



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 04:53 pm BST

PDB ID : 3IKL
Title : Crystal structure of Pol gB delta-I4.
Authors : Lee, Y.S.; Kennedy, W.D.; Yin, Y.W.
Deposited on : 2009-08-06
Resolution : 3.10 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
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

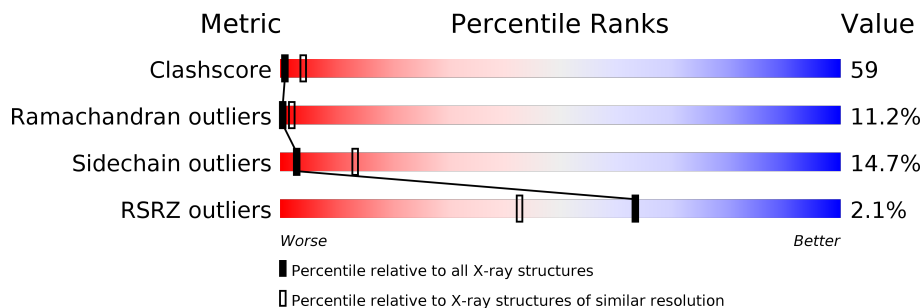
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	459	 2% 22% 44% 12% • 21%
1	B	459	 2% 23% 42% 13% • 21%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5866 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 DNA polymerase subunit gamma-2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	364	2931	1877	515	523	16	0	0	0
1	B	364	2935	1880	517	522	16	0	0	0

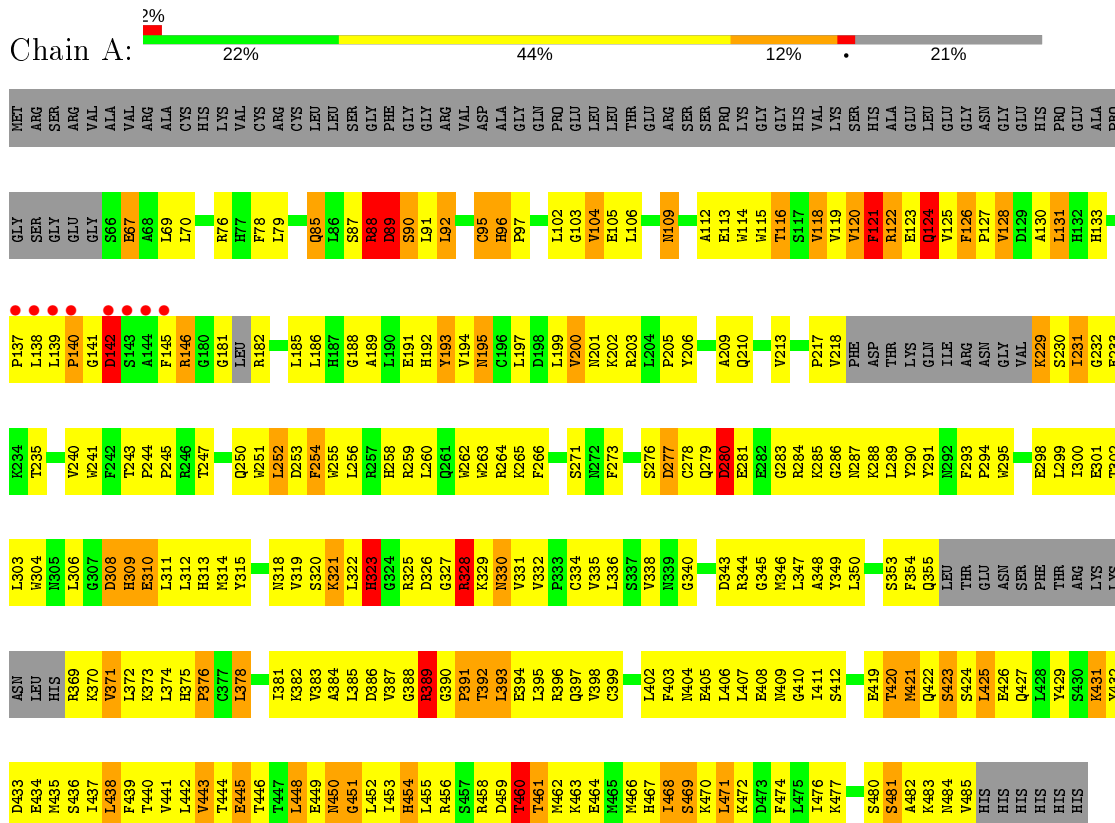
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	180	GLY	-	linker	UNP Q9UHN1
A	181	GLY	-	linker	UNP Q9UHN1
A	486	HIS	-	expression tag	UNP Q9UHN1
A	487	HIS	-	expression tag	UNP Q9UHN1
A	488	HIS	-	expression tag	UNP Q9UHN1
A	489	HIS	-	expression tag	UNP Q9UHN1
A	490	HIS	-	expression tag	UNP Q9UHN1
A	491	HIS	-	expression tag	UNP Q9UHN1
B	180	GLY	-	linker	UNP Q9UHN1
B	181	GLY	-	linker	UNP Q9UHN1
B	486	HIS	-	expression tag	UNP Q9UHN1
B	487	HIS	-	expression tag	UNP Q9UHN1
B	488	HIS	-	expression tag	UNP Q9UHN1
B	489	HIS	-	expression tag	UNP Q9UHN1
B	490	HIS	-	expression tag	UNP Q9UHN1
B	491	HIS	-	expression tag	UNP Q9UHN1

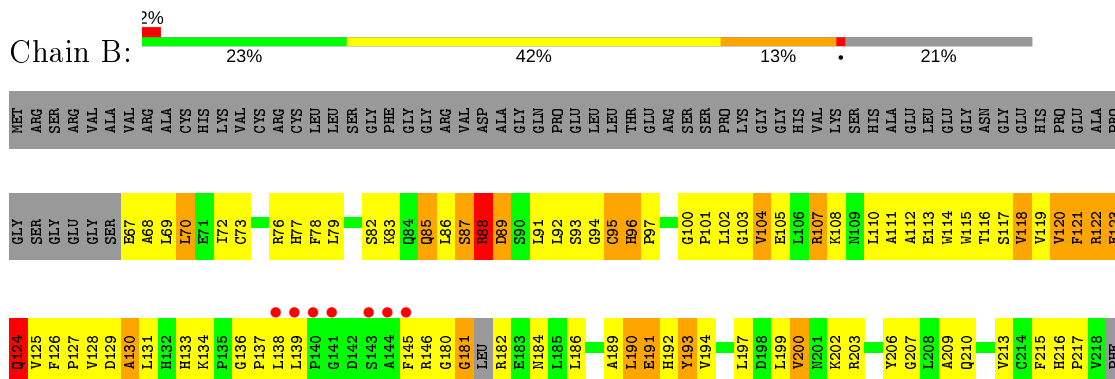
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: DNA polymerase subunit gamma-2, mitochondrial



- Molecule 1: DNA polymerase subunit gamma-2, mitochondrial



V485	HIS
HIS	
HIS	
HIS	
HIS	
HIS	
V413	
W414	
P415	
G416	
Y417	
L418	
E419	
T420	
M421	
Q422	
S423	
S424	
L425	
E426	
Q427	
L428	
K431	
Y432	
D433	
I437	
L438	
F439	
T440	
V441	
L442	
V443	
T444	
E445	
T446	
T447	
L448	
E449	
L452	
I453	
H454	
L455	
R456	
S457	
R458	
D459	
T460	
T461	
M462	
M465	
M466	
K472	
D473	
K477	
Y478	
I479	
S480	
S481	
N484	
A348	
Y351	
D352	
S353	
F354	
Q355	
LEU	
THR	
GLU	
ASN	
SER	
PHE	
THR	
ARG	
LYS	
ASN	
LYS	
LEU	
H366	
R369	
K370	
V371	
L372	
K373	
L374	
H375	
P376	
C377	
L378	
K382	
V383	
A384	
L385	
D386	
V387	
C388	
R389	
G390	
P391	
T392	
L393	
E394	
L395	
R396	
Q397	
V398	
C399	
L402	
F403	
N404	
E405	
L406	
L407	
E408	
I411	
S412	
R284	
K285	
G286	
N287	
K288	
L289	
Y290	
Y291	
P294	
W295	
G296	
K297	
E298	
L299	
I300	
E301	
T302	
L303	
M304	
M305	
L306	
H309	
E310	
L311	
L312	
H313	
M314	
Y315	
M318	
V319	
S320	
K321	
L322	
H323	
G324	
R325	
D326	
G327	
R328	
K329	
M330	
V331	
V332	
P333	
C334	
V335	
L336	
S337	
V338	
N339	
G340	
D341	
R344	
G345	
M346	
L347	
ASP	
THR	
LYS	
GLN	
ILE	
ARG	
ASN	
GLY	
VAL	
K229	
S230	
I231	
G232	
E233	
K234	
V240	
W241	
F242	
T243	
P244	
P245	
R246	
T247	
S248	
N249	
Q250	
W251	
L252	
D253	
F254	
W255	
L256	
R257	
H258	
R259	
L260	
Q261	
W262	
W263	
R264	
K265	
F266	
A267	
L268	
S269	
P270	
S271	
N272	
F273	
S274	
S275	
S276	
D277	
C278	
Q279	
D280	
E281	
G283	

4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	64.43Å 64.43Å 260.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.82 - 3.10 45.82 - 3.10	Depositor EDS
% Data completeness (in resolution range)	74.6 (45.82-3.10) 74.7 (45.82-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 3.12Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.257 , 0.294 0.259 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	56.5	Xtrriage
Anisotropy	0.591	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 14.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.450 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	5866	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.46	0/3006	0.78	1/4067 (0.0%)
1	B	0.46	0/3011	0.76	1/4074 (0.0%)
All	All	0.46	0/6017	0.77	2/8141 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	GLN	N-CA-C	-6.04	94.69	111.00
1	B	455	LEU	CA-CB-CG	5.72	128.46	115.30

There are no chirality outliers.

