Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2021 – 11:23 PM EDT

PDB ID	:	1S6P
Title	:	CRYSTAL STRUCTURE OF HUMAN IMMUNODEFICIENCY VIRUS TYPE 1 REVERSE TRANSCRIPTASE (RT) IN COMPLEX WITH JANSSEN-R100943
Authors	:	Das, K.; Arnold, E.
Deposited on	:	2004-01-26
Resolution	:	2.90 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 following versions of software and data (see references ⓘ) were used in the production of this report:

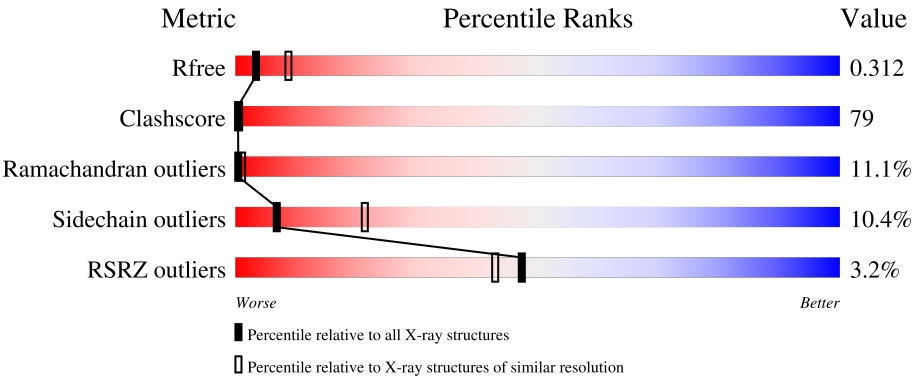
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	560	3% 21% 62% 15%
2	B	430	3% 19% 59% 20%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8202 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 POL polyprotein [Contains: Reverse transcriptase].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	18	0	0
			4498	2913	748	830	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 2 is a protein called POL polyprotein [Contains: Reverse transcriptase].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	17	0	0
			3529	2300	584	638	7			

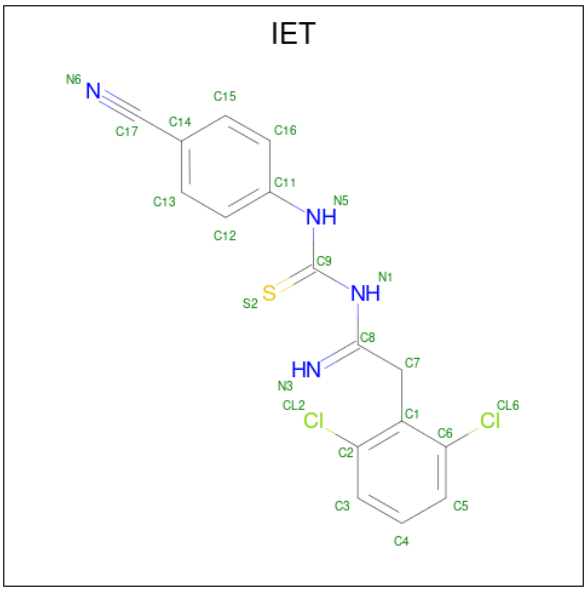
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 1-(4-CYANO-PHENYL)-3-[2-(2,6-DICHLORO-PHENYL)-1-IMINO-ETHYL] -THIOUREA (three-letter code: IET) (formula: $C_{16}H_{12}Cl_2N_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	S	0	0
			23	16	2	4	1		

- Molecule 5 is water.

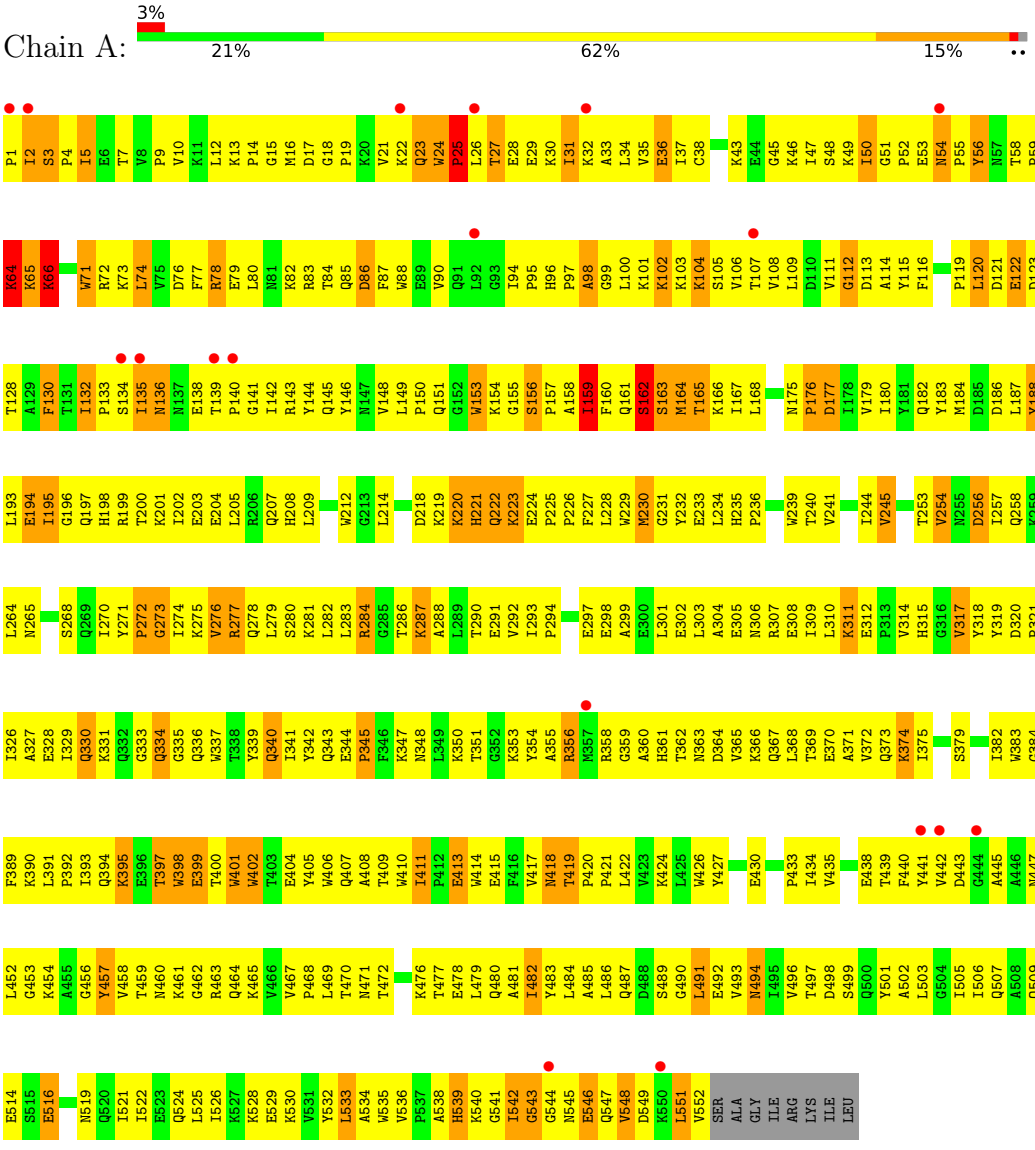
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	81	Total	O	0	0
			81	81		
5	B	70	Total	O	0	0
			70	70		

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.

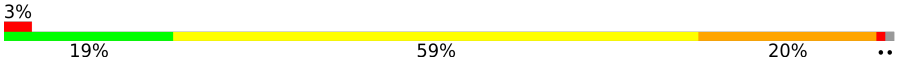
• Molecule 1: POL polyprotein [Contains: Reverse transcriptase]

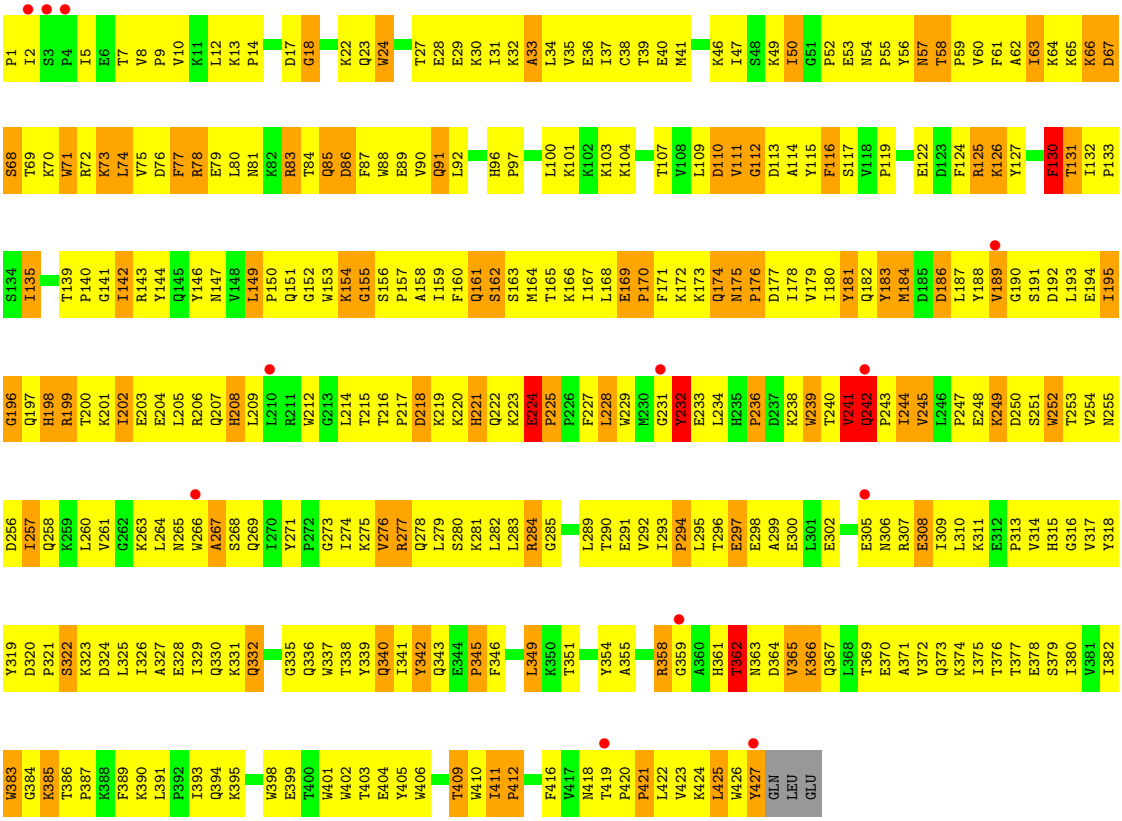
Chain A:



• Molecule 2: POL polyprotein [Contains: Reverse transcriptase]

Chain B:




P1 I2 S3 P4 I5 E6 T7 V8 P9 V10 K11 L12 K13 P14 D17 G18 K22 Q23 W24 T27 E28 E29 K30 I31 K32 A33 L34 V35 E36 I37 C38 T39 E40 M41 K46 I47 S48 K49 I50 G51 P52 E53 N54 P55 Y56 N57 T58 P59 V60 F61 A62 I63 K64 K65 K66 D67
S68 T69 K70 W71 R72 K73 L74 V75 D76 F77 R78 E79 L80 N81 K82 R83 T84 Q85 D86 F87 W88 E89 V90 Q91 L92 H96 P97 L100 K101 K102 K103 K104 T107 V108 L109 D110 V111 G112 D113 A114 Y115 F116 S117 V118 P119 E122 D123 F124 R125 K126 Y127 F130 T131 I132 P133
S134 I135 T139 P140 G141 I142 R143 Y144 Q145 Y146 N147 V148 L149 P150 Q151 G152 W153 K154 G155 S156 P157 A158 I159 F160 Q161 S162 S163 M164 T165 K166 I167 L168 E169 P170 F171 K172 K173 Q174 N175 P176 D177 I178 V179 I180 Y181 Q182 Y183 M184 D185 D186 L187 Y188 V189 G190 S191 D192 L193 E194 I195
G196 Q197 H198 R199 T200 K201 I202 E203 E204 L205 R206 Q207 H208 L209 L210 R211 W212 G213 L214 T215 T216 P217 D218 K219 K220 H221 Q222 K223 E224 P225 P226 F227 L228 W229 M230 G231 Y232 E233 L234 H235 P236 D237 K238 W239 T240 V241 Q242 P243 I244 V245 L246 P247 E248 K249 D250 S251 W252 T253 V254 N255
D256 I257 Q258 K259 L260 V261 G262 K263 L264 N265 W266 A267 S268 Q269 Y270 Y271 P272 G273 I274 K275 V276 R277 Q278 L279 S280 K281 L282 L283 R284 G285 L289 T290 E291 V292 I293 P294 L295 T296 E297 E298 A299 E300 L301 E302 E305 N306 R307 E308 I309 L310 K311 E312 P313 V314 H315 G316 V317 Y318
Y319 D320 P321 S322 K323 D324 L325 I326 A327 E328 I329 Q330 K331 Q332 G335 Q336 W337 T338 Y339 Q340 I341 Y342 Q343 E344 P345 F346 L349 K350 T351 Y354 A355 R358 G359 A360 H361 T362 N363 D364 V365 K366 Q367 L368 T369 E370 A371 V372 Q373 K374 I375 T376 T377 E378 S379 I380 V381 I382
W383 G384 K385 T386 P387 K388 F389 K390 L391 P392 I393 Q394 K395 W398 E399 T400 W401 W402 T403 E404 Y405 W406 T409 W410 I411 P412 F416 V417 N418 T419 P420 P421 I422 V423 K424 L425 W426 Y427 GLN LEU GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	226.70Å 67.40Å 104.30Å 90.00° 107.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 19.95 – 2.82	Depositor EDS
% Data completeness (in resolution range)	89.8 (20.00-2.90) 87.2 (19.95-2.82)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 2.83Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.245 , 0.312 0.249 , 0.312	Depositor DCC
R_{free} test set	1616 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	67.3	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 97.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	8202	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.67	1/4616 (0.0%)	0.90	8/6271 (0.1%)
2	B	0.66	2/3634 (0.1%)	0.95	9/4940 (0.2%)
All	All	0.67	3/8250 (0.0%)	0.92	17/11211 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0
2	B	0	1
All	All	1	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	31	ILE	CG1-CD1	23.29	3.11	1.50
2	B	224	GLU	C-N	-5.33	1.24	1.34
2	B	225	PRO	N-CD	-5.15	1.40	1.47

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	31	ILE	CB-CG1-CD1	-20.89	55.42	113.90
1	A	72	ARG	NE-CZ-NH2	7.40	124.00	120.30
2	B	242	GLN	N-CA-C	7.12	130.24	111.00
1	A	287	LYS	O-C-N	6.82	133.61	122.70
2	B	83	ARG	NE-CZ-NH2	6.67	123.63	120.30
1	A	284	ARG	NE-CZ-NH2	6.49	123.55	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	241	VAL	N-CA-C	6.30	128.01	111.00
1	A	221	HIS	N-CA-CB	-6.23	99.38	110.60
2	B	225	PRO	O-C-N	-6.10	109.51	121.10
2	B	225	PRO	CB-CA-C	-6.10	96.76	112.00
2	B	78	ARG	NE-CZ-NH2	-5.93	117.34	120.30
2	B	225	PRO	CA-N-CD	5.91	119.98	111.70
1	A	273	GLY	N-CA-C	5.87	127.78	113.10
1	A	162	SER	N-CA-C	-5.36	96.54	111.00
1	A	220	LYS	O-C-N	5.23	131.07	122.70
2	B	130	PHE	N-CA-C	-5.17	97.05	111.00
2	B	411	ILE	C-N-CD	5.10	139.11	128.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	31	ILE	CB

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	130	PHE	Sidechain

5.2 Too-close contacts (i)

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	4498	0	4560	697	0
2	B	3529	0	3568	615	0
3	A	1	0	0	0	0
4	A	23	0	12	5	0
5	A	81	0	0	8	0
5	B	70	0	0	5	0
All	All	8202	0	8140	1277	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 79.

