



## Full wwPDB EM Validation Report ⓘ

Feb 25, 2024 – 07:29 AM EST

PDB ID : 6XF7  
EMDB ID : EMD-22165  
Title : SLP  
Authors : Sutton, G.; Sun, D.P.; Fu, X.F.; Kotecha, A.; Hecksel, G.W.; Clare, D.K.;  
Zhang, P.; Stuart, D.; Boyce, M.  
Deposited on : 2020-06-15  
Resolution : 6.60 Å(reported)

This is a Full wwPDB EM 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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

EMDB validation analysis : 0.0.1.dev70  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

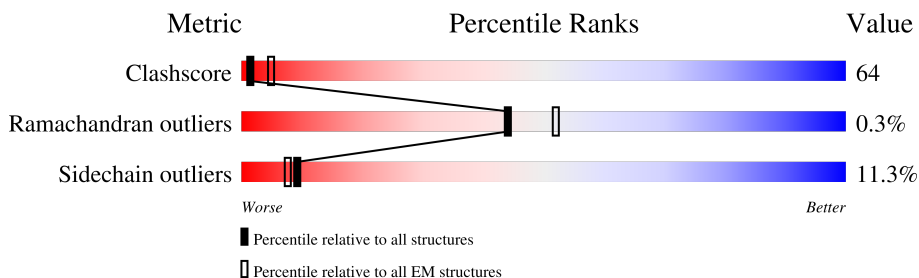
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.60 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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 EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	1059	
1	C	1059	

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 16454 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

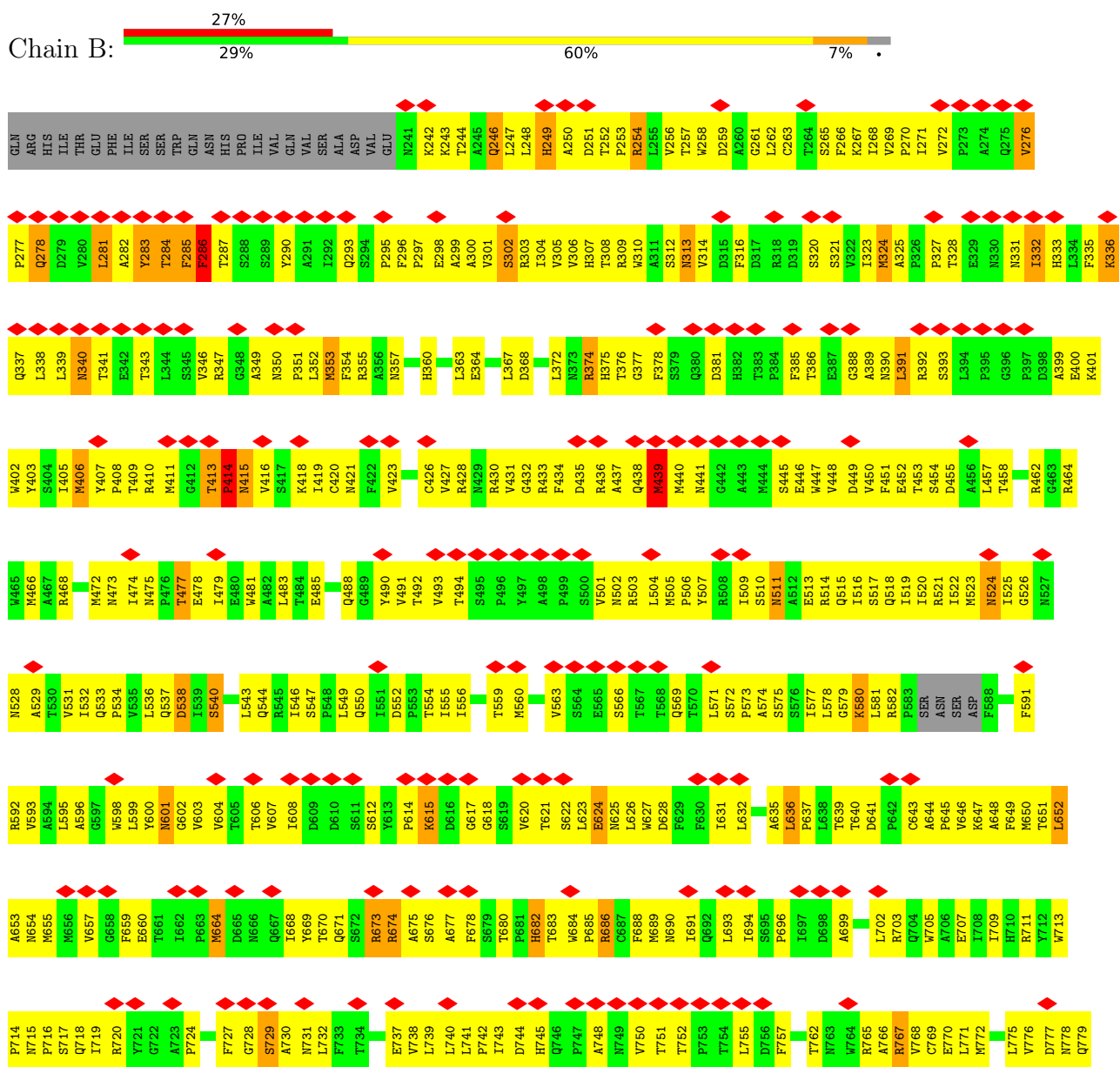
- Molecule 1 is a protein called Lambda 1 protein.

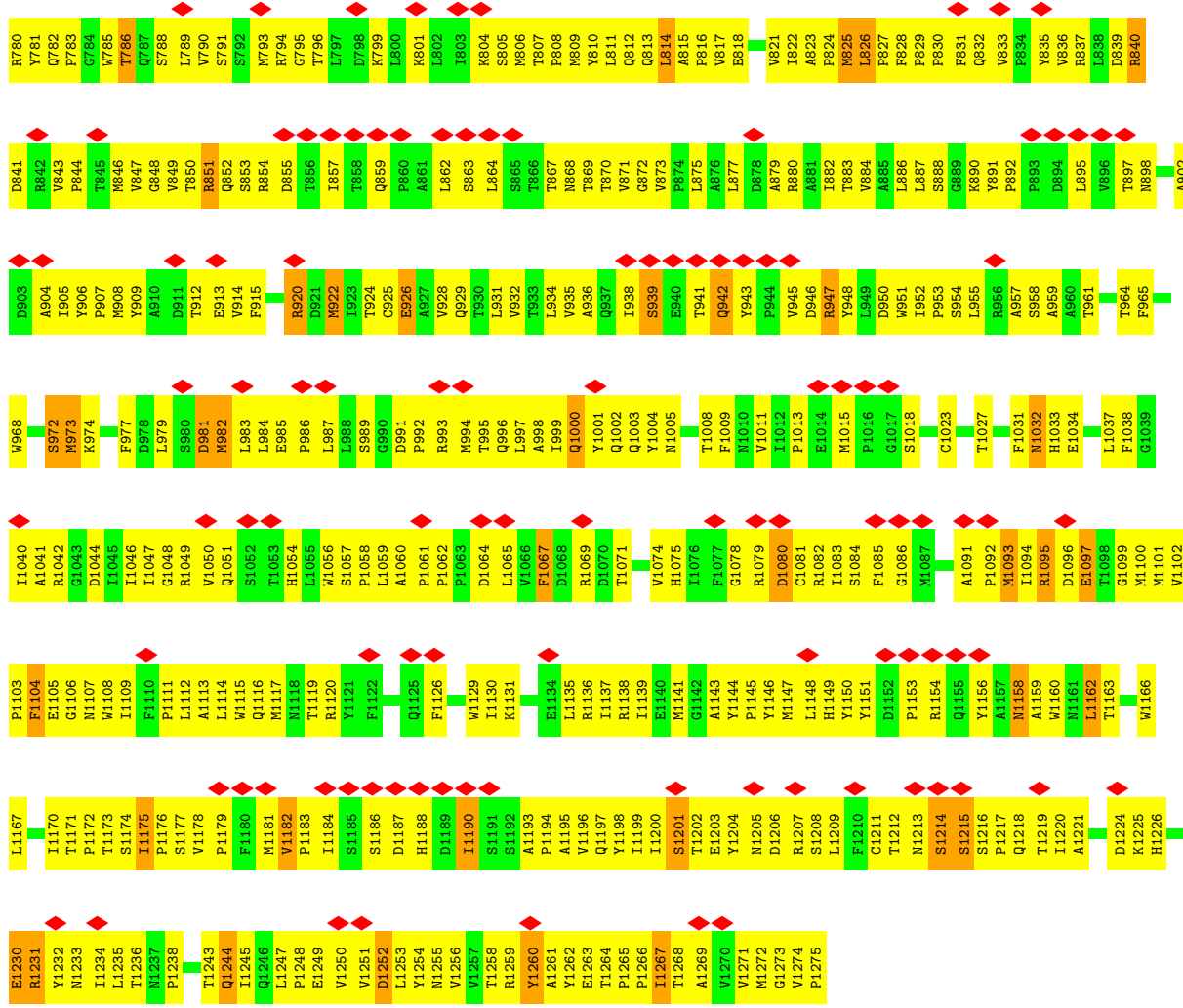
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	1031	Total	C	N	O	S	0	0
			8143	5208	1375	1510	50		
1	C	1051	Total	C	N	O	S	0	0
			8311	5314	1407	1540	50		

### 3 Residue-property plots

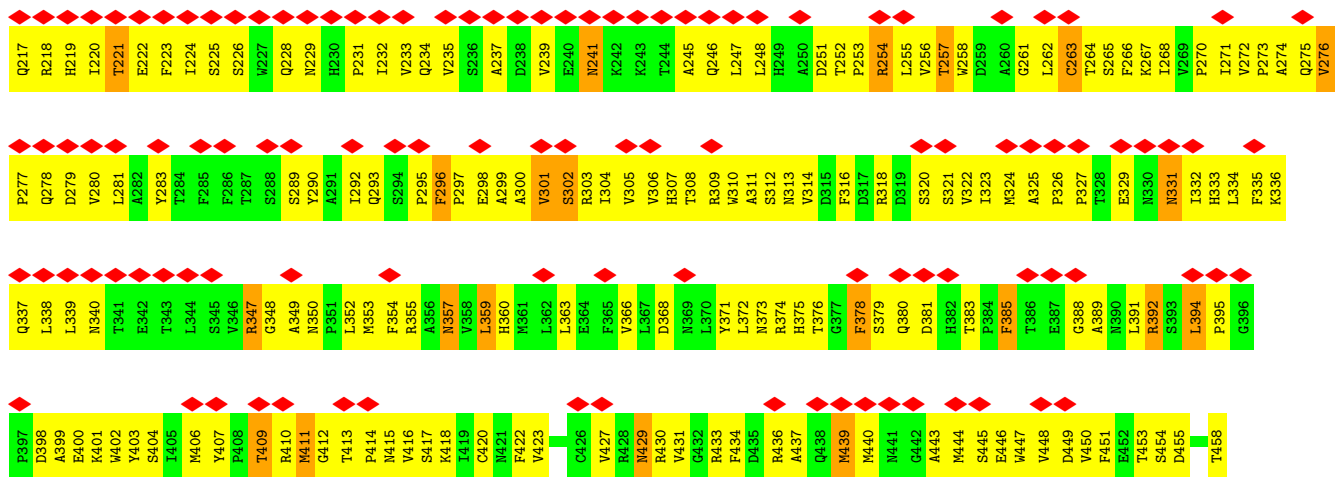
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

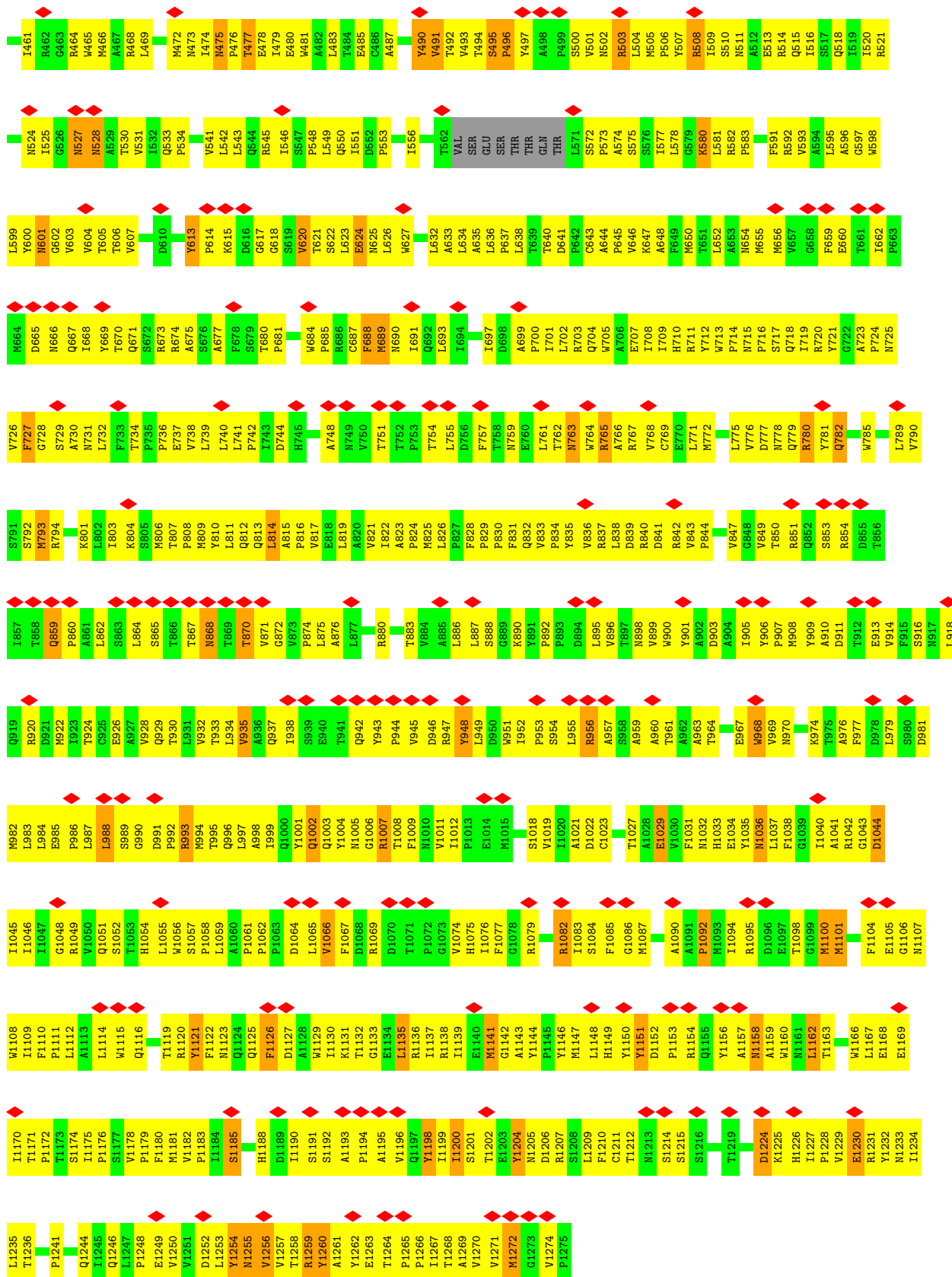
#### • Molecule 1: Lambda 1 protein





• Molecule 1: Lambda 1 protein





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of subtomograms used	2683	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	10.927	Depositor
Minimum map value	-5.906	Depositor
Average map value	0.059	Depositor
Map value standard deviation	0.498	Depositor
Recommended contour level	3.0	Depositor
Map size ( $\text{\AA}$ )	696.6, 696.6, 696.6	wwPDB
Map dimensions	387, 387, 387	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.8, 1.8, 1.8	Depositor

## 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	B	0.61	0/8363	0.70	1/11454 (0.0%)
1	C	0.61	0/8537	0.71	1/11693 (0.0%)
All	All	0.61	0/16900	0.70	2/23147 (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	B	284	THR	N-CA-C	-8.20	88.85	111.00
1	C	496	PRO	N-CA-C	-5.60	97.54	112.10

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	B	8143	0	8063	999	0
1	C	8311	0	8215	1116	0
All	All	16454	0	16278	2095	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 64.

All (2095) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:LEU:HD22	1:C:395:PRO:CD	1.28	1.60
1:C:276:VAL:CG2	1:C:277:PRO:HD2	1.50	1.40
1:C:276:VAL:HG23	1:C:277:PRO:CD	1.65	1.26
1:C:394:LEU:CD2	1:C:395:PRO:HD2	1.67	1.22
1:C:713:TRP:CE3	1:C:714:PRO:CD	2.24	1.20
1:C:713:TRP:CE3	1:C:714:PRO:HD2	1.77	1.20
1:C:394:LEU:CD2	1:C:395:PRO:CD	2.22	1.17
1:C:348:GLY:HA2	1:C:1176:PRO:HA	1.29	1.15
1:C:268:ILE:HA	1:C:304:ILE:HA	1.24	1.14
1:C:253:PRO:HB3	1:C:977:PHE:HB3	1.26	1.14
1:C:833:VAL:HG12	1:C:834:PRO:HD2	1.33	1.10
1:C:1171:THR:HG23	1:C:1172:PRO:HD2	1.29	1.10
1:B:717:SER:HB3	1:B:744:ASP:HA	1.20	1.09
1:C:502:ASN:HB2	1:C:1262:TYR:HA	1.31	1.09
1:C:713:TRP:CD2	1:C:714:PRO:HD2	1.87	1.09
1:B:636:LEU:HD12	1:B:648:ALA:HB2	1.35	1.08
1:B:1212:THR:HG23	1:B:1225:LYS:HB3	1.32	1.08
1:B:617:GLY:HA3	1:B:654:ASN:HB3	1.35	1.07
1:C:841:ASP:HB3	1:C:1005:ASN:HB3	1.33	1.07
1:C:276:VAL:CG2	1:C:277:PRO:CD	2.28	1.07
1:C:268:ILE:HG12	1:C:304:ILE:HG12	1.36	1.07
1:B:524:ASN:HB3	1:B:986:PRO:HG3	1.37	1.06
1:C:394:LEU:HD22	1:C:395:PRO:HD3	1.29	1.06
1:C:278:GLN:HG2	1:C:415:ASN:HB3	1.37	1.06
1:C:833:VAL:CG1	1:C:834:PRO:HD2	1.85	1.06
1:C:713:TRP:CE3	1:C:714:PRO:HD3	1.92	1.05
1:C:494:THR:HG22	1:C:496:PRO:HD3	1.39	1.05
1:B:375:HIS:HB3	1:B:1261:ALA:HB2	1.39	1.05
1:C:602:GLY:H	1:C:832:GLN:HA	1.19	1.04
1:C:755:LEU:HD11	1:C:804:LYS:HE3	1.34	1.04
1:B:1079:ARG:HA	1:B:1114:LEU:HD21	1.39	1.03
1:C:1241:PRO:HG2	1:C:1244:GLN:HB2	1.35	1.02
1:C:754:THR:HG22	1:C:806:MET:HG2	1.42	1.02
1:C:1056:TRP:HB2	1:C:1061:PRO:HA	1.38	1.02
1:B:282:ALA:HB1	1:C:1084:SER:HA	1.40	1.01
1:B:303:ARG:HG2	1:B:1209:LEU:HA	1.43	1.00
1:B:1049:ARG:HB3	1:B:1049:ARG:NH1	1.73	1.00
1:B:434:PHE:H	1:B:450:VAL:HA	1.22	1.00
1:C:375:HIS:HB3	1:C:1261:ALA:HB2	1.41	0.99
1:B:327:PRO:HB2	1:B:1148:LEU:HG	1.44	0.99
1:C:731:ASN:HB2	1:C:736:PRO:HA	1.44	0.99
1:C:543:LEU:HA	1:C:546:ILE:HG22	1.40	0.99

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:724:PRO:HA	1:C:728:GLY:HA2	1.40	0.99
1:B:827:PRO:HA	1:B:914:VAL:HG13	1.45	0.98
1:B:338:LEU:HD23	1:B:339:LEU:HG	1.41	0.98
1:B:1069:ARG:HA	1:B:1109:ILE:HG13	1.43	0.98
1:C:1211:CYS:HA	1:C:1225:LYS:HG3	1.45	0.98
1:C:276:VAL:HB	1:C:277:PRO:HD3	1.44	0.98
1:B:1171:THR:HG23	1:B:1172:PRO:HD2	1.43	0.97
1:C:352:LEU:HD22	1:C:955:LEU:HB3	1.46	0.97
1:C:219:HIS:HA	1:C:235:VAL:HG12	1.43	0.97
1:C:339:LEU:HD12	1:C:353:MET:HB3	1.45	0.97
1:C:810:TYR:HA	1:C:814:LEU:HD23	1.43	0.97
1:B:256:VAL:HG11	1:B:1264:THR:HG21	1.42	0.96
1:C:854:ARG:NH1	1:C:854:ARG:HA	1.78	0.96
1:B:298:GLU:HA	1:B:1214:SER:HB2	1.44	0.96
1:B:1156:TYR:HB2	1:B:1194:PRO:HG2	1.47	0.96
1:C:982:MET:HB2	1:C:985:GLU:HG3	1.47	0.96
1:C:270:PRO:HG3	1:C:297:PRO:HB2	1.46	0.95
1:B:436:ARG:HB2	1:B:448:VAL:HG12	1.46	0.95
1:B:621:THR:HA	1:B:781:TYR:HE1	1.28	0.95
1:B:852:GLN:HA	1:B:995:THR:HA	1.48	0.95
1:B:1163:THR:HG21	1:B:1198:TYR:HB2	1.47	0.95
1:B:409:THR:HG22	1:B:423:VAL:HG13	1.47	0.95
1:B:892:PRO:HD2	1:B:895:LEU:HD22	1.49	0.95
1:C:418:LYS:HD2	1:C:1214:SER:HA	1.48	0.95
1:B:474:ILE:HD13	1:B:507:TYR:HB2	1.49	0.94
1:B:1230:GLU:HB2	1:B:1250:VAL:HG11	1.49	0.94
1:C:276:VAL:CB	1:C:277:PRO:CD	2.45	0.94
1:C:1082:ARG:HG2	1:C:1082:ARG:HH11	1.33	0.94
1:B:691:ILE:H	1:B:691:ILE:HD12	1.30	0.94
1:B:953:PRO:HD2	1:B:1143:ALA:HB3	1.49	0.93
1:B:516:ILE:HG12	1:B:1013:PRO:HB3	1.51	0.93
1:C:453:THR:HA	1:C:1254:TYR:HA	1.48	0.93
1:C:634:LEU:HD23	1:C:883:THR:HG23	1.49	0.93
1:C:360:HIS:CD2	1:C:969:VAL:HG22	2.04	0.92
1:B:446:GLU:HB3	1:B:1262:TYR:HE1	1.32	0.92
1:B:690:ASN:HB3	1:B:693:LEU:HD12	1.51	0.92
1:C:1230:GLU:HB2	1:C:1250:VAL:HG11	1.52	0.91
1:B:478:GLU:HA	1:B:481:TRP:CE3	2.05	0.91
1:C:991:ASP:HA	1:C:993:ARG:NH2	1.85	0.91
1:B:332:ILE:CG2	1:B:347:ARG:HA	2.01	0.91
1:C:278:GLN:HA	1:C:416:VAL:H	1.36	0.90

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:483:LEU:HD13	1:C:493:VAL:HG11	1.52	0.90
1:C:577:ILE:HD13	1:C:627:TRP:HB3	1.50	0.90
1:B:992:PRO:HA	1:B:995:THR:HG23	1.54	0.90
1:B:1145:PRO:HG2	1:B:1177:SER:HA	1.51	0.89
1:C:1035:TYR:HA	1:C:1038:PHE:HB2	1.52	0.89
1:B:608:ILE:HD12	1:B:879:ALA:HB2	1.52	0.89
1:C:1105:GLU:HA	1:C:1135:LEU:HB2	1.53	0.89
1:B:243:LYS:NZ	1:B:828:PHE:HB3	1.87	0.89
1:C:924:THR:HG23	1:C:984:LEU:CD2	2.02	0.89
1:B:256:VAL:HG13	1:B:372:LEU:HD12	1.52	0.89
1:B:295:PRO:HB3	1:B:405:ILE:HA	1.55	0.89
1:C:306:VAL:HB	1:C:324:MET:HB3	1.54	0.89
1:C:602:GLY:N	1:C:832:GLN:HA	1.86	0.88
1:C:1212:THR:HG23	1:C:1225:LYS:HB3	1.53	0.88
1:C:332:ILE:HG13	1:C:336:LYS:HD2	1.52	0.88
1:B:278:GLN:HG2	1:B:281:LEU:HB2	1.56	0.88
1:C:303:ARG:HG2	1:C:1209:LEU:HA	1.55	0.88
1:C:483:LEU:HD12	1:C:493:VAL:HG21	1.53	0.88
1:C:224:ILE:HG23	1:C:1270:VAL:HG13	1.53	0.87
1:C:520:ILE:HD12	1:C:987:LEU:HD21	1.56	0.87
1:C:277:PRO:HG2	1:C:416:VAL:HG21	1.57	0.87
1:B:751:THR:HG21	1:B:898:ASN:HD22	1.40	0.87
1:B:1093:MET:HB2	1:B:1101:MET:HB3	1.57	0.87
1:B:1211:CYS:HA	1:B:1225:LYS:HG3	1.57	0.87
1:C:338:LEU:HD11	1:C:360:HIS:CG	2.09	0.86
1:C:853:SER:H	1:C:995:THR:HB	1.39	0.86
1:C:1075:HIS:HB2	1:C:1108:TRP:CD1	2.10	0.86
1:C:1126:PHE:HA	1:C:1129:TRP:HD1	1.38	0.86
1:B:769:CYS:HA	1:B:772:MET:HE2	1.58	0.86
1:C:277:PRO:HG2	1:C:416:VAL:CG2	2.05	0.86
1:B:600:TYR:CE2	1:B:830:PRO:HA	2.12	0.85
1:B:854:ARG:HG3	1:B:863:SER:HB2	1.57	0.85
1:C:1171:THR:HG23	1:C:1172:PRO:CD	2.05	0.85
1:B:307:HIS:HA	1:B:323:ILE:HG12	1.58	0.85
1:C:280:VAL:HB	1:C:414:PRO:HB3	1.59	0.85
1:C:983:LEU:HG	1:C:984:LEU:HG	1.56	0.84
1:C:1082:ARG:HB2	1:C:1095:ARG:HD3	1.59	0.84
1:C:276:VAL:HB	1:C:277:PRO:CD	2.04	0.84
1:C:1175:ILE:CG1	1:C:1176:PRO:HD2	2.08	0.84
1:B:1108:TRP:HB2	1:B:1137:ILE:HG12	1.60	0.84
1:C:1171:THR:CG2	1:C:1172:PRO:HD2	2.07	0.84

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1056:TRP:HB2	1:B:1061:PRO:HA	1.60	0.84
1:C:1260:TYR:HB2	1:C:1262:TYR:CE1	2.13	0.84
1:B:389:ALA:CB	1:B:431:VAL:HG22	2.08	0.83
1:B:840:ARG:HA	1:B:843:VAL:HG23	1.59	0.83
1:B:259:ASP:HA	1:B:314:VAL:HG12	1.60	0.83
1:B:491:VAL:HG21	1:B:905:ILE:HG21	1.60	0.83
1:B:717:SER:CB	1:B:744:ASP:HA	2.04	0.83
1:B:602:GLY:HA2	1:B:833:VAL:HG13	1.58	0.83
1:C:360:HIS:HD2	1:C:969:VAL:HG22	1.40	0.83
1:B:283:TYR:CD1	1:B:286:PHE:HB2	2.14	0.83
1:C:263:CYS:O	1:C:263:CYS:SG	2.36	0.83
1:B:778:ASN:HB3	1:B:781:TYR:HB3	1.60	0.83
1:C:691:ILE:H	1:C:691:ILE:HD12	1.43	0.82
1:B:285:PHE:HB2	1:C:1083:ILE:HG13	1.60	0.82
1:C:268:ILE:CA	1:C:304:ILE:HA	2.09	0.82
1:C:500:SER:HB3	1:C:503:ARG:HB2	1.61	0.82
1:C:394:LEU:CD2	1:C:395:PRO:HD3	2.00	0.82
1:C:1031:PHE:HA	1:C:1038:PHE:CE1	2.15	0.82
1:B:283:TYR:HB2	1:B:286:PHE:CD1	2.15	0.81
1:B:1074:VAL:CG1	1:B:1109:ILE:HG12	2.09	0.81
1:B:685:PRO:HG2	1:B:688:PHE:CB	2.10	0.81
1:C:754:THR:HA	1:C:809:MET:HE1	1.63	0.81
1:C:1252:ASP:HB2	1:C:1255:ASN:ND2	1.96	0.81
1:B:448:VAL:O	1:B:1258:THR:HA	1.79	0.81
1:C:434:PHE:HB2	1:C:1256:VAL:HG11	1.61	0.81
1:B:246:GLN:HG3	1:B:250:ALA:HB2	1.62	0.81
1:B:283:TYR:CD1	1:B:283:TYR:O	2.34	0.81
1:C:621:THR:HG22	1:C:782:GLN:HA	1.61	0.81
1:B:272:VAL:HG12	1:B:300:ALA:HB3	1.62	0.80
1:C:514:ARG:HB2	1:C:730:ALA:HB2	1.63	0.80
1:B:351:PRO:HA	1:B:354:PHE:CD1	2.16	0.80
1:C:265:SER:CB	1:C:308:THR:HA	2.12	0.80
1:B:778:ASN:HD21	1:B:780:ARG:HG3	1.46	0.80
1:B:1092:PRO:O	1:B:1103:PRO:HA	1.82	0.80
1:C:278:GLN:HA	1:C:416:VAL:N	1.97	0.80
1:C:573:PRO:HB2	1:C:627:TRP:HZ2	1.46	0.80
1:C:982:MET:HB2	1:C:985:GLU:CG	2.12	0.80
1:C:417:SER:HG	1:C:420:CYS:HG	1.28	0.80
1:C:305:VAL:HA	1:C:324:MET:HE1	1.64	0.80
1:C:474:ILE:HD11	1:C:726:VAL:HG22	1.63	0.80
1:C:754:THR:HA	1:C:809:MET:CE	2.11	0.79

