIS:C	1:A:226:LEU:HD23	2.32	0.54
2:B:170:ARG:HG2	2:B:170:ARG:NH1	2.21	0.54
2:B:96:LYS:HB2	2:B:118:SER:OG	2.08	0.54
2:B:598:LYS:HE2	2:B:613:THR:N	2.23	0.54
1:A:252:PHE:HA	1:A:289:GLY:CA	2.38	0.54
1:A:292:PRO:C	1:A:333:LEU:HD23	2.32	0.54
2:B:136:SER:CB	2:B:174:THR:HB	2.38	0.54
2:B:448:ILE:HG22	2:B:452:ILE:CD1	2.37	0.54
2:B:76:VAL:N	2:B:178:LEU:O	2.38	0.54
2:B:532:VAL:CG2	2:B:533:LYS:N	2.70	0.54
1:A:75:ALA:O	1:A:78:LEU:HB2	2.08	0.54
2:B:25:ASN:HB3	2:B:28:ILE:CG2	2.38	0.54
2:B:90:ILE:HG12	2:B:147:TYR:HD2	1.73	0.54
2:B:137:LYS:HD3	2:B:137:LYS:N	2.23	0.54
2:B:170:ARG:N	2:B:171:PRO:HD3	2.23	0.54
2:B:518:ILE:HG22	2:B:526:VAL:HG22	1.90	0.54
1:A:181:ILE:HD13	1:A:237:ILE:HG13	1.89	0.54
2:B:184:TYR:O	2:B:186:LYS:N	2.41	0.54
2:B:212:ASP:CG	2:B:216:ASN:OD1	2.51	0.54
2:B:26:ARG:HG2	2:B:26:ARG:O	2.07	0.53
2:B:375:ARG:HH11	2:B:382:LEU:HD23	1.68	0.53
1:A:158:THR:O	1:A:189:GLU:HB3	2.08	0.53
2:B:373:ILE:O	2:B:373:ILE:CG1	2.55	0.53
2:B:398:ILE:HG13	2:B:449:ASP:OD1	2.09	0.53
2:B:400:TRP:CE3	2:B:407:GLN:O	2.61	0.53
2:B:539:ALA:HA	2:B:577:SER:HB2	1.90	0.53
1:A:28:TYR:O	1:A:29:ASN:C	2.51	0.53
1:A:305:LEU:HD21	1:A:339:LYS:N	2.23	0.53
2:B:168:TRP:O	2:B:169:PHE:CB	2.53	0.53
2:B:528:VAL:CG1	2:B:584:LEU:HD12	2.37	0.53
2:B:544:VAL:HG22	2:B:601:GLN:HG3	1.91	0.53
1:A:28:TYR:CE2	2:B:492:HIS:HB3	2.43	0.53
1:A:149:ALA:HA	1:A:180:GLN:HG3	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:184:TYR:CE1	2:B:192:ILE:HG12	2.39	0.53
2:B:511:ASN:O	2:B:512:LEU:HB3	2.09	0.53
1:A:85:THR:C	1:A:87:PHE:H	2.16	0.53
1:A:87:PHE:HD2	1:A:111:TRP:HZ3	1.56	0.53
1:A:203:THR:C	1:A:205:GLY:N	2.67	0.53
1:A:248:PRO:O	1:A:249:VAL:HG23	2.08	0.53
2:B:78:ILE:HG22	2:B:78:ILE:O	2.07	0.53
2:B:167:ASP:O	2:B:168:TRP:HB3	2.08	0.53
2:B:77:ILE:N	2:B:77:ILE:CD1	2.72	0.53
2:B:139:SER:CB	2:B:140:PRO:HD2	2.36	0.53
2:B:302:GLU:HA	2:B:305:GLU:HG2	1.91	0.53
2:B:360:ALA:HB3	2:B:418:ILE:HG21	1.88	0.53
1:A:181:ILE:HD11	1:A:234:THR:HA	1.91	0.53
2:B:77:ILE:O	2:B:78:ILE:HD12	2.05	0.53
1:A:100:THR:HG22	1:A:143:ARG:O	2.09	0.53
1:A:140:PHE:O	1:A:141:HIS:CB	2.57	0.53
1:A:251:VAL:HG21	1:A:263:TYR:HD1	1.74	0.53
2:B:44:GLU:OE2	2:B:44:GLU:HA	2.09	0.53
2:B:263:ARG:HD2	2:B:271:LEU:CD2	2.39	0.53
2:B:449:ASP:C	2:B:451:ALA:N	2.66	0.53
2:B:593:GLU:O	2:B:596:LEU:HD12	2.09	0.53
1:A:31:PHE:HB2	2:B:489:LYS:CE	2.38	0.53
1:A:145:GLU:O	1:A:146:GLU:CB	2.57	0.53
1:A:185:VAL:HG11	1:A:236:ARG:HB2	1.90	0.53
1:A:281:ALA:HB1	1:A:283:PRO:HD3	1.91	0.53
2:B:289:PRO:O	2:B:292:LEU:HG	2.09	0.53
2:B:515:HIS:CE1	2:B:529:ALA:HB3	2.44	0.53
2:B:151:ILE:O	2:B:152:ASN:O	2.27	0.53
2:B:448:ILE:O	2:B:452:ILE:HG13	2.09	0.53
2:B:455:VAL:C	2:B:457:ARG:H	2.17	0.53
2:B:27:GLN:OE1	2:B:32:ASP:HB2	2.09	0.52
2:B:61:ASP:HA	2:B:207:ARG:O	2.09	0.52
2:B:65:GLN:HE21	2:B:67:GLU:CG	2.22	0.52
2:B:150:MET:CE	2:B:152:ASN:HB2	2.39	0.52
2:B:381:PRO:O	2:B:382:LEU:CB	2.49	0.52
2:B:550:CYS:O	2:B:551:LYS:CB	2.57	0.52
1:A:69:ALA:O	1:A:70:LYS:CB	2.56	0.52
1:A:317:LEU:C	1:A:319:ASP:H	2.17	0.52
2:B:513:LEU:O	2:B:513:LEU:HD12	2.09	0.52
2:B:557:PRO:O	2:B:558:GLU:HB2	2.09	0.52
2:B:16:ILE:O	2:B:17:SER:HB2	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:ASN:O	2:B:27:GLN:N	2.41	0.52
2:B:53:CYS:C	2:B:55:GLU:N	2.66	0.52
2:B:65:GLN:HE21	2:B:67:GLU:HG2	1.75	0.52
2:B:90:ILE:HD13	2:B:147:TYR:HE2	1.74	0.52
2:B:348:TYR:CZ	2:B:351:ASN:HB2	2.44	0.52
2:B:428:VAL:HB	2:B:430:PHE:HE2	1.73	0.52
1:A:206:MET:O	1:A:210:LEU:HB2	2.10	0.52
2:B:44:GLU:O	2:B:45:ALA:C	2.52	0.52
2:B:152:ASN:O	2:B:153:THR:O	2.28	0.52
2:B:418:ILE:HG23	2:B:418:ILE:O	2.09	0.52
2:B:322:GLU:HG3	2:B:342:THR:HB	1.92	0.52
1:A:83:TYR:CG	2:B:488:ALA:HB1	2.44	0.52
1:A:183:PHE:CD1	1:A:183:PHE:N	2.75	0.52
1:A:323:GLU:OE2	1:A:328:LYS:HD2	2.09	0.52
2:B:337:PHE:HB2	2:B:462:TYR:CE1	2.45	0.52
2:B:359:MET:HE1	2:B:456:ALA:HA	1.91	0.52
2:B:392:THR:O	2:B:395:VAL:HB	2.10	0.52
2:B:449:ASP:C	2:B:451:ALA:H	2.16	0.52
1:A:338:GLY:C	1:A:339:LYS:HG3	2.35	0.52
1:A:359:LEU:HB2	1:A:360:PRO:CD	2.40	0.52
2:B:190:GLN:HG2	2:B:383:LEU:CD2	2.30	0.52
2:B:453:LYS:HA	2:B:456:ALA:HB3	1.92	0.52
2:B:493:VAL:O	2:B:495:GLU:N	2.39	0.52