There are no planarity outliers.

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	2931	0	2915	376	0
1	B	2935	0	2917	326	0
All	All	5866	0	5832	691	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 59.

All (691) 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:231:ILE:H	1:A:231:ILE:HD12	1.16	1.10
1:B:392:THR:HG22	1:B:393:LEU:H	1.24	1.03
1:A:280:ASP:H	1:A:284:ARG:HA	1.23	1.03
1:A:448:LEU:HD23	1:A:448:LEU:H	1.23	1.02
1:A:450:ASN:HD21	1:A:452:LEU:HB2	1.24	1.01
1:B:303:LEU:HG	1:B:338:VAL:HG22	1.43	0.99
1:B:454:HIS:HE1	1:B:465:MET:HG2	1.27	0.99
1:A:88:ARG:HA	1:A:91:LEU:HD12	1.44	0.96
1:A:441:VAL:HG12	1:A:455:LEU:HB3	1.43	0.95
1:B:395:LEU:O	1:B:398:VAL:HG12	1.66	0.94
1:A:320:SER:HA	1:A:323:HIS:NE2	1.81	0.94
1:A:197:LEU:HD11	1:A:202:LYS:HG3	1.48	0.94
1:B:438:LEU:O	1:B:458:ARG:HB2	1.68	0.93
1:A:186:LEU:HD11	1:A:306:LEU:HD11	1.51	0.91
1:A:391:PRO:HD2	1:A:395:LEU:HD21	1.51	0.91
1:A:303:LEU:HD11	1:A:338:VAL:HG13	1.52	0.89
1:A:88:ARG:N	1:A:88:ARG:HD2	1.88	0.88
1:A:201:ASN:HD22	1:A:203:ARG:NH2	1.69	0.88
1:A:369:ARG:HH21	1:A:371:VAL:HG21	1.37	0.88
1:A:388:GLY:O	1:A:390:GLY:N	2.07	0.87
1:B:454:HIS:CE1	1:B:465:MET:HG2	2.10	0.86
1:A:431:LYS:NZ	1:A:431:LYS:HB2	1.92	0.85
1:A:389:ARG:HH11	1:A:444:THR:HG21	1.39	0.84
1:B:121:PHE:O	1:B:122:ARG:HG2	1.78	0.84
1:B:406:LEU:HD12	1:B:406:LEU:H	1.39	0.84
1:B:252:LEU:HB2	1:B:336:LEU:HD11	1.57	0.84
1:B:406:LEU:H	1:B:406:LEU:CD1	1.90	0.83
1:A:450:ASN:ND2	1:A:452:LEU:HB2	1.92	0.83
1:A:67:GLU:HG2	1:A:69:LEU:H	1.42	0.83
1:B:280:ASP:HA	1:B:284:ARG:HH21	1.43	0.83
1:A:393:LEU:HD23	1:A:397:GLN:HG3	1.60	0.83
1:A:256:LEU:HD22	1:A:287:ASN:ND2	1.94	0.82
1:A:421:MET:HG3	1:A:422:GLN:H	1.43	0.82
1:A:201:ASN:HD22	1:A:203:ARG:HH22	1.24	0.82
1:B:445:GLU:C	1:B:447:THR:H	1.82	0.82
1:A:116:THR:HA	1:A:120:VAL:CG2	2.10	0.82
1:A:243:THR:HG23	1:A:334:CYS:HB2	1.62	0.81
1:A:394:GLU:O	1:A:397:GLN:HB2	1.81	0.81
1:B:134:LYS:H	1:B:180:GLY:HA2	1.46	0.81
1:A:381:ILE:HD11	1:A:437:ILE:HD12	1.62	0.81
1:A:448:LEU:HD23	1:A:448:LEU:N	1.96	0.80
1:B:320:SER:HA	1:B:323:HIS:CD2	2.17	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ARG:NH1	1:B:122:ARG:HB3	1.97	0.80
1:A:450:ASN:HD22	1:A:452:LEU:HD23	1.46	0.80
1:B:128:VAL:HG13	1:B:210:GLN:HB2	1.65	0.79
1:A:385:LEU:HD23	1:A:385:LEU:H	1.45	0.79
1:A:419:GLU:HG3	1:A:420:THR:H	1.49	0.77
1:A:231:ILE:CD1	1:A:231:ILE:H	1.96	0.77
1:B:301:GLU:OE2	1:B:340:GLY:HA3	1.85	0.77
1:B:122:ARG:HB3	1:B:122:ARG:HH11	1.48	0.77
1:B:445:GLU:HA	1:B:445:GLU:OE1	1.83	0.77
1:A:353:SER:HB3	1:A:374:LEU:HD23	1.67	0.77
1:B:406:LEU:N	1:B:406:LEU:HD12	1.98	0.77
1:A:396:ARG:HA	1:A:399:CYS:HB2	1.65	0.77
1:B:122:ARG:O	1:B:124:GLN:HG3	1.85	0.77
1:A:455:LEU:HD11	1:A:474:PHE:HE2	1.49	0.77
1:A:231:ILE:HD12	1:A:231:ILE:N	1.97	0.76
1:A:389:ARG:NH1	1:A:444:THR:HG21	1.98	0.76
1:B:373:LYS:HE2	1:B:459:ASP:HA	1.64	0.76
1:A:303:LEU:HG	1:A:338:VAL:HG22	1.66	0.76
1:A:421:MET:CG	1:A:422:GLN:H	1.95	0.76
1:B:477:LYS:HA	1:B:480:SER:HB3	1.68	0.75
1:B:122:ARG:HB2	1:B:124:GLN:NE2	2.00	0.75
1:A:389:ARG:HD2	1:A:444:THR:HB	1.69	0.75
1:B:384:ALA:O	1:B:385:LEU:HB3	1.86	0.75
1:B:229:LYS:HE2	1:B:229:LYS:HA	1.70	0.74
1:B:392:THR:HG22	1:B:393:LEU:N	2.02	0.74
1:A:131:LEU:HD21	1:B:97:PRO:O	1.88	0.74
1:B:280:ASP:O	1:B:281:GLU:HB2	1.87	0.74
1:A:69:LEU:HD13	1:A:354:PHE:CD2	2.23	0.74
1:A:116:THR:HG23	1:A:120:VAL:HG21	1.71	0.73
1:A:280:ASP:N	1:A:284:ARG:HA	2.00	0.73
1:B:389:ARG:HG2	1:B:444:THR:HB	1.69	0.73
1:A:370:LYS:O	1:A:371:VAL:HG12	1.87	0.72
1:B:257:ARG:HB3	1:B:257:ARG:NH2	2.04	0.72
1:B:128:VAL:HG22	1:B:129:ASP:N	2.05	0.71
1:A:441:VAL:CG1	1:A:455:LEU:HB3	2.20	0.71
1:A:444:THR:OG1	1:A:446:THR:HG22	1.91	0.71
1:B:256:LEU:HD22	1:B:287:ASN:ND2	2.06	0.71
1:B:134:LYS:H	1:B:180:GLY:CA	2.03	0.71
1:B:289:LEU:HB2	1:B:301:GLU:HB3	1.72	0.71
1:B:310:GLU:CD	1:B:310:GLU:H	1.94	0.71
1:B:257:ARG:HB3	1:B:257:ARG:HH21	1.54	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:ARG:HA	1:B:329:LYS:O	1.90	0.71
1:B:420:THR:HG23	1:B:421:MET:H	1.54	0.71
1:B:249:ASN:CG	1:B:250:GLN:N	2.44	0.71
1:A:303:LEU:CD1	1:A:338:VAL:HG13	2.20	0.71
1:A:243:THR:HG22	1:A:334:CYS:O	1.91	0.71
1:A:325:ARG:HG2	1:A:325:ARG:HH11	1.56	0.70
1:A:432:TYR:O	1:A:437:ILE:HG12	1.91	0.70
1:A:391:PRO:CD	1:A:395:LEU:HD21	2.21	0.70
1:A:116:THR:HA	1:A:120:VAL:HG23	1.73	0.69
1:A:133:HIS:HA	1:A:181:GLY:HA2	1.74	0.69
1:A:327:GLY:O	1:A:328:ARG:HB2	1.91	0.69
1:B:197:LEU:HD11	1:B:202:LYS:HA	1.72	0.69
1:A:393:LEU:O	1:A:397:GLN:HG2	1.92	0.69
1:A:375:HIS:ND1	1:A:376:PRO:HD2	2.07	0.69
1:B:291:TYR:OH	1:B:352:ASP:HB2	1.91	0.69
1:B:294:PRO:HD2	1:B:295:TRP:CZ3	2.28	0.69
1:B:91:LEU:HD13	1:B:96:HIS:HB3	1.75	0.69
1:A:318:ASN:ND2	1:A:319:VAL:H	1.91	0.69
1:B:420:THR:HG23	1:B:421:MET:N	2.08	0.69
1:A:262:TRP:O	1:A:265:LYS:HB3	1.93	0.69
1:A:231:ILE:HG22	1:A:232:GLY:H	1.59	0.68
1:A:421:MET:HG3	1:A:422:GLN:N	2.07	0.68
1:B:422:GLN:HG3	1:B:423:SER:N	2.07	0.68
1:A:251:TRP:O	1:A:254:PHE:HB3	1.93	0.68
1:A:382:LYS:HD2	1:A:382:LYS:N	2.08	0.68
1:B:260:LEU:HD13	1:B:275:SER:HB3	1.76	0.68
1:A:411:ILE:HD11	1:A:476:ILE:CD1	2.23	0.68
1:A:431:LYS:HZ2	1:A:431:LYS:HB2	1.56	0.68
1:B:416:GLY:O	1:B:418:LEU:N	2.27	0.68
1:A:468:ILE:HD12	1:A:469:SER:N	2.09	0.68
1:B:128:VAL:CG1	1:B:210:GLN:HB2	2.23	0.67
1:B:415:PRO:HB2	1:B:418:LEU:HD13	1.76	0.67
1:A:217:PRO:HB2	1:A:229:LYS:HD3	1.76	0.67
1:A:460:THR:O	1:A:462:MET:N	2.27	0.67
1:B:91:LEU:N	1:B:91:LEU:HD22	2.09	0.67
1:B:112:ALA:O	1:B:116:THR:HG23	1.93	0.67
1:A:393:LEU:HD23	1:A:397:GLN:CG	2.25	0.67
1:B:131:LEU:O	1:B:182:ARG:HD3	1.94	0.67
1:B:460:THR:HB	1:B:462:MET:HG2	1.77	0.67
1:A:92:LEU:HD22	1:A:344:ARG:CZ	2.25	0.66
1:B:405:GLU:O	1:B:408:GLU:HB2	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ARG:HH11	1:A:146:ARG:HA	1.60	0.66
1:A:263:TRP:CZ3	1:A:300:ILE:HD12	2.29	0.66
1:A:450:ASN:ND2	1:A:452:LEU:HD23	2.11	0.66
1:A:420:THR:OG1	1:A:421:MET:N	2.29	0.66
1:B:193:TYR:CZ	1:B:333:PRO:HG3	2.31	0.66
1:B:402:LEU:O	1:B:406:LEU:HD13	1.96	0.66
1:A:453:ILE:HD12	1:A:454:HIS:N	2.09	0.65
1:A:477:LYS:HA	1:A:480:SER:HB3	1.77	0.65