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:807:THR:HG21	1:C:886:LEU:HA	1.63	0.79
1:C:717:SER:HB3	1:C:744:ASP:HA	1.64	0.79
1:B:563:VAL:HG22	1:B:799:LYS:HD3	1.64	0.79
1:C:268:ILE:HA	1:C:304:ILE:CA	2.10	0.79
1:C:363:LEU:HD21	1:C:969:VAL:HG13	1.63	0.79
1:C:378:PHE:HA	1:C:392:ARG:HA	1.63	0.79
1:C:436:ARG:HD2	1:C:440:MET:CE	2.13	0.79
1:C:833:VAL:HG12	1:C:834:PRO:CD	2.12	0.79
1:C:1110:PHE:HB2	1:C:1139:ILE:HD13	1.64	0.79
1:B:569:GLN:HA	1:B:569:GLN:NE2	1.97	0.79
1:B:685:PRO:HG2	1:B:688:PHE:HB2	1.64	0.79
1:C:295:PRO:HG3	1:C:404:SER:HB2	1.63	0.79
1:C:732:LEU:HD13	1:C:1011:VAL:HG11	1.63	0.79
1:C:253:PRO:CB	1:C:977:PHE:HB3	2.11	0.79
1:C:1095:ARG:HA	1:C:1101:MET:HA	1.64	0.79
1:B:243:LYS:HZ3	1:B:828:PHE:HB3	1.48	0.79
1:B:806:MET:HB3	1:B:891:TYR:CZ	2.18	0.79
1:C:394:LEU:HD22	1:C:395:PRO:HD2	0.81	0.79
1:C:502:ASN:CB	1:C:1262:TYR:HA	2.12	0.79
1:B:300:ALA:HA	1:B:1213:ASN:H	1.48	0.79
1:B:836:VAL:HB	1:B:839:ASP:HB3	1.65	0.79
1:B:283:TYR:HA	1:B:286:PHE:H	1.47	0.78
1:B:578:LEU:HA	1:B:581:LEU:HD12	1.65	0.78
1:C:232:ILE:HG13	1:C:906:TYR:CE2	2.18	0.78
1:C:300:ALA:HB1	1:C:1185:SER:HB3	1.65	0.78
1:C:1029:GLU:OE1	1:C:1029:GLU:HA	1.82	0.78
1:C:984:LEU:HB3	1:C:987:LEU:HD12	1.65	0.78
1:C:1166:TRP:CD1	1:C:1179:PRO:HD3	2.19	0.78
1:B:266:PHE:CD2	1:B:306:VAL:HG22	2.17	0.78
1:B:283:TYR:HD1	1:B:286:PHE:HB2	1.45	0.78
1:B:446:GLU:HB3	1:B:1262:TYR:CE1	2.16	0.78
1:C:350:ASN:HA	1:C:1174:SER:HB2	1.66	0.78
1:C:892:PRO:HD2	1:C:895:LEU:HD22	1.65	0.78
1:C:1045:ILE:HD12	1:C:1199:ILE:HG23	1.63	0.78
1:B:849:VAL:HG12	1:B:999:ILE:HG13	1.64	0.78
1:C:635:ALA:HA	1:C:638:LEU:HG	1.64	0.78
1:C:656:MET:HA	1:C:656:MET:CE	2.13	0.78
1:C:1162:LEU:CD1	1:C:1162:LEU:H	1.96	0.78
1:B:982:MET:O	1:B:982:MET:HG2	1.84	0.78
1:B:1079:ARG:HA	1:B:1114:LEU:CD2	2.14	0.78
1:C:1046:ILE:HD12	1:C:1066:VAL:HB	1.66	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:664:MET:HA	1:B:664:MET:CE	2.14	0.78
1:C:1162:LEU:HD12	1:C:1162:LEU:N	1.97	0.78
1:B:266:PHE:HD2	1:B:306:VAL:HG22	1.46	0.77
1:B:328:THR:HA	1:B:1148:LEU:O	1.83	0.77
1:B:598:TRP:CD2	1:B:742:PRO:HG3	2.19	0.77
1:B:905:ILE:HG23	1:B:909:TYR:CD1	2.19	0.77
1:C:854:ARG:HA	1:C:854:ARG:HH11	1.46	0.77
1:B:1266:PRO:HG2	1:B:1269:ALA:CB	2.13	0.77
1:C:280:VAL:HB	1:C:414:PRO:CB	2.14	0.77
1:B:332:ILE:HG23	1:B:347:ARG:HA	1.65	0.77
1:B:902:ALA:HB1	1:B:1275:PRO:HB2	1.64	0.77
1:B:906:TYR:CE1	1:B:1275:PRO:HD3	2.19	0.77
1:C:436:ARG:HD2	1:C:440:MET:HE2	1.65	0.77
1:C:600:TYR:CD2	1:C:830:PRO:HA	2.19	0.77
1:C:219:HIS:HA	1:C:235:VAL:CG1	2.14	0.77
1:C:380:GLN:HG3	1:C:388:GLY:HA2	1.67	0.77
1:B:1074:VAL:HG11	1:B:1109:ILE:HG12	1.66	0.77
1:B:1166:TRP:CD1	1:B:1176:PRO:HG2	2.20	0.77
1:B:293:GLN:HE22	1:B:401:LYS:HA	1.50	0.77
1:B:491:VAL:HG22	1:B:1275:PRO:HA	1.65	0.76
1:B:1049:ARG:HB3	1:B:1049:ARG:HH11	1.48	0.76
1:B:1049:ARG:HH11	1:B:1049:ARG:CB	1.97	0.76
1:B:283:TYR:O	1:B:283:TYR:CG	2.38	0.76
1:C:814:LEU:HD22	1:C:814:LEU:H	1.50	0.76
1:B:602:GLY:HA3	1:B:831:PHE:HD2	1.51	0.76
1:B:503:ARG:HD2	1:B:1265:PRO:HG3	1.68	0.76
1:C:279:ASP:HB2	1:C:414:PRO:O	1.85	0.76
1:B:847:VAL:O	1:B:870:THR:HA	1.86	0.76
1:C:1076:ILE:HG12	1:C:1109:ILE:HB	1.67	0.76
1:C:1101:MET:N	1:C:1101:MET:SD	2.60	0.75
1:B:617:GLY:HA3	1:B:654:ASN:CB	2.14	0.75
1:B:436:ARG:HA	1:B:448:VAL:HA	1.66	0.75
1:C:430:ARG:HD2	1:C:1234:ILE:HB	1.67	0.75
1:C:491:VAL:HB	1:C:1271:VAL:CG1	2.17	0.75
1:B:999:ILE:HG23	1:B:1011:VAL:HB	1.69	0.75
1:B:332:ILE:HG21	1:B:347:ARG:HA	1.67	0.75
1:B:992:PRO:HA	1:B:995:THR:CG2	2.17	0.75
1:C:258:TRP:HH2	1:C:1262:TYR:HB2	1.50	0.75
1:C:573:PRO:HB3	1:C:623:LEU:HD21	1.67	0.75
1:C:235:VAL:HG21	1:C:239:VAL:HG11	1.69	0.75
1:C:352:LEU:O	1:C:954:SER:HA	1.87	0.75

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:430:ARG:HD3	1:C:451:PHE:CE2	2.21	0.75
1:C:699:ALA:HB1	1:C:702:LEU:HB2	1.67	0.75
1:C:272:VAL:O	1:C:300:ALA:N	2.20	0.74
1:C:336:LYS:HB2	1:C:340:ASN:HB2	1.67	0.74
1:C:493:VAL:HG12	1:C:1269:ALA:HB1	1.68	0.74
1:B:298:GLU:CA	1:B:1214:SER:HB2	2.17	0.74
1:B:813:GLN:C	1:B:816:PRO:HD2	2.08	0.74
1:B:1212:THR:HG23	1:B:1225:LYS:CB	2.16	0.74
1:C:1075:HIS:H	1:C:1108:TRP:HA	1.53	0.74
1:B:338:LEU:CD2	1:B:339:LEU:HG	2.17	0.74
1:C:841:ASP:CB	1:C:1005:ASN:HB3	2.13	0.74
1:C:375:HIS:CE1	1:C:445:SER:H	2.06	0.74
1:B:265:SER:HB3	1:B:308:THR:HG22	1.70	0.74
1:B:1049:ARG:NH1	1:B:1049:ARG:CB	2.50	0.74
1:B:1000:GLN:HA	1:B:1009:PHE:O	1.88	0.74
1:C:220:ILE:O	1:C:1266:PRO:HB2	1.87	0.74
1:C:246:GLN:HB3	1:C:911:ASP:CG	2.08	0.74
1:C:263:CYS:SG	1:C:458:THR:HG21	2.28	0.74
1:B:243:LYS:HB2	1:B:538:ASP:OD2	1.87	0.74
1:B:1074:VAL:HG22	1:B:1107:ASN:CB	2.17	0.74
1:C:221:THR:HA	1:C:1267:ILE:O	1.87	0.74
1:C:1002:GLN:CB	1:C:1008:THR:HG22	2.18	0.74
1:C:1111:PRO:HG2	1:C:1114:LEU:HB2	1.68	0.74
1:C:262:LEU:HB2	1:C:311:ALA:HB3	1.69	0.73
1:C:270:PRO:HB2	1:C:299:ALA:HB2	1.68	0.73
1:C:814:LEU:HD22	1:C:814:LEU:N	2.02	0.73
1:B:352:LEU:HA	1:B:954:SER:HA	1.70	0.73
1:B:1058:PRO:HB3	1:B:1200:ILE:HA	1.69	0.73
1:B:1078:GLY:HA3	1:B:1097:GLU:HB3	1.70	0.73
1:C:1232:TYR:CE1	1:C:1253:LEU:HD12	2.22	0.73
1:C:985:GLU:N	1:C:986:PRO:HD2	2.03	0.73
1:B:1170:ILE:HG12	1:B:1176:PRO:HD2	1.70	0.73
1:B:263:CYS:O	1:B:263:CYS:SG	2.47	0.73
1:C:336:LYS:CB	1:C:340:ASN:HB2	2.19	0.73
1:B:984:LEU:HD22	1:B:987:LEU:HD12	1.70	0.73
1:C:1049:ARG:HG3	1:C:1196:VAL:HG13	1.69	0.73
1:B:1041:ALA:HB2	1:B:1146:TYR:HD2	1.52	0.73
1:C:265:SER:HB3	1:C:308:THR:HA	1.71	0.73
1:C:836:VAL:HB	1:C:839:ASP:HB3	1.69	0.73
1:B:491:VAL:HG21	1:B:905:ILE:CG2	2.19	0.73
1:B:591:PHE:CE1	1:B:811:LEU:HD21	2.24	0.73

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:999:ILE:CG2	1:B:1011:VAL:HB	2.19	0.73
1:B:385:PHE:HB3	1:B:410:ARG:HA	1.69	0.72
1:C:318:ARG:HG2	1:C:371:TYR:CE1	2.24	0.72
1:C:322:VAL:HG13	1:C:334:LEU:HD22	1.71	0.72
1:C:1229:VAL:HA	1:C:1236:THR:HG21	1.70	0.72
1:B:652:LEU:HD12	1:B:652:LEU:O	1.89	0.72
1:C:636:LEU:HD22	1:C:648:ALA:HB2	1.70	0.72
1:C:543:LEU:HA	1:C:546:ILE:CG2	2.17	0.72
1:C:1175:ILE:HG13	1:C:1176:PRO:HD2	1.70	0.72
1:C:234:GLN:HB2	1:C:910:ALA:O	1.89	0.72
1:C:633:ALA:HA	1:C:636:LEU:HD12	1.70	0.72
1:C:1108:TRP:HB2	1:C:1137:ILE:HG12	1.69	0.72
1:B:438:GLN:HA	1:C:862:LEU:HB3	1.70	0.72
1:C:403:TYR:HD1	1:C:407:TYR:HE1	1.35	0.72
1:C:1054:HIS:HB2	1:C:1056:TRP:CD1	2.25	0.72
1:C:1131:LYS:HD2	1:C:1131:LYS:O	1.89	0.72
1:C:1151:TYR:HD2	1:C:1181:MET:HG2	1.54	0.72
1:C:258:TRP:HB3	1:C:374:ARG:HB2	1.72	0.72
1:C:276:VAL:HG13	1:C:1215:SER:HB2	1.72	0.72
1:C:447:TRP:HA	1:C:1260:TYR:HA	1.70	0.72
1:C:493:VAL:CG1	1:C:1269:ALA:HB1	2.19	0.72
1:C:508:ARG:HA	1:C:508:ARG:HE	1.54	0.72
1:B:848:GLY:CA	1:B:868:ASN:HB2	2.19	0.72
1:B:1002:GLN:HB2	1:B:1008:THR:HG22	1.72	0.72
1:B:434:PHE:N	1:B:450:VAL:HA	2.03	0.72
1:C:755:LEU:HD11	1:C:804:LYS:CE	2.18	0.72
1:C:847:VAL:HG23	1:C:871:VAL:HG11	1.70	0.72
1:B:1074:VAL:HG22	1:B:1107:ASN:HB3	1.72	0.71
1:B:1203:GLU:HG3	1:B:1205:ASN:HD21	1.54	0.71
1:B:333:HIS:HB3	1:B:346:VAL:CB	2.20	0.71
1:B:1086:GLY:CA	1:B:1092:PRO:HA	2.19	0.71
1:C:483:LEU:CD1	1:C:493:VAL:HG11	2.21	0.71
1:C:851:ARG:HD2	1:C:991:ASP:HB3	1.72	0.71
1:B:389:ALA:HB1	1:B:432:GLY:HA3	1.72	0.71
1:C:352:LEU:CD2	1:C:955:LEU:HB3	2.20	0.71
1:B:281:LEU:HB3	1:B:286:PHE:HE1	1.53	0.71
1:B:659:PHE:HZ	1:B:778:ASN:ND2	1.87	0.71
1:B:691:ILE:HD12	1:B:691:ILE:N	2.04	0.71
1:B:1266:PRO:HG2	1:B:1269:ALA:HB3	1.70	0.71
1:C:601:ASN:H	1:C:832:GLN:HG2	1.56	0.71
1:C:748:ALA:HA	1:C:813:GLN:HB3	1.73	0.71

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1154:ARG:HA	1:C:1192:SER:HA	1.73	0.71
1:B:892:PRO:HG2	1:B:895:LEU:HD13	1.72	0.71
1:B:1046:ILE:HB	1:B:1200:ILE:HG12	1.73	0.71
1:C:350:ASN:HB3	1:C:353:MET:HG3	1.71	0.71
1:C:518:GLN:HG3	1:C:521:ARG:HE	1.56	0.71
1:C:669:TYR:HA	1:C:673:ARG:HD2	1.72	0.71
1:C:806:MET:HB3	1:C:809:MET:HE3	1.72	0.71
1:C:851:ARG:HB3	1:C:994:MET:HB2	1.71	0.71
1:C:418:LYS:HB2	1:C:1214:SER:HA	1.71	0.71
1:C:766:ALA:HB1	1:C:801:LYS:HE3	1.73	0.71
1:C:1051:GLN:HE21	1:C:1194:PRO:HA	1.54	0.71
1:B:882:ILE:O	1:B:886:LEU:HG	1.91	0.70
1:C:338:LEU:HB2	1:C:357:ASN:CG	2.11	0.70
1:C:375:HIS:HE2	1:C:448:VAL:HB	1.56	0.70
1:B:261:GLY:HA3	1:B:312:SER:HA	1.72	0.70
1:B:415:ASN:HB3	1:B:420:CYS:SG	2.31	0.70
1:B:621:THR:HA	1:B:781:TYR:CE1	2.20	0.70
1:C:603:VAL:HG13	1:C:831:PHE:CD2	2.25	0.70
1:B:529:ALA:O	1:B:532:ILE:HG22	1.92	0.70
1:B:929:GLN:HB2	1:B:1015:MET:HB3	1.72	0.70
1:C:600:TYR:CE2	1:C:830:PRO:HA	2.27	0.70
1:C:1151:TYR:N	1:C:1182:VAL:O	2.23	0.70
1:B:1049:ARG:HB2	1:B:1198:TYR:CE2	2.27	0.70
1:C:413:THR:HG21	1:C:423:VAL:HB	1.72	0.70
1:C:623:LEU:HA	1:C:626:LEU:HD12	1.71	0.70
1:B:707:GLU:HB3	1:B:711:ARG:HH12	1.55	0.70
1:B:840:ARG:HA	1:B:843:VAL:CG2	2.20	0.70
1:C:1056:TRP:CG	1:C:1062:PRO:HD3	2.27	0.70
1:B:509:ILE:HG21	1:B:922:MET:HG3	1.73	0.70
1:C:500:SER:HB3	1:C:503:ARG:CB	2.21	0.70
1:B:295:PRO:HG2	1:B:408:PRO:HB3	1.72	0.70
1:C:516:ILE:O	1:C:520:ILE:HG12	1.91	0.70
1:C:261:GLY:HA3	1:C:313:ASN:N	2.06	0.70
1:C:647:LYS:HA	1:C:675:ALA:HB1	1.72	0.70
1:C:699:ALA:HB1	1:C:702:LEU:HD12	1.73	0.70
1:C:920:ARG:HH22	1:C:981:ASP:HB2	1.56	0.70
1:B:778:ASN:ND2	1:B:780:ARG:HG3	2.07	0.69
1:B:973:MET:HA	1:B:973:MET:CE	2.21	0.69
1:B:339:LEU:HD12	1:B:357:ASN:HD21	1.56	0.69
1:C:433:ARG:HA	1:C:450:VAL:HA	1.73	0.69
1:C:1126:PHE:HA	1:C:1129:TRP:CD1	2.25	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:LYS:HB2	1:B:340:ASN:HB2	1.75	0.69
1:B:716:PRO:HA	1:B:743:ILE:HA	1.73	0.69
1:C:283:TYR:HD1	1:C:290:TYR:HB2	1.57	0.69
1:C:418:LYS:HB2	1:C:1214:SER:CA	2.22	0.69
1:C:434:PHE:HB2	1:C:1256:VAL:CG1	2.22	0.69
1:C:814:LEU:H	1:C:814:LEU:CD2	2.05	0.69
1:B:651:THR:HA	1:B:654:ASN:HD22	1.57	0.69
1:B:724:PRO:HA	1:B:728:GLY:HA2	1.73	0.69
1:C:527:ASN:HB3	1:C:868:ASN:OD1	1.91	0.69
1:C:646:VAL:HG22	1:C:688:PHE:CZ	2.26	0.69
1:B:340:ASN:HD22	1:B:340:ASN:N	1.91	0.69
1:C:262:LEU:HD11	1:C:402:TRP:CE3	2.27	0.69
1:C:278:GLN:CG	1:C:415:ASN:HB3	2.19	0.69
1:C:607:VAL:O	1:C:876:ALA:HA	1.92	0.69
1:B:399:ALA:HA	1:B:402:TRP:HD1	1.58	0.69
1:C:394:LEU:HD12	1:C:402:TRP:CG	2.27	0.69
1:B:242:LYS:HD3	1:B:534:PRO:HB2	1.74	0.69
1:B:285:PHE:C	1:B:285:PHE:CD2	2.66	0.69
1:B:664:MET:HA	1:B:664:MET:HE2	1.72	0.69
1:B:1151:TYR:CD2	1:B:1181:MET:HG2	2.28	0.69
1:B:285:PHE:CB	1:C:1083:ILE:HG13	2.22	0.69
1:C:524:ASN:ND2	1:C:982:MET:SD	2.61	0.69
1:C:659:PHE:CE2	1:C:781:TYR:HA	2.28	0.69
1:B:352:LEU:HB3	1:B:955:LEU:CB	2.23	0.69
1:C:813:GLN:O	1:C:816:PRO:HD2	1.93	0.68
1:B:381:ASP:HB3	1:B:388:GLY:HA2	1.73	0.68
1:C:409:THR:HG21	1:C:1235:LEU:HD21	1.74	0.68
1:B:1074:VAL:HA	1:B:1107:ASN:O	1.93	0.68
1:C:556:ILE:HD11	1:C:888:SER:HB3	1.76	0.68
1:C:573:PRO:HA	1:C:623:LEU:HD21	1.74	0.68
1:B:284:THR:HB	1:C:1083:ILE:HB	1.74	0.68
1:B:617:GLY:O	1:B:655:MET:HG3	1.94	0.68
1:C:543:LEU:CA	1:C:546:ILE:HG22	2.19	0.68
1:C:656:MET:HA	1:C:656:MET:HE2	1.74	0.68
1:B:327:PRO:CB	1:B:1148:LEU:HG	2.21	0.68
1:C:811:LEU:O	1:C:816:PRO:HD3	1.94	0.68
1:B:631:ILE:CD1	1:B:883:THR:HG21	2.23	0.68
1:B:1229:VAL:HG13	1:B:1236:THR:HG21	1.75	0.68
1:C:474:ILE:HG21	1:C:507:TYR:HB2	1.76	0.68
1:C:1260:TYR:HB2	1:C:1262:TYR:HE1	1.57	0.68
1:B:853:SER:HB2	1:B:996:GLN:HB3	1.75	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1175:ILE:HG12	1:C:1176:PRO:HD2	1.73	0.68
1:B:468:ARG:HD2	1:B:468:ARG:O	1.94	0.68
1:B:848:GLY:HA3	1:B:868:ASN:HB2	1.76	0.68
1:C:273:PRO:HA	1:C:298:GLU:C	2.15	0.68
1:B:333:HIS:HB3	1:B:346:VAL:HB	1.75	0.67
1:B:776:VAL:HA	1:B:781:TYR:HE2	1.59	0.67
1:B:807:THR:HG21	1:B:886:LEU:HD23	1.75	0.67
1:B:959:ALA:HB2	1:B:993:ARG:HH22	1.60	0.67
1:B:300:ALA:HA	1:B:1213:ASN:N	2.08	0.67
1:B:552:ASP:HB3	1:B:555:ILE:HG13	1.77	0.67
1:C:684:TRP:CE3	1:C:840:ARG:HD3	2.30	0.67
1:B:332:ILE:HG12	1:B:347:ARG:O	1.93	0.67
1:B:300:ALA:CA	1:B:1213:ASN:H	2.06	0.67
1:B:303:ARG:HH11	1:B:1208:SER:HB3	1.59	0.67
1:B:413:THR:N	1:B:414:PRO:HD2	2.09	0.67
1:B:776:VAL:HA	1:B:781:TYR:CE2	2.30	0.67
1:C:1212:THR:HG23	1:C:1225:LYS:CB	2.23	0.67
1:C:851:ARG:HB3	1:C:994:MET:CB	2.25	0.67
1:B:1041:ALA:HB2	1:B:1146:TYR:CD2	2.30	0.67
1:C:273:PRO:CB	1:C:298:GLU:HB2	2.25	0.67
1:C:833:VAL:HG13	1:C:834:PRO:HD2	1.75	0.67
1:B:409:THR:CG2	1:B:423:VAL:HG13	2.24	0.67
1:B:782:GLN:HG3	1:B:790:VAL:HG21	1.77	0.67
1:B:1023:CYS:O	1:B:1027:THR:HG23	1.95	0.67
1:C:494:THR:CG2	1:C:496:PRO:HD3	2.22	0.67
1:C:573:PRO:CA	1:C:623:LEU:HD21	2.24	0.67
1:C:1002:GLN:HB2	1:C:1008:THR:HG22	1.77	0.67
1:B:516:ILE:HG12	1:B:1013:PRO:CB	2.24	0.66
1:B:518:GLN:HG3	1:B:829:PRO:HG2	1.77	0.66
1:B:1086:GLY:N	1:B:1092:PRO:HA	2.10	0.66
1:B:852:GLN:HA	1:B:996:GLN:H	1.58	0.66
1:B:1105:GLU:HA	1:B:1135:LEU:HB2	1.76	0.66
1:B:1171:THR:HG23	1:B:1172:PRO:CD	2.24	0.66
1:C:502:ASN:HB2	1:C:1262:TYR:CA	2.16	0.66
1:B:649:PHE:HA	1:B:705:TRP:HE1	1.61	0.66
1:C:849:VAL:HG22	1:C:999:ILE:HG13	1.76	0.66
1:C:1107:ASN:HA	1:C:1136:ARG:O	1.95	0.66
1:B:518:GLN:NE2	1:B:829:PRO:HD2	2.09	0.66
1:C:398:ASP:HB3	1:C:401:LYS:HD3	1.77	0.66
1:C:418:LYS:HB2	1:C:1214:SER:CB	2.25	0.66
1:C:949:LEU:HA	1:C:951:TRP:CD1	2.29	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1162:LEU:H	1:C:1162:LEU:HD12	1.59	0.66
1:C:1260:TYR:N	1:C:1260:TYR:CD1	2.61	0.66
1:B:324:MET:HA	1:B:335:PHE:HZ	1.60	0.66
1:B:327:PRO:HB2	1:B:1148:LEU:CG	2.21	0.66
1:B:716:PRO:HA	1:B:743:ILE:CA	2.26	0.66
1:B:849:VAL:H	1:B:869:THR:H	1.42	0.66
1:C:306:VAL:HB	1:C:324:MET:CB	2.25	0.66
1:B:603:VAL:HG23	1:B:604:VAL:HG23	1.78	0.66
1:B:647:LYS:HB3	1:B:675:ALA:HB1	1.77	0.66
1:B:806:MET:HB3	1:B:891:TYR:CE2	2.29	0.66
1:B:1034:GLU:HB3	1:B:1037:LEU:HB2	1.77	0.66
1:B:1060:ALA:HB2	1:B:1204:TYR:HD1	1.60	0.66
1:C:732:LEU:HB3	1:C:1011:VAL:HG11	1.76	0.66
1:C:1152:ASP:OD1	1:C:1154:ARG:HG2	1.95	0.66
1:B:1075:HIS:H	1:B:1108:TRP:HA	1.60	0.66
1:C:490:TYR:CE2	1:C:898:ASN:HA	2.31	0.66
1:C:515:GLN:HG3	1:C:730:ALA:HB1	1.76	0.66
1:B:472:MET:O	1:B:506:PRO:HA	1.96	0.66
1:B:516:ILE:CG1	1:B:1013:PRO:HB3	2.25	0.66
1:B:955:LEU:HD11	1:B:961:THR:HG21	1.78	0.66
1:C:490:TYR:CE2	1:C:901:TYR:HB2	2.30	0.66
1:C:1162:LEU:CD1	1:C:1162:LEU:N	2.55	0.66
1:B:1156:TYR:HA	1:B:1194:PRO:O	1.96	0.66
1:C:807:THR:N	1:C:808:PRO:HD2	2.11	0.66
1:B:268:ILE:HA	1:B:304:ILE:HA	1.77	0.66
1:C:1171:THR:CG2	1:C:1172:PRO:CD	2.72	0.66
1:B:1231:ARG:HB3	1:B:1253:LEU:HG	1.77	0.65
1:C:276:VAL:HG23	1:C:277:PRO:HD2	0.72	0.65
1:B:298:GLU:HA	1:B:1214:SER:CB	2.25	0.65
1:B:352:LEU:HB3	1:B:955:LEU:HB3	1.78	0.65
1:B:724:PRO:HA	1:B:728:GLY:CA	2.26	0.65
1:B:713:TRP:HD1	1:B:837:ARG:HG3	1.60	0.65
1:C:331:ASN:N	1:C:331:ASN:OD1	2.29	0.65
1:C:813:GLN:C	1:C:816:PRO:HD2	2.17	0.65
1:C:1230:GLU:HB2	1:C:1250:VAL:CG1	2.25	0.65
1:B:437:ALA:O	1:B:445:SER:HA	1.96	0.65
1:B:1093:MET:HB2	1:B:1101:MET:CB	2.27	0.65
1:C:480:GLU:HA	1:C:493:VAL:CG2	2.26	0.65
1:C:851:ARG:O	1:C:994:MET:HB2	1.96	0.65
1:C:1166:TRP:CZ3	1:C:1170:ILE:HD11	2.32	0.65
1:B:474:ILE:CD1	1:B:507:TYR:HB2	2.25	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:569:GLN:OE1	1:B:789:LEU:HB2	1.96	0.65
1:B:1083:ILE:HG23	1:B:1104:PHE:HZ	1.62	0.65
1:C:272:VAL:C	1:C:299:ALA:HA	2.16	0.65
1:C:896:VAL:HB	1:C:899:VAL:HB	1.78	0.65
1:B:426:CYS:HB3	1:B:1235:LEU:HB3	1.77	0.65
1:C:573:PRO:CB	1:C:623:LEU:HD21	2.26	0.65
1:B:433:ARG:HD2	1:B:436:ARG:HB3	1.77	0.65
1:C:258:TRP:CH2	1:C:1262:TYR:HB2	2.31	0.65
1:C:453:THR:HA	1:C:1254:TYR:CA	2.25	0.65
1:C:636:LEU:HD13	1:C:648:ALA:HB1	1.78	0.65
1:B:438:GLN:HB3	1:B:445:SER:CA	2.27	0.65
1:B:673:ARG:HD3	1:B:677:ALA:CB	2.26	0.65
1:B:719:ILE:HB	1:B:741:LEU:HD11	1.79	0.65
1:B:814:LEU:HD11	1:B:897:THR:HG21	1.77	0.65
1:C:264:THR:HG22	1:C:311:ALA:HB3	1.79	0.65
1:C:755:LEU:CD1	1:C:804:LYS:HE3	2.19	0.65
1:B:1082:ARG:O	1:B:1095:ARG:N	2.30	0.65
1:B:375:HIS:NE2	1:B:448:VAL:HG11	2.12	0.64
1:B:1095:ARG:HG2	1:B:1099:GLY:HA2	1.78	0.64
1:B:1104:PHE:N	1:B:1104:PHE:CD1	2.61	0.64
1:C:524:ASN:HB2	1:C:986:PRO:HG3	1.78	0.64
1:C:599:LEU:HD21	1:C:819:LEU:HD22	1.79	0.64
1:C:221:THR:HB	1:C:234:GLN:HB3	1.79	0.64
1:C:363:LEU:CD2	1:C:969:VAL:HG13	2.26	0.64
1:C:399:ALA:O	1:C:403:TYR:N	2.27	0.64
1:C:531:VAL:O	1:C:534:PRO:HD2	1.97	0.64
1:B:1049:ARG:HB3	1:B:1049:ARG:CZ	2.28	0.64
1:C:348:GLY:CA	1:C:1176:PRO:HA	2.19	0.64
1:C:383:THR:HG22	1:C:385:PHE:CD1	2.32	0.64
1:B:332:ILE:HG13	1:B:332:ILE:O	1.96	0.64
1:B:1112:LEU:HG	1:B:1116:GLN:NE2	2.12	0.64
1:C:465:TRP:CZ2	1:C:469:LEU:HD21	2.32	0.64
1:B:647:LYS:CB	1:B:675:ALA:HB1	2.27	0.64
1:C:332:ILE:HA	1:C:335:PHE:HD1	1.62	0.64
1:C:691:ILE:HD12	1:C:691:ILE:N	2.11	0.64
1:C:713:TRP:CZ3	1:C:714:PRO:HD2	2.29	0.64
1:C:283:TYR:HB2	1:C:290:TYR:HB2	1.80	0.64
1:B:332:ILE:HD11	1:B:349:ALA:HB2	1.78	0.64
1:B:492:THR:OG1	1:B:1274:VAL:HB	1.98	0.64
1:B:685:PRO:HG2	1:B:688:PHE:HB3	1.78	0.64
1:C:334:LEU:HA	1:C:337:GLN:HG3	1.78	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:375:HIS:ND1	1:C:444:MET:HG2	2.12	0.64
1:B:450:VAL:O	1:B:1256:VAL:HA	1.97	0.64
1:B:483:LEU:HB2	1:B:493:VAL:HG21	1.79	0.64
1:B:719:ILE:CG2	1:B:739:LEU:HB3	2.28	0.64
1:B:1109:ILE:CD1	1:B:1138:ARG:HB3	2.28	0.64
1:C:254:ARG:HB2	1:C:254:ARG:HH11	1.63	0.64
1:C:765:ARG:HG3	1:C:765:ARG:HH11	1.63	0.64
1:C:439:MET:SD	1:C:501:VAL:HG11	2.38	0.64
1:C:713:TRP:CD2	1:C:714:PRO:CD	2.63	0.64
1:B:307:HIS:CG	1:B:310:TRP:HB3	2.32	0.63
1:C:234:GLN:HG3	1:C:246:GLN:HB2	1.80	0.63
1:C:491:VAL:HB	1:C:1271:VAL:HG13	1.80	0.63
1:C:573:PRO:HB2	1:C:627:TRP:CZ2	2.32	0.63
1:C:1045:ILE:HG22	1:C:1201:SER:HA	1.79	0.63
1:B:268:ILE:HG13	1:B:304:ILE:HG12	1.79	0.63
1:B:352:LEU:HD13	1:B:955:LEU:HB3	1.79	0.63
1:B:389:ALA:HB1	1:B:432:GLY:CA	2.28	0.63
1:C:272:VAL:O	1:C:299:ALA:HA	1.98	0.63
1:C:718:GLN:HB2	1:C:738:VAL:CG1	2.29	0.63
1:B:491:VAL:CG2	1:B:905:ILE:HG21	2.29	0.63
1:B:822:ILE:O	1:B:826:LEU:HD22	1.98	0.63
1:C:493:VAL:HA	1:C:1270:VAL:O	1.98	0.63
1:C:477:THR:HA	1:C:480:GLU:OE2	1.98	0.63
1:C:765:ARG:CD	1:C:801:LYS:HA	2.28	0.63
1:B:401:LYS:HE3	1:B:402:TRP:CZ2	2.34	0.63
1:B:1171:THR:HG22	1:B:1173:THR:H	1.63	0.63
1:C:403:TYR:HD1	1:C:407:TYR:CE1	2.16	0.63
1:C:701:ILE:HD13	1:C:704:GLN:HE22	1.63	0.63
1:C:1046:ILE:HB	1:C:1200:ILE:HG12	1.81	0.63
1:C:360:HIS:NE2	1:C:969:VAL:HA	2.13	0.63
1:B:243:LYS:HZ1	1:B:828:PHE:HB3	1.63	0.63
1:B:493:VAL:HA	1:B:1273:GLY:HA2	1.81	0.63
1:B:1147:MET:HE2	1:B:1179:PRO:HB3	1.80	0.63
1:C:527:ASN:HD21	1:C:864:LEU:C	2.01	0.63
1:C:740:LEU:HB3	1:C:835:TYR:CE1	2.34	0.63
1:C:844:PRO:HA	1:C:1003:GLN:HA	1.81	0.63
1:B:657:VAL:HG22	1:B:671:GLN:HG2	1.81	0.63
1:B:1153:PRO:O	1:B:1193:ALA:HB3	1.99	0.63
1:C:381:ASP:N	1:C:389:ALA:O	2.32	0.63
1:C:617:GLY:O	1:C:655:MET:HG2	1.98	0.63
1:B:751:THR:HG21	1:B:898:ASN:ND2	2.13	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:VAL:HG13	1:C:1209:LEU:HD13	1.80	0.63
1:C:434:PHE:N	1:C:449:ASP:O	2.32	0.63
1:C:765:ARG:HD2	1:C:801:LYS:HA	1.79	0.63
1:C:836:VAL:HB	1:C:839:ASP:CB	2.28	0.63
1:B:266:PHE:HA	1:B:306:VAL:HA	1.81	0.62
1:B:433:ARG:HA	1:B:450:VAL:HB	1.81	0.62
1:B:947:ARG:HB3	1:B:950:ASP:OD1	1.99	0.62
1:B:1094:ILE:HG22	1:B:1102:VAL:O	1.99	0.62
1:C:391:LEU:HB3	1:C:403:TYR:CE1	2.34	0.62
1:C:905:ILE:HG23	1:C:909:TYR:CD1	2.33	0.62
1:B:281:LEU:HB3	1:B:286:PHE:CE1	2.33	0.62
1:B:399:ALA:HA	1:B:402:TRP:CD1	2.34	0.62
1:B:646:VAL:HG22	1:B:688:PHE:CD2	2.34	0.62
1:B:810:TYR:HB2	1:B:891:TYR:HE1	1.64	0.62
1:C:223:PHE:HA	1:C:1269:ALA:O	1.99	0.62
1:C:394:LEU:CG	1:C:395:PRO:HD2	2.29	0.62
1:C:502:ASN:OD1	1:C:502:ASN:N	2.33	0.62
1:C:632:LEU:O	1:C:636:LEU:HG	1.99	0.62
1:C:1066:VAL:HB	1:C:1200:ILE:HD11	1.81	0.62
1:B:815:ALA:HB3	1:B:816:PRO:HD3	1.81	0.62
1:B:1131:LYS:HD2	1:B:1160:TRP:NE1	2.14	0.62
1:C:233:VAL:O	1:C:245:ALA:HB1	1.99	0.62
1:C:932:VAL:O	1:C:935:VAL:HG12	1.99	0.62
1:C:1210:PHE:CE1	1:C:1228:PRO:HD2	2.35	0.62
1:B:272:VAL:O	1:B:299:ALA:HB1	1.98	0.62
1:B:591:PHE:CZ	1:B:811:LEU:HD21	2.34	0.62
1:B:813:GLN:O	1:B:816:PRO:HD2	1.98	0.62
1:B:857:ILE:CG2	1:B:862:LEU:HB2	2.29	0.62
1:B:983:LEU:HG	1:B:984:LEU:HG	1.82	0.62
1:C:1151:TYR:C	1:C:1151:TYR:CD1	2.73	0.62
1:C:1246:GLN:HB2	1:C:1250:VAL:HB	1.80	0.62
1:B:807:THR:N	1:B:808:PRO:HD2	2.14	0.62
1:B:1150:TYR:HA	1:B:1182:VAL:O	1.99	0.62
1:C:332:ILE:HG12	1:C:347:ARG:HA	1.81	0.62
1:C:713:TRP:CZ3	1:C:714:PRO:CD	2.82	0.62
1:C:716:PRO:HD2	1:C:837:ARG:HD2	1.81	0.62
1:C:1082:ARG:HG2	1:C:1082:ARG:NH1	2.07	0.62
1:B:852:GLN:HA	1:B:995:THR:CA	2.27	0.62
1:C:451:PHE:HB3	1:C:1254:TYR:OH	1.99	0.62
1:C:1129:TRP:HA	1:C:1133:GLY:HA3	1.80	0.62
1:C:1231:ARG:HB3	1:C:1253:LEU:HG	1.81	0.62

