



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:01 pm GMT

PDB ID : 1CR6  
Title : CRYSTAL STRUCTURE OF MURINE SOLUBLE EPOXIDE HYDROLASE  
COMPLEXED WITH CPU INHIBITOR  
Authors : Argiriadi, M.A.; Morisseau, C.; Hammock, B.D.; Christianson, D.W.  
Deposited on : 1999-08-13  
Resolution : 2.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

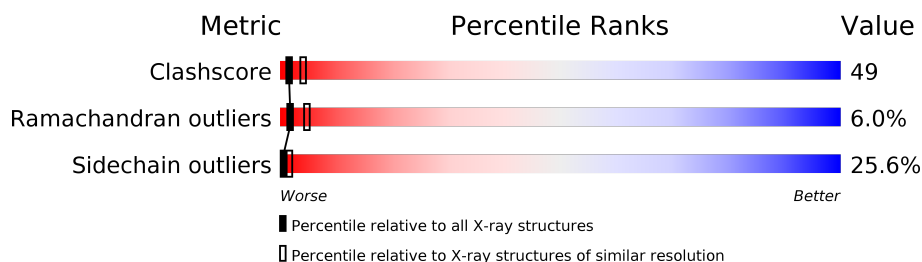
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	554	
1	B	554	

## 2 Entry composition [i](#)

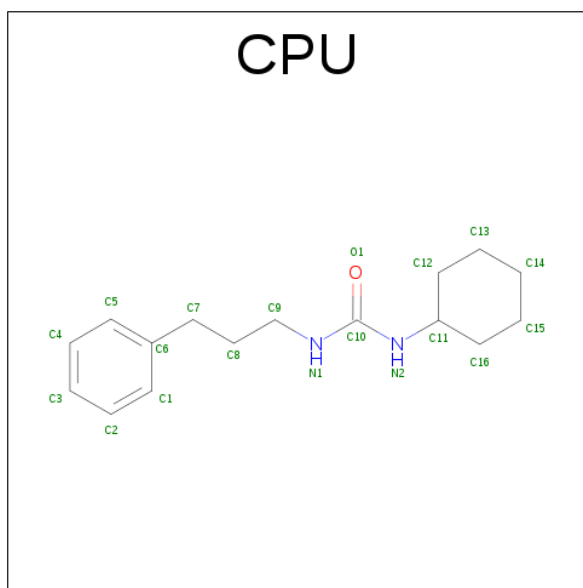
There are 3 unique types of molecules in this entry. The entry contains 8237 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 EPOXIDE HYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	61	0	0
			3879	2501	648	701	29			
1	B	541	Total	C	N	O	S	71	0	0
			4299	2766	719	783	31			

- Molecule 2 is N-CYCLOHEXYL-N'-(PROPYL)PHENYL UREA (three-letter code: CPU) (formula:  $C_{16}H_{24}N_2O$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			19	16	2	1		
2	B	1	Total	C	N	O	0	0
			19	16	2	1		

- Molecule 3 is water.

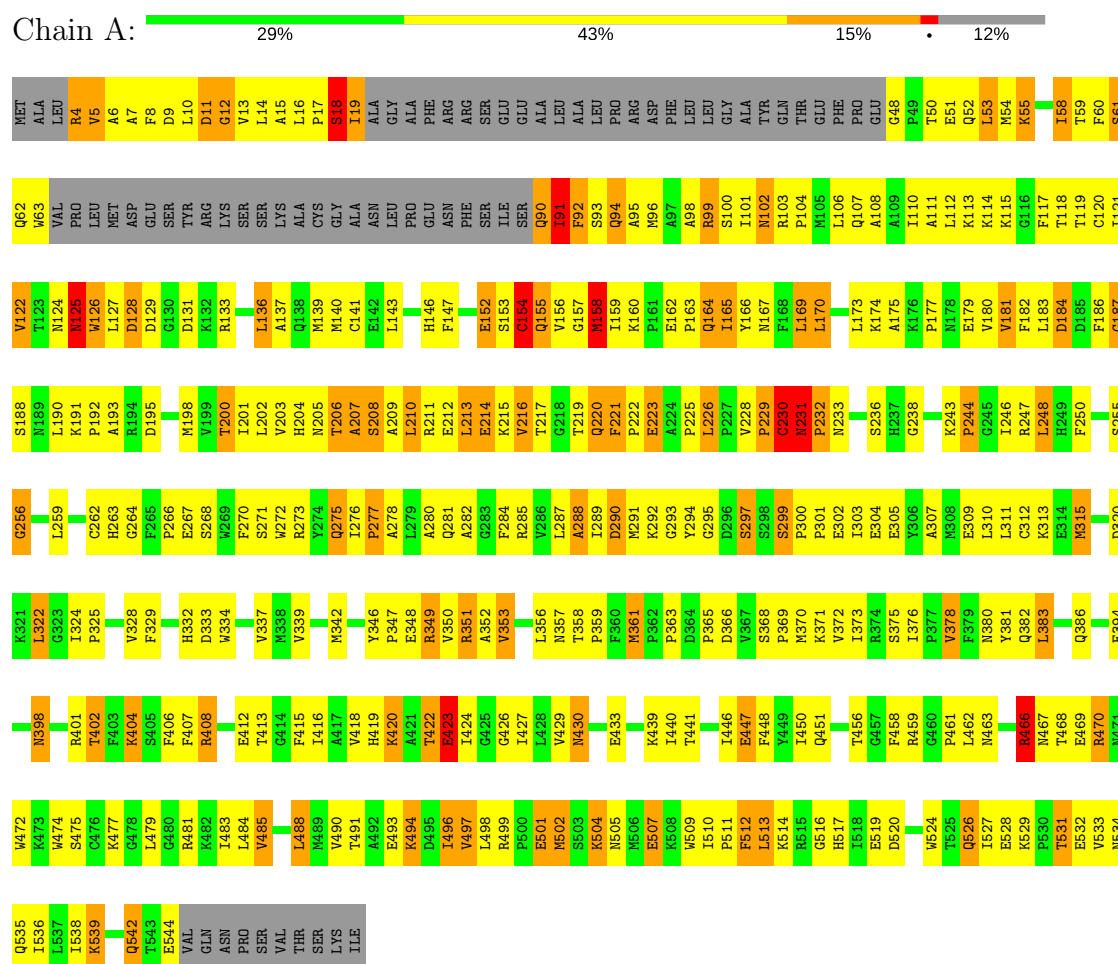
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total	O	0	0
			12	12		
3	B	9	Total	O	0	0
			9	9		

### 3 Residue-property plots

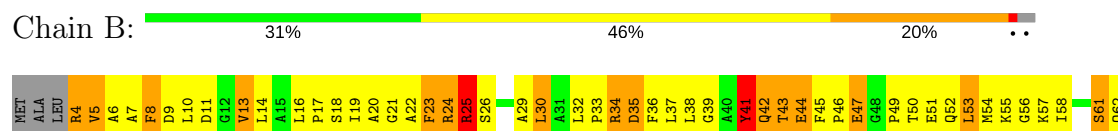
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

#### • Molecule 1: EPOXIDE HYDROLASE



#### • Molecule 1: EPOXIDE HYDROLASE



Q536	M471	G323	L259	L190	M125	M63
I536	W472	I324	L259	K191	W125	V64
L537	K473	P325	C262	A193	D127	P65
I538	K404	V328	C262	D195	D128	L66
K539	S405	F329	H263	D195	D129	M67
	S476		G264	D196	G130	D68
	G476		F265	M196	D131	E69
	K477		P266	G197	K132	S70
	G478		E267	M198	K133	Y71
	L479		E268	V199	D134	R72
VAL	G480		W269	T200	S135	K73
GLN	T413		F270	I201	L136	S74
ASN	G414		S271	L202	A137	S75
PRO	T483		W272	V203	Q138	K76
SER	F415		R273	H204	M139	A77
VAL	I416		Y274	N205	M140	C78
	A417		Q275	T206		G79
	V418		I276	A207	S144	A80
	V419		Q277	S208	Q145	N81
L488	K420		A278	A209	H146	L82
N489	A421		L279	L210	F147	P83
V490	T422		A280	R211	D148	E84
T491	E423		Q281	E212	F149	N85
	I424			L213	L150	F86
K494	G425		F284	E214	I151	S87
D495	G426		R285	K215	E152	T88
T496	A352		L286	V216	S153	S89
V497	L428		L287	T217	C154	Q90
L498	V429		A288	G218	Q155	I91
R499	N430		I289	T219	V156	F92
P500	T431		D290	Q220	G157	S93
E501	P432		M291	F221	M158	Q94
M502	P432		K292	A222	I159	A95
S503	E433		G293	E223	K160	N96
K504	D434		G295	P225	E161	
N505	P435		D296	V228	P163	R99
M506	S438		S297	P229	Q164	S100
K508	K439		S298	N231	I165	I101
E507	I440		S299	N231	Y166	N102
N509	I440		P300	N232	N167	R103
T510	T441		P301	P232		P104
P511	I446		E302	N233	L170	M105
F512	E447		I303	D234	D171	L106
L513	F448		E304	V235	T172	Q107
K514	F448		E305	H237	L173	A108
R515	Y449		Y306	S236	K174	A109
G516	I450		A307	G238	A175	I110
G517	Q451		M308		K176	A111
T518	T456		E309	K243	P177	L112
E519	G457		L310	P244		K115
D520	F458		L311	G245	V180	G116
	R459		C312	P246	V181	F117
	G460		K313	R247	F182	T118
	P461		E314	L248	L183	T119
	L462		M315	H249	C120	C120
	N463		D320	F250	I121	I121
	N463		K321	S255	T122	V122
	R466		L322	G256	T123	T123
	N467				F186	
	T468				G187	
	E469				S188	
	R470				N189	
						N124

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	151.90Å 143.00Å 60.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	91.0 (20.00-2.80)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, $R_{free}$	0.201 , 0.312	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8237	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.60	0/3981	0.79	1/5397 (0.0%)
1	B	0.60	0/4413	0.80	3/5984 (0.1%)
All	All	0.60	0/8394	0.80	4/11381 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	231	ASN	C-N-CD	-11.76	94.72	120.60
1	B	231	ASN	C-N-CA	7.25	152.46	122.00
1	A	488	LEU	CA-CB-CG	5.33	127.55	115.30
1	B	488	LEU	CA-CB-CG	5.32	127.53	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	3879	0	3863	370	0
1	B	4299	0	4270	434	0
2	A	19	0	24	5	0
2	B	19	0	24	5	0
3	A	12	0	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	9	0	0	0	0
All	All	8237	0	8181	786	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 49.

