



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 10:35 am BST

PDB ID : 4DJK  
Title : Structure of glutamate-GABA antiporter GadC  
Authors : Ma, D.; Lu, P.L.; Yan, C.Y.; Fan, C.; Yin, P.; Wang, J.W.; Shi, Y.G.  
Deposited on : 2012-02-02  
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

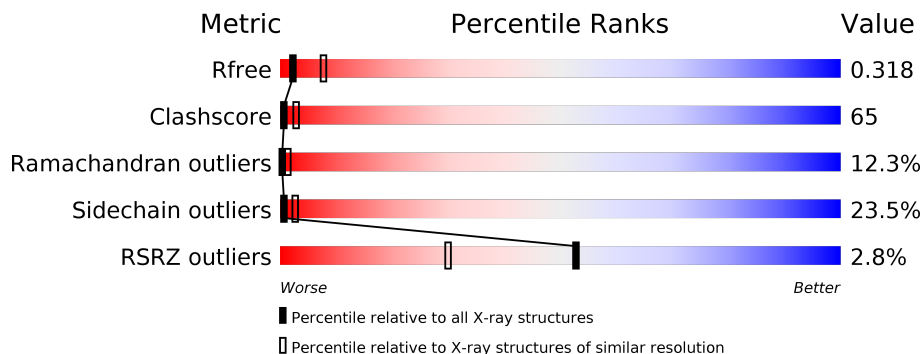
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	511	 2% 22% 47% 17% • 12%
1	B	511	 3% 20% 47% 19% • 11%

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6891 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

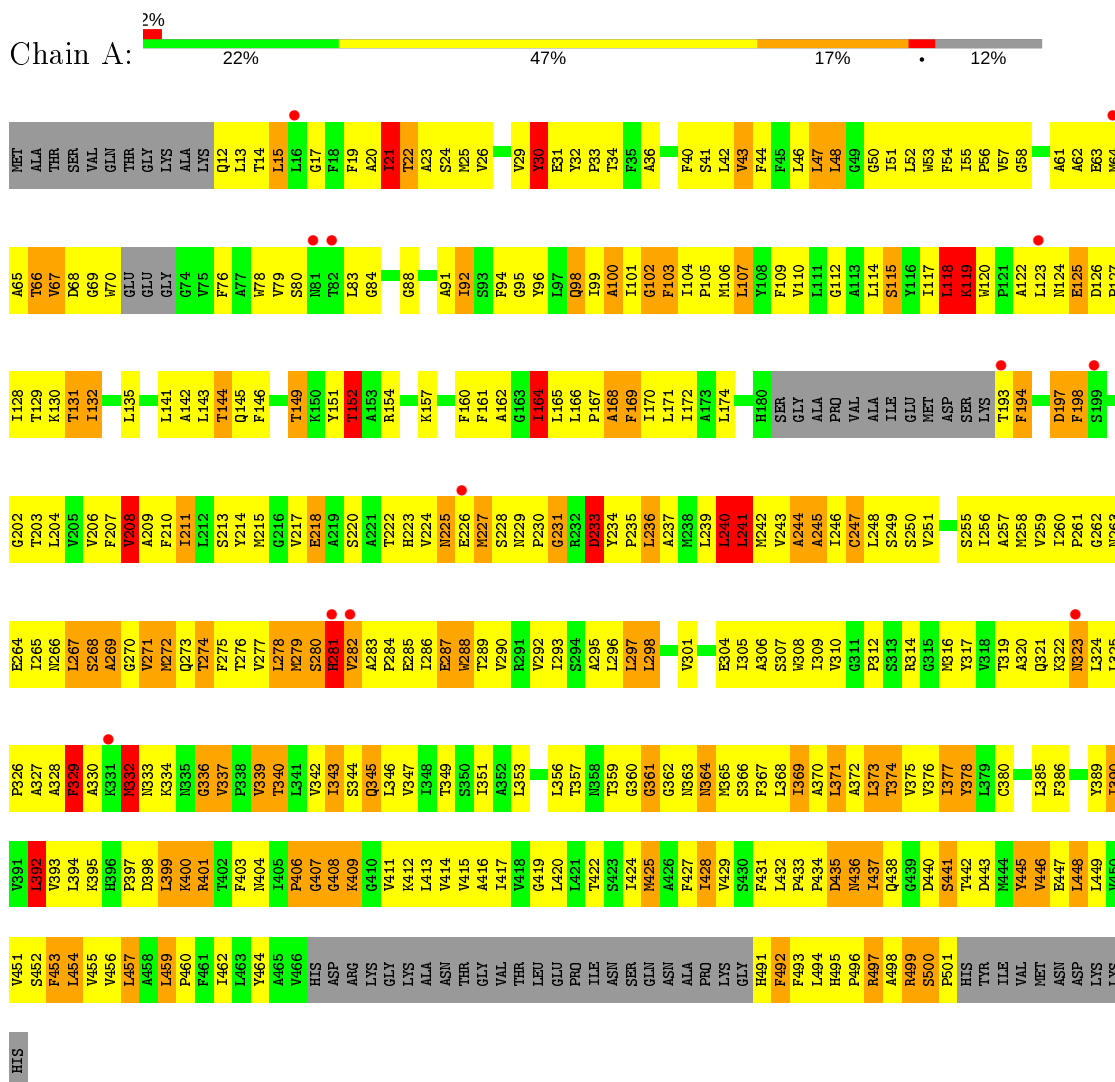
- Molecule 1 is a protein called Probable glutamate/gamma-aminobutyrate antiporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	451	Total 3436	C 2314	N 528	O 574	S 20	0	0	0
1	B	453	Total 3455	C 2324	N 532	O 579	S 20	0	0	0

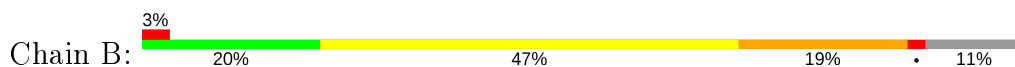
### 3 Residue-property plots i

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

- Molecule 1: Probable glutamate/gamma-aminobutyrate antiporter



- Molecule 1: Probable glutamate/gamma-aminobutyrate antiporter





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.96 Å 106.41 Å 185.98 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.14 – 3.10 33.14 – 3.10	Depositor EDS
% Data completeness (in resolution range)	79.7 (33.14-3.10) 79.8 (33.14-3.10)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.62 (at 3.12 Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.282 , 0.325 0.270 , 0.318	Depositor DCC
$R_{free}$ test set	1146 reflections (5.38%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	102.0	Xtrriage
Anisotropy	0.794	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 87.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6891	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	142.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.49	0/3524	0.72	2/4812 (0.0%)
1	B	0.49	0/3543	0.72	0/4836
All	All	0.49	0/7067	0.72	2/9648 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	392	LEU	CA-CB-CG	5.75	128.52	115.30
1	A	118	LEU	CB-CG-CD2	5.35	120.10	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	337	VAL	Peptide

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3436	0	3595	439	0
1	B	3455	0	3605	486	0
All	All	6891	0	7200	918	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 65.