1:A:383:VAL:HG22	1:A:384:ALA:N	2.12	0.65
1:B:445:GLU:O	1:B:447:THR:N	2.30	0.65
1:B:325:ARG:HH11	1:B:325:ARG:HG2	1.61	0.65
1:A:88:ARG:N	1:A:88:ARG:CD	2.53	0.65
1:B:91:LEU:HD22	1:B:91:LEU:H	1.61	0.65
1:B:88:ARG:HD2	1:B:89:ASP:N	2.12	0.64
1:A:123:GLU:O	1:A:124:GLN:HG3	1.97	0.64
1:B:303:LEU:HG	1:B:338:VAL:CG2	2.22	0.64
1:A:325:ARG:NH1	1:A:330:ASN:HD21	1.94	0.64
1:A:96:HIS:CD2	1:A:96:HIS:H	2.15	0.64
1:B:115:TRP:CZ2	1:B:119:VAL:HG11	2.33	0.64
1:B:197:LEU:C	1:B:199:LEU:H	2.00	0.64
1:B:445:GLU:C	1:B:447:THR:N	2.52	0.64
1:A:122:ARG:HG3	1:A:122:ARG:O	1.99	0.64
1:A:448:LEU:CD2	1:A:448:LEU:H	1.91	0.63
1:B:392:THR:CG2	1:B:393:LEU:H	2.05	0.63
1:B:128:VAL:HG12	1:B:209:ALA:O	1.98	0.63
1:A:424:SER:OG	1:A:427:GLN:HG3	1.98	0.63
1:B:424:SER:HB3	1:B:427:GLN:CG	2.28	0.63
1:A:76:ARG:HB3	1:A:435:MET:HG2	1.79	0.63
1:B:145:PHE:CZ	1:B:217:PRO:HB3	2.34	0.63
1:B:457:SER:HB2	1:B:462:MET:HG3	1.80	0.63
1:B:94:GLY:O	1:B:232:GLY:HA2	1.98	0.63
1:B:193:TYR:OH	1:B:333:PRO:HG3	1.97	0.63
1:A:199:LEU:HD21	1:B:101:PRO:HG2	1.81	0.62
1:A:182:ARG:HD2	1:A:213:VAL:O	1.99	0.62
1:A:303:LEU:CD1	1:A:338:VAL:HG22	2.29	0.62
1:A:460:THR:C	1:A:462:MET:H	2.02	0.62
1:A:290:TYR:HD1	1:A:299:LEU:HA	1.63	0.62
1:B:69:LEU:HA	1:B:72:ILE:HD12	1.81	0.62
1:A:404:ASN:O	1:A:408:GLU:HG2	1.99	0.62
1:B:256:LEU:C	1:B:256:LEU:HD12	2.20	0.62
1:B:253:ASP:HB3	1:B:257:ARG:HH12	1.65	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:HIS:ND1	1:B:259:ARG:N	2.48	0.62
1:B:88:ARG:CD	1:B:89:ASP:H	2.13	0.61
1:A:323:HIS:HB2	1:A:331:VAL:C	2.21	0.61
1:A:231:ILE:HB	1:B:133:HIS:NE2	2.16	0.61
1:B:249:ASN:CG	1:B:250:GLN:H	2.03	0.61
1:A:69:LEU:HD13	1:A:354:PHE:CG	2.36	0.61
1:A:325:ARG:NH1	1:A:330:ASN:ND2	2.49	0.61
1:A:422:GLN:HG3	1:A:424:SER:H	1.66	0.61
1:B:252:LEU:HA	1:B:336:LEU:HD21	1.83	0.61
1:A:201:ASN:ND2	1:A:203:ARG:HH22	1.98	0.60
1:A:303:LEU:CG	1:A:338:VAL:HG22	2.31	0.60
1:A:405:GLU:O	1:A:408:GLU:HB2	2.00	0.60
1:B:301:GLU:OE2	1:B:340:GLY:CA	2.49	0.60
1:A:391:PRO:HG2	1:A:395:LEU:HD23	1.83	0.60
1:A:327:GLY:O	1:A:328:ARG:CB	2.49	0.60
1:A:385:LEU:HD23	1:A:385:LEU:N	2.16	0.60
1:A:404:ASN:O	1:A:408:GLU:CG	2.49	0.60
1:A:466:MET:HE1	1:A:471:LEU:HA	1.84	0.60
1:A:389:ARG:HD2	1:A:444:THR:CB	2.31	0.60
1:A:453:ILE:C	1:A:453:ILE:HD12	2.22	0.60
1:A:455:LEU:HD11	1:A:474:PHE:CE2	2.33	0.60
1:A:88:ARG:CA	1:A:91:LEU:HD12	2.26	0.60
1:B:457:SER:OG	1:B:458:ARG:N	2.28	0.60
1:A:199:LEU:HD13	1:B:77:HIS:CD2	2.37	0.60
1:B:107:ARG:HG3	1:B:108:LYS:N	2.17	0.59
1:A:306:LEU:HD12	1:A:335:VAL:HG12	1.83	0.59
1:B:322:LEU:HD23	1:B:322:LEU:N	2.18	0.59
1:A:423:SER:O	1:A:427:GLN:HB2	2.03	0.59
1:B:311:LEU:O	1:B:314:MET:HB2	2.03	0.59
1:A:233:GLU:HG3	1:B:133:HIS:HE1	1.68	0.59
1:A:411:ILE:HD11	1:A:476:ILE:HD13	1.84	0.59
1:B:441:VAL:HG12	1:B:455:LEU:CB	2.32	0.59
1:A:445:GLU:HA	1:A:448:LEU:HD21	1.85	0.59
1:A:262:TRP:O	1:A:265:LYS:CB	2.51	0.58
1:B:376:PRO:C	1:B:378:LEU:H	2.06	0.58
1:A:277:ASP:OD2	1:A:277:ASP:N	2.36	0.58
1:B:286:GLY:HA3	1:B:304:TRP:CE3	2.38	0.58
1:B:325:ARG:NH1	1:B:325:ARG:HG2	2.16	0.58
1:B:331:VAL:HG22	1:B:332:VAL:N	2.18	0.58
1:A:309:HIS:O	1:A:311:LEU:N	2.36	0.58
1:A:432:TYR:CD2	1:A:440:THR:HG23	2.39	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:ILE:O	1:A:469:SER:HB3	2.03	0.58
1:B:290:TYR:CD1	1:B:299:LEU:HA	2.38	0.58
1:B:110:LEU:HD13	1:B:378:LEU:HD11	1.85	0.58
1:A:459:ASP:C	1:A:461:THR:H	2.07	0.58
1:B:447:THR:O	1:B:449:GLU:N	2.37	0.58
1:A:279:GLN:HB3	1:A:285:LYS:H	1.68	0.58
1:A:455:LEU:HD23	1:A:455:LEU:H	1.68	0.58
1:B:453:ILE:HD12	1:B:453:ILE:C	2.23	0.58
1:A:299:LEU:HD23	1:A:299:LEU:C	2.24	0.58
1:A:381:ILE:HA	1:A:412:SER:OG	2.03	0.58
1:A:395:LEU:N	1:A:395:LEU:HD22	2.18	0.58
1:B:371:VAL:HA	1:B:433:ASP:HB3	1.85	0.58
1:A:243:THR:OG1	1:A:244:PRO:HD2	2.03	0.58
1:A:259:ARG:HH21	1:A:301:GLU:CD	2.07	0.58
1:A:310:GLU:O	1:A:313:HIS:HB3	2.04	0.58
1:A:87:SER:O	1:A:89:ASP:N	2.37	0.58
1:B:87:SER:HB2	1:B:88:ARG:CZ	2.34	0.58
1:A:466:MET:CE	1:A:471:LEU:HA	2.34	0.57
1:A:395:LEU:CD2	1:A:395:LEU:H	2.16	0.57
1:A:437:ILE:O	1:A:438:LEU:C	2.42	0.57
1:A:139:LEU:HB2	1:A:140:PRO:HD2	1.86	0.57
1:A:197:LEU:O	1:A:197:LEU:HD12	2.05	0.57
1:B:391:PRO:HG2	1:B:395:LEU:HD13	1.86	0.57
1:A:431:LYS:CG	1:A:432:TYR:N	2.67	0.57
1:B:420:THR:CG2	1:B:421:MET:H	2.14	0.57
1:B:438:LEU:HD23	1:B:458:ARG:NH1	2.19	0.57
1:A:389:ARG:O	1:A:389:ARG:HG2	2.05	0.57
1:A:402:LEU:O	1:A:406:LEU:HD23	2.05	0.57
1:A:306:LEU:HD12	1:A:335:VAL:CG1	2.35	0.57
1:B:180:GLY:O	1:B:181:GLY:C	2.43	0.57
1:B:424:SER:HB3	1:B:427:GLN:CD	2.25	0.57
1:A:244:PRO:HG2	1:A:247:THR:OG1	2.05	0.57
1:A:260:LEU:HD21	1:A:264:ARG:NH2	2.20	0.57
1:B:92:LEU:HD22	1:B:298:GLU:HG2	1.87	0.57
1:A:130:ALA:HB1	1:A:188:GLY:HA3	1.86	0.56
1:B:121:PHE:O	1:B:122:ARG:CG	2.52	0.56
1:B:302:THR:C	1:B:303:LEU:HD12	2.26	0.56
1:A:122:ARG:HH11	1:A:122:ARG:HG2	1.70	0.56
1:B:392:THR:O	1:B:394:GLU:N	2.38	0.56
1:A:321:LYS:C	1:A:322:LEU:HD23	2.26	0.56
1:B:128:VAL:CG2	1:B:129:ASP:N	2.67	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ILE:HG22	1:A:232:GLY:N	2.20	0.56
1:A:411:ILE:HD11	1:A:476:ILE:HD11	1.86	0.56
1:A:456:ARG:HA	1:A:462:MET:O	2.06	0.56
1:B:115:TRP:CE3	1:B:119:VAL:HG21	2.41	0.56
1:B:241:TRP:CD1	1:B:243:THR:CG2	2.88	0.56
1:A:265:LYS:HD2	1:A:266:PHE:CZ	2.40	0.56
1:A:309:HIS:O	1:A:310:GLU:C	2.44	0.56
1:A:381:ILE:CD1	1:A:437:ILE:HD12	2.32	0.56
1:B:116:THR:HA	1:B:120:VAL:CG2	2.35	0.56
1:B:251:TRP:O	1:B:254:PHE:HB3	2.05	0.56
1:B:120:VAL:HG12	1:B:121:PHE:N	2.20	0.56
1:B:280:ASP:HA	1:B:284:ARG:NH2	2.17	0.56
1:B:384:ALA:HB2	1:B:437:ILE:HG21	1.87	0.56
1:A:432:TYR:HD2	1:A:440:THR:HG23	1.71	0.56
1:B:122:ARG:HB2	1:B:124:GLN:HE21	1.71	0.56
1:A:460:THR:OG1	1:A:462:MET:HB2	2.06	0.56
1:A:123:GLU:C	1:A:124:GLN:HG3	2.26	0.56
1:B:382:LYS:HE3	1:B:479:ILE:HD13	1.88	0.56
1:B:252:LEU:C	1:B:252:LEU:HD13	2.26	0.55
1:A:445:GLU:O	1:A:448:LEU:HG	2.05	0.55
1:A:450:ASN:CG	1:A:451:GLY:H	2.09	0.55
1:B:428:LEU:N	1:B:428:LEU:HD12	2.22	0.55
1:B:189:ALA:CB	1:B:240:VAL:HG21	2.36	0.55
1:B:100:GLY:O	1:B:104:VAL:HG23	2.07	0.55
1:B:128:VAL:HG22	1:B:129:ASP:H	1.71	0.55
1:B:88:ARG:O	1:B:91:LEU:N	2.40	0.55