All (786) 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:B:232:PRO:HD2	1:B:233:ASN:H	1.11	1.11
1:B:5:VAL:HG21	1:B:173:LEU:HD21	1.35	1.08
1:A:101:ILE:HG21	1:A:106:LEU:HD12	1.38	1.06
1:B:300:PRO:HG2	1:B:305:GLU:HG2	1.36	1.05
1:B:496:ILE:H	1:B:496:ILE:HD12	1.19	1.04
1:B:424:ILE:HD13	1:B:424:ILE:H	1.19	1.04
1:A:300:PRO:HG2	1:A:305:GLU:HG2	1.36	1.02
1:A:90:GLN:HG3	1:A:91:ILE:HD13	1.37	1.02
1:A:496:ILE:HD12	1:A:496:ILE:H	1.20	1.01
1:A:193:ALA:HA	1:A:198:MET:HE3	1.44	1.00
1:A:232:PRO:HD2	1:A:233:ASN:H	1.27	0.99
1:A:166:TYR:O	1:A:170:LEU:HD12	1.60	0.98
1:A:52:GLN:HG3	1:A:58:ILE:HD11	1.44	0.98
1:B:19:ILE:HD11	1:B:96:MET:HA	1.45	0.98
1:B:263:HIS:CD2	1:B:291:MET:HG2	2.00	0.96
1:A:263:HIS:CD2	1:A:291:MET:HG2	2.01	0.94
1:A:430:ASN:HD22	1:A:430:ASN:H	1.06	0.94
1:A:193:ALA:O	1:A:198:MET:HB2	1.68	0.94
1:A:13:VAL:HG22	1:A:203:VAL:HG21	1.48	0.94
1:B:155:GLN:HA	1:B:155:GLN:OE1	1.69	0.93
1:A:155:GLN:OE1	1:A:155:GLN:HA	1.69	0.92
1:A:447:GLU:HA	1:A:450:ILE:HD13	1.51	0.92
1:B:447:GLU:HA	1:B:450:ILE:HD13	1.51	0.92
1:A:322:LEU:HB3	1:A:324:ILE:CD1	2.00	0.92
1:B:106:LEU:HD21	1:B:146:HIS:CD2	2.06	0.91
1:A:205:ASN:ND2	1:A:209:ALA:H	1.69	0.91
1:B:322:LEU:HB3	1:B:324:ILE:CD1	2.00	0.90
1:A:205:ASN:HD21	1:A:209:ALA:HB3	1.36	0.90
1:B:13:VAL:HB	1:B:203:VAL:HG11	1.54	0.88
1:B:72:ARG:HA	1:B:75:SER:HB3	1.53	0.88
1:A:17:PRO:HD2	1:A:99:ARG:HA	1.54	0.88
1:B:232:PRO:CD	1:B:233:ASN:H	1.87	0.87

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:PRO:CD	1:A:233:ASN:H	1.87	0.87
1:B:424:ILE:H	1:B:424:ILE:CD1	1.87	0.86
1:B:158:MET:HE3	1:B:165:ILE:HA	1.57	0.86
1:B:127:LEU:HD12	1:B:127:LEU:H	1.40	0.86
1:B:5:VAL:HG23	1:B:118:THR:O	1.75	0.85
1:A:230:CYS:O	1:A:231:ASN:HB3	1.75	0.85
1:B:122:VAL:HB	1:B:151:ILE:HG13	1.56	0.85
1:A:211:ARG:HA	1:A:214:GLU:HB2	1.59	0.85
1:A:48:GLY:N	1:A:51:GLU:HB2	1.91	0.85
1:A:102:ASN:HD22	1:A:104:PRO:HD2	1.41	0.84
1:B:496:ILE:H	1:B:496:ILE:CD1	1.90	0.84
1:A:529:LYS:O	1:A:533:VAL:HG23	1.78	0.84
1:B:404:LYS:O	1:B:408:ARG:HD2	1.77	0.84
1:B:232:PRO:O	1:B:235:VAL:HG22	1.78	0.83
1:A:404:LYS:O	1:A:408:ARG:HD2	1.78	0.83
1:A:422:THR:O	1:A:423:GLU:HB2	1.77	0.83
1:A:94:GLN:H	1:A:94:GLN:CD	1.82	0.82
1:A:215:LYS:HG2	1:A:220:GLN:HA	1.61	0.82
1:A:496:ILE:H	1:A:496:ILE:CD1	1.91	0.82
1:B:322:LEU:HB3	1:B:324:ILE:HD13	1.61	0.81
1:B:424:ILE:HD13	1:B:424:ILE:N	1.95	0.81
1:B:529:LYS:O	1:B:533:VAL:HG23	1.81	0.81
1:B:339:VAL:HG13	1:B:353:VAL:HG12	1.62	0.81
1:B:5:VAL:HG13	1:B:180:VAL:HB	1.61	0.81
1:A:140:MET:HE3	1:A:140:MET:HA	1.62	0.81
1:A:369:PRO:O	1:A:372:VAL:HG22	1.80	0.81
1:B:232:PRO:HD2	1:B:233:ASN:N	1.92	0.81
1:B:369:PRO:O	1:B:372:VAL:HG22	1.80	0.80
1:B:58:ILE:HD12	1:B:63:TRP:HB2	1.64	0.80
1:A:463:ASN:HA	1:A:466:ARG:HG3	1.62	0.80
1:A:96:MET:SD	1:A:136:LEU:HD23	2.21	0.80
1:A:446:ILE:O	1:A:450:ILE:HD12	1.81	0.80
1:B:463:ASN:HA	1:B:466:ARG:HG3	1.62	0.80
1:A:535:GLN:O	1:A:539:LYS:HD3	1.82	0.80
1:B:270:PHE:CE1	1:B:273:ARG:HD3	2.17	0.80
1:B:50:THR:CG2	1:B:63:TRP:HE1	1.95	0.80
1:A:62:GLN:O	1:A:63:TRP:HD1	1.64	0.80
1:A:102:ASN:ND2	1:A:104:PRO:HD2	1.97	0.79
1:A:133:ARG:HG2	1:B:348:GLU:HA	1.63	0.79
1:A:339:VAL:HG13	1:A:353:VAL:HG12	1.63	0.79
1:A:205:ASN:HD21	1:A:209:ALA:CB	1.94	0.79