2:B:222:ARG:NH2	2:B:332:GLU:N	2.58	0.51
2:B:559:PRO:O	2:B:560:LYS:HB2	2.10	0.51
1:A:188:ILE:CG1	1:A:240:ARG:NH2	2.70	0.51
2:B:36:ARG:HA	2:B:39:ILE:CG2	2.39	0.51
2:B:31:PHE:O	2:B:32:ASP:C	2.52	0.51
2:B:53:CYS:C	2:B:55:GLU:H	2.19	0.51
2:B:235:LEU:HB2	2:B:267:CYS:SG	2.50	0.51
2:B:423:VAL:HG21	2:B:438:ILE:CD1	2.40	0.51
1:A:149:ALA:HB2	1:A:180:GLN:OE1	2.11	0.51
2:B:133:LYS:HE3	2:B:146:TYR:HE1	1.74	0.51
2:B:391:THR:O	2:B:395:VAL:HG23	2.10	0.51
2:B:496:LYS:O	2:B:497:ASP:HB2	2.09	0.51
2:B:539:ALA:HA	2:B:577:SER:CB	2.41	0.51
1:A:31:PHE:CB	2:B:489:LYS:NZ	2.74	0.51
2:B:112:GLN:HB2	2:B:435:LYS:CD	2.40	0.51
2:B:190:GLN:O	2:B:383:LEU:HD21	2.11	0.51
2:B:201:ILE:HG13	2:B:328:GLY:C	2.35	0.51
2:B:325:ILE:O	2:B:326:TYR:C	2.53	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:LEU:H	1:A:305:LEU:CD1	1.96	0.51
2:B:27:GLN:C	2:B:29:LEU:H	2.17	0.51
2:B:78:ILE:N	2:B:78:ILE:CD1	2.74	0.51
2:B:405:LEU:HD11	2:B:415:GLY:HA3	1.91	0.51
2:B:90:ILE:HG22	2:B:91:PRO:CD	2.40	0.51
2:B:154:SER:O	2:B:156:ASN:N	2.44	0.51
2:B:232:GLU:CD	2:B:316:CYS:CA	2.73	0.51
1:A:362:ARG:HG3	1:A:362:ARG:HH11	1.75	0.51
2:B:348:TYR:O	2:B:349:SER:C	2.54	0.51
1:A:32:GLU:C	1:A:34:GLU:H	2.20	0.51
1:A:75:ALA:HB1	2:B:481:LYS:HD2	1.92	0.51
2:B:36:ARG:CG	2:B:384:TYR:OH	2.59	0.51
2:B:417:VAL:O	2:B:418:ILE:HB	2.11	0.51
2:B:548:LEU:O	2:B:568:TYR:N	2.45	0.51
1:A:305:LEU:HD11	1:A:338:GLY:C	2.36	0.50
2:B:233:GLU:HG2	2:B:234:ILE:H	1.75	0.50
2:B:396:GLU:HG2	2:B:412:ILE:N	2.26	0.50
2:B:543:ARG:O	2:B:601:GLN:HA	2.11	0.50
1:A:138:GLU:HG3	1:A:236:ARG:HH12	1.76	0.50
1:A:156:GLU:O	1:A:157:ILE:CG1	2.53	0.50
2:B:451:ALA:O	2:B:454:GLU:HB2	2.11	0.50
2:B:528:VAL:HG12	2:B:528:VAL:O	2.11	0.50
2:B:402:GLN:O	2:B:403:TYR:HD1	1.94	0.50
2:B:423:VAL:HG21	2:B:438:ILE:HD11	1.93	0.50
2:B:532:VAL:CG2	2:B:533:LYS:H	2.25	0.50
1:A:35:VAL:O	1:A:36:VAL:C	2.55	0.50
1:A:147:ASP:O	1:A:147:ASP:OD2	2.29	0.50
2:B:310:MET:HE3	2:B:310:MET:HA	1.94	0.50
1:A:31:PHE:HB2	2:B:489:LYS:HZ2	1.77	0.50
2:B:354:VAL:HG22	2:B:424:ALA:HB3	1.93	0.50
2:B:27:GLN:O	2:B:29:LEU:N	2.45	0.50
2:B:58:ILE:O	2:B:59:LEU:C	2.55	0.50
2:B:58:ILE:O	2:B:60:PRO:N	2.44	0.50
2:B:65:GLN:CG	2:B:211:ILE:HG13	2.37	0.50
2:B:251:HIS:HA	2:B:290:HIS:CE1	2.47	0.50
2:B:382:LEU:HD11	2:B:436:ASP:C	2.36	0.50
1:A:98:GLY:HA3	1:A:141:HIS:ND1	2.26	0.50
2:B:171:PRO:O	2:B:172:HIS:CB	2.58	0.50
2:B:115:ILE:O	2:B:116:GLY:O	2.29	0.50
2:B:253:THR:CG2	2:B:254:GLU:N	2.75	0.50
2:B:508:ILE:HG23	2:B:509:MET:N	2.25	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:PRO:HD2	1:A:221:ALA:O	2.12	0.50
1:A:346:PHE:HB2	1:A:354:VAL:HG22	1.94	0.50
2:B:431:THR:O	2:B:432:SER:C	2.55	0.50
1:A:136:GLN:O	1:A:137:ARG:C	2.55	0.49
2:B:66:VAL:O	2:B:213:PRO:CD	2.61	0.49
2:B:145:HIS:HB3	2:B:147:TYR:HE1	1.73	0.49
2:B:198:ALA:HB1	2:B:376:PHE:CZ	2.46	0.49
2:B:235:LEU:O	2:B:267:CYS:SG	2.70	0.49
2:B:335:VAL:CG2	2:B:360:ALA:HB1	2.39	0.49
1:A:72:VAL:HG21	2:B:474:GLU:HG2	1.94	0.49
1:A:150:THR:HB	1:A:225:HIS:HB3	1.93	0.49
1:A:206:MET:HE1	1:A:354:VAL:CG1	2.36	0.49
2:B:43:LYS:O	2:B:47:ASP:OD2	2.30	0.49
2:B:110:ARG:O	2:B:111:GLY:C	2.55	0.49
2:B:428:VAL:HB	2:B:430:PHE:CE2	2.47	0.49
2:B:445:LYS:HA	2:B:448:ILE:HD12	1.94	0.49
1:A:96:ASN:O	1:A:97:ARG:O	2.31	0.49
2:B:399:LYS:O	2:B:400:TRP:CG	2.66	0.49
2:B:401:LYS:O	2:B:403:TYR:N	2.46	0.49
2:B:430:PHE:CE1	2:B:435:LYS:HG2	2.47	0.49
2:B:550:CYS:N	2:B:589:GLU:OE2	2.46	0.49
1:A:125:LEU:O	1:A:128:ASP:HB2	2.12	0.49
2:B:338:ILE:CG2	2:B:339:ALA:N	2.75	0.49
2:B:346:ALA:HB3	2:B:353:PHE:CE1	2.47	0.49
1:A:117:LYS:HB2	1:A:117:LYS:HZ3	1.75	0.49
1:A:149:ALA:HB2	1:A:180:GLN:HG3	1.94	0.49
2:B:61:ASP:CB	2:B:207:ARG:HH11	2.16	0.49
2:B:132:THR:HG23	2:B:178:LEU:HD11	1.95	0.49
2:B:342:THR:HG23	2:B:356:GLU:CG	2.41	0.49
1:A:154:PRO:O	1:A:155:ILE:CG2	2.59	0.49
2:B:107:LYS:NZ	2:B:424:ALA:HB1	2.28	0.49
2:B:337:PHE:CE2	2:B:459:LEU:HA	2.47	0.49
2:B:361:TYR:C	2:B:361:TYR:CD2	2.90	0.49
1:A:231:ALA:C	1:A:235:ARG:HE	2.20	0.49
2:B:417:VAL:HG12	2:B:418:ILE:N	2.27	0.49
2:B:508:ILE:HG22	2:B:509:MET:N	2.24	0.49
1:A:138:GLU:O	1:A:139:TYR:C	2.55	0.49
1:A:145:GLU:O	1:A:146:GLU:HB2	2.13	0.49