All (1277) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:LYS:O	1:A:66:LYS:HG2	1.34	1.25
2:B:139:THR:CG2	2:B:140:PRO:HD2	1.66	1.24
1:A:222:GLN:O	1:A:224:GLU:HG3	1.41	1.16
1:A:497:THR:HG22	1:A:499:SER:H	1.09	1.16
2:B:358:ARG:HG2	2:B:359:GLY:H	1.09	1.16
2:B:139:THR:HG23	2:B:140:PRO:HD2	1.23	1.15
2:B:206:ARG:HE	2:B:218:ASP:HB2	1.09	1.14
2:B:296:THR:HG22	2:B:297:GLU:H	1.10	1.14
1:A:90:VAL:HG11	1:A:161:GLN:HE22	1.13	1.13
1:A:362:THR:HG22	1:A:363:ASN:H	0.97	1.13
2:B:135:ILE:H	2:B:135:ILE:CD1	1.61	1.12
2:B:195:ILE:HG23	2:B:196:GLY:H	1.10	1.11
2:B:104:LYS:HB2	2:B:192:ASP:HA	1.28	1.10
2:B:135:ILE:HD12	2:B:135:ILE:N	1.66	1.09
1:A:454:LYS:HB2	1:A:552:VAL:HG13	1.16	1.07
2:B:220:LYS:HE3	2:B:231:GLY:HA2	1.35	1.07
1:A:288:ALA:HB1	1:A:291:GLU:HB2	1.38	1.06
2:B:85:GLN:HG3	2:B:154:LYS:HB3	1.33	1.06
1:A:442:VAL:HG22	1:A:481:ALA:HB1	1.38	1.05
1:A:397:THR:HG21	1:A:424:LYS:HA	1.36	1.03
1:A:84:THR:HG23	1:A:154:LYS:HE2	1.35	1.03
1:A:411:ILE:HD13	1:A:411:ILE:H	1.23	1.02
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.42	1.02
1:A:64:LYS:C	1:A:66:LYS:HG2	1.78	1.02
2:B:297:GLU:HG3	2:B:298:GLU:H	1.22	1.00
2:B:326:ILE:HB	2:B:342:TYR:CE1	1.96	1.00
2:B:295:LEU:HD12	2:B:300:GLU:HG2	1.43	1.00
1:A:492:GLU:HG3	1:A:530:LYS:HB2	1.44	0.99
2:B:216:THR:HB	2:B:218:ASP:OD2	1.62	0.98
2:B:74:LEU:HD21	2:B:411:ILE:HD11	1.47	0.97
1:A:108:VAL:HG12	1:A:188:TYR:CG	1.99	0.97
2:B:221:HIS:ND1	2:B:229:TRP:HB2	1.80	0.97
2:B:358:ARG:HA	2:B:362:THR:HB	1.47	0.96
2:B:135:ILE:H	2:B:135:ILE:HD12	0.81	0.95
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.44	0.95
2:B:326:ILE:HB	2:B:342:TYR:HE1	1.30	0.94
1:A:362:THR:HG22	1:A:363:ASN:N	1.80	0.94
2:B:373:GLN:HE22	2:B:406:TRP:HA	1.30	0.94
1:A:19:PRO:O	1:A:56:TYR:HB3	1.67	0.93
2:B:253:THR:O	2:B:257:ILE:HG22	1.68	0.93
1:A:362:THR:CG2	1:A:363:ASN:H	1.80	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:363:ASN:O	2:B:367:GLN:HG3	1.68	0.92
2:B:139:THR:HG22	2:B:140:PRO:HD2	1.49	0.92
2:B:296:THR:CG2	2:B:297:GLU:H	1.82	0.92
1:A:411:ILE:H	1:A:411:ILE:CD1	1.82	0.91
2:B:174:GLN:O	2:B:176:PRO:HD3	1.70	0.91
1:A:90:VAL:HG11	1:A:161:GLN:NE2	1.85	0.91
1:A:422:LEU:HD23	1:A:424:LYS:HD3	1.51	0.91
2:B:171:PHE:HB2	2:B:208:HIS:HD2	1.35	0.90
1:A:449:GLU:HG3	1:A:450:THR:N	1.83	0.90
2:B:31:ILE:O	2:B:35:VAL:HG23	1.72	0.90
2:B:275:LYS:HG2	2:B:277:ARG:HH21	1.35	0.90
2:B:358:ARG:HG2	2:B:359:GLY:N	1.87	0.89
2:B:139:THR:CG2	2:B:140:PRO:CD	2.50	0.88
1:A:53:GLU:HG3	1:A:54:ASN:H	1.38	0.88
1:A:288:ALA:CB	1:A:291:GLU:HB2	2.04	0.88
1:A:442:VAL:CG2	1:A:481:ALA:HB1	2.02	0.88
2:B:12:LEU:HD12	2:B:83:ARG:O	1.73	0.88
1:A:64:LYS:O	1:A:66:LYS:N	2.06	0.88
1:A:115:TYR:OH	1:A:151:GLN:HG3	1.74	0.88
2:B:115:TYR:HE2	2:B:157:PRO:HA	1.37	0.88
2:B:260:LEU:HG	2:B:264:LEU:HD11	1.56	0.87
1:A:38:CYS:HB3	1:A:144:TYR:CE1	2.10	0.87
1:A:240:THR:HG22	1:A:241:VAL:N	1.90	0.87
1:A:34:LEU:CD2	1:A:62:ALA:HB2	2.05	0.86
1:A:134:SER:OG	1:A:139:THR:HB	1.75	0.86
1:A:258:GLN:HG2	1:A:283:LEU:HD22	1.56	0.86
1:A:441:TYR:HB3	1:A:548:VAL:HG11	1.56	0.86
1:A:254:VAL:HG23	1:A:293:ILE:HD11	1.58	0.86
2:B:261:VAL:HG13	2:B:276:VAL:HG11	1.56	0.86
2:B:248:GLU:HG2	2:B:307:ARG:HH12	1.39	0.85
2:B:373:GLN:NE2	2:B:406:TRP:HA	1.90	0.85
2:B:183:TYR:HD1	2:B:380:ILE:HG23	1.40	0.85
2:B:221:HIS:CE1	2:B:229:TRP:HB2	2.11	0.85
2:B:296:THR:HG22	2:B:297:GLU:N	1.89	0.85
1:A:291:GLU:O	1:A:293:ILE:HD12	1.77	0.85
1:A:497:THR:HG22	1:A:499:SER:N	1.92	0.84
1:A:195:ILE:O	1:A:199:ARG:HG2	1.74	0.84
1:A:483:TYR:HB2	1:A:521:ILE:CG1	2.07	0.84
2:B:195:ILE:HG23	2:B:196:GLY:N	1.91	0.84
2:B:380:ILE:O	2:B:384:GLY:HA2	1.78	0.84
2:B:298:GLU:O	2:B:302:GLU:N	2.11	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:THR:HG22	1:A:241:VAL:H	1.39	0.84
1:A:254:VAL:HA	1:A:257:ILE:HG22	1.57	0.84
2:B:1:PRO:HD3	2:B:117:SER:HA	1.59	0.84
2:B:104:LYS:CB	2:B:192:ASP:HA	2.07	0.83
1:A:218:ASP:O	1:A:221:HIS:HB2	1.77	0.83
1:A:27:THR:HB	1:A:29:GLU:HG2	1.61	0.83
1:A:545:ASN:O	1:A:548:VAL:HG22	1.79	0.82
1:A:479:LEU:O	1:A:521:ILE:HD11	1.79	0.82
2:B:174:GLN:HA	2:B:174:GLN:HE21	1.44	0.82
2:B:101:LYS:O	2:B:236:PRO:HB2	1.80	0.82
2:B:206:ARG:NE	2:B:218:ASP:HB2	1.93	0.82
1:A:31:ILE:O	1:A:35:VAL:HG23	1.79	0.81
1:A:60:VAL:HG22	1:A:130:PHE:HB2	1.62	0.81
1:A:447:ASN:HB3	1:A:450:THR:HB	1.60	0.81
2:B:332:GLN:HG2	2:B:338:THR:HG23	1.60	0.81
1:A:130:PHE:CE1	1:A:144:TYR:HB2	2.16	0.81
2:B:206:ARG:HB3	2:B:206:ARG:NH1	1.95	0.81
1:A:79:GLU:HG3	1:A:83:ARG:HH12	1.45	0.81
2:B:178:ILE:HD13	2:B:191:SER:HB3	1.61	0.81
1:A:356:ARG:CZ	1:A:358:ARG:HG3	2.11	0.81
1:A:258:GLN:HG2	1:A:283:LEU:CD2	2.09	0.81
1:A:368:LEU:O	1:A:372:VAL:HG23	1.80	0.81
1:A:96:HIS:HB3	1:A:382:ILE:HD12	1.63	0.81
1:A:288:ALA:HB1	1:A:291:GLU:CB	2.11	0.81
1:A:108:VAL:CG1	1:A:188:TYR:CD2	2.64	0.81
1:A:320:ASP:H	1:A:343:GLN:HE22	1.27	0.81
1:A:441:TYR:HB3	1:A:548:VAL:CG1	2.10	0.80
2:B:27:THR:HG22	2:B:29:GLU:H	1.47	0.80
1:A:10:VAL:HG11	1:A:153:TRP:HZ2	1.47	0.80
2:B:171:PHE:HB2	2:B:208:HIS:CD2	2.16	0.80
1:A:29:GLU:HG3	1:A:30:LYS:N	1.97	0.79
2:B:326:ILE:CB	2:B:342:TYR:HE1	1.94	0.79
1:A:434:ILE:HG21	1:A:492:GLU:HG2	1.61	0.79
2:B:103:LYS:HG3	2:B:190:GLY:O	1.83	0.79
1:A:64:LYS:O	1:A:66:LYS:CG	2.26	0.79
1:A:23:GLN:O	1:A:25:PRO:HD3	1.81	0.79
2:B:201:LYS:HE2	2:B:201:LYS:HA	1.64	0.79
1:A:540:LYS:HD3	2:B:265:ASN:HD21	1.48	0.78
1:A:476:LYS:HE3	1:A:516:GLU:OE2	1.83	0.78
1:A:503:LEU:CD2	1:A:535:TRP:HB2	2.12	0.78
1:A:28:GLU:HG2	1:A:135:ILE:O	1.83	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:295:LEU:HG	2:B:295:LEU:O	1.83	0.78
2:B:339:TYR:CG	2:B:375:ILE:HD11	2.19	0.78
1:A:2:ILE:HG22	1:A:3:SER:H	1.47	0.77
1:A:458:VAL:HG22	1:A:464:GLN:HG2	1.64	0.77
2:B:376:THR:HG22	2:B:380:ILE:CD1	2.14	0.77
1:A:132:ILE:CG2	1:A:142:ILE:HB	2.15	0.77
2:B:195:ILE:CG2	2:B:196:GLY:H	1.96	0.77
2:B:335:GLY:O	2:B:355:ALA:HA	1.85	0.77
1:A:12:LEU:HG	1:A:124:PHE:HE1	1.47	0.77
2:B:175:ASN:H	2:B:175:ASN:HD22	1.31	0.77
1:A:28:GLU:HA	1:A:31:ILE:CG2	2.14	0.77
1:A:189:VAL:HG21	1:A:205:LEU:CD2	2.15	0.77
1:A:439:THR:O	1:A:459:THR:HG22	1.85	0.77
2:B:69:THR:O	2:B:70:LYS:HG3	1.84	0.76
2:B:139:THR:HG23	2:B:140:PRO:CD	2.12	0.76
2:B:23:GLN:CG	2:B:133:PRO:HG3	2.14	0.76
1:A:331:LYS:HE2	1:A:333:GLY:HA2	1.68	0.76
2:B:261:VAL:HG13	2:B:276:VAL:CG1	2.14	0.76
1:A:198:HIS:NE2	1:A:202:ILE:HD11	2.01	0.76
2:B:66:LYS:HD3	2:B:69:THR:HB	1.67	0.76
1:A:104:LYS:HD3	1:A:192:ASP:O	1.84	0.76
2:B:23:GLN:HG2	2:B:133:PRO:HG3	1.68	0.76
2:B:221:HIS:N	2:B:221:HIS:CD2	2.53	0.76
1:A:156:SER:H	1:A:157:PRO:HD2	1.51	0.76
1:A:193:LEU:HB3	1:A:197:GLN:HB3	1.65	0.76
2:B:131:THR:OG1	2:B:143:ARG:HG2	1.86	0.75
1:A:286:THR:HG22	1:A:287:LYS:N	2.00	0.75
2:B:267:ALA:HB2	2:B:426:TRP:CZ2	2.21	0.75
1:A:29:GLU:HG3	1:A:30:LYS:H	1.51	0.75
2:B:76:ASP:OD1	2:B:78:ARG:NE	2.17	0.75
2:B:282:LEU:O	2:B:293:ILE:HD11	1.85	0.75
1:A:101:LYS:O	1:A:103:LYS:HG2	1.86	0.75
2:B:183:TYR:CE2	2:B:184:MET:HG3	2.20	0.75
1:A:132:ILE:HG22	1:A:142:ILE:HB	1.68	0.75
1:A:286:THR:CG2	1:A:287:LYS:N	2.49	0.75
1:A:7:THR:HG22	1:A:119:PRO:HB2	1.69	0.75
1:A:195:ILE:HD12	1:A:199:ARG:HH21	1.51	0.75
1:A:53:GLU:HG3	1:A:54:ASN:N	2.00	0.75
1:A:34:LEU:HD21	1:A:62:ALA:CB	2.16	0.74
1:A:209:LEU:HD22	1:A:214:LEU:HD12	1.69	0.74
2:B:85:GLN:HG3	2:B:154:LYS:CB	2.12	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:TYR:HB3	2:B:274:ILE:HD13	1.67	0.74
1:A:331:LYS:HE3	1:A:364:ASP:OD1	1.87	0.74
2:B:139:THR:HG22	2:B:140:PRO:CD	2.14	0.74
2:B:351:THR:HG22	2:B:351:THR:O	1.87	0.74
2:B:31:ILE:HG22	2:B:35:VAL:CG2	2.18	0.74
1:A:84:THR:CG2	1:A:154:LYS:HE2	2.17	0.74
2:B:33:ALA:O	2:B:37:ILE:HG13	1.88	0.74
1:A:108:VAL:CG1	1:A:188:TYR:CG	2.70	0.73
1:A:339:TYR:O	1:A:340:GLN:HG3	1.88	0.73
2:B:69:THR:HG23	2:B:70:LYS:N	2.03	0.73
2:B:358:ARG:CG	2:B:359:GLY:H	1.96	0.73
1:A:108:VAL:HG12	1:A:188:TYR:CB	2.18	0.73
1:A:132:ILE:HD13	1:A:133:PRO:HD2	1.70	0.73
1:A:139:THR:CG2	1:A:140:PRO:HD2	2.17	0.73
2:B:60:VAL:HG11	2:B:130:PHE:CD2	2.22	0.73
1:A:240:THR:CG2	1:A:241:VAL:H	2.00	0.73
2:B:244:ILE:HD13	2:B:244:ILE:H	1.53	0.73
2:B:393:ILE:HG12	2:B:398:TRP:HB2	1.70	0.73
2:B:61:PHE:HE1	2:B:76:ASP:HB2	1.54	0.73
2:B:369:THR:O	2:B:373:GLN:HG3	1.89	0.73
1:A:64:LYS:HA	1:A:66:LYS:HD3	1.70	0.73
2:B:80:LEU:HD11	2:B:124:PHE:HZ	1.54	0.73
2:B:277:ARG:H	2:B:277:ARG:HD3	1.53	0.73
2:B:302:GLU:O	2:B:306:ASN:HB2	1.89	0.73
2:B:380:ILE:HD12	2:B:380:ILE:H	1.54	0.73
1:A:10:VAL:HG11	1:A:153:TRP:CZ2	2.23	0.72
1:A:442:VAL:HG12	1:A:496:VAL:O	1.87	0.72
2:B:103:LYS:HG3	2:B:190:GLY:C	2.09	0.72
1:A:17:ASP:O	1:A:83:ARG:HD3	1.89	0.72
1:A:64:LYS:HG3	1:A:66:LYS:HG3	1.71	0.72
2:B:358:ARG:CA	2:B:362:THR:HB	2.19	0.72
1:A:139:THR:HG23	1:A:140:PRO:HD2	1.71	0.72
1:A:427:TYR:CE1	1:A:525:LEU:HD13	2.25	0.72
1:A:483:TYR:HB2	1:A:521:ILE:HG12	1.70	0.72
1:A:164:MET:HE3	1:A:168:LEU:HD11	1.72	0.72
1:A:64:LYS:O	1:A:64:LYS:CG	2.37	0.72
1:A:84:THR:HG21	1:A:154:LYS:HB3	1.71	0.72
1:A:328:GLU:HG2	1:A:390:LYS:HB2	1.69	0.72
1:A:356:ARG:NE	1:A:358:ARG:HG3	2.05	0.72
2:B:278:GLN:NE2	2:B:297:GLU:HG3	2.04	0.72
2:B:311:LYS:O	2:B:313:PRO:HD3	1.89	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:257:ILE:HG23	2:B:283:LEU:HD21	1.71	0.72
1:A:3:SER:OG	1:A:5:ILE:HG13	1.90	0.71
2:B:96:HIS:HD1	2:B:181:TYR:HE2	1.38	0.71
2:B:297:GLU:CG	2:B:298:GLU:H	2.01	0.71
2:B:195:ILE:HD11	2:B:199:ARG:HE	1.54	0.71
1:A:23:GLN:CD	1:A:23:GLN:H	1.93	0.71
1:A:30:LYS:O	1:A:33:ALA:HB3	1.91	0.71
2:B:146:TYR:CG	2:B:150:PRO:HB3	2.25	0.71
1:A:10:VAL:HG21	1:A:153:TRP:HH2	1.56	0.71
1:A:122:GLU:HA	1:A:125:ARG:HD2	1.71	0.71
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.26	0.71
2:B:109:LEU:HB2	2:B:218:ASP:OD2	1.91	0.71
1:A:50:ILE:HA	5:A:1095:HOH:O	1.91	0.71
1:A:399:GLU:CD	1:A:402:TRP:HE1	1.92	0.71
2:B:109:LEU:HD13	2:B:206:ARG:HG2	1.73	0.71
2:B:278:GLN:HE21	2:B:298:GLU:HB2	1.55	0.71
2:B:146:TYR:CD1	2:B:150:PRO:HB3	2.26	0.71
2:B:365:VAL:HG12	2:B:365:VAL:O	1.90	0.70
2:B:174:GLN:HA	2:B:174:GLN:NE2	2.06	0.70
1:A:96:HIS:HB3	1:A:382:ILE:CD1	2.21	0.70
2:B:1:PRO:HD3	2:B:117:SER:CA	2.20	0.70
2:B:91:GLN:HE21	2:B:91:GLN:C	1.95	0.70
2:B:266:TRP:CD1	2:B:422:LEU:HD23	2.27	0.70
2:B:278:GLN:NE2	2:B:297:GLU:CG	2.54	0.70
2:B:297:GLU:HG3	2:B:298:GLU:N	2.02	0.70
2:B:332:GLN:O	2:B:424:LYS:HE2	1.90	0.70
1:A:64:LYS:O	1:A:64:LYS:HG2	1.92	0.70
2:B:339:TYR:CD1	2:B:375:ILE:HD11	2.26	0.70
1:A:55:PRO:HG2	1:A:143:ARG:HH22	1.57	0.70
2:B:1:PRO:O	2:B:2:ILE:HD13	1.91	0.70
1:A:124:PHE:CE2	1:A:153:TRP:CZ2	2.79	0.69
1:A:290:THR:O	1:A:290:THR:HG22	1.91	0.69
2:B:168:LEU:HD11	2:B:180:ILE:HG21	1.74	0.69
1:A:34:LEU:HD12	1:A:132:ILE:HG12	1.75	0.69
1:A:326:ILE:HD12	1:A:326:ILE:N	2.07	0.69
2:B:340:GLN:HE21	2:B:340:GLN:N	1.90	0.69
2:B:69:THR:HG23	2:B:70:LYS:H	1.57	0.69
1:A:491:LEU:O	1:A:529:GLU:HB3	1.93	0.69
1:A:84:THR:HG23	1:A:154:LYS:CE	2.19	0.69
1:A:363:ASN:ND2	1:A:365:VAL:H	1.90	0.69
1:A:399:GLU:HA	1:A:402:TRP:CD1	2.28	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:TYR:HB3	2:B:274:ILE:CD1	2.22	0.69
2:B:295:LEU:O	2:B:295:LEU:CG	2.41	0.69
2:B:241:VAL:O	2:B:243:PRO:HD3	1.91	0.69
1:A:108:VAL:HG23	1:A:222:GLN:HB3	1.75	0.69
1:A:128:THR:HB	1:A:146:TYR:HB2	1.75	0.69
1:A:197:GLN:O	1:A:200:THR:HG22	1.92	0.69
1:A:222:GLN:O	1:A:223:LYS:C	2.31	0.69
2:B:260:LEU:HG	2:B:264:LEU:CD1	2.23	0.69
1:A:74:LEU:HD23	1:A:74:LEU:O	1.92	0.69
1:A:388:LYS:HE2	5:A:1092:HOH:O	1.93	0.69
1:A:395:LYS:HA	1:A:414:TRP:HZ2	1.56	0.69
1:A:483:TYR:HB2	1:A:521:ILE:HG13	1.74	0.69
2:B:376:THR:HG22	2:B:380:ILE:HD11	1.74	0.69
2:B:393:ILE:HG23	2:B:416:PHE:HD1	1.57	0.68
1:A:433:PRO:HB3	2:B:255:ASN:ND2	2.08	0.68
1:A:76:ASP:OD2	1:A:78:ARG:NH1	2.27	0.68
1:A:87:PHE:CE2	1:A:159:ILE:HD11	2.29	0.68
2:B:76:ASP:CG	2:B:78:ARG:HH21	1.96	0.68
1:A:97:PRO:HA	1:A:100:LEU:CD1	2.24	0.68
2:B:181:TYR:HD1	2:B:182:GLN:N	1.92	0.68
1:A:208:HIS:CE1	1:A:212:TRP:HE1	2.11	0.68
2:B:111:VAL:O	2:B:113:ASP:N	2.27	0.68
2:B:125:ARG:O	2:B:127:TYR:N	2.27	0.68
2:B:248:GLU:HB2	5:B:1086:HOH:O	1.95	0.67
1:A:34:LEU:HD22	1:A:73:LYS:HB2	1.76	0.67
1:A:96:HIS:HD1	1:A:97:PRO:N	1.92	0.67
1:A:193:LEU:HD22	1:A:197:GLN:NE2	2.09	0.67
2:B:206:ARG:HH11	2:B:206:ARG:CB	2.07	0.67
1:A:17:ASP:OD2	1:A:56:TYR:HE2	1.77	0.67
1:A:64:LYS:HB3	1:A:71:TRP:CD1	2.29	0.67
1:A:406:TRP:CZ2	2:B:418:ASN:O	2.47	0.67
1:A:422:LEU:CD2	1:A:424:LYS:HD3	2.24	0.67
1:A:438:GLU:OE1	1:A:463:ARG:NH2	2.28	0.67
2:B:254:VAL:O	2:B:258:GLN:HG3	1.95	0.67
2:B:377:THR:O	2:B:378:GLU:C	2.30	0.67
1:A:95:PRO:HG2	1:A:229:TRP:HH2	1.59	0.67
1:A:497:THR:CG2	1:A:499:SER:HB3	2.25	0.67
1:A:87:PHE:HE2	1:A:159:ILE:HD11	1.59	0.67
2:B:175:ASN:H	2:B:175:ASN:ND2	1.92	0.67
1:A:453:GLY:O	1:A:454:LYS:HD3	1.95	0.66
1:A:96:HIS:HD1	1:A:98:ALA:H	1.42	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:GLU:HB2	1:A:532:TYR:HB2	1.76	0.66
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.34	0.66
2:B:260:LEU:CG	2:B:264:LEU:HD11	2.25	0.66
1:A:38:CYS:HB3	1:A:144:TYR:HE1	1.58	0.66
2:B:69:THR:CG2	2:B:70:LYS:H	2.08	0.66
2:B:168:LEU:CD1	2:B:180:ILE:HG21	2.25	0.66
2:B:206:ARG:HE	2:B:218:ASP:CB	1.99	0.66
2:B:277:ARG:O	2:B:281:LYS:HG3	1.96	0.66
2:B:326:ILE:CG2	2:B:342:TYR:HE1	2.08	0.66
1:A:108:VAL:HG11	1:A:188:TYR:CD2	2.30	0.66
2:B:206:ARG:NH1	2:B:206:ARG:CB	2.58	0.66
1:A:363:ASN:HB3	1:A:366:LYS:HG3	1.78	0.66
2:B:176:PRO:O	2:B:178:ILE:N	2.28	0.66
1:A:219:LYS:O	1:A:220:LYS:C	2.34	0.66
1:A:435:VAL:HA	2:B:290:THR:OG1	1.96	0.65
2:B:340:GLN:HG2	2:B:427:TYR:CE1	2.31	0.65
2:B:341:ILE:O	2:B:349:LEU:HB2	1.96	0.65
1:A:29:GLU:CG	1:A:30:LYS:H	2.08	0.65
2:B:109:LEU:HB2	2:B:218:ASP:CG	2.17	0.65
2:B:252:TRP:O	2:B:292:VAL:HG13	1.95	0.65
1:A:254:VAL:HG23	1:A:293:ILE:CD1	2.26	0.65
1:A:254:VAL:O	1:A:258:GLN:HG3	1.96	0.65
1:A:340:GLN:HA	1:A:351:THR:HA	1.78	0.65
2:B:100:LEU:HD13	2:B:179:VAL:HG21	1.79	0.65
2:B:202:ILE:O	2:B:205:LEU:N	2.30	0.65
2:B:358:ARG:H	2:B:358:ARG:HE	1.43	0.65
2:B:376:THR:CG2	2:B:380:ILE:HD11	2.26	0.65
2:B:308:GLU:HG3	2:B:309:ILE:N	2.12	0.65
1:A:539:HIS:O	1:A:542:ILE:HG12	1.97	0.65
2:B:60:VAL:CG1	2:B:130:PHE:HB2	2.27	0.65
1:A:434:ILE:HG12	1:A:530:LYS:HB3	1.79	0.65
2:B:115:TYR:HE2	2:B:157:PRO:CA	2.09	0.65
2:B:220:LYS:HE3	2:B:231:GLY:CA	2.21	0.65
1:A:27:THR:CB	1:A:29:GLU:HG2	2.27	0.65
1:A:28:GLU:HA	1:A:31:ILE:HG23	1.78	0.65
2:B:324:ASP:O	2:B:343:GLN:HG2	1.96	0.65
1:A:10:VAL:HG21	1:A:153:TRP:CH2	2.31	0.65
2:B:232:TYR:HE2	2:B:234:LEU:HD21	1.60	0.65
1:A:254:VAL:HG13	1:A:283:LEU:HD13	1.79	0.65
1:A:356:ARG:HD2	1:A:362:THR:OG1	1.97	0.65
1:A:398:TRP:CZ2	1:A:411:ILE:HD12	2.32	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:THR:CG2	1:A:424:LYS:HA	2.23	0.64
2:B:66:LYS:HD3	2:B:69:THR:CB	2.27	0.64
2:B:191:SER:OG	2:B:198:HIS:ND1	2.30	0.64
1:A:542:ILE:O	1:A:546:GLU:HB2	1.98	0.64
2:B:299:ALA:HA	2:B:302:GLU:HB2	1.78	0.64
2:B:366:LYS:HG3	2:B:405:TYR:CD2	2.32	0.64
1:A:406:TRP:CE3	2:B:420:PRO:HD2	2.33	0.64
2:B:78:ARG:HD3	2:B:412:PRO:O	1.96	0.64
2:B:274:ILE:HG23	2:B:306:ASN:CG	2.18	0.64
2:B:100:LEU:O	2:B:100:LEU:HD12	1.98	0.64
1:A:108:VAL:CG2	1:A:222:GLN:HB3	2.27	0.64
2:B:342:TYR:HD1	2:B:342:TYR:O	1.81	0.64
1:A:420:PRO:HA	1:A:421:PRO:C	2.19	0.64
1:A:95:PRO:HG2	1:A:229:TRP:CH2	2.33	0.63
2:B:358:ARG:O	2:B:362:THR:CB	2.45	0.63
2:B:364:ASP:O	2:B:366:LYS:N	2.31	0.63
1:A:64:LYS:HG3	1:A:66:LYS:CG	2.29	0.63
2:B:85:GLN:O	2:B:89:GLU:HB2	1.98	0.63
1:A:130:PHE:HD1	1:A:130:PHE:H	1.46	0.63
1:A:224:GLU:O	1:A:226:PRO:O	2.17	0.63
1:A:301:LEU:O	1:A:304:ALA:HB3	1.97	0.63
2:B:31:ILE:C	2:B:35:VAL:HG23	2.18	0.63
2:B:85:GLN:CG	2:B:154:LYS:HB3	2.22	0.63
2:B:197:GLN:O	2:B:200:THR:HB	1.97	0.63
1:A:175:ASN:N	1:A:176:PRO:CD	2.60	0.63
1:A:405:TYR:CE2	1:A:407:GLN:HB3	2.34	0.63
2:B:110:ASP:C	2:B:110:ASP:OD1	2.36	0.63
1:A:443:ASP:HB2	1:A:548:VAL:HG23	1.81	0.63
1:A:539:HIS:O	1:A:542:ILE:HG23	1.98	0.63
1:A:282:LEU:C	1:A:284:ARG:H	2.02	0.63
2:B:220:LYS:HG3	2:B:231:GLY:HA3	1.79	0.63
1:A:99:GLY:HA3	1:A:382:ILE:CG2	2.29	0.63
1:A:163:SER:O	1:A:167:ILE:HG12	1.99	0.63
2:B:5:ILE:HB	2:B:119:PRO:HD2	1.80	0.63
2:B:221:HIS:HD1	2:B:229:TRP:HB2	1.61	0.62
1:A:276:VAL:HG12	1:A:276:VAL:O	1.99	0.62
1:A:51:GLY:O	1:A:53:GLU:N	2.31	0.62
1:A:319:TYR:OH	1:A:385:LYS:HD3	1.98	0.62
1:A:55:PRO:HG2	1:A:143:ARG:NH2	2.14	0.62
1:A:198:HIS:CD2	1:A:202:ILE:HD11	2.35	0.62
2:B:275:LYS:HA	2:B:277:ARG:NH2	2.14	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:223:LYS:O	2:B:224:GLU:OE1	2.17	0.62
1:A:254:VAL:H	1:A:293:ILE:HD13	1.64	0.62
1:A:142:ILE:HD12	1:A:142:ILE:H	1.63	0.62
1:A:319:TYR:CD1	1:A:325:LEU:HD21	2.35	0.62
2:B:65:LYS:HD3	2:B:72:ARG:HD2	1.80	0.62
2:B:175:ASN:ND2	2:B:175:ASN:N	2.48	0.61
2:B:220:LYS:CE	2:B:231:GLY:HA2	2.22	0.61
1:A:32:LYS:HA	1:A:35:VAL:CG2	2.31	0.61
1:A:244:ILE:HG23	1:A:263:LYS:HE2	1.82	0.61
1:A:434:ILE:HD13	1:A:494:ASN:ND2	2.14	0.61
1:A:479:LEU:HD21	1:A:502:ALA:HA	1.83	0.61
2:B:24:TRP:HE1	2:B:399:GLU:HG3	1.63	0.61
2:B:115:TYR:O	2:B:117:SER:N	2.29	0.61
1:A:33:ALA:O	1:A:37:ILE:HG12	2.01	0.61
1:A:189:VAL:HG21	1:A:205:LEU:HD23	1.81	0.61
1:A:434:ILE:HB	1:A:494:ASN:HD21	1.63	0.61
1:A:298:GLU:N	1:A:298:GLU:CD	2.53	0.61
2:B:195:ILE:HG13	2:B:199:ARG:CD	2.30	0.61
1:A:97:PRO:HA	1:A:100:LEU:HG	1.83	0.61
1:A:142:ILE:HD12	1:A:142:ILE:N	2.16	0.61
2:B:183:TYR:CD2	2:B:184:MET:HG3	2.36	0.61
2:B:195:ILE:O	2:B:197:GLN:N	2.33	0.61
1:A:469:LEU:HD12	1:A:477:THR:HG22	1.83	0.61
2:B:194:GLU:O	2:B:195:ILE:C	2.37	0.61
2:B:281:LYS:O	2:B:284:ARG:HB2	1.99	0.61
2:B:402:TRP:CH2	2:B:411:ILE:HD12	2.36	0.60
1:A:2:ILE:HG22	1:A:3:SER:N	2.14	0.60
1:A:98:ALA:CB	1:A:350:LYS:HB2	2.31	0.60
1:A:122:GLU:HA	1:A:125:ARG:CD	2.31	0.60
1:A:226:PRO:HB2	1:A:233:GLU:HG2	1.84	0.60
2:B:160:PHE:O	2:B:161:GLN:O	2.19	0.60
2:B:252:TRP:HA	2:B:252:TRP:CE3	2.37	0.60
1:A:417:VAL:HG12	1:A:419:THR:H	1.66	0.60
2:B:76:ASP:CG	2:B:76:ASP:O	2.39	0.60
2:B:221:HIS:N	2:B:221:HIS:HD2	1.98	0.60
2:B:282:LEU:HD11	2:B:293:ILE:HG12	1.83	0.60
2:B:364:ASP:C	2:B:366:LYS:H	2.05	0.60
1:A:56:TYR:N	1:A:56:TYR:CD1	2.70	0.60
1:A:253:THR:OG1	1:A:290:THR:HA	2.01	0.60
2:B:242:GLN:CG	2:B:242:GLN:O	2.49	0.60
1:A:23:GLN:H	1:A:23:GLN:NE2	1.98	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:VAL:HG21	1:A:347:LYS:HD3	1.83	0.60
2:B:391:LEU:HB3	2:B:393:ILE:HG22	1.84	0.60
2:B:149:LEU:CD1	2:B:159:ILE:HB	2.32	0.60
2:B:349:LEU:HD12	2:B:383:TRP:CZ2	2.37	0.60
1:A:286:THR:CG2	1:A:287:LYS:H	2.14	0.60
2:B:30:LYS:HG3	2:B:62:ALA:HB3	1.82	0.60
2:B:252:TRP:HA	2:B:252:TRP:HE3	1.66	0.59
2:B:336:GLN:HA	2:B:354:TYR:O	2.02	0.59
1:A:126:LYS:HG3	1:A:127:TYR:CE2	2.38	0.59
2:B:194:GLU:O	2:B:195:ILE:O	2.20	0.59
2:B:198:HIS:O	2:B:201:LYS:N	2.35	0.59
2:B:244:ILE:HG12	2:B:244:ILE:O	2.01	0.59
1:A:433:PRO:HB3	2:B:255:ASN:HD22	1.65	0.59
2:B:282:LEU:HD11	2:B:294:PRO:HD2	1.83	0.59
2:B:161:GLN:O	2:B:162:SER:C	2.40	0.59
2:B:332:GLN:HA	2:B:332:GLN:OE1	2.01	0.59
1:A:64:LYS:C	1:A:66:LYS:N	2.50	0.59
1:A:109:LEU:HD21	1:A:202:ILE:CG2	2.33	0.59
2:B:66:LYS:HB3	2:B:69:THR:HG22	1.84	0.59
2:B:80:LEU:HD11	2:B:124:PHE:CZ	2.36	0.59
1:A:116:PHE:O	1:A:148:VAL:HG21	2.03	0.59
2:B:326:ILE:HB	2:B:342:TYR:CD1	2.38	0.59
1:A:128:THR:CB	1:A:146:TYR:HB2	2.33	0.59
1:A:341:ILE:HG21	1:A:383:TRP:CH2	2.38	0.59
2:B:69:THR:CG2	2:B:70:LYS:N	2.63	0.59
2:B:277:ARG:H	2:B:277:ARG:CD	2.11	0.59
1:A:254:VAL:H	1:A:293:ILE:CD1	2.16	0.59
2:B:13:LYS:HG3	2:B:14:PRO:HD2	1.85	0.59
2:B:171:PHE:CE2	2:B:205:LEU:HB2	2.38	0.59
2:B:282:LEU:HG	2:B:293:ILE:HD13	1.84	0.59
2:B:385:LYS:HB3	2:B:385:LYS:NZ	2.17	0.59
1:A:108:VAL:HA	1:A:188:TYR:HA	1.84	0.59
2:B:10:VAL:HG22	2:B:88:TRP:CH2	2.38	0.59
2:B:242:GLN:O	2:B:242:GLN:HG2	2.02	0.59
1:A:356:ARG:HG3	1:A:367:GLN:HG2	1.85	0.58
1:A:58:THR:HG22	1:A:76:ASP:O	2.03	0.58
1:A:64:LYS:C	1:A:66:LYS:H	2.05	0.58
1:A:134:SER:HB3	1:A:138:GLU:HB3	1.84	0.58
1:A:513:SER:N	1:A:519:ASN:HD21	2.01	0.58
2:B:206:ARG:HB3	2:B:206:ARG:CZ	2.34	0.58
2:B:266:TRP:HD1	2:B:422:LEU:HD23	1.65	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:VAL:HG22	1:A:279:LEU:HD22	1.86	0.58
2:B:18:GLY:HA3	2:B:127:TYR:CD1	2.38	0.58
2:B:171:PHE:CZ	2:B:205:LEU:HB2	2.38	0.58
1:A:200:THR:HG23	1:A:201:LYS:N	2.18	0.58
1:A:229:TRP:CE3	1:A:234:LEU:HD11	2.37	0.58
1:A:354:TYR:HB2	1:A:374:LYS:HZ1	1.69	0.58
1:A:410:TRP:HB3	2:B:365:VAL:HG21	1.85	0.58
1:A:430:GLU:OE1	1:A:430:GLU:HA	2.03	0.58
2:B:46:LYS:NZ	2:B:116:PHE:HD2	2.01	0.58
2:B:340:GLN:N	2:B:340:GLN:NE2	2.51	0.58
1:A:61:PHE:HB2	1:A:74:LEU:O	2.04	0.58
1:A:342:TYR:OH	1:A:390:LYS:HD2	2.04	0.58
2:B:273:GLY:C	2:B:274:ILE:HD12	2.23	0.58
1:A:132:ILE:HG22	1:A:142:ILE:O	2.04	0.58
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.39	0.58
1:A:130:PHE:HD1	1:A:130:PHE:N	2.02	0.58
1:A:245:VAL:H	1:A:263:LYS:NZ	2.01	0.58
1:A:506:ILE:HG21	1:A:533:LEU:CD1	2.33	0.58
2:B:217:PRO:O	2:B:219:LYS:N	2.36	0.57
2:B:366:LYS:O	2:B:370:GLU:HG3	2.04	0.57
1:A:363:ASN:HD22	1:A:365:VAL:H	1.52	0.57
2:B:149:LEU:HD23	2:B:149:LEU:H	1.69	0.57
2:B:206:ARG:NH2	2:B:216:THR:O	2.37	0.57
1:A:402:TRP:HE3	1:A:402:TRP:O	1.88	0.57
2:B:192:ASP:O	2:B:193:LEU:HD23	2.03	0.57
2:B:369:THR:HG22	2:B:373:GLN:HE21	1.68	0.57
1:A:297:GLU:CD	1:A:297:GLU:H	2.07	0.57
2:B:168:LEU:O	2:B:172:LYS:HG3	2.04	0.57
2:B:379:SER:O	2:B:380:ILE:C	2.43	0.57
2:B:395:LYS:O	2:B:399:GLU:HB2	2.04	0.57
2:B:169:GLU:C	2:B:171:PHE:H	2.06	0.57
2:B:80:LEU:HD12	2:B:80:LEU:O	2.03	0.57
2:B:161:GLN:O	2:B:164:MET:N	2.35	0.57
1:A:88:TRP:CD1	2:B:143:ARG:HD2	2.39	0.57
1:A:179:VAL:HG21	4:A:701:IET:N3	2.20	0.57
1:A:203:GLU:OE2	1:A:207:GLN:NE2	2.37	0.57
1:A:353:LYS:O	1:A:374:LYS:NZ	2.38	0.57
1:A:447:ASN:CB	1:A:450:THR:HB	2.32	0.57
2:B:195:ILE:HD11	2:B:199:ARG:NE	2.19	0.57
1:A:195:ILE:HG13	1:A:196:GLY:N	2.19	0.57
1:A:411:ILE:HD13	1:A:411:ILE:N	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:VAL:O	2:B:91:GLN:C	2.43	0.57
2:B:206:ARG:HH11	2:B:206:ARG:HB2	1.70	0.57
1:A:493:VAL:C	1:A:494:ASN:HD22	2.09	0.57
1:A:497:THR:HG21	1:A:499:SER:HB3	1.87	0.57
2:B:238:LYS:O	2:B:240:THR:N	2.38	0.57
1:A:77:PHE:CZ	1:A:150:PRO:HB3	2.40	0.56
1:A:254:VAL:N	1:A:293:ILE:HD13	2.20	0.56
1:A:360:ALA:HA	1:A:514:GLU:CD	2.26	0.56
2:B:183:TYR:CE2	2:B:184:MET:HE2	2.40	0.56
2:B:59:PRO:HB2	2:B:76:ASP:HB3	1.87	0.56
2:B:116:PHE:CE1	2:B:151:GLN:HG3	2.41	0.56
2:B:253:THR:HA	2:B:292:VAL:HA	1.86	0.56
2:B:376:THR:O	2:B:379:SER:HB2	2.05	0.56
1:A:227:PHE:HB2	1:A:234:LEU:HB2	1.87	0.56
1:A:438:GLU:OE2	1:A:461:LYS:HB2	2.05	0.56
1:A:492:GLU:OE2	1:A:530:LYS:HD2	2.05	0.56
1:A:524:GLN:O	1:A:528:LYS:HG2	2.06	0.56
2:B:149:LEU:HD23	2:B:149:LEU:N	2.20	0.56
2:B:198:HIS:O	2:B:200:THR:N	2.39	0.56
2:B:201:LYS:HE2	2:B:201:LYS:CA	2.34	0.56
1:A:7:THR:HG22	1:A:119:PRO:CB	2.36	0.56
1:A:182:GLN:HB3	5:A:1044:HOH:O	2.05	0.56
1:A:28:GLU:HA	1:A:31:ILE:HG21	1.87	0.56
2:B:111:VAL:C	2:B:113:ASP:N	2.58	0.56
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.87	0.56
1:A:32:LYS:HA	1:A:35:VAL:HG23	1.86	0.56
1:A:218:ASP:O	1:A:221:HIS:CB	2.50	0.56
1:A:454:LYS:HB2	1:A:552:VAL:CG1	2.11	0.56
1:A:511:ASP:OD1	1:A:512:LYS:HG2	2.05	0.56
2:B:402:TRP:CZ3	2:B:411:ILE:HD12	2.40	0.56
1:A:180:ILE:N	1:A:180:ILE:HD12	2.21	0.56
1:A:545:ASN:O	1:A:549:ASP:OD2	2.24	0.56
2:B:41:MET:HE3	2:B:46:LYS:HD3	1.88	0.56
2:B:279:LEU:HD13	2:B:299:ALA:HB1	1.87	0.56
1:A:121:ASP:C	1:A:123:ASP:H	2.09	0.56
1:A:130:PHE:N	1:A:130:PHE:CD1	2.73	0.56
1:A:198:HIS:CE1	1:A:202:ILE:HD11	2.40	0.56
2:B:13:LYS:HG2	2:B:14:PRO:O	2.06	0.56
2:B:111:VAL:O	2:B:112:GLY:C	2.44	0.56
1:A:426:TRP:O	1:A:427:TYR:HB3	2.06	0.56
2:B:328:GLU:HG2	2:B:390:LYS:HD3	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ILE:HA	1:A:263:LYS:HE2	1.87	0.56
1:A:543:GLY:HA2	2:B:284:ARG:HA	1.88	0.56
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.41	0.56
1:A:79:GLU:HG3	1:A:83:ARG:NH1	2.18	0.55
2:B:377:THR:HA	2:B:380:ILE:HD13	1.88	0.55
2:B:205:LEU:O	2:B:208:HIS:HB3	2.05	0.55
2:B:315:HIS:HB3	5:B:1076:HOH:O	2.06	0.55
1:A:324:ASP:OD2	1:A:324:ASP:N	2.38	0.55
2:B:393:ILE:HG23	2:B:416:PHE:CD1	2.41	0.55
1:A:339:TYR:CD1	1:A:375:ILE:HD11	2.41	0.55
1:A:362:THR:CG2	1:A:363:ASN:N	2.51	0.55
2:B:332:GLN:OE1	2:B:424:LYS:HG2	2.06	0.55
1:A:3:SER:OG	1:A:4:PRO:HD2	2.05	0.55
1:A:543:GLY:O	2:B:284:ARG:HA	2.07	0.55
1:A:183:TYR:N	1:A:186:ASP:O	2.40	0.55
1:A:282:LEU:C	1:A:284:ARG:N	2.59	0.55
1:A:86:ASP:OD2	1:A:86:ASP:N	2.40	0.55
1:A:112:GLY:O	1:A:115:TYR:CE2	2.60	0.55
1:A:226:PRO:CB	1:A:233:GLU:HG2	2.36	0.55
1:A:320:ASP:N	1:A:343:GLN:HE22	2.02	0.55
1:A:434:ILE:H	1:A:434:ILE:HD12	1.71	0.55
1:A:401:TRP:HA	1:A:401:TRP:CE3	2.42	0.55
1:A:1:PRO:HA	1:A:46:LYS:NZ	2.22	0.55
1:A:244:ILE:CG2	1:A:310:LEU:HD21	2.37	0.55
2:B:183:TYR:CD2	2:B:183:TYR:C	2.78	0.55
2:B:296:THR:CG2	2:B:297:GLU:N	2.57	0.55
2:B:342:TYR:CD1	2:B:342:TYR:C	2.77	0.55
1:A:532:TYR:HE1	2:B:255:ASN:HD21	1.52	0.54
2:B:283:LEU:O	2:B:285:GLY:N	2.40	0.54
1:A:258:GLN:HE21	1:A:283:LEU:HD11	1.73	0.54
2:B:38:CYS:O	2:B:39:THR:C	2.45	0.54
2:B:149:LEU:HB2	2:B:156:SER:HB3	1.89	0.54
2:B:345:PRO:HB2	2:B:346:PHE:HD1	1.72	0.54
2:B:168:LEU:CD2	2:B:209:LEU:HD21	2.38	0.54
1:A:106:VAL:HA	1:A:190:GLY:HA2	1.89	0.54
1:A:490:GLY:C	1:A:492:GLU:H	2.11	0.54
2:B:193:LEU:HD12	2:B:198:HIS:HA	1.90	0.54
1:A:509:GLN:N	1:A:510:PRO:HD3	2.21	0.54
2:B:100:LEU:HD13	2:B:179:VAL:CG2	2.38	0.54
2:B:169:GLU:O	2:B:171:PHE:N	2.34	0.54
2:B:266:TRP:CZ3	2:B:426:TRP:CD1	2.95	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LYS:NZ	1:A:130:PHE:CE2	2.70	0.54
1:A:7:THR:CG2	1:A:119:PRO:HB2	2.36	0.54
1:A:58:THR:HG22	1:A:59:PRO:HD2	1.90	0.54
1:A:325:LEU:HD13	1:A:383:TRP:CE3	2.42	0.54
2:B:156:SER:N	2:B:157:PRO:HD2	2.22	0.54
2:B:183:TYR:O	2:B:184:MET:HB2	2.07	0.54
1:A:194:GLU:O	1:A:197:GLN:N	2.41	0.54
1:A:401:TRP:CZ3	1:A:509:GLN:NE2	2.76	0.54
2:B:214:LEU:N	2:B:214:LEU:HD23	2.23	0.54
1:A:55:PRO:HG2	1:A:143:ARG:HH12	1.73	0.54
2:B:47:ILE:CG2	2:B:146:TYR:CD1	2.91	0.54
2:B:371:ALA:O	2:B:375:ILE:HD12	2.08	0.54
1:A:24:TRP:O	1:A:25:PRO:C	2.45	0.54
1:A:363:ASN:HB3	1:A:366:LYS:CG	2.38	0.54
1:A:434:ILE:HD13	1:A:494:ASN:HD21	1.73	0.54
1:A:450:THR:HG22	1:A:452:LEU:CG	2.38	0.54
2:B:12:LEU:CD1	2:B:83:ARG:O	2.53	0.54
2:B:180:ILE:CG2	2:B:187:LEU:HD22	2.37	0.54
2:B:198:HIS:O	2:B:199:ARG:C	2.44	0.54
1:A:373:GLN:HG2	2:B:394:GLN:NE2	2.23	0.53
2:B:183:TYR:CE1	2:B:380:ILE:HG13	2.43	0.53
2:B:314:VAL:O	2:B:314:VAL:HG23	2.08	0.53
1:A:288:ALA:CB	1:A:291:GLU:CB	2.78	0.53
1:A:503:LEU:HD12	1:A:507:GLN:HG2	1.90	0.53
2:B:110:ASP:HA	2:B:186:ASP:HA	1.90	0.53
2:B:171:PHE:CE2	2:B:205:LEU:HA	2.42	0.53
2:B:220:LYS:HG3	2:B:231:GLY:CA	2.39	0.53
2:B:257:ILE:CD1	2:B:279:LEU:HG	2.38	0.53
2:B:326:ILE:HG22	2:B:327:ALA:N	2.23	0.53
2:B:331:LYS:HE3	2:B:364:ASP:OD1	2.08	0.53
1:A:47:ILE:HG22	1:A:146:TYR:HA	1.89	0.53
1:A:82:LYS:O	1:A:82:LYS:HD3	2.08	0.53
1:A:164:MET:HE3	1:A:187:LEU:HD13	1.89	0.53
1:A:272:PRO:O	1:A:274:ILE:N	2.41	0.53
1:A:298:GLU:CD	1:A:298:GLU:H	2.11	0.53
1:A:401:TRP:HA	1:A:401:TRP:HE3	1.72	0.53
1:A:108:VAL:HG12	1:A:188:TYR:HA	1.90	0.53
2:B:205:LEU:O	2:B:208:HIS:N	2.35	0.53
2:B:261:VAL:O	2:B:265:ASN:HB2	2.08	0.53
1:A:253:THR:HG22	1:A:256:ASP:OD2	2.08	0.53
1:A:369:THR:O	1:A:372:VAL:N	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:LYS:O	2:B:36:GLU:HG3	2.09	0.53
2:B:73:LYS:HE2	2:B:75:VAL:CG2	2.39	0.53
2:B:116:PHE:HE1	2:B:151:GLN:HG3	1.72	0.53
2:B:168:LEU:HD13	2:B:180:ILE:HD12	1.91	0.53
2:B:183:TYR:CE2	2:B:184:MET:CE	2.92	0.53
1:A:201:LYS:HD3	1:A:204:GLU:OE1	2.09	0.53
2:B:111:VAL:O	2:B:114:ALA:N	2.36	0.53
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.91	0.53
1:A:12:LEU:HD21	1:A:127:TYR:CD1	2.44	0.53
1:A:279:LEU:N	1:A:302:GLU:OE2	2.32	0.53
1:A:458:VAL:HG23	1:A:551:LEU:HD11	1.90	0.53
1:A:94:ILE:HD12	1:A:94:ILE:N	2.24	0.53
2:B:150:PRO:O	2:B:156:SER:OG	2.19	0.53
1:A:162:SER:O	1:A:163:SER:C	2.46	0.53
2:B:164:MET:O	2:B:166:LYS:N	2.42	0.53
2:B:174:GLN:HE21	2:B:174:GLN:CA	2.11	0.53
2:B:366:LYS:HG3	2:B:405:TYR:CE2	2.44	0.53
1:A:194:GLU:O	1:A:196:GLY:N	2.42	0.52
1:A:244:ILE:HG23	1:A:263:LYS:HG2	1.89	0.52
1:A:398:TRP:O	1:A:400:THR:N	2.42	0.52
1:A:543:GLY:C	2:B:284:ARG:HA	2.28	0.52