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:MET:O	1:B:165:ILE:HG12	1.82	0.79
1:B:5:VAL:HG21	1:B:173:LEU:CD2	2.11	0.79
1:B:535:GLN:O	1:B:539:LYS:HD3	1.83	0.79
1:B:431:THR:HG22	1:B:432:PRO:HD2	1.63	0.78
1:A:270:PHE:CE1	1:A:273:ARG:HD3	2.19	0.78
1:A:124:ASN:HA	1:A:153:SER:HB3	1.65	0.77
1:B:529:LYS:HB3	1:B:532:GLU:HG3	1.66	0.77
1:A:497:VAL:O	1:A:498:LEU:HB2	1.84	0.77
1:B:300:PRO:CG	1:B:305:GLU:HG2	2.13	0.77
1:B:112:LEU:O	1:B:117:PHE:HB2	1.85	0.77
1:A:159:ILE:O	1:A:159:ILE:HD12	1.85	0.76
1:B:50:THR:HG23	1:B:63:TRP:HE1	1.49	0.76
1:A:13:VAL:CG2	1:A:203:VAL:HG21	2.15	0.76
1:B:320:ASP:OD1	1:B:349:ARG:NH2	2.19	0.76
1:B:483:ILE:HB	1:B:510:ILE:HG12	1.67	0.76
1:B:446:ILE:O	1:B:450:ILE:HD12	1.86	0.76
1:A:322:LEU:HB3	1:A:324:ILE:HD13	1.66	0.75
1:A:52:GLN:CG	1:A:58:ILE:HD11	2.17	0.75
1:A:529:LYS:HB3	1:A:532:GLU:HG3	1.66	0.75
1:A:91:ILE:C	1:A:94:GLN:HE22	1.90	0.75
1:B:424:ILE:HB	1:B:429:VAL:HG11	1.67	0.75
1:A:162:GLU:HB3	1:A:164:GLN:HE21	1.51	0.75
1:A:292:LYS:NZ	1:A:305:GLU:HG3	2.03	0.74
1:A:446:ILE:HG22	1:A:450:ILE:HD11	1.68	0.74
1:B:292:LYS:NZ	1:B:305:GLU:HG3	2.02	0.74
1:B:446:ILE:HG22	1:B:450:ILE:HD11	1.69	0.74
1:B:9:ASP:O	1:B:13:VAL:HG22	1.87	0.74
1:A:499:ARG:O	1:A:502:MET:HG3	1.88	0.74
1:A:320:ASP:OD1	1:A:349:ARG:NH2	2.19	0.73
1:B:177:PRO:O	1:B:198:MET:HA	1.89	0.73
1:A:300:PRO:CG	1:A:305:GLU:HG2	2.14	0.73
1:A:231:ASN:HB2	1:A:232:PRO:HA	1.69	0.73
1:A:205:ASN:ND2	1:A:209:ALA:HB3	2.03	0.73
1:A:483:ILE:HB	1:A:510:ILE:HG12	1.69	0.73
1:B:127:LEU:HD12	1:B:127:LEU:N	2.03	0.73
1:B:497:VAL:O	1:B:498:LEU:HB2	1.86	0.73
1:B:73:LYS:HZ2	1:B:73:LYS:HA	1.53	0.73
1:B:177:PRO:O	1:B:198:MET:HG3	1.87	0.72
1:B:499:ARG:O	1:B:502:MET:HG3	1.89	0.72
1:B:510:ILE:HG22	1:B:513:LEU:HB2	1.71	0.72
1:B:64:VAL:HB	1:B:65:PRO:CD	2.19	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:ILE:CD1	1:B:63:TRP:HB2	2.19	0.72
1:B:8:PHE:N	1:B:8:PHE:CD1	2.57	0.72
1:B:121:ILE:O	1:B:151:ILE:HG12	1.89	0.71
1:A:348:GLU:HA	1:B:133:ARG:CG	2.19	0.71
1:B:83:PRO:HG2	1:B:86:PHE:HB2	1.69	0.71
1:B:201:ILE:HD12	1:B:201:ILE:N	2.05	0.71
1:B:420:LYS:HB3	1:B:424:ILE:HD12	1.72	0.71
1:A:159:ILE:O	1:A:165:ILE:HD11	1.91	0.71
1:B:8:PHE:CE1	1:B:147:PHE:HE2	2.08	0.71
1:A:162:GLU:O	1:A:165:ILE:HG13	1.90	0.71
1:A:10:LEU:O	1:A:12:GLY:N	2.24	0.70
1:B:232:PRO:HD2	1:B:233:ASN:HD22	1.55	0.70
1:B:531:THR:HG23	1:B:532:GLU:OE2	1.90	0.70
1:B:103:ARG:O	1:B:107:GLN:HB2	1.92	0.70
1:A:58:ILE:HG22	1:A:62:GLN:HB3	1.73	0.70
1:B:158:MET:CE	1:B:165:ILE:HA	2.22	0.70
1:B:5:VAL:HG11	1:B:173:LEU:HD23	1.74	0.70
1:A:136:LEU:O	1:A:140:MET:HG2	1.92	0.69
1:B:496:ILE:N	1:B:496:ILE:HD12	2.01	0.69
1:A:324:ILE:HD12	1:A:324:ILE:N	2.08	0.69
1:B:7:ALA:HA	1:B:120:CYS:O	1.91	0.69
1:B:128:ASP:O	1:B:133:ARG:HG3	1.92	0.69
1:B:181:VAL:HG23	1:B:201:ILE:CD1	2.22	0.69
1:B:259:LEU:O	1:B:259:LEU:HD12	1.92	0.69
1:A:187:GLY:HA2	1:A:190:LEU:HD12	1.74	0.69
1:A:416:ILE:HG23	1:A:427:ILE:CG1	2.23	0.69
1:B:497:VAL:HG13	2:B:1200:CPU:C12	2.21	0.69
1:B:229:PRO:HB2	1:B:231:ASN:HD21	1.56	0.69
1:B:77:ALA:O	1:B:78:CYS:HB2	1.92	0.69
1:A:348:GLU:HA	1:B:133:ARG:HG2	1.72	0.69
1:B:124:ASN:HA	1:B:153:SER:HB3	1.75	0.69
1:B:529:LYS:HB3	1:B:532:GLU:CG	2.22	0.69
1:A:510:ILE:HG22	1:A:513:LEU:HB2	1.74	0.69
1:A:216:VAL:CG1	1:A:217:THR:N	2.56	0.68
1:B:103:ARG:HB2	1:B:104:PRO:HD3	1.75	0.68
1:B:49:PRO:HB2	1:B:67:MET:HG2	1.74	0.68
1:A:430:ASN:ND2	1:A:430:ASN:H	1.84	0.68
1:A:52:GLN:HG3	1:A:58:ILE:CD1	2.22	0.68
1:B:159:ILE:O	1:B:165:ILE:HD11	1.92	0.68
1:B:222:PRO:HG2	1:B:225:PRO:HG3	1.73	0.68
1:A:496:ILE:N	1:A:496:ILE:HD12	2.03	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:PHE:CD1	1:A:147:PHE:HE2	2.11	0.68
1:B:427:ILE:HG13	1:B:428:LEU:HD13	1.75	0.68
1:A:214:GLU:OE1	1:A:214:GLU:HA	1.91	0.68
1:A:5:VAL:HB	1:A:118:THR:HB	1.76	0.68
1:B:93:SER:HB2	1:B:132:LYS:HE2	1.76	0.68
1:A:158:MET:HE3	1:A:165:ILE:HA	1.76	0.67
1:A:529:LYS:HB3	1:A:532:GLU:CG	2.23	0.67
1:A:92:PHE:N	1:A:94:GLN:HE22	1.90	0.67
1:A:157:GLY:O	1:A:158:MET:HG2	1.95	0.67
1:B:72:ARG:HD3	1:B:73:LYS:HZ1	1.59	0.67
1:B:72:ARG:CA	1:B:75:SER:HB3	2.25	0.67
1:A:206:THR:O	1:A:207:ALA:HB3	1.95	0.67
1:A:159:ILE:C	1:A:159:ILE:HD12	2.15	0.67
1:A:223:GLU:O	1:A:225:PRO:HD3	1.94	0.67
1:A:513:LEU:HD22	1:A:514:LYS:O	1.93	0.67
1:A:205:ASN:ND2	1:A:209:ALA:N	2.43	0.67
1:A:216:VAL:HG12	1:A:217:THR:HG23	1.76	0.67
1:A:5:VAL:HG22	1:A:180:VAL:HB	1.77	0.66
1:B:19:ILE:HD11	1:B:96:MET:CA	2.23	0.66
1:B:513:LEU:HD22	1:B:514:LYS:O	1.95	0.66
1:A:531:THR:HG23	1:A:532:GLU:OE2	1.95	0.66
1:A:124:ASN:HD21	1:A:160:LYS:HB2	1.60	0.66
1:B:181:VAL:HA	1:B:199:VAL:HB	1.76	0.66
1:A:259:LEU:O	1:A:259:LEU:HD12	1.96	0.66
1:B:532:GLU:O	1:B:536:ILE:HG13	1.96	0.65
1:A:137:ALA:O	1:A:141:CYS:N	2.27	0.65
1:A:108:ALA:O	1:A:111:ALA:HB3	1.96	0.65
1:A:15:ALA:O	1:A:16:LEU:HD23	1.97	0.65
1:B:499:ARG:HB3	1:B:501:GLU:HG3	1.79	0.65
1:A:272:TRP:HA	1:A:275:GLN:HE21	1.60	0.65
1:B:272:TRP:HA	1:B:275:GLN:HE21	1.61	0.65
1:B:497:VAL:HG13	2:B:1200:CPU:H121	1.79	0.65
1:B:324:ILE:HD12	1:B:324:ILE:N	2.10	0.65
1:A:264:GLY:HA3	1:A:333:ASP:HB3	1.78	0.65
1:A:416:ILE:HG23	1:A:427:ILE:HG13	1.77	0.64
1:A:532:GLU:O	1:A:536:ILE:HG13	1.97	0.64
1:B:25:ARG:O	1:B:29:ALA:HB2	1.97	0.64
1:B:264:GLY:HA3	1:B:333:ASP:HB3	1.78	0.64
1:A:177:PRO:O	1:A:198:MET:HG3	1.97	0.64
1:A:211:ARG:CA	1:A:214:GLU:HB2	2.26	0.64
1:A:255:SER:O	1:A:256:GLY:O	2.16	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:VAL:HB	1:B:65:PRO:HD3	1.79	0.64
1:A:101:ILE:CG2	1:A:106:LEU:HD12	2.21	0.64
1:A:499:ARG:HB3	1:A:501:GLU:HG3	1.80	0.64
1:B:255:SER:O	1:B:256:GLY:O	2.16	0.64
1:A:169:LEU:O	1:A:173:LEU:HB2	1.97	0.64
1:B:420:LYS:C	1:B:424:ILE:HD11	2.18	0.64
1:A:193:ALA:CA	1:A:198:MET:HE3	2.22	0.64
1:B:119:THR:HG23	1:B:148:ASP:H	1.61	0.63
1:B:212:GLU:C	1:B:214:GLU:H	2.00	0.63
1:B:469:GLU:O	1:B:472:TRP:HB3	1.98	0.63
1:A:5:VAL:HG21	1:A:173:LEU:CD2	2.28	0.63
1:A:190:LEU:HD22	1:A:200:THR:HG22	1.79	0.63
1:B:458:PHE:C	1:B:461:PRO:HD2	2.19	0.63
1:B:72:ARG:HD3	1:B:73:LYS:NZ	2.13	0.63
1:A:9:ASP:OD1	1:A:11:ASP:HB2	1.98	0.63
1:A:458:PHE:C	1:A:461:PRO:HD2	2.19	0.63
1:B:248:LEU:HA	1:B:297:SER:HB3	1.79	0.63
1:A:106:LEU:HD22	1:A:110:ILE:HD11	1.80	0.63
1:B:124:ASN:HA	1:B:153:SER:CB	2.29	0.63
1:B:292:LYS:CE	1:B:305:GLU:HG3	2.28	0.63
1:A:205:ASN:ND2	1:A:209:ALA:CB	2.61	0.63
1:A:248:LEU:HA	1:A:297:SER:HB3	1.79	0.63
1:A:125:ASN:OD1	1:A:152:GLU:HB3	1.99	0.63
1:A:214:GLU:HB3	1:A:221:PHE:CZ	2.33	0.63
1:A:292:LYS:CE	1:A:305:GLU:HG3	2.29	0.62
1:B:535:GLN:HB3	1:B:539:LYS:HZ2	1.64	0.62
1:A:158:MET:O	1:A:165:ILE:HG12	1.99	0.62
1:A:433:GLU:HA	1:A:433:GLU:OE1	1.99	0.62
1:B:32:LEU:HB3	1:B:33:PRO:HD2	1.82	0.62
1:A:497:VAL:HG13	2:A:1100:CPU:H122	1.81	0.62
1:A:232:PRO:CD	1:A:233:ASN:N	2.60	0.62
1:B:232:PRO:HG2	1:B:233:ASN:ND2	2.14	0.62
1:B:26:SER:HA	1:B:29:ALA:HB3	1.81	0.62
1:B:75:SER:OG	1:B:76:LYS:N	2.31	0.62
1:B:180:VAL:HG22	1:B:198:MET:CG	2.30	0.62
1:B:181:VAL:HG23	1:B:201:ILE:HD13	1.80	0.62
1:A:62:GLN:HE22	1:B:481:ARG:HA	1.63	0.62
1:A:216:VAL:HG12	1:A:217:THR:N	2.14	0.62
1:A:230:CYS:HB3	1:A:277:PRO:HG3	1.82	0.62
1:A:206:THR:O	1:A:207:ALA:CB	2.47	0.61
1:A:276:ILE:HD11	1:A:288:ALA:CB	2.29	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:LEU:CD2	1:A:200:THR:HG22	2.30	0.61
1:A:157:GLY:C	1:A:158:MET:HG2	2.20	0.61
1:A:124:ASN:ND2	1:A:160:LYS:HB2	2.14	0.61
1:A:205:ASN:HD21	1:A:209:ALA:N	1.98	0.61
1:B:524:TRP:HB3	1:B:527:ILE:HD12	1.81	0.61
1:A:205:ASN:C	1:A:207:ALA:H	2.04	0.61
1:B:32:LEU:HD22	1:B:36:PHE:CD2	2.35	0.61
1:B:380:ASN:ND2	1:B:422:THR:OG1	2.32	0.61
1:A:163:PRO:O	1:A:167:ASN:ND2	2.34	0.61
1:A:183:LEU:HD13	1:A:201:ILE:HB	1.82	0.61
1:A:294:TYR:CZ	1:A:461:PRO:HB3	2.36	0.61
1:B:119:THR:HG23	1:B:147:PHE:HA	1.83	0.61
1:B:276:ILE:HD11	1:B:288:ALA:CB	2.30	0.61
1:B:62:GLN:O	1:B:65:PRO:HD2	2.01	0.61
1:A:339:VAL:CG1	1:A:353:VAL:HG12	2.30	0.60
1:A:469:GLU:O	1:A:472:TRP:HB3	2.01	0.60
1:A:153:SER:OG	1:A:154:CYS:N	2.31	0.60
1:A:205:ASN:HD21	1:A:209:ALA:H	1.48	0.60
1:A:524:TRP:HB3	1:A:527:ILE:HD12	1.84	0.60
1:B:339:VAL:CG1	1:B:353:VAL:HG12	2.31	0.60
1:B:194:ARG:HB2	1:B:200:THR:HG21	1.84	0.60
1:B:107:GLN:HA	1:B:107:GLN:NE2	2.17	0.60
1:B:39:GLY:HA2	1:B:43:THR:CG2	2.31	0.60
1:A:4:ARG:HA	1:A:179:GLU:O	2.01	0.60
1:B:119:THR:HG21	1:B:146:HIS:O	2.01	0.60
1:B:122:VAL:CB	1:B:151:ILE:HG13	2.31	0.60
1:A:201:ILE:HD13	1:A:213:LEU:HB3	1.84	0.60
1:A:287:LEU:O	1:A:289:ILE:HG13	2.02	0.60
1:A:293:GLY:HA2	1:A:299:SER:HA	1.84	0.60
1:B:122:VAL:HG11	1:B:182:PHE:HE1	1.67	0.60
1:B:4:ARG:HB3	1:B:4:ARG:CZ	2.32	0.60
1:A:177:PRO:O	1:A:198:MET:HA	2.02	0.59
1:B:73:LYS:HA	1:B:73:LYS:NZ	2.17	0.59
1:B:421:ALA:N	1:B:424:ILE:HD11	2.18	0.59
1:A:216:VAL:HG12	1:A:217:THR:H	1.67	0.59
1:B:183:LEU:CD1	1:B:201:ILE:HB	2.33	0.59
1:B:467:ASN:OD1	1:B:470:ARG:HD2	2.02	0.59
1:B:72:ARG:HA	1:B:75:SER:CB	2.30	0.59
1:B:20:ALA:O	1:B:23:PHE:HB2	2.03	0.59
1:B:45:PHE:CE1	1:B:47:GLU:HB2	2.36	0.59
1:A:90:GLN:HG3	1:A:91:ILE:N	2.18	0.59