1:A:223:LEU:O	1:A:224:VAL:HG13	2.13	0.49
1:A:359:LEU:O	1:A:363:LEU:HB2	2.12	0.49
2:B:327:ARG:O	2:B:328:GLY:C	2.55	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:348:TYR:OH	2:B:429:PRO:HD3	2.13	0.49
2:B:594:GLU:O	2:B:596:LEU:N	2.45	0.49
2:B:273:THR:O	2:B:277:ILE:HG13	2.12	0.49
2:B:284:ASP:HB2	2:B:287:ILE:CG2	2.43	0.49
2:B:369:GLU:HG2	2:B:414:VAL:HG23	1.95	0.49
2:B:444:ILE:HG22	2:B:445:LYS:N	2.27	0.49
1:A:137:ARG:HH11	1:A:137:ARG:HB2	1.78	0.49
2:B:224:THR:O	2:B:226:LYS:N	2.46	0.49
2:B:302:GLU:C	2:B:304:PHE:H	2.21	0.49
2:B:550:CYS:HB2	2:B:589:GLU:OE2	2.13	0.49
2:B:396:GLU:CG	2:B:412:ILE:HG23	2.42	0.48
2:B:400:TRP:HZ3	2:B:408:PRO:CA	2.25	0.48
2:B:560:LYS:HB3	2:B:571:VAL:O	2.12	0.48
1:A:21:LEU:HD12	1:A:93:LEU:HD13	1.94	0.48
1:A:28:TYR:CE1	2:B:489:LYS:HA	2.48	0.48
1:A:198:ILE:HD12	1:A:249:VAL:CG2	2.44	0.48
1:A:331:ILE:O	1:A:334:GLN:N	2.41	0.48
2:B:180:MET:O	2:B:180:MET:CG	2.59	0.48
2:B:398:ILE:CG2	2:B:399:LYS:N	2.76	0.48
2:B:425:SER:O	2:B:427:ASN:N	2.46	0.48
1:A:176:GLU:CD	1:A:176:GLU:N	2.71	0.48
2:B:75:THR:HA	2:B:178:LEU:O	2.14	0.48
2:B:193:TYR:CE1	2:B:218:GLU:HG2	2.48	0.48
1:A:156:GLU:HA	1:A:170:CYS:HB3	1.95	0.48
1:A:288:LEU:HD12	1:A:288:LEU:O	2.13	0.48
1:A:305:LEU:HD12	1:A:305:LEU:N	2.05	0.48
2:B:202:VAL:C	2:B:204:PRO:CD	2.85	0.48
2:B:234:ILE:C	2:B:234:ILE:HD12	2.39	0.48
2:B:42:VAL:C	2:B:44:GLU:N	2.71	0.48
2:B:401:LYS:HZ2	2:B:406:ASN:ND2	2.10	0.48
2:B:551:LYS:HG2	2:B:552:VAL:H	1.74	0.48
1:A:151:MET:HG3	1:A:224:VAL:CG1	2.44	0.48
2:B:20:GLU:O	2:B:22:PHE:N	2.47	0.48
2:B:361:TYR:CD2	2:B:362:GLY:N	2.82	0.48
1:A:217:GLU:C	1:A:219:TYR:H	2.21	0.48
1:A:235:ARG:C	1:A:237:ILE:N	2.71	0.48
2:B:137:LYS:CE	2:B:173:GLY:H	2.26	0.48
2:B:239:GLU:CD	2:B:239:GLU:H	2.19	0.48
1:A:151:MET:HG3	1:A:224:VAL:HG12	1.95	0.48
1:A:296:VAL:HG22	1:A:337:ILE:HD11	1.94	0.48
1:A:365:GLU:HG2	1:A:367:GLY:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:GLU:O	2:B:21:PHE:C	2.56	0.48
2:B:85:ILE:HG13	2:B:90:ILE:CD1	2.44	0.48
1:A:30:GLN:O	1:A:34:GLU:CD	2.56	0.48
1:A:76:PHE:C	1:A:78:LEU:N	2.71	0.48
2:B:46:VAL:O	2:B:50:LEU:HG	2.14	0.48
2:B:91:PRO:O	2:B:95:ALA:HB3	2.14	0.48
1:A:30:GLN:O	1:A:34:GLU:HB2	2.13	0.48
2:B:237:HIS:ND1	2:B:239:GLU:OE1	2.42	0.48
2:B:591:ALA:O	2:B:593:GLU:N	2.47	0.48
1:A:130:GLU:CD	1:A:136:GLN:HE22	2.22	0.47
1:A:192:LYS:HD2	1:A:192:LYS:HA	1.73	0.47
2:B:23:GLU:OE1	2:B:26:ARG:HD2	2.14	0.47
2:B:80:ASP:HB3	2:B:81:ASN:H	1.57	0.47
2:B:345:PRO:HB3	2:B:354:VAL:HG12	1.95	0.47
2:B:402:GLN:O	2:B:403:TYR:CD1	2.67	0.47
2:B:505:VAL:O	2:B:508:ILE:HG22	2.14	0.47
1:A:122:SER:O	1:A:123:ASP:O	2.32	0.47
2:B:65:GLN:HA	2:B:211:ILE:O	2.14	0.47
2:B:169:PHE:O	2:B:169:PHE:CD1	2.67	0.47
2:B:338:ILE:HG22	2:B:339:ALA:N	2.30	0.47
2:B:534:ASN:ND2	2:B:539:ALA:HB3	2.29	0.47
1:A:96:ASN:O	1:A:97:ARG:C	2.57	0.47
1:A:101:LEU:C	1:A:103:GLU:H	2.22	0.47
2:B:168:TRP:CZ3	2:B:169:PHE:HA	2.46	0.47
1:A:98:GLY:CA	1:A:141:HIS:CE1	2.97	0.47
1:A:106:TYR:C	1:A:108:SER:N	2.70	0.47
1:A:149:ALA:HB2	1:A:180:GLN:CG	2.44	0.47
1:A:155:ILE:HD13	1:A:222:ILE:CD1	2.45	0.47
2:B:190:GLN:HG3	2:B:194:GLU:HG2	1.95	0.47
2:B:191:SER:OG	2:B:192:ILE:N	2.45	0.47
2:B:430:PHE:CD2	2:B:435:LYS:HG2	2.49	0.47
1:A:84:ALA:HB1	1:A:111:TRP:CZ2	2.50	0.47
1:A:118:GLU:C	1:A:120:GLY:N	2.73	0.47
2:B:311:ALA:O	2:B:312:PRO:O	2.33	0.47
2:B:359:MET:HB2	2:B:419:LEU:CD2	2.44	0.47
1:A:99:SER:HB3	1:A:103:GLU:OE1	2.15	0.47
1:A:159:GLU:HG3	1:A:160:GLN:N	2.29	0.47
2:B:375:ARG:NH1	2:B:382:LEU:CD2	2.76	0.47
2:B:389:CYS:O	2:B:390:VAL:C	2.56	0.47
2:B:543:ARG:O	2:B:601:GLN:CA	2.63	0.47
1:A:126:ILE:HD13	1:A:129:LEU:HD12	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ALA:HA	1:A:267:ALA:CB	2.42	0.47
2:B:58:ILE:O	2:B:60:PRO:HD3	2.15	0.47
2:B:81:ASN:CG	2:B:81:ASN:O	2.56	0.47
2:B:136:SER:HB2	2:B:174:THR:HB	1.97	0.47
2:B:203:ASN:O	2:B:204:PRO:C	2.57	0.47
2:B:263:ARG:O	2:B:263:ARG:HG2	2.15	0.47
2:B:308:LYS:HD2	2:B:308:LYS:O	2.15	0.47
2:B:355:VAL:HA	2:B:422:HIS:O	2.14	0.47
2:B:386:GLN:O	2:B:387:GLY:C	2.56	0.47
2:B:91:PRO:HB3	2:B:158:PRO:HG3	1.97	0.47
1:A:155:ILE:C	1:A:170:CYS:HB3	2.40	0.47
2:B:21:PHE:C	2:B:21:PHE:CD1	2.92	0.47