1:A:96:HIS:HD1	1:A:96:HIS:C	2.13	0.52
1:A:179:VAL:HG11	4:A:701:IET:N3	2.25	0.52
1:A:331:LYS:HG2	1:A:333:GLY:H	1.75	0.52
1:A:363:ASN:HD22	1:A:365:VAL:N	2.08	0.52
1:A:545:ASN:ND2	1:A:549:ASP:OD2	2.42	0.52
2:B:421:PRO:HG2	2:B:422:LEU:H	1.74	0.52
1:A:19:PRO:O	1:A:56:TYR:CB	2.49	0.52
1:A:58:THR:CG2	1:A:59:PRO:HD2	2.40	0.52
1:A:275:LYS:O	1:A:276:VAL:HG23	2.09	0.52
1:A:331:LYS:HE2	1:A:333:GLY:CA	2.36	0.52
1:A:434:ILE:HD12	1:A:434:ILE:N	2.24	0.52
2:B:263:LYS:HB3	2:B:426:TRP:CE3	2.45	0.52
2:B:277:ARG:HA	2:B:280:SER:OG	2.10	0.52
1:A:254:VAL:HA	1:A:257:ILE:CG2	2.32	0.52
2:B:282:LEU:O	2:B:293:ILE:CD1	2.55	0.52
1:A:540:LYS:HD3	2:B:265:ASN:ND2	2.21	0.52
2:B:56:TYR:O	2:B:57:ASN:HB2	2.10	0.52
2:B:149:LEU:HD13	2:B:159:ILE:HB	1.91	0.52
2:B:241:VAL:C	2:B:243:PRO:HD3	2.29	0.52
2:B:278:GLN:HG2	2:B:299:ALA:N	2.25	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:VAL:HG12	1:A:188:TYR:CA	2.40	0.52
1:A:121:ASP:O	1:A:123:ASP:N	2.41	0.52
1:A:225:PRO:HG3	1:A:227:PHE:CE2	2.45	0.52
2:B:268:SER:HA	2:B:271:TYR:O	2.09	0.52
2:B:23:GLN:HE21	2:B:24:TRP:N	2.07	0.52
2:B:46:LYS:CE	2:B:116:PHE:HD2	2.23	0.52
2:B:391:LEU:HB3	2:B:393:ILE:CG2	2.39	0.52
1:A:208:HIS:O	1:A:212:TRP:HD1	1.91	0.52
1:A:371:ALA:O	1:A:375:ILE:HD13	2.10	0.52
2:B:376:THR:HG21	2:B:410:TRP:CH2	2.45	0.52
1:A:96:HIS:CE1	1:A:98:ALA:H	2.28	0.52
1:A:271:TYR:CE2	1:A:314:VAL:HG23	2.45	0.52
1:A:276:VAL:O	1:A:276:VAL:CG1	2.58	0.52
1:A:456:GLY:HA2	1:A:484:LEU:HD23	1.91	0.52
2:B:17:ASP:O	2:B:18:GLY:O	2.27	0.52
1:A:164:MET:CE	1:A:187:LEU:HD13	2.39	0.51
1:A:354:TYR:HB2	1:A:374:LYS:NZ	2.25	0.51
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.93	0.51
1:A:151:GLN:O	1:A:151:GLN:HG2	2.09	0.51
1:A:277:ARG:HB2	1:A:336:GLN:CD	2.31	0.51
1:A:450:THR:HG22	1:A:452:LEU:HB2	1.92	0.51
2:B:295:LEU:O	2:B:295:LEU:CD2	2.59	0.51
1:A:258:GLN:HG2	1:A:283:LEU:HD21	1.91	0.51
1:A:329:ILE:HG12	1:A:391:LEU:CD2	2.40	0.51
2:B:183:TYR:HE2	2:B:184:MET:HE2	1.76	0.51
2:B:247:PRO:HB2	2:B:252:TRP:CZ2	2.45	0.51
2:B:253:THR:H	2:B:256:ASP:HB2	1.74	0.51
2:B:379:SER:HA	2:B:383:TRP:CE3	2.45	0.51
1:A:406:TRP:HZ2	2:B:418:ASN:O	1.93	0.51
1:A:460:ASN:C	1:A:462:GLY:H	2.14	0.51
1:A:490:GLY:O	1:A:492:GLU:N	2.44	0.51
2:B:319:TYR:CE2	2:B:321:PRO:HG3	2.45	0.51
2:B:361:HIS:O	2:B:363:ASN:N	2.43	0.51
2:B:395:LYS:NZ	2:B:399:GLU:OE1	2.34	0.51
1:A:369:THR:O	1:A:370:GLU:C	2.49	0.51
1:A:506:ILE:HG21	1:A:533:LEU:HD11	1.92	0.51
1:A:101:LYS:O	1:A:102:LYS:C	2.49	0.51
1:A:125:ARG:O	1:A:145:GLN:HG3	2.10	0.51
1:A:244:ILE:HG22	1:A:310:LEU:HD21	1.92	0.51
1:A:411:ILE:CD1	1:A:411:ILE:N	2.59	0.51
1:A:513:SER:CA	1:A:519:ASN:HD21	2.24	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ILE:O	1:A:198:HIS:HB3	2.10	0.51
2:B:263:LYS:HB3	2:B:426:TRP:HE3	1.75	0.51
1:A:32:LYS:O	1:A:36:GLU:HG2	2.11	0.51
1:A:408:ALA:CB	2:B:337:TRP:HH2	2.24	0.51
1:A:481:ALA:O	1:A:482:ILE:C	2.48	0.51
2:B:63:ILE:O	2:B:71:TRP:HE3	1.93	0.51
1:A:186:ASP:HB3	1:A:188:TYR:CE1	2.46	0.51
2:B:104:LYS:HB2	2:B:192:ASP:CA	2.21	0.51
2:B:263:LYS:HE2	2:B:425:LEU:HD13	1.92	0.51
2:B:275:LYS:O	2:B:276:VAL:HG23	2.11	0.51
2:B:317:VAL:HG23	2:B:317:VAL:O	2.11	0.51
1:A:55:PRO:HG2	1:A:143:ARG:NH1	2.26	0.51
2:B:66:LYS:CB	2:B:69:THR:CG2	2.89	0.51
2:B:84:THR:O	2:B:87:PHE:N	2.43	0.51
2:B:178:ILE:CG2	2:B:189:VAL:HG12	2.41	0.51
2:B:221:HIS:CD2	2:B:221:HIS:H	2.26	0.51
1:A:38:CYS:CB	1:A:144:TYR:HE1	2.23	0.50
1:A:162:SER:O	1:A:164:MET:N	2.44	0.50
1:A:318:TYR:CE1	4:A:701:IET:H16	2.45	0.50
1:A:501:TYR:O	1:A:505:ILE:HG12	2.11	0.50
2:B:295:LEU:O	2:B:295:LEU:HD23	2.11	0.50
2:B:380:ILE:HD11	2:B:386:THR:HG22	1.93	0.50
1:A:34:LEU:CG	1:A:62:ALA:HB2	2.40	0.50
1:A:86:ASP:HA	1:A:154:LYS:HZ2	1.75	0.50
2:B:8:VAL:O	2:B:10:VAL:HG23	2.11	0.50
2:B:257:ILE:CG2	2:B:283:LEU:HD21	2.40	0.50
2:B:284:ARG:HH11	2:B:284:ARG:HG3	1.77	0.50
1:A:450:THR:HG22	1:A:452:LEU:HG	1.93	0.50
2:B:49:LYS:HE2	2:B:142:ILE:HG22	1.93	0.50
2:B:79:GLU:C	2:B:81:ASN:N	2.64	0.50
2:B:278:GLN:HG3	2:B:299:ALA:HB2	1.92	0.50
1:A:28:GLU:CG	1:A:135:ILE:O	2.57	0.50
1:A:29:GLU:CG	1:A:30:LYS:N	2.64	0.50
1:A:318:TYR:OH	4:A:701:IET:H15	2.11	0.50
1:A:360:ALA:O	1:A:514:GLU:HG2	2.11	0.50
2:B:257:ILE:HD11	2:B:279:LEU:HG	1.93	0.50
2:B:342:TYR:HD1	2:B:342:TYR:C	2.14	0.50
2:B:365:VAL:O	2:B:365:VAL:CG1	2.59	0.50
1:A:139:THR:C	1:A:141:GLY:N	2.65	0.50
2:B:146:TYR:CD2	2:B:150:PRO:HB3	2.46	0.50
1:A:51:GLY:C	1:A:53:GLU:H	2.13	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:THR:O	1:A:154:LYS:NZ	2.33	0.50
1:A:153:TRP:CE3	1:A:155:GLY:O	2.65	0.50
2:B:325:LEU:HD23	2:B:343:GLN:HG3	1.94	0.50
1:A:55:PRO:CG	1:A:143:ARG:NH1	2.75	0.50
1:A:77:PHE:CZ	1:A:150:PRO:CB	2.94	0.50
1:A:391:LEU:O	1:A:393:ILE:N	2.41	0.50
2:B:156:SER:H	2:B:157:PRO:HD2	1.77	0.50
2:B:329:ILE:HD11	2:B:389:PHE:CD2	2.47	0.50
1:A:97:PRO:HA	1:A:100:LEU:CG	2.41	0.50
1:A:150:PRO:HG2	1:A:153:TRP:HB2	1.94	0.50
1:A:430:GLU:HG3	1:A:434:ILE:HD11	1.94	0.50
1:A:457:TYR:C	1:A:457:TYR:CD2	2.86	0.50
1:A:497:THR:HG22	1:A:498:ASP:N	2.26	0.50
2:B:183:TYR:HE2	2:B:184:MET:HG3	1.74	0.50
1:A:90:VAL:HG22	1:A:90:VAL:O	2.12	0.50
2:B:149:LEU:HB3	2:B:156:SER:HA	1.94	0.50
2:B:169:GLU:CB	2:B:170:PRO:HD3	2.42	0.50
2:B:181:TYR:CD1	2:B:182:GLN:N	2.77	0.50
2:B:330:GLN:HG2	2:B:338:THR:OG1	2.12	0.50
1:A:55:PRO:CG	1:A:143:ARG:HH12	2.24	0.49
1:A:261:VAL:HG21	1:A:280:SER:HB3	1.93	0.49
1:A:496:VAL:HG22	1:A:534:ALA:HB3	1.93	0.49
2:B:18:GLY:HA3	2:B:127:TYR:HD1	1.76	0.49
1:A:135:ILE:O	1:A:136:ASN:ND2	2.44	0.49
1:A:356:ARG:NH1	1:A:358:ARG:HB2	2.26	0.49
1:A:481:ALA:O	1:A:484:LEU:HB3	2.12	0.49
1:A:513:SER:HB3	1:A:519:ASN:ND2	2.27	0.49
1:A:50:ILE:N	1:A:50:ILE:HD12	2.26	0.49
1:A:229:TRP:O	1:A:231:GLY:N	2.44	0.49
1:A:319:TYR:CE2	1:A:321:PRO:HA	2.47	0.49
2:B:245:VAL:HG13	2:B:245:VAL:O	2.12	0.49
2:B:385:LYS:HB3	2:B:385:LYS:HZ3	1.77	0.49
1:A:139:THR:HG22	1:A:141:GLY:H	1.77	0.49
1:A:200:THR:HG23	1:A:201:LYS:H	1.76	0.49
1:A:543:GLY:CA	2:B:284:ARG:HA	2.42	0.49
2:B:372:VAL:HG12	2:B:373:GLN:N	2.27	0.49
1:A:339:TYR:C	1:A:340:GLN:HG3	2.33	0.49
1:A:408:ALA:HB2	2:B:337:TRP:HH2	1.78	0.49
2:B:66:LYS:CB	2:B:69:THR:HG22	2.42	0.49
2:B:46:LYS:HZ3	2:B:116:PHE:HD2	1.56	0.49
2:B:160:PHE:O	2:B:161:GLN:C	2.49	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:CYS:CB	1:A:144:TYR:CE1	2.92	0.49
1:A:224:GLU:O	1:A:225:PRO:C	2.50	0.49
1:A:384:GLY:HA3	2:B:135:ILE:CG2	2.43	0.49
2:B:47:ILE:HG13	2:B:47:ILE:O	2.12	0.49
2:B:125:ARG:HD3	2:B:146:TYR:O	2.12	0.49
2:B:255:ASN:HB2	2:B:289:LEU:O	2.12	0.49
1:A:12:LEU:HB3	1:A:83:ARG:O	2.13	0.49
1:A:179:VAL:C	1:A:180:ILE:HD12	2.32	0.49
1:A:413:GLU:H	1:A:413:GLU:HG2	1.33	0.49
2:B:282:LEU:CD1	2:B:293:ILE:HG12	2.41	0.49
2:B:358:ARG:O	2:B:359:GLY:C	2.51	0.49
1:A:104:LYS:HG3	1:A:192:ASP:HA	1.95	0.49
1:A:290:THR:O	1:A:290:THR:CG2	2.61	0.49
1:A:402:TRP:O	1:A:402:TRP:CE3	2.65	0.49
2:B:153:TRP:CZ2	2:B:155:GLY:HA3	2.47	0.49
2:B:191:SER:HG	2:B:198:HIS:HD1	1.53	0.49
1:A:97:PRO:HA	1:A:100:LEU:HD12	1.95	0.49
2:B:274:ILE:HA	2:B:306:ASN:HD21	1.78	0.49
1:A:49:LYS:HG2	1:A:144:TYR:CE2	2.48	0.48
1:A:58:THR:CG2	1:A:76:ASP:O	2.61	0.48
1:A:149:LEU:HA	1:A:150:PRO:HD2	1.72	0.48
2:B:172:LYS:NZ	5:B:1070:HOH:O	2.46	0.48
2:B:305:GLU:HA	2:B:308:GLU:HG2	1.95	0.48
1:A:478:GLU:HB3	1:A:499:SER:HB2	1.95	0.48
2:B:84:THR:HG22	2:B:85:GLN:N	2.28	0.48
1:A:200:THR:O	1:A:204:GLU:HG3	2.13	0.48
1:A:502:ALA:O	1:A:506:ILE:HG12	2.12	0.48
2:B:76:ASP:O	2:B:78:ARG:N	2.42	0.48
2:B:248:GLU:O	2:B:249:LYS:C	2.52	0.48
2:B:319:TYR:OH	2:B:385:LYS:HD2	2.13	0.48
1:A:1:PRO:HA	1:A:46:LYS:HZ1	1.78	0.48
1:A:76:ASP:OD2	1:A:78:ARG:HG3	2.14	0.48
2:B:37:ILE:O	2:B:40:GLU:HB3	2.12	0.48
2:B:354:TYR:CG	2:B:355:ALA:N	2.81	0.48
1:A:43:LYS:C	1:A:45:GLY:H	2.16	0.48
1:A:64:LYS:HA	1:A:66:LYS:CD	2.41	0.48
1:A:218:ASP:N	5:A:1036:HOH:O	2.36	0.48
1:A:260:LEU:HD23	1:A:279:LEU:HD21	1.95	0.48
1:A:320:ASP:H	1:A:343:GLN:NE2	2.02	0.48
1:A:379:SER:HA	1:A:383:TRP:CE3	2.48	0.48
1:A:458:VAL:CG2	1:A:551:LEU:HD11	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:PRO:CG	1:A:80:LEU:HA	2.44	0.48
1:A:161:GLN:O	1:A:161:GLN:HG2	2.13	0.48
1:A:283:LEU:O	1:A:283:LEU:HD12	2.14	0.48
2:B:57:ASN:C	2:B:57:ASN:ND2	2.66	0.48
2:B:85:GLN:HA	2:B:88:TRP:HB2	1.96	0.48
2:B:425:LEU:HD23	2:B:425:LEU:O	2.14	0.48
1:A:64:LYS:CA	1:A:66:LYS:HG2	2.44	0.48
1:A:239:TRP:O	1:A:240:THR:OG1	2.30	0.48
1:A:261:VAL:HG13	1:A:276:VAL:CG1	2.43	0.48
2:B:216:THR:C	2:B:218:ASP:H	2.17	0.48
2:B:332:GLN:HG2	2:B:338:THR:CG2	2.39	0.48
1:A:335:GLY:HA2	1:A:367:GLN:OE1	2.14	0.48
2:B:426:TRP:HD1	2:B:427:TYR:CD2	2.32	0.48
1:A:34:LEU:HD12	1:A:132:ILE:CG1	2.44	0.48
1:A:111:VAL:O	1:A:114:ALA:N	2.47	0.48
1:A:162:SER:HB2	2:B:52:PRO:HG3	1.95	0.48
1:A:331:LYS:CE	1:A:333:GLY:HA2	2.42	0.48
1:A:402:TRP:CE3	1:A:402:TRP:C	2.86	0.48
1:A:441:TYR:CE1	1:A:544:GLY:HA3	2.49	0.48
2:B:75:VAL:HG11	2:B:77:PHE:CE2	2.48	0.48
1:A:107:THR:HG1	1:A:198:HIS:CD2	2.32	0.47
2:B:115:TYR:CE2	2:B:157:PRO:HA	2.30	0.47
2:B:183:TYR:C	2:B:183:TYR:HD2	2.17	0.47
1:A:139:THR:HG22	1:A:140:PRO:HD2	1.94	0.47
2:B:54:ASN:ND2	2:B:126:LYS:HA	2.29	0.47
1:A:270:ILE:HD12	1:A:351:THR:HG23	1.95	0.47
1:A:410:TRP:HB3	2:B:365:VAL:CG2	2.44	0.47
1:A:494:ASN:HD22	1:A:494:ASN:N	2.12	0.47
2:B:354:TYR:CD1	2:B:355:ALA:N	2.83	0.47
1:A:120:LEU:O	1:A:121:ASP:C	2.52	0.47
1:A:122:GLU:O	1:A:122:GLU:CG	2.62	0.47
1:A:375:ILE:HG21	1:A:389:PHE:CE1	2.48	0.47
1:A:485:ALA:O	1:A:486:LEU:C	2.50	0.47
2:B:267:ALA:O	2:B:271:TYR:HB2	2.15	0.47
1:A:107:THR:CB	1:A:202:ILE:HD13	2.45	0.47
1:A:160:PHE:CE1	1:A:182:GLN:OE1	2.68	0.47
1:A:458:VAL:HG11	1:A:547:GLN:HG2	1.96	0.47
1:A:188:TYR:CD2	4:A:701:IET:H5	2.50	0.47
1:A:435:VAL:HG22	2:B:290:THR:CG2	2.31	0.47
1:A:445:ALA:H	1:A:552:VAL:HG11	1.80	0.47
1:A:513:SER:H	1:A:519:ASN:HD21	1.62	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:217:PRO:C	2:B:219:LYS:H	2.18	0.47
1:A:244:ILE:HA	1:A:263:LYS:CE	2.44	0.47
1:A:274:ILE:HG23	1:A:306:ASN:OD1	2.14	0.47
1:A:281:LYS:O	1:A:284:ARG:HB3	2.15	0.47
1:A:406:TRP:CZ3	2:B:420:PRO:HD2	2.49	0.47
1:A:439:THR:HG21	1:A:441:TYR:CE2	2.49	0.47
1:A:506:ILE:HD11	1:A:521:ILE:HG21	1.96	0.47
2:B:60:VAL:HG13	2:B:130:PHE:HB2	1.97	0.47
2:B:320:ASP:OD1	2:B:322:SER:HB3	2.13	0.47
2:B:369:THR:O	2:B:369:THR:HG22	2.14	0.47
2:B:401:TRP:O	2:B:402:TRP:C	2.50	0.47
2:B:418:ASN:O	2:B:419:THR:HB	2.15	0.47
1:A:97:PRO:HG2	1:A:232:TYR:CD2	2.49	0.47
1:A:102:LYS:N	1:A:318:TYR:HD1	2.13	0.47
1:A:108:VAL:HG12	1:A:188:TYR:CD2	2.35	0.47
1:A:139:THR:HG22	1:A:140:PRO:CD	2.45	0.47
1:A:363:ASN:ND2	1:A:365:VAL:HB	2.29	0.47
2:B:130:PHE:CZ	2:B:144:TYR:CB	2.97	0.47
2:B:179:VAL:HG23	2:B:179:VAL:O	2.15	0.47
2:B:195:ILE:CG1	2:B:199:ARG:NE	2.77	0.47
2:B:307:ARG:O	2:B:307:ARG:HG2	2.14	0.47
2:B:380:ILE:O	2:B:384:GLY:CA	2.58	0.47
2:B:380:ILE:HD12	2:B:380:ILE:N	2.28	0.47
1:A:7:THR:HG22	1:A:119:PRO:CG	2.45	0.47
1:A:34:LEU:CD1	1:A:132:ILE:HG12	2.44	0.47
1:A:124:PHE:CD2	1:A:124:PHE:O	2.68	0.47
2:B:157:PRO:HG3	2:B:184:MET:HA	1.96	0.47
1:A:229:TRP:O	1:A:232:TYR:N	2.48	0.46
2:B:168:LEU:HD23	2:B:209:LEU:HD21	1.97	0.46
2:B:195:ILE:HG13	2:B:199:ARG:HD2	1.96	0.46
1:A:85:GLN:HE22	2:B:53:GLU:HA	1.80	0.46
1:A:208:HIS:CE1	1:A:212:TRP:NE1	2.82	0.46
1:A:309:ILE:HG22	1:A:310:LEU:N	2.30	0.46
1:A:326:ILE:HB	1:A:342:TYR:CD1	2.50	0.46
1:A:458:VAL:HG21	1:A:547:GLN:HG3	1.97	0.46
2:B:195:ILE:HD11	2:B:233:GLU:OE1	2.15	0.46
1:A:164:MET:CE	1:A:168:LEU:HD11	2.42	0.46
1:A:301:LEU:O	1:A:305:GLU:HG3	2.16	0.46
2:B:13:LYS:CG	2:B:14:PRO:N	2.78	0.46
2:B:76:ASP:C	2:B:78:ARG:H	2.19	0.46
2:B:274:ILE:HA	2:B:306:ASN:ND2	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:GLU:O	1:A:299:ALA:C	2.53	0.46
1:A:334:GLN:C	1:A:336:GLN:N	2.69	0.46
1:A:418:ASN:O	1:A:420:PRO:HD3	2.16	0.46
2:B:178:ILE:HG23	2:B:189:VAL:HG12	1.98	0.46
2:B:223:LYS:HA	2:B:223:LYS:HD3	1.70	0.46
2:B:366:LYS:HB2	2:B:405:TYR:CZ	2.50	0.46
1:A:373:GLN:HG2	2:B:394:GLN:HE21	1.80	0.46
1:A:450:THR:O	1:A:451:LYS:C	2.53	0.46
2:B:47:ILE:HG22	2:B:146:TYR:CD1	2.50	0.46
2:B:124:PHE:O	2:B:125:ARG:C	2.54	0.46
2:B:221:HIS:HD2	2:B:221:HIS:H	1.61	0.46
1:A:9:PRO:O	1:A:9:PRO:HG2	2.16	0.46
1:A:64:LYS:O	1:A:65:LYS:C	2.52	0.46
1:A:180:ILE:CG2	1:A:187:LEU:HD11	2.46	0.46
1:A:228:LEU:HD23	1:A:232:TYR:O	2.15	0.46
1:A:433:PRO:CB	2:B:255:ASN:ND2	2.78	0.46
1:A:470:THR:O	1:A:471:ASN:HB3	2.14	0.46
2:B:168:LEU:HD13	2:B:180:ILE:CD1	2.45	0.46
2:B:245:VAL:O	2:B:245:VAL:HG22	2.15	0.46
1:A:24:TRP:O	1:A:26:LEU:N	2.49	0.46
1:A:175:ASN:O	1:A:177:ASP:N	2.48	0.46
1:A:440:PHE:CD2	1:A:459:THR:HG23	2.51	0.46
2:B:31:ILE:HG22	2:B:35:VAL:HG22	1.97	0.46
2:B:109:LEU:HD12	2:B:218:ASP:OD2	2.14	0.46
2:B:161:GLN:O	2:B:163:SER:N	2.48	0.46
1:A:98:ALA:HB2	1:A:350:LYS:HB2	1.98	0.46
1:A:335:GLY:O	1:A:355:ALA:HA	2.15	0.46
1:A:401:TRP:HE3	1:A:404:GLU:HG3	1.81	0.46
1:A:480:GLN:O	1:A:481:ALA:C	2.54	0.46
2:B:54:ASN:OD1	2:B:56:TYR:HB2	2.16	0.46
2:B:263:LYS:O	2:B:426:TRP:CZ3	2.68	0.46
2:B:331:LYS:O	2:B:424:LYS:HG3	2.16	0.46
1:A:339:TYR:CE2	1:A:375:ILE:HG13	2.51	0.46
2:B:201:LYS:O	2:B:205:LEU:N	2.49	0.46
2:B:330:GLN:N	2:B:330:GLN:OE1	2.49	0.46
2:B:358:ARG:H	2:B:358:ARG:NE	2.13	0.46
2:B:378:GLU:O	2:B:382:ILE:HG13	2.16	0.46
1:A:111:VAL:O	1:A:113:ASP:N	2.49	0.46
1:A:219:LYS:HB3	5:A:1088:HOH:O	2.16	0.46
1:A:311:LYS:NZ	5:A:1040:HOH:O	2.49	0.46
1:A:348:ASN:ND2	1:A:351:THR:HG22	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:HIS:CD2	1:A:505:ILE:HD12	2.51	0.46
1:A:490:GLY:C	1:A:492:GLU:N	2.70	0.46
2:B:66:LYS:HB2	2:B:69:THR:CG2	2.46	0.46
2:B:202:ILE:O	2:B:205:LEU:HB3	2.16	0.46
2:B:254:VAL:O	2:B:257:ILE:HG23	2.16	0.46
2:B:329:ILE:CD1	2:B:389:PHE:HD2	2.29	0.46
1:A:64:LYS:CA	1:A:66:LYS:HD3	2.43	0.45
1:A:319:TYR:CE1	1:A:325:LEU:HD21	2.52	0.45
1:A:379:SER:OG	1:A:387:PRO:HD3	2.16	0.45
1:A:394:GLN:O	1:A:397:THR:N	2.44	0.45
1:A:503:LEU:HD23	1:A:535:TRP:HB2	1.98	0.45
2:B:22:LYS:HA	2:B:22:LYS:HD3	1.68	0.45
2:B:61:PHE:CE1	2:B:76:ASP:HB2	2.42	0.45
2:B:72:ARG:NH2	2:B:409:THR:HG22	2.31	0.45
2:B:205:LEU:O	2:B:206:ARG:C	2.53	0.45
1:A:12:LEU:HG	1:A:124:PHE:CE1	2.38	0.45
1:A:434:ILE:CG1	1:A:530:LYS:HD3	2.46	0.45
2:B:23:GLN:HG2	2:B:133:PRO:CG	2.43	0.45
1:A:12:LEU:HD12	1:A:12:LEU:H	1.80	0.45
1:A:94:ILE:HG21	1:A:230:MET:HE2	1.98	0.45
1:A:107:THR:HG21	1:A:202:ILE:HD13	1.97	0.45
1:A:124:PHE:CE2	1:A:153:TRP:CE2	3.04	0.45
1:A:306:ASN:O	1:A:310:LEU:HB2	2.15	0.45
1:A:408:ALA:HB2	2:B:337:TRP:CH2	2.52	0.45
1:A:491:LEU:HD12	1:A:491:LEU:H	1.80	0.45
1:A:513:SER:N	1:A:519:ASN:ND2	2.64	0.45
2:B:115:TYR:C	2:B:117:SER:H	2.19	0.45
2:B:181:TYR:CD1	2:B:181:TYR:C	2.88	0.45
2:B:227:PHE:O	2:B:228:LEU:HG	2.16	0.45
1:A:13:LYS:HD2	1:A:16:MET:HE1	1.98	0.45
1:A:27:THR:C	1:A:29:GLU:H	2.18	0.45
1:A:34:LEU:CD2	1:A:62:ALA:CB	2.85	0.45
1:A:203:GLU:O	1:A:207:GLN:HG2	2.16	0.45
1:A:491:LEU:O	1:A:529:GLU:CB	2.63	0.45
2:B:41:MET:HE2	2:B:41:MET:HB3	1.86	0.45
2:B:146:TYR:CE1	2:B:150:PRO:HB3	2.52	0.45
2:B:164:MET:C	2:B:166:LYS:N	2.70	0.45
2:B:266:TRP:O	2:B:268:SER:N	2.49	0.45
2:B:376:THR:CG2	2:B:380:ILE:CD1	2.87	0.45
1:A:134:SER:HB3	1:A:138:GLU:OE1	2.16	0.45
1:A:409:THR:OG1	1:A:410:TRP:N	2.48	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:TYR:C	1:A:457:TYR:HD2	2.18	0.45
2:B:279:LEU:HD12	2:B:279:LEU:HA	1.82	0.45
2:B:358:ARG:O	2:B:362:THR:HB	2.16	0.45
1:A:12:LEU:HD12	1:A:12:LEU:N	2.31	0.45
2:B:31:ILE:O	2:B:32:LYS:C	2.55	0.45
2:B:139:THR:HG22	2:B:140:PRO:N	2.29	0.45
2:B:220:LYS:CB	2:B:221:HIS:HD2	2.29	0.45
1:A:265:ASN:O	1:A:268:SER:N	2.47	0.45
1:A:286:THR:HG23	1:A:287:LYS:H	1.81	0.45
1:A:450:THR:HG22	1:A:450:THR:O	2.17	0.45
2:B:47:ILE:HG21	2:B:146:TYR:CD1	2.52	0.45
2:B:66:LYS:HB2	2:B:69:THR:HG21	1.98	0.45
1:A:229:TRP:HE3	1:A:234:LEU:HD11	1.82	0.45
1:A:307:ARG:O	1:A:308:GLU:C	2.55	0.45
1:A:379:SER:CB	1:A:387:PRO:HD3	2.47	0.45
1:A:398:TRP:CD1	1:A:399:GLU:N	2.85	0.45
1:A:483:TYR:HA	1:A:486:LEU:HD12	1.98	0.45
2:B:54:ASN:HD21	2:B:126:LYS:CA	2.30	0.45
2:B:60:VAL:HG23	2:B:60:VAL:O	2.16	0.45
2:B:208:HIS:CE1	2:B:212:TRP:HD1	2.34	0.45
1:A:105:SER:OG	1:A:198:HIS:CG	2.70	0.45
1:A:195:ILE:HA	1:A:198:HIS:HB3	1.97	0.45
1:A:270:ILE:O	1:A:272:PRO:HD3	2.17	0.45
1:A:426:TRP:HB3	1:A:526:ILE:HD12	1.99	0.45
2:B:320:ASP:OD2	2:B:323:LYS:HE2	2.17	0.45
2:B:402:TRP:O	2:B:403:THR:C	2.54	0.45
1:A:77:PHE:O	1:A:78:ARG:C	2.56	0.45
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.52	0.45
2:B:266:TRP:C	2:B:268:SER:H	2.20	0.45
1:A:120:LEU:HD23	1:A:125:ARG:CG	2.48	0.44
1:A:467:VAL:HA	1:A:468:PRO:HD3	1.79	0.44
2:B:38:CYS:O	2:B:40:GLU:N	2.50	0.44
2:B:66:LYS:HA	5:B:1037:HOH:O	2.17	0.44
2:B:88:TRP:HZ3	2:B:159:ILE:HG13	1.81	0.44
2:B:112:GLY:HA2	2:B:115:TYR:CE1	2.52	0.44
2:B:168:LEU:HD21	2:B:209:LEU:HD21	1.99	0.44
2:B:200:THR:O	2:B:204:GLU:N	2.34	0.44
2:B:374:LYS:O	2:B:375:ILE:C	2.54	0.44
2:B:376:THR:HG22	2:B:380:ILE:HD13	1.97	0.44
1:A:18:GLY:HA3	1:A:56:TYR:CD2	2.53	0.44
2:B:27:THR:HG22	2:B:28:GLU:N	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:THR:HG22	2:B:59:PRO:HD2	1.98	0.44
2:B:96:HIS:HA	2:B:97:PRO:HD2	1.88	0.44
2:B:109:LEU:HD12	2:B:216:THR:HG21	1.99	0.44
2:B:220:LYS:HB2	2:B:221:HIS:HD2	1.83	0.44
2:B:346:PHE:N	2:B:346:PHE:CD1	2.85	0.44
1:A:43:LYS:C	1:A:45:GLY:N	2.71	0.44
1:A:161:GLN:O	1:A:162:SER:O	2.36	0.44
1:A:469:LEU:HD11	1:A:480:GLN:HG2	1.99	0.44
2:B:54:ASN:HD21	2:B:126:LYS:HA	1.82	0.44
1:A:62:ALA:O	1:A:63:ILE:CG2	2.66	0.44
1:A:121:ASP:C	1:A:123:ASP:N	2.71	0.44
2:B:376:THR:HG21	2:B:410:TRP:CZ3	2.53	0.44
1:A:96:HIS:C	1:A:96:HIS:ND1	2.71	0.44
1:A:127:TYR:CD2	1:A:127:TYR:N	2.84	0.44
1:A:132:ILE:HD13	1:A:133:PRO:CD	2.44	0.44
1:A:148:VAL:O	1:A:150:PRO:CD	2.66	0.44
1:A:194:GLU:O	1:A:195:ILE:C	2.56	0.44
1:A:328:GLU:HG2	1:A:390:LYS:CB	2.44	0.44
1:A:536:VAL:HG12	1:A:541:GLY:HA3	1.99	0.44
2:B:72:ARG:NH2	2:B:409:THR:CG2	2.81	0.44
1:A:452:LEU:HD23	1:A:470:THR:HA	1.99	0.44
1:A:482:ILE:CD1	1:A:502:ALA:HB1	2.47	0.44
2:B:53:GLU:OE1	2:B:53:GLU:N	2.37	0.44
2:B:169:GLU:O	2:B:172:LYS:N	2.50	0.44
2:B:195:ILE:O	2:B:196:GLY:C	2.54	0.44
1:A:2:ILE:HD11	1:A:45:GLY:O	2.18	0.44
1:A:17:ASP:CG	1:A:18:GLY:H	2.21	0.44
1:A:254:VAL:CA	1:A:257:ILE:HG22	2.38	0.44
1:A:282:LEU:O	1:A:284:ARG:N	2.51	0.44
1:A:450:THR:O	1:A:452:LEU:HG	2.17	0.44
1:A:499:SER:OG	1:A:502:ALA:CB	2.65	0.44
2:B:79:GLU:O	2:B:81:ASN:N	2.51	0.44
2:B:86:ASP:O	2:B:89:GLU:HB3	2.17	0.44
2:B:107:THR:HA	2:B:232:TYR:O	2.18	0.44
2:B:228:LEU:HD23	2:B:228:LEU:HA	1.85	0.44
1:A:469:LEU:CD1	1:A:477:THR:HG22	2.46	0.44
2:B:13:LYS:HG2	2:B:14:PRO:N	2.30	0.44
2:B:73:LYS:HE2	2:B:75:VAL:HG23	1.99	0.44
1:A:19:PRO:HG3	1:A:80:LEU:HA	2.00	0.44
1:A:55:PRO:HG2	1:A:143:ARG:CZ	2.48	0.44
1:A:122:GLU:O	1:A:122:GLU:HG2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ILE:CA	1:A:263:LYS:HE2	2.48	0.44
1:A:320:ASP:HB3	1:A:323:LYS:HZ2	1.83	0.44
2:B:60:VAL:HG11	2:B:130:PHE:HD2	1.76	0.44
1:A:292:VAL:O	1:A:294:PRO:HD3	2.18	0.43
1:A:513:SER:H	1:A:519:ASN:ND2	2.16	0.43
2:B:58:THR:HA	2:B:59:PRO:HD3	1.75	0.43
2:B:278:GLN:HE22	2:B:297:GLU:CG	2.30	0.43
2:B:364:ASP:C	2:B:366:LYS:N	2.65	0.43
1:A:27:THR:C	1:A:29:GLU:N	2.71	0.43
2:B:72:ARG:HH21	2:B:151:GLN:HE22	1.65	0.43
2:B:308:GLU:C	2:B:310:LEU:N	2.71	0.43
1:A:102:LYS:O	1:A:103:LYS:HD3	2.18	0.43
1:A:139:THR:C	1:A:141:GLY:H	2.21	0.43
1:A:175:ASN:C	1:A:177:ASP:H	2.22	0.43
1:A:326:ILE:N	1:A:326:ILE:CD1	2.76	0.43
1:A:433:PRO:CB	2:B:255:ASN:HD22	2.31	0.43
2:B:103:LYS:HE3	2:B:179:VAL:HG13	1.98	0.43
2:B:300:GLU:OE1	2:B:300:GLU:O	2.36	0.43
2:B:311:LYS:NZ	5:B:1079:HOH:O	2.50	0.43
1:A:130:PHE:HE1	1:A:144:TYR:HB2	1.77	0.43
1:A:315:HIS:CD2	5:A:1029:HOH:O	2.71	0.43
2:B:92:LEU:HB2	2:B:158:ALA:HB1	1.99	0.43
2:B:142:ILE:H	2:B:142:ILE:HG12	1.58	0.43
2:B:198:HIS:C	2:B:198:HIS:CD2	2.90	0.43
2:B:209:LEU:HB3	2:B:214:LEU:HB2	2.00	0.43
2:B:269:GLN:HB3	2:B:346:PHE:CD2	2.53	0.43
1:A:50:ILE:HD12	1:A:50:ILE:H	1.83	0.43
1:A:54:ASN:N	1:A:55:PRO:CD	2.81	0.43
1:A:156:SER:O	1:A:157:PRO:C	2.56	0.43
1:A:363:ASN:HD22	1:A:366:LYS:H	1.67	0.43
2:B:329:ILE:HD11	2:B:389:PHE:HD2	1.83	0.43
1:A:23:GLN:O	1:A:23:GLN:NE2	2.44	0.43
1:A:482:ILE:HD11	1:A:502:ALA:HB1	2.01	0.43
2:B:115:TYR:OH	2:B:184:MET:O	2.16	0.43
2:B:425:LEU:O	2:B:425:LEU:CD2	2.66	0.43
1:A:97:PRO:C	1:A:99:GLY:H	2.22	0.43
1:A:165:THR:HG22	1:A:166:LYS:N	2.32	0.43
1:A:312:GLU:H	1:A:312:GLU:HG2	1.59	0.43
1:A:406:TRP:CE3	1:A:406:TRP:C	2.91	0.43
1:A:408:ALA:HB1	2:B:364:ASP:HB3	2.00	0.43
2:B:164:MET:O	2:B:167:ILE:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:426:TRP:CD1	2:B:427:TYR:N	2.86	0.43
1:A:325:LEU:CD1	1:A:383:TRP:CE3	3.02	0.43
1:A:395:LYS:HA	1:A:414:TRP:CZ2	2.45	0.43
1:A:477:THR:C	1:A:479:LEU:N	2.72	0.43
2:B:274:ILE:HD12	2:B:274:ILE:N	2.33	0.43
2:B:316:GLY:HA2	2:B:318:TYR:HE1	1.84	0.43
1:A:497:THR:HG22	1:A:499:SER:HB3	2.01	0.43
2:B:231:GLY:O	2:B:233:GLU:HG3	2.19	0.43
2:B:277:ARG:HD3	2:B:277:ARG:N	2.27	0.43
1:A:261:VAL:CG2	1:A:279:LEU:HD22	2.48	0.42
1:A:264:LEU:CD1	1:A:279:LEU:HD13	2.49	0.42
1:A:330:GLN:NE2	1:A:340:GLN:OE1	2.51	0.42
1:A:334:GLN:C	1:A:336:GLN:H	2.21	0.42
2:B:79:GLU:O	2:B:80:LEU:C	2.57	0.42
2:B:203:GLU:OE2	2:B:207:GLN:HG2	2.19	0.42
2:B:220:LYS:CB	2:B:221:HIS:CD2	3.02	0.42
1:A:134:SER:O	1:A:135:ILE:C	2.58	0.42
1:A:142:ILE:H	1:A:142:ILE:CD1	2.29	0.42
1:A:200:THR:CG2	1:A:201:LYS:N	2.82	0.42
1:A:279:LEU:HB2	1:A:302:GLU:OE2	2.18	0.42
1:A:398:TRP:NE1	1:A:402:TRP:HD1	2.18	0.42
2:B:349:LEU:HD12	2:B:383:TRP:CE2	2.53	0.42
2:B:358:ARG:C	2:B:362:THR:HB	2.39	0.42
1:A:193:LEU:O	1:A:198:HIS:HB2	2.19	0.42
1:A:460:ASN:C	1:A:462:GLY:N	2.73	0.42
1:A:477:THR:O	1:A:480:GLN:N	2.53	0.42
2:B:218:ASP:O	2:B:220:LYS:N	2.51	0.42
1:A:319:TYR:HD1	1:A:325:LEU:HD21	1.84	0.42
1:A:433:PRO:HG3	2:B:255:ASN:ND2	2.34	0.42
1:A:434:ILE:HG13	1:A:530:LYS:HD3	2.01	0.42
2:B:183:TYR:HE1	2:B:380:ILE:HG13	1.83	0.42
2:B:202:ILE:O	2:B:203:GLU:C	2.57	0.42
2:B:345:PRO:HB2	2:B:346:PHE:CD1	2.51	0.42
1:A:85:GLN:O	1:A:154:LYS:CE	2.67	0.42
1:A:126:LYS:HG3	1:A:127:TYR:CD2	2.55	0.42
1:A:433:PRO:CG	2:B:255:ASN:ND2	2.82	0.42
1:A:541:GLY:O	1:A:545:ASN:HB3	2.19	0.42
2:B:34:LEU:HD21	2:B:61:PHE:O	2.20	0.42
2:B:53:GLU:O	2:B:55:PRO:HD3	2.20	0.42
2:B:111:VAL:C	2:B:113:ASP:H	2.23	0.42
1:A:139:THR:CG2	1:A:140:PRO:CD	2.92	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:THR:O	1:A:254:VAL:C	2.56	0.42
1:A:369:THR:O	1:A:373:GLN:N	2.45	0.42
2:B:23:GLN:HG3	2:B:133:PRO:HG3	1.95	0.42
2:B:64:LYS:HG3	2:B:71:TRP:CE3	2.55	0.42
2:B:68:SER:O	2:B:69:THR:C	2.57	0.42
2:B:96:HIS:CE1	2:B:384:GLY:N	2.88	0.42
2:B:156:SER:N	2:B:157:PRO:CD	2.82	0.42
2:B:208:HIS:ND1	2:B:208:HIS:C	2.73	0.42
1:A:390:LYS:HA	1:A:415:GLU:O	2.20	0.42
1:A:541:GLY:C	1:A:543:GLY:H	2.23	0.42
2:B:49:LYS:HE3	2:B:144:TYR:CZ	2.55	0.42
2:B:85:GLN:HG3	2:B:154:LYS:HD2	2.01	0.42
2:B:198:HIS:C	2:B:200:THR:N	2.71	0.42
2:B:257:ILE:HG23	2:B:258:GLN:N	2.35	0.42
2:B:366:LYS:CG	2:B:405:TYR:CD2	3.01	0.42
1:A:47:ILE:HB	1:A:145:GLN:O	2.19	0.42
1:A:341:ILE:HG12	1:A:383:TRP:CH2	2.55	0.42
2:B:171:PHE:CE2	2:B:205:LEU:CA	3.03	0.42
2:B:257:ILE:CD1	2:B:261:VAL:HG23	2.50	0.42
2:B:278:GLN:HG3	2:B:278:GLN:O	2.19	0.42
2:B:345:PRO:C	2:B:346:PHE:HD1	2.22	0.42
1:A:73:LYS:HE3	1:A:130:PHE:CE2	2.55	0.42
1:A:98:ALA:HB1	1:A:350:LYS:HB2	2.02	0.42
1:A:120:LEU:HD13	1:A:150:PRO:HD2	2.01	0.42
1:A:278:GLN:HB2	1:A:302:GLU:CD	2.40	0.42
1:A:331:LYS:HG3	1:A:337:TRP:CZ2	2.55	0.42
2:B:7:THR:HG22	2:B:119:PRO:HB2	2.01	0.42
2:B:60:VAL:O	2:B:60:VAL:CG2	2.67	0.42
2:B:358:ARG:CG	2:B:359:GLY:N	2.63	0.42
2:B:386:THR:HA	2:B:387:PRO:HD3	1.78	0.42
1:A:122:GLU:HA	1:A:125:ARG:NE	2.34	0.42
1:A:233:GLU:N	1:A:240:THR:O	2.44	0.42
1:A:442:VAL:HG22	1:A:443:ASP:N	2.35	0.42
1:A:456:GLY:HA2	1:A:484:LEU:CD2	2.50	0.42
2:B:34:LEU:HD21	2:B:62:ALA:HB2	2.01	0.42
2:B:320:ASP:O	2:B:343:GLN:NE2	2.51	0.42
1:A:543:GLY:O	2:B:284:ARG:O	2.37	0.41
2:B:253:THR:HB	2:B:291:GLU:O	2.20	0.41
1:A:96:HIS:HD1	1:A:98:ALA:N	2.13	0.41
1:A:126:LYS:H	1:A:126:LYS:HG2	1.71	0.41
1:A:344:GLU:HA	1:A:345:PRO:HD2	1.58	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:GLU:O	1:A:373:GLN:HB3	2.20	0.41
1:A:441:TYR:HB2	1:A:458:VAL:O	2.21	0.41
1:A:164:MET:CE	1:A:187:LEU:HD22	2.50	0.41
1:A:434:ILE:CD1	1:A:494:ASN:HD21	2.33	0.41
2:B:92:LEU:CB	2:B:158:ALA:HB1	2.50	0.41
2:B:151:GLN:O	2:B:152:GLY:C	2.57	0.41
2:B:195:ILE:CG2	2:B:196:GLY:N	2.64	0.41
2:B:375:ILE:CG2	2:B:389:PHE:HE2	2.33	0.41
1:A:499:SER:OG	1:A:499:SER:O	2.36	0.41
2:B:269:GLN:HG2	2:B:346:PHE:CG	2.56	0.41
2:B:385:LYS:NZ	2:B:385:LYS:CB	2.83	0.41
1:A:183:TYR:CD2	1:A:229:TRP:CD1	3.08	0.41
1:A:315:HIS:CD2	1:A:315:HIS:H	2.38	0.41
2:B:244:ILE:HD13	2:B:244:ILE:N	2.30	0.41
2:B:372:VAL:O	2:B:374:LYS:N	2.53	0.41
1:A:48:SER:O	1:A:144:TYR:HA	2.21	0.41
1:A:168:LEU:HD13	1:A:180:ILE:HG21	2.02	0.41
1:A:183:TYR:CD2	1:A:229:TRP:HD1	2.39	0.41
1:A:278:GLN:HG3	1:A:298:GLU:HB3	2.03	0.41
1:A:435:VAL:HG13	2:B:290:THR:OG1	2.20	0.41
1:A:482:ILE:O	1:A:483:TYR:C	2.57	0.41
2:B:75:VAL:HG11	2:B:77:PHE:CZ	2.56	0.41
2:B:275:LYS:HA	2:B:277:ARG:CZ	2.50	0.41
2:B:328:GLU:OE1	2:B:342:TYR:OH	2.30	0.41
1:A:32:LYS:O	1:A:36:GLU:CG	2.69	0.41
1:A:224:GLU:N	1:A:225:PRO:HD3	2.34	0.41
1:A:229:TRP:C	1:A:231:GLY:N	2.73	0.41
1:A:483:TYR:CB	1:A:521:ILE:HG12	2.43	0.41
1:A:503:LEU:HD21	1:A:535:TRP:HB2	1.98	0.41
1:A:309:ILE:O	1:A:312:GLU:CG	2.68	0.41
1:A:325:LEU:C	1:A:326:ILE:HD12	2.41	0.41
1:A:339:TYR:CG	1:A:375:ILE:HD11	2.56	0.41
2:B:50:ILE:HG13	2:B:143:ARG:HB3	2.03	0.41
2:B:72:ARG:HH22	2:B:409:THR:CG2	2.34	0.41
2:B:78:ARG:CZ	2:B:411:ILE:HG21	2.51	0.41
2:B:91:GLN:O	2:B:91:GLN:NE2	2.48	0.41
2:B:149:LEU:HD12	2:B:156:SER:O	2.20	0.41
2:B:269:GLN:HG2	2:B:346:PHE:CD2	2.56	0.41
2:B:283:LEU:O	2:B:285:GLY:O	2.39	0.41
1:A:107:THR:O	1:A:189:VAL:N	2.33	0.41
1:A:162:SER:CB	2:B:52:PRO:HG3	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:GLY:C	1:A:198:HIS:N	2.74	0.41
1:A:219:LYS:HA	5:A:1088:HOH:O	2.21	0.41
1:A:229:TRP:C	1:A:231:GLY:H	2.24	0.41
1:A:253:THR:OG1	1:A:290:THR:CA	2.68	0.41
1:A:275:LYS:O	1:A:276:VAL:CG2	2.68	0.41
1:A:277:ARG:HA	1:A:277:ARG:HD2	1.92	0.41
1:A:472:THR:OG1	1:A:476:LYS:HB3	2.21	0.41
2:B:38:CYS:HA	2:B:41:MET:HG3	2.02	0.41
2:B:260:LEU:CD1	2:B:264:LEU:HD11	2.50	0.41
2:B:261:VAL:HG21	2:B:283:LEU:CD1	2.50	0.41
2:B:276:VAL:O	2:B:276:VAL:HG12	2.21	0.41
2:B:295:LEU:HD23	2:B:295:LEU:N	2.36	0.41
2:B:375:ILE:HG21	2:B:389:PHE:HE2	1.84	0.41
1:A:21:VAL:HG12	1:A:22:LYS:N	2.36	0.41
1:A:261:VAL:HG13	1:A:276:VAL:HG11	2.01	0.41
1:A:307:ARG:C	1:A:309:ILE:N	2.74	0.41
1:A:356:ARG:NE	1:A:358:ARG:CG	2.79	0.41
1:A:443:ASP:HB2	1:A:548:VAL:CG2	2.50	0.41
2:B:23:GLN:HG3	2:B:24:TRP:O	2.20	0.41
2:B:85:GLN:O	2:B:88:TRP:C	2.59	0.41
2:B:306:ASN:HD22	2:B:306:ASN:HA	1.64	0.41
2:B:371:ALA:O	2:B:375:ILE:HB	2.21	0.41
1:A:142:ILE:N	1:A:142:ILE:CD1	2.84	0.40
1:A:257:ILE:O	1:A:261:VAL:HG23	2.21	0.40
1:A:326:ILE:HG22	1:A:327:ALA:N	2.36	0.40
1:A:485:ALA:O	1:A:487:GLN:N	2.54	0.40
2:B:66:LYS:HB3	2:B:67:ASP:H	1.62	0.40
2:B:183:TYR:HD1	2:B:380:ILE:CG2	2.23	0.40
1:A:438:GLU:CD	1:A:463:ARG:HH21	2.23	0.40
1:A:450:THR:HG22	1:A:452:LEU:CB	2.52	0.40
2:B:198:HIS:CD2	2:B:199:ARG:N	2.89	0.40
1:A:2:ILE:CG2	1:A:3:SER:H	2.25	0.40
1:A:15:GLY:O	1:A:16:MET:C	2.60	0.40
2:B:156:SER:HB2	2:B:157:PRO:CD	2.51	0.40
2:B:253:THR:HG22	2:B:292:VAL:HG22	2.03	0.40
1:A:193:LEU:CB	1:A:197:GLN:HB3	2.46	0.40
1:A:303:LEU:O	1:A:307:ARG:HG2	2.21	0.40
1:A:481:ALA:O	1:A:484:LEU:N	2.54	0.40
2:B:171:PHE:CD1	2:B:171:PHE:O	2.74	0.40
2:B:232:TYR:CE2	2:B:234:LEU:HD21	2.48	0.40
1:A:104:LYS:CG	1:A:192:ASP:HA	2.52	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ILE:HG22	1:A:136:ASN:N	2.37	0.40
2:B:125:ARG:HD3	2:B:147:ASN:OD1	2.21	0.40
2:B:125:ARG:HD3	2:B:147:ASN:HA	2.03	0.40
2:B:149:LEU:C	2:B:150:PRO:O	2.60	0.40
2:B:181:TYR:O	2:B:188:TYR:N	2.51	0.40
2:B:187:LEU:HD23	2:B:187:LEU:HA	1.90	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	550/560 (98%)	404 (74%)	92 (17%)	54 (10%)	0 1
2	B	425/430 (99%)	277 (65%)	94 (22%)	54 (13%)	0 0
All	All	975/990 (98%)	681 (70%)	186 (19%)	108 (11%)	0 1