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LYS:HG3	1:A:221:PHE:CE1	2.38	0.59
1:B:54:MET:HB2	1:B:159:ILE:CG2	2.33	0.58
1:A:232:PRO:HG2	1:A:233:ASN:OD1	2.03	0.58
1:A:213:LEU:O	1:A:216:VAL:HG12	2.03	0.58
1:A:359:PRO:HD2	1:A:361:MET:HE3	1.86	0.58
1:B:201:ILE:HD12	1:B:201:ILE:H	1.69	0.58
1:B:294:TYR:CZ	1:B:461:PRO:HB3	2.38	0.58
1:A:236:SER:HB2	1:B:322:LEU:HD12	1.85	0.58
1:B:8:PHE:CD1	1:B:147:PHE:HE2	2.21	0.58
1:B:293:GLY:HA2	1:B:299:SER:HA	1.83	0.58
1:A:347:PRO:O	1:B:133:ARG:HD2	2.04	0.58
1:A:309:GLU:HB2	1:A:474:TRP:CD2	2.38	0.58
1:B:228:VAL:O	1:B:277:PRO:HG2	2.03	0.57
1:B:158:MET:HE1	1:B:164:GLN:O	2.04	0.57
1:B:420:LYS:HB3	1:B:424:ILE:CD1	2.33	0.57
1:B:309:GLU:HB2	1:B:474:TRP:CD2	2.38	0.57
1:B:287:LEU:O	1:B:289:ILE:HG13	2.03	0.57
1:B:432:PRO:HB2	1:B:434:ASP:OD1	2.04	0.57
1:A:535:GLN:HB3	1:A:539:LYS:HZ2	1.68	0.57
1:B:75:SER:HB2	1:B:82:LEU:HB3	1.86	0.57
1:A:169:LEU:HD11	1:A:173:LEU:HD22	1.85	0.57
1:B:160:LYS:HA	1:B:165:ILE:CD1	2.34	0.57
1:B:272:TRP:HE3	1:B:275:GLN:HG3	1.69	0.57
1:B:102:ASN:O	1:B:105:MET:HB2	2.04	0.57
1:B:417:ALA:HB3	1:B:427:ILE:HA	1.85	0.57
1:B:434:ASP:N	1:B:435:PRO:CD	2.68	0.57
1:B:91:ILE:HG13	1:B:92:PHE:N	2.19	0.56
1:A:467:ASN:OD1	1:A:470:ARG:HD2	2.05	0.56
1:A:53:LEU:HD23	1:A:59:THR:O	2.05	0.56
1:B:222:PRO:CG	1:B:225:PRO:HG3	2.35	0.56
1:B:46:PRO:HG2	1:B:159:ILE:HD11	1.87	0.56
1:B:102:ASN:OD1	1:B:105:MET:HG3	2.05	0.56
1:B:44:GLU:O	1:B:46:PRO:HD3	2.05	0.56
1:B:51:GLU:O	1:B:55:LYS:HG3	2.04	0.56
1:A:106:LEU:HD21	1:A:146:HIS:CD2	2.40	0.56
1:A:272:TRP:HE3	1:A:275:GLN:HG3	1.70	0.56
1:B:270:PHE:CZ	1:B:273:ARG:HD3	2.40	0.56
1:B:458:PHE:HB3	1:B:462:LEU:HD12	1.87	0.56
1:A:510:ILE:O	1:A:513:LEU:HB2	2.05	0.56
1:A:230:CYS:O	1:A:231:ASN:CB	2.52	0.56
1:B:426:GLY:HA3	1:B:429:VAL:HG23	1.88	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:PRO:O	1:A:195:ASP:HB2	2.05	0.56
1:A:214:GLU:HB3	1:A:221:PHE:HZ	1.69	0.56
1:A:292:LYS:HZ3	1:A:305:GLU:HG3	1.68	0.56
1:A:270:PHE:CZ	1:A:273:ARG:HD3	2.41	0.56
1:A:307:ALA:O	1:A:311:LEU:HG	2.05	0.56
1:B:292:LYS:HE2	1:B:305:GLU:HG3	1.88	0.56
1:B:8:PHE:O	1:B:121:ILE:HG23	2.05	0.56
1:A:426:GLY:HA3	1:A:429:VAL:CG2	2.36	0.56
1:B:421:ALA:HA	1:B:426:GLY:O	2.05	0.56
1:A:446:ILE:HG22	1:A:450:ILE:CD1	2.36	0.55
1:B:232:PRO:CD	1:B:233:ASN:HD22	2.19	0.55
1:B:535:GLN:CB	1:B:539:LYS:HZ2	2.19	0.55
1:A:230:CYS:HB3	1:A:277:PRO:CG	2.36	0.55
1:B:170:LEU:O	1:B:174:LYS:N	2.39	0.55
1:B:26:SER:O	1:B:30:LEU:HB2	2.06	0.55
1:B:292:LYS:HZ3	1:B:305:GLU:HG3	1.70	0.55
1:B:337:VAL:HG21	2:B:1200:CPU:H4	1.88	0.55
1:B:529:LYS:O	1:B:532:GLU:HG2	2.06	0.55
1:A:186:PHE:O	1:A:188:SER:N	2.39	0.55
1:B:50:THR:O	1:B:54:MET:HG2	2.06	0.55
1:A:426:GLY:HA3	1:A:429:VAL:HG23	1.89	0.55
1:B:359:PRO:HD2	1:B:361:MET:HE3	1.88	0.55
1:A:231:ASN:HB2	1:A:232:PRO:CA	2.36	0.55
1:A:351:ARG:O	1:A:351:ARG:HD2	2.07	0.55
1:B:181:VAL:HG23	1:B:201:ILE:HD11	1.88	0.55
1:B:446:ILE:HG22	1:B:450:ILE:CD1	2.37	0.55
1:B:37:LEU:C	1:B:39:GLY:H	2.09	0.54
1:B:222:PRO:HB2	1:B:225:PRO:HG3	1.89	0.54
1:B:351:ARG:O	1:B:351:ARG:HD2	2.06	0.54
1:A:292:LYS:HE2	1:A:305:GLU:HG3	1.89	0.54
1:B:510:ILE:O	1:B:513:LEU:HB2	2.06	0.54
1:B:203:VAL:O	1:B:203:VAL:HG12	2.06	0.54
1:B:372:VAL:CG2	1:B:373:ILE:HD12	2.37	0.54
1:A:264:GLY:HA3	1:A:333:ASP:CB	2.38	0.54
1:B:186:PHE:HB2	1:B:189:ASN:HD22	1.71	0.54
1:A:458:PHE:HB3	1:A:462:LEU:HD12	1.89	0.54
1:A:359:PRO:HD2	1:A:361:MET:CE	2.38	0.54
1:A:304:GLU:H	1:A:304:GLU:CD	2.12	0.54
1:A:398:ASN:OD1	1:A:398:ASN:C	2.45	0.54
1:B:136:LEU:O	1:B:140:MET:HG2	2.08	0.54
1:A:484:LEU:HD13	1:B:61:SER:OG	2.08	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:MET:O	1:A:154:CYS:CA	2.56	0.53
1:B:134:ASP:O	1:B:137:ALA:N	2.41	0.53
1:B:264:GLY:HA3	1:B:333:ASP:CB	2.38	0.53
1:A:170:LEU:HD23	1:A:175:ALA:O	2.07	0.53
1:A:211:ARG:C	1:A:214:GLU:HB2	2.28	0.53
1:A:497:VAL:CG1	2:A:1100:CPU:H122	2.38	0.53
1:B:106:LEU:O	1:B:110:ILE:HG13	2.08	0.53
1:B:24:ARG:C	1:B:26:SER:H	2.11	0.53
1:B:30:LEU:HB3	1:B:32:LEU:CD1	2.39	0.53
1:B:359:PRO:HD2	1:B:361:MET:CE	2.38	0.53
1:B:9:ASP:OD1	1:B:11:ASP:O	2.26	0.53
1:A:5:VAL:HG21	1:A:173:LEU:HD21	1.89	0.53
1:B:497:VAL:CG1	2:B:1200:CPU:H122	2.38	0.53
1:B:497:VAL:HG13	2:B:1200:CPU:H122	1.90	0.53
1:A:140:MET:CE	1:A:140:MET:HA	2.34	0.53
1:A:529:LYS:O	1:A:532:GLU:HG2	2.08	0.53
1:A:535:GLN:CB	1:A:539:LYS:HZ2	2.21	0.53
1:B:125:ASN:HB2	1:B:152:GLU:HB3	1.89	0.53
1:B:212:GLU:C	1:B:214:GLU:N	2.61	0.53
1:B:304:GLU:CD	1:B:304:GLU:H	2.12	0.53
1:B:187:GLY:HA2	1:B:190:LEU:HD12	1.89	0.53
1:B:212:GLU:HA	1:B:215:LYS:HG3	1.89	0.53
1:A:334:TRP:CZ3	2:A:1100:CPU:H4	2.44	0.53
1:A:48:GLY:O	1:A:52:GLN:HG2	2.09	0.53
1:B:375:SER:OG	1:B:376:ILE:N	2.42	0.53
1:B:45:PHE:CZ	1:B:47:GLU:HB2	2.44	0.53
1:B:20:ALA:O	1:B:23:PHE:N	2.42	0.52
1:A:122:VAL:O	1:A:122:VAL:HG22	2.08	0.52
1:A:156:VAL:HG23	1:A:158:MET:HG3	1.91	0.52
1:A:236:SER:HB2	1:B:322:LEU:CD1	2.39	0.52
1:B:441:THR:OG1	1:B:446:ILE:HD11	2.09	0.52
1:B:511:PRO:C	1:B:513:LEU:H	2.12	0.52
1:A:372:VAL:CG2	1:A:373:ILE:HD12	2.39	0.52
1:B:398:ASN:C	1:B:398:ASN:OD1	2.48	0.52
1:B:86:PHE:CD1	1:B:87:SER:N	2.77	0.52
1:B:11:ASP:HB2	1:B:99:ARG:NH1	2.24	0.52
1:A:159:ILE:O	1:A:162:GLU:HB2	2.09	0.52
1:A:441:THR:OG1	1:A:446:ILE:HD11	2.10	0.52
1:A:160:LYS:HA	1:A:165:ILE:CD1	2.39	0.52
1:A:300:PRO:HG2	1:A:305:GLU:CG	2.26	0.52
1:B:75:SER:HB2	1:B:82:LEU:CB	2.39	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:VAL:HG22	1:B:352:ALA:HB3	1.92	0.52
1:A:301:PRO:HG2	1:A:302:GLU:OE1	2.10	0.52
1:A:538:ILE:O	1:A:542:GLN:HG2	2.10	0.52