2:B:229:GLU:CG	2:B:230:PRO:HD2	2.45	0.47
1:A:85:THR:C	1:A:87:PHE:N	2.72	0.47
1:A:260:TYR:HE1	1:A:287:PHE:CE2	2.33	0.47
1:A:279:PHE:O	1:A:280:MET:CG	2.61	0.47
2:B:62:ILE:HG23	2:B:79:GLU:O	2.15	0.47
2:B:281:ALA:HB2	2:B:300:LEU:HA	1.96	0.47
2:B:455:VAL:O	2:B:456:ALA:C	2.58	0.47
2:B:561:VAL:HG21	2:B:570:TYR:HE1	1.79	0.47
1:A:362:ARG:HG3	1:A:362:ARG:NH1	2.29	0.46
2:B:180:MET:O	2:B:180:MET:HG2	2.15	0.46
2:B:197:LYS:O	2:B:201:ILE:HG22	2.14	0.46
2:B:277:ILE:HG22	2:B:300:LEU:HD11	1.97	0.46
2:B:430:PHE:CZ	2:B:435:LYS:HE3	2.49	0.46
2:B:439:ALA:O	2:B:441:ILE:N	2.48	0.46
2:B:534:ASN:HD21	2:B:539:ALA:HB3	1.81	0.46
1:A:76:PHE:CD2	2:B:481:LYS:HE2	2.50	0.46
2:B:135:LEU:CD1	2:B:146:TYR:HB2	2.45	0.46
1:A:231:ALA:HA	1:A:235:ARG:HH21	1.80	0.46
2:B:106:LEU:HB3	2:B:233:GLU:HA	1.97	0.46
2:B:318:SER:OG	2:B:379:ARG:NH2	2.48	0.46
2:B:205:HIS:CG	2:B:205:HIS:O	2.68	0.46
2:B:445:LYS:C	2:B:447:GLU:N	2.73	0.46
2:B:448:ILE:CG2	2:B:452:ILE:HD11	2.45	0.46
1:A:138:GLU:CG	1:A:236:ARG:HH12	2.29	0.46
2:B:50:LEU:O	2:B:54:GLU:HB2	2.15	0.46
2:B:329:LEU:O	2:B:330:GLU:C	2.59	0.46
2:B:390:VAL:CG2	2:B:440:ASP:HA	2.43	0.46
2:B:434:SER:O	2:B:435:LYS:C	2.59	0.46
2:B:457:ARG:HG3	2:B:458:LYS:N	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ARG:CD	1:A:265:SER:O	2.63	0.46
2:B:478:ILE:C	2:B:479:ILE:HG13	2.41	0.46
1:A:157:ILE:HD11	1:A:190:PHE:CD1	2.50	0.46
1:A:73:LYS:O	1:A:77:GLN:HB2	2.15	0.46
1:A:162:LYS:O	1:A:163:ARG:C	2.58	0.46
2:B:36:ARG:O	2:B:36:ARG:HG2	2.16	0.46
2:B:58:ILE:CG2	2:B:59:LEU:H	2.22	0.46
2:B:216:ASN:OD1	2:B:216:ASN:N	2.47	0.46
2:B:523:ASP:O	2:B:588:ILE:CD1	2.63	0.46
1:A:78:LEU:O	1:A:79:LEU:C	2.57	0.46
2:B:167:ASP:O	2:B:168:TRP:CB	2.64	0.46
2:B:168:TRP:HE3	2:B:169:PHE:HA	1.72	0.46
2:B:510:GLY:O	2:B:533:LYS:O	2.34	0.46
1:A:263:TYR:CE2	1:A:327:TRP:CH2	3.03	0.46
2:B:19:ALA:O	2:B:22:PHE:HB3	2.15	0.46
2:B:561:VAL:CG2	2:B:570:TYR:CE1	2.99	0.46
1:A:291:GLN:HB2	1:A:330:GLN:OE1	2.16	0.45
2:B:27:GLN:C	2:B:27:GLN:HE21	2.24	0.45
2:B:65:GLN:NE2	2:B:67:GLU:HG2	2.30	0.45
1:A:76:PHE:CD2	2:B:481:LYS:NZ	2.83	0.45
1:A:252:PHE:HA	1:A:289:GLY:HA3	1.98	0.45
1:A:360:PRO:O	1:A:363:LEU:N	2.48	0.45
2:B:48:ASN:O	2:B:51:ASP:HB2	2.16	0.45
2:B:94:PHE:O	2:B:121:VAL:HG21	2.16	0.45
2:B:203:ASN:O	2:B:205:HIS:N	2.50	0.45
2:B:512:LEU:HD11	2:B:542:PHE:CZ	2.50	0.45
1:A:21:LEU:HD23	1:A:21:LEU:C	2.41	0.45
1:A:180:GLN:O	1:A:181:ILE:C	2.58	0.45
2:B:267:CYS:O	2:B:268:LYS:C	2.59	0.45
2:B:361:TYR:O	2:B:362:GLY:O	2.35	0.45
2:B:396:GLU:HG2	2:B:412:ILE:H	1.82	0.45
2:B:518:ILE:HG22	2:B:526:VAL:CG1	2.44	0.45
1:A:29:ASN:O	1:A:31:PHE:N	2.48	0.45
1:A:353:PHE:CE1	1:A:357:VAL:HG21	2.51	0.45
1:A:356:GLU:O	1:A:360:PRO:CG	2.63	0.45
2:B:18:VAL:HG23	2:B:19:ALA:H	1.81	0.45
2:B:309:ILE:O	2:B:310:MET:C	2.59	0.45
2:B:450:LEU:O	2:B:454:GLU:HG2	2.16	0.45
2:B:42:VAL:C	2:B:44:GLU:H	2.24	0.45
2:B:425:SER:O	2:B:426:ILE:C	2.59	0.45
1:A:291:GLN:OE1	1:A:294:ASP:OD2	2.35	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:PHE:O	2:B:21:PHE:CD1	2.68	0.45
1:A:17:ARG:HH12	1:A:141:HIS:CD2	2.34	0.45
1:A:155:ILE:HG22	1:A:192:LYS:O	2.17	0.45
1:A:238:ILE:HG22	1:A:282:THR:OG1	2.17	0.45
2:B:36:ARG:NH1	2:B:40:THR:OG1	2.49	0.45
2:B:148:GLU:HB2	2:B:162:VAL:CG2	2.47	0.45
2:B:284:ASP:C	2:B:286:GLU:H	2.25	0.45
2:B:468:ASN:O	2:B:471:LYS:N	2.50	0.45
2:B:552:VAL:HB	2:B:587:LYS:CB	2.36	0.45
1:A:86:ASP:O	2:B:492:HIS:CE1	2.69	0.45
2:B:170:ARG:N	2:B:171:PRO:CD	2.79	0.45
2:B:222:ARG:NH1	2:B:222:ARG:HB2	2.31	0.45
1:A:108:SER:C	1:A:110:GLY:N	2.74	0.45
1:A:112:ASP:O	1:A:113:TYR:C	2.60	0.45
1:A:281:ALA:O	1:A:282:THR:OG1	2.20	0.45
2:B:27:GLN:HG2	2:B:32:ASP:CB	2.41	0.45
2:B:130:ARG:O	2:B:131:HIS:C	2.60	0.45
2:B:234:ILE:HD12	2:B:234:ILE:O	2.17	0.45
2:B:309:ILE:CG2	2:B:310:MET:H	2.29	0.45
2:B:543:ARG:O	2:B:601:GLN:CB	2.65	0.45
1:A:101:LEU:O	1:A:104:LEU:HB3	2.17	0.45
2:B:22:PHE:O	2:B:26:ARG:N	2.50	0.45
2:B:114:GLY:O	2:B:115:ILE:C	2.59	0.45
2:B:212:ASP:CB	2:B:213:PRO:HD2	2.46	0.45
2:B:545:HIS:ND1	2:B:571:VAL:HG22	2.32	0.44
1:A:32:GLU:O	1:A:34:GLU:N	2.50	0.44
1:A:155:ILE:HD13	1:A:222:ILE:HD11	1.99	0.44
1:A:202:GLU:HA	1:A:225:HIS:CD2	2.52	0.44