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:680:THR:OG1	1:B:683:THR:HG23	2.00	0.62
1:B:267:LYS:N	1:B:305:VAL:O	2.29	0.62
1:B:618:GLY:O	1:B:655:MET:HA	2.00	0.62
1:B:928:VAL:HG22	1:B:987:LEU:HD11	1.81	0.62
1:C:924:THR:HG23	1:C:984:LEU:HD21	1.82	0.62
1:B:540:SER:HA	1:B:592:ARG:HB3	1.81	0.62
1:B:1156:TYR:HD1	1:B:1194:PRO:HB2	1.64	0.62
1:C:515:GLN:CG	1:C:730:ALA:HB1	2.29	0.62
1:B:518:GLN:CG	1:B:829:PRO:HG2	2.30	0.62
1:B:601:ASN:ND2	1:B:832:GLN:HA	2.15	0.62
1:B:631:ILE:HD12	1:B:883:THR:HG21	1.80	0.62
1:B:1091:ALA:HB3	1:B:1103:PRO:HB3	1.81	0.62
1:C:223:PHE:HB2	1:C:232:ILE:O	1.99	0.62
1:C:551:ILE:HG22	1:C:553:PRO:HD3	1.81	0.62
1:C:1157:ALA:HB3	1:C:1195:ALA:CB	2.29	0.62
1:B:351:PRO:O	1:B:354:PHE:HB2	1.98	0.61
1:B:1094:ILE:HB	1:B:1104:PHE:CE1	2.34	0.61
1:B:1159:ALA:O	1:B:1163:THR:HG23	1.99	0.61
1:C:851:ARG:NH2	1:C:986:PRO:O	2.32	0.61
1:B:493:VAL:HB	1:B:1271:VAL:HG13	1.82	0.61
1:B:578:LEU:HD23	1:B:581:LEU:HD12	1.81	0.61
1:C:274:ALA:O	1:C:1214:SER:OG	2.15	0.61
1:C:666:ASN:OD1	1:C:668:ILE:HB	2.00	0.61
1:C:731:ASN:HB2	1:C:736:PRO:CA	2.26	0.61
1:C:996:GLN:OE1	1:C:998:ALA:HB2	2.00	0.61
1:C:1049:ARG:HG3	1:C:1196:VAL:CG1	2.30	0.61
1:C:1087:MET:H	1:C:1090:ALA:HB3	1.64	0.61
1:B:272:VAL:O	1:B:300:ALA:N	2.34	0.61
1:B:375:HIS:CD2	1:B:448:VAL:HG11	2.35	0.61
1:B:987:LEU:N	1:B:987:LEU:HD23	2.15	0.61
1:B:1083:ILE:HG23	1:B:1104:PHE:CZ	2.34	0.61
1:C:933:THR:HG21	1:C:1021:ALA:HB1	1.81	0.61
1:B:257:THR:HG22	1:B:316:PHE:HB3	1.81	0.61
1:B:438:GLN:HG3	1:B:439:MET:N	2.14	0.61
1:B:591:PHE:O	1:B:595:LEU:HG	2.01	0.61
1:B:719:ILE:HG23	1:B:739:LEU:HB3	1.82	0.61
1:B:836:VAL:HB	1:B:839:ASP:CB	2.31	0.61
1:B:849:VAL:HG12	1:B:999:ILE:CG1	2.29	0.61
1:C:283:TYR:CD1	1:C:290:TYR:HB2	2.35	0.61
1:C:1149:HIS:N	1:C:1180:PHE:O	2.32	0.61
1:B:303:ARG:HG2	1:B:1209:LEU:CA	2.26	0.61