1:A:54:MET:O	1:A:154:CYS:HA	2.09	0.52
1:A:211:ARG:HA	1:A:214:GLU:CB	2.37	0.52
1:A:458:PHE:O	1:A:461:PRO:HD2	2.10	0.52
1:B:356:LEU:O	1:B:357:ASN:HB2	2.10	0.52
1:A:246:ILE:HD12	1:A:246:ILE:N	2.25	0.52
1:B:276:ILE:HB	1:B:277:PRO:HD3	1.90	0.52
1:B:332:HIS:CD2	1:B:333:ASP:HB2	2.45	0.52
1:A:375:SER:OG	1:A:376:ILE:N	2.39	0.51
1:B:301:PRO:HG2	1:B:302:GLU:OE1	2.10	0.51
1:A:381:TYR:CE1	1:A:382:GLN:HG3	2.45	0.51
1:A:91:ILE:HA	1:A:94:GLN:OE1	2.09	0.51
1:B:479:LEU:O	1:B:509:TRP:HZ3	1.94	0.51
1:B:77:ALA:O	1:B:78:CYS:CB	2.58	0.51
1:A:112:LEU:HD23	1:A:117:PHE:CD2	2.45	0.51
1:B:64:VAL:CG1	1:B:89:SER:HB2	2.41	0.51
1:B:322:LEU:C	1:B:324:ILE:HD12	2.30	0.51
1:B:458:PHE:O	1:B:461:PRO:HD2	2.11	0.51
1:A:62:GLN:NE2	1:B:481:ARG:HA	2.25	0.51
1:B:37:LEU:C	1:B:39:GLY:N	2.63	0.51
1:B:381:TYR:CE1	1:B:382:GLN:HG3	2.46	0.51
1:A:289:ILE:HG22	1:A:290:ASP:N	2.25	0.51
1:B:39:GLY:HA2	1:B:43:THR:HG23	1.91	0.51
1:A:192:PRO:HA	1:A:195:ASP:HB2	1.92	0.51
1:A:407:PHE:C	1:A:408:ARG:HG2	2.30	0.51
1:A:363:PRO:HB2	1:A:472:TRP:CD1	2.46	0.51
1:A:91:ILE:H	1:A:91:ILE:HD13	1.75	0.51
1:B:299:SER:HB2	1:B:456:THR:HG22	1.93	0.51
1:B:33:PRO:O	1:B:34:ARG:C	2.48	0.51
1:B:434:ASP:H	1:B:435:PRO:CD	2.24	0.51
1:A:158:MET:SD	1:A:164:GLN:HB2	2.51	0.51
1:B:34:ARG:O	1:B:35:ASP:HB2	2.11	0.51
1:B:50:THR:HA	1:B:53:LEU:HB2	1.92	0.51
1:B:11:ASP:HB2	1:B:99:ARG:HH12	1.75	0.51
1:A:5:VAL:HG21	1:A:173:LEU:HD23	1.91	0.50
1:A:191:LYS:CB	1:A:192:PRO:HD3	2.41	0.50
1:B:122:VAL:HA	1:B:151:ILE:HG13	1.92	0.50
1:B:307:ALA:O	1:B:311:LEU:HG	2.12	0.50
1:B:36:PHE:HE2	1:B:82:LEU:HD13	1.75	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ILE:HB	1:A:277:PRO:HD3	1.92	0.50
1:A:332:HIS:CD2	1:A:333:ASP:HB2	2.45	0.50
1:A:485:VAL:HB	1:B:133:ARG:NH1	2.26	0.50
1:B:363:PRO:HB2	1:B:472:TRP:CD1	2.46	0.50
1:B:72:ARG:HG2	1:B:72:ARG:O	2.11	0.50
1:B:8:PHE:CE1	1:B:147:PHE:CE2	2.96	0.50
1:A:128:ASP:O	1:A:133:ARG:HG3	2.10	0.50
1:A:159:ILE:CD1	1:A:159:ILE:C	2.79	0.50
1:A:60:PHE:C	1:A:62:GLN:N	2.64	0.50
1:A:328:VAL:HG22	1:A:352:ALA:HB3	1.94	0.50
1:A:511:PRO:C	1:A:513:LEU:H	2.14	0.50
1:B:155:GLN:CA	1:B:155:GLN:OE1	2.51	0.50
1:B:246:ILE:N	1:B:246:ILE:HD12	2.25	0.50
1:B:372:VAL:HG22	1:B:373:ILE:HD12	1.93	0.50
1:B:160:LYS:HA	1:B:165:ILE:HD11	1.94	0.50
1:A:90:GLN:CG	1:A:91:ILE:HD13	2.26	0.50
1:B:21:GLY:O	1:B:25:ARG:HD3	2.11	0.50
1:A:231:ASN:CB	1:A:232:PRO:HA	2.34	0.50
1:A:299:SER:HB2	1:A:456:THR:HG22	1.94	0.50
1:B:157:GLY:C	1:B:158:MET:HG2	2.33	0.50
1:A:61:SER:C	1:A:63:TRP:H	2.15	0.50
1:A:62:GLN:O	1:A:63:TRP:CD1	2.55	0.50
1:A:121:ILE:HG13	1:A:147:PHE:CD2	2.46	0.49
1:A:325:PRO:O	1:A:349:ARG:NH1	2.45	0.49
1:B:180:VAL:HG23	1:B:181:VAL:N	2.26	0.49
1:B:229:PRO:O	1:B:231:ASN:ND2	2.33	0.49
1:B:43:THR:O	1:B:44:GLU:CB	2.60	0.49
1:A:124:ASN:HA	1:A:153:SER:CB	2.37	0.49
1:B:63:TRP:O	1:B:67:MET:HB2	2.12	0.49
1:B:194:ARG:HB2	1:B:200:THR:CG2	2.42	0.49
1:B:402:THR:O	1:B:406:PHE:HD2	1.96	0.49
1:A:92:PHE:C	1:A:92:PHE:CD2	2.86	0.49
1:B:20:ALA:O	1:B:21:GLY:C	2.51	0.49
1:A:61:SER:HB2	1:B:484:LEU:HD13	1.95	0.49
1:A:106:LEU:CD2	1:A:110:ILE:HD11	2.41	0.49
1:A:55:LYS:HG3	1:A:159:ILE:HG23	1.93	0.49
1:B:106:LEU:HD22	1:B:110:ILE:HD11	1.94	0.49
1:B:192:PRO:O	1:B:196:MET:HB2	2.12	0.49
1:B:125:ASN:CB	1:B:152:GLU:HB3	2.43	0.49
1:B:229:PRO:C	1:B:231:ASN:HD22	2.13	0.49
1:B:278:ALA:HA	1:B:281:GLN:HE21	1.77	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:PRO:O	1:B:349:ARG:NH1	2.45	0.49
1:B:535:GLN:HB3	1:B:539:LYS:NZ	2.27	0.49
1:A:501:GLU:O	1:A:504:LYS:HD3	2.13	0.48
1:A:9:ASP:OD2	1:A:160:LYS:NZ	2.44	0.48
1:B:229:PRO:HA	1:B:273:ARG:O	2.13	0.48
1:A:322:LEU:C	1:A:324:ILE:HD12	2.33	0.48
1:A:53:LEU:HA	1:A:58:ILE:HD12	1.95	0.48
1:B:186:PHE:C	1:B:188:SER:H	2.15	0.48
1:B:407:PHE:C	1:B:408:ARG:HG2	2.32	0.48
1:B:428:LEU:N	1:B:428:LEU:CD1	2.76	0.48
1:A:356:LEU:O	1:A:357:ASN:HB2	2.13	0.48
1:B:186:PHE:HB3	1:B:188:SER:OG	2.12	0.48
1:B:8:PHE:H	1:B:8:PHE:HD1	1.61	0.48
1:A:15:ALA:HA	1:A:100:SER:O	2.14	0.48
1:A:479:LEU:O	1:A:509:TRP:HZ3	1.97	0.48
1:B:339:VAL:O	1:B:342:MET:HB2	2.13	0.48
1:B:534:ASN:O	1:B:535:GLN:C	2.52	0.48
1:A:205:ASN:HD21	1:A:209:ALA:CA	2.26	0.48
1:B:182:PHE:HD2	1:B:190:LEU:HD23	1.78	0.48
1:B:267:GLU:HB3	1:B:271:SER:OG	2.13	0.48
1:A:339:VAL:O	1:A:342:MET:HB2	2.13	0.48
1:A:231:ASN:CB	1:A:232:PRO:CA	2.91	0.48
1:B:434:ASP:O	1:B:435:PRO:C	2.51	0.48
1:A:17:PRO:O	1:A:18:SER:O	2.32	0.48
1:A:256:GLY:N	1:A:285:ARG:HB2	2.29	0.48
1:B:238:GLY:HA3	1:B:250:PHE:CE1	2.49	0.48
1:A:474:TRP:O	1:A:477:LYS:HG3	2.14	0.48
1:B:215:LYS:NZ	1:B:221:PHE:O	2.47	0.48
1:B:290:ASP:HB3	1:B:297:SER:OG	2.14	0.48
1:B:160:LYS:HB3	1:B:189:ASN:OD1	2.14	0.47
1:B:431:THR:CG2	1:B:432:PRO:HD2	2.41	0.47
1:A:193:ALA:O	1:A:198:MET:CB	2.51	0.47
1:A:290:ASP:HB3	1:A:297:SER:OG	2.14	0.47
1:A:278:ALA:HA	1:A:281:GLN:HE21	1.79	0.47
1:B:210:LEU:O	1:B:214:GLU:HB2	2.13	0.47
1:B:491:THR:OG1	1:B:517:HIS:HD2	1.98	0.47
1:B:538:ILE:O	1:B:542:GLN:HG2	2.15	0.47
1:A:9:ASP:O	1:A:13:VAL:HB	2.15	0.47
1:B:102:ASN:HB3	1:B:105:MET:HB2	1.96	0.47
1:B:125:ASN:C	1:B:154:CYS:HB3	2.35	0.47
1:B:270:PHE:HB2	1:B:448:PHE:CE2	2.50	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:VAL:HG22	1:A:373:ILE:HD12	1.95	0.47
1:B:124:ASN:HA	1:B:153:SER:OG	2.14	0.47
1:B:233:ASN:H	1:B:233:ASN:HD22	1.61	0.47
1:B:329:PHE:O	1:B:353:VAL:HA	2.15	0.47
1:B:474:TRP:O	1:B:477:LYS:HG3	2.14	0.47
1:A:7:ALA:HA	1:A:120:CYS:O	2.15	0.47
1:A:8:PHE:HD1	1:A:147:PHE:HE2	1.58	0.47
1:A:402:THR:O	1:A:406:PHE:HD2	1.97	0.47
1:B:204:HIS:O	1:B:205:ASN:CB	2.62	0.47