1:A:237:ILE:CG2	1:A:241:MET:HE2	2.40	0.44
1:A:251:VAL:CG2	1:A:263:TYR:HD1	2.30	0.44
2:B:194:GLU:HG2	2:B:383:LEU:HD11	1.99	0.44
2:B:378:ASN:O	2:B:379:ARG:HB2	2.16	0.44
2:B:531:LYS:HG2	2:B:581:SER:CA	2.48	0.44
1:A:207:TYR:HE1	1:A:223:LEU:HB3	1.83	0.44
1:A:268:TYR:HB2	1:A:322:PHE:CE2	2.47	0.44
2:B:61:ASP:O	2:B:61:ASP:OD2	2.35	0.44
2:B:89:GLN:O	2:B:93:VAL:HG23	2.17	0.44
2:B:152:ASN:ND2	2:B:155:THR:OG1	2.50	0.44
2:B:329:LEU:HD12	2:B:329:LEU:H	1.82	0.44
2:B:459:LEU:O	2:B:462:TYR:N	2.51	0.44
2:B:470:LYS:C	2:B:472:ARG:N	2.75	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:531:LYS:HG2	2:B:581:SER:HB2	1.99	0.44
2:B:320:ILE:HD11	2:B:379:ARG:HH11	1.80	0.44
1:A:351:LEU:HD12	1:A:351:LEU:H	1.79	0.44
2:B:87:ARG:HG3	2:B:88:GLU:HG3	1.98	0.44
2:B:386:GLN:CD	2:B:386:GLN:H	2.20	0.44
2:B:484:PRO:HA	2:B:487:ALA:HB3	1.99	0.44
2:B:531:LYS:HD3	2:B:581:SER:HB2	2.00	0.44
1:A:149:ALA:CB	1:A:180:GLN:HG3	2.48	0.44
1:A:216:ASP:OD2	1:A:216:ASP:N	2.50	0.44
2:B:20:GLU:C	2:B:22:PHE:N	2.75	0.44
2:B:37:SER:HB2	2:B:182:ALA:CB	2.45	0.44
2:B:53:CYS:SG	2:B:60:PRO:HB3	2.57	0.44
2:B:120:ALA:O	2:B:121:VAL:C	2.59	0.44
2:B:195:TYR:HE1	2:B:381:PRO:HD2	1.82	0.44
2:B:198:ALA:HB1	2:B:376:PHE:HZ	1.81	0.44
2:B:440:ASP:OD1	2:B:440:ASP:O	2.35	0.44
2:B:444:ILE:O	2:B:447:GLU:HB3	2.18	0.44
2:B:521:ASN:HB2	2:B:522:GLY:H	1.50	0.44
1:A:20:LEU:HD12	1:A:20:LEU:C	2.41	0.44
1:A:231:ALA:O	1:A:235:ARG:HB2	2.18	0.44
2:B:44:GLU:CD	2:B:116:GLY:HA2	2.42	0.44
2:B:150:MET:HG2	2:B:151:ILE:N	2.33	0.44
2:B:345:PRO:CB	2:B:354:VAL:HG12	2.48	0.44
1:A:151:MET:HE3	1:A:224:VAL:CG1	2.48	0.44
1:A:233:SER:OG	1:A:234:THR:N	2.49	0.44
1:A:263:TYR:CZ	1:A:327:TRP:CH2	3.06	0.44
1:A:330:GLN:O	1:A:333:LEU:HB3	2.18	0.44
2:B:90:ILE:CG2	2:B:91:PRO:N	2.76	0.44
2:B:137:LYS:HG2	2:B:173:GLY:H	1.81	0.44
1:A:117:LYS:HB2	1:A:117:LYS:HZ2	1.82	0.43
2:B:514:VAL:HA	2:B:530:ILE:HG12	2.00	0.43
2:B:603:ILE:O	2:B:604:VAL:CB	2.66	0.43
1:A:201:ILE:HA	1:A:252:PHE:O	2.18	0.43
2:B:30:GLY:O	2:B:31:PHE:CG	2.71	0.43
2:B:337:PHE:HE2	2:B:459:LEU:HA	1.83	0.43
2:B:473:ARG:HE	2:B:477:ILE:HD11	1.83	0.43
1:A:125:LEU:O	1:A:128:ASP:N	2.51	0.43
1:A:155:ILE:O	1:A:170:CYS:CB	2.66	0.43
2:B:195:TYR:CE1	2:B:381:PRO:HG2	2.54	0.43
2:B:485:LYS:C	2:B:487:ALA:N	2.72	0.43
1:A:100:THR:OG1	1:A:103:GLU:CD	2.61	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:VAL:HA	2:B:77:ILE:O	2.19	0.43
2:B:82:GLY:O	2:B:172:HIS:O	2.36	0.43
2:B:355:VAL:CG2	2:B:423:VAL:HG12	2.47	0.43
2:B:400:TRP:HZ2	2:B:411:GLY:CA	2.31	0.43
1:A:24:ALA:HA	1:A:27:ILE:CD1	2.48	0.43
1:A:84:ALA:CB	1:A:111:TRP:CE2	3.00	0.43
2:B:65:GLN:OE1	2:B:211:ILE:HD12	2.19	0.43
1:A:96:ASN:O	1:A:141:HIS:NE2	2.52	0.43
1:A:161:THR:O	1:A:162:LYS:HB2	2.19	0.43
1:A:214:GLY:O	1:A:215:PHE:CB	2.65	0.43
2:B:36:ARG:HG2	2:B:36:ARG:HH11	1.84	0.43
2:B:80:ASP:O	2:B:81:ASN:HB2	2.19	0.43
2:B:158:PRO:HB2	2:B:159:ASP:H	1.58	0.43
1:A:32:GLU:O	1:A:33:GLU:C	2.62	0.43
1:A:79:LEU:HD22	1:A:114:ALA:CB	2.48	0.43
2:B:135:LEU:HD12	2:B:135:LEU:HA	1.87	0.43
2:B:153:THR:C	2:B:154:SER:HG	2.23	0.43
2:B:284:ASP:O	2:B:286:GLU:N	2.48	0.43
2:B:347:VAL:C	2:B:353:PHE:HE2	2.27	0.43
2:B:394:ALA:CA	2:B:445:LYS:HE3	2.49	0.43
2:B:443:VAL:O	2:B:443:VAL:HG12	2.17	0.43
2:B:551:LYS:HZ3	2:B:586:TYR:HB3	1.84	0.43
1:A:15:LEU:HD11	1:A:141:HIS:CD2	2.53	0.43
1:A:206:MET:N	1:A:344:GLN:NE2	2.66	0.43
1:A:206:MET:HE3	1:A:252:PHE:CE2	2.54	0.43
2:B:90:ILE:CD1	2:B:147:TYR:CE2	3.02	0.43
2:B:222:ARG:NH2	2:B:332:GLU:CB	2.67	0.43
2:B:302:GLU:HA	2:B:305:GLU:HG3	2.00	0.43
2:B:445:LYS:C	2:B:447:GLU:H	2.26	0.43
2:B:502:ASN:HB3	2:B:503:PRO:HD3	2.00	0.43
2:B:541:SER:HA	2:B:575:SER:OG	2.19	0.43
2:B:551:LYS:HB3	2:B:570:TYR:OH	2.19	0.43
1:A:145:GLU:O	1:A:146:GLU:HG3	2.18	0.43
2:B:33:SER:C	2:B:35:PRO:HD2	2.43	0.43
2:B:311:ALA:C	2:B:312:PRO:O	2.61	0.43
2:B:411:GLY:O	2:B:412:ILE:CG1	2.57	0.43
2:B:500:ASP:HB3	2:B:503:PRO:HD3	2.01	0.43
1:A:32:GLU:O	1:A:35:VAL:N	2.52	0.43
2:B:235:LEU:HB2	2:B:267:CYS:H	1.84	0.43
2:B:314:THR:O	2:B:316:CYS:N	2.51	0.43
2:B:357:VAL:CG2	2:B:421:ILE:HG12	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:375:ARG:HD2	2:B:382:LEU:CD2	2.45	0.43