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:851:ARG:HG3	1:B:851:ARG:HH11	1.64	0.61
1:B:928:VAL:O	1:B:932:VAL:HG13	2.00	0.61
1:C:278:GLN:CA	1:C:415:ASN:HA	2.31	0.61
1:C:577:ILE:O	1:C:581:LEU:HG	2.01	0.61
1:C:1037:LEU:HD21	1:C:1207:ARG:HG2	1.82	0.61
1:C:521:ARG:O	1:C:525:ILE:HG13	2.01	0.61
1:C:527:ASN:ND2	1:C:864:LEU:O	2.32	0.61
1:C:1170:ILE:HG12	1:C:1175:ILE:HG13	1.82	0.61
1:B:363:LEU:O	1:B:367:LEU:HG	2.01	0.61
1:B:636:LEU:N	1:B:637:PRO:HD2	2.16	0.61
1:B:1171:THR:CG2	1:B:1172:PRO:HD2	2.25	0.61
1:B:391:LEU:HD23	1:B:403:TYR:CD2	2.36	0.61
1:B:490:TYR:CE2	1:B:817:VAL:HG13	2.36	0.61
1:B:622:SER:HB3	1:B:625:ASN:HB2	1.82	0.61
1:C:283:TYR:CE2	1:C:385:PHE:HZ	2.18	0.61
1:C:622:SER:HB3	1:C:625:ASN:HB2	1.82	0.61
1:B:258:TRP:HA	1:B:372:LEU:O	2.01	0.60
1:B:1032:ASN:HD21	1:B:1042:ARG:HH12	1.48	0.60
1:B:1147:MET:N	1:B:1178:VAL:O	2.33	0.60
1:C:1151:TYR:CD2	1:C:1181:MET:HG2	2.35	0.60
1:C:1154:ARG:HB3	1:C:1191:SER:O	2.00	0.60
1:B:1069:ARG:HG2	1:B:1109:ILE:HG21	1.83	0.60
1:C:732:LEU:HD13	1:C:1011:VAL:CG1	2.31	0.60
1:C:984:LEU:O	1:C:988:LEU:HG	2.01	0.60
1:B:522:ILE:HA	1:B:525:ILE:HG12	1.83	0.60
1:C:603:VAL:C	1:C:872:GLY:HA2	2.21	0.60
1:C:1034:GLU:OE2	1:C:1034:GLU:HA	2.01	0.60
1:B:243:LYS:O	1:B:247:LEU:HG	2.02	0.60
1:B:883:THR:HA	1:B:886:LEU:HD12	1.83	0.60
1:C:231:PRO:HA	1:C:906:TYR:OH	2.01	0.60
1:C:1209:LEU:HD21	1:C:1212:THR:HG22	1.82	0.60
1:B:246:GLN:HG3	1:B:250:ALA:CB	2.31	0.60
1:B:440:MET:HG3	1:C:864:LEU:HG	1.83	0.60
1:B:1217:PRO:HG2	1:B:1218:GLN:OE1	2.02	0.60
1:B:1231:ARG:HG2	1:B:1250:VAL:HG13	1.84	0.60
1:C:708:ILE:HA	1:C:711:ARG:NH1	2.16	0.60
1:C:1041:ALA:HB3	1:C:1144:TYR:CE1	2.35	0.60
1:C:1074:VAL:HA	1:C:1107:ASN:O	2.01	0.60
1:B:438:GLN:HB3	1:B:445:SER:HA	1.84	0.60
1:B:936:ALA:O	1:B:945:VAL:HG21	2.02	0.60
1:C:327:PRO:O	1:C:1148:LEU:HB2	2.02	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:ARG:HB3	1:B:312:SER:HB2	1.84	0.60
1:B:321:SER:HA	1:B:368:ASP:OD1	2.01	0.60
1:B:413:THR:HG23	1:B:420:CYS:HB3	1.83	0.60
1:B:691:ILE:H	1:B:691:ILE:CD1	2.07	0.60
1:B:823:ALA:HA	1:B:826:LEU:HD23	1.84	0.60
1:C:375:HIS:NE2	1:C:448:VAL:HB	2.17	0.60
1:C:721:TYR:N	1:C:737:GLU:O	2.32	0.60
1:C:1126:PHE:O	1:C:1130:ILE:N	2.29	0.60
1:B:811:LEU:O	1:B:816:PRO:HD3	2.00	0.60
1:B:1044:ASP:H	1:B:1202:THR:HB	1.65	0.60
1:B:1094:ILE:HD12	1:B:1126:PHE:HZ	1.67	0.60
1:C:400:GLU:CD	1:C:400:GLU:H	2.04	0.60
1:C:681:PRO:HA	1:C:684:TRP:CD1	2.37	0.60
1:C:277:PRO:C	1:C:416:VAL:HG13	2.21	0.60
1:B:277:PRO:HB3	1:B:286:PHE:HE2	1.67	0.59
1:B:620:VAL:HB	1:B:775:LEU:HD11	1.84	0.59
1:B:1266:PRO:HG2	1:B:1269:ALA:HB2	1.82	0.59
1:C:270:PRO:CB	1:C:299:ALA:HB2	2.32	0.59
1:B:284:THR:N	1:C:1085:PHE:HB2	2.16	0.59
1:B:1078:GLY:CA	1:B:1097:GLU:HB3	2.32	0.59
1:C:478:GLU:HA	1:C:481:TRP:CE3	2.37	0.59
1:C:1042:ARG:HA	1:C:1143:ALA:HA	1.85	0.59
1:C:1110:PHE:O	1:C:1139:ILE:HA	2.01	0.59
1:B:825:MET:HA	1:B:825:MET:CE	2.32	0.59
1:B:854:ARG:HB2	1:B:857:ILE:HB	1.82	0.59
1:B:1093:MET:HB3	1:B:1101:MET:C	2.23	0.59
1:C:892:PRO:HB2	1:C:895:LEU:HB2	1.82	0.59
1:C:440:MET:HA	1:C:445:SER:HA	1.84	0.59
1:C:937:GLN:OE1	1:C:937:GLN:HA	2.01	0.59
1:C:949:LEU:HB3	1:C:952:ILE:HD12	1.83	0.59
1:B:1001:TYR:O	1:B:1008:THR:HA	2.03	0.59
1:B:1078:GLY:HA3	1:B:1097:GLU:CB	2.30	0.59
1:C:717:SER:O	1:C:741:LEU:N	2.34	0.59
1:B:427:VAL:HG21	1:B:1238:PRO:HA	1.84	0.59
1:C:914:VAL:O	1:C:918:LEU:HG	2.01	0.59
1:C:1115:TRP:HA	1:C:1122:PHE:CE2	2.38	0.59
1:B:353:MET:N	1:B:353:MET:SD	2.76	0.59
1:B:855:ASP:HA	1:B:994:MET:CE	2.33	0.59
1:B:883:THR:O	1:B:887:LEU:HG	2.03	0.59
1:B:1059:LEU:HD22	1:B:1205:ASN:HB2	1.85	0.59
1:B:646:VAL:HG13	1:B:685:PRO:HD2	1.85	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:959:ALA:HA	1:B:993:ARG:HH12	1.68	0.59
1:B:1034:GLU:HB3	1:B:1037:LEU:HG	1.85	0.59
1:C:466:MET:HE3	1:C:469:LEU:HB2	1.84	0.59
1:C:681:PRO:HB3	1:C:840:ARG:HG3	1.84	0.59
1:C:956:ARG:C	1:C:956:ARG:HD2	2.23	0.59
1:B:624:GLU:OE1	1:B:624:GLU:HA	2.02	0.59
1:C:1252:ASP:HB2	1:C:1255:ASN:HD21	1.68	0.59
1:B:295:PRO:CG	1:B:408:PRO:HA	2.33	0.58
1:B:352:LEU:HB3	1:B:955:LEU:CG	2.33	0.58
1:B:391:LEU:HD23	1:B:403:TYR:HD2	1.68	0.58
1:B:643:CYS:HB2	1:B:647:LYS:HE3	1.85	0.58
1:C:375:HIS:HB3	1:C:1261:ALA:CB	2.24	0.58
1:C:713:TRP:HE3	1:C:714:PRO:HD3	1.62	0.58
1:B:503:ARG:HA	1:B:1263:GLU:O	2.02	0.58
1:B:979:LEU:HB3	1:B:981:ASP:OD2	2.03	0.58
1:C:283:TYR:CZ	1:C:292:ILE:HG12	2.37	0.58
1:C:350:ASN:HA	1:C:1174:SER:CB	2.32	0.58
1:C:403:TYR:CD1	1:C:407:TYR:HE1	2.19	0.58
1:C:691:ILE:H	1:C:691:ILE:CD1	2.16	0.58
1:C:1054:HIS:HB2	1:C:1056:TRP:NE1	2.18	0.58
1:B:254:ARG:HG2	1:B:316:PHE:CG	2.37	0.58
1:B:332:ILE:HD12	1:B:335:PHE:HB2	1.86	0.58
1:B:407:TYR:CE2	1:B:431:VAL:HG23	2.39	0.58
1:B:559:THR:O	1:B:563:VAL:HG23	2.03	0.58
1:B:852:GLN:CA	1:B:996:GLN:H	2.16	0.58
1:B:1059:LEU:HB3	1:B:1205:ASN:H	1.66	0.58
1:C:724:PRO:HA	1:C:728:GLY:CA	2.24	0.58
1:B:646:VAL:HG22	1:B:688:PHE:CE2	2.38	0.58
1:B:685:PRO:O	1:B:689:MET:HG2	2.03	0.58
1:C:318:ARG:O	1:C:976:ALA:HA	2.02	0.58
1:C:974:LYS:HD3	1:C:983:LEU:HB3	1.85	0.58
1:C:413:THR:HG23	1:C:423:VAL:HG11	1.86	0.58
1:C:580:LYS:HE2	1:C:624:GLU:CG	2.34	0.58
1:C:974:LYS:NZ	1:C:982:MET:HA	2.18	0.58
1:B:478:GLU:HA	1:B:481:TRP:CZ3	2.39	0.58
1:B:825:MET:HA	1:B:825:MET:HE3	1.85	0.58
1:B:1104:PHE:HA	1:B:1108:TRP:CZ2	2.39	0.58
1:C:278:GLN:HB3	1:C:415:ASN:HA	1.85	0.58
1:C:690:ASN:HB3	1:C:693:LEU:HD12	1.86	0.58
1:C:1075:HIS:HB3	1:C:1077:PHE:CE1	2.37	0.58
1:B:852:GLN:O	1:B:996:GLN:HG2	2.03	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:VAL:HG22	1:C:326:PRO:HA	1.85	0.58
1:C:383:THR:HG22	1:C:385:PHE:HD1	1.68	0.58
1:C:763:ASN:C	1:C:763:ASN:HD22	2.07	0.58
1:C:1112:LEU:HG	1:C:1116:GLN:HE21	1.69	0.58
1:B:985:GLU:N	1:B:986:PRO:CD	2.66	0.58
1:C:277:PRO:HG2	1:C:416:VAL:HG22	1.83	0.58
1:C:591:PHE:HE1	1:C:811:LEU:HD21	1.68	0.58
1:C:1121:TYR:O	1:C:1125:GLN:HG2	2.04	0.58
1:B:1111:PRO:HG2	1:B:1114:LEU:HB2	1.86	0.58
1:C:273:PRO:HB3	1:C:298:GLU:HB2	1.85	0.58
1:C:333:HIS:HA	1:C:336:LYS:HG2	1.85	0.58
1:C:732:LEU:HB3	1:C:1011:VAL:HG21	1.86	0.58
1:C:1131:LYS:HG3	1:C:1132:THR:HG23	1.85	0.58
1:C:1131:LYS:HD3	1:C:1160:TRP:CD2	2.39	0.58
1:C:1151:TYR:HB3	1:C:1181:MET:HG2	1.86	0.58
1:B:841:ASP:HA	1:B:1004:TYR:HB3	1.85	0.58
1:C:464:ARG:HD3	1:C:1023:CYS:SG	2.44	0.58
1:B:364:GLU:OE1	1:B:972:SER:HB3	2.04	0.57
1:B:707:GLU:HB3	1:B:711:ARG:NH1	2.18	0.57
1:C:429:ASN:HD22	1:C:429:ASN:N	2.01	0.57
1:C:754:THR:HA	1:C:809:MET:HE2	1.86	0.57
1:B:256:VAL:HG13	1:B:372:LEU:CD1	2.32	0.57
1:B:566:SER:HB3	1:B:788:SER:OG	2.04	0.57
1:B:1056:TRP:HB3	1:B:1062:PRO:HD3	1.84	0.57
1:B:1059:LEU:HB3	1:B:1204:TYR:HA	1.86	0.57
1:B:1156:TYR:CD1	1:B:1194:PRO:HB2	2.38	0.57
1:B:1187:ASP:O	1:B:1220:ILE:HB	2.03	0.57
1:C:465:TRP:CH2	1:C:469:LEU:HD21	2.39	0.57
1:C:810:TYR:CD1	1:C:814:LEU:HB2	2.39	0.57
1:C:853:SER:HA	1:C:996:GLN:HB3	1.86	0.57
1:B:243:LYS:HB2	1:B:538:ASP:CG	2.24	0.57
1:B:768:VAL:O	1:B:772:MET:HG3	2.04	0.57
1:B:1166:TRP:NE1	1:B:1176:PRO:HG2	2.18	0.57
1:C:380:GLN:HE21	1:C:388:GLY:HA2	1.69	0.57
1:C:1059:LEU:HD22	1:C:1205:ASN:HD22	1.68	0.57
1:B:262:LEU:HD11	1:B:402:TRP:CE3	2.39	0.57
1:C:261:GLY:C	1:C:312:SER:HA	2.25	0.57
1:B:320:SER:O	1:B:368:ASP:HB2	2.04	0.57
1:C:265:SER:HA	1:C:308:THR:HA	1.85	0.57
1:C:321:SER:HA	1:C:368:ASP:OD1	2.05	0.57
1:C:336:LYS:HA	1:C:340:ASN:HB2	1.86	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1241:PRO:CG	1:C:1244:GLN:HB2	2.22	0.57
1:B:1093:MET:CE	1:B:1103:PRO:HG3	2.35	0.57
1:B:1245:ILE:HD12	1:B:1247:LEU:HB2	1.87	0.57
1:C:270:PRO:HG3	1:C:297:PRO:CB	2.30	0.57
1:C:754:THR:HG22	1:C:806:MET:CG	2.24	0.57
1:B:338:LEU:HG	1:B:968:TRP:CZ2	2.40	0.57
1:B:543:LEU:HA	1:B:546:ILE:HG22	1.87	0.57
1:B:574:ALA:HA	1:B:577:ILE:HG22	1.86	0.57
1:C:221:THR:OG1	1:C:1267:ILE:HB	2.04	0.57
1:C:277:PRO:O	1:C:416:VAL:N	2.37	0.57
1:C:418:LYS:HB2	1:C:1214:SER:HB2	1.86	0.57
1:C:490:TYR:HE2	1:C:898:ASN:HA	1.68	0.57
1:B:338:LEU:HG	1:B:968:TRP:CE2	2.39	0.57
1:B:375:HIS:HA	1:B:1259:ARG:HB3	1.86	0.57
1:B:844:PRO:HA	1:B:1003:GLN:HA	1.87	0.57
1:B:913:GLU:OE2	1:B:913:GLU:N	2.31	0.57
1:B:955:LEU:HD12	1:B:955:LEU:O	2.04	0.57
1:B:1163:THR:HG21	1:B:1198:TYR:CB	2.29	0.57
1:C:806:MET:CB	1:C:809:MET:HE3	2.35	0.57
1:C:1170:ILE:HA	1:C:1176:PRO:HD3	1.87	0.57
1:C:844:PRO:HB3	1:C:1001:TYR:CE1	2.40	0.57
1:C:775:LEU:HD23	1:C:775:LEU:C	2.24	0.57
1:B:1051:GLN:HB2	1:B:1196:VAL:HG22	1.87	0.56
1:C:807:THR:O	1:C:811:LEU:HG	2.05	0.56
1:B:622:SER:O	1:B:626:LEU:HG	2.05	0.56
1:B:952:ILE:HA	1:B:1143:ALA:CB	2.35	0.56
1:B:1207:ARG:HH21	1:B:1231:ARG:HH12	1.52	0.56
1:C:254:ARG:CZ	1:C:316:PHE:HB2	2.35	0.56
1:C:723:ALA:O	1:C:728:GLY:N	2.28	0.56
1:C:1130:ILE:HG22	1:C:1160:TRP:HZ3	1.70	0.56
1:B:603:VAL:O	1:B:873:VAL:N	2.37	0.56
1:B:905:ILE:O	1:B:909:TYR:N	2.37	0.56
1:C:278:GLN:CB	1:C:415:ASN:HA	2.36	0.56
1:C:1048:GLY:HA3	1:C:1136:ARG:HE	1.70	0.56
1:B:254:ARG:HG3	1:B:254:ARG:O	2.05	0.56
1:B:265:SER:CB	1:B:308:THR:HA	2.36	0.56
1:B:295:PRO:HG2	1:B:408:PRO:CB	2.35	0.56
1:B:336:LYS:HB2	1:B:340:ASN:CB	2.34	0.56
1:B:533:GLN:N	1:B:534:PRO:HD2	2.21	0.56
1:B:598:TRP:CE2	1:B:742:PRO:HG3	2.40	0.56
1:B:857:ILE:HG21	1:B:862:LEU:HB2	1.87	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:454:SER:N	1:C:1253:LEU:O	2.35	0.56
1:C:814:LEU:N	1:C:814:LEU:CD2	2.68	0.56
1:C:823:ALA:N	1:C:824:PRO:HD2	2.20	0.56
1:C:836:VAL:HG23	1:C:836:VAL:O	2.05	0.56
1:C:906:TYR:HD1	1:C:1271:VAL:HG21	1.71	0.56
1:C:1086:GLY:N	1:C:1092:PRO:HG3	2.21	0.56
1:B:472:MET:HE2	1:B:506:PRO:HB2	1.88	0.56
1:B:682:HIS:CE1	1:B:1004:TYR:HE1	2.24	0.56
1:B:436:ARG:O	1:C:859:GLN:NE2	2.39	0.56
1:C:451:PHE:CG	1:C:1256:VAL:HG13	2.41	0.56
1:C:740:LEU:HB3	1:C:835:TYR:CD1	2.40	0.56
1:B:515:GLN:NE2	1:B:731:ASN:O	2.38	0.56
1:C:255:LEU:HB3	1:C:465:TRP:CH2	2.40	0.56
1:C:596:ALA:HA	1:C:599:LEU:HD12	1.87	0.56
1:C:1043:GLY:N	1:C:1142:GLY:O	2.29	0.56
1:B:699:ALA:HB1	1:B:702:LEU:CB	2.36	0.56
1:B:757:PHE:CZ	1:B:804:LYS:HA	2.40	0.56
1:B:782:GLN:N	1:B:783:PRO:CD	2.69	0.56
1:C:323:ILE:C	1:C:334:LEU:HD11	2.26	0.56
1:C:673:ARG:NH2	1:C:677:ALA:HB1	2.21	0.56
1:B:696:PRO:HG3	1:B:703:ARG:HD3	1.88	0.56
1:B:973:MET:HA	1:B:973:MET:HE3	1.87	0.56
1:B:1186:SER:C	1:B:1221:ALA:HB3	2.27	0.56
1:C:306:VAL:O	1:C:324:MET:N	2.31	0.56
1:C:301:VAL:HG22	1:C:1209:LEU:HD21	1.87	0.55
1:C:468:ARG:HD2	1:C:468:ARG:O	2.06	0.55
1:C:1056:TRP:CE3	1:C:1056:TRP:O	2.59	0.55
1:B:549:LEU:HD12	1:B:890:LYS:O	2.05	0.55
1:B:659:PHE:HZ	1:B:778:ASN:HD21	1.54	0.55
1:B:941:THR:HG22	1:B:993:ARG:HB3	1.89	0.55
1:C:267:LYS:HD3	1:C:310:TRP:CD2	2.41	0.55
1:C:508:ARG:HA	1:C:508:ARG:NE	2.21	0.55
1:B:494:THR:OG1	1:B:1272:MET:HB2	2.06	0.55
1:B:1046:ILE:HB	1:B:1200:ILE:CG1	2.36	0.55
1:C:449:ASP:HA	1:C:1257:VAL:O	2.07	0.55
1:C:928:VAL:HG22	1:C:987:LEU:HD13	1.88	0.55
1:C:1211:CYS:HA	1:C:1225:LYS:CG	2.29	0.55
1:B:295:PRO:CB	1:B:405:ILE:HA	2.33	0.55
1:B:1074:VAL:HG12	1:B:1109:ILE:HG12	1.88	0.55
1:B:1153:PRO:HG3	1:B:1183:PRO:HB2	1.87	0.55
1:B:1170:ILE:HA	1:B:1176:PRO:HD3	1.88	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:ARG:HG2	1:C:347:ARG:HH11	1.70	0.55
1:C:815:ALA:HB3	1:C:816:PRO:HD3	1.88	0.55
1:B:407:TYR:CD2	1:B:431:VAL:HG23	2.42	0.55
1:B:696:PRO:HG3	1:B:703:ARG:CD	2.37	0.55
1:B:929:GLN:O	1:B:932:VAL:HG22	2.07	0.55
1:C:1051:GLN:NE2	1:C:1194:PRO:HA	2.21	0.55
1:C:1230:GLU:CB	1:C:1250:VAL:HG11	2.31	0.55
1:B:285:PHE:O	1:B:286:PHE:C	2.43	0.55
1:B:378:PHE:HA	1:B:391:LEU:O	2.06	0.55
1:B:973:MET:HA	1:B:973:MET:HE2	1.88	0.55
1:B:1081:CYS:HA	1:B:1095:ARG:O	2.06	0.55
1:C:811:LEU:HA	1:C:815:ALA:CB	2.37	0.55
1:B:670:THR:O	1:B:673:ARG:HB3	2.07	0.55
1:B:821:VAL:O	1:B:824:PRO:HD2	2.07	0.55
1:B:850:THR:CG2	1:B:998:ALA:HB3	2.37	0.55
1:B:1059:LEU:HB3	1:B:1205:ASN:N	2.22	0.55
1:C:232:ILE:HD12	1:C:907:PRO:HB3	1.89	0.55
1:C:635:ALA:HA	1:C:638:LEU:CG	2.36	0.55
1:C:1131:LYS:HD3	1:C:1160:TRP:CG	2.41	0.55
1:B:483:LEU:CB	1:B:493:VAL:HG21	2.35	0.55
1:B:556:ILE:O	1:B:559:THR:HG22	2.07	0.55
1:B:1115:TRP:O	1:B:1119:THR:N	2.40	0.55
1:C:253:PRO:HD3	1:C:979:LEU:HD21	1.87	0.55
1:C:527:ASN:OD1	1:C:865:SER:HA	2.07	0.55
1:C:853:SER:N	1:C:995:THR:HB	2.14	0.55
1:B:265:SER:O	1:B:307:HIS:N	2.40	0.55
1:B:389:ALA:HB3	1:B:431:VAL:HG22	1.89	0.55
1:B:906:TYR:CD1	1:B:1275:PRO:HD3	2.41	0.55
1:B:1094:ILE:N	1:B:1102:VAL:O	2.30	0.55
1:C:922:MET:C	1:C:922:MET:SD	2.85	0.55
1:B:243:LYS:CB	1:B:538:ASP:OD2	2.52	0.55
1:B:333:HIS:HB3	1:B:346:VAL:HG12	1.89	0.55
1:B:415:ASN:HD22	1:B:416:VAL:H	1.55	0.55
1:B:757:PHE:HZ	1:B:804:LYS:HA	1.72	0.55
1:C:277:PRO:CD	1:C:416:VAL:HG22	2.37	0.55
1:C:381:ASP:HB2	1:C:391:LEU:HG	1.89	0.55
1:C:480:GLU:CD	1:C:495:SER:HB2	2.26	0.55
1:B:378:PHE:HB3	1:B:390:ASN:HB3	1.89	0.54
1:B:436:ARG:HB2	1:B:448:VAL:CG1	2.29	0.54
1:B:920:ARG:HH11	1:B:920:ARG:HG3	1.72	0.54
1:B:1096:ASP:N	1:B:1100:MET:O	2.40	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:THR:CG2	1:C:311:ALA:HB3	2.36	0.54
1:C:391:LEU:HD11	1:C:410:ARG:HD2	1.88	0.54
1:C:620:VAL:HG21	1:C:659:PHE:CE1	2.42	0.54
1:C:1074:VAL:CG1	1:C:1109:ILE:HG13	2.38	0.54
1:C:265:SER:CA	1:C:308:THR:HA	2.37	0.54
1:C:601:ASN:ND2	1:C:833:VAL:O	2.37	0.54
1:C:930:THR:HG1	1:C:1018:SER:HG	1.55	0.54
1:C:1057:SER:OG	1:C:1058:PRO:HD2	2.07	0.54
1:B:906:TYR:N	1:B:907:PRO:HD2	2.23	0.54
1:B:1231:ARG:HH21	1:B:1251:VAL:H	1.55	0.54
1:C:232:ILE:HG13	1:C:906:TYR:HE2	1.69	0.54
1:C:670:THR:H	1:C:673:ARG:HB2	1.72	0.54
1:C:960:ALA:O	1:C:964:THR:HG23	2.07	0.54
1:B:336:LYS:HB2	1:B:340:ASN:CG	2.28	0.54
1:B:416:VAL:O	1:B:416:VAL:HG22	2.08	0.54
1:B:1233:ASN:HA	1:B:1236:THR:OG1	2.07	0.54
1:C:418:LYS:CD	1:C:1214:SER:HA	2.29	0.54
1:C:709:ILE:O	1:C:713:TRP:N	2.40	0.54
1:B:259:ASP:CA	1:B:314:VAL:HG12	2.36	0.54
1:C:278:GLN:CA	1:C:416:VAL:H	2.15	0.54
1:C:1115:TRP:HA	1:C:1122:PHE:CD2	2.41	0.54
1:C:300:ALA:O	1:C:1212:THR:HA	2.08	0.54
1:C:955:LEU:HD12	1:C:955:LEU:C	2.28	0.54
1:B:1033:HIS:CD2	1:B:1248:PRO:HG2	2.43	0.54
1:C:494:THR:HB	1:C:1270:VAL:HB	1.89	0.54
1:C:543:LEU:HB3	1:C:592:ARG:HD2	1.90	0.54
1:C:844:PRO:HB3	1:C:1001:TYR:CD1	2.43	0.54
1:B:556:ILE:HD11	1:B:884:VAL:HG13	1.90	0.54
1:C:1151:TYR:O	1:C:1183:PRO:HA	2.08	0.54
1:B:242:LYS:N	1:B:242:LYS:HD2	2.23	0.54
1:B:285:PHE:HB2	1:C:1083:ILE:CG1	2.36	0.54
1:C:433:ARG:HB2	1:C:450:VAL:HG12	1.89	0.54
1:C:446:GLU:O	1:C:1261:ALA:N	2.25	0.54
1:C:1157:ALA:HB3	1:C:1195:ALA:HB1	1.88	0.54
1:B:433:ARG:HA	1:B:450:VAL:CB	2.38	0.54
1:B:591:PHE:HE1	1:B:811:LEU:HD21	1.69	0.54
1:C:603:VAL:HG22	1:C:831:PHE:HB3	1.89	0.54
1:C:822:ILE:HA	1:C:825:MET:HB2	1.90	0.54
1:C:1087:MET:N	1:C:1090:ALA:HB3	2.23	0.54
1:C:1147:MET:O	1:C:1180:PHE:N	2.38	0.54
1:B:265:SER:HA	1:B:308:THR:HA	1.89	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:ARG:NH1	1:B:1208:SER:HB3	2.23	0.53
1:B:352:LEU:HB3	1:B:955:LEU:HG	1.90	0.53
1:B:418:LYS:HB3	1:B:1226:HIS:CD2	2.44	0.53
1:C:417:SER:OG	1:C:420:CYS:SG	2.48	0.53
1:C:508:ARG:HH21	1:C:726:VAL:HA	1.73	0.53
1:C:715:ASN:O	1:C:744:ASP:N	2.41	0.53
1:B:852:GLN:HA	1:B:996:GLN:N	2.22	0.53
1:C:474:ILE:HD11	1:C:726:VAL:CG2	2.37	0.53
1:C:542:LEU:O	1:C:546:ILE:N	2.41	0.53
1:C:573:PRO:HB3	1:C:623:LEU:CD2	2.38	0.53
1:C:279:ASP:N	1:C:414:PRO:O	2.37	0.53
1:C:303:ARG:CG	1:C:1209:LEU:HA	2.33	0.53
1:C:307:HIS:CG	1:C:310:TRP:HB3	2.44	0.53
1:C:652:LEU:HD23	1:C:702:LEU:HD23	1.89	0.53
1:B:301:VAL:HG11	1:B:1150:TYR:OH	2.09	0.53
1:B:339:LEU:HD21	1:B:964:THR:HG21	1.89	0.53
1:B:809:MET:HB3	1:B:891:TYR:OH	2.08	0.53
1:B:851:ARG:HG3	1:B:851:ARG:NH1	2.22	0.53
1:B:1002:GLN:CB	1:B:1008:THR:HG22	2.38	0.53
1:B:1106:GLY:O	1:B:1136:ARG:N	2.38	0.53
1:C:305:VAL:CG2	1:C:326:PRO:HA	2.39	0.53
1:C:494:THR:CB	1:C:1270:VAL:HB	2.38	0.53
1:C:708:ILE:HG12	1:C:711:ARG:HH12	1.74	0.53
1:B:378:PHE:CB	1:B:390:ASN:HB3	2.39	0.53
1:B:591:PHE:CE2	1:B:595:LEU:HD11	2.43	0.53
1:B:653:ALA:HB1	1:B:671:GLN:HG3	1.90	0.53
1:C:427:VAL:HG22	1:C:1235:LEU:HA	1.90	0.53
1:C:494:THR:OG1	1:C:1272:MET:SD	2.55	0.53
1:C:636:LEU:HD13	1:C:648:ALA:CB	2.38	0.53
1:C:1146:TYR:HB2	1:C:1180:PHE:CE1	2.44	0.53
1:C:1230:GLU:O	1:C:1246:GLN:NE2	2.37	0.53
1:B:507:TYR:CZ	1:B:1267:ILE:HD11	2.44	0.53
1:B:847:VAL:HG22	1:B:1001:TYR:HB2	1.89	0.53
1:C:278:GLN:HA	1:C:415:ASN:HA	1.89	0.53
1:C:403:TYR:HA	1:C:406:MET:HE3	1.90	0.53
1:C:1136:ARG:HH22	1:C:1200:ILE:HD13	1.74	0.53
1:B:511:ASN:HB2	1:B:729:SER:O	2.08	0.53
1:B:536:LEU:HD13	1:B:593:VAL:HG13	1.91	0.53
1:B:857:ILE:HB	1:B:863:SER:HB3	1.91	0.53
1:C:307:HIS:HB3	1:C:310:TRP:HB3	1.90	0.53
1:C:654:ASN:ND2	1:C:671:GLN:O	2.41	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:435:ASP:O	1:B:449:ASP:N	2.34	0.53
1:B:631:ILE:HD13	1:B:883:THR:HG21	1.91	0.53
1:C:413:THR:HB	1:C:420:CYS:HB3	1.90	0.53
1:C:920:ARG:NH2	1:C:981:ASP:HB2	2.24	0.53
1:C:1029:GLU:OE1	1:C:1029:GLU:CA	2.56	0.53
1:C:1156:TYR:HA	1:C:1194:PRO:O	2.08	0.53
1:B:674:ARG:HD3	1:B:674:ARG:N	2.22	0.53
1:B:912:THR:CG2	1:B:1268:THR:HG23	2.39	0.53
1:B:952:ILE:HA	1:B:1143:ALA:HB3	1.91	0.53
1:C:223:PHE:CZ	1:C:1269:ALA:HB3	2.43	0.53
1:C:336:LYS:CA	1:C:340:ASN:HB2	2.39	0.53
1:C:591:PHE:CZ	1:C:595:LEU:HD11	2.44	0.53
1:B:439:MET:C	1:B:439:MET:SD	2.87	0.53
1:C:487:ALA:HB1	1:C:491:VAL:H	1.74	0.53
1:C:1101:MET:H	1:C:1101:MET:CE	2.21	0.53
1:C:1233:ASN:HA	1:C:1236:THR:OG1	2.09	0.53
1:B:377:GLY:O	1:B:392:ARG:HA	2.09	0.52
1:B:955:LEU:HD12	1:B:955:LEU:C	2.29	0.52
1:B:1061:PRO:HB2	1:B:1062:PRO:HD2	1.90	0.52
1:B:1096:ASP:HB3	1:B:1100:MET:H	1.73	0.52
1:C:262:LEU:HD11	1:C:402:TRP:CZ3	2.43	0.52
1:C:851:ARG:HA	1:C:997:LEU:HD23	1.91	0.52
1:B:295:PRO:HG3	1:B:408:PRO:HA	1.91	0.52
1:B:401:LYS:HE3	1:B:402:TRP:CE2	2.44	0.52
1:B:905:ILE:HG23	1:B:909:TYR:CE1	2.45	0.52
1:B:1149:HIS:O	1:B:1181:MET:HA	2.08	0.52
1:C:375:HIS:CE1	1:C:445:SER:N	2.76	0.52
1:C:732:LEU:CD1	1:C:1011:VAL:HG11	2.36	0.52
1:C:929:GLN:O	1:C:932:VAL:HG22	2.09	0.52
1:C:967:GLU:OE1	1:C:988:LEU:HD13	2.08	0.52
1:C:1150:TYR:HA	1:C:1182:VAL:O	2.09	0.52
1:C:1157:ALA:HB3	1:C:1195:ALA:HA	1.91	0.52
1:B:327:PRO:O	1:B:1147:MET:HG3	2.09	0.52
1:B:1084:SER:HB3	1:B:1101:MET:HE2	1.91	0.52
1:C:436:ARG:HD2	1:C:440:MET:HE1	1.91	0.52
1:C:504:LEU:N	1:C:1263:GLU:O	2.42	0.52
1:C:637:PRO:HB3	1:C:714:PRO:HG2	1.91	0.52
1:C:1074:VAL:HG11	1:C:1109:ILE:HG13	1.90	0.52
1:C:1158:ASN:ND2	1:C:1160:TRP:H	2.08	0.52
1:B:436:ARG:CB	1:B:448:VAL:HG12	2.31	0.52
1:B:750:VAL:HG12	1:B:752:THR:H	1.75	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:ARG:HB3	1:C:312:SER:OG	2.10	0.52
1:C:335:PHE:CD2	1:C:1040:ILE:HD11	2.43	0.52
1:C:338:LEU:HB2	1:C:357:ASN:ND2	2.23	0.52
1:C:1002:GLN:NE2	1:C:1006:GLY:HA2	2.24	0.52
1:C:1112:LEU:HG	1:C:1116:GLN:NE2	2.24	0.52
1:C:1131:LYS:HD2	1:C:1131:LYS:C	2.29	0.52
1:B:607:VAL:N	1:B:875:LEU:O	2.40	0.52
1:B:627:TRP:O	1:B:631:ILE:HG12	2.09	0.52
1:C:256:VAL:HG13	1:C:372:LEU:HD12	1.92	0.52
1:C:636:LEU:N	1:C:637:PRO:CD	2.73	0.52
1:C:922:MET:SD	1:C:922:MET:O	2.67	0.52
1:C:934:LEU:O	1:C:938:ILE:HG12	2.09	0.52
1:C:1023:CYS:O	1:C:1027:THR:HG23	2.10	0.52
1:B:333:HIS:HB3	1:B:346:VAL:CG1	2.39	0.52
1:B:457:LEU:HD12	1:B:457:LEU:O	2.10	0.52
1:B:850:THR:HG22	1:B:998:ALA:HB3	1.91	0.52
1:B:1095:ARG:HB2	1:B:1101:MET:HE3	1.91	0.52
1:C:515:GLN:CD	1:C:732:LEU:HD21	2.30	0.52
1:C:521:ARG:HD2	1:C:828:PHE:CE1	2.45	0.52
1:C:581:LEU:HA	1:C:880:ARG:HD2	1.92	0.52
1:C:948:TYR:CD2	1:C:948:TYR:N	2.78	0.52
1:C:1204:TYR:C	1:C:1204:TYR:CD2	2.82	0.52
1:C:1231:ARG:HA	1:C:1252:ASP:HA	1.91	0.52
1:B:287:THR:HA	1:B:290:TYR:CD1	2.45	0.52
1:B:574:ALA:O	1:B:577:ILE:HG22	2.10	0.52
1:C:278:GLN:HB3	1:C:415:ASN:OD1	2.10	0.52
1:C:598:TRP:CD1	1:C:742:PRO:HG3	2.44	0.52
1:C:685:PRO:HB2	1:C:688:PHE:HB3	1.92	0.52
1:C:1041:ALA:N	1:C:1144:TYR:O	2.37	0.52
1:B:272:VAL:CG1	1:B:300:ALA:HB3	2.39	0.52
1:B:434:PHE:N	1:B:449:ASP:O	2.43	0.52
1:B:646:VAL:CG1	1:B:685:PRO:HD2	2.39	0.52
1:B:664:MET:HG3	1:B:670:THR:C	2.31	0.52
1:B:1171:THR:N	1:B:1174:SER:O	2.39	0.52
1:C:277:PRO:CG	1:C:416:VAL:HG22	2.40	0.52
1:C:354:PHE:HB2	1:C:953:PRO:HG2	1.91	0.52
1:C:647:LYS:CA	1:C:675:ALA:HB1	2.40	0.52
1:B:696:PRO:HA	1:B:703:ARG:HB2	1.92	0.52
1:B:713:TRP:CD2	1:B:714:PRO:HD2	2.45	0.52
1:C:246:GLN:HG3	1:C:911:ASP:HB2	1.90	0.52
1:C:333:HIS:HA	1:C:336:LYS:CD	2.40	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:605:THR:HB	1:C:874:PRO:HA	1.90	0.52
1:C:985:GLU:N	1:C:986:PRO:CD	2.73	0.52
1:C:1166:TRP:HB2	1:C:1179:PRO:HG3	1.92	0.52
1:B:934:LEU:O	1:B:938:ILE:HG23	2.10	0.52
1:B:1074:VAL:HG22	1:B:1107:ASN:HB2	1.89	0.52
1:C:1159:ALA:HA	1:C:1162:LEU:HD22	1.91	0.52
1:B:381:ASP:HB3	1:B:388:GLY:CA	2.39	0.51
1:B:479:ILE:HD12	1:B:505:MET:CE	2.40	0.51
1:B:775:LEU:HD12	1:B:775:LEU:O	2.10	0.51
1:B:827:PRO:HG3	1:B:914:VAL:HG22	1.92	0.51
1:C:473:ASN:HA	1:C:506:PRO:HA	1.91	0.51
1:C:1095:ARG:HA	1:C:1101:MET:CA	2.38	0.51
1:B:543:LEU:HB3	1:B:592:ARG:HG2	1.92	0.51
1:B:643:CYS:O	1:B:647:LYS:HG3	2.10	0.51
1:B:812:GLN:O	1:B:816:PRO:HG2	2.11	0.51
1:B:859:GLN:HB2	1:B:862:LEU:HG	1.92	0.51
1:B:939:SER:HA	1:B:957:ALA:HB1	1.91	0.51
1:C:905:ILE:HG23	1:C:909:TYR:CE1	2.46	0.51
1:C:949:LEU:HB3	1:C:952:ILE:CD1	2.40	0.51
1:B:628:ASP:O	1:B:632:LEU:HG	2.10	0.51
1:C:355:ARG:HA	1:C:952:ILE:HG21	1.92	0.51
1:C:1046:ILE:N	1:C:1200:ILE:O	2.35	0.51
1:C:1111:PRO:HG2	1:C:1114:LEU:CB	2.39	0.51
1:B:836:VAL:CG2	1:B:836:VAL:O	2.58	0.51
1:B:985:GLU:OE1	1:B:985:GLU:HA	2.11	0.51
1:C:352:LEU:HB3	1:C:955:LEU:N	2.25	0.51
1:C:378:PHE:CZ	1:C:448:VAL:HG21	2.46	0.51
1:B:847:VAL:HG11	1:B:871:VAL:HB	1.91	0.51
1:B:1069:ARG:HA	1:B:1109:ILE:CG1	2.30	0.51
1:B:1113:ALA:O	1:B:1117:MET:HG2	2.11	0.51