1:B:64:VAL:HG11	1:B:89:SER:HB2	1.97	0.47
1:B:5:VAL:HB	1:B:118:THR:HB	1.95	0.47
1:B:232:PRO:CD	1:B:233:ASN:N	2.55	0.47
1:B:501:GLU:O	1:B:504:LYS:HD3	2.14	0.47
1:A:270:PHE:HB2	1:A:448:PHE:CE2	2.50	0.47
1:A:301:PRO:HA	1:A:459:ARG:HD3	1.96	0.47
1:B:229:PRO:HB2	1:B:231:ASN:ND2	2.25	0.47
1:B:428:LEU:HA	1:B:431:THR:OG1	2.15	0.47
1:B:483:ILE:HD12	1:B:510:ILE:HD11	1.97	0.47
1:A:262:CYS:O	1:A:272:TRP:HZ2	1.98	0.47
1:B:256:GLY:N	1:B:285:ARG:HB2	2.30	0.47
1:B:201:ILE:N	1:B:201:ILE:CD1	2.74	0.47
1:B:38:LEU:HD23	1:B:38:LEU:O	2.15	0.47
1:B:45:PHE:O	1:B:45:PHE:CG	2.68	0.47
1:B:524:TRP:O	1:B:528:GLU:HB2	2.15	0.47
1:B:53:LEU:HA	1:B:53:LEU:HD23	1.67	0.47
1:A:230:CYS:CB	1:A:277:PRO:HG3	2.44	0.46
1:B:107:GLN:CA	1:B:107:GLN:NE2	2.78	0.46
1:B:24:ARG:O	1:B:26:SER:N	2.48	0.46
1:B:4:ARG:HB2	1:B:117:PHE:CE2	2.50	0.46
1:A:512:PHE:N	1:A:512:PHE:CD2	2.82	0.46
1:B:7:ALA:HB2	1:B:120:CYS:SG	2.55	0.46
1:B:207:ALA:O	1:B:210:LEU:N	2.46	0.46
1:A:182:PHE:HD2	1:A:190:LEU:CD2	2.28	0.46
1:A:186:PHE:C	1:A:188:SER:H	2.18	0.46
1:A:91:ILE:CD1	1:A:91:ILE:H	2.28	0.46
1:B:289:ILE:HG22	1:B:290:ASP:N	2.28	0.46
1:B:301:PRO:HA	1:B:459:ARG:HD3	1.96	0.46
1:B:52:GLN:HB3	1:B:58:ILE:HG12	1.98	0.46
1:B:50:THR:HG22	1:B:63:TRP:HE1	1.79	0.46
1:A:108:ALA:O	1:A:112:LEU:HD12	2.16	0.46
1:A:497:VAL:HG13	2:A:1100:CPU:C12	2.45	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:TRP:O	1:A:528:GLU:HB2	2.14	0.46
1:B:101:ILE:HG22	1:B:102:ASN:N	2.31	0.46
1:B:312:CYS:O	1:B:315:MET:HB2	2.15	0.46
1:B:5:VAL:HG13	1:B:180:VAL:CB	2.37	0.46
1:A:378:VAL:HG13	1:A:378:VAL:O	2.15	0.46
1:B:170:LEU:HD23	1:B:175:ALA:O	2.16	0.46
1:B:428:LEU:N	1:B:428:LEU:HD13	2.31	0.46
1:B:22:ALA:HA	1:B:25:ARG:HD3	1.97	0.46
1:A:182:PHE:CE2	1:A:184:ASP:HB2	2.51	0.45
1:B:106:LEU:HD23	1:B:106:LEU:O	2.16	0.45
1:A:312:CYS:O	1:A:315:MET:HB2	2.16	0.45
1:A:535:GLN:HB3	1:A:539:LYS:NZ	2.31	0.45
1:B:119:THR:HG23	1:B:148:ASP:N	2.29	0.45
1:B:49:PRO:O	1:B:52:GLN:HB2	2.17	0.45
1:A:115:LYS:NZ	1:A:219:THR:HG23	2.30	0.45
1:A:267:GLU:HB3	1:A:271:SER:OG	2.16	0.45
1:B:43:THR:O	1:B:44:GLU:HB2	2.16	0.45
1:B:50:THR:CG2	1:B:63:TRP:NE1	2.72	0.45
1:B:30:LEU:HB3	1:B:32:LEU:HD11	1.98	0.45
1:B:39:GLY:HA2	1:B:43:THR:HG21	1.98	0.45
1:B:61:SER:O	1:B:65:PRO:HD2	2.16	0.45
1:B:84:GLU:HG3	1:B:84:GLU:H	1.42	0.45
1:A:58:ILE:HG22	1:A:62:GLN:OE1	2.17	0.45
1:B:125:ASN:N	1:B:153:SER:OG	2.50	0.45
1:B:25:ARG:O	1:B:29:ALA:CB	2.63	0.45
1:A:19:ILE:HD12	1:A:126:TRP:HH2	1.82	0.45
1:B:125:ASN:O	1:B:154:CYS:HB3	2.16	0.45
1:A:325:PRO:HB3	1:B:138:GLN:HA	1.99	0.45
1:B:364:ASP:HA	1:B:365:PRO:HD3	1.76	0.45
1:A:491:THR:OG1	1:A:517:HIS:HD2	2.00	0.45
1:B:17:PRO:O	1:B:18:SER:C	2.53	0.45
1:B:26:SER:CA	1:B:29:ALA:HB3	2.46	0.45
1:A:238:GLY:HA3	1:A:250:PHE:CE1	2.51	0.45
1:A:507:GLU:H	1:A:507:GLU:HG2	1.41	0.45
1:A:60:PHE:C	1:A:62:GLN:H	2.20	0.45
1:B:112:LEU:HD23	1:B:117:PHE:CE1	2.51	0.45
1:A:484:LEU:HD12	1:B:129:ASP:OD1	2.16	0.45
1:A:430:ASN:HD22	1:A:430:ASN:N	1.87	0.45
1:A:8:PHE:HB2	1:A:14:LEU:HD11	1.99	0.44
1:A:215:LYS:HA	1:A:219:THR:O	2.17	0.44
1:A:275:GLN:NE2	1:A:526:GLN:HB3	2.32	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:TYR:HB2	1:A:427:ILE:HD12	1.99	0.44
1:A:52:GLN:HA	1:A:55:LYS:HB2	1.99	0.44
1:B:275:GLN:NE2	1:B:526:GLN:HB3	2.32	0.44
1:A:139:MET:HG2	1:A:143:LEU:HD12	1.98	0.44
1:A:183:LEU:CD1	1:A:201:ILE:HB	2.46	0.44
1:B:334:TRP:O	1:B:337:VAL:HB	2.17	0.44
1:A:127:LEU:N	1:A:127:LEU:HD12	2.32	0.44
1:A:155:GLN:CA	1:A:155:GLN:OE1	2.51	0.44
1:A:322:LEU:HD12	1:B:236:SER:HB2	1.99	0.44
1:A:380:ASN:CB	1:A:419:HIS:O	2.65	0.44
1:B:216:VAL:HG12	1:B:217:THR:OG1	2.17	0.44
1:B:71:TYR:HE1	1:B:88:ILE:HD13	1.83	0.44
1:A:165:ILE:H	1:A:165:ILE:HG13	1.33	0.44
1:A:133:ARG:CG	1:B:348:GLU:HA	2.42	0.44
1:B:54:MET:HB2	1:B:159:ILE:HG21	1.99	0.44
1:A:125:ASN:O	1:A:126:TRP:HB3	2.16	0.44
1:B:144:SER:OG	1:B:145:GLN:NE2	2.44	0.44
1:B:162:GLU:O	1:B:165:ILE:CD1	2.66	0.44
1:B:206:THR:O	1:B:207:ALA:CB	2.66	0.44
1:B:230:CYS:HB3	1:B:277:PRO:HG3	2.00	0.44
1:B:262:CYS:O	1:B:272:TRP:HZ2	2.00	0.44
1:B:30:LEU:HD11	1:B:83:PRO:CG	2.48	0.44
1:A:346:TYR:O	1:A:350:VAL:HG23	2.17	0.44
1:A:381:TYR:CB	1:A:427:ILE:HD12	2.48	0.44
1:B:121:ILE:HB	1:B:150:LEU:HD12	2.00	0.44
1:B:154:CYS:SG	1:B:154:CYS:O	2.76	0.44
1:B:190:LEU:HD11	1:B:202:LEU:HA	2.00	0.44
1:B:512:PHE:N	1:B:512:PHE:CD2	2.84	0.44
1:B:76:LYS:HE2	1:B:76:LYS:O	2.17	0.44
1:A:210:LEU:C	1:A:212:GLU:H	2.22	0.44
1:A:420:LYS:O	1:A:424:ILE:HG12	2.17	0.44
1:B:210:LEU:O	1:B:214:GLU:CB	2.66	0.44
1:B:68:ASP:O	1:B:71:TYR:HB2	2.18	0.44
1:A:122:VAL:HG13	1:A:182:PHE:HE1	1.82	0.44
1:A:394:GLU:OE1	1:A:427:ILE:HG22	2.17	0.44
1:A:534:ASN:O	1:A:535:GLN:C	2.54	0.44
1:B:107:GLN:CA	1:B:107:GLN:HE21	2.30	0.44
1:B:5:VAL:CG1	1:B:180:VAL:HB	2.41	0.44
1:A:16:LEU:HB3	1:A:17:PRO:HA	1.99	0.43
1:A:208:SER:C	1:A:210:LEU:N	2.66	0.43
1:A:334:TRP:O	1:A:337:VAL:HB	2.18	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:VAL:HG23	1:A:6:ALA:N	2.32	0.43
1:B:19:ILE:HA	1:B:19:ILE:HD13	1.89	0.43
1:B:300:PRO:HG2	1:B:305:GLU:CG	2.26	0.43
1:A:102:ASN:HD22	1:A:102:ASN:C	2.22	0.43
1:A:158:MET:HB3	1:A:164:GLN:HG3	2.00	0.43
1:B:183:LEU:HD13	1:B:201:ILE:HB	2.00	0.43
1:A:209:ALA:HA	1:A:212:GLU:HB2	2.01	0.43
1:A:60:PHE:O	1:A:62:GLN:N	2.50	0.43
1:B:215:LYS:O	1:B:219:THR:O	2.37	0.43
1:B:466:ARG:H	1:B:466:ARG:HG2	1.49	0.43
1:A:113:LYS:HE2	1:A:113:LYS:HB3	1.86	0.43
1:A:329:PHE:O	1:A:353:VAL:HA	2.18	0.43
1:A:365:PRO:HG3	1:A:479:LEU:HD13	2.00	0.43
1:B:50:THR:HG22	1:B:63:TRP:NE1	2.33	0.43
1:A:276:ILE:HD11	1:A:288:ALA:HB2	1.99	0.43