2:B:382:LEU:HD11	2:B:436:ASP:O	2.19	0.43
2:B:61:ASP:OD1	2:B:207:ARG:NH1	2.52	0.42
2:B:204:PRO:HA	2:B:222:ARG:HD3	2.01	0.42
2:B:337:PHE:HB2	2:B:462:TYR:CD1	2.54	0.42
2:B:591:ALA:O	2:B:592:SER:C	2.61	0.42
1:A:79:LEU:HD21	1:A:114:ALA:HB2	1.98	0.42
1:A:133:THR:O	1:A:134:SER:C	2.62	0.42
2:B:300:LEU:HD12	2:B:303:ALA:HB3	2.01	0.42
2:B:302:GLU:C	2:B:304:PHE:N	2.76	0.42
1:A:268:TYR:HB3	1:A:269:GLY:H	1.61	0.42
2:B:48:ASN:ND2	2:B:117:ILE:HG12	2.32	0.42
2:B:117:ILE:O	2:B:121:VAL:HG23	2.20	0.42
2:B:263:ARG:HD2	2:B:271:LEU:CG	2.47	0.42
2:B:376:PHE:CD2	2:B:381:PRO:HA	2.54	0.42
2:B:475:LYS:O	2:B:479:ILE:HG13	2.18	0.42
2:B:479:ILE:HG23	2:B:505:VAL:HG11	2.01	0.42
2:B:576:ALA:HB2	2:B:582:LYS:CE	2.49	0.42
1:A:79:LEU:CD2	1:A:79:LEU:C	2.92	0.42
1:A:135:LEU:CB	1:A:140:PHE:HE1	2.30	0.42
1:A:155:ILE:O	1:A:155:ILE:HG13	2.20	0.42
2:B:353:PHE:CA	2:B:424:ALA:O	2.61	0.42
2:B:479:ILE:HG22	2:B:479:ILE:O	2.19	0.42
2:B:576:ALA:CB	2:B:582:LYS:HE3	2.48	0.42
1:A:102:ARG:O	1:A:106:TYR:HD1	2.01	0.42
2:B:382:LEU:HD11	2:B:436:ASP:CA	2.49	0.42
1:A:169:HIS:HD2	1:A:172:LYS:H	1.68	0.42
1:A:300:LEU:HD11	1:A:346:PHE:HE2	1.84	0.42
2:B:65:GLN:OE1	2:B:211:ILE:CD1	2.68	0.42
2:B:184:TYR:CE2	2:B:212:ASP:HB2	2.54	0.42
2:B:507:LYS:HA	2:B:533:LYS:HD2	2.01	0.42
2:B:47:ASP:O	2:B:48:ASN:C	2.62	0.42
2:B:342:THR:HA	2:B:356:GLU:HG2	2.02	0.42
1:A:20:LEU:C	1:A:22:GLU:N	2.73	0.42
1:A:100:THR:HG22	1:A:143:ARG:C	2.44	0.42
1:A:169:HIS:O	1:A:174:VAL:N	2.53	0.42
2:B:18:VAL:CG1	2:B:156:ASN:OD1	2.68	0.42
2:B:46:VAL:O	2:B:46:VAL:CG1	2.64	0.42
2:B:46:VAL:O	2:B:46:VAL:HG12	2.20	0.42
2:B:222:ARG:HB2	2:B:222:ARG:HH11	1.85	0.42
2:B:453:LYS:CE	2:B:457:ARG:HH21	2.29	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:490:VAL:HG21	2:B:498:VAL:HG22	2.02	0.42
2:B:65:GLN:HG2	2:B:66:VAL:N	2.30	0.42
2:B:190:GLN:NE2	2:B:383:LEU:HD11	2.35	0.42
2:B:405:LEU:HD22	2:B:417:VAL:HG21	2.02	0.42
1:A:26:LYS:HB2	1:A:26:LYS:HE3	1.78	0.42
1:A:107:ILE:HG22	1:A:107:ILE:O	2.19	0.42
1:A:193:HIS:CD2	1:A:193:HIS:C	2.98	0.42
1:A:206:MET:HG2	1:A:343:GLN:NE2	2.34	0.42
2:B:27:GLN:CD	2:B:32:ASP:HB2	2.44	0.42
2:B:232:GLU:OE2	2:B:316:CYS:CA	2.65	0.42
2:B:500:ASP:HB3	2:B:503:PRO:CD	2.50	0.42
2:B:480:THR:O	2:B:480:THR:HG22	2.20	0.41
1:A:71:THR:HA	2:B:478:ILE:HD13	2.02	0.41
1:A:137:ARG:O	1:A:138:GLU:C	2.62	0.41
1:A:180:GLN:O	1:A:182:PRO:HD3	2.19	0.41
2:B:34:ALA:N	2:B:35:PRO:CD	2.83	0.41
2:B:90:ILE:O	2:B:91:PRO:C	2.63	0.41
2:B:260:PRO:C	2:B:262:LEU:H	2.28	0.41
2:B:323:ASP:O	2:B:326:TYR:HB3	2.19	0.41
2:B:531:LYS:CG	2:B:581:SER:HB2	2.49	0.41
1:A:118:GLU:O	1:A:120:GLY:N	2.54	0.41
1:A:151:MET:HE3	1:A:224:VAL:HG11	2.02	0.41
1:A:255:GLY:O	1:A:256:ASP:C	2.63	0.41
1:A:256:ASP:C	1:A:258:TRP:N	2.78	0.41
1:A:309:ASP:O	1:A:312:ALA:HB3	2.20	0.41
2:B:39:ILE:HG23	2:B:40:THR:N	2.35	0.41
2:B:93:VAL:C	2:B:94:PHE:HD2	2.28	0.41
2:B:263:ARG:HH11	2:B:271:LEU:HD11	1.83	0.41
2:B:307:VAL:O	2:B:307:VAL:CG1	2.67	0.41
2:B:309:ILE:O	2:B:310:MET:O	2.37	0.41
1:A:41:LEU:HD22	1:A:68:SER:O	2.20	0.41
1:A:159:GLU:HG3	1:A:160:GLN:H	1.83	0.41
1:A:185:VAL:HG21	1:A:236:ARG:CB	2.40	0.41
2:B:22:PHE:C	2:B:24:LYS:N	2.78	0.41
2:B:131:HIS:HB2	2:B:132:THR:H	1.74	0.41
2:B:323:ASP:O	2:B:324:LEU:C	2.62	0.41
2:B:417:VAL:O	2:B:418:ILE:CB	2.68	0.41
2:B:543:ARG:HB2	2:B:602:LEU:HB2	2.03	0.41
1:A:135:LEU:O	1:A:140:PHE:HE1	2.03	0.41
1:A:154:PRO:C	1:A:155:ILE:HG23	2.45	0.41
2:B:30:GLY:O	2:B:31:PHE:CD1	2.73	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:110:ARG:HB3	2:B:111:GLY:H	1.51	0.41
2:B:178:LEU:HD12	2:B:178:LEU:HA	1.83	0.41
2:B:343:ARG:NH1	2:B:447:GLU:OE2	2.54	0.41
2:B:508:ILE:C	2:B:510:GLY:N	2.77	0.41
1:A:138:GLU:HB2	1:A:236:ARG:HH12	1.86	0.41
1:A:154:PRO:HA	1:A:171:GLN:HA	2.02	0.41
1:A:158:THR:H	1:A:189:GLU:HB3	1.84	0.41
1:A:215:PHE:CE2	1:A:219:TYR:HD2	2.38	0.41
1:A:300:LEU:C	1:A:301:SER:O	2.61	0.41
1:A:321:ARG:HD3	1:A:321:ARG:HA	1.89	0.41
2:B:118:SER:O	2:B:121:VAL:HG23	2.21	0.41
2:B:234:ILE:C	2:B:234:ILE:CD1	2.94	0.41
2:B:425:SER:C	2:B:427:ASN:N	2.78	0.41
2:B:455:VAL:HG23	2:B:456:ALA:N	2.35	0.41
2:B:483:LEU:HB3	2:B:484:PRO:CD	2.51	0.41