All (918) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:LEU:HD11	1:B:204:LEU:HD12	1.40	1.04
1:A:491:HIS:C	1:A:493:PHE:H	1.58	1.01
1:A:101:ILE:HD13	1:A:373:LEU:HD21	1.43	1.00
1:B:400:LYS:H	1:B:400:LYS:HD2	1.24	1.00
1:B:279:MET:O	1:B:281:HIS:N	1.94	1.00
1:A:128:ILE:HG22	1:A:132:ILE:HG22	1.44	0.99
1:B:377:ILE:HD11	1:B:456:VAL:HG11	1.44	0.99
1:A:12:GLN:HG2	1:A:228:SER:HB3	1.45	0.98
1:A:21:ILE:HG13	1:A:492:PHE:CD1	1.99	0.97
1:B:283:ALA:HB1	1:B:284:PRO:HA	1.44	0.97
1:A:17:GLY:O	1:A:21:ILE:HG22	1.64	0.96
1:A:336:GLY:HA3	1:A:337:VAL:HB	1.46	0.96
1:B:178:TYR:O	1:B:178:TYR:HD2	1.48	0.96
1:B:219:ALA:HB3	1:B:220:SER:HB2	1.48	0.95
1:B:22:THR:O	1:B:24:SER:N	1.98	0.95
1:B:398:ASP:HA	1:B:399:LEU:HG	1.48	0.95
1:B:377:ILE:CD1	1:B:456:VAL:HG11	1.96	0.95
1:A:491:HIS:HD1	1:A:492:PHE:HD2	1.01	0.95
1:B:254:LEU:HA	1:B:257:ALA:HB3	1.49	0.94
1:A:260:ILE:HD11	1:A:277:VAL:HG21	1.51	0.93
1:A:94:PHE:CE1	1:A:460:PRO:HG2	2.03	0.93
1:B:92:ILE:HD12	1:B:316:MET:HG3	1.52	0.91
1:B:219:ALA:HB3	1:B:220:SER:CB	2.01	0.91
1:B:495:HIS:CD2	1:B:497:ARG:HG3	2.05	0.91
1:A:40:PHE:HD2	1:A:194:PHE:HB2	1.35	0.90
1:A:406:PRO:O	1:A:408:GLY:N	2.03	0.90
1:A:441:SER:O	1:A:443:ASP:N	2.05	0.89
1:B:67:VAL:CG2	1:B:400:LYS:HB2	2.02	0.89
1:A:233:ASP:H	1:A:235:PRO:HD2	1.34	0.88
1:B:284:PRO:HA	1:B:287:GLU:HB2	1.56	0.88
1:A:168:ALA:O	1:A:171:LEU:N	2.06	0.88
1:B:253:GLY:O	1:B:257:ALA:HB2	1.74	0.87

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:PHE:O	1:B:23:ALA:HB2	1.72	0.87
1:A:157:LYS:HE3	1:A:491:HIS:N	1.88	0.87
1:A:436:ASN:ND2	1:A:436:ASN:O	2.08	0.87
1:A:491:HIS:O	1:A:494:LEU:HD23	1.75	0.87
1:B:399:LEU:H	1:B:400:LYS:HD2	1.40	0.87
1:A:117:ILE:O	1:A:119:LYS:N	2.08	0.86
1:B:276:THR:HG22	1:B:290:VAL:HG11	1.56	0.85
1:B:80:SER:HA	1:B:84:GLY:O	1.75	0.85
1:B:364:ASN:HD22	1:B:438:GLN:HB2	1.42	0.84
1:B:68:ASP:CB	1:B:69:GLY:HA2	2.08	0.84
1:B:29:VAL:HA	1:B:32:TYR:CD1	2.12	0.84
1:A:314:ARG:HH21	1:A:337:VAL:HA	1.44	0.83
1:B:222:THR:O	1:B:224:VAL:N	2.11	0.83
1:B:67:VAL:HG23	1:B:400:LYS:HB2	1.60	0.83
1:B:451:VAL:O	1:B:455:VAL:HG23	1.79	0.83
1:B:79:VAL:HG13	1:B:83:LEU:HD12	1.60	0.83
1:B:162:ALA:O	1:B:167:PRO:HD3	1.80	0.82
1:B:68:ASP:HB2	1:B:69:GLY:HA2	1.62	0.81
1:A:174:LEU:HG	1:A:278:LEU:HD23	1.60	0.81
1:B:257:ALA:O	1:B:261:PRO:HG2	1.80	0.80
1:B:110:VAL:HG11	1:B:137:ILE:HD13	1.62	0.80
1:A:364:ASN:HD22	1:A:438:GLN:HB2	1.47	0.80
1:B:240:LEU:O	1:B:243:VAL:N	2.15	0.80
1:A:451:VAL:O	1:A:455:VAL:HG23	1.81	0.80
1:B:436:ASN:HA	1:B:441:SER:CB	2.11	0.80
1:B:281:HIS:C	1:B:283:ALA:H	1.81	0.79
1:A:225:ASN:C	1:A:227:MET:H	1.86	0.79
1:A:279:MET:O	1:A:281:HIS:N	2.15	0.79
1:A:198:PHE:O	1:B:395:LYS:HG3	1.82	0.79
1:A:126:ASP:O	1:A:129:THR:OG1	1.99	0.79
1:B:258:MET:O	1:B:259:VAL:HG13	1.83	0.79
1:B:250:SER:O	1:B:254:LEU:HB2	1.82	0.79
1:A:29:VAL:O	1:A:32:TYR:N	2.15	0.78
1:B:464:TYR:HD2	1:B:464:TYR:O	1.65	0.78
1:B:491:HIS:C	1:B:493:PHE:H	1.87	0.78
1:A:283:ALA:HA	1:A:286:ILE:HB	1.64	0.78
1:B:208:VAL:HG13	1:B:375:VAL:HG21	1.66	0.78
1:B:339:VAL:O	1:B:343:ILE:HB	1.83	0.77
1:A:495:HIS:HD2	1:A:497:ARG:HB2	1.47	0.77
1:A:19:PHE:O	1:A:23:ALA:HB2	1.83	0.77
1:A:47:LEU:O	1:A:51:ILE:HG12	1.84	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:HIS:C	1:A:493:PHE:N	2.32	0.77
1:A:459:LEU:HD13	1:A:462:ILE:HD11	1.66	0.77
1:B:331:LYS:O	1:B:332:MET:HG2	1.84	0.77
1:A:19:PHE:HE1	1:A:241:LEU:HA	1.50	0.76
1:B:120:TRP:NE1	1:B:122:ALA:HB3	2.00	0.76
1:B:425:MET:O	1:B:429:VAL:HG23	1.85	0.76
1:A:322:LYS:O	1:A:325:LEU:HD13	1.85	0.76
1:A:222:THR:O	1:A:224:VAL:N	2.16	0.76
1:A:276:THR:HG22	1:A:290:VAL:HG11	1.67	0.76
1:A:491:HIS:O	1:A:493:PHE:N	2.18	0.76
1:B:279:MET:C	1:B:281:HIS:H	1.90	0.75
1:A:411:VAL:HA	1:A:414:VAL:HG12	1.68	0.75
1:B:398:ASP:HA	1:B:399:LEU:CG	2.16	0.75
1:B:83:LEU:HB3	1:B:87:TRP:HE3	1.52	0.75
1:B:94:PHE:CE1	1:B:460:PRO:HG2	2.21	0.75
1:A:52:LEU:HB3	1:A:422:THR:HG21	1.67	0.74
1:B:491:HIS:O	1:B:494:LEU:HD23	1.86	0.74
1:B:500:SER:H	1:B:501:PRO:HD3	1.53	0.74
1:A:106:MET:HB3	1:A:305:ILE:HD11	1.69	0.74
1:B:306:ALA:HA	1:B:309:ILE:HG12	1.70	0.74
1:B:414:VAL:O	1:B:418:VAL:HG23	1.88	0.73
1:A:325:LEU:HB2	1:A:326:PRO:HD3	1.71	0.73
1:A:491:HIS:ND1	1:A:492:PHE:CD2	2.55	0.73
1:B:361:GLY:N	1:B:442:THR:OG1	2.19	0.73
1:B:68:ASP:OD1	1:B:81:ASN:ND2	2.20	0.73
1:B:229:ASN:O	1:B:229:ASN:ND2	2.22	0.73
1:B:41:SER:CB	1:B:196:PRO:HB3	2.19	0.73
1:A:44:PHE:HB2	1:A:193:THR:HG22	1.71	0.72
1:B:157:LYS:HE3	1:B:491:HIS:N	2.03	0.72
1:A:286:ILE:C	1:A:288:TRP:H	1.93	0.72
1:B:392:LEU:O	1:B:392:LEU:HD12	1.88	0.72
1:B:491:HIS:O	1:B:493:PHE:N	2.22	0.72
1:B:202:GLY:HA3	1:B:434:PRO:CA	2.19	0.72
1:A:327:ALA:O	1:A:329:PHE:N	2.23	0.72
1:A:64:MET:CE	1:A:78:TRP:HB3	2.19	0.72
1:B:436:ASN:HA	1:B:441:SER:OG	1.88	0.72
1:B:202:GLY:HA3	1:B:434:PRO:N	2.05	0.72
1:A:293:ILE:HA	1:A:296:LEU:HD13	1.71	0.72
1:B:464:TYR:HE2	1:B:468:ASP:O	1.72	0.71
1:A:292:VAL:O	1:A:296:LEU:HD12	1.89	0.71
1:A:395:LYS:HG3	1:B:201:VAL:HG21	1.70	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:MET:HG2	1:A:316:MET:O	1.91	0.71