All (108) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	25	PRO
1	A	52	PRO
1	A	65	LYS
1	A	112	GLY
1	A	153	TRP
1	A	162	SER
1	A	163	SER
1	A	273	GLY
1	A	359	GLY
1	A	538	ALA
2	B	66	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	68	SER
2	B	71	TRP
2	B	77	PHE
2	B	116	PHE
2	B	126	LYS
2	B	161	GLN
2	B	176	PRO
2	B	177	ASP
2	B	195	ILE
2	B	218	ASP
2	B	242	GLN
2	B	267	ALA
2	B	284	ARG
2	B	297	GLU
2	B	362	THR
2	B	365	VAL
2	B	404	GLU
2	B	421	PRO
1	A	98	ALA
1	A	122	GLU
1	A	164	MET
1	A	195	ILE
1	A	223	LYS
1	A	230	MET
1	A	276	VAL
1	A	277	ARG
1	A	399	GLU
1	A	491	LEU
1	A	546	GLU
2	B	18	GLY
2	B	85	GLN
2	B	112	GLY
2	B	154	LYS
2	B	162	SER
2	B	165	THR
2	B	174	GLN
2	B	196	GLY
2	B	202	ILE
2	B	228	LEU
2	B	232	TYR
2	B	239	TRP
2	B	250	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	345	PRO
1	A	2	ILE
1	A	64	LYS
1	A	66	LYS
1	A	78	ARG
1	A	102	LYS
1	A	156	SER
1	A	158	ALA
1	A	222	GLN
1	A	272	PRO
1	A	311	LYS
1	A	324	ASP
1	A	398	TRP
1	A	539	HIS
2	B	125	ARG
2	B	173	LYS
2	B	199	ARG
2	B	249	LYS
2	B	294	PRO
1	A	14	PRO
1	A	27	THR
1	A	104	LYS
1	A	176	PRO
1	A	254	VAL
1	A	465	LYS
1	A	482	ILE
2	B	122	GLU
2	B	170	PRO
2	B	251	SER
2	B	276	VAL
1	A	184	MET
1	A	194	GLU
1	A	345	PRO
1	A	392	PRO
1	A	542	ILE
2	B	184	MET
2	B	222	GLN
2	B	236	PRO
2	B	33	ALA
2	B	141	GLY
1	A	159	ILE
1	A	543	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	24	TRP
1	A	54	ASN
1	A	135	ILE
1	A	236	PRO
2	B	111	VAL
2	B	155	GLY
1	A	419	THR
2	B	241	VAL
2	B	245	VAL
2	B	225	PRO
2	B	412	PRO
2	B	423	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	494/500 (99%)	449 (91%)	45 (9%)	9 28
2	B	389/392 (99%)	342 (88%)	47 (12%)	5 15
All	All	883/892 (99%)	791 (90%)	92 (10%)	7 21