2:B:556:LYS:HD3	2:B:556:LYS:N	2.36	0.41
1:A:104:LEU:C	1:A:106:TYR:N	2.78	0.41
2:B:44:GLU:O	2:B:47:ASP:N	2.42	0.41
2:B:117:ILE:O	2:B:118:SER:C	2.63	0.41
2:B:167:ASP:O	2:B:168:TRP:CD1	2.73	0.41
2:B:381:PRO:HB2	2:B:382:LEU:H	1.61	0.41
2:B:391:THR:O	2:B:392:THR:C	2.62	0.41
1:A:31:PHE:HE1	1:A:32:GLU:HG3	1.77	0.41
1:A:194:ASP:OD1	1:A:194:ASP:N	2.53	0.41
1:A:240:ARG:O	1:A:240:ARG:HG2	2.20	0.41
2:B:116:GLY:O	2:B:117:ILE:C	2.62	0.41
2:B:153:THR:O	2:B:155:THR:N	2.54	0.41
2:B:188:ARG:CG	2:B:189:ARG:H	2.32	0.41
2:B:309:ILE:CG2	2:B:310:MET:N	2.81	0.41
2:B:365:LEU:CD1	2:B:417:VAL:O	2.69	0.41
2:B:392:THR:O	2:B:393:HIS:C	2.63	0.41
2:B:459:LEU:O	2:B:460:LYS:C	2.63	0.41
2:B:615:ALA:O	2:B:616:LYS:CB	2.68	0.41
1:A:20:LEU:HB2	1:A:135:LEU:HD11	2.01	0.41
1:A:193:HIS:O	1:A:193:HIS:CG	2.73	0.41
1:A:245:LEU:HD13	1:A:247:ILE:HD12	2.02	0.41
1:A:254:ASP:CG	1:A:343:GLN:HB2	2.46	0.41
1:A:300:LEU:HD11	1:A:346:PHE:CD2	2.56	0.41
1:A:340:LYS:O	1:A:341:ALA:HB2	2.21	0.41
1:A:346:PHE:CB	1:A:354:VAL:HG22	2.50	0.41
2:B:52:ALA:O	2:B:53:CYS:C	2.64	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:161:LEU:O	2:B:162:VAL:HG22	2.20	0.41
2:B:262:LEU:HD13	2:B:274:ALA:HA	2.02	0.41
2:B:307:VAL:CG2	2:B:309:ILE:HD11	2.34	0.41
2:B:345:PRO:HB3	2:B:354:VAL:CG1	2.51	0.41
2:B:462:TYR:O	2:B:466:GLN:N	2.28	0.41
2:B:470:LYS:O	2:B:472:ARG:N	2.50	0.41
2:B:512:LEU:N	2:B:512:LEU:HD23	2.36	0.41
2:B:544:VAL:O	2:B:544:VAL:HG12	2.19	0.41
2:B:561:VAL:HG22	2:B:570:TYR:CE1	2.56	0.41
1:A:245:LEU:HB3	1:A:247:ILE:CD1	2.51	0.41
1:A:357:VAL:O	1:A:361:ASN:HB2	2.20	0.41
2:B:31:PHE:CE2	2:B:123:TYR:CG	3.09	0.41
2:B:36:ARG:HB2	2:B:384:TYR:OH	2.21	0.41
2:B:355:VAL:HG13	2:B:422:HIS:O	2.21	0.41
2:B:390:VAL:HB	2:B:438:ILE:HB	2.02	0.41
1:A:258:TRP:CZ3	1:A:261:ARG:CZ	3.05	0.40
2:B:80:ASP:HB2	2:B:174:THR:H	1.85	0.40
2:B:417:VAL:CG1	2:B:418:ILE:H	2.24	0.40
2:B:490:VAL:C	2:B:492:HIS:N	2.50	0.40
1:A:17:ARG:NH1	1:A:17:ARG:HG3	2.36	0.40
1:A:231:ALA:HA	1:A:235:ARG:CZ	2.51	0.40
2:B:44:GLU:OE1	2:B:116:GLY:HA2	2.20	0.40
2:B:96:LYS:CB	2:B:118:SER:OG	2.70	0.40
2:B:484:PRO:O	2:B:487:ALA:HB3	2.21	0.40
2:B:516:ARG:NH2	2:B:546:GLU:OE1	2.54	0.40
2:B:576:ALA:HB1	2:B:580:SER:CB	2.48	0.40
1:A:68:SER:O	1:A:69:ALA:HB3	2.20	0.40
1:A:360:PRO:O	1:A:361:ASN:C	2.63	0.40
2:B:58:ILE:O	2:B:60:PRO:CD	2.68	0.40
2:B:148:GLU:HG3	2:B:162:VAL:HG21	2.02	0.40
2:B:246:LEU:O	2:B:250:LEU:HG	2.22	0.40
2:B:466:GLN:O	2:B:467:SER:C	2.65	0.40
1:A:76:PHE:CE2	2:B:481:LYS:HE2	2.56	0.40
1:A:235:ARG:O	1:A:237:ILE:N	2.54	0.40
2:B:27:GLN:O	2:B:28:ILE:C	2.64	0.40
2:B:208:ILE:HB	2:B:220:PHE:HB2	2.04	0.40
2:B:224:THR:O	2:B:224:THR:HG22	2.22	0.40
2:B:320:ILE:HD13	2:B:320:ILE:HA	1.91	0.40
2:B:333:THR:HB	2:B:334:THR:H	1.47	0.40
2:B:497:ASP:O	2:B:499:PRO:CD	2.51	0.40
1:A:80:LYS:HG2	1:A:114:ALA:O	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ASP:HB2	1:A:180:GLN:NE2	2.37	0.40
1:A:346:PHE:HB2	1:A:354:VAL:CG2	2.52	0.40
1:A:357:VAL:O	1:A:360:PRO:HG2	2.21	0.40
2:B:57:GLY:C	2:B:58:ILE:HG12	2.45	0.40
2:B:65:GLN:HB3	2:B:77:ILE:HD13	2.02	0.40
2:B:425:SER:OG	2:B:427:ASN:O	2.31	0.40
2:B:430:PHE:CD1	2:B:435:LYS:HG2	2.57	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	303/369 (82%)	163 (54%)	78 (26%)	62 (20%)	0	1
2	B	566/621 (91%)	339 (60%)	122 (22%)	105 (19%)	0	2
All	All	869/990 (88%)	502 (58%)	200 (23%)	167 (19%)	0	2

All (167) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	72	VAL
1	A	97	ARG
1	A	112	ASP
1	A	113	TYR
1	A	115	LYS
1	A	123	ASP
1	A	124	ARG
1	A	137	ARG
1	A	146	GLU
1	A	160	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	192	LYS
1	A	215	PHE
1	A	280	MET
1	A	282	THR
1	A	300	LEU
2	B	12	LYS
2	B	14	LYS
2	B	26	ARG
2	B	58	ILE
2	B	66	VAL
2	B	81	ASN
2	B	115	ILE
2	B	116	GLY
2	B	117	ILE
2	B	131	HIS
2	B	132	THR
2	B	152	ASN
2	B	153	THR
2	B	158	PRO
2	B	159	ASP
2	B	168	TRP
2	B	169	PHE
2	B	171	PRO
2	B	172	HIS
2	B	185	VAL
2	B	189	ARG
2	B	190	GLN
2	B	224	THR
2	B	225	ASP
2	B	251	HIS
2	B	267	CYS
2	B	310	MET
2	B	349	SER
2	B	362	GLY
2	B	367	LYS
2	B	381	PRO
2	B	382	LEU
2	B	385	GLN
2	B	400	TRP
2	B	418	ILE
2	B	440	ASP