1:C:255:LEU:HB3	1:C:465:TRP:CZ2	2.45	0.51
1:C:331:ASN:HA	1:C:333:HIS:CE1	2.46	0.51
1:C:338:LEU:HD11	1:C:360:HIS:CD2	2.46	0.51
1:C:1066:VAL:HG12	1:C:1200:ILE:HD12	1.92	0.51
1:B:864:LEU:HD12	1:B:868:ASN:HB3	1.92	0.51
1:C:277:PRO:HD2	1:C:416:VAL:HG22	1.92	0.51
1:C:543:LEU:CB	1:C:592:ARG:HD2	2.41	0.51
1:C:732:LEU:CB	1:C:1011:VAL:HG11	2.41	0.51
1:C:951:TRP:CZ3	1:C:1042:ARG:HB2	2.46	0.51
1:C:1104:PHE:HA	1:C:1108:TRP:HH2	1.75	0.51
1:C:1207:ARG:HH21	1:C:1231:ARG:HH22	1.59	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:762:THR:HG23	1:B:765:ARG:NH2	2.25	0.51
1:B:864:LEU:CD1	1:B:868:ASN:HB3	2.40	0.51
1:C:807:THR:CG2	1:C:886:LEU:HA	2.38	0.51
1:B:303:ARG:CG	1:B:1209:LEU:HA	2.29	0.51
1:B:418:LYS:HB3	1:B:1226:HIS:HD2	1.76	0.51
1:B:501:VAL:HG23	1:B:1263:GLU:OE1	2.11	0.51
1:C:607:VAL:HG23	1:C:876:ALA:HB2	1.93	0.51
1:C:1106:GLY:O	1:C:1135:LEU:HD12	2.10	0.51
1:B:413:THR:O	1:B:415:ASN:N	2.44	0.51
1:B:924:THR:O	1:B:928:VAL:HG23	2.11	0.51
1:C:776:VAL:HG22	1:C:776:VAL:O	2.11	0.51
1:C:811:LEU:HA	1:C:815:ALA:HB2	1.93	0.51
1:C:1112:LEU:HD13	1:C:1141:MET:HE1	1.92	0.51
1:B:253:PRO:N	1:B:979:LEU:HD21	2.25	0.51
1:B:446:GLU:O	1:B:1260:TYR:HA	2.11	0.51
1:B:598:TRP:CE3	1:B:742:PRO:HG3	2.46	0.51
1:B:811:LEU:HA	1:B:815:ALA:CB	2.41	0.51
1:B:854:ARG:HD3	1:B:857:ILE:HD12	1.93	0.51
1:B:985:GLU:OE1	1:B:985:GLU:CA	2.59	0.51
1:B:1034:GLU:HB3	1:B:1037:LEU:CG	2.41	0.51
1:B:1093:MET:CB	1:B:1101:MET:CB	2.89	0.51
1:B:1158:ASN:HA	1:B:1196:VAL:HB	1.92	0.51
1:C:336:LYS:HA	1:C:340:ASN:HD22	1.76	0.51
1:C:373:ASN:HB3	1:C:1259:ARG:CZ	2.41	0.51
1:C:440:MET:HB3	1:C:445:SER:OG	2.11	0.51
1:C:755:LEU:HG	1:C:804:LYS:HG3	1.93	0.51
1:C:870:THR:HB	1:C:872:GLY:O	2.11	0.51
1:C:556:ILE:CD1	1:C:888:SER:HB3	2.41	0.50
1:C:638:LEU:N	1:C:638:LEU:HD23	2.26	0.50
1:B:271:ILE:HB	1:B:301:VAL:HG12	1.93	0.50
1:C:1035:TYR:CA	1:C:1038:PHE:HB2	2.35	0.50
1:B:300:ALA:HA	1:B:1213:ASN:CA	2.41	0.50
1:B:355:ARG:NH2	1:B:950:ASP:HA	2.26	0.50
1:B:430:ARG:HD3	1:B:1234:ILE:HG23	1.93	0.50
1:B:946:ASP:HB3	1:B:948:TYR:CE1	2.46	0.50
1:C:267:LYS:O	1:C:305:VAL:N	2.44	0.50
1:C:598:TRP:CG	1:C:742:PRO:HG3	2.46	0.50
1:C:641:ASP:OD2	1:C:643:CYS:N	2.44	0.50
1:C:719:ILE:O	1:C:739:LEU:N	2.32	0.50
1:C:1147:MET:CE	1:C:1179:PRO:HB3	2.41	0.50
1:C:1159:ALA:O	1:C:1163:THR:HG23	2.10	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:PRO:HG2	1:B:408:PRO:HA	1.93	0.50
1:B:427:VAL:HG23	1:B:1235:LEU:O	2.11	0.50
1:B:647:LYS:CA	1:B:675:ALA:HB1	2.42	0.50
1:B:823:ALA:HB3	1:B:824:PRO:HD3	1.94	0.50
1:C:265:SER:HB3	1:C:308:THR:HG22	1.93	0.50
1:C:333:HIS:HA	1:C:336:LYS:HD3	1.93	0.50
1:C:339:LEU:CD1	1:C:353:MET:HB3	2.30	0.50
1:C:413:THR:HB	1:C:420:CYS:CB	2.41	0.50
1:C:509:ILE:HD11	1:C:727:PHE:HA	1.94	0.50
1:C:1112:LEU:HD22	1:C:1141:MET:HE2	1.93	0.50
1:C:1229:VAL:HG13	1:C:1236:THR:OG1	2.12	0.50
1:B:254:ARG:CZ	1:B:316:PHE:HB2	2.41	0.50
1:B:375:HIS:CD2	1:B:448:VAL:CG1	2.93	0.50
1:B:474:ILE:N	1:B:505:MET:O	2.44	0.50
1:B:612:SER:HB3	1:B:632:LEU:HD21	1.93	0.50
1:B:1059:LEU:CB	1:B:1204:TYR:HA	2.41	0.50
1:C:224:ILE:CG2	1:C:1270:VAL:HG22	2.42	0.50
1:C:622:SER:O	1:C:626:LEU:HG	2.11	0.50
1:C:719:ILE:HG23	1:C:739:LEU:HB3	1.92	0.50
1:C:1076:ILE:HA	1:C:1109:ILE:O	2.12	0.50
1:C:1110:PHE:HB2	1:C:1139:ILE:CD1	2.39	0.50
1:C:1163:THR:O	1:C:1167:LEU:HG	2.12	0.50
1:B:284:THR:CB	1:C:1083:ILE:HB	2.40	0.50
1:B:601:ASN:HD22	1:B:601:ASN:N	2.09	0.50
1:B:684:TRP:HB3	1:B:689:MET:HE1	1.94	0.50
1:B:686:ARG:HA	1:B:689:MET:HG3	1.93	0.50
1:B:849:VAL:O	1:B:868:ASN:HA	2.12	0.50
1:B:1213:ASN:HB3	1:B:1216:SER:HB2	1.92	0.50
1:C:276:VAL:HG13	1:C:1215:SER:CB	2.39	0.50
1:C:433:ARG:HD3	1:C:448:VAL:CG2	2.42	0.50
1:C:437:ALA:HB2	1:C:447:TRP:CD1	2.47	0.50
1:C:595:LEU:O	1:C:599:LEU:HG	2.11	0.50
1:B:440:MET:HG3	1:C:864:LEU:CD2	2.41	0.50
1:B:740:LEU:HB3	1:B:835:TYR:CE1	2.46	0.50
1:B:1058:PRO:CB	1:B:1200:ILE:HA	2.41	0.50
1:B:1094:ILE:N	1:B:1104:PHE:HE1	2.10	0.50
1:B:1131:LYS:HD2	1:B:1160:TRP:CD1	2.46	0.50
1:C:338:LEU:HD13	1:C:968:TRP:CE3	2.47	0.50
1:C:430:ARG:HD3	1:C:451:PHE:CZ	2.46	0.50
1:C:591:PHE:CE1	1:C:811:LEU:HD21	2.46	0.50
1:B:540:SER:HA	1:B:592:ARG:CB	2.42	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:PRO:HA	1:C:302:SER:HB3	1.92	0.50
1:C:601:ASN:N	1:C:832:GLN:HG2	2.25	0.50
1:C:844:PRO:HA	1:C:1002:GLN:O	2.12	0.50
1:C:1147:MET:HB3	1:C:1179:PRO:HA	1.94	0.50
1:B:333:HIS:O	1:B:337:GLN:N	2.44	0.50
1:B:522:ILE:O	1:B:526:GLY:N	2.45	0.50
1:B:627:TRP:CH2	1:B:796:THR:HG21	2.47	0.50
1:B:1050:VAL:N	1:B:1197:GLN:O	2.38	0.50
1:B:1083:ILE:HD11	1:B:1126:PHE:CZ	2.46	0.50
1:C:374:ARG:O	1:C:1259:ARG:HD3	2.12	0.50
1:C:375:HIS:ND1	1:C:444:MET:CG	2.75	0.50
1:C:641:ASP:HB3	1:C:644:ALA:HB2	1.94	0.50
1:C:937:GLN:NE2	1:C:945:VAL:HB	2.26	0.50
1:C:1041:ALA:HB2	1:C:1146:TYR:CD2	2.47	0.50
1:B:1060:ALA:HB2	1:B:1204:TYR:CD1	2.45	0.49
1:B:1170:ILE:HG23	1:B:1175:ILE:HG22	1.93	0.49
1:C:448:VAL:O	1:C:1258:THR:HA	2.12	0.49
1:B:472:MET:C	1:B:506:PRO:HA	2.33	0.49
1:B:507:TYR:CE1	1:B:1267:ILE:HD11	2.47	0.49
1:B:1147:MET:HB3	1:B:1179:PRO:HA	1.95	0.49
1:C:277:PRO:O	1:C:416:VAL:HG13	2.12	0.49
1:C:338:LEU:HD21	1:C:360:HIS:HB3	1.95	0.49
1:C:430:ARG:HG3	1:C:1234:ILE:O	2.11	0.49
1:C:551:ILE:HA	1:C:888:SER:O	2.12	0.49
1:C:1082:ARG:HH11	1:C:1082:ARG:CG	2.12	0.49
1:C:234:GLN:HA	1:C:246:GLN:O	2.12	0.49
1:C:528:ASN:ND2	1:C:530:THR:H	2.10	0.49
1:C:669:TYR:HA	1:C:673:ARG:CD	2.41	0.49
1:C:1002:GLN:HE22	1:C:1006:GLY:HA2	1.76	0.49
1:C:1046:ILE:HD12	1:C:1200:ILE:HD11	1.94	0.49
1:C:1198:TYR:N	1:C:1198:TYR:CD1	2.80	0.49
1:C:1204:TYR:CD2	1:C:1204:TYR:O	2.65	0.49
1:B:389:ALA:HB2	1:B:431:VAL:HG22	1.91	0.49
1:B:543:LEU:CB	1:B:592:ARG:HG2	2.42	0.49
1:B:1091:ALA:CB	1:B:1103:PRO:HB3	2.42	0.49
1:B:1166:TRP:CZ3	1:B:1170:ILE:HD11	2.47	0.49
1:C:283:TYR:O	1:C:289:SER:HA	2.12	0.49
1:C:577:ILE:HD13	1:C:627:TRP:CB	2.34	0.49
1:C:644:ALA:N	1:C:645:PRO:CD	2.75	0.49
1:C:725:ASN:ND2	1:C:726:VAL:HG23	2.27	0.49
1:C:1051:GLN:HA	1:C:1195:ALA:O	2.12	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1104:PHE:HA	1:C:1108:TRP:CH2	2.47	0.49
1:B:477:THR:HG22	1:B:481:TRP:CZ2	2.47	0.49
1:B:569:GLN:NE2	1:B:786:THR:OG1	2.41	0.49
1:B:608:ILE:HG12	1:B:639:THR:HG21	1.93	0.49
1:B:652:LEU:HD23	1:B:705:TRP:CD2	2.47	0.49
1:C:276:VAL:CB	1:C:277:PRO:HD3	2.15	0.49
1:C:278:GLN:HG2	1:C:415:ASN:CB	2.27	0.49
1:C:398:ASP:O	1:C:402:TRP:N	2.31	0.49
1:C:413:THR:HG21	1:C:420:CYS:HA	1.93	0.49
1:C:508:ARG:NH2	1:C:726:VAL:HG22	2.27	0.49
1:C:597:GLY:CA	1:C:604:VAL:HG11	2.41	0.49
1:C:606:THR:H	1:C:640:THR:HG1	1.61	0.49
1:C:690:ASN:HB3	1:C:693:LEU:CG	2.42	0.49
1:B:433:ARG:HD2	1:B:436:ARG:HD3	1.95	0.49
1:B:437:ALA:N	1:B:445:SER:HB3	2.28	0.49
1:B:474:ILE:O	1:B:505:MET:HB2	2.11	0.49
1:C:474:ILE:CG2	1:C:507:TYR:HB2	2.42	0.49
1:C:685:PRO:HB2	1:C:688:PHE:H	1.77	0.49
1:C:906:TYR:N	1:C:907:PRO:HD2	2.27	0.49
1:C:1130:ILE:HG22	1:C:1160:TRP:CZ3	2.48	0.49
1:B:433:ARG:CD	1:B:436:ARG:HD3	2.43	0.49
1:B:601:ASN:ND2	1:B:832:GLN:HG2	2.28	0.49
1:B:840:ARG:CA	1:B:843:VAL:HG23	2.38	0.49
1:B:1171:THR:HG22	1:B:1173:THR:N	2.28	0.49
1:C:476:PRO:O	1:C:480:GLU:HG3	2.12	0.49
1:C:957:ALA:HB1	1:C:961:THR:HB	1.94	0.49
1:C:1156:TYR:CE2	1:C:1158:ASN:HB2	2.47	0.49
1:B:331:ASN:ND2	1:B:335:PHE:HE1	2.10	0.49
1:B:1047:ILE:HG12	1:B:1199:ILE:HG12	1.95	0.49
1:B:1108:TRP:CG	1:B:1135:LEU:HD11	2.47	0.49
1:C:434:PHE:H	1:C:450:VAL:HA	1.78	0.49
1:C:542:LEU:HD11	1:C:546:ILE:HD12	1.93	0.49
1:C:1044:ASP:HA	1:C:1141:MET:CG	2.43	0.49
1:C:1138:ARG:NH2	1:C:1202:THR:HG21	2.28	0.49
1:B:284:THR:CG2	1:C:1083:ILE:HB	2.43	0.49
1:B:430:ARG:HH11	1:B:1234:ILE:HG23	1.78	0.49
1:B:569:GLN:HA	1:B:569:GLN:HE21	1.73	0.49
1:B:600:TYR:CD1	1:B:830:PRO:HB3	2.47	0.49
1:B:939:SER:OG	1:B:993:ARG:HD3	2.12	0.49
1:B:1009:PHE:N	1:B:1009:PHE:CD1	2.81	0.49
1:B:1186:SER:O	1:B:1221:ALA:HB3	2.12	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:HIS:CE1	1:C:233:VAL:HG21	2.47	0.49
1:C:222:GLU:HB2	1:C:1268:THR:HG22	1.95	0.49
1:B:340:ASN:HB3	1:B:343:THR:OG1	2.12	0.49
1:C:262:LEU:HB2	1:C:311:ALA:CB	2.41	0.49
1:C:303:ARG:HD2	1:C:327:PRO:HG2	1.95	0.49
1:C:383:THR:OG1	1:C:410:ARG:NH2	2.46	0.49
1:C:768:VAL:O	1:C:772:MET:HG3	2.12	0.49
1:C:772:MET:O	1:C:776:VAL:HG12	2.12	0.49
1:C:1003:GLN:N	1:C:1007:ARG:O	2.38	0.49
1:C:1115:TRP:O	1:C:1119:THR:N	2.46	0.49
1:B:285:PHE:HD2	1:B:286:PHE:N	2.10	0.48
1:B:514:ARG:HH12	1:B:727:PHE:HD2	1.60	0.48
1:B:673:ARG:HD3	1:B:677:ALA:HB3	1.93	0.48
1:B:718:GLN:HE22	1:B:738:VAL:HG22	1.78	0.48
1:B:850:THR:HG23	1:B:850:THR:O	2.13	0.48
1:B:1049:ARG:HG3	1:B:1196:VAL:HG13	1.95	0.48
1:B:1162:LEU:HD23	1:B:1162:LEU:N	2.28	0.48
1:C:277:PRO:O	1:C:416:VAL:CA	2.61	0.48
1:C:436:ARG:HB3	1:C:448:VAL:HG23	1.95	0.48
1:C:607:VAL:HG22	1:C:875:LEU:C	2.33	0.48
1:C:614:PRO:HB2	1:C:618:GLY:CA	2.43	0.48
1:C:1041:ALA:O	1:C:1144:TYR:N	2.45	0.48
1:C:1159:ALA:HA	1:C:1162:LEU:HD13	1.95	0.48
1:B:690:ASN:ND2	1:B:693:LEU:HG	2.28	0.48
1:B:1188:HIS:HA	1:B:1220:ILE:HG22	1.95	0.48
1:C:391:LEU:HD11	1:C:410:ARG:CD	2.43	0.48
1:C:859:GLN:OE1	1:C:860:PRO:HD2	2.13	0.48
1:C:928:VAL:HG22	1:C:987:LEU:CD1	2.42	0.48
1:B:374:ARG:HA	1:B:1260:TYR:O	2.13	0.48
1:B:550:GLN:HB2	1:B:890:LYS:HE3	1.94	0.48
1:B:602:GLY:HA2	1:B:833:VAL:CG1	2.37	0.48
1:B:847:VAL:HA	1:B:1001:TYR:HA	1.94	0.48
1:C:257:THR:O	1:C:372:LEU:HB2	2.12	0.48
1:C:403:TYR:HB3	1:C:410:ARG:NH1	2.29	0.48
1:C:451:PHE:CE2	1:C:1256:VAL:HG22	2.48	0.48
1:C:465:TRP:O	1:C:469:LEU:HG	2.13	0.48
1:C:1120:ARG:HH12	1:C:1168:GLU:HA	1.78	0.48
1:C:1159:ALA:O	1:C:1163:THR:N	2.35	0.48
1:B:543:LEU:HD12	1:B:592:ARG:HB3	1.95	0.48
1:B:674:ARG:HD3	1:B:674:ARG:H	1.77	0.48
1:B:777:ASP:HA	1:B:782:GLN:NE2	2.27	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:795:GLY:O	1:B:799:LYS:HG3	2.14	0.48
1:B:1034:GLU:HB3	1:B:1037:LEU:CB	2.43	0.48
1:C:821:VAL:O	1:C:825:MET:HG2	2.13	0.48
1:C:850:THR:O	1:C:997:LEU:HA	2.13	0.48
1:C:1200:ILE:O	1:C:1200:ILE:CG1	2.61	0.48
1:B:267:LYS:HD2	1:B:310:TRP:CG	2.48	0.48
1:B:515:GLN:CG	1:B:730:ALA:HA	2.42	0.48
1:B:591:PHE:CZ	1:B:595:LEU:HD11	2.48	0.48
1:B:606:THR:N	1:B:640:THR:OG1	2.40	0.48
1:B:1231:ARG:HA	1:B:1252:ASP:HA	1.95	0.48
1:C:333:HIS:HA	1:C:336:LYS:CG	2.43	0.48
1:C:580:LYS:HE2	1:C:624:GLU:HG2	1.94	0.48
1:C:1170:ILE:HA	1:C:1176:PRO:CD	2.43	0.48
1:B:890:LYS:HB3	1:B:890:LYS:HE2	1.68	0.48
1:B:1094:ILE:HD12	1:B:1126:PHE:CZ	2.46	0.48
1:C:527:ASN:ND2	1:C:867:THR:OG1	2.47	0.48
1:C:970:ASN:ND2	1:C:988:LEU:HD11	2.29	0.48
1:C:974:LYS:HD3	1:C:983:LEU:CB	2.43	0.48
1:C:1084:SER:O	1:C:1092:PRO:HB2	2.13	0.48
1:C:1098:THR:OG1	1:C:1100:MET:HG2	2.14	0.48
1:B:650:MET:O	1:B:654:ASN:N	2.42	0.48
1:B:699:ALA:HB1	1:B:702:LEU:HB3	1.94	0.48
1:B:1095:ARG:NE	1:B:1096:ASP:O	2.39	0.48
1:B:1166:TRP:O	1:B:1170:ILE:HG13	2.13	0.48
1:B:1219:THR:HG21	1:B:1224:ASP:HA	1.96	0.48
1:C:373:ASN:HB3	1:C:1259:ARG:NE	2.29	0.48
1:B:271:ILE:HG12	1:B:302:SER:HA	1.96	0.48
1:B:503:ARG:HB3	1:B:1265:PRO:CD	2.43	0.48
1:B:906:TYR:HE1	1:B:1275:PRO:HD3	1.74	0.48
1:B:1051:GLN:HA	1:B:1195:ALA:O	2.13	0.48
1:C:232:ILE:CD1	1:C:907:PRO:HB3	2.43	0.48
1:C:281:LEU:C	1:C:292:ILE:HD12	2.34	0.48
1:C:1154:ARG:HA	1:C:1192:SER:CA	2.42	0.48
1:B:399:ALA:O	1:B:403:TYR:HD1	1.97	0.48
1:B:627:TRP:HA	1:B:627:TRP:CE3	2.49	0.48
1:B:849:VAL:CG1	1:B:999:ILE:HG13	2.40	0.48
1:B:1031:PHE:HA	1:B:1038:PHE:CE1	2.49	0.48
1:C:475:ASN:OD1	1:C:475:ASN:C	2.52	0.48
1:C:504:LEU:O	1:C:1265:PRO:HD2	2.14	0.48
1:C:833:VAL:CG1	1:C:834:PRO:CD	2.75	0.48
1:C:994:MET:CE	1:C:997:LEU:HD21	2.44	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:LEU:HD13	1:B:391:LEU:N	2.29	0.48
1:B:432:GLY:C	1:B:450:VAL:HG23	2.34	0.48
1:B:755:LEU:HD21	1:B:757:PHE:CZ	2.48	0.48
1:B:1229:VAL:HG13	1:B:1236:THR:CG2	2.44	0.48
1:C:322:VAL:CG1	1:C:334:LEU:HD13	2.43	0.48
1:C:530:THR:O	1:C:534:PRO:HD3	2.14	0.48
1:B:547:SER:HA	1:B:818:GLU:OE2	2.13	0.47
1:B:600:TYR:HE2	1:B:828:PHE:CE2	2.32	0.47
1:B:931:LEU:O	1:B:935:VAL:HG23	2.14	0.47
1:C:637:PRO:HG3	1:C:764:TRP:CE2	2.49	0.47
1:C:790:VAL:O	1:C:794:ARG:HG3	2.14	0.47
1:C:1147:MET:N	1:C:1178:VAL:O	2.34	0.47
1:C:1166:TRP:NE1	1:C:1179:PRO:HD3	2.28	0.47
1:B:601:ASN:HD22	1:B:601:ASN:H	1.61	0.47
1:B:822:ILE:HG22	1:B:826:LEU:HD21	1.95	0.47
1:C:271:ILE:HD13	1:C:301:VAL:HG12	1.96	0.47
1:C:699:ALA:HB1	1:C:702:LEU:CD1	2.42	0.47
1:C:1149:HIS:O	1:C:1182:VAL:N	2.39	0.47
1:B:579:GLY:O	1:B:582:ARG:HG3	2.15	0.47
1:B:623:LEU:HB2	1:B:785:TRP:CH2	2.49	0.47
1:B:947:ARG:HG2	1:B:947:ARG:HH11	1.78	0.47
1:C:283:TYR:O	1:C:290:TYR:N	2.45	0.47
1:C:295:PRO:HG3	1:C:404:SER:CB	2.38	0.47
1:C:413:THR:HG21	1:C:423:VAL:CB	2.41	0.47
1:C:521:ARG:HD2	1:C:828:PHE:CD1	2.48	0.47
1:C:543:LEU:HB3	1:C:592:ARG:HH11	1.79	0.47
1:B:261:GLY:N	1:B:313:ASN:H	2.13	0.47
1:B:569:GLN:NE2	1:B:569:GLN:CA	2.64	0.47
1:B:752:THR:HG22	1:B:895:LEU:O	2.15	0.47
1:B:778:ASN:HD22	1:B:781:TYR:CB	2.27	0.47
1:B:955:LEU:CD1	1:B:961:THR:HG21	2.43	0.47
1:B:1106:GLY:O	1:B:1135:LEU:HA	2.13	0.47
1:B:1108:TRP:O	1:B:1137:ILE:HA	2.14	0.47
1:C:366:VAL:HG22	1:C:461:ILE:HD13	1.95	0.47
1:C:697:ILE:O	1:C:700:PRO:HD3	2.15	0.47
1:C:1167:LEU:O	1:C:1170:ILE:HB	2.14	0.47
1:B:1104:PHE:N	1:B:1104:PHE:HD1	2.08	0.47
1:B:1182:VAL:HG23	1:B:1183:PRO:HD2	1.97	0.47
1:B:1260:TYR:HB3	1:B:1262:TYR:CE2	2.50	0.47
1:C:237:ALA:HA	1:C:247:LEU:HD13	1.96	0.47
1:C:472:MET:HA	1:C:508:ARG:HB3	1.97	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:PRO:HD3	1:B:979:LEU:HD11	1.97	0.47
1:B:332:ILE:O	1:B:336:LYS:HG2	2.14	0.47
1:B:520:ILE:HG23	1:B:986:PRO:HG2	1.96	0.47
1:C:601:ASN:HB3	1:C:832:GLN:HG2	1.96	0.47
1:C:803:ILE:HG21	1:C:887:LEU:HG	1.97	0.47
1:C:817:VAL:O	1:C:821:VAL:HG23	2.14	0.47
1:C:920:ARG:NE	1:C:979:LEU:HD22	2.30	0.47
1:C:943:TYR:CD1	1:C:944:PRO:HD2	2.49	0.47
1:C:1076:ILE:CG1	1:C:1109:ILE:HB	2.40	0.47
1:B:299:ALA:O	1:B:1213:ASN:N	2.47	0.47
1:B:445:SER:HB2	1:B:448:VAL:CG1	2.44	0.47
1:B:533:GLN:HE21	1:B:537:GLN:NE2	2.11	0.47
1:B:699:ALA:HB1	1:B:702:LEU:HB2	1.97	0.47
1:B:766:ALA:HB1	1:B:801:LYS:HE3	1.97	0.47
1:B:777:ASP:HA	1:B:782:GLN:HE21	1.80	0.47
1:B:1057:SER:CB	1:B:1060:ALA:H	2.28	0.47
1:B:1163:THR:CG2	1:B:1198:TYR:HB2	2.33	0.47
1:B:1211:CYS:HA	1:B:1225:LYS:CG	2.39	0.47
1:C:274:ALA:HB1	1:C:1215:SER:HB3	1.95	0.47
1:C:515:GLN:HG2	1:C:730:ALA:O	2.15	0.47
1:C:623:LEU:O	1:C:626:LEU:HB2	2.15	0.47
1:C:699:ALA:CB	1:C:702:LEU:HB2	2.40	0.47
1:C:963:ALA:HB2	1:C:992:PRO:HG3	1.97	0.47
1:C:1079:ARG:HG2	1:C:1079:ARG:HH11	1.78	0.47
1:B:475:ASN:ND2	1:B:478:GLU:H	2.11	0.47
1:B:920:ARG:HH11	1:B:920:ARG:CG	2.27	0.47
1:B:935:VAL:HA	1:B:938:ILE:HG12	1.96	0.47
1:B:1058:PRO:HB2	1:B:1201:SER:H	1.79	0.47
1:C:225:SER:OG	1:C:228:GLN:HG2	2.15	0.47
1:C:782:GLN:HB2	1:C:785:TRP:CE2	2.49	0.47
1:C:541:VAL:HG13	1:C:545:ARG:CZ	2.45	0.47
1:C:646:VAL:HG21	1:C:684:TRP:CD1	2.50	0.47
1:C:765:ARG:HG3	1:C:765:ARG:NH1	2.30	0.47
1:C:1151:TYR:C	1:C:1151:TYR:HD1	2.16	0.47
1:C:1254:TYR:C	1:C:1254:TYR:CD2	2.89	0.47
1:B:572:SER:HB3	1:B:575:SER:HB3	1.97	0.47
1:B:604:VAL:HA	1:B:873:VAL:O	2.15	0.47
1:B:606:THR:H	1:B:640:THR:HG1	1.58	0.47
1:B:852:GLN:C	1:B:996:GLN:HG2	2.35	0.47
1:B:1104:PHE:HA	1:B:1108:TRP:CH2	2.50	0.47
1:C:254:ARG:HH11	1:C:254:ARG:CB	2.26	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:MET:HB2	1:C:334:LEU:HD12	1.95	0.47
1:C:477:THR:HA	1:C:480:GLU:CD	2.35	0.47
1:C:620:VAL:HG21	1:C:659:PHE:CZ	2.50	0.47
1:C:1036:ASN:C	1:C:1036:ASN:HD22	2.18	0.47
1:C:1051:GLN:HG2	1:C:1195:ALA:H	1.79	0.47
1:C:1249:GLU:CD	1:C:1249:GLU:H	2.18	0.47
1:B:298:GLU:HB3	1:B:1215:SER:N	2.30	0.46
1:B:351:PRO:HA	1:B:354:PHE:CG	2.48	0.46
1:B:437:ALA:H	1:B:445:SER:HB3	1.79	0.46
1:B:811:LEU:HA	1:B:815:ALA:HB2	1.97	0.46
1:C:301:VAL:HG22	1:C:1209:LEU:CD2	2.45	0.46
1:C:305:VAL:HA	1:C:324:MET:CE	2.41	0.46
1:C:472:MET:HE2	1:C:506:PRO:HB2	1.96	0.46
1:C:514:ARG:NH1	1:C:729:SER:HA	2.29	0.46
1:C:723:ALA:HB3	1:C:727:PHE:CD2	2.50	0.46
1:C:1127:ASP:HA	1:C:1130:ILE:HD12	1.97	0.46
1:B:846:MET:HB3	1:B:1002:GLN:HB3	1.96	0.46
1:B:867:THR:HG22	1:B:867:THR:O	2.16	0.46
1:B:1057:SER:O	1:B:1061:PRO:N	2.48	0.46
1:C:301:VAL:HG13	1:C:1209:LEU:CD1	2.45	0.46
1:C:674:ARG:HA	1:C:674:ARG:HD3	1.57	0.46
1:C:690:ASN:HB3	1:C:693:LEU:CD1	2.45	0.46
1:C:1033:HIS:CD2	1:C:1248:PRO:HG2	2.51	0.46
1:C:1062:PRO:HB2	1:C:1065:LEU:HG	1.96	0.46
1:C:1108:TRP:CD2	1:C:1135:LEU:HD11	2.51	0.46
1:B:823:ALA:HA	1:B:826:LEU:CD2	2.45	0.46
1:B:942:GLN:H	1:B:942:GLN:HG3	1.35	0.46
1:B:1062:PRO:HG2	1:B:1065:LEU:HB2	1.96	0.46
1:C:219:HIS:ND1	1:C:233:VAL:HG11	2.31	0.46
1:C:267:LYS:HB3	1:C:310:TRP:CE2	2.51	0.46
1:C:270:PRO:CG	1:C:297:PRO:HB2	2.33	0.46
1:C:379:SER:N	1:C:391:LEU:O	2.45	0.46
1:C:400:GLU:HA	1:C:403:TYR:HB2	1.97	0.46
1:B:242:LYS:HD3	1:B:534:PRO:CB	2.44	0.46
1:B:1031:PHE:HZ	1:B:1040:ILE:HG13	1.80	0.46
1:B:1137:ILE:HG22	1:B:1139:ILE:HD12	1.97	0.46
1:C:582:ARG:N	1:C:583:PRO:HD3	2.29	0.46
1:C:920:ARG:HH22	1:C:981:ASP:CB	2.27	0.46
1:C:991:ASP:N	1:C:992:PRO:CD	2.78	0.46
1:C:1075:HIS:O	1:C:1109:ILE:N	2.42	0.46
1:B:324:MET:H	1:B:324:MET:HE2	1.80	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:SER:HB2	1:B:448:VAL:HG13	1.98	0.46
1:B:474:ILE:HG12	1:B:505:MET:HB2	1.98	0.46
1:B:503:ARG:CD	1:B:1265:PRO:HG3	2.40	0.46
1:B:891:TYR:HB3	1:B:895:LEU:HD22	1.96	0.46
1:C:349:ALA:CB	1:C:354:PHE:HE2	2.29	0.46
1:C:785:TRP:CZ3	1:C:789:LEU:HD22	2.50	0.46
1:B:261:GLY:H	1:B:313:ASN:H	1.63	0.46
1:B:352:LEU:HB3	1:B:955:LEU:H	1.80	0.46
1:B:617:GLY:CA	1:B:654:ASN:CB	2.90	0.46
1:B:707:GLU:HB3	1:B:711:ARG:HH22	1.79	0.46
1:B:974:LYS:HD3	1:B:983:LEU:HB3	1.98	0.46
1:C:271:ILE:HG22	1:C:272:VAL:HG23	1.97	0.46
1:C:378:PHE:H	1:C:443:ALA:HB1	1.80	0.46
1:C:464:ARG:HH12	1:C:1022:ASP:HB2	1.81	0.46
1:C:533:GLN:N	1:C:534:PRO:CD	2.78	0.46
1:C:636:LEU:CD2	1:C:648:ALA:HB2	2.43	0.46
1:C:1147:MET:HE2	1:C:1179:PRO:HB3	1.97	0.46
1:C:1157:ALA:O	1:C:1196:VAL:N	2.41	0.46
1:B:307:HIS:ND1	1:B:310:TRP:HB3	2.30	0.46
1:B:515:GLN:O	1:B:519:ILE:HG13	2.14	0.46
1:B:573:PRO:HB3	1:B:623:LEU:HD21	1.98	0.46
1:B:1203:GLU:HG3	1:B:1205:ASN:ND2	2.27	0.46
1:C:248:LEU:HA	1:C:913:GLU:OE1	2.16	0.46
1:C:854:ARG:HA	1:C:854:ARG:CZ	2.43	0.46
1:B:325:ALA:H	1:B:331:ASN:HD21	1.64	0.46
1:B:520:ILE:CG2	1:B:986:PRO:HG2	2.46	0.46
1:B:1069:ARG:HG2	1:B:1109:ILE:CG2	2.44	0.46
1:B:1218:GLN:HG2	1:B:1220:ILE:HG13	1.98	0.46
1:C:261:GLY:HA3	1:C:313:ASN:H	1.79	0.46
1:C:378:PHE:HE2	1:C:433:ARG:HB2	1.80	0.46
1:C:385:PHE:CE2	1:C:412:GLY:HA3	2.51	0.46
1:C:392:ARG:NH1	1:C:406:MET:SD	2.89	0.46
1:C:417:SER:H	1:C:420:CYS:HB2	1.80	0.46
1:C:450:VAL:O	1:C:1256:VAL:HA	2.16	0.46
1:C:528:ASN:HD21	1:C:530:THR:HB	1.81	0.46
1:C:854:ARG:NH1	1:C:854:ARG:CA	2.67	0.46
1:C:985:GLU:O	1:C:989:SER:N	2.49	0.46
1:C:1042:ARG:HG2	1:C:1043:GLY:N	2.30	0.46
1:C:1170:ILE:HG12	1:C:1175:ILE:CG1	2.43	0.46
1:B:244:THR:O	1:B:248:LEU:HG	2.16	0.46
1:B:298:GLU:HG2	1:B:1214:SER:HB2	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:LEU:HG	1:B:506:PRO:HD3	1.98	0.46
1:B:573:PRO:HA	1:B:623:LEU:HD21	1.97	0.46
1:B:732:LEU:HD12	1:B:831:PHE:CE1	2.50	0.46
1:C:246:GLN:HG3	1:C:907:PRO:O	2.15	0.46
1:C:258:TRP:O	1:C:314:VAL:HG12	2.15	0.46
1:C:307:HIS:HA	1:C:323:ILE:HA	1.97	0.46
1:C:593:VAL:CG1	1:C:875:LEU:HD21	2.45	0.46
1:C:843:VAL:O	1:C:1004:TYR:N	2.48	0.46
1:C:1111:PRO:HG2	1:C:1114:LEU:CG	2.45	0.46
1:B:270:PRO:HG3	1:B:297:PRO:HB3	1.98	0.46
1:B:406:MET:HG3	1:B:452:GLU:HB2	1.98	0.46
1:B:637:PRO:CB	1:B:714:PRO:HG2	2.46	0.46
1:B:657:VAL:CG2	1:B:671:GLN:HG2	2.46	0.46
1:B:1160:TRP:HB2	1:B:1198:TYR:CZ	2.51	0.46
1:C:302:SER:O	1:C:1209:LEU:HD12	2.16	0.46
1:C:836:VAL:HG23	1:C:843:VAL:HG22	1.96	0.46
1:C:1249:GLU:CD	1:C:1249:GLU:N	2.69	0.46
1:B:437:ALA:HB3	1:B:447:TRP:H	1.79	0.45
1:B:778:ASN:HD22	1:B:781:TYR:HB2	1.81	0.45
1:B:439:MET:HE1	1:C:989:SER:O	2.17	0.45
1:B:645:PRO:HG3	1:B:713:TRP:CZ2	2.51	0.45
1:B:1220:ILE:HG22	1:B:1220:ILE:O	2.17	0.45
1:C:822:ILE:O	1:C:825:MET:HB2	2.16	0.45
1:B:544:GLN:HA	1:B:592:ARG:HH21	1.81	0.45
1:B:573:PRO:CB	1:B:623:LEU:HD21	2.46	0.45
1:B:596:ALA:HA	1:B:599:LEU:HD12	1.98	0.45
1:B:659:PHE:CZ	1:B:778:ASN:ND2	2.78	0.45
1:B:668:ILE:O	1:B:673:ARG:NE	2.49	0.45
1:B:852:GLN:CA	1:B:995:THR:HA	2.34	0.45
1:B:1231:ARG:NH2	1:B:1250:VAL:HA	2.30	0.45
1:C:1232:TYR:HE1	1:C:1253:LEU:HD12	1.79	0.45
1:B:283:TYR:HB2	1:B:286:PHE:CG	2.50	0.45
1:B:644:ALA:N	1:B:645:PRO:CD	2.79	0.45
1:C:472:MET:HA	1:C:508:ARG:CB	2.47	0.45
1:C:708:ILE:HG23	1:C:712:TYR:HD1	1.81	0.45
1:C:769:CYS:SG	1:C:801:LYS:HB2	2.55	0.45
1:C:1064:ASP:N	1:C:1064:ASP:OD1	2.49	0.45
1:B:418:LYS:H	1:B:418:LYS:HG3	1.60	0.45
1:B:939:SER:CB	1:B:993:ARG:HD3	2.47	0.45
1:B:1084:SER:HB3	1:B:1101:MET:CE	2.45	0.45
1:C:226:SER:OG	1:C:1272:MET:HA	2.17	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:TYR:HD1	1:C:290:TYR:CB	2.28	0.45
1:C:347:ARG:HG2	1:C:347:ARG:NH1	2.32	0.45
1:C:528:ASN:ND2	1:C:530:THR:HB	2.31	0.45
1:C:685:PRO:HD2	1:C:688:PHE:HB3	1.98	0.45
1:C:716:PRO:HB3	1:C:742:PRO:HA	1.99	0.45
1:C:789:LEU:O	1:C:793:MET:HB2	2.16	0.45
1:B:515:GLN:HG2	1:B:730:ALA:HA	1.97	0.45
1:C:635:ALA:HA	1:C:638:LEU:CD1	2.47	0.45
1:C:703:ARG:O	1:C:707:GLU:HG3	2.17	0.45
1:C:949:LEU:HA	1:C:951:TRP:NE1	2.31	0.45
1:C:1031:PHE:O	1:C:1035:TYR:N	2.50	0.45
1:C:1233:ASN:HB2	1:C:1246:GLN:HE22	1.82	0.45
1:B:381:ASP:O	1:B:388:GLY:HA2	2.17	0.45
1:B:454:SER:O	1:B:1255:ASN:ND2	2.49	0.45
1:B:748:ALA:HB2	1:B:813:GLN:CG	2.47	0.45
1:C:279:ASP:CB	1:C:414:PRO:O	2.60	0.45
1:C:812:GLN:O	1:C:816:PRO:HG2	2.16	0.45
1:C:1136:ARG:NH2	1:C:1200:ILE:HD13	2.30	0.45