1:A:66:THR:HG21	1:A:403:PHE:HB3	1.73	0.71
1:A:66:THR:O	1:A:67:VAL:HB	1.91	0.71
1:B:66:THR:HG22	1:B:224:VAL:HG11	1.73	0.71
1:A:339:VAL:HG13	1:A:340:THR:N	2.05	0.70
1:B:29:VAL:O	1:B:31:GLU:N	2.24	0.70
1:B:262:GLY:O	1:B:264:GLU:N	2.23	0.70
1:B:62:ALA:O	1:B:66:THR:HG23	1.90	0.70
1:A:117:ILE:C	1:A:119:LYS:H	1.93	0.70
1:A:101:ILE:HG22	1:A:374:THR:OG1	1.91	0.70
1:B:67:VAL:HG21	1:B:400:LYS:HB2	1.72	0.70
1:B:103:PHE:HZ	1:B:309:ILE:HD13	1.57	0.70
1:B:398:ASP:HA	1:B:399:LEU:CB	2.21	0.70
1:A:222:THR:C	1:A:224:VAL:H	1.95	0.70
1:B:283:ALA:HB1	1:B:284:PRO:CA	2.21	0.70
1:A:149:THR:OG1	1:A:149:THR:O	2.10	0.69
1:B:227:MET:CE	1:B:234:TYR:HB2	2.22	0.69
1:A:30:TYR:N	1:A:30:TYR:CD2	2.59	0.69
1:A:284:PRO:C	1:A:286:ILE:H	1.94	0.69
1:B:178:TYR:O	1:B:178:TYR:CD2	2.38	0.69
1:A:46:LEU:HD23	1:A:246:ILE:HA	1.72	0.69
1:B:68:ASP:HB2	1:B:69:GLY:CA	2.22	0.69
1:A:118:LEU:O	1:A:118:LEU:HD23	1.93	0.69
1:B:304:GLU:O	1:B:307:SER:OG	2.09	0.69
1:B:495:HIS:NE2	1:B:497:ARG:HG3	2.08	0.69
1:B:174:LEU:HG	1:B:278:LEU:HD22	1.74	0.69
1:B:314:ARG:HB2	1:B:337:VAL:HG21	1.75	0.69
1:B:350:SER:O	1:B:354:ILE:HG13	1.92	0.69
1:B:276:THR:CG2	1:B:290:VAL:HG11	2.22	0.69
1:A:46:LEU:HD12	1:A:210:PHE:CD1	2.27	0.69
1:A:101:ILE:HD13	1:A:373:LEU:CD2	2.21	0.68
1:B:43:VAL:O	1:B:47:LEU:HG	1.94	0.68
1:B:21:ILE:HB	1:B:492:PHE:CD1	2.29	0.68
1:B:68:ASP:CB	1:B:69:GLY:CA	2.71	0.68
1:A:307:SER:HB2	1:A:494:LEU:HD12	1.74	0.68
1:A:67:VAL:HG11	1:A:400:LYS:HB2	1.76	0.68
1:A:365:MET:HA	1:A:437:ILE:HD11	1.74	0.68
1:B:38:SER:O	1:B:41:SER:OG	2.10	0.68
1:B:99:ILE:O	1:B:101:ILE:N	2.27	0.68
1:A:274:THR:O	1:A:278:LEU:HB2	1.94	0.68
1:A:98:GLN:HG3	1:A:378:TYR:CD2	2.28	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:PHE:O	1:B:340:THR:HG21	1.93	0.68
1:A:46:LEU:HD12	1:A:210:PHE:HD1	1.59	0.68
1:A:128:ILE:N	1:A:128:ILE:HD12	2.08	0.67
1:A:66:THR:OG1	1:A:66:THR:O	2.10	0.67
1:A:433:PRO:HG3	1:A:445:TYR:CD2	2.30	0.67
1:A:237:ALA:O	1:A:241:LEU:HB2	1.95	0.67
1:A:215:MET:HE3	1:A:375:VAL:HG13	1.76	0.67
1:B:491:HIS:C	1:B:493:PHE:N	2.46	0.67
1:B:314:ARG:HG2	1:B:500:SER:OG	1.95	0.67
1:B:64:MET:CE	1:B:78:TRP:HB3	2.25	0.67
1:A:166:LEU:HB3	1:A:167:PRO:HD3	1.76	0.67
1:B:86:ARG:HA	1:B:464:TYR:CE1	2.30	0.67
1:A:240:LEU:O	1:A:243:VAL:N	2.28	0.67
1:A:101:ILE:O	1:A:103:PHE:N	2.28	0.67
1:A:124:ASN:HD21	1:A:268:SER:HB2	1.59	0.67
1:A:333:ASN:O	1:A:334:LYS:HG3	1.95	0.67
1:A:361:GLY:O	1:A:440:ASP:HB3	1.95	0.66
1:B:282:VAL:HG13	1:B:286:ILE:HG21	1.76	0.66
1:A:369:ILE:HG13	1:A:445:TYR:CE1	2.30	0.66
1:B:243:VAL:HA	1:B:246:ILE:HD12	1.77	0.66
1:B:364:ASN:HD22	1:B:438:GLN:CB	2.08	0.66
1:A:408:GLY:O	1:A:412:LYS:HE3	1.95	0.66
1:B:42:LEU:HD12	1:B:43:VAL:N	2.10	0.66
1:A:25:MET:HB2	1:A:495:HIS:HE1	1.61	0.66
1:A:67:VAL:HG11	1:A:401:ARG:H	1.60	0.66
1:B:157:LYS:HZ1	1:B:491:HIS:N	1.94	0.66
1:A:269:ALA:O	1:A:271:VAL:N	2.29	0.66
1:A:29:VAL:O	1:A:31:GLU:N	2.28	0.65
1:A:336:GLY:CA	1:A:337:VAL:HB	2.22	0.65
1:B:233:ASP:H	1:B:235:PRO:HD2	1.60	0.65
1:B:365:MET:HA	1:B:437:ILE:CD1	2.25	0.65
1:B:83:LEU:HB3	1:B:87:TRP:CE3	2.31	0.65
1:B:284:PRO:C	1:B:286:ILE:H	1.98	0.65
1:A:171:LEU:HB2	1:A:275:PHE:CZ	2.31	0.65
1:A:377:ILE:HG12	1:A:456:VAL:HG11	1.78	0.65
1:B:274:THR:O	1:B:278:LEU:HB2	1.97	0.65
1:B:283:ALA:HB1	1:B:287:GLU:HB2	1.77	0.65
1:B:222:THR:C	1:B:224:VAL:H	1.99	0.65
1:B:46:LEU:HD23	1:B:246:ILE:HA	1.79	0.65
1:B:94:PHE:HE1	1:B:460:PRO:HG2	1.62	0.65
1:B:175:ALA:HB2	1:B:278:LEU:HD11	1.77	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:TRP:C	1:A:56:PRO:HD2	2.17	0.65
1:B:120:TRP:CD1	1:B:122:ALA:HB3	2.31	0.65
1:B:286:ILE:O	1:B:289:THR:HG22	1.97	0.65
1:B:233:ASP:OD2	1:B:234:TYR:N	2.29	0.65
1:B:356:LEU:HD11	1:B:369:ILE:HD13	1.79	0.65
1:B:365:MET:HA	1:B:437:ILE:HD11	1.78	0.65
1:A:431:PHE:C	1:A:432:LEU:HD23	2.18	0.65
1:B:209:ALA:HB2	1:B:371:LEU:HD12	1.79	0.65
1:B:448:LEU:O	1:B:452:SER:HB2	1.96	0.65
1:B:433:PRO:HG3	1:B:445:TYR:HD2	1.62	0.64
1:A:323:ASN:HB3	1:A:325:LEU:CD1	2.26	0.64
1:B:34:THR:HG22	1:B:267:LEU:HD12	1.79	0.64
1:A:99:ILE:O	1:A:101:ILE:N	2.30	0.64
1:B:411:VAL:HA	1:B:414:VAL:HG12	1.80	0.64
1:A:197:ASP:O	1:A:203:THR:HG21	1.96	0.64
1:A:295:ALA:O	1:A:298:LEU:HD23	1.97	0.64
1:B:98:GLN:HB2	1:B:378:TYR:HB2	1.80	0.64
1:B:117:ILE:HD11	1:B:295:ALA:HA	1.78	0.64
1:B:103:PHE:CZ	1:B:309:ILE:HD13	2.32	0.64
1:B:317:TYR:CE1	1:B:330:ALA:HB1	2.32	0.64
1:A:356:LEU:HD11	1:A:369:ILE:HD13	1.80	0.64
1:B:127:PRO:O	1:B:131:THR:HG22	1.97	0.64
1:A:409:LYS:HA	1:A:412:LYS:HB2	1.79	0.64
1:A:101:ILE:C	1:A:103:PHE:H	1.99	0.64
1:A:440:ASP:N	1:A:441:SER:OG	2.26	0.64
1:B:219:ALA:HB3	1:B:220:SER:HB3	1.80	0.64
1:A:347:VAL:O	1:A:351:ILE:CG1	2.46	0.64
1:B:12:GLN:N	1:B:12:GLN:OE1	2.31	0.64
1:B:22:THR:OG1	1:B:241:LEU:HD11	1.98	0.63
1:A:356:LEU:HD11	1:A:369:ILE:HG21	1.79	0.63
1:A:373:LEU:HB2	1:A:449:LEU:HD12	1.81	0.63
1:A:104:ILE:N	1:A:105:PRO:HD2	2.14	0.63
1:B:124:ASN:ND2	1:B:269:ALA:HB2	2.14	0.63
1:B:30:TYR:N	1:B:30:TYR:CD2	2.65	0.63
1:B:400:LYS:CD	1:B:400:LYS:H	1.97	0.63
1:A:333:ASN:CG	1:A:334:LYS:H	2.02	0.63