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	23	GLN
1	A	25	PRO
1	A	36	GLU
1	A	50	ILE
1	A	56	TYR
1	A	64	LYS
1	A	66	LYS
1	A	71	TRP
1	A	74	LEU
1	A	86	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	120	LEU
1	A	126	LYS
1	A	130	PHE
1	A	132	ILE
1	A	136	ASN
1	A	159	ILE
1	A	165	THR
1	A	177	ASP
1	A	188	TYR
1	A	245	VAL
1	A	256	ASP
1	A	317	VAL
1	A	330	GLN
1	A	334	GLN
1	A	340	GLN
1	A	356	ARG
1	A	374	LYS
1	A	385	LYS
1	A	386	THR
1	A	395	LYS
1	A	397	THR
1	A	401	TRP
1	A	402	TRP
1	A	411	ILE
1	A	413	GLU
1	A	418	ASN
1	A	449	GLU
1	A	457	TYR
1	A	494	ASN
1	A	516	GLU
1	A	522	ILE
1	A	533	LEU
1	A	548	VAL
1	A	551	LEU
2	B	9	PRO
2	B	24	TRP
2	B	50	ILE
2	B	57	ASN
2	B	58	THR
2	B	63	ILE
2	B	67	ASP
2	B	73	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	74	LEU
2	B	86	ASP
2	B	91	GLN
2	B	110	ASP
2	B	131	THR
2	B	135	ILE
2	B	142	ILE
2	B	149	LEU
2	B	169	GLU
2	B	175	ASN
2	B	181	TYR
2	B	183	TYR
2	B	186	ASP
2	B	189	VAL
2	B	198	HIS
2	B	208	HIS
2	B	215	THR
2	B	221	HIS
2	B	224	GLU
2	B	232	TYR
2	B	239	TRP
2	B	244	ILE
2	B	252	TRP
2	B	257	ILE
2	B	277	ARG
2	B	308	GLU
2	B	322	SER
2	B	332	GLN
2	B	340	GLN
2	B	342	TYR
2	B	349	LEU
2	B	358	ARG
2	B	362	THR
2	B	366	LYS
2	B	383	TRP
2	B	385	LYS
2	B	409	THR
2	B	425	LEU
2	B	427	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	A	161	GLN
1	A	182	GLN
1	A	197	GLN
1	A	235	HIS
1	A	258	GLN
1	A	315	HIS
1	A	330	GLN
1	A	343	GLN
1	A	363	ASN
1	A	471	ASN
1	A	487	GLN
1	A	494	ASN
1	A	500	GLN
1	A	507	GLN
1	A	519	ASN
2	B	23	GLN
2	B	91	GLN
2	B	136	ASN
2	B	151	GLN
2	B	174	GLN
2	B	175	ASN
2	B	208	HIS
2	B	221	HIS
2	B	255	ASN
2	B	258	GLN
2	B	278	GLN
2	B	306	ASN
2	B	330	GLN
2	B	336	GLN
2	B	340	GLN
2	B	348	ASN
2	B	394	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	IET	A	701	-	24,24,24	5.19	11 (45%)	29,32,32	2.40	7 (24%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	IET	A	701	-	-	5/12/14/14	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	IET	C7-C8	-18.81	1.39	1.51
4	A	701	IET	C6-CL6	-9.49	1.51	1.73
4	A	701	IET	C2-CL2	-9.45	1.51	1.73
4	A	701	IET	C2-C1	4.16	1.46	1.39
4	A	701	IET	C16-C11	4.00	1.46	1.39
4	A	701	IET	C16-C15	3.52	1.45	1.38
4	A	701	IET	C8-N3	3.17	1.35	1.27
4	A	701	IET	C7-C1	3.10	1.58	1.51
4	A	701	IET	C6-C1	2.72	1.44	1.39
4	A	701	IET	C9-N1	-2.67	1.34	1.39
4	A	701	IET	C3-C2	2.47	1.44	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	701	IET	C9-N1-C8	-6.76	121.42	128.74
4	A	701	IET	C1-C7-C8	6.49	124.82	113.85
4	A	701	IET	N5-C9-N1	5.27	123.15	115.34
4	A	701	IET	C7-C1-C6	-3.84	116.63	121.84
4	A	701	IET	C7-C1-C2	3.35	126.39	121.84
4	A	701	IET	S2-C9-N5	-2.64	116.50	124.26
4	A	701	IET	C1-C2-CL2	2.10	123.56	119.60