1:B:265:SER:CA	1:B:308:THR:HA	2.46	0.45
1:B:415:ASN:HD22	1:B:416:VAL:N	2.14	0.45
1:B:812:GLN:HG2	1:B:813:GLN:HG3	1.98	0.45
1:B:815:ALA:N	1:B:816:PRO:CD	2.80	0.45
1:B:1105:GLU:CA	1:B:1135:LEU:HB2	2.45	0.45
1:C:218:ARG:NH2	1:C:241:ASN:HB2	2.31	0.45
1:C:574:ALA:O	1:C:578:LEU:HG	2.17	0.45
1:C:926:GLU:OE1	1:C:926:GLU:C	2.55	0.45
1:C:1086:GLY:H	1:C:1092:PRO:HG3	1.82	0.45
1:C:1157:ALA:HB3	1:C:1195:ALA:CA	2.47	0.45
1:B:242:LYS:HD2	1:B:242:LYS:H	1.82	0.45
1:C:433:ARG:HA	1:C:450:VAL:HG12	1.97	0.45
1:C:708:ILE:HG23	1:C:712:TYR:CD1	2.52	0.45
1:B:521:ARG:O	1:B:524:ASN:ND2	2.50	0.45
1:B:945:VAL:HG22	1:B:946:ASP:N	2.32	0.45
1:C:479:ILE:O	1:C:483:LEU:HG	2.17	0.45
1:C:1158:ASN:HD21	1:C:1160:TRP:HB3	1.81	0.45
1:B:268:ILE:HD12	1:B:268:ILE:N	2.32	0.44
1:B:767:ARG:HD3	1:B:767:ARG:HA	1.71	0.44
1:B:805:SER:OG	1:B:886:LEU:O	2.32	0.44
1:B:810:TYR:HB2	1:B:891:TYR:CE1	2.49	0.44
1:B:1071:THR:HB	1:B:1074:VAL:HG21	2.00	0.44
1:B:1093:MET:HE1	1:B:1103:PRO:CD	2.47	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:ARG:H	1:C:218:ARG:HG3	1.59	0.44
1:C:503:ARG:HG2	1:C:1265:PRO:HG3	1.99	0.44
1:C:505:MET:CG	1:C:1265:PRO:HG2	2.47	0.44
1:C:690:ASN:ND2	1:C:693:LEU:HG	2.32	0.44
1:C:959:ALA:CB	1:C:993:ARG:HD3	2.47	0.44
1:C:1036:ASN:C	1:C:1036:ASN:ND2	2.70	0.44
1:B:602:GLY:HA3	1:B:831:PHE:CD2	2.42	0.44
1:B:652:LEU:HD12	1:B:652:LEU:C	2.37	0.44
1:B:654:ASN:HA	1:B:657:VAL:HG23	1.99	0.44
1:B:670:THR:HG23	1:B:673:ARG:N	2.32	0.44
1:B:720:ARG:HA	1:B:737:GLU:O	2.16	0.44
1:B:851:ARG:HA	1:B:997:LEU:HD23	2.00	0.44
1:C:353:MET:H	1:C:353:MET:HG2	1.61	0.44
1:C:394:LEU:HD23	1:C:394:LEU:HA	1.63	0.44
1:C:413:THR:CG2	1:C:420:CYS:HA	2.47	0.44
1:C:633:ALA:O	1:C:637:PRO:HD3	2.17	0.44
1:B:253:PRO:HA	1:B:977:PHE:O	2.17	0.44
1:B:517:SER:HB3	1:B:925:CYS:SG	2.56	0.44
1:B:603:VAL:HG13	1:B:831:PHE:CG	2.52	0.44
1:B:1046:ILE:HG23	1:B:1067:PHE:HE2	1.81	0.44
1:C:223:PHE:CE2	1:C:1269:ALA:HB3	2.53	0.44
1:C:283:TYR:CZ	1:C:385:PHE:HZ	2.35	0.44
1:C:359:LEU:N	1:C:359:LEU:HD23	2.33	0.44
1:C:394:LEU:HD12	1:C:402:TRP:CD1	2.52	0.44
1:C:716:PRO:CD	1:C:837:ARG:HD2	2.47	0.44
1:B:340:ASN:N	1:B:340:ASN:ND2	2.61	0.44
1:B:543:LEU:HD13	1:B:595:LEU:HD12	2.00	0.44
1:B:1091:ALA:HB1	1:B:1092:PRO:HD2	1.98	0.44
1:B:1093:MET:HE1	1:B:1103:PRO:HG3	1.99	0.44
1:C:296:PHE:HZ	1:C:422:PHE:HE2	1.65	0.44
1:C:433:ARG:HD2	1:C:436:ARG:HB3	1.99	0.44
1:C:806:MET:HE3	1:C:809:MET:HE1	1.99	0.44
1:B:376:THR:HG23	1:B:1259:ARG:HD3	1.98	0.44
1:B:595:LEU:O	1:B:599:LEU:HG	2.18	0.44
1:B:1057:SER:HB3	1:B:1060:ALA:HB3	1.99	0.44
1:C:248:LEU:C	1:C:248:LEU:HD23	2.38	0.44
1:C:300:ALA:CB	1:C:1185:SER:HB3	2.42	0.44
1:C:338:LEU:HG	1:C:357:ASN:HA	2.00	0.44
1:C:1077:PHE:CE2	1:C:1094:ILE:HD13	2.52	0.44
1:B:268:ILE:HG22	1:B:297:PRO:HG2	2.00	0.44
1:B:352:LEU:HB3	1:B:955:LEU:N	2.33	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:ASN:N	1:B:421:ASN:ND2	2.66	0.44
1:B:647:LYS:NZ	1:B:676:SER:HA	2.32	0.44
1:B:1056:TRP:HB2	1:B:1061:PRO:CA	2.38	0.44
1:B:1131:LYS:HB2	1:B:1160:TRP:CE2	2.52	0.44
1:C:473:ASN:ND2	1:C:505:MET:H	2.15	0.44
1:C:494:THR:H	1:C:1270:VAL:HB	1.82	0.44
1:C:748:ALA:CA	1:C:813:GLN:HB3	2.46	0.44
1:C:779:GLN:CD	1:C:785:TRP:HB2	2.38	0.44
1:C:1166:TRP:NE1	1:C:1176:PRO:HG2	2.33	0.44
1:B:939:SER:HA	1:B:957:ALA:CB	2.47	0.44
1:C:637:PRO:HB3	1:C:714:PRO:CG	2.48	0.44
1:C:763:ASN:ND2	1:C:767:ARG:HG2	2.32	0.44
1:C:933:THR:HG21	1:C:1021:ALA:CB	2.47	0.44
1:C:1151:TYR:CE1	1:C:1183:PRO:HB3	2.53	0.44
1:B:272:VAL:O	1:B:301:VAL:N	2.38	0.44
1:B:432:GLY:O	1:B:450:VAL:HG23	2.18	0.44
1:B:477:THR:CG2	1:B:481:TRP:CZ2	3.01	0.44
1:B:660:GLU:OE2	1:B:702:LEU:HB2	2.18	0.44
1:C:713:TRP:CE3	1:C:713:TRP:HA	2.53	0.44
1:C:731:ASN:HB3	1:C:734:THR:O	2.18	0.44
1:C:821:VAL:HG13	1:C:909:TYR:OH	2.18	0.44
1:C:974:LYS:HZ2	1:C:982:MET:HA	1.81	0.44
1:C:1067:PHE:HE2	1:C:1136:ARG:HB3	1.82	0.44
1:B:252:THR:C	1:B:979:LEU:HD21	2.37	0.44
1:B:375:HIS:HE1	1:B:438:GLN:OE1	1.99	0.44
1:B:438:GLN:HB3	1:B:445:SER:OG	2.16	0.44
1:B:1095:ARG:CG	1:B:1099:GLY:HA2	2.45	0.44
1:B:1107:ASN:O	1:B:1108:TRP:HD1	2.00	0.44
1:C:307:HIS:O	1:C:310:TRP:HB3	2.18	0.44
1:C:308:THR:HG1	1:C:321:SER:HA	1.83	0.44
1:C:574:ALA:O	1:C:577:ILE:HG22	2.18	0.44
1:C:779:GLN:HA	1:C:782:GLN:HG2	2.00	0.44
1:C:851:ARG:NH1	1:C:994:MET:SD	2.90	0.44
1:C:1041:ALA:HB2	1:C:1146:TYR:HD2	1.83	0.44
1:C:1170:ILE:HG23	1:C:1175:ILE:HG13	2.00	0.44
1:B:295:PRO:HG2	1:B:408:PRO:CA	2.48	0.43
1:B:593:VAL:CG1	1:B:875:LEU:HD21	2.47	0.43
1:B:871:VAL:HG12	1:B:872:GLY:N	2.33	0.43
1:C:740:LEU:HB3	1:C:835:TYR:HE1	1.81	0.43
1:C:807:THR:N	1:C:808:PRO:CD	2.80	0.43
1:C:841:ASP:HB3	1:C:1005:ASN:CB	2.24	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:635:ALA:O	1:B:639:THR:HG23	2.19	0.43
1:B:854:ARG:HB2	1:B:863:SER:HB3	2.00	0.43
1:C:380:GLN:CG	1:C:388:GLY:HA2	2.44	0.43
1:C:504:LEU:HB3	1:C:1264:THR:OG1	2.17	0.43
1:C:591:PHE:O	1:C:595:LEU:HG	2.19	0.43
1:C:691:ILE:HD11	1:C:710:HIS:CE1	2.53	0.43
1:C:1034:GLU:OE2	1:C:1034:GLU:CA	2.66	0.43
1:B:522:ILE:HA	1:B:525:ILE:CG1	2.48	0.43
1:B:848:GLY:C	1:B:868:ASN:HB2	2.39	0.43
1:B:1111:PRO:HG2	1:B:1114:LEU:CB	2.48	0.43
1:B:1230:GLU:CB	1:B:1250:VAL:HG21	2.48	0.43
1:C:1009:PHE:N	1:C:1009:PHE:CD1	2.86	0.43
1:C:1049:ARG:HB2	1:C:1198:TYR:CD2	2.53	0.43
1:B:419:ILE:HD11	1:B:1214:SER:HB3	1.99	0.43
1:B:1041:ALA:HB3	1:B:1144:TYR:O	2.18	0.43
1:B:1145:PRO:CG	1:B:1177:SER:HA	2.36	0.43
1:C:492:THR:O	1:C:1272:MET:N	2.49	0.43
1:C:622:SER:HB3	1:C:625:ASN:HD22	1.83	0.43
1:C:729:SER:HB3	1:C:736:PRO:HB2	2.00	0.43
1:C:839:ASP:CG	1:C:842:ARG:HB2	2.39	0.43
1:C:924:THR:HG23	1:C:984:LEU:HD22	1.94	0.43
1:C:1067:PHE:CD1	1:C:1107:ASN:HB3	2.54	0.43
1:B:440:MET:HG3	1:C:864:LEU:CG	2.48	0.43
1:B:520:ILE:HD13	1:B:523:MET:SD	2.58	0.43
1:B:578:LEU:HD23	1:B:581:LEU:CD1	2.48	0.43
1:B:825:MET:O	1:B:914:VAL:HG21	2.18	0.43
1:B:855:ASP:HA	1:B:994:MET:HE2	2.00	0.43
1:C:851:ARG:HB3	1:C:994:MET:HB3	1.99	0.43
1:B:246:GLN:HE21	1:B:246:GLN:HB2	1.53	0.43
1:B:391:LEU:HG	1:B:407:TYR:CE1	2.53	0.43
1:B:600:TYR:CD2	1:B:830:PRO:HA	2.52	0.43
1:B:600:TYR:CE1	1:B:830:PRO:HB3	2.52	0.43
1:B:603:VAL:HG12	1:B:871:VAL:CG1	2.47	0.43
1:B:652:LEU:HD21	1:B:771:LEU:HD21	2.01	0.43
1:B:807:THR:N	1:B:808:PRO:CD	2.81	0.43
1:B:846:MET:SD	1:B:846:MET:C	2.96	0.43
1:B:951:TRP:CE3	1:B:1042:ARG:HG3	2.54	0.43
1:B:1034:GLU:O	1:B:1038:PHE:HD1	2.02	0.43
1:B:1153:PRO:HD3	1:B:1184:ILE:H	1.84	0.43
1:C:705:TRP:CE3	1:C:771:LEU:HD22	2.53	0.43
1:C:806:MET:CE	1:C:809:MET:HE1	2.48	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:828:PHE:CD1	1:C:829:PRO:HD2	2.54	0.43
1:C:1166:TRP:CG	1:C:1179:PRO:HD3	2.51	0.43
1:B:360:HIS:CE1	1:B:364:GLU:HG3	2.53	0.43
1:B:852:GLN:HG2	1:B:867:THR:CG2	2.49	0.43
1:B:926:GLU:OE2	1:B:1018:SER:HA	2.19	0.43
1:B:945:VAL:CG1	1:B:947:ARG:HE	2.31	0.43
1:B:1130:ILE:HG22	1:B:1160:TRP:HZ3	1.82	0.43
1:B:1139:ILE:HG22	1:B:1141:MET:HG2	2.01	0.43
1:B:1188:HIS:C	1:B:1221:ALA:HB2	2.39	0.43
1:B:1212:THR:OG1	1:B:1225:LYS:N	2.39	0.43
1:C:262:LEU:CD1	1:C:402:TRP:CZ3	3.00	0.43
1:C:326:PRO:HD2	1:C:329:GLU:HB2	2.01	0.43
1:C:349:ALA:HB1	1:C:354:PHE:HE2	1.82	0.43
1:C:597:GLY:HA3	1:C:604:VAL:HG11	1.99	0.43
1:C:813:GLN:HB2	1:C:814:LEU:HD22	2.01	0.43
1:C:1156:TYR:HD1	1:C:1194:PRO:HG2	1.82	0.43
1:B:265:SER:HB3	1:B:308:THR:HA	2.01	0.43
1:B:324:MET:HE3	1:B:324:MET:HB2	1.88	0.43
1:B:437:ALA:HB2	1:B:447:TRP:CE2	2.53	0.43
1:B:439:MET:HE3	1:C:990:GLY:HA3	2.00	0.43
1:B:959:ALA:CB	1:B:993:ARG:HH22	2.30	0.43
1:C:641:ASP:OD2	1:C:641:ASP:C	2.57	0.43
1:C:685:PRO:CB	1:C:688:PHE:HB3	2.49	0.43
1:C:720:ARG:HA	1:C:737:GLU:O	2.19	0.43
1:C:824:PRO:HG2	1:C:825:MET:HE3	2.00	0.43
1:C:937:GLN:O	1:C:947:ARG:NE	2.48	0.43
1:C:1129:TRP:O	1:C:1133:GLY:N	2.52	0.43
1:B:261:GLY:HA3	1:B:313:ASN:N	2.34	0.43
1:B:466:MET:HE1	1:B:1262:TYR:HE2	1.82	0.43
1:B:485:GLU:O	1:B:488:GLN:NE2	2.52	0.43
1:B:1108:TRP:CD2	1:B:1135:LEU:HD11	2.54	0.43
1:C:274:ALA:C	1:C:1215:SER:HB3	2.39	0.43
1:C:305:VAL:HG13	1:C:324:MET:O	2.19	0.43
1:C:406:MET:O	1:C:1254:TYR:HE1	2.01	0.43
1:C:500:SER:HB3	1:C:503:ARG:CG	2.49	0.43
1:C:613:TYR:CD1	1:C:613:TYR:N	2.87	0.43
1:C:687:CYS:SG	1:C:688:PHE:N	2.92	0.43
1:C:1149:HIS:O	1:C:1181:MET:HA	2.19	0.43
1:B:560:MET:HE1	1:B:577:ILE:HG21	2.01	0.43
1:B:702:LEU:HA	1:B:702:LEU:HD12	1.80	0.43
1:B:769:CYS:HA	1:B:772:MET:CE	2.41	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:920:ARG:CG	1:B:920:ARG:NH1	2.81	0.43
1:B:922:MET:HE1	1:B:926:GLU:HB2	2.00	0.43
1:B:1059:LEU:HD13	1:B:1205:ASN:C	2.39	0.43
1:B:1092:PRO:HG3	1:B:1129:TRP:CZ2	2.54	0.43
1:C:480:GLU:HA	1:C:493:VAL:HG21	2.01	0.43
1:C:600:TYR:HE2	1:C:828:PHE:CD2	2.36	0.43
1:C:930:THR:HG22	1:C:934:LEU:HD22	2.01	0.43
1:C:1031:PHE:HA	1:C:1038:PHE:CD1	2.53	0.43
1:C:1052:SER:HB3	1:C:1056:TRP:CZ2	2.54	0.43
1:C:1069:ARG:NH1	1:C:1138:ARG:HD3	2.33	0.43
1:C:548:PRO:HB3	1:C:900:TRP:CD2	2.54	0.42
1:C:778:ASN:OD1	1:C:780:ARG:HB3	2.19	0.42
1:C:994:MET:O	1:C:994:MET:CG	2.66	0.42
1:B:350:ASN:ND2	1:B:1173:THR:O	2.52	0.42
1:B:627:TRP:HH2	1:B:796:THR:CG2	2.32	0.42
1:B:669:TYR:HB3	1:B:678:PHE:CE2	2.53	0.42
1:B:941:THR:HG22	1:B:993:ARG:CB	2.49	0.42
1:B:1229:VAL:HG13	1:B:1236:THR:CB	2.49	0.42
1:C:235:VAL:CG2	1:C:239:VAL:HG11	2.42	0.42
1:C:375:HIS:HB2	1:C:1260:TYR:C	2.39	0.42
1:B:446:GLU:OE1	1:B:446:GLU:HA	2.19	0.42
1:B:477:THR:HB	1:B:481:TRP:CH2	2.54	0.42
1:B:891:TYR:HB3	1:B:892:PRO:HD2	2.02	0.42
1:B:991:ASP:O	1:B:995:THR:HG23	2.19	0.42
1:C:293:GLN:O	1:C:411:MET:HG3	2.18	0.42
1:C:302:SER:O	1:C:1210:PHE:N	2.50	0.42
1:C:307:HIS:CB	1:C:310:TRP:HB3	2.49	0.42
1:C:602:GLY:N	1:C:831:PHE:O	2.51	0.42
1:C:650:MET:O	1:C:654:ASN:ND2	2.52	0.42
1:C:685:PRO:O	1:C:689:MET:N	2.46	0.42
1:C:754:THR:CG2	1:C:806:MET:HE3	2.50	0.42
1:C:1044:ASP:HB3	1:C:1141:MET:HG2	2.01	0.42
1:C:1094:ILE:HG23	1:C:1094:ILE:O	2.19	0.42
1:B:375:HIS:HB3	1:B:1261:ALA:CB	2.27	0.42
1:B:385:PHE:HB3	1:B:410:ARG:CA	2.45	0.42
1:B:552:ASP:O	1:B:888:SER:HB2	2.19	0.42
1:B:644:ALA:HB3	1:B:645:PRO:HD3	2.00	0.42
1:B:646:VAL:HG21	1:B:684:TRP:CG	2.55	0.42
1:B:652:LEU:HA	1:B:655:MET:SD	2.59	0.42
1:B:1048:GLY:O	1:B:1198:TYR:HA	2.19	0.42
1:B:1059:LEU:H	1:B:1059:LEU:HG	1.57	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1144:TYR:OH	1:B:1201:SER:HB2	2.19	0.42
1:B:1154:ARG:HD3	1:B:1190:ILE:HD12	2.01	0.42
1:C:375:HIS:CB	1:C:1261:ALA:HB2	2.30	0.42
1:C:466:MET:HE3	1:C:466:MET:HA	2.01	0.42
1:C:515:GLN:HG3	1:C:730:ALA:CB	2.48	0.42
1:C:705:TRP:CE2	1:C:709:ILE:HD11	2.53	0.42
1:C:957:ALA:HB1	1:C:961:THR:CG2	2.49	0.42
1:C:1002:GLN:HA	1:C:1008:THR:HA	2.01	0.42
1:C:1005:ASN:OD1	1:C:1006:GLY:N	2.52	0.42
1:B:400:GLU:H	1:B:400:GLU:CD	2.22	0.42
1:B:464:ARG:NH1	1:B:1023:CYS:HA	2.35	0.42
1:B:641:ASP:HB3	1:B:644:ALA:HB2	2.01	0.42
1:B:922:MET:CE	1:B:922:MET:O	2.67	0.42
1:B:1267:ILE:O	1:B:1271:VAL:HG23	2.19	0.42
1:C:313:ASN:C	1:C:313:ASN:OD1	2.57	0.42
1:C:418:LYS:NZ	1:C:1224:ASP:OD1	2.46	0.42
1:C:451:PHE:HA	1:C:1256:VAL:HA	2.00	0.42
1:C:495:SER:O	1:C:497:TYR:HD2	2.03	0.42
1:C:1260:TYR:N	1:C:1260:TYR:HD1	2.14	0.42
1:B:627:TRP:HA	1:B:627:TRP:HE3	1.82	0.42
1:B:968:TRP:O	1:B:972:SER:OG	2.36	0.42
1:C:320:SER:HB2	1:C:368:ASP:HB2	2.00	0.42
1:C:690:ASN:HB3	1:C:693:LEU:HG	2.00	0.42
1:C:713:TRP:CD1	1:C:838:LEU:HD21	2.55	0.42
1:C:1041:ALA:HB3	1:C:1144:TYR:CD1	2.54	0.42
1:B:984:LEU:HA	1:B:987:LEU:HG	2.02	0.42
1:B:1046:ILE:HG12	1:B:1138:ARG:HB2	2.01	0.42
1:B:1096:ASP:HB3	1:B:1100:MET:N	2.35	0.42
1:B:1096:ASP:HB2	1:B:1100:MET:O	2.19	0.42
1:C:303:ARG:CZ	1:C:1209:LEU:HB2	2.49	0.42
1:C:660:GLU:OE2	1:C:701:ILE:HB	2.20	0.42
1:B:272:VAL:HB	1:B:301:VAL:HB	2.02	0.42
1:B:276:VAL:HG13	1:B:277:PRO:CA	2.49	0.42
1:B:408:PRO:O	1:B:411:MET:HB3	2.19	0.42
1:B:438:GLN:HA	1:C:862:LEU:CB	2.46	0.42
1:B:647:LYS:HA	1:B:675:ALA:HB1	2.02	0.42
1:B:847:VAL:CG1	1:B:871:VAL:HB	2.48	0.42
1:C:221:THR:N	1:C:234:GLN:O	2.52	0.42
1:C:378:PHE:N	1:C:378:PHE:CD1	2.87	0.42
1:C:708:ILE:HA	1:C:711:ARG:HH12	1.85	0.42
1:C:1002:GLN:HB3	1:C:1008:THR:HG22	2.01	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1230:GLU:O	1:C:1233:ASN:HB2	2.19	0.42
1:C:1246:GLN:CB	1:C:1250:VAL:HB	2.46	0.42
1:B:451:PHE:CD2	1:B:1256:VAL:HG22	2.55	0.42
1:B:510:SER:OG	1:B:513:GLU:HG3	2.19	0.42
1:B:904:ALA:O	1:B:907:PRO:HG2	2.19	0.42
1:B:938:ILE:HD13	1:B:965:PHE:CD2	2.55	0.42
1:B:1033:HIS:NE2	1:B:1248:PRO:HG2	2.35	0.42
1:B:1232:TYR:O	1:B:1236:THR:HG23	2.20	0.42
1:C:327:PRO:HB3	1:C:1148:LEU:HD12	2.02	0.42
1:C:409:THR:CG2	1:C:1235:LEU:HD21	2.46	0.42
1:C:466:MET:CE	1:C:469:LEU:HB2	2.48	0.42
1:C:605:THR:O	1:C:875:LEU:N	2.52	0.42
1:C:635:ALA:CA	1:C:638:LEU:HG	2.44	0.42
1:C:701:ILE:HD13	1:C:704:GLN:NE2	2.31	0.42
1:C:937:GLN:HA	1:C:945:VAL:HG21	2.02	0.42
1:C:1001:TYR:CD1	1:C:1001:TYR:C	2.93	0.42
1:C:1212:THR:OG1	1:C:1225:LYS:N	2.37	0.42
1:B:435:ASP:OD2	1:C:859:GLN:HB2	2.20	0.42
1:B:437:ALA:N	1:B:447:TRP:O	2.41	0.42
1:B:447:TRP:HB2	1:B:1258:THR:CG2	2.50	0.42
1:B:543:LEU:HA	1:B:546:ILE:CG2	2.48	0.42
1:B:799:LYS:NZ	1:B:799:LYS:HB3	2.35	0.42
1:B:939:SER:HB3	1:B:993:ARG:HD3	2.01	0.42
1:B:1109:ILE:HD13	1:B:1138:ARG:HB3	2.02	0.42
1:B:1171:THR:HB	1:B:1174:SER:O	2.20	0.42
1:C:265:SER:O	1:C:307:HIS:N	2.44	0.42
1:C:500:SER:HB3	1:C:503:ARG:HG3	2.02	0.42
1:C:550:GLN:O	1:C:890:LYS:HG2	2.19	0.42
1:C:613:TYR:H	1:C:613:TYR:HD1	1.68	0.42
1:C:822:ILE:O	1:C:826:LEU:N	2.52	0.42
1:C:1051:GLN:HG2	1:C:1195:ALA:N	2.34	0.42
1:C:1082:ARG:NH1	1:C:1082:ARG:CG	2.74	0.42
1:C:1162:LEU:H	1:C:1162:LEU:HD13	1.78	0.42
1:C:1230:GLU:CB	1:C:1250:VAL:HG21	2.50	0.42
1:C:1241:PRO:HG2	1:C:1244:GLN:CB	2.27	0.42
1:B:333:HIS:O	1:B:337:GLN:HB2	2.20	0.41
1:B:338:LEU:HD11	1:B:968:TRP:CD2	2.55	0.41
1:B:473:ASN:HD21	1:B:504:LEU:HA	1.85	0.41
1:B:627:TRP:CH2	1:B:796:THR:CG2	3.03	0.41
1:B:707:GLU:HB3	1:B:711:ARG:NH2	2.35	0.41
1:B:1080:ASP:HB3	1:B:1095:ARG:HH21	1.85	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1149:HIS:O	1:B:1182:VAL:N	2.44	0.41
1:C:988:LEU:HG	1:C:988:LEU:H	1.71	0.41
1:B:580:LYS:HD2	1:B:624:GLU:OE1	2.20	0.41
1:C:276:VAL:HG23	1:C:416:VAL:HG22	2.02	0.41
1:C:429:ASN:HD22	1:C:429:ASN:H	1.69	0.41
1:B:246:GLN:HA	1:B:249:HIS:O	2.21	0.41
1:B:406:MET:CG	1:B:452:GLU:HB2	2.50	0.41
1:B:603:VAL:HG13	1:B:831:PHE:CB	2.50	0.41
1:B:607:VAL:O	1:B:877:LEU:N	2.45	0.41
1:B:719:ILE:HG22	1:B:739:LEU:HB3	2.01	0.41
1:C:275:GLN:OE1	1:C:275:GLN:N	2.53	0.41
1:C:281:LEU:O	1:C:292:ILE:HD12	2.21	0.41
1:C:839:ASP:O	1:C:843:VAL:HG23	2.20	0.41
1:C:1106:GLY:O	1:C:1136:ARG:N	2.43	0.41
1:B:269:VAL:HG22	1:B:305:VAL:HG23	2.03	0.41
1:B:285:PHE:CD2	1:B:286:PHE:N	2.88	0.41
1:B:409:THR:HA	1:B:423:VAL:HG13	2.02	0.41
1:B:694:ILE:O	1:B:703:ARG:NH1	2.46	0.41
1:B:791:SER:HA	1:B:794:ARG:HD2	2.03	0.41
1:C:383:THR:HG22	1:C:385:PHE:CE1	2.55	0.41
1:C:427:VAL:HG22	1:C:1235:LEU:O	2.21	0.41
1:C:494:THR:N	1:C:1270:VAL:O	2.54	0.41
1:C:525:ILE:HG22	1:C:527:ASN:N	2.35	0.41
1:C:982:MET:O	1:C:982:MET:HG3	2.20	0.41
1:C:993:ARG:H	1:C:993:ARG:HG3	1.65	0.41
1:C:1044:ASP:HA	1:C:1141:MET:HB2	2.02	0.41
1:C:1158:ASN:ND2	1:C:1160:TRP:HB3	2.35	0.41
1:C:1207:ARG:NH2	1:C:1231:ARG:HH22	2.19	0.41
1:B:377:GLY:O	1:B:393:SER:N	2.40	0.41
1:B:615:LYS:C	1:B:615:LYS:HD3	2.40	0.41
1:B:985:GLU:HB2	1:B:986:PRO:HD3	2.02	0.41
1:B:1131:LYS:HD2	1:B:1160:TRP:CE2	2.55	0.41
1:B:1170:ILE:HG23	1:B:1175:ILE:CG2	2.49	0.41
1:B:1220:ILE:O	1:B:1220:ILE:CG2	2.69	0.41
1:C:413:THR:HB	1:C:420:CYS:HA	2.02	0.41
1:C:418:LYS:HE2	1:C:1226:HIS:CE1	2.55	0.41
1:C:474:ILE:HG22	1:C:505:MET:O	2.19	0.41
1:C:503:ARG:CZ	1:C:503:ARG:HB3	2.50	0.41
1:C:510:SER:OG	1:C:513:GLU:HG3	2.20	0.41
1:C:1049:ARG:HB2	1:C:1198:TYR:CE2	2.55	0.41
1:C:1175:ILE:HG12	1:C:1176:PRO:CD	2.46	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:GLN:NE2	1:B:401:LYS:HA	2.27	0.41
1:B:385:PHE:CB	1:B:410:ARG:HA	2.44	0.41
1:C:318:ARG:HG2	1:C:371:TYR:CZ	2.53	0.41
1:C:433:ARG:HD3	1:C:448:VAL:HG21	2.01	0.41
1:C:656:MET:CE	1:C:656:MET:CA	2.91	0.41
1:C:840:ARG:HG2	1:C:1004:TYR:CD2	2.55	0.41
1:B:1046:ILE:HG23	1:B:1067:PHE:CE2	2.55	0.41
1:B:1231:ARG:HG2	1:B:1250:VAL:CG1	2.50	0.41
1:C:503:ARG:CD	1:C:1265:PRO:HG3	2.51	0.41
1:C:822:ILE:HA	1:C:825:MET:CG	2.50	0.41
1:C:826:LEU:CD1	1:C:830:PRO:HG3	2.51	0.41
1:C:850:THR:N	1:C:998:ALA:O	2.49	0.41
1:C:998:ALA:CB	1:C:1012:ILE:HG12	2.51	0.41
1:C:1055:LEU:HD23	1:C:1055:LEU:HA	1.86	0.41
1:C:1062:PRO:HG2	1:C:1065:LEU:HD12	2.03	0.41
1:B:306:VAL:O	1:B:323:ILE:HG23	2.21	0.41
1:B:375:HIS:CB	1:B:1261:ALA:HB2	2.30	0.41
1:B:439:MET:CE	1:C:990:GLY:HA3	2.50	0.41
1:B:494:THR:HG1	1:B:1272:MET:HB2	1.86	0.41
1:B:905:ILE:HA	1:B:908:MET:HE3	2.02	0.41
1:B:1044:ASP:O	1:B:1202:THR:N	2.51	0.41
1:C:403:TYR:CD1	1:C:407:TYR:CE1	3.01	0.41
1:C:451:PHE:CD2	1:C:1256:VAL:HG13	2.55	0.41
1:C:542:LEU:HD11	1:C:908:MET:SD	2.61	0.41
1:C:654:ASN:HD22	1:C:654:ASN:N	2.18	0.41
1:C:748:ALA:HA	1:C:813:GLN:CB	2.48	0.41
1:C:757:PHE:HA	1:C:762:THR:CG2	2.51	0.41
1:C:1169:GLU:HB2	1:C:1176:PRO:HG3	2.03	0.41
1:B:278:GLN:HE21	1:B:281:LEU:HG	1.85	0.41
1:B:313:ASN:ND2	1:B:313:ASN:C	2.73	0.41
1:B:364:GLU:HA	1:B:367:LEU:HD12	2.03	0.41
1:B:475:ASN:O	1:B:478:GLU:HB2	2.21	0.41
1:B:522:ILE:CA	1:B:525:ILE:HG12	2.51	0.41
1:B:604:VAL:CG1	1:B:875:LEU:HB2	2.50	0.41
1:B:636:LEU:N	1:B:637:PRO:CD	2.84	0.41
1:B:645:PRO:HG3	1:B:713:TRP:CE2	2.55	0.41
1:B:836:VAL:O	1:B:836:VAL:HG23	2.20	0.41
1:B:843:VAL:O	1:B:1004:TYR:N	2.54	0.41
1:B:1075:HIS:HB2	1:B:1108:TRP:CD1	2.56	0.41
1:C:333:HIS:O	1:C:336:LYS:HG2	2.20	0.41
1:C:355:ARG:CZ	1:C:954:SER:HB3	2.51	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:511:ASN:OD1	1:C:728:GLY:HA3	2.21	0.41
1:C:533:GLN:HB3	1:C:534:PRO:HD3	2.03	0.41
1:C:572:SER:HB3	1:C:575:SER:HB2	2.03	0.41
1:C:597:GLY:HA2	1:C:604:VAL:HG11	2.03	0.41
1:C:811:LEU:HA	1:C:815:ALA:HB3	2.03	0.41
1:C:1036:ASN:ND2	1:C:1036:ASN:O	2.52	0.41
1:C:1175:ILE:CG1	1:C:1176:PRO:CD	2.91	0.41
1:C:1193:ALA:HB1	1:C:1194:PRO:HD2	2.03	0.41
1:B:391:LEU:N	1:B:391:LEU:CD1	2.83	0.41
1:B:518:GLN:HE21	1:B:521:ARG:CZ	2.34	0.41
1:B:592:ARG:HH11	1:B:592:ARG:HG3	1.86	0.41
1:B:614:PRO:HB2	1:B:617:GLY:CA	2.50	0.41
1:B:755:LEU:CD2	1:B:804:LYS:HB3	2.51	0.41
1:B:952:ILE:HA	1:B:1143:ALA:HB2	2.01	0.41
1:B:998:ALA:HA	1:B:1011:VAL:O	2.21	0.41
1:B:1080:ASP:HB3	1:B:1095:ARG:NH2	2.35	0.41
1:C:224:ILE:HG22	1:C:1270:VAL:HG22	2.03	0.41
1:C:258:TRP:HA	1:C:372:LEU:O	2.20	0.41
1:C:277:PRO:O	1:C:278:GLN:HG3	2.20	0.41
1:C:514:ARG:NH1	1:C:728:GLY:O	2.54	0.41
1:C:1077:PHE:CD2	1:C:1094:ILE:HD13	2.56	0.41
1:C:1123:ASN:O	1:C:1127:ASP:N	2.54	0.41
1:C:1153:PRO:HG3	1:C:1183:PRO:CB	2.51	0.41
1:C:1260:TYR:HD1	1:C:1260:TYR:H	1.67	0.41
1:B:290:TYR:HE2	1:C:1121:TYR:CE1	2.39	0.40
1:B:705:TRP:O	1:B:709:ILE:HG13	2.22	0.40
1:B:1003:GLN:HB2	1:B:1005:ASN:OD1	2.21	0.40
1:B:1046:ILE:HA	1:B:1138:ARG:HA	2.04	0.40
1:B:1151:TYR:CD2	1:B:1181:MET:CG	3.02	0.40
1:B:1167:LEU:HA	1:B:1170:ILE:HD12	2.03	0.40
1:B:1244:GLN:HG2	1:B:1245:ILE:N	2.33	0.40
1:C:503:ARG:HA	1:C:1263:GLU:O	2.21	0.40
1:C:600:TYR:CD1	1:C:600:TYR:N	2.89	0.40
1:C:620:VAL:HB	1:C:781:TYR:O	2.21	0.40
1:C:684:TRP:HA	1:C:685:PRO:HD3	1.95	0.40
1:C:906:TYR:HB3	1:C:907:PRO:CD	2.51	0.40
1:C:1147:MET:HB3	1:C:1147:MET:HE2	1.93	0.40
1:C:1210:PHE:CZ	1:C:1227:ILE:HG23	2.56	0.40
1:B:281:LEU:HD13	1:B:282:ALA:N	2.36	0.40
1:B:1031:PHE:CZ	1:B:1040:ILE:HG13	2.56	0.40
1:B:1054:HIS:HB2	1:B:1056:TRP:HD1	1.86	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1059:LEU:HD23	1:B:1201:SER:HB3	2.03	0.40
1:B:1103:PRO:O	1:B:1108:TRP:HZ2	2.05	0.40
1:B:1151:TYR:O	1:B:1183:PRO:HA	2.21	0.40
1:C:492:THR:CG2	1:C:1274:VAL:HG22	2.51	0.40
1:C:643:CYS:O	1:C:647:LYS:HG3	2.21	0.40
1:C:949:LEU:O	1:C:952:ILE:HB	2.20	0.40
1:C:1120:ARG:HA	1:C:1120:ARG:HD3	1.43	0.40
1:B:409:THR:HA	1:B:423:VAL:CG1	2.51	0.40
1:B:423:VAL:O	1:B:428:ARG:NH2	2.50	0.40
1:B:528:ASN:CG	1:B:531:VAL:HG23	2.41	0.40
1:B:823:ALA:N	1:B:824:PRO:CD	2.84	0.40
1:B:905:ILE:HG23	1:B:909:TYR:CG	2.56	0.40
1:B:1170:ILE:HG12	1:B:1176:PRO:CD	2.47	0.40
1:C:325:ALA:HB1	1:C:326:PRO:HD2	2.03	0.40
1:C:636:LEU:HB2	1:C:637:PRO:HD3	2.03	0.40
1:C:779:GLN:HG2	1:C:782:GLN:HG2	2.04	0.40
1:C:1151:TYR:HB3	1:C:1181:MET:CG	2.50	0.40
1:B:284:THR:CA	1:C:1085:PHE:HB2	2.51	0.40
1:B:355:ARG:CZ	1:B:954:SER:HB3	2.51	0.40
1:B:439:MET:HG3	1:B:440:MET:N	2.36	0.40
1:B:514:ARG:NH1	1:B:727:PHE:HB3	2.37	0.40
1:B:569:GLN:HG3	1:B:571:LEU:O	2.21	0.40
1:B:755:LEU:HA	1:B:809:MET:CE	2.52	0.40
1:B:836:VAL:HG21	1:B:839:ASP:O	2.22	0.40
1:C:422:PHE:CD2	1:C:1227:ILE:HD12	2.55	0.40
1:C:448:VAL:N	1:C:1259:ARG:O	2.52	0.40
1:C:1076:ILE:HG12	1:C:1109:ILE:CB	2.44	0.40
1:C:1138:ARG:CZ	1:C:1202:THR:HG21	2.51	0.40
1:C:1212:THR:N	1:C:1225:LYS:HB3	2.37	0.40
1:B:346:VAL:HG23	1:B:347:ARG:HG2	2.03	0.40
1:B:453:THR:HA	1:B:1254:TYR:HA	2.03	0.40
1:B:458:THR:O	1:B:462:ARG:HG3	2.21	0.40
1:B:518:GLN:HE21	1:B:829:PRO:HD2	1.83	0.40
1:B:546:ILE:HD13	1:B:818:GLU:HB3	2.03	0.40
1:B:651:THR:HG22	1:B:655:MET:CE	2.51	0.40
1:B:669:TYR:HE2	1:B:678:PHE:HA	1.87	0.40
1:B:715:ASN:O	1:B:744:ASP:N	2.50	0.40
1:B:809:MET:HE3	1:B:891:TYR:CE2	2.57	0.40
1:B:983:LEU:O	1:B:984:LEU:HB2	2.21	0.40
1:C:472:MET:O	1:C:508:ARG:N	2.47	0.40
1:C:732:LEU:CG	1:C:1011:VAL:HG11	2.52	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:892:PRO:HD2	1:C:895:LEU:CD2	2.42	0.40
1:C:1046:ILE:HB	1:C:1200:ILE:CG1	2.50	0.40
1:C:1188:HIS:O	1:C:1190:ILE:HG23	2.21	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 PDB entries followed by that with respect to all EM entries.