1:A:80:SER:HA	1:A:84:GLY:O	1.99	0.63
1:B:117:ILE:HG22	1:B:118:LEU:HD12	1.79	0.63
1:B:92:ILE:HD12	1:B:316:MET:CG	2.27	0.63
1:A:339:VAL:CG1	1:A:340:THR:N	2.62	0.62
1:B:317:TYR:O	1:B:320:ALA:N	2.32	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:PHE:CD2	1:A:492:PHE:N	2.68	0.62
1:B:194:PHE:O	1:B:196:PRO:N	2.32	0.62
1:B:208:VAL:CG1	1:B:371:LEU:HB3	2.29	0.62
1:B:281:HIS:C	1:B:283:ALA:N	2.50	0.62
1:B:240:LEU:O	1:B:242:MET:N	2.32	0.62
1:A:19:PHE:CE1	1:A:241:LEU:HA	2.33	0.62
1:B:41:SER:HB2	1:B:196:PRO:HB3	1.82	0.62
1:A:119:LYS:HE3	1:A:119:LYS:HA	1.81	0.62
1:A:347:VAL:O	1:A:351:ILE:HG13	1.99	0.62
1:A:368:LEU:HD23	1:A:437:ILE:HG21	1.80	0.62
1:A:492:PHE:HD2	1:A:492:PHE:N	1.96	0.62
1:A:67:VAL:HG21	1:A:400:LYS:HB3	1.80	0.62
1:B:22:THR:C	1:B:24:SER:H	2.01	0.62
1:B:18:PHE:CD1	1:B:21:ILE:HD11	2.34	0.62
1:B:376:VAL:HG23	1:B:453:PHE:HD1	1.65	0.62
1:A:356:LEU:HD11	1:A:369:ILE:CG2	2.30	0.62
1:B:244:ALA:O	1:B:246:ILE:N	2.33	0.62
1:B:377:ILE:HG22	1:B:378:TYR:N	2.15	0.62
1:B:365:MET:HG3	1:B:437:ILE:HD11	1.82	0.62
1:A:317:TYR:OH	1:A:330:ALA:HB1	2.00	0.61
1:A:40:PHE:HD2	1:A:194:PHE:CB	2.11	0.61
1:A:377:ILE:HD11	1:A:456:VAL:HG21	1.81	0.61
1:B:260:ILE:H	1:B:261:PRO:HD2	1.65	0.61
1:B:431:PHE:O	1:B:432:LEU:HD23	1.99	0.61
1:A:215:MET:CE	1:A:375:VAL:HG13	2.31	0.61
1:B:362:GLY:HA3	1:B:440:ASP:HB3	1.82	0.61
1:B:255:SER:O	1:B:259:VAL:HG22	2.00	0.61
1:B:417:ILE:O	1:B:421:LEU:HD13	2.00	0.61
1:A:259:VAL:HG21	1:A:278:LEU:HD12	1.83	0.61
1:A:117:ILE:HD11	1:A:295:ALA:N	2.15	0.61
1:A:40:PHE:O	1:A:43:VAL:HG23	1.99	0.61
1:A:229:ASN:O	1:A:230:PRO:C	2.37	0.61
1:A:64:MET:HE2	1:A:78:TRP:HB3	1.81	0.61
1:B:104:ILE:HG12	1:B:353:LEU:HD23	1.83	0.61
1:A:386:PHE:O	1:A:390:ILE:HG12	2.00	0.61
1:B:104:ILE:HG22	1:B:105:PRO:N	2.16	0.61
1:B:128:ILE:O	1:B:132:ILE:HG23	2.01	0.61
1:B:453:PHE:C	1:B:453:PHE:CD2	2.73	0.61
1:A:32:TYR:N	1:A:33:PRO:HD2	2.16	0.61
1:A:64:MET:HE1	1:A:78:TRP:HB3	1.81	0.61
1:B:234:TYR:CD2	1:B:234:TYR:C	2.74	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:VAL:HG12	1:B:457:LEU:N	2.15	0.61
1:A:142:ALA:O	1:A:146:PHE:HD2	1.84	0.61
1:A:152:THR:HG21	1:A:307:SER:HA	1.83	0.61
1:B:227:MET:HE3	1:B:234:TYR:HB2	1.83	0.61
1:B:76:PHE:O	1:B:80:SER:OG	2.10	0.61
1:B:433:PRO:HG3	1:B:445:TYR:CD2	2.36	0.60
1:B:307:SER:HB2	1:B:494:LEU:HD12	1.83	0.60
1:A:112:GLY:O	1:A:115:SER:HB3	2.01	0.60
1:B:256:ILE:HG23	1:B:274:THR:OG1	2.01	0.60
1:B:64:MET:HE1	1:B:78:TRP:HB3	1.81	0.60
1:B:113:ALA:HA	1:B:272:MET:SD	2.42	0.60
1:B:371:LEU:O	1:B:375:VAL:HG23	2.01	0.60
1:B:53:TRP:C	1:B:56:PRO:HD2	2.21	0.60
1:A:120:TRP:CD1	1:A:122:ALA:HB3	2.36	0.60
1:A:368:LEU:O	1:A:371:LEU:HB2	2.01	0.60
1:A:12:GLN:HG2	1:A:228:SER:CB	2.28	0.60
1:B:253:GLY:O	1:B:257:ALA:CB	2.48	0.60
1:B:47:LEU:O	1:B:51:ILE:HG12	2.02	0.60
1:B:174:LEU:HG	1:B:278:LEU:CD2	2.31	0.60
1:A:225:ASN:C	1:A:227:MET:N	2.54	0.60
1:A:244:ALA:O	1:A:246:ILE:N	2.35	0.59
1:A:306:ALA:O	1:A:309:ILE:HG12	2.02	0.59
1:A:21:ILE:HG13	1:A:492:PHE:CE1	2.37	0.59
1:A:124:ASN:O	1:A:363:ASN:ND2	2.35	0.59
1:B:55:ILE:HA	1:B:238:MET:CE	2.33	0.59
1:A:361:GLY:HA3	1:A:441:SER:HA	1.84	0.59
1:A:496:PRO:C	1:A:498:ALA:H	2.05	0.59
1:A:30:TYR:CE2	1:A:301:VAL:HG23	2.37	0.59
1:B:365:MET:O	1:B:366:SER:C	2.41	0.59
1:B:367:PHE:O	1:B:370:ALA:N	2.35	0.59
1:B:98:GLN:HG3	1:B:378:TYR:CD2	2.38	0.59
1:A:128:ILE:O	1:A:131:THR:HG23	2.01	0.59
1:A:256:ILE:HA	1:A:274:THR:OG1	2.03	0.59
1:B:499:ARG:O	1:B:500:SER:HB2	2.02	0.59
1:A:54:PHE:CD1	1:A:214:TYR:HD1	2.21	0.59
1:B:29:VAL:HA	1:B:32:TYR:CE1	2.37	0.59
1:B:361:GLY:H	1:B:442:THR:HG1	1.46	0.59
1:B:233:ASP:O	1:B:236:LEU:HB2	2.03	0.59
1:A:399:LEU:C	1:A:400:LYS:HD2	2.22	0.59
1:A:491:HIS:HA	1:A:494:LEU:HD22	1.85	0.58
1:A:79:VAL:CG1	1:A:88:GLY:HA2	2.33	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:ALA:O	1:A:499:ARG:O	2.21	0.58
1:B:44:PHE:HA	1:B:193:THR:HG22	1.85	0.58
1:A:227:MET:CE	1:A:234:TYR:HB2	2.33	0.58
1:A:314:ARG:NH2	1:A:336:GLY:HA3	2.18	0.58
1:A:61:ALA:HB2	1:A:385:LEU:HD11	1.84	0.58
1:B:236:LEU:HA	1:B:239:LEU:HB2	1.85	0.58
1:A:98:GLN:HG3	1:A:378:TYR:CG	2.38	0.58
1:B:314:ARG:NH2	1:B:335:ASN:HB3	2.19	0.58
1:B:94:PHE:C	1:B:96:TYR:H	2.07	0.58
1:B:234:TYR:HD2	1:B:234:TYR:C	2.06	0.58
1:B:31:GLU:O	1:B:32:TYR:C	2.42	0.58
1:B:163:GLY:O	1:B:164:ILE:HG13	2.03	0.58
1:B:208:VAL:HG12	1:B:209:ALA:N	2.18	0.58
1:B:225:ASN:C	1:B:227:MET:N	2.57	0.58
1:B:145:GLN:NE2	1:B:152:THR:HG21	2.19	0.58
1:B:283:ALA:HA	1:B:285:GLU:N	2.18	0.58
1:B:101:ILE:HG22	1:B:374:THR:OG1	2.04	0.58
1:A:52:LEU:CB	1:A:422:THR:HG21	2.34	0.58
1:B:407:GLY:HA3	1:B:411:VAL:HB	1.85	0.58
1:A:332:MET:HA	1:A:337:VAL:O	2.04	0.58
1:B:45:PHE:HD2	1:B:210:PHE:CE2	2.22	0.58
1:B:225:ASN:C	1:B:227:MET:H	2.07	0.58
1:A:245:ALA:O	1:A:249:SER:OG	2.16	0.57
1:A:286:ILE:C	1:A:288:TRP:N	2.57	0.57
1:B:99:ILE:HG21	1:B:312:PRO:HG2	1.85	0.57
1:A:101:ILE:C	1:A:103:PHE:N	2.56	0.57
1:A:40:PHE:CD2	1:A:194:PHE:HB2	2.27	0.57
1:A:21:ILE:O	1:A:499:ARG:NH2	2.36	0.57
1:A:79:VAL:HG12	1:A:88:GLY:HA2	1.86	0.57
1:B:365:MET:CG	1:B:437:ILE:HD11	2.34	0.57