1:A:426:GLY:CA	1:A:429:VAL:HG23	2.49	0.43
1:B:119:THR:CG2	1:B:147:PHE:HA	2.46	0.43
1:B:41:TYR:HB3	1:B:42:GLN:H	1.63	0.43
1:A:8:PHE:HB2	1:A:14:LEU:CD1	2.49	0.43
1:A:222:PRO:HG2	1:A:225:PRO:HB3	1.99	0.43
1:A:230:CYS:HB3	1:A:277:PRO:HD3	2.01	0.43
1:B:105:MET:O	1:B:108:ALA:HB3	2.19	0.43
1:B:276:ILE:CB	1:B:277:PRO:HD3	2.49	0.43
1:B:263:HIS:HD2	1:B:291:MET:HG2	1.74	0.43
1:B:5:VAL:CG2	1:B:6:ALA:N	2.81	0.43
1:B:278:ALA:HA	1:B:281:GLN:NE2	2.34	0.43
1:B:373:ILE:HG22	1:B:383:LEU:HD11	2.00	0.43
1:A:207:ALA:HA	1:A:210:LEU:HB3	2.00	0.43
1:B:222:PRO:CB	1:B:225:PRO:HG3	2.47	0.43
1:B:358:THR:HG22	1:B:359:PRO:O	2.19	0.43
1:B:511:PRO:C	1:B:513:LEU:N	2.72	0.43
1:A:481:ARG:HG2	1:B:57:LYS:O	2.19	0.43
1:B:265:PHE:HA	1:B:266:PRO:HA	1.87	0.43
1:A:373:ILE:HG22	1:A:383:LEU:HD11	2.00	0.42
1:B:222:PRO:HA	1:B:223:GLU:OE2	2.19	0.42
1:A:107:GLN:O	1:A:108:ALA:C	2.57	0.42
1:A:127:LEU:HD12	1:A:127:LEU:H	1.84	0.42
1:A:220:GLN:HB2	1:A:220:GLN:HE21	1.58	0.42
1:B:6:ALA:HA	1:B:181:VAL:HG13	2.01	0.42
1:A:111:ALA:O	1:A:114:LYS:N	2.53	0.42
1:A:483:ILE:HD12	1:A:510:ILE:HD11	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:PHE:O	1:A:63:TRP:HB2	2.20	0.42
1:A:50:THR:HA	1:A:63:TRP:HZ2	1.83	0.42
1:B:33:PRO:HG3	1:B:80:ALA:HB2	2.01	0.42
1:A:205:ASN:O	1:A:207:ALA:N	2.52	0.42
1:A:303:ILE:C	1:A:305:GLU:N	2.72	0.42
1:A:90:GLN:CG	1:A:91:ILE:N	2.82	0.42
1:B:30:LEU:HD11	1:B:83:PRO:HG3	2.01	0.42
1:A:226:LEU:CD2	1:A:226:LEU:N	2.82	0.42
1:A:490:VAL:HA	1:A:516:GLY:O	2.20	0.42
1:B:119:THR:HG22	1:B:148:ASP:OD1	2.20	0.42
1:B:122:VAL:HG22	1:B:160:LYS:HE2	2.01	0.42
1:B:187:GLY:HA2	1:B:190:LEU:HB2	2.01	0.42
1:B:8:PHE:HD1	1:B:120:CYS:O	2.03	0.42
1:A:181:VAL:HG22	1:A:181:VAL:O	2.19	0.42
1:B:13:VAL:CG2	1:B:14:LEU:N	2.83	0.42
1:B:64:VAL:CB	1:B:65:PRO:CD	2.88	0.42
1:B:36:PHE:CE2	1:B:82:LEU:HD13	2.54	0.42
1:A:232:PRO:HD2	1:A:233:ASN:N	2.11	0.42
1:A:243:LYS:O	1:A:244:PRO:C	2.58	0.42
1:B:63:TRP:CE2	1:B:67:MET:HG3	2.55	0.42
1:B:112:LEU:HA	1:B:115:LYS:HB3	2.02	0.42
1:B:367:VAL:O	1:B:368:SER:C	2.58	0.42
1:B:180:VAL:HG22	1:B:198:MET:HG2	2.01	0.42
1:B:187:GLY:O	1:B:190:LEU:HB2	2.19	0.42
1:B:214:GLU:HG3	1:B:221:PHE:CE1	2.54	0.42
1:B:25:ARG:HH11	1:B:25:ARG:HG2	1.84	0.42
1:B:511:PRO:O	1:B:513:LEU:N	2.52	0.42
1:A:8:PHE:O	1:A:121:ILE:HA	2.20	0.42
1:A:276:ILE:CB	1:A:277:PRO:HD3	2.50	0.42
1:B:303:ILE:C	1:B:305:GLU:N	2.73	0.42
1:B:350:VAL:HG13	1:B:352:ALA:O	2.20	0.42
1:B:369:PRO:O	1:B:373:ILE:CD1	2.68	0.42
1:A:277:PRO:O	1:A:280:ALA:N	2.53	0.41
1:A:422:THR:O	1:A:423:GLU:CB	2.56	0.41
1:A:61:SER:C	1:A:63:TRP:N	2.73	0.41
1:A:92:PHE:O	1:A:95:ALA:HB3	2.20	0.41
1:B:490:VAL:HA	1:B:516:GLY:O	2.20	0.41
1:A:137:ALA:HB1	1:B:325:PRO:O	2.20	0.41
1:A:180:VAL:HG22	1:A:198:MET:HG2	2.02	0.41
1:A:380:ASN:OD1	1:A:422:THR:N	2.48	0.41
1:B:122:VAL:HG22	1:B:122:VAL:O	2.20	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:ALA:O	1:B:209:ALA:N	2.53	0.41
1:B:21:GLY:C	1:B:25:ARG:HD3	2.40	0.41
1:B:243:LYS:O	1:B:244:PRO:C	2.58	0.41
1:A:10:LEU:HD12	1:A:10:LEU:HA	1.80	0.41
1:A:511:PRO:C	1:A:513:LEU:N	2.74	0.41
1:B:122:VAL:CA	1:B:151:ILE:HG13	2.50	0.41
1:B:230:CYS:SG	1:B:230:CYS:O	2.77	0.41
1:B:303:ILE:HG21	1:B:466:ARG:HB2	2.03	0.41
1:B:346:TYR:O	1:B:350:VAL:HG23	2.19	0.41
1:B:380:ASN:HB3	1:B:418:VAL:O	2.20	0.41
1:B:481:ARG:HH11	1:B:481:ARG:HD2	1.70	0.41
1:A:358:THR:HG22	1:A:359:PRO:O	2.19	0.41
1:A:380:ASN:HB3	1:A:418:VAL:O	2.20	0.41
1:B:167:ASN:O	1:B:171:ASP:OD2	2.39	0.41
1:A:205:ASN:C	1:A:207:ALA:N	2.70	0.41
1:B:263:HIS:HE1	1:B:294:TYR:CD2	2.38	0.41
1:A:303:ILE:HG21	1:A:466:ARG:HB2	2.03	0.41
1:B:198:MET:HE2	1:B:198:MET:HB2	2.00	0.41
1:B:378:VAL:HG13	1:B:378:VAL:O	2.20	0.41
1:B:54:MET:HA	1:B:125:ASN:O	2.21	0.41
1:A:228:VAL:HA	1:A:229:PRO:HD3	1.79	0.41
1:A:280:ALA:HA	1:A:284:PHE:O	2.20	0.41
1:B:56:GLY:HA2	1:B:127:LEU:HD11	2.03	0.41
1:B:206:THR:O	1:B:207:ALA:HB3	2.20	0.41
1:B:199:VAL:HG12	1:B:201:ILE:HD11	2.03	0.41
1:B:281:GLN:HE21	1:B:281:GLN:HB2	1.62	0.41
1:B:396:GLU:OE1	1:B:458:PHE:N	2.54	0.41
1:B:420:LYS:O	1:B:421:ALA:C	2.59	0.41
1:B:71:TYR:CE1	1:B:88:ILE:HD13	2.55	0.41
1:A:110:ILE:HD13	1:A:228:VAL:HG12	2.03	0.41
1:A:484:LEU:CD1	1:B:61:SER:OG	2.69	0.41
1:B:20:ALA:HA	1:B:23:PHE:HB2	2.03	0.41
1:A:170:LEU:HD21	1:A:177:PRO:HA	2.03	0.40
1:A:191:LYS:CB	1:A:192:PRO:CD	2.99	0.40
1:A:191:LYS:HB2	1:A:192:PRO:HD3	2.03	0.40
1:A:289:ILE:CG2	1:A:290:ASP:N	2.84	0.40
1:B:11:ASP:OD2	1:B:19:ILE:HG12	2.22	0.40
1:B:30:LEU:HA	1:B:30:LEU:HD23	1.77	0.40
1:B:380:ASN:CB	1:B:419:HIS:O	2.69	0.40
1:B:73:LYS:O	1:B:77:ALA:HB3	2.20	0.40
1:A:278:ALA:O	1:A:282:ALA:N	2.53	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:ILE:HA	1:A:325:PRO:HD3	1.94	0.40
1:A:58:ILE:HG22	1:A:62:GLN:CB	2.47	0.40
1:B:280:ALA:HA	1:B:284:PHE:O	2.20	0.40
1:B:408:ARG:HA	1:B:438:SER:OG	2.21	0.40
1:B:54:MET:HB2	1:B:159:ILE:HG22	2.03	0.40
1:A:4:ARG:HH11	1:A:4:ARG:HB2	1.86	0.40
1:B:303:ILE:CG2	1:B:466:ARG:HB2	2.52	0.40
1:A:334:TRP:CE3	2:A:1100:CPU:H4	2.55	0.40
1:A:278:ALA:HA	1:A:281:GLN:NE2	2.36	0.40
1:A:493:GLU:HG2	1:A:494:LYS:HG2	2.03	0.40
1:A:496:ILE:N	1:A:496:ILE:CD1	2.70	0.40
1:B:277:PRO:O	1:B:280:ALA:N	2.54	0.40
1:B:538:ILE:O	1:B:539:LYS:C	2.59	0.40
1:A:401:ARG:O	1:A:402:THR:C	2.60	0.40
1:A:303:ILE:CG2	1:A:466:ARG:HB2	2.52	0.40
1:A:511:PRO:O	1:A:513:LEU:N	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	481/554 (87%)	392 (82%)	59 (12%)	30 (6%)	2	4
1	B	539/554 (97%)	431 (80%)	77 (14%)	31 (6%)	2	5
All	All	1020/1108 (92%)	823 (81%)	136 (13%)	61 (6%)	2	5