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	701	IET	C7-C8-N1-C9
4	A	701	IET	N5-C9-N1-C8
4	A	701	IET	S2-C9-N1-C8
4	A	701	IET	C6-C1-C7-C8
4	A	701	IET	C1-C7-C8-N1

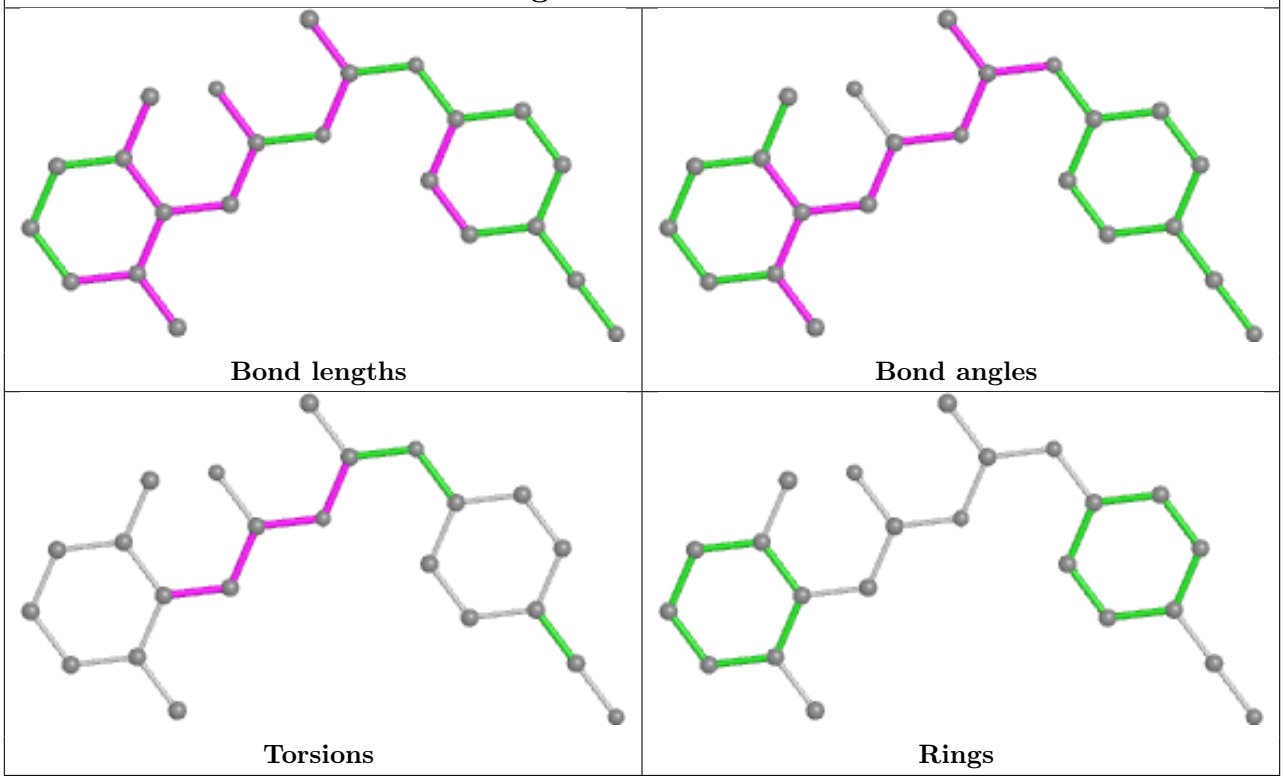
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	701	IET	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand IET A 701