1:A:325:ARG:HH12	1:A:330:ASN:HD21	1.53	0.55
1:A:395:LEU:N	1:A:395:LEU:CD2	2.70	0.55
1:B:111:ALA:O	1:B:114:TRP:HB3	2.06	0.55
1:A:102:LEU:N	1:A:102:LEU:HD12	2.22	0.55
1:A:424:SER:OG	1:A:425:LEU:N	2.39	0.55
1:A:87:SER:HB3	1:A:88:ARG:NH2	2.22	0.55
1:B:472:LYS:HD3	1:B:473:ASP:N	2.21	0.55
1:A:113:GLU:HG2	1:A:266:PHE:CZ	2.41	0.55
1:B:395:LEU:C	1:B:397:GLN:H	2.10	0.55
1:B:405:GLU:HB3	1:B:406:LEU:HD12	1.89	0.55
1:B:86:LEU:N	1:B:86:LEU:HD22	2.22	0.55
1:A:197:LEU:HD21	1:A:202:LYS:HE3	1.89	0.54
1:B:113:GLU:OE2	1:B:266:PHE:HZ	1.90	0.54
1:A:105:GLU:O	1:A:109:ASN:HB2	2.07	0.54
1:A:381:ILE:HG13	1:A:381:ILE:O	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:PRO:HG2	1:A:395:LEU:CD2	2.37	0.54
1:B:122:ARG:HH11	1:B:122:ARG:CB	2.17	0.54
1:A:273:PHE:CE1	1:A:291:TYR:HD1	2.25	0.54
1:A:419:GLU:HG3	1:A:420:THR:N	2.19	0.54
1:B:128:VAL:CG2	1:B:129:ASP:H	2.21	0.54
1:B:87:SER:HB2	1:B:88:ARG:NE	2.22	0.54
1:A:78:PHE:CE1	1:A:102:LEU:HB3	2.43	0.54
1:A:197:LEU:HD12	1:A:202:LYS:HA	1.89	0.54
1:A:435:MET:HB3	1:A:437:ILE:HD11	1.89	0.54
1:B:441:VAL:HG12	1:B:455:LEU:HB2	1.89	0.54
1:B:69:LEU:HD13	1:B:354:PHE:CD2	2.43	0.54
1:B:88:ARG:HD2	1:B:89:ASP:H	1.70	0.54
1:A:116:THR:HA	1:A:120:VAL:HG21	1.89	0.54
1:A:286:GLY:HA3	1:A:304:TRP:CE3	2.43	0.54
1:A:323:HIS:HB3	1:A:332:VAL:HG22	1.90	0.54
1:A:67:GLU:HG2	1:A:69:LEU:N	2.19	0.54
1:B:114:TRP:O	1:B:117:SER:HB3	2.08	0.54
1:B:91:LEU:O	1:B:92:LEU:C	2.47	0.54
1:A:127:PRO:HB2	1:B:104:VAL:HG11	1.90	0.54
1:B:303:LEU:HD12	1:B:303:LEU:N	2.22	0.54
1:A:145:PHE:HE2	1:A:229:LYS:HD2	1.73	0.53
1:A:260:LEU:HD13	1:A:289:LEU:HD12	1.90	0.53
1:A:145:PHE:HE2	1:A:229:LYS:HZ3	1.56	0.53
1:A:373:LYS:HA	1:A:458:ARG:CZ	2.38	0.53
1:A:320:SER:C	1:A:322:LEU:H	2.11	0.53
1:A:466:MET:CE	1:A:471:LEU:HD22	2.39	0.53
1:B:87:SER:OG	1:B:88:ARG:CZ	2.56	0.53
1:A:321:LYS:O	1:A:322:LEU:HD23	2.07	0.53
1:A:431:LYS:HZ3	1:A:431:LYS:HB2	1.72	0.53
1:B:252:LEU:O	1:B:252:LEU:HD13	2.08	0.53
1:B:95:CYS:O	1:B:96:HIS:C	2.47	0.53
1:A:243:THR:CG2	1:A:334:CYS:HB2	2.37	0.53
1:B:192:HIS:O	1:B:194:VAL:N	2.42	0.53
1:B:351:TYR:C	1:B:353:SER:H	2.12	0.53
1:A:320:SER:O	1:A:322:LEU:N	2.42	0.53
1:A:455:LEU:O	1:A:463:LYS:HA	2.09	0.53
1:B:193:TYR:O	1:B:197:LEU:HB2	2.08	0.53
1:A:320:SER:HA	1:A:323:HIS:CE1	2.43	0.52
1:A:199:LEU:CD2	1:B:101:PRO:HG2	2.39	0.52
1:B:121:PHE:C	1:B:122:ARG:HG2	2.30	0.52
1:A:279:GLN:CB	1:A:285:LYS:H	2.22	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:LEU:HD12	1:B:385:LEU:C	2.30	0.52
1:A:394:GLU:C	1:A:397:GLN:HB2	2.30	0.52
1:A:126:PHE:HB3	1:A:127:PRO:HD2	1.91	0.52
1:B:289:LEU:HD12	1:B:301:GLU:HG2	1.90	0.52
1:B:368:HIS:HB3	1:B:370:LYS:HE2	1.90	0.52
1:B:115:TRP:CE2	1:B:119:VAL:HG11	2.44	0.52
1:A:407:LEU:HD23	1:A:411:ILE:O	2.10	0.52
1:A:468:ILE:O	1:A:469:SER:CB	2.57	0.52
1:B:116:THR:HA	1:B:120:VAL:HG23	1.91	0.52
1:B:332:VAL:CG1	1:B:333:PRO:HD2	2.40	0.52
1:A:120:VAL:O	1:A:121:PHE:C	2.48	0.52
1:B:252:LEU:CB	1:B:336:LEU:HD11	2.35	0.52
1:B:438:LEU:HA	1:B:458:ARG:HD3	1.92	0.52
1:A:146:ARG:NH1	1:A:146:ARG:O	2.43	0.52
1:A:460:THR:C	1:A:462:MET:N	2.61	0.51
1:A:405:GLU:OE2	1:A:472:LYS:HB2	2.10	0.51
1:A:218:VAL:C	1:A:229:LYS:HG3	2.30	0.51
1:A:369:ARG:HE	1:A:371:VAL:CG1	2.23	0.51
1:A:397:GLN:OE1	1:A:397:GLN:HA	2.09	0.51
1:B:421:MET:O	1:B:422:GLN:C	2.48	0.51
1:A:146:ARG:CA	1:A:146:ARG:HH11	2.24	0.51
1:A:369:ARG:NH2	1:A:458:ARG:O	2.40	0.51
1:B:114:TRP:O	1:B:117:SER:N	2.40	0.51
1:B:321:LYS:HG2	1:B:321:LYS:O	2.09	0.51
1:B:87:SER:H	1:B:91:LEU:HD21	1.75	0.51
1:B:369:ARG:HH11	1:B:369:ARG:HG3	1.74	0.51
1:A:369:ARG:NH2	1:A:371:VAL:HG21	2.16	0.51
1:B:251:TRP:HA	1:B:254:PHE:HB3	1.92	0.51
1:B:389:ARG:HG2	1:B:389:ARG:O	2.10	0.51
1:A:450:ASN:ND2	1:A:452:LEU:CB	2.71	0.51
1:A:471:LEU:O	1:A:474:PHE:HB3	2.10	0.51
1:B:287:ASN:HB2	1:B:303:LEU:HB2	1.91	0.51
1:B:424:SER:HB3	1:B:427:GLN:HB2	1.93	0.51
1:B:87:SER:CB	1:B:88:ARG:CZ	2.88	0.51
1:A:410:GLY:O	1:A:411:ILE:HD13	2.10	0.51
1:A:470:LYS:HE2	1:A:470:LYS:HA	1.92	0.51
1:A:309:HIS:O	1:A:312:LEU:N	2.41	0.51
1:B:87:SER:O	1:B:88:ARG:C	2.50	0.51
1:B:297:LYS:O	1:B:298:GLU:OE1	2.29	0.50
1:A:116:THR:CG2	1:A:120:VAL:HG21	2.41	0.50
1:A:484:ASN:O	1:A:485:VAL:C	2.50	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:VAL:HG12	1:A:121:PHE:N	2.24	0.50
1:A:76:ARG:HG3	1:A:434:GLU:O	2.11	0.50
1:B:182:ARG:NH2	1:B:213:VAL:O	2.32	0.50
1:A:128:VAL:HG12	1:A:209:ALA:O	2.11	0.50
1:A:302:THR:O	1:A:303:LEU:HD12	2.11	0.50
1:A:456:ARG:HH11	1:A:456:ARG:HG2	1.77	0.50
1:B:253:ASP:C	1:B:257:ARG:NH1	2.64	0.50
1:B:306:LEU:HB2	1:B:335:VAL:HG23	1.92	0.50
1:A:189:ALA:CB	1:A:240:VAL:HG21	2.42	0.50
1:A:456:ARG:HG2	1:A:456:ARG:NH1	2.27	0.50
1:B:345:GLY:O	1:B:348:ALA:N	2.44	0.50
1:A:197:LEU:CD1	1:A:202:LYS:HG3	2.33	0.50
1:A:326:ASP:C	1:A:326:ASP:OD1	2.49	0.50
1:A:419:GLU:HG3	1:A:420:THR:HG22	1.94	0.50
1:B:73:CYS:O	1:B:78:PHE:HB2	2.11	0.50
1:A:114:TRP:O	1:A:118:VAL:HG13	2.11	0.50
1:A:325:ARG:NH1	1:A:325:ARG:HG2	2.25	0.50
1:A:320:SER:C	1:A:322:LEU:N	2.65	0.49
1:A:466:MET:HG2	1:A:467:HIS:N	2.27	0.49
1:B:389:ARG:CG	1:B:389:ARG:O	2.59	0.49
1:A:306:LEU:HB2	1:A:335:VAL:HB	1.94	0.49
1:A:345:GLY:O	1:A:348:ALA:N	2.44	0.49
1:B:318:ASN:ND2	1:B:318:ASN:N	2.59	0.49
1:B:136:GLY:O	1:B:138:LEU:HD22	2.12	0.49
1:B:281:GLU:C	1:B:283:GLY:H	2.15	0.49
1:B:110:LEU:CD1	1:B:378:LEU:HD11	2.42	0.49
1:A:310:GLU:O	1:A:313:HIS:N	2.46	0.49
1:B:371:VAL:CA	1:B:433:ASP:HB3	2.41	0.49
1:B:460:THR:O	1:B:462:MET:N	2.45	0.49
1:B:254:PHE:CD2	1:B:255:TRP:N	2.81	0.49
1:B:386:ASP:HB3	1:B:417:TYR:N	2.28	0.49
1:B:134:LYS:N	1:B:180:GLY:HA2	2.21	0.49
1:B:277:ASP:HA	1:B:287:ASN:OD1	2.12	0.49
1:A:252:LEU:HD11	1:A:287:ASN:HD22	1.78	0.49
1:B:421:MET:O	1:B:423:SER:N	2.45	0.49
1:A:383:VAL:CG2	1:A:384:ALA:N	2.76	0.49
1:B:437:ILE:O	1:B:438:LEU:C	2.51	0.49
1:B:255:TRP:O	1:B:256:LEU:C	2.51	0.48
1:B:314:MET:HE1	1:B:315:TYR:OH	2.13	0.48
1:B:405:GLU:O	1:B:408:GLU:N	2.46	0.48
1:B:78:PHE:C	1:B:79:LEU:HD22	2.34	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:SER:O	1:B:88:ARG:HD2	2.13	0.48
1:A:106:LEU:HD12	1:A:106:LEU:O	2.14	0.48