1:B:307:SER:HB2	1:B:494:LEU:CD1	2.35	0.57
1:B:145:GLN:HG3	1:B:309:ILE:HB	1.85	0.57
1:B:204:LEU:O	1:B:206:VAL:N	2.37	0.57
1:B:215:MET:CE	1:B:378:TYR:HB3	2.35	0.57
1:B:227:MET:HE1	1:B:234:TYR:HB2	1.86	0.57
1:B:377:ILE:HD11	1:B:456:VAL:CG1	2.27	0.57
1:A:92:ILE:HG23	1:A:316:MET:SD	2.45	0.57
1:B:63:GLU:OE2	1:B:404:ASN:HA	2.03	0.57
1:B:405:ILE:HG23	1:B:406:PRO:HD2	1.87	0.57
1:B:431:PHE:O	1:B:433:PRO:HD3	2.04	0.57
1:A:20:ALA:O	1:A:23:ALA:N	2.33	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:ILE:O	1:A:431:PHE:N	2.36	0.57
1:B:463:LEU:O	1:B:466:VAL:HG22	2.04	0.57
1:A:247:CYS:O	1:A:251:VAL:HG23	2.05	0.57
1:A:327:ALA:C	1:A:329:PHE:H	2.07	0.57
1:B:240:LEU:O	1:B:241:LEU:C	2.43	0.57
1:A:225:ASN:O	1:A:227:MET:N	2.38	0.57
1:B:431:PHE:C	1:B:432:LEU:HD23	2.25	0.57
1:B:21:ILE:HB	1:B:492:PHE:HD1	1.69	0.57
1:B:349:THR:O	1:B:353:LEU:HB2	2.05	0.56
1:A:209:ALA:HB2	1:A:371:LEU:CD1	2.35	0.56
1:B:40:PHE:HD1	1:B:40:PHE:O	1.88	0.56
1:A:145:GLN:NE2	1:A:145:GLN:HA	2.20	0.56
1:A:161:PHE:CE2	1:A:493:PHE:HE1	2.24	0.56
1:A:68:ASP:HB2	1:A:69:GLY:HA2	1.88	0.56
1:A:411:VAL:HA	1:A:414:VAL:CG1	2.35	0.56
1:B:46:LEU:HD12	1:B:210:PHE:CD1	2.41	0.56
1:A:228:SER:HA	1:A:230:PRO:HD3	1.87	0.56
1:A:392:LEU:HD12	1:A:401:ARG:HH21	1.70	0.56
1:B:92:ILE:HG23	1:B:316:MET:HG3	1.86	0.56
1:B:458:ALA:O	1:B:462:ILE:HG23	2.05	0.56
1:B:207:PHE:O	1:B:208:VAL:C	2.44	0.56
1:B:284:PRO:HA	1:B:287:GLU:CB	2.34	0.56
1:A:456:VAL:HG12	1:A:457:LEU:N	2.19	0.56
1:B:27:MET:HG2	1:B:164:ILE:CG2	2.35	0.56
1:B:369:ILE:HG13	1:B:445:TYR:CE1	2.41	0.56
1:B:229:ASN:O	1:B:230:PRO:O	2.24	0.56
1:B:94:PHE:CD2	1:B:380:CYS:HB2	2.40	0.56
1:B:145:GLN:HA	1:B:145:GLN:OE1	2.05	0.55
1:B:365:MET:CB	1:B:437:ILE:HD11	2.36	0.55
1:B:411:VAL:HA	1:B:414:VAL:CG1	2.35	0.55
1:A:25:MET:HB2	1:A:495:HIS:CE1	2.40	0.55
1:B:149:THR:HG21	1:B:314:ARG:HH22	1.71	0.55
1:A:227:MET:HE3	1:A:234:TYR:HB2	1.89	0.55
1:B:400:LYS:N	1:B:400:LYS:HD2	2.08	0.55
1:A:339:VAL:CG1	1:A:340:THR:H	2.19	0.55
1:B:157:LYS:CE	1:B:491:HIS:N	2.70	0.55
1:B:337:VAL:N	1:B:338:PRO:HD3	2.22	0.55
1:B:351:ILE:O	1:B:355:ILE:HD12	2.07	0.55
1:B:436:ASN:HA	1:B:441:SER:HB2	1.88	0.55
1:A:209:ALA:HB2	1:A:371:LEU:HD12	1.89	0.55
1:A:500:SER:H	1:A:501:PRO:HD2	1.72	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:TYR:CD1	1:B:272:MET:HB2	2.42	0.55
1:B:31:GLU:O	1:B:33:PRO:N	2.40	0.55
1:A:398:ASP:HA	1:A:399:LEU:HB2	1.89	0.55
1:A:365:MET:HA	1:A:437:ILE:CD1	2.37	0.55
1:A:22:THR:HA	1:A:499:ARG:HH22	1.72	0.55
1:A:168:ALA:O	1:A:170:ILE:N	2.40	0.54
1:A:261:PRO:O	1:A:263:ASN:N	2.39	0.54
1:A:41:SER:HB3	1:A:194:PHE:O	2.07	0.54
1:B:31:GLU:HB2	1:B:35:PHE:CE2	2.41	0.54
1:B:362:GLY:CA	1:B:440:ASP:HB3	2.37	0.54
1:B:131:THR:O	1:B:135:LEU:HB2	2.07	0.54
1:B:279:MET:C	1:B:281:HIS:N	2.51	0.54
1:B:330:ALA:O	1:B:331:LYS:HD3	2.07	0.54
1:A:124:ASN:HD21	1:A:269:ALA:H	1.55	0.54
1:B:218:GLU:OE2	1:B:378:TYR:OH	2.12	0.54
1:B:301:VAL:O	1:B:305:ILE:HG13	2.07	0.54
1:A:124:ASN:ND2	1:A:268:SER:HB2	2.22	0.54
1:A:44:PHE:HB2	1:A:193:THR:CG2	2.38	0.54
1:A:377:ILE:CD1	1:A:456:VAL:HG11	2.37	0.54
1:B:70:TRP:CD1	1:B:222:THR:HB	2.43	0.54
1:A:36:ALA:HB1	1:A:257:ALA:HA	1.90	0.54
1:B:358:ASN:O	1:B:359:THR:HG23	2.07	0.54
1:A:46:LEU:HD22	1:A:250:SER:HB3	1.90	0.54
1:A:284:PRO:C	1:A:286:ILE:N	2.61	0.54
1:A:79:VAL:HG12	1:A:88:GLY:CA	2.37	0.54
1:A:120:TRP:NE1	1:A:122:ALA:HB3	2.23	0.53
1:A:206:VAL:HG13	1:A:210:PHE:HE2	1.73	0.53
1:B:142:ALA:HB2	1:B:346:LEU:HD11	1.89	0.53
1:A:12:GLN:CG	1:A:228:SER:HB3	2.30	0.53
1:A:296:LEU:HD12	1:A:296:LEU:H	1.73	0.53
1:A:312:PRO:HG3	1:A:498:ALA:HA	1.90	0.53
1:A:323:ASN:HB3	1:A:325:LEU:HD12	1.89	0.53
1:A:389:TYR:O	1:A:393:VAL:HG23	2.07	0.53
1:B:166:LEU:HB3	1:B:167:PRO:HD3	1.88	0.53
1:A:168:ALA:O	1:A:169:PHE:C	2.47	0.53
1:B:44:PHE:HB2	1:B:193:THR:HG22	1.91	0.53
1:B:304:GLU:O	1:B:307:SER:N	2.42	0.53
1:B:86:ARG:HA	1:B:464:TYR:CD1	2.43	0.53
1:A:376:VAL:HG23	1:A:453:PHE:HD1	1.74	0.53
1:A:204:LEU:HB3	1:A:429:VAL:CG1	2.39	0.53
1:A:441:SER:O	1:A:443:ASP:OD1	2.26	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:GLU:HB2	1:B:35:PHE:CD2	2.43	0.53
1:A:119:LYS:CE	1:A:119:LYS:HA	2.38	0.53
1:A:131:THR:HG22	1:A:357:THR:HG21	1.89	0.53
1:A:267:LEU:HB3	1:A:367:PHE:CD2	2.44	0.53
1:A:41:SER:O	1:A:44:PHE:HB3	2.08	0.53
1:B:329:PHE:C	1:B:329:PHE:CD2	2.82	0.53
1:A:106:MET:O	1:A:110:VAL:HG23	2.08	0.53
1:B:317:TYR:OH	1:B:330:ALA:HB1	2.08	0.53
1:B:373:LEU:HD23	1:B:373:LEU:O	2.09	0.53
1:B:351:ILE:HG22	1:B:355:ILE:HD12	1.91	0.53
1:B:219:ALA:CB	1:B:220:SER:CB	2.82	0.52
1:B:66:THR:HG22	1:B:224:VAL:CG1	2.39	0.52
1:B:366:SER:O	1:B:369:ILE:HG22	2.08	0.52
1:A:271:VAL:O	1:A:274:THR:HB	2.09	0.52
1:A:130:LYS:NZ	1:A:363:ASN:HB2	2.25	0.52
1:B:175:ALA:CB	1:B:278:LEU:HD11	2.40	0.52
1:B:70:TRP:N	1:B:70:TRP:CE3	2.78	0.52
1:A:110:VAL:HG22	1:A:301:VAL:HG11	1.90	0.52
1:A:361:GLY:H	1:A:365:MET:HE3	1.74	0.52
1:A:377:ILE:CG1	1:A:456:VAL:HG11	2.39	0.52
1:A:491:HIS:ND1	1:A:492:PHE:CE2	2.78	0.52
1:B:442:THR:HG21	1:B:444:MET:CE	2.40	0.52