2	B	491	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	494	LEU
2	B	496	LYS
2	B	498	VAL
2	B	551	LYS
2	B	560	LYS
2	B	589	GLU
2	B	592	SER
2	B	603	ILE
1	A	16	ALA
1	A	39	VAL
1	A	70	LYS
1	A	83	TYR
1	A	84	ALA
1	A	85	THR
1	A	119	GLN
1	A	141	HIS
1	A	149	ALA
1	A	150	THR
1	A	155	ILE
1	A	175	GLY
1	A	183	PHE
1	A	205	GLY
1	A	227	LYS
1	A	232	ARG
1	A	233	SER
1	A	254	ASP
1	A	290	LEU
1	A	299	GLU
1	A	366	MET
2	B	17	SER
2	B	31	PHE
2	B	52	ALA
2	B	54	GLU
2	B	104	HIS
2	B	111	GLY
2	B	114	GLY
2	B	140	PRO
2	B	155	THR
2	B	289	PRO
2	B	312	PRO
2	B	365	LEU
2	B	403	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	431	THR
2	B	435	LYS
2	B	456	ALA
2	B	497	ASP
2	B	500	ASP
2	B	512	LEU
2	B	524	GLY
2	B	546	GLU
2	B	593	GLU
2	B	598	LYS
2	B	604	VAL
1	A	102	ARG
1	A	144	PRO
1	A	203	THR
1	A	341	ALA
1	A	342	GLU
2	B	23	GLU
2	B	32	ASP
2	B	45	ALA
2	B	238	PRO
2	B	426	ILE
2	B	432	SER
2	B	449	ASP
2	B	454	GLU
2	B	586	TYR
2	B	595	GLU
2	B	596	LEU
1	A	37	PRO
1	A	42	PRO
1	A	86	ASP
1	A	96	ASN
1	A	114	ALA
1	A	184	ASN
1	A	234	THR
1	A	236	ARG
1	A	268	TYR
2	B	21	PHE
2	B	80	ASP
2	B	113	GLN
2	B	188	ARG
2	B	250	LEU
2	B	285	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	333	THR
2	B	402	GLN
2	B	471	LYS
2	B	499	PRO
2	B	521	ASN
2	B	557	PRO
2	B	558	GLU
1	A	30	GLN
1	A	89	ILE
1	A	212	GLU
1	A	218	ALA
1	A	336	ASP
2	B	15	SER
2	B	204	PRO
2	B	313	PRO
2	B	334	THR
2	B	433	GLU
2	B	550	CYS
2	B	588	ILE
1	A	190	PHE
1	A	320	PRO
2	B	483	LEU
2	B	412	ILE
2	B	417	VAL
1	A	182	PRO
1	A	337	ILE
2	B	559	PRO
1	A	295	ILE
1	A	292	PRO
2	B	478	ILE

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	268/315 (85%)	239 (89%)	29 (11%)	6 24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	486/527 (92%)	427 (88%)	59 (12%)	5	21
All	All	754/842 (90%)	666 (88%)	88 (12%)	5	21

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	18	GLU
1	A	28	TYR
1	A	39	VAL
1	A	77	GLN
1	A	93	LEU
1	A	111	TRP
1	A	117	LYS
1	A	118	GLU
1	A	140	PHE
1	A	143	ARG
1	A	145	GLU
1	A	174	VAL
1	A	176	GLU
1	A	182	PRO
1	A	183	PHE
1	A	187	ASN
1	A	194	ASP
1	A	203	THR
1	A	210	LEU
1	A	211	MET
1	A	219	TYR
1	A	286	LYS
1	A	292	PRO
1	A	299	GLU
1	A	305	LEU
1	A	319	ASP
1	A	323	GLU
1	A	355	THR
2	B	27	GLN
2	B	29	LEU
2	B	58	ILE
2	B	64	VAL
2	B	77	ILE
2	B	79	GLU
2	B	83	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	89	GLN
2	B	90	ILE
2	B	97	LEU
2	B	99	TYR
2	B	109	SER
2	B	112	GLN
2	B	115	ILE
2	B	117	ILE
2	B	121	VAL
2	B	127	THR
2	B	137	LYS
2	B	141	THR
2	B	159	ASP
2	B	161	LEU
2	B	170	ARG
2	B	171	PRO
2	B	175	GLN
2	B	178	LEU
2	B	179	GLU
2	B	185	VAL
2	B	210	LEU
2	B	214	ASP
2	B	216	ASN
2	B	218	GLU
2	B	310	MET
2	B	315	ASP
2	B	325	ILE
2	B	333	THR
2	B	334	THR
2	B	357	VAL
2	B	366	PRO
2	B	373	ILE
2	B	375	ARG
2	B	383	LEU
2	B	391	THR
2	B	397	ASP
2	B	399	LYS
2	B	403	TYR
2	B	406	ASN
2	B	436	ASP
2	B	444	ILE
2	B	473	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	508	ILE
2	B	521	ASN
2	B	528	VAL
2	B	540	TYR
2	B	548	LEU
2	B	551	LYS
2	B	561	VAL
2	B	564	MET
2	B	584	LEU
2	B	599	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	77	GLN
1	A	90	ASN
1	A	119	GLN
1	A	136	GLN
1	A	187	ASN
1	A	193	HIS
1	A	229	GLN
1	A	332	GLN
1	A	344	GLN
2	B	25	ASN
2	B	48	ASN
2	B	81	ASN
2	B	89	GLN
2	B	152	ASN
2	B	190	GLN
2	B	251	HIS
2	B	378	ASN
2	B	406	ASN
2	B	502	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 oligosaccharides 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	315/369 (85%)	0.33	12 (3%) 44 34	139, 217, 258, 265	0
2	B	582/621 (93%)	0.10	11 (1%) 66 49	93, 175, 248, 265	0
All	All	897/990 (90%)	0.18	23 (2%) 57 42	93, 192, 254, 265	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	594	GLU	3.6
2	B	515	HIS	3.4
1	A	179	TYR	3.0
1	A	25	GLU	2.9
1	A	82	THR	2.7
2	B	289	PRO	2.7
1	A	297	GLU	2.7
1	A	86	ASP	2.6
1	A	147	ASP	2.6
2	B	254	GLU	2.6
2	B	605	GLU	2.6
1	A	260	TYR	2.4
2	B	231	ALA	2.3
2	B	28	ILE	2.3
1	A	202	GLU	2.3
1	A	270	ALA	2.2
2	B	369	GLU	2.2
2	B	260	PRO	2.2
1	A	85	THR	2.1
1	A	83	TYR	2.1
2	B	19	ALA	2.1
1	A	23	ILE	2.0
2	B	181	ARG	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 oligosaccharides 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.