1:B:424:SER:O	1:B:428:LEU:CD1	2.61	0.48
1:A:254:PHE:CD2	1:A:255:TRP:N	2.81	0.48
1:A:459:ASP:O	1:A:461:THR:N	2.46	0.48
1:B:416:GLY:HA2	1:B:419:GLU:OE1	2.13	0.48
1:B:415:PRO:HB2	1:B:418:LEU:CD1	2.44	0.48
1:B:441:VAL:HG12	1:B:455:LEU:HB3	1.94	0.48
1:A:266:PHE:HB2	1:A:349:TYR:CE1	2.49	0.48
1:A:420:THR:HG23	1:A:421:MET:N	2.28	0.48
1:B:256:LEU:HG	1:B:257:ARG:N	2.29	0.48
1:B:415:PRO:O	1:B:418:LEU:HD13	2.14	0.48
1:A:451:GLY:O	1:A:467:HIS:HA	2.13	0.48
1:B:137:PRO:O	1:B:138:LEU:HD13	2.14	0.48
1:B:280:ASP:CA	1:B:284:ARG:HH21	2.22	0.48
1:A:314:MET:HG2	1:A:315:TYR:CE1	2.48	0.48
1:A:372:LEU:HD12	1:A:434:GLU:C	2.34	0.48
1:A:186:LEU:HD11	1:A:306:LEU:CD1	2.35	0.48
1:B:290:TYR:HD1	1:B:299:LEU:HA	1.77	0.48
1:B:373:LYS:HE2	1:B:459:ASP:CA	2.40	0.48
1:A:200:VAL:C	1:A:202:LYS:N	2.67	0.47
1:B:77:HIS:O	1:B:102:LEU:HB2	2.13	0.47
1:A:189:ALA:HB3	1:A:240:VAL:HG21	1.96	0.47
1:B:286:GLY:HA2	1:B:303:LEU:O	2.14	0.47
1:B:452:LEU:CD2	1:B:452:LEU:N	2.77	0.47
1:B:102:LEU:O	1:B:103:GLY:C	2.52	0.47
1:B:326:ASP:O	1:B:329:LYS:HB2	2.14	0.47
1:A:87:SER:O	1:A:88:ARG:C	2.53	0.47
1:B:190:LEU:C	1:B:192:HIS:H	2.16	0.47
1:B:256:LEU:HB2	1:B:287:ASN:HD22	1.79	0.47
1:A:255:TRP:O	1:A:256:LEU:C	2.52	0.47
1:A:382:LYS:N	1:A:412:SER:OG	2.46	0.47
1:A:306:LEU:HB2	1:A:335:VAL:O	2.14	0.47
1:A:394:GLU:HA	1:A:394:GLU:OE2	2.14	0.47
1:A:477:LYS:O	1:A:481:SER:HB3	2.14	0.47
1:A:130:ALA:HB3	1:A:210:GLN:HE22	1.79	0.47
1:A:288:LYS:HD3	1:A:299:LEU:HD12	1.97	0.47
1:A:371:VAL:HG23	1:A:433:ASP:HB3	1.96	0.47
1:A:437:ILE:O	1:A:439:PHE:N	2.48	0.47
1:A:459:ASP:C	1:A:461:THR:N	2.67	0.47
1:A:121:PHE:CD2	1:A:121:PHE:N	2.77	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:HIS:O	1:A:194:VAL:N	2.48	0.47
1:A:308:ASP:O	1:A:309:HIS:O	2.32	0.47
1:A:390:GLY:HA2	1:A:445:GLU:HB3	1.97	0.47
1:B:332:VAL:HG13	1:B:333:PRO:HD2	1.97	0.47
1:B:145:PHE:CE1	1:B:217:PRO:HB3	2.48	0.47
1:B:88:ARG:O	1:B:89:ASP:C	2.53	0.47
1:A:385:LEU:HB3	1:A:441:VAL:HG23	1.97	0.47
1:B:234:LYS:HD3	1:B:341:ASP:OD2	2.15	0.47
1:A:88:ARG:H	1:A:88:ARG:CD	2.24	0.47
1:B:115:TRP:HH2	1:B:127:PRO:HB3	1.80	0.47
1:B:385:LEU:HD12	1:B:385:LEU:O	2.14	0.47
1:B:387:VAL:HG12	1:B:443:VAL:HG12	1.97	0.47
1:B:120:VAL:HG12	1:B:121:PHE:CD2	2.50	0.46
1:B:458:ARG:HB3	1:B:459:ASP:H	1.59	0.46
1:A:259:ARG:NH2	1:A:301:GLU:OE2	2.38	0.46
1:A:429:TYR:CE2	1:A:456:ARG:HD3	2.51	0.46
1:A:463:LYS:HD2	1:A:463:LYS:N	2.30	0.46
1:A:229:LYS:HG2	1:A:230:SER:N	2.30	0.46
1:B:370:LYS:O	1:B:371:VAL:O	2.32	0.46
1:A:291:TYR:CG	1:A:348:ALA:HB1	2.51	0.46
1:A:266:PHE:HB2	1:A:349:TYR:HE1	1.80	0.46
1:A:89:ASP:O	1:A:91:LEU:N	2.49	0.46
1:A:381:ILE:HD11	1:A:437:ILE:CD1	2.42	0.46
1:B:244:PRO:HG2	1:B:247:THR:OG1	2.16	0.46
1:B:258:HIS:ND1	1:B:258:HIS:C	2.69	0.46
1:B:447:THR:O	1:B:448:LEU:C	2.53	0.46
1:A:141:GLY:O	1:A:142:ASP:O	2.34	0.46
1:B:197:LEU:HD21	1:B:202:LYS:HG3	1.98	0.46
1:A:95:CYS:SG	1:A:218:VAL:HG21	2.56	0.46
1:B:422:GLN:CG	1:B:423:SER:N	2.77	0.46
1:A:244:PRO:O	1:A:245:PRO:C	2.53	0.46
1:A:303:LEU:HD11	1:A:338:VAL:CG1	2.36	0.46
1:A:468:ILE:HD12	1:A:468:ILE:C	2.35	0.46
1:B:125:VAL:HA	1:B:207:GLY:O	2.15	0.46
1:A:112:ALA:O	1:A:116:THR:OG1	2.33	0.46
1:A:392:THR:O	1:A:393:LEU:C	2.54	0.46
1:B:369:ARG:HG3	1:B:369:ARG:NH1	2.31	0.46
1:B:376:PRO:C	1:B:378:LEU:N	2.69	0.46
1:A:392:THR:HG22	1:A:393:LEU:N	2.31	0.46
1:A:481:SER:O	1:A:482:ALA:C	2.54	0.46
1:B:318:ASN:HD22	1:B:318:ASN:N	2.13	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:THR:HB	1:B:462:MET:CG	2.45	0.46
1:A:293:PHE:O	1:A:295:TRP:N	2.50	0.45
1:A:290:TYR:CD1	1:A:299:LEU:HA	2.49	0.45
1:A:301:GLU:OE2	1:A:340:GLY:HA3	2.16	0.45
1:A:369:ARG:HE	1:A:371:VAL:HG11	1.81	0.45
1:B:455:LEU:HD12	1:B:455:LEU:O	2.16	0.45
1:B:460:THR:HB	1:B:462:MET:SD	2.56	0.45
1:A:128:VAL:HG23	1:A:192:HIS:CD2	2.52	0.45
1:A:318:ASN:OD1	1:A:320:SER:HB2	2.16	0.45
1:B:126:PHE:HB3	1:B:127:PRO:HD2	1.97	0.45
1:B:197:LEU:C	1:B:199:LEU:N	2.69	0.45
1:A:115:TRP:CZ2	1:A:119:VAL:HG11	2.51	0.45
1:A:119:VAL:O	1:A:123:GLU:HG3	2.15	0.45
1:A:263:TRP:CH2	1:A:300:ILE:HD12	2.51	0.45
1:A:454:HIS:N	1:A:454:HIS:ND1	2.63	0.45
1:A:481:SER:OG	1:A:482:ALA:N	2.46	0.45
1:B:424:SER:O	1:B:428:LEU:HD13	2.17	0.45
1:B:437:ILE:HG22	1:B:439:PHE:O	2.16	0.45
1:B:465:MET:O	1:B:466:MET:HB2	2.16	0.45
1:A:255:TRP:O	1:A:258:HIS:HB3	2.17	0.45
1:A:394:GLU:O	1:A:398:VAL:HG12	2.16	0.45
1:A:403:PHE:HZ	1:B:123:GLU:HB2	1.82	0.45
1:B:320:SER:HA	1:B:323:HIS:NE2	2.31	0.45
1:A:218:VAL:C	1:A:229:LYS:CG	2.85	0.45
1:A:279:GLN:HB2	1:A:284:ARG:HA	1.99	0.45
1:B:305:ASN:HB2	1:B:336:LEU:HD12	1.99	0.45
1:B:420:THR:O	1:B:422:GLN:N	2.50	0.45
1:B:426:GLU:OE1	1:B:426:GLU:HA	2.17	0.45
1:A:281:GLU:OE2	1:A:304:TRP:CD1	2.70	0.45
1:A:395:LEU:C	1:A:397:GLN:H	2.20	0.45
1:A:89:ASP:O	1:A:90:SER:C	2.55	0.45
1:B:263:TRP:CZ3	1:B:300:ILE:HD12	2.51	0.45
1:A:313:HIS:C	1:A:313:HIS:CD2	2.90	0.45
1:A:394:GLU:HA	1:A:397:GLN:HB2	1.99	0.45
1:A:205:PRO:HG3	1:A:251:TRP:CZ2	2.52	0.45
1:A:326:ASP:HB3	1:A:329:LYS:O	2.16	0.45
1:A:126:PHE:N	1:A:126:PHE:CD1	2.84	0.45
1:B:115:TRP:CH2	1:B:127:PRO:HB3	2.52	0.45
1:A:137:PRO:O	1:A:138:LEU:HG	2.17	0.44
1:A:145:PHE:CE2	1:A:229:LYS:HD2	2.51	0.44
1:A:318:ASN:ND2	1:A:319:VAL:N	2.60	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:ARG:HG3	1:A:370:LYS:H	1.82	0.44
1:B:191:GLU:N	1:B:314:MET:HE2	2.32	0.44
1:B:264:ARG:HB3	1:B:270:PRO:HB3	1.99	0.44
1:A:254:PHE:O	1:A:255:TRP:C	2.56	0.44
1:A:299:LEU:O	1:A:344:ARG:HD2	2.17	0.44
1:B:256:LEU:O	1:B:256:LEU:HD12	2.16	0.44
1:B:392:THR:HG22	1:B:393:LEU:HD22	1.98	0.44
1:A:241:TRP:HB3	1:A:336:LEU:HD22	2.00	0.44
1:A:409:ASN:ND2	1:A:472:LYS:HD2	2.32	0.44
1:B:73:CYS:CB	1:B:79:LEU:HD23	2.48	0.44
1:A:85:GLN:HG2	1:A:85:GLN:H	1.49	0.44
1:B:200:VAL:O	1:B:203:ARG:HG3	2.17	0.44
1:B:73:CYS:HB3	1:B:79:LEU:HD23	2.00	0.44
1:B:266:PHE:HB3	1:B:378:LEU:HD22	2.00	0.44
1:B:264:ARG:HB3	1:B:270:PRO:CB	2.47	0.44
1:B:290:TYR:HE1	1:B:299:LEU:HB2	1.83	0.44
1:B:319:VAL:O	1:B:319:VAL:HG22	2.17	0.44
1:B:396:ARG:HA	1:B:399:CYS:HB2	2.00	0.44
1:B:402:LEU:O	1:B:403:PHE:C	2.55	0.44
1:B:93:SER:O	1:B:94:GLY:C	2.54	0.44