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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	552/560 (98%)	-0.11	19 (3%)	45	40	37, 83, 109, 111	5 (0%)
2	B	427/430 (99%)	-0.18	12 (2%)	53	49	19, 69, 110, 111	4 (0%)
All	All	979/990 (98%)	-0.14	31 (3%)	47	43	19, 78, 110, 111	9 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	231	GLY	6.6
1	A	444	GLY	5.8
2	B	3	SER	4.0
1	A	107	THR	3.6
1	A	442	VAL	3.5
2	B	4	PRO	3.4
2	B	2	ILE	3.4
2	B	419	THR	3.4
1	A	550	LYS	3.3
1	A	26	LEU	3.2
2	B	305	GLU	3.1
1	A	134	SER	2.9
2	B	427	TYR	2.8
1	A	357	MET	2.8
1	A	139	THR	2.7
1	A	140	PRO	2.6
1	A	92	LEU	2.5
2	B	266	TRP	2.4
1	A	54	ASN	2.4
2	B	242	GLN	2.4
2	B	210	LEU	2.4
1	A	449	GLU	2.2
1	A	544	GLY	2.2
1	A	135	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	22	LYS	2.1
2	B	189	VAL	2.1
1	A	2	ILE	2.1
1	A	441	TYR	2.1
2	B	359	GLY	2.0
1	A	32	LYS	2.0
1	A	1	PRO	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 monosaccharides in this entry.