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	B	1027/1059 (97%)	1012 (98%)	11 (1%)	4 (0%)	34 72
1	C	1047/1059 (99%)	1028 (98%)	17 (2%)	2 (0%)	47 81
All	All	2074/2118 (98%)	2040 (98%)	28 (1%)	6 (0%)	44 76

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	414	PRO
1	C	276	VAL
1	B	286	PHE
1	B	439	MET
1	B	502	ASN
1	C	1092	PRO

### 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 PDB entries followed by that with respect to all EM entries.

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	B	911/938 (97%)	810 (89%)	101 (11%)	6	22
1	C	930/938 (99%)	823 (88%)	107 (12%)	5	21
All	All	1841/1876 (98%)	1633 (89%)	208 (11%)	9	21

All (208) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	246	GLN
1	B	249	HIS
1	B	251	ASP
1	B	254	ARG
1	B	276	VAL
1	B	278	GLN
1	B	281	LEU
1	B	283	TYR
1	B	285	PHE
1	B	286	PHE
1	B	296	PHE
1	B	302	SER
1	B	313	ASN
1	B	324	MET
1	B	332	ILE
1	B	336	LYS
1	B	340	ASN
1	B	341	THR
1	B	353	MET
1	B	374	ARG
1	B	386	THR
1	B	391	LEU
1	B	406	MET
1	B	413	THR
1	B	414	PRO
1	B	415	ASN
1	B	439	MET
1	B	441	ASN
1	B	455	ASP
1	B	477	THR
1	B	511	ASN
1	B	524	ASN
1	B	538	ASP
1	B	540	SER
1	B	554	THR

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	580	LYS
1	B	601	ASN
1	B	615	LYS
1	B	624	GLU
1	B	636	LEU
1	B	652	LEU
1	B	664	MET
1	B	673	ARG
1	B	674	ARG
1	B	682	HIS
1	B	686	ARG
1	B	729	SER
1	B	745	HIS
1	B	767	ARG
1	B	770	GLU
1	B	779	GLN
1	B	786	THR
1	B	793	MET
1	B	814	LEU
1	B	825	MET
1	B	826	LEU
1	B	840	ARG
1	B	851	ARG
1	B	880	ARG
1	B	915	PHE
1	B	920	ARG
1	B	922	MET
1	B	926	GLU
1	B	939	SER
1	B	942	GLN
1	B	943	TYR
1	B	947	ARG
1	B	958	SER
1	B	972	SER
1	B	973	MET
1	B	981	ASP
1	B	982	MET
1	B	989	SER
1	B	1000	GLN
1	B	1032	ASN
1	B	1064	ASP
1	B	1067	PHE

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	1080	ASP
1	B	1085	PHE
1	B	1093	MET
1	B	1095	ARG
1	B	1097	GLU
1	B	1104	PHE
1	B	1120	ARG
1	B	1158	ASN
1	B	1162	LEU
1	B	1175	ILE
1	B	1182	VAL
1	B	1190	ILE
1	B	1201	SER
1	B	1206	ASP
1	B	1214	SER
1	B	1215	SER
1	B	1230	GLU
1	B	1231	ARG
1	B	1243	THR
1	B	1244	GLN
1	B	1249	GLU
1	B	1252	ASP
1	B	1260	TYR
1	B	1267	ILE
1	C	217	GLN
1	C	221	THR
1	C	229	ASN
1	C	241	ASN
1	C	251	ASP
1	C	252	THR
1	C	254	ARG
1	C	257	THR
1	C	263	CYS
1	C	266	PHE
1	C	296	PHE
1	C	301	VAL
1	C	302	SER
1	C	331	ASN
1	C	347	ARG
1	C	357	ASN
1	C	359	LEU
1	C	376	THR

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	378	PHE
1	C	385	PHE
1	C	392	ARG
1	C	394	LEU
1	C	409	THR
1	C	411	MET
1	C	429	ASN
1	C	431	VAL
1	C	439	MET
1	C	455	ASP
1	C	475	ASN
1	C	477	THR
1	C	485	GLU
1	C	490	TYR
1	C	491	VAL
1	C	495	SER
1	C	503	ARG
1	C	508	ARG
1	C	527	ASN
1	C	528	ASN
1	C	549	LEU
1	C	580	LYS
1	C	601	ASN
1	C	613	TYR
1	C	615	LYS
1	C	620	VAL
1	C	624	GLU
1	C	662	ILE
1	C	665	ASP
1	C	667	GLN
1	C	680	THR
1	C	688	PHE
1	C	689	MET
1	C	727	PHE
1	C	751	THR
1	C	759	ASN
1	C	761	LEU
1	C	763	ASN
1	C	765	ARG
1	C	777	ASP
1	C	780	ARG
1	C	782	GLN

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	792	SER
1	C	793	MET
1	C	814	LEU
1	C	859	GLN
1	C	868	ASN
1	C	870	THR
1	C	903	ASP
1	C	916	SER
1	C	935	VAL
1	C	942	GLN
1	C	946	ASP
1	C	948	TYR
1	C	956	ARG
1	C	968	TRP
1	C	988	LEU
1	C	993	ARG
1	C	1002	GLN
1	C	1007	ARG
1	C	1019	VAL
1	C	1029	GLU
1	C	1032	ASN
1	C	1036	ASN
1	C	1044	ASP
1	C	1066	VAL
1	C	1082	ARG
1	C	1100	MET
1	C	1101	MET
1	C	1121	TYR
1	C	1126	PHE
1	C	1135	LEU
1	C	1141	MET
1	C	1151	TYR
1	C	1158	ASN
1	C	1162	LEU
1	C	1185	SER
1	C	1198	TYR
1	C	1200	ILE
1	C	1204	TYR
1	C	1206	ASP
1	C	1224	ASP
1	C	1230	GLU
1	C	1254	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	1255	ASN
1	C	1256	VAL
1	C	1259	ARG
1	C	1260	TYR
1	C	1272	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	241	ASN
1	B	246	GLN
1	B	278	GLN
1	B	293	GLN
1	B	313	ASN
1	B	340	ASN
1	B	357	ASN
1	B	360	HIS
1	B	375	HIS
1	B	415	ASN
1	B	421	ASN
1	B	502	ASN
1	B	518	GLN
1	B	524	ASN
1	B	527	ASN
1	B	537	GLN
1	B	601	ASN
1	B	654	ASN
1	B	704	GLN
1	B	718	GLN
1	B	731	ASN
1	B	745	HIS
1	B	774	ASN
1	B	778	ASN
1	B	782	GLN
1	B	813	GLN
1	B	917	ASN
1	B	996	GLN
1	B	1000	GLN
1	B	1032	ASN
1	B	1116	GLN
1	B	1149	HIS
1	B	1188	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	1205	ASN
1	B	1213	ASN
1	B	1226	HIS
1	C	229	ASN
1	C	380	GLN
1	C	390	ASN
1	C	429	ASN
1	C	438	GLN
1	C	473	ASN
1	C	518	GLN
1	C	528	ASN
1	C	544	GLN
1	C	625	ASN
1	C	654	ASN
1	C	682	HIS
1	C	704	GLN
1	C	731	ASN
1	C	763	ASN
1	C	774	ASN
1	C	970	ASN
1	C	1002	GLN
1	C	1051	GLN
1	C	1075	HIS
1	C	1116	GLN
1	C	1125	GLN
1	C	1149	HIS
1	C	1158	ASN
1	C	1205	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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.