1:A:259:ARG:O	1:A:262:TRP:HB3	2.18	0.44
1:A:306:LEU:HB3	1:A:310:GLU:OE1	2.18	0.44
1:A:369:ARG:CG	1:A:370:LYS:N	2.80	0.44
1:A:431:LYS:HA	1:A:434:GLU:HB2	2.00	0.44
1:A:130:ALA:CB	1:A:210:GLN:HE22	2.30	0.44
1:A:322:LEU:O	1:A:323:HIS:HD2	2.01	0.44
1:A:76:ARG:HB3	1:A:435:MET:CG	2.46	0.44
1:B:259:ARG:O	1:B:263:TRP:HD1	2.00	0.44
1:B:190:LEU:C	1:B:314:MET:HE2	2.39	0.44
1:B:82:SER:OG	1:B:83:LYS:N	2.51	0.44
1:A:195:ASN:C	1:A:197:LEU:H	2.21	0.44
1:A:393:LEU:HD21	1:A:397:GLN:HE21	1.83	0.44
1:B:197:LEU:CD1	1:B:202:LYS:HA	2.45	0.44
1:B:252:LEU:C	1:B:252:LEU:CD1	2.86	0.44
1:B:424:SER:HB3	1:B:427:GLN:CB	2.48	0.44
1:A:252:LEU:O	1:A:253:ASP:C	2.56	0.43
1:A:403:PHE:CZ	1:B:123:GLU:HB2	2.53	0.43
1:B:122:ARG:O	1:B:124:GLN:N	2.51	0.43
1:B:395:LEU:C	1:B:397:GLN:N	2.71	0.43
1:A:106:LEU:HG	1:A:346:MET:HG2	1.99	0.43
1:A:443:VAL:HG22	1:A:453:ILE:HG22	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:HIS:O	1:A:470:LYS:HB2	2.18	0.43
1:B:130:ALA:CB	1:B:210:GLN:HE22	2.31	0.43
1:B:259:ARG:HA	1:B:259:ARG:HD2	1.72	0.43
1:B:347:LEU:HA	1:B:347:LEU:HD23	1.62	0.43
1:B:472:LYS:C	1:B:472:LYS:HD3	2.39	0.43
1:A:231:ILE:HD13	1:B:133:HIS:CD2	2.53	0.43
1:A:350:LEU:HA	1:A:350:LEU:HD23	1.72	0.43
1:B:130:ALA:HB3	1:B:210:GLN:HE22	1.83	0.43
1:A:200:VAL:O	1:A:202:LYS:N	2.52	0.43
1:A:432:TYR:HD2	1:A:440:THR:CG2	2.31	0.43
1:B:92:LEU:CD2	1:B:298:GLU:HG2	2.47	0.43
1:B:439:PHE:HD1	1:B:456:ARG:O	2.01	0.43
1:B:87:SER:H	1:B:91:LEU:CD2	2.31	0.43
1:B:95:CYS:O	1:B:96:HIS:O	2.35	0.43
1:A:103:GLY:O	1:A:104:VAL:C	2.57	0.43
1:A:441:VAL:HG11	1:A:471:LEU:HD21	2.00	0.43
1:B:215:PHE:CD1	1:B:215:PHE:N	2.86	0.43
1:B:286:GLY:CA	1:B:303:LEU:O	2.66	0.43
1:B:373:LYS:HA	1:B:458:ARG:NH2	2.33	0.43
1:A:96:HIS:H	1:A:96:HIS:HD2	1.61	0.43
1:A:235:THR:N	1:A:343:ASP:OD2	2.38	0.43
1:A:436:SER:C	1:A:437:ILE:HD13	2.38	0.43
1:A:102:LEU:CD1	1:A:102:LEU:N	2.80	0.43
1:A:393:LEU:C	1:A:397:GLN:HG2	2.38	0.43
1:A:450:ASN:N	1:A:450:ASN:OD1	2.51	0.43
1:A:466:MET:CG	1:A:467:HIS:N	2.82	0.43
1:B:108:LYS:O	1:B:111:ALA:HB3	2.19	0.43
1:B:118:VAL:HG13	1:B:119:VAL:H	1.84	0.43
1:B:87:SER:C	1:B:88:ARG:HD2	2.38	0.43
1:A:381:ILE:CG1	1:A:437:ILE:HD12	2.49	0.43
1:B:299:LEU:HD13	1:B:299:LEU:C	2.39	0.43
1:B:82:SER:N	1:B:85:GLN:OE1	2.42	0.43
1:A:466:MET:HE1	1:A:471:LEU:HD13	2.00	0.42
1:B:331:VAL:CG2	1:B:332:VAL:N	2.80	0.42
1:B:252:LEU:HD23	1:B:336:LEU:HD11	2.01	0.42
1:B:406:LEU:HB3	1:B:411:ILE:HB	2.00	0.42
1:A:122:ARG:CG	1:A:122:ARG:O	2.67	0.42
1:A:87:SER:C	1:A:88:ARG:HD2	2.38	0.42
1:B:265:LYS:HB2	1:B:265:LYS:HE3	1.90	0.42
1:B:287:ASN:N	1:B:303:LEU:O	2.51	0.42
1:B:278:CYS:SG	1:B:304:TRP:CZ2	3.12	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:LEU:O	1:B:374:LEU:N	2.52	0.42
1:B:289:LEU:CB	1:B:301:GLU:HB3	2.45	0.42
1:B:281:GLU:OE1	1:B:304:TRP:CE2	2.72	0.42
1:B:397:GLN:HG2	1:B:397:GLN:O	2.13	0.42
1:A:354:PHE:CG	1:A:355:GLN:N	2.87	0.42
1:B:87:SER:N	1:B:91:LEU:HD21	2.35	0.42
1:A:322:LEU:O	1:A:323:HIS:C	2.58	0.42
1:A:431:LYS:HG2	1:A:432:TYR:N	2.34	0.42
1:B:119:VAL:HG22	1:B:209:ALA:HB3	2.01	0.42
1:A:188:GLY:HA2	1:A:191:GLU:OE2	2.20	0.42
1:A:372:LEU:CB	1:A:436:SER:HB2	2.49	0.42
1:A:407:LEU:HD13	1:B:120:VAL:HG12	2.01	0.42
1:A:407:LEU:O	1:A:408:GLU:C	2.58	0.42
1:B:258:HIS:O	1:B:261:GLN:N	2.53	0.42
1:B:107:ARG:HG2	1:B:107:ARG:HH11	1.85	0.42
1:B:193:TYR:O	1:B:193:TYR:CD1	2.73	0.42
1:B:269:SER:HB2	1:B:272:ASN:HD22	1.84	0.42
1:A:139:LEU:CD1	1:A:142:ASP:HB2	2.50	0.42
1:A:385:LEU:CB	1:A:441:VAL:HG23	2.49	0.42
1:A:481:SER:O	1:A:483:LYS:N	2.53	0.42
1:B:186:LEU:HD21	1:B:306:LEU:HD11	2.01	0.42
1:B:481:SER:O	1:B:484:ASN:HB2	2.20	0.42
1:A:202:LYS:HG2	1:A:202:LYS:O	2.20	0.41
1:A:389:ARG:HD2	1:A:444:THR:CG2	2.50	0.41
1:B:244:PRO:HA	1:B:245:PRO:HD3	1.91	0.41
1:B:82:SER:HB3	1:B:85:GLN:OE1	2.20	0.41
1:A:375:HIS:HA	1:A:376:PRO:HD3	1.92	0.41
1:B:76:ARG:HD3	1:B:76:ARG:HA	1.64	0.41
1:A:121:PHE:HB2	1:A:122:ARG:H	1.72	0.41
1:A:442:LEU:HA	1:A:442:LEU:HD23	1.73	0.41
1:B:385:LEU:HD23	1:B:413:VAL:CG1	2.51	0.41
1:B:115:TRP:CZ3	1:B:119:VAL:HG21	2.55	0.41
1:B:391:PRO:HG2	1:B:392:THR:H	1.84	0.41
1:B:460:THR:CB	1:B:462:MET:HG2	2.48	0.41
1:A:127:PRO:HA	1:A:209:ALA:O	2.21	0.41
1:A:385:LEU:CD2	1:A:385:LEU:N	2.83	0.41
1:A:435:MET:HB3	1:A:435:MET:HE2	1.93	0.41
1:A:185:LEU:HD23	1:A:185:LEU:HA	1.82	0.41
1:A:448:LEU:N	1:A:448:LEU:CD2	2.65	0.41
1:A:96:HIS:HB2	1:A:97:PRO:HD2	2.03	0.41
1:B:192:HIS:O	1:B:193:TYR:C	2.58	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:ALA:HB2	1:B:273:PHE:HE2	1.86	0.41
1:B:69:LEU:O	1:B:72:ILE:HB	2.21	0.41
1:A:243:THR:OG1	1:A:244:PRO:CD	2.68	0.41
1:A:308:ASP:OD2	1:A:308:ASP:N	2.26	0.41
1:A:353:SER:HB2	1:A:373:LYS:C	2.40	0.41
1:A:420:THR:CG2	1:A:421:MET:N	2.84	0.41
1:A:423:SER:HB3	1:A:427:GLN:NE2	2.35	0.41
1:B:104:VAL:O	1:B:107:ARG:N	2.52	0.41
1:B:368:HIS:ND1	1:B:368:HIS:O	2.54	0.41
1:B:69:LEU:O	1:B:70:LEU:C	2.59	0.41
1:A:139:LEU:CB	1:A:140:PRO:HD2	2.50	0.41
1:A:355:GLN:NE2	1:A:355:GLN:HA	2.35	0.41
1:B:122:ARG:O	1:B:122:ARG:HG3	2.20	0.41
1:B:260:LEU:CD1	1:B:275:SER:HB3	2.48	0.41
1:B:392:THR:HG22	1:B:393:LEU:CD2	2.51	0.41
1:A:260:LEU:HD21	1:A:264:ARG:CZ	2.51	0.41
1:B:387:VAL:HG12	1:B:443:VAL:O	2.20	0.41
1:A:266:PHE:HB3	1:A:378:LEU:HD22	2.02	0.40
1:A:372:LEU:HB3	1:A:436:SER:HB2	2.01	0.40
1:B:294:PRO:HD2	1:B:295:TRP:CE3	2.56	0.40
1:B:395:LEU:O	1:B:397:GLN:N	2.54	0.40
1:A:375:HIS:O	1:A:378:LEU:HB2	2.22	0.40
1:B:202:LYS:HB3	1:B:324:GLY:HA2	2.04	0.40
1:A:193:TYR:O	1:A:197:LEU:HB2	2.21	0.40
1:A:200:VAL:C	1:A:202:LYS:H	2.24	0.40
1:A:263:TRP:CE3	1:A:300:ILE:HD12	2.56	0.40
1:B:122:ARG:CB	1:B:124:GLN:HE21	2.34	0.40
1:B:193:TYR:HB2	1:B:242:PHE:CZ	2.56	0.40
1:A:425:LEU:HA	1:A:425:LEU:HD23	1.86	0.40
1:A:87:SER:C	1:A:89:ASP:N	2.74	0.40
1:A:280:ASP:HA	1:A:283:GLY:C	2.42	0.40
1:A:323:HIS:CB	1:A:331:VAL:C	2.89	0.40
1:B:273:PHE:CE1	1:B:291:TYR:HD1	2.40	0.40
1:B:299:LEU:O	1:B:344:ARG:HD2	2.22	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	358/459 (78%)	246 (69%)	75 (21%)	37 (10%)	0	3
1	B	358/459 (78%)	242 (68%)	73 (20%)	43 (12%)	0	1
All	All	716/918 (78%)	488 (68%)	148 (21%)	80 (11%)	0	2