1:A:29:VAL:C	1:A:31:GLU:N	2.63	0.52
1:B:120:TRP:HE1	1:B:122:ALA:HB3	1.71	0.52
1:B:18:PHE:HD1	1:B:21:ILE:HD11	1.74	0.52
1:B:260:ILE:HD11	1:B:274:THR:HA	1.91	0.52
1:A:42:LEU:HD12	1:A:42:LEU:C	2.30	0.52
1:B:68:ASP:HB3	1:B:69:GLY:HA2	1.89	0.52
1:A:500:SER:H	1:A:501:PRO:CD	2.23	0.52
1:B:124:ASN:HD22	1:B:269:ALA:HB2	1.75	0.52
1:B:132:ILE:HD12	1:B:132:ILE:O	2.09	0.52
1:B:308:TRP:CD1	1:B:308:TRP:N	2.78	0.52
1:B:393:VAL:HG11	1:B:413:LEU:HD13	1.91	0.52
1:A:141:LEU:HA	1:A:144:THR:CG2	2.39	0.52
1:A:222:THR:C	1:A:224:VAL:N	2.63	0.52
1:A:401:ARG:HH12	1:A:412:LYS:NZ	2.07	0.52
1:B:104:ILE:O	1:B:107:LEU:N	2.42	0.52
1:B:289:THR:O	1:B:292:VAL:HB	2.10	0.52
1:A:307:SER:HB2	1:A:494:LEU:CD1	2.40	0.52
1:A:152:THR:CG2	1:A:307:SER:HA	2.40	0.51
1:A:360:GLY:O	1:A:362:GLY:N	2.37	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:ILE:O	1:B:258:MET:N	2.43	0.51
1:A:117:ILE:C	1:A:119:LYS:N	2.60	0.51
1:A:395:LYS:HG3	1:B:201:VAL:CG2	2.39	0.51
1:A:495:HIS:ND1	1:A:496:PRO:HD2	2.25	0.51
1:B:149:THR:O	1:B:149:THR:OG1	2.28	0.51
1:B:336:GLY:HA3	1:B:338:PRO:HG3	1.92	0.51
1:A:160:PHE:CE1	1:A:165:LEU:HD21	2.46	0.51
1:B:20:ALA:O	1:B:22:THR:N	2.44	0.51
1:B:46:LEU:CD1	1:B:210:PHE:CD1	2.94	0.51
1:B:435:ASP:N	1:B:435:ASP:OD2	2.43	0.51
1:A:65:ALA:HB2	1:A:78:TRP:CZ2	2.46	0.51
1:B:22:THR:HA	1:B:499:ARG:HH22	1.76	0.51
1:B:317:TYR:HE1	1:B:330:ALA:HB1	1.76	0.51
1:A:398:ASP:OD2	1:A:398:ASP:N	2.42	0.51
1:A:99:ILE:C	1:A:101:ILE:N	2.64	0.51
1:B:272:MET:O	1:B:273:GLN:C	2.47	0.51
1:B:338:PRO:O	1:B:339:VAL:C	2.48	0.51
1:A:243:VAL:HG12	1:A:244:ALA:N	2.23	0.51
1:B:209:ALA:HB2	1:B:371:LEU:CD1	2.41	0.51
1:B:270:GLY:O	1:B:273:GLN:HB3	2.11	0.51
1:B:464:TYR:CD2	1:B:464:TYR:C	2.84	0.51
1:B:495:HIS:HD2	1:B:497:ARG:HG3	1.70	0.51
1:A:233:ASP:OD2	1:A:234:TYR:N	2.44	0.51
1:A:373:LEU:HB2	1:A:449:LEU:CD1	2.41	0.51
1:A:54:PHE:CD1	1:A:214:TYR:CD1	2.99	0.51
1:A:110:VAL:HG22	1:A:301:VAL:CG1	2.40	0.51
1:A:229:ASN:O	1:A:229:ASN:CG	2.49	0.51
1:A:26:VAL:HG13	1:A:245:ALA:HA	1.93	0.50
1:A:325:LEU:CB	1:A:326:PRO:HD3	2.40	0.50
1:A:67:VAL:HG11	1:A:401:ARG:N	2.25	0.50
1:B:240:LEU:HA	1:B:243:VAL:HG12	1.93	0.50
1:A:286:ILE:O	1:A:288:TRP:N	2.36	0.50
1:A:66:THR:O	1:A:67:VAL:CB	2.59	0.50
1:B:94:PHE:CD2	1:B:380:CYS:CB	2.93	0.50
1:B:42:LEU:O	1:B:46:LEU:HD13	2.11	0.50
1:A:304:GLU:O	1:A:307:SER:N	2.44	0.50
1:A:67:VAL:HG21	1:A:400:LYS:CB	2.41	0.50
1:A:25:MET:CB	1:A:495:HIS:CE1	2.94	0.50
1:A:361:GLY:H	1:A:365:MET:CE	2.23	0.50
1:A:453:PHE:CD2	1:A:453:PHE:C	2.84	0.50
1:A:66:THR:O	1:A:401:ARG:HA	2.12	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:CYS:O	1:B:383:PHE:HB2	2.11	0.50
1:B:377:ILE:HD11	1:B:456:VAL:HG21	1.93	0.50
1:B:96:TYR:O	1:B:99:ILE:HB	2.11	0.50
1:B:99:ILE:C	1:B:101:ILE:N	2.65	0.50
1:B:40:PHE:CD1	1:B:40:PHE:O	2.64	0.50
1:B:48:LEU:HD12	1:B:207:PHE:CE2	2.47	0.50
1:B:281:HIS:O	1:B:283:ALA:N	2.44	0.50
1:B:292:VAL:O	1:B:295:ALA:HB3	2.11	0.50
1:B:365:MET:CA	1:B:437:ILE:HD11	2.41	0.49
1:A:114:LEU:CD2	1:A:298:LEU:HD13	2.42	0.49
1:A:128:ILE:HD12	1:A:128:ILE:H	1.75	0.49
1:A:208:VAL:HG12	1:A:209:ALA:N	2.27	0.49
1:B:464:TYR:HD2	1:B:464:TYR:C	2.16	0.49
1:A:128:ILE:N	1:A:128:ILE:CD1	2.75	0.49
1:A:19:PHE:HE1	1:A:241:LEU:CA	2.23	0.49
1:A:361:GLY:HA3	1:A:441:SER:CA	2.42	0.49
1:A:417:ILE:HG21	1:B:425:MET:HE3	1.94	0.49
1:B:464:TYR:CD2	1:B:464:TYR:O	2.55	0.49
1:B:51:ILE:O	1:B:56:PRO:HD3	2.12	0.49
1:A:103:PHE:HE2	1:A:308:TRP:HB2	1.76	0.49
1:A:30:TYR:CE2	1:A:301:VAL:CG2	2.95	0.49
1:A:393:VAL:HG11	1:A:413:LEU:HD13	1.94	0.49
1:A:202:GLY:HA3	1:A:434:PRO:HG3	1.94	0.49
1:B:20:ALA:O	1:B:21:ILE:C	2.51	0.49
1:B:240:LEU:HD23	1:B:243:VAL:HG12	1.94	0.49
1:A:29:VAL:O	1:A:30:TYR:C	2.51	0.49
1:B:163:GLY:O	1:B:164:ILE:CG1	2.60	0.49
1:B:321:GLN:OE1	1:B:321:GLN:HA	2.13	0.49
1:B:324:LEU:HD13	1:B:467:HIS:HE1	1.78	0.49
1:A:496:PRO:C	1:A:498:ALA:N	2.66	0.49
1:A:286:ILE:HA	1:A:288:TRP:HD1	1.78	0.49
1:B:306:ALA:HA	1:B:309:ILE:CG1	2.40	0.49
1:A:218:GLU:HG3	1:A:218:GLU:H	1.31	0.49
1:A:411:VAL:O	1:A:412:LYS:C	2.51	0.49
1:B:244:ALA:O	1:B:245:ALA:C	2.51	0.49
1:A:317:TYR:O	1:A:319:THR:N	2.45	0.49
1:A:343:ILE:HG22	1:A:344:SER:N	2.28	0.49
1:A:124:ASN:HD21	1:A:269:ALA:N	2.10	0.48
1:A:322:LYS:O	1:A:324:LEU:N	2.45	0.48
1:A:76:PHE:O	1:A:80:SER:HB2	2.13	0.48
1:B:92:ILE:CG2	1:B:316:MET:HG3	2.43	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:ILE:C	1:B:288:TRP:H	2.17	0.48
1:B:275:PHE:O	1:B:276:THR:C	2.51	0.48
1:B:48:LEU:HD12	1:B:207:PHE:CZ	2.48	0.48
1:A:48:LEU:HD12	1:A:207:PHE:CE2	2.48	0.48
1:A:364:ASN:HB2	1:A:440:ASP:OD2	2.13	0.48
1:B:104:ILE:N	1:B:105:PRO:HD2	2.28	0.48
1:B:44:PHE:CA	1:B:193:THR:HG22	2.42	0.48
1:B:66:THR:CG2	1:B:224:VAL:HG11	2.43	0.48
1:B:275:PHE:HB3	1:B:290:VAL:HG22	1.94	0.48
1:A:500:SER:O	1:A:501:PRO:C	2.51	0.48
1:B:316:MET:O	1:B:316:MET:HG2	2.13	0.48
1:A:385:LEU:HD23	1:A:385:LEU:C	2.33	0.48
1:A:432:LEU:HD23	1:A:432:LEU:N	2.28	0.48
1:A:53:TRP:O	1:A:56:PRO:HD2	2.14	0.48
1:B:13:LEU:HB2	1:B:226:GLU:O	2.13	0.48
1:B:42:LEU:CD1	1:B:250:SER:HB2	2.43	0.48