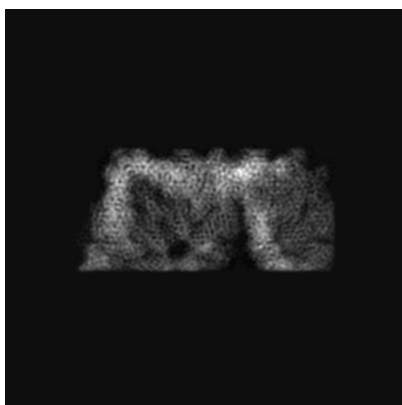
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22165. These allow visual inspection of the internal detail of the map and identification of artifacts.

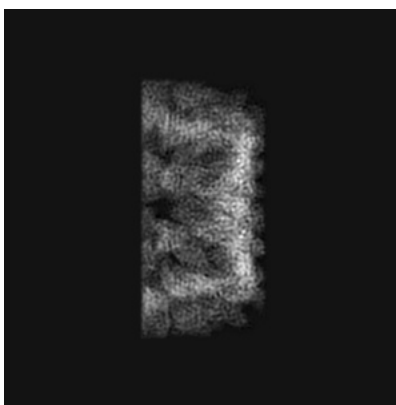
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

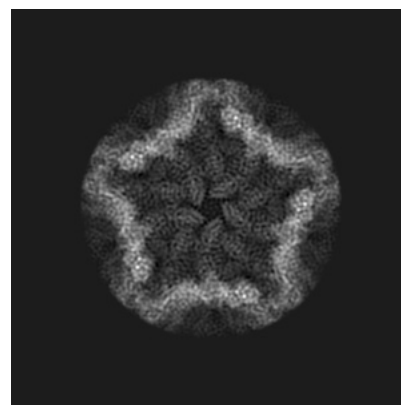
#### 6.1.1 Primary map



X



Y



Z

The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

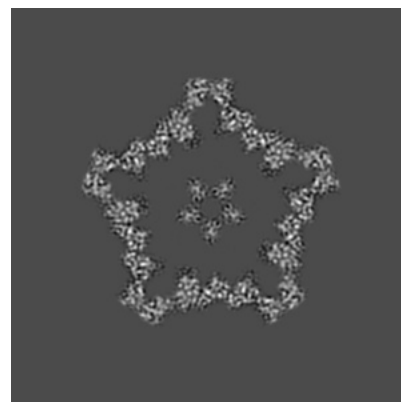
#### 6.2.1 Primary map



X Index: 193



Y Index: 193

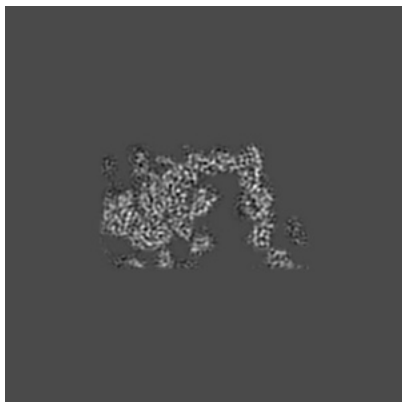


Z Index: 193

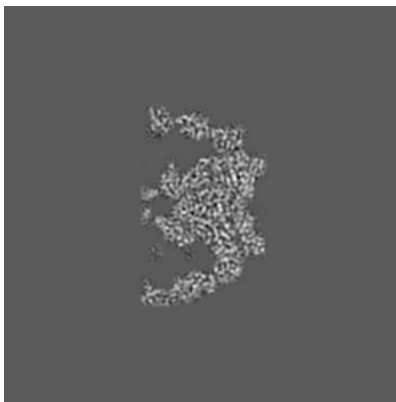
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

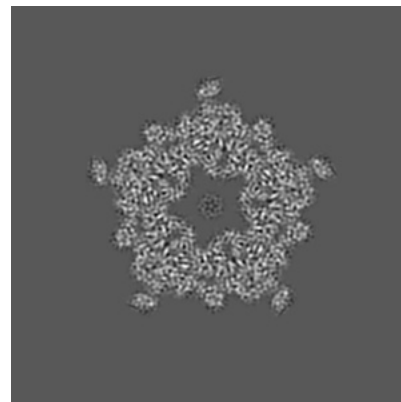
### 6.3.1 Primary map



X Index: 117



Y Index: 112

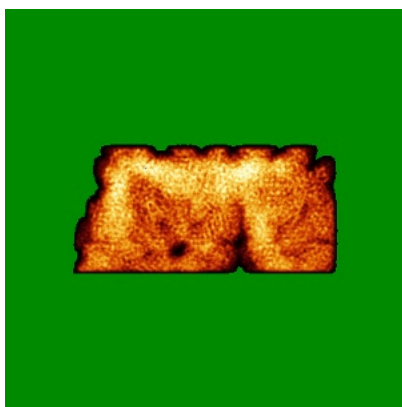


Z Index: 230

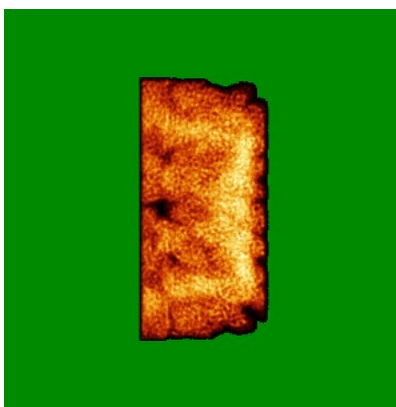
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

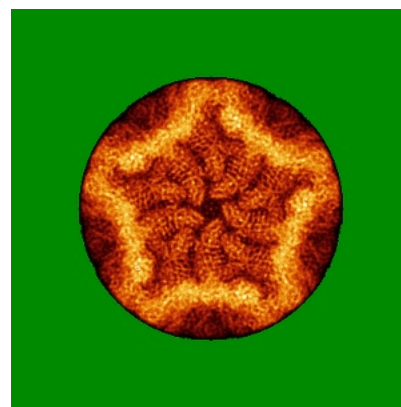
### 6.4.1 Primary map



X



Y

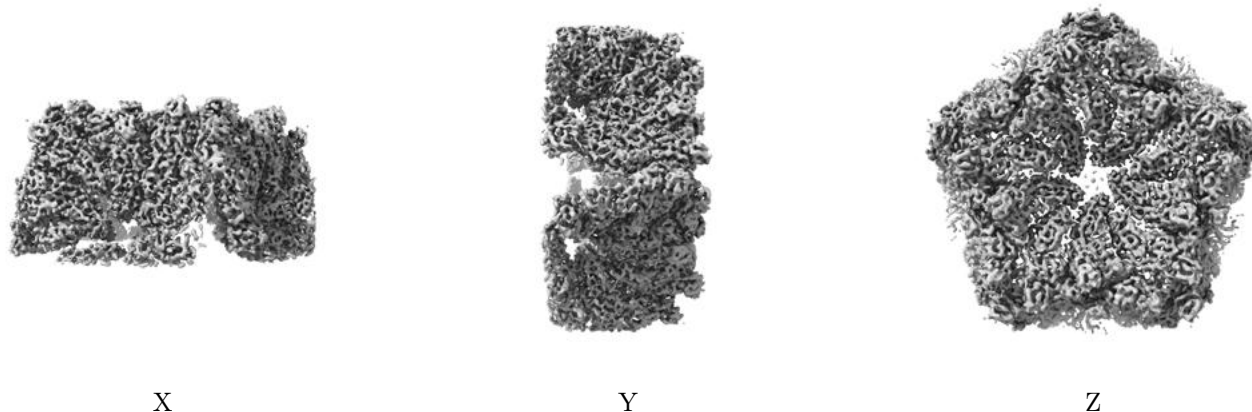


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

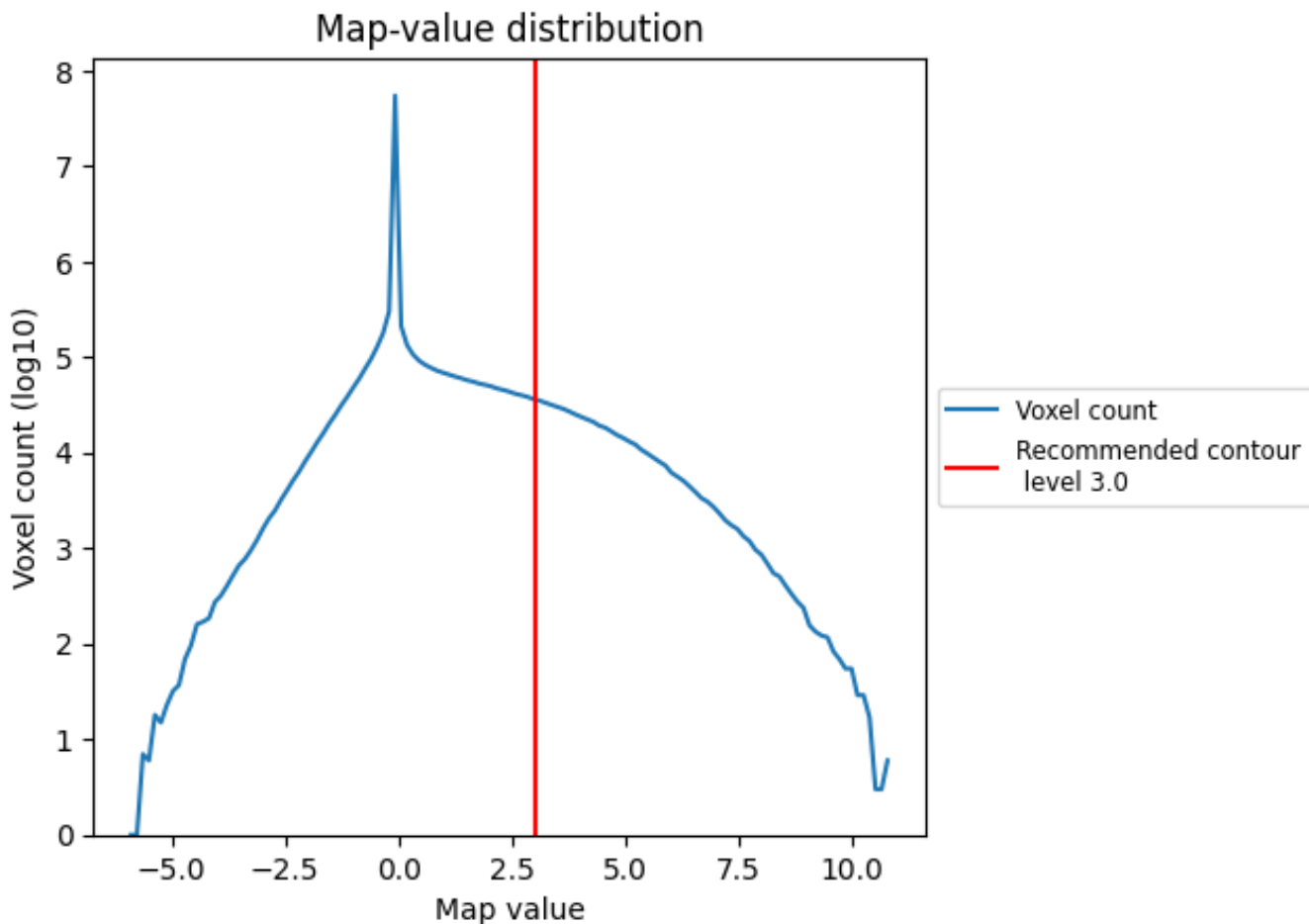
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

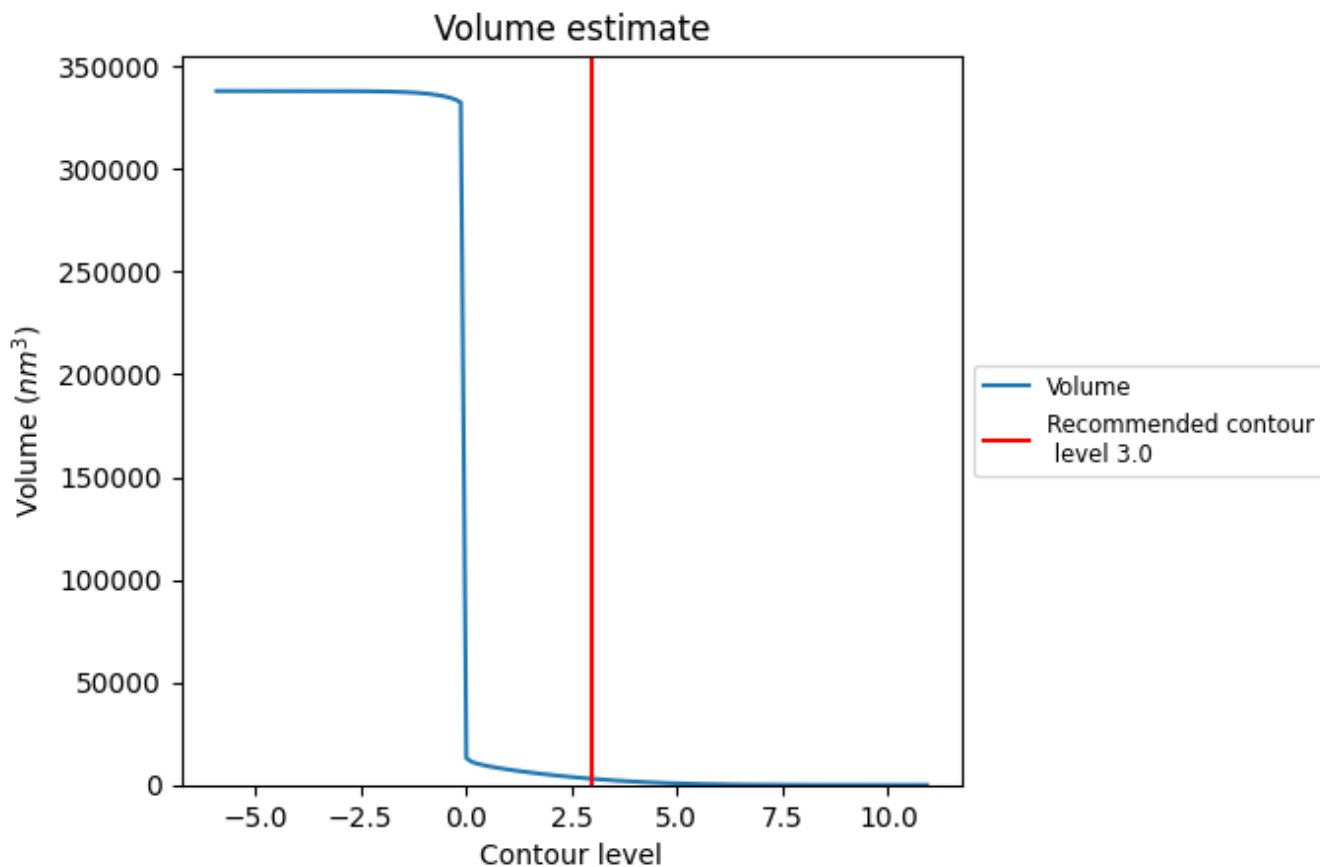
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

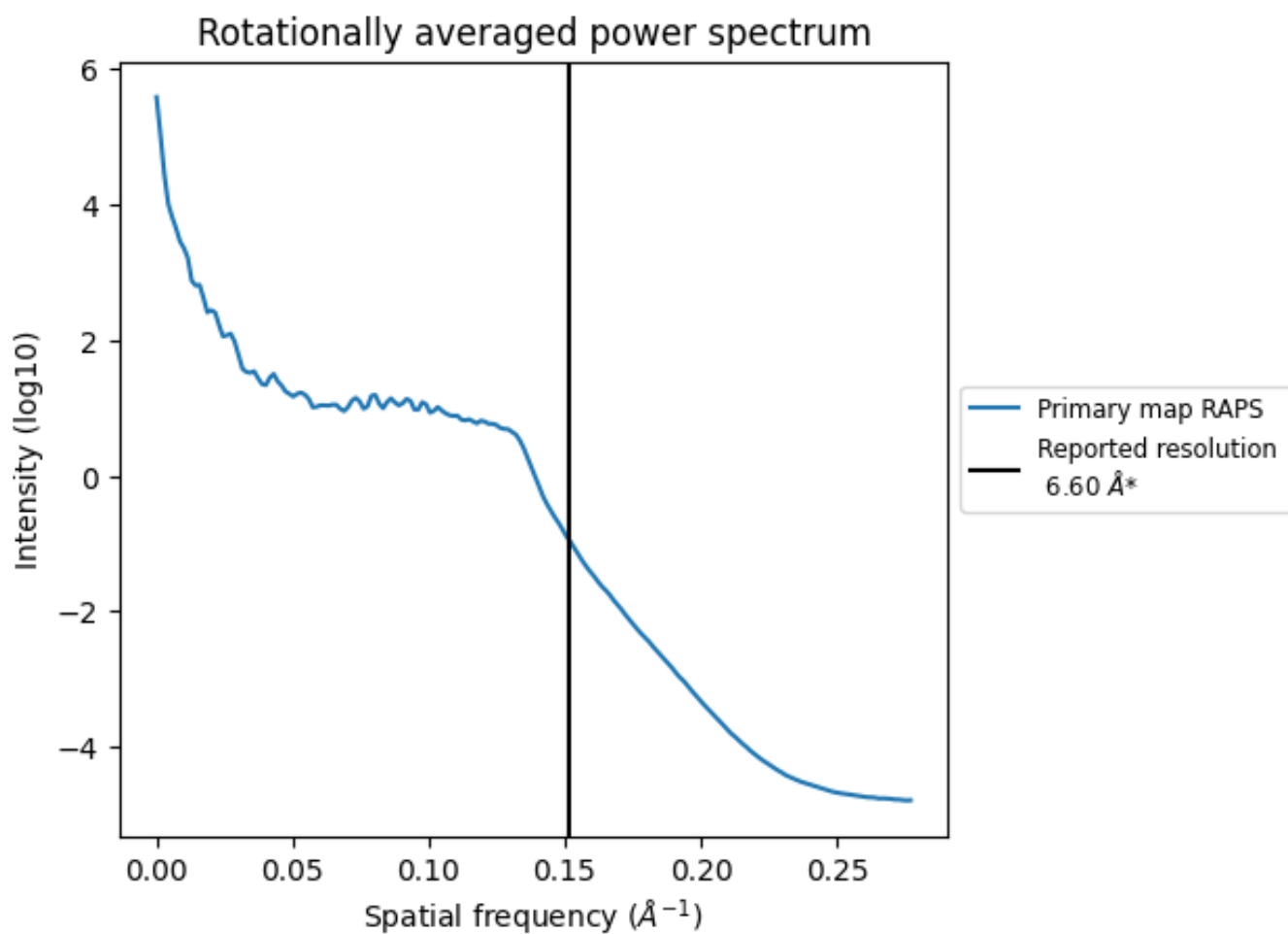
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 2987  $\text{nm}^3$ ; this corresponds to an approximate mass of 2698 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)



\*Reported resolution corresponds to spatial frequency of 0.152 Å<sup>-1</sup>

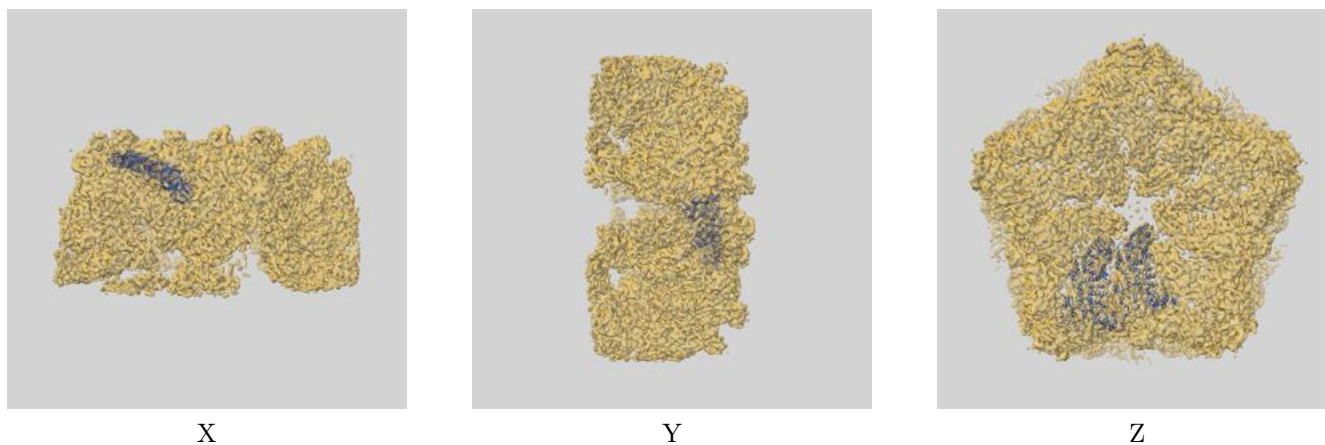
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22165 and PDB model 6XF7. Per-residue inclusion information can be found in section [3](#) on page [4](#).

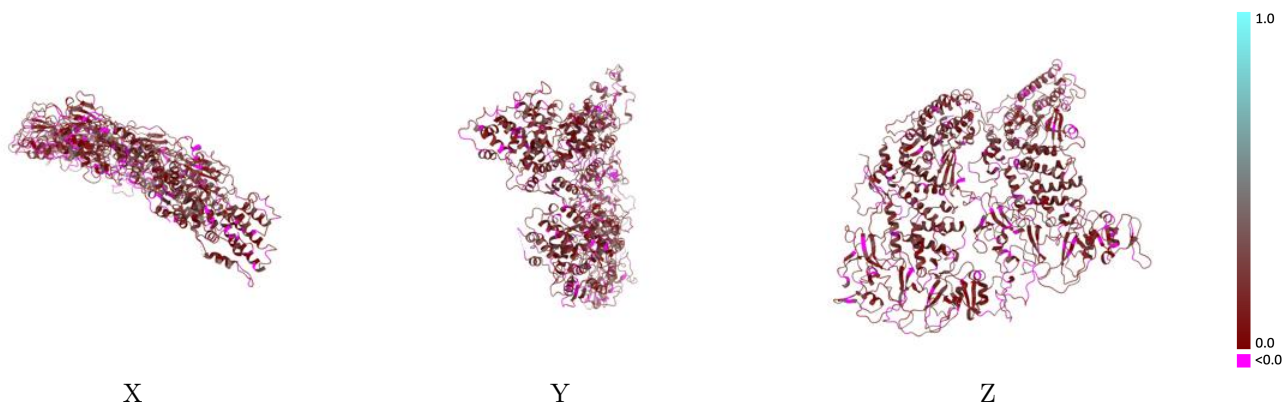
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

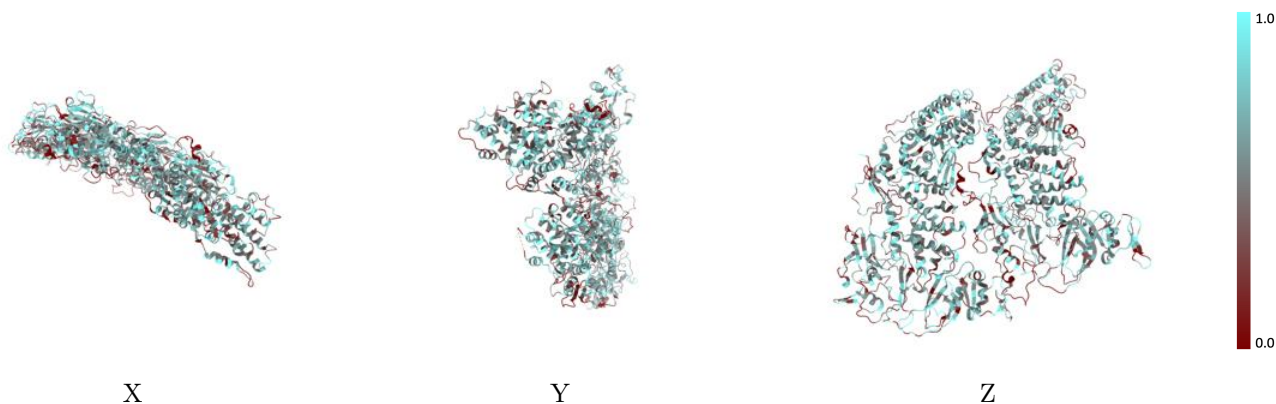


## 9.2 Q-score mapped to coordinate model [i](#)



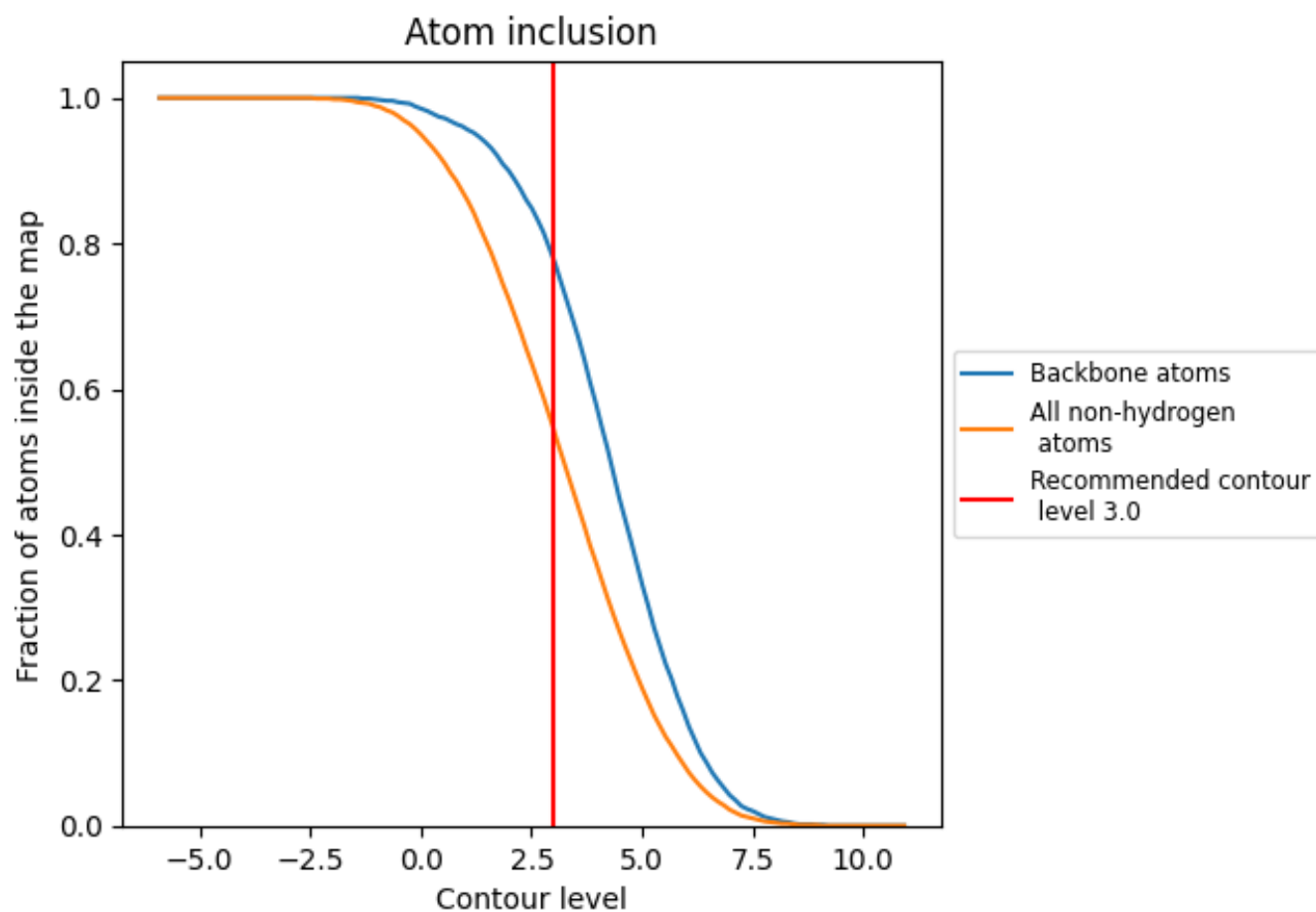
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.0).







## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 55% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (3.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5450	 0.1500
B	 0.5390	 0.1500
C	 0.5500	 0.1500