All (80) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	ARG
1	A	120	VAL
1	A	124	GLN
1	A	131	LEU
1	A	142	ASP
1	A	193	TYR
1	A	309	HIS
1	A	310	GLU
1	A	323	HIS
1	A	389	ARG
1	A	420	THR
1	A	421	MET
1	A	461	THR
1	B	68	ALA
1	B	88	ARG
1	B	104	VAL
1	B	120	VAL
1	B	181	GLY
1	B	281	GLU
1	B	371	VAL
1	B	391	PRO
1	B	393	LEU
1	B	417	TYR
1	B	423	SER
1	B	424	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	448	LEU
1	B	461	THR
1	A	90	SER
1	A	121	PHE
1	A	328	ARG
1	A	371	VAL
1	A	391	PRO
1	A	438	LEU
1	A	450	ASN
1	A	469	SER
1	B	121	PHE
1	B	130	ALA
1	B	146	ARG
1	B	191	GLU
1	B	193	TYR
1	B	309	HIS
1	B	421	MET
1	B	438	LEU
1	B	446	THR
1	A	89	ASP
1	A	254	PHE
1	A	271	SER
1	A	321	LYS
1	A	393	LEU
1	A	460	THR
1	B	123	GLU
1	B	124	GLN
1	B	258	HIS
1	B	259	ARG
1	B	285	LYS
1	B	373	LYS
1	B	385	LEU
1	B	396	ARG
1	B	422	GLN
1	B	466	MET
1	A	146	ARG
1	A	294	PRO
1	A	392	THR
1	A	464	GLU
1	B	87	SER
1	B	105	GLU
1	B	321	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	352	ASP
1	B	419	GLU
1	A	280	ASP
1	B	190	LEU
1	B	354	PHE
1	A	140	PRO
1	A	425	LEU
1	B	118	VAL
1	A	376	PRO
1	A	451	GLY
1	B	376	PRO
1	A	104	VAL
1	B	96	HIS