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	207	ALA

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	231	ASN
1	A	244	PRO
1	A	256	GLY
1	A	415	PHE
1	A	423	GLU
1	B	41	TYR
1	B	75	SER
1	B	78	CYS
1	B	207	ALA
1	B	208	SER
1	B	222	PRO
1	B	232	PRO
1	B	244	PRO
1	B	256	GLY
1	B	415	PHE
1	B	421	ALA
1	A	18	SER
1	A	98	ALA
1	A	158	MET
1	A	466	ARG
1	A	520	ASP
1	B	25	ARG
1	B	44	GLU
1	B	80	ALA
1	B	205	ASN
1	B	386	GLN
1	B	466	ARG
1	B	520	ASP
1	A	154	CYS
1	A	288	ALA
1	A	402	THR
1	B	63	TRP
1	A	126	TRP
1	A	210	LEU
1	A	232	PRO
1	A	386	GLN
1	A	496	ILE
1	B	288	ALA
1	B	402	THR
1	B	434	ASP
1	A	125	ASN
1	A	206	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	230	CYS
1	A	277	PRO
1	B	34	ARG
1	B	203	VAL
1	B	219	THR
1	B	277	PRO
1	B	432	PRO
1	B	496	ILE
1	A	187	GLY
1	A	295	GLY
1	B	295	GLY
1	A	229	PRO
1	A	12	GLY
1	B	216	VAL
1	A	91	ILE
1	A	266	PRO
1	B	266	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	424/480 (88%)	322 (76%)	102 (24%)	1	2
1	B	468/480 (98%)	342 (73%)	126 (27%)	0	1
All	All	892/960 (93%)	664 (74%)	228 (26%)	0	2

All (228) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	5	VAL
1	A	18	SER
1	A	19	ILE
1	A	53	LEU
1	A	55	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	58	ILE
1	A	61	SER
1	A	90	GLN
1	A	91	ILE
1	A	92	PHE
1	A	93	SER
1	A	94	GLN
1	A	99	ARG
1	A	102	ASN
1	A	103	ARG
1	A	119	THR
1	A	122	VAL
1	A	125	ASN
1	A	128	ASP
1	A	129	ASP
1	A	131	ASP
1	A	136	LEU
1	A	152	GLU
1	A	154	CYS
1	A	155	GLN
1	A	158	MET
1	A	164	GLN
1	A	165	ILE
1	A	169	LEU
1	A	170	LEU
1	A	174	LYS
1	A	181	VAL
1	A	184	ASP
1	A	200	THR
1	A	202	LEU
1	A	204	HIS
1	A	208	SER
1	A	213	LEU
1	A	214	GLU
1	A	216	VAL
1	A	220	GLN
1	A	221	PHE
1	A	223	GLU
1	A	226	LEU
1	A	230	CYS
1	A	231	ASN
1	A	247	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	248	LEU
1	A	268	SER
1	A	275	GLN
1	A	290	ASP
1	A	297	SER
1	A	299	SER
1	A	310	LEU
1	A	313	LYS
1	A	315	MET
1	A	322	LEU
1	A	349	ARG
1	A	351	ARG
1	A	353	VAL
1	A	361	MET
1	A	366	ASP
1	A	368	SER
1	A	370	MET
1	A	371	LYS
1	A	378	VAL
1	A	383	LEU
1	A	398	ASN
1	A	404	LYS
1	A	408	ARG
1	A	412	GLU
1	A	413	THR
1	A	420	LYS
1	A	422	THR
1	A	423	GLU
1	A	430	ASN
1	A	439	LYS
1	A	440	ILE
1	A	447	GLU
1	A	451	GLN
1	A	466	ARG
1	A	468	THR
1	A	470	ARG
1	A	475	SER
1	A	485	VAL
1	A	488	LEU
1	A	494	LYS
1	A	497	VAL
1	A	501	GLU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	502	MET
1	A	504	LYS
1	A	505	ASN
1	A	507	GLU
1	A	512	PHE
1	A	513	LEU
1	A	519	GLU
1	A	526	GLN
1	A	531	THR
1	A	539	LYS
1	A	542	GLN
1	A	544	GLU
1	B	4	ARG
1	B	5	VAL
1	B	8	PHE
1	B	10	LEU
1	B	13	VAL
1	B	16	LEU
1	B	23	PHE
1	B	24	ARG
1	B	25	ARG
1	B	30	LEU
1	B	35	ASP
1	B	41	TYR
1	B	42	GLN
1	B	43	THR
1	B	47	GLU
1	B	53	LEU
1	B	61	SER
1	B	67	MET
1	B	69	GLU
1	B	70	SER
1	B	71	TYR
1	B	72	ARG
1	B	73	LYS
1	B	74	SER
1	B	76	LYS
1	B	78	CYS
1	B	81	ASN
1	B	84	GLU
1	B	85	ASN
1	B	91	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	94	GLN
1	B	99	ARG
1	B	100	SER
1	B	101	ILE
1	B	102	ASN
1	B	103	ARG
1	B	106	LEU
1	B	107	GLN
1	B	110	ILE
1	B	118	THR
1	B	122	VAL
1	B	125	ASN
1	B	127	LEU
1	B	131	ASP
1	B	132	LYS
1	B	133	ARG
1	B	135	SER
1	B	136	LEU
1	B	151	ILE
1	B	154	CYS
1	B	155	GLN
1	B	158	MET
1	B	159	ILE
1	B	164	GLN
1	B	165	ILE
1	B	180	VAL
1	B	181	VAL
1	B	183	LEU
1	B	198	MET
1	B	200	THR
1	B	201	ILE
1	B	202	LEU
1	B	206	THR
1	B	208	SER
1	B	210	LEU
1	B	213	LEU
1	B	217	THR
1	B	219	THR
1	B	228	VAL
1	B	233	ASN
1	B	247	ARG
1	B	248	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	268	SER
1	B	275	GLN
1	B	290	ASP
1	B	297	SER
1	B	299	SER
1	B	310	LEU
1	B	313	LYS
1	B	315	MET
1	B	322	LEU
1	B	349	ARG
1	B	351	ARG
1	B	353	VAL
1	B	361	MET
1	B	366	ASP
1	B	368	SER
1	B	370	MET
1	B	371	LYS
1	B	378	VAL
1	B	383	LEU
1	B	398	ASN
1	B	404	LYS
1	B	408	ARG
1	B	412	GLU
1	B	413	THR
1	B	422	THR
1	B	424	ILE
1	B	427	ILE
1	B	428	LEU
1	B	431	THR
1	B	439	LYS
1	B	440	ILE
1	B	447	GLU
1	B	451	GLN
1	B	466	ARG
1	B	468	THR
1	B	470	ARG
1	B	475	SER
1	B	485	VAL
1	B	488	LEU
1	B	494	LYS
1	B	497	VAL
1	B	501	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	502	MET
1	B	504	LYS
1	B	505	ASN
1	B	507	GLU
1	B	512	PHE
1	B	513	LEU
1	B	519	GLU
1	B	526	GLN
1	B	531	THR
1	B	539	LYS
1	B	542	GLN
1	B	544	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	102	ASN
1	A	107	GLN
1	A	125	ASN
1	A	146	HIS
1	A	164	GLN
1	A	205	ASN
1	A	220	GLN
1	A	275	GLN
1	A	281	GLN
1	A	332	HIS
1	A	386	GLN
1	A	430	ASN
1	A	517	HIS
1	B	81	ASN
1	B	90	GLN
1	B	107	GLN
1	B	146	HIS
1	B	167	ASN
1	B	178	ASN
1	B	204	HIS
1	B	231	ASN
1	B	233	ASN
1	B	275	GLN
1	B	281	GLN
1	B	332	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	517	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	CPU	A	1100	-	20,20,20	1.78	8 (40%)	23,24,24	1.40	3 (13%)
2	CPU	B	1200	-	20,20,20	1.94	10 (50%)	23,24,24	1.69	5 (21%)

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
2	CPU	A	1100	-	-	0/11/19/19	0/2/2/2
2	CPU	B	1200	-	-	0/11/19/19	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1200	CPU	C15-C16	2.03	1.58	1.53
2	A	1100	CPU	C14-C13	2.05	1.59	1.51
2	B	1200	CPU	C5-C6	2.07	1.43	1.38
2	A	1100	CPU	C4-C3	2.08	1.43	1.38
2	B	1200	CPU	C3-C2	2.10	1.43	1.38
2	B	1200	CPU	C15-C14	2.17	1.60	1.51
2	B	1200	CPU	C16-C11	2.23	1.57	1.51
2	A	1100	CPU	C13-C12	2.24	1.59	1.53
2	B	1200	CPU	C13-C12	2.26	1.59	1.53
2	A	1100	CPU	C15-C16	2.27	1.59	1.53
2	B	1200	CPU	C4-C5	2.28	1.43	1.38
2	A	1100	CPU	C12-C11	2.31	1.57	1.51
2	A	1100	CPU	C16-C11	2.38	1.57	1.51
2	B	1200	CPU	C12-C11	2.42	1.57	1.51
2	B	1200	CPU	C4-C3	2.78	1.44	1.38
2	A	1100	CPU	C4-C5	2.87	1.44	1.38
2	A	1100	CPU	C1-C6	3.26	1.45	1.38
2	B	1200	CPU	C1-C6	3.75	1.46	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1200	CPU	O1-C10-N1	-3.88	115.55	122.62
2	A	1100	CPU	O1-C10-N1	-3.60	116.06	122.62
2	B	1200	CPU	N1-C10-N2	2.03	121.07	115.83
2	B	1200	CPU	C8-C7-C6	2.18	121.85	113.67
2	A	1100	CPU	N1-C10-N2	2.25	121.64	115.83
2	A	1100	CPU	C8-C7-C6	2.79	124.15	113.67
2	B	1200	CPU	C13-C12-C11	3.04	115.56	111.11
2	B	1200	CPU	C11-N2-C10	3.50	129.44	123.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1100	CPU	5	0
2	B	1200	CPU	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.