1:A:141:LEU:HA	1:A:144:THR:HG22	1.94	0.48
1:A:204:LEU:HB3	1:A:429:VAL:HG11	1.96	0.48
1:B:31:GLU:O	1:B:34:THR:N	2.47	0.48
1:B:46:LEU:CD1	1:B:210:PHE:CE1	2.97	0.48
1:B:99:ILE:C	1:B:101:ILE:H	2.16	0.48
1:A:101:ILE:HG22	1:A:374:THR:HG1	1.78	0.48
1:B:258:MET:O	1:B:259:VAL:CG1	2.58	0.48
1:B:171:LEU:HB2	1:B:275:PHE:CZ	2.49	0.48
1:A:415:VAL:HG12	1:A:416:ALA:N	2.28	0.48
1:B:167:PRO:CB	1:B:297:LEU:HD21	2.44	0.48
1:B:53:TRP:O	1:B:56:PRO:HD2	2.14	0.48
1:A:162:ALA:O	1:A:167:PRO:HD3	2.14	0.47
1:B:262:GLY:C	1:B:264:GLU:H	2.16	0.47
1:B:149:THR:CG2	1:B:314:ARG:HH22	2.26	0.47
1:B:326:PRO:HB2	1:B:329:PHE:CE2	2.48	0.47
1:A:33:PRO:HB2	1:A:267:LEU:HA	1.96	0.47
1:A:385:LEU:HD23	1:A:386:PHE:N	2.29	0.47
1:A:53:TRP:CZ2	1:A:57:VAL:HG21	2.50	0.47
1:B:208:VAL:HG11	1:B:371:LEU:HB3	1.96	0.47
1:B:389:TYR:CD2	1:B:389:TYR:C	2.88	0.47
1:A:193:THR:HG22	1:A:193:THR:O	2.15	0.47
1:B:204:LEU:O	1:B:205:VAL:C	2.52	0.47
1:B:29:VAL:C	1:B:31:GLU:N	2.67	0.47
1:B:368:LEU:HD23	1:B:437:ILE:HG21	1.96	0.47
1:B:113:ALA:HB2	1:B:272:MET:HE1	1.95	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:TYR:CD1	1:A:106:MET:HG2	2.50	0.47
1:A:297:LEU:HD22	1:A:297:LEU:HA	1.80	0.47
1:A:42:LEU:HD12	1:A:43:VAL:N	2.30	0.47
1:B:27:MET:HG2	1:B:164:ILE:HG23	1.95	0.47
1:B:315:GLY:O	1:B:318:VAL:HG23	2.14	0.47
1:A:117:ILE:HG22	1:A:118:LEU:N	2.30	0.47
1:A:14:THR:O	1:A:17:GLY:N	2.48	0.47
1:A:314:ARG:HH22	1:A:336:GLY:HA3	1.79	0.47
1:A:101:ILE:HG21	1:A:373:LEU:HD23	1.96	0.47
1:B:142:ALA:CB	1:B:346:LEU:HD11	2.45	0.47
1:B:212:LEU:HA	1:B:215:MET:SD	2.54	0.47
1:A:293:ILE:HA	1:A:296:LEU:CD1	2.43	0.47
1:B:284:PRO:C	1:B:286:ILE:N	2.62	0.47
1:B:67:VAL:HB	1:B:401:ARG:HA	1.96	0.47
1:A:123:LEU:O	1:A:130:LYS:HG3	2.14	0.47
1:A:397:PRO:HD2	1:A:398:ASP:OD2	2.14	0.47
1:B:157:LYS:NZ	1:B:491:HIS:N	2.62	0.47
1:B:47:LEU:HD12	1:B:193:THR:CG2	2.44	0.47
1:B:208:VAL:HG13	1:B:375:VAL:CG2	2.40	0.47
1:B:219:ALA:CB	1:B:220:SER:HB2	2.34	0.47
1:B:274:THR:O	1:B:278:LEU:CB	2.62	0.47
1:B:114:LEU:HD23	1:B:298:LEU:HD22	1.95	0.47
1:B:317:TYR:CZ	1:B:330:ALA:HB1	2.50	0.47
1:B:48:LEU:HD22	1:B:52:LEU:HD12	1.96	0.47
1:B:500:SER:H	1:B:501:PRO:CD	2.24	0.47
1:A:389:TYR:CD2	1:A:416:ALA:HB2	2.49	0.47
1:A:431:PHE:HD1	1:A:446:VAL:HG12	1.79	0.47
1:A:496:PRO:O	1:A:498:ALA:N	2.48	0.47
1:B:129:THR:O	1:B:130:LYS:C	2.52	0.47
1:B:101:ILE:HD13	1:B:373:LEU:HD13	1.97	0.47
1:A:99:ILE:C	1:A:101:ILE:H	2.17	0.47
1:B:111:LEU:HD12	1:B:130:LYS:HG3	1.97	0.46
1:B:357:THR:HG22	1:B:358:ASN:ND2	2.31	0.46
1:B:398:ASP:CA	1:B:399:LEU:CB	2.92	0.46
1:B:47:LEU:HD12	1:B:193:THR:HG23	1.97	0.46
1:A:127:PRO:HA	1:A:128:ILE:C	2.36	0.46
1:A:433:PRO:HG3	1:A:445:TYR:HD2	1.79	0.46
1:A:373:LEU:CD1	1:A:452:SER:HB3	2.44	0.46
1:A:94:PHE:HE1	1:A:460:PRO:HG2	1.69	0.46
1:A:88:GLY:O	1:A:91:ALA:HB3	2.15	0.46
1:B:275:PHE:O	1:B:278:LEU:N	2.48	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:HIS:O	1:A:494:LEU:CD2	2.57	0.46
1:A:491:HIS:CE1	1:A:492:PHE:CE2	3.04	0.46
1:A:259:VAL:HG21	1:A:278:LEU:CD1	2.45	0.46
1:A:92:ILE:HD12	1:A:316:MET:HG3	1.97	0.46
1:B:175:ALA:O	1:B:178:TYR:N	2.48	0.46
1:B:337:VAL:N	1:B:338:PRO:CD	2.78	0.46
1:B:67:VAL:HG21	1:B:401:ARG:H	1.80	0.46
1:A:283:ALA:HB1	1:A:287:GLU:HG2	1.97	0.46
1:A:94:PHE:CD2	1:A:380:CYS:HB3	2.49	0.46
1:B:118:LEU:O	1:B:119:LYS:C	2.53	0.46
1:B:138:LEU:HD11	1:B:346:LEU:HD22	1.97	0.46
1:B:378:TYR:CE1	1:B:382:TYR:HE2	2.34	0.46
1:B:462:ILE:O	1:B:466:VAL:HG13	2.16	0.46
1:A:207:PHE:CE1	1:A:211:ILE:HG13	2.51	0.46
1:A:210:PHE:O	1:A:213:SER:HB3	2.16	0.46
1:A:46:LEU:CD1	1:A:210:PHE:CD1	2.97	0.46
1:B:224:VAL:HG23	1:B:227:MET:SD	2.55	0.46
1:A:109:PHE:HZ	1:A:297:LEU:CD1	2.28	0.46
1:A:233:ASP:O	1:A:236:LEU:HB2	2.16	0.46
1:B:261:PRO:C	1:B:264:GLU:OE1	2.54	0.46
1:A:172:ILE:HG12	1:A:251:VAL:CG1	2.46	0.46
1:B:120:TRP:CE3	1:B:123:LEU:HG	2.51	0.46
1:B:162:ALA:O	1:B:166:LEU:HB3	2.16	0.46
1:B:22:THR:HG22	1:B:220:SER:OG	2.15	0.46
1:B:325:LEU:HB2	1:B:326:PRO:HD3	1.97	0.46
1:B:442:THR:HG21	1:B:444:MET:HE3	1.98	0.46
1:B:103:PHE:HA	1:B:106:MET:HE2	1.97	0.46
1:B:224:VAL:HG13	1:B:225:ASN:OD1	2.16	0.46
1:A:114:LEU:HD23	1:A:114:LEU:HA	1.73	0.45
1:A:48:LEU:HD22	1:A:52:LEU:HD12	1.96	0.45
1:B:365:MET:HA	1:B:437:ILE:HD12	1.98	0.45
1:B:64:MET:HE2	1:B:78:TRP:HB3	1.98	0.45
1:A:204:LEU:HD23	1:A:204:LEU:HA	1.67	0.45
1:A:46:LEU:CD1	1:A:210:PHE:HD1	2.27	0.45
1:A:240:LEU:O	1:A:241:LEU:C	2.55	0.45
1:A:94:PHE:C	1:A:96:TYR:H	2.20	0.45
1:B:46:LEU:HD12	1:B:210:PHE:HD1	1.80	0.45
1:A:342:VAL:HG12	1:A:343:ILE:N	2.32	0.45
1:A:459:LEU:O	1:A:462:ILE:HG12	2.16	0.45
1:B:123:LEU:HA	1:B:123:LEU:HD23	1.56	0.45
1:B:204:LEU:C	1:B:206:VAL:N	2.69	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:VAL:HG12	1:B:248:LEU:HG	1.99	0.45
1:B:283:ALA:HA	1:B:285:GLU:H	1.81	0.45
1:A:491:HIS:O	1:A:494:LEU:N	2.44	0.45
1:B:172:ILE:HG12	1:B:251:VAL:CG1	2.46	0.45
1:B:428:ILE:HG13	1:B:428:ILE:H	1.62	0.45
1:B:63:GLU:HA	1:B:403:PHE:HD2	1.81	0.45
1:B:27:MET:SD	1:B:248:LEU:HD11	2.57	0.45
1:B:29:VAL:C	1:B:31:GLU:H	2.20	0.45
1:A:118:LEU:O	1:A:118:LEU:CD2	2.64	0.45