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	323/401 (80%)	271 (84%)	52 (16%)	2	10
1	B	323/401 (80%)	280 (87%)	43 (13%)	4	16
All	All	646/802 (80%)	551 (85%)	95 (15%)	3	13

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	GLU
1	A	70	LEU
1	A	79	LEU
1	A	85	GLN
1	A	88	ARG
1	A	89	ASP
1	A	92	LEU
1	A	95	CYS
1	A	96	HIS
1	A	109	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	116	THR
1	A	118	VAL
1	A	121	PHE
1	A	122	ARG
1	A	124	GLN
1	A	125	VAL
1	A	126	PHE
1	A	128	VAL
1	A	142	ASP
1	A	195	ASN
1	A	200	VAL
1	A	206	TYR
1	A	229	LYS
1	A	231	ILE
1	A	250	GLN
1	A	252	LEU
1	A	276	SER
1	A	277	ASP
1	A	278	CYS
1	A	280	ASP
1	A	298	GLU
1	A	308	ASP
1	A	323	HIS
1	A	328	ARG
1	A	330	ASN
1	A	347	LEU
1	A	378	LEU
1	A	386	ASP
1	A	387	VAL
1	A	389	ARG
1	A	423	SER
1	A	426	GLU
1	A	431	LYS
1	A	443	VAL
1	A	445	GLU
1	A	448	LEU
1	A	449	GLU
1	A	454	HIS
1	A	460	THR
1	A	468	ILE
1	A	471	LEU
1	A	481	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	67	GLU
1	B	70	LEU
1	B	85	GLN
1	B	88	ARG
1	B	89	ASP
1	B	95	CYS
1	B	107	ARG
1	B	122	ARG
1	B	124	GLN
1	B	139	LEU
1	B	184	ASN
1	B	200	VAL
1	B	206	TYR
1	B	216	HIS
1	B	230	SER
1	B	234	LYS
1	B	248	SER
1	B	256	LEU
1	B	257	ARG
1	B	271	SER
1	B	284	ARG
1	B	298	GLU
1	B	311	LEU
1	B	312	LEU
1	B	322	LEU
1	B	328	ARG
1	B	335	VAL
1	B	374	LEU
1	B	377	CYS
1	B	389	ARG
1	B	397	GLN
1	B	426	GLU
1	B	431	LYS
1	B	445	GLU
1	B	448	LEU
1	B	455	LEU
1	B	456	ARG
1	B	459	ASP
1	B	460	THR
1	B	462	MET
1	B	472	LYS
1	B	473	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	481	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	96	HIS
1	A	192	HIS
1	A	201	ASN
1	A	210	GLN
1	A	216	HIS
1	A	287	ASN
1	A	313	HIS
1	A	323	HIS
1	A	355	GLN
1	A	400	GLN
1	A	422	GLN
1	A	427	GLN
1	A	450	ASN
1	A	454	HIS
1	B	77	HIS
1	B	124	GLN
1	B	192	HIS
1	B	201	ASN
1	B	210	GLN
1	B	272	ASN
1	B	287	ASN
1	B	305	ASN
1	B	313	HIS
1	B	318	ASN
1	B	323	HIS
1	B	375	HIS
1	B	400	GLN
1	B	454	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	364/459 (79%)	-0.09	8 (2%) 62 41	41, 74, 102, 136	0
1	B	364/459 (79%)	-0.09	7 (1%) 66 46	48, 73, 108, 127	0
All	All	728/918 (79%)	-0.09	15 (2%) 63 43	41, 73, 107, 136	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	138	LEU	9.6
1	A	139	LEU	9.1
1	B	140	PRO	7.7
1	A	140	PRO	6.7
1	B	139	LEU	4.4
1	B	143	SER	3.7
1	B	144	ALA	3.5
1	B	141	GLY	3.2
1	A	144	ALA	3.1
1	A	143	SER	3.0
1	A	142	ASP	2.7
1	A	137	PRO	2.6
1	B	138	LEU	2.4
1	B	145	PHE	2.3
1	A	145	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.