6.4 Ligands (i)

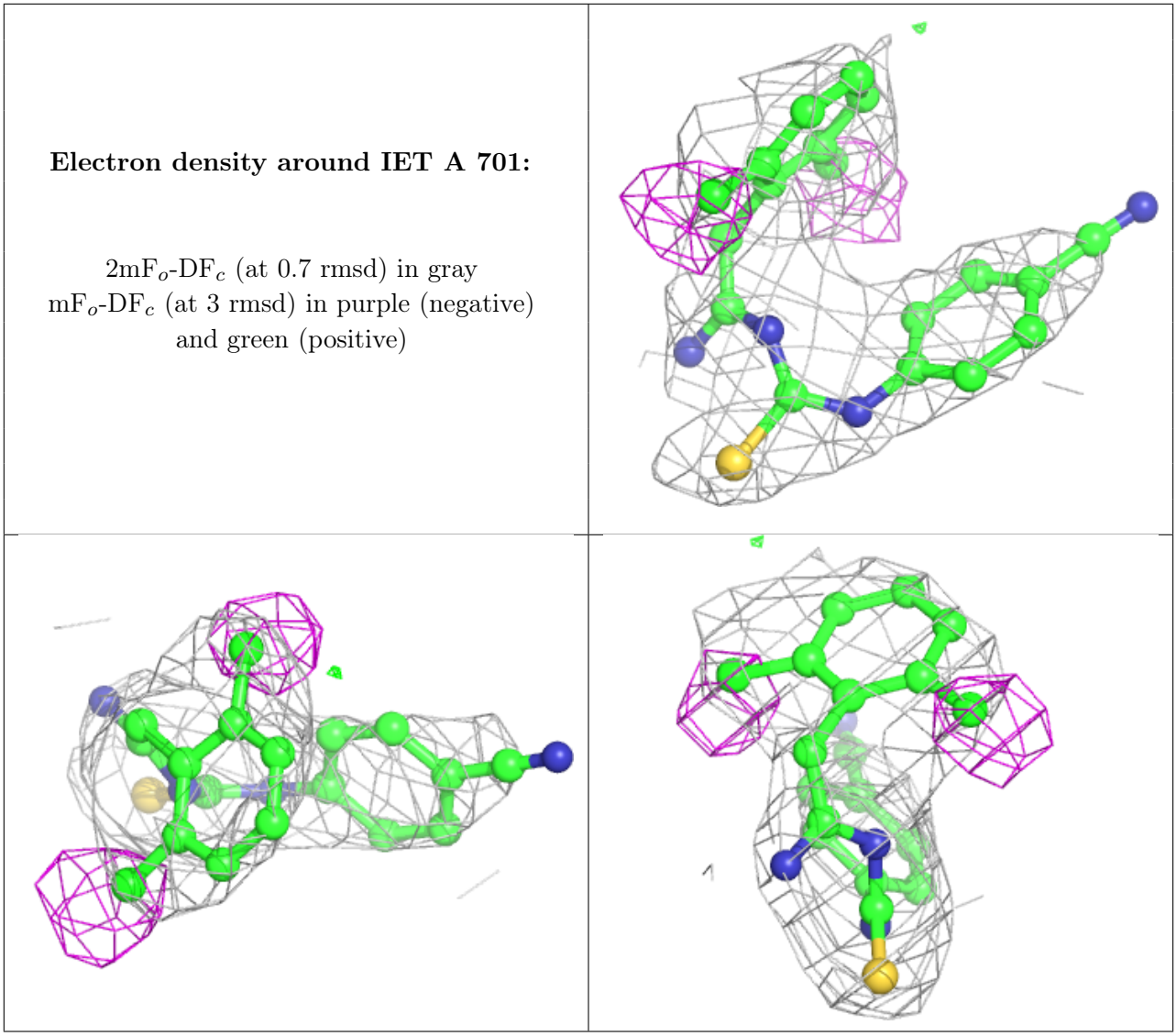
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	IET	A	701	23/23	0.86	0.24	63,78,84,92	0
3	MG	A	601	1/1	0.90	0.14	79,79,79,79	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around IET A 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.