1:A:128:ILE:H	1:A:128:ILE:CD1	2.29	0.45
1:A:164:ILE:HG22	1:A:165:LEU:N	2.32	0.45
1:B:142:ALA:HA	1:B:309:ILE:HG21	1.98	0.45
1:B:178:TYR:C	1:B:178:TYR:CD2	2.91	0.45
1:B:337:VAL:HG12	1:B:341:LEU:HD12	1.97	0.45
1:A:124:ASN:ND2	1:A:266:ASN:ND2	2.65	0.45
1:A:20:ALA:O	1:A:22:THR:N	2.50	0.45
1:A:345:GLN:O	1:A:345:GLN:HG3	2.15	0.45
1:B:279:MET:CE	1:B:289:THR:HG21	2.47	0.45
1:B:371:LEU:O	1:B:372:ALA:C	2.55	0.45
1:B:85:PRO:CD	1:B:86:ARG:H	2.30	0.45
1:A:275:PHE:O	1:A:276:THR:C	2.55	0.45
1:A:44:PHE:HA	1:A:193:THR:HG21	1.98	0.45
1:B:267:LEU:HB3	1:B:367:PHE:CD2	2.52	0.45
1:A:119:LYS:CA	1:A:119:LYS:HE3	2.44	0.44
1:B:101:ILE:C	1:B:103:PHE:N	2.69	0.44
1:B:442:THR:CG2	1:B:444:MET:HG3	2.47	0.44
1:B:46:LEU:HD22	1:B:250:SER:HB3	1.99	0.44
1:A:26:VAL:HG13	1:A:245:ALA:CA	2.47	0.44
1:A:157:LYS:CE	1:A:491:HIS:N	2.72	0.44
1:B:202:GLY:HA3	1:B:434:PRO:CB	2.47	0.44
1:B:216:GLY:HA3	1:B:497:ARG:HG2	1.99	0.44
1:B:67:VAL:CG2	1:B:401:ARG:H	2.31	0.44
1:A:229:ASN:N	1:A:230:PRO:CD	2.81	0.44
1:A:63:GLU:HA	1:A:403:PHE:HD2	1.82	0.44
1:B:114:LEU:CD2	1:B:298:LEU:HD22	2.46	0.44
1:B:346:LEU:O	1:B:349:THR:HG22	2.18	0.44
1:B:98:GLN:HG3	1:B:378:TYR:CG	2.52	0.44
1:B:377:ILE:CG1	1:B:456:VAL:HG11	2.47	0.44
1:B:66:THR:OG1	1:B:66:THR:O	2.33	0.44
1:A:377:ILE:HD11	1:A:456:VAL:HG11	2.00	0.44
1:A:431:PHE:CD1	1:A:449:LEU:HD23	2.52	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:LEU:O	1:B:144:THR:HG22	2.17	0.44
1:B:30:TYR:CD1	1:B:106:MET:HG2	2.51	0.44
1:A:15:LEU:HD12	1:A:15:LEU:O	2.17	0.44
1:A:193:THR:O	1:A:194:PHE:C	2.56	0.44
1:A:365:MET:CB	1:A:437:ILE:HD11	2.48	0.44
1:A:369:ILE:CG2	1:A:370:ALA:N	2.80	0.44
1:A:454:LEU:HA	1:A:454:LEU:HD12	1.69	0.44
1:B:311:GLY:O	1:B:312:PRO:C	2.55	0.44
1:B:314:ARG:N	1:B:337:VAL:HG11	2.33	0.44
1:B:57:VAL:HG12	1:B:58:GLY:N	2.33	0.44
1:A:101:ILE:HG21	1:A:373:LEU:CD2	2.48	0.44
1:A:333:ASN:CG	1:A:334:LYS:N	2.70	0.44
1:A:364:ASN:HD22	1:A:438:GLN:CB	2.25	0.44
1:B:433:PRO:HB3	1:B:445:TYR:CE2	2.52	0.44
1:A:407:GLY:HA3	1:A:411:VAL:HB	1.99	0.44
1:A:42:LEU:O	1:A:46:LEU:HD13	2.18	0.44
1:B:47:LEU:CD1	1:B:193:THR:HG23	2.48	0.44
1:A:141:LEU:HA	1:A:141:LEU:HD23	1.74	0.44
1:A:40:PHE:CD2	1:A:194:PHE:CB	2.97	0.44
1:A:342:VAL:O	1:A:346:LEU:HG	2.18	0.44
1:A:364:ASN:ND2	1:A:438:GLN:HB2	2.24	0.44
1:B:254:LEU:HA	1:B:257:ALA:CB	2.33	0.44
1:B:346:LEU:HA	1:B:346:LEU:HD23	1.79	0.44
1:A:285:GLU:O	1:A:288:TRP:HB3	2.18	0.44
1:A:101:ILE:CD1	1:A:373:LEU:HD21	2.29	0.44
1:A:198:PHE:O	1:B:395:LYS:HE2	2.18	0.43
1:A:314:ARG:NH2	1:A:337:VAL:HA	2.23	0.43
1:A:64:MET:HE1	1:A:78:TRP:CB	2.46	0.43
1:B:149:THR:HG21	1:B:314:ARG:NH2	2.33	0.43
1:B:92:ILE:HG21	1:B:319:THR:CG2	2.48	0.43
1:A:198:PHE:CD2	1:A:198:PHE:N	2.83	0.43
1:B:141:LEU:HA	1:B:144:THR:HG22	1.99	0.43
1:A:327:ALA:C	1:A:329:PHE:N	2.68	0.43
1:B:111:LEU:HD12	1:B:130:LYS:CG	2.49	0.43
1:B:222:THR:O	1:B:224:VAL:HG12	2.18	0.43
1:A:166:LEU:O	1:A:170:ILE:HD13	2.17	0.43
1:A:227:MET:HE1	1:A:234:TYR:HB2	2.00	0.43
1:A:347:VAL:O	1:A:351:ILE:HG12	2.18	0.43
1:A:495:HIS:CG	1:A:496:PRO:HD2	2.54	0.43
1:B:62:ALA:HB2	1:B:234:TYR:OH	2.18	0.43
1:B:420:LEU:HA	1:B:420:LEU:HD12	1.75	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:LEU:C	1:A:15:LEU:HD12	2.39	0.43
1:A:230:PRO:O	1:A:231:GLY:O	2.37	0.43
1:B:94:PHE:CE2	1:B:380:CYS:HB3	2.53	0.43
1:B:392:LEU:C	1:B:392:LEU:HD12	2.39	0.43
1:B:65:ALA:HB2	1:B:78:TRP:CZ2	2.54	0.43
1:A:13:LEU:HB3	1:A:227:MET:HA	2.00	0.43
1:A:246:ILE:O	1:A:250:SER:OG	2.24	0.43
1:A:376:VAL:HB	1:A:427:PHE:CE1	2.54	0.43
1:A:464:TYR:C	1:A:464:TYR:CD2	2.92	0.43
1:A:394:LEU:CD1	1:B:204:LEU:HD12	2.28	0.43
1:B:222:THR:C	1:B:224:VAL:N	2.61	0.43
1:B:365:MET:O	1:B:367:PHE:N	2.52	0.43
1:B:46:LEU:CD2	1:B:250:SER:HB3	2.48	0.43
1:A:124:ASN:OD1	1:A:268:SER:HB2	2.18	0.43
1:A:260:ILE:HG22	1:A:265:ILE:HG12	1.99	0.43
1:A:339:VAL:O	1:A:340:THR:C	2.56	0.43
1:B:64:MET:SD	1:B:389:TYR:HB2	2.59	0.43
1:A:50:GLY:HA2	1:A:54:PHE:HB3	2.00	0.43
1:B:29:VAL:O	1:B:32:TYR:N	2.51	0.43
1:B:413:LEU:HD12	1:B:413:LEU:HA	1.89	0.43
1:B:442:THR:O	1:B:443:ASP:C	2.56	0.43
1:B:44:PHE:CB	1:B:193:THR:HG22	2.48	0.43
1:A:125:GLU:O	1:A:127:PRO:CD	2.67	0.43
1:B:333:ASN:O	1:B:333:ASN:ND2	2.52	0.43
1:A:107:LEU:HD12	1:A:107:LEU:HA	1.66	0.42
1:A:109:PHE:HZ	1:A:297:LEU:HD13	1.84	0.42
1:A:356:LEU:CD2	1:A:370:ALA:HB2	2.49	0.42
1:A:435:ASP:N	1:A:435:ASP:OD1	2.50	0.42
1:A:445:TYR:O	1:A:448:LEU:N	2.52	0.42
1:A:94:PHE:O	1:A:98:GLN:HB3	2.18	0.42
1:B:217:VAL:C	1:B:219:ALA:H	2.22	0.42
1:B:336:GLY:O	1:B:337:VAL:HB	2.19	0.42
1:B:369:ILE:CD1	1:B:448:LEU:HD22	2.49	0.42
1:B:500:SER:N	1:B:501:PRO:CD	2.82	0.42
1:A:224:VAL:HG22	1:A:227:MET:SD	2.59	0.42
1:A:376:VAL:HG23	1:A:453:PHE:CD1	2.54	0.42
1:A:386:PHE:CZ	1:A:419:GLY:HA3	2.54	0.42
1:B:101:ILE:C	1:B:103:PHE:H	2.21	0.42
1:B:436:ASN:OD1	1:B:436:ASN:O	2.37	0.42
1:A:389:TYR:CE2	1:A:416:ALA:HB2	2.54	0.42
1:A:500:SER:N	1:A:501:PRO:HD2	2.34	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:GLU:O	1:B:126:ASP:C	2.58	0.42
1:B:326:PRO:HB2	1:B:329:PHE:CZ	2.53	0.42
1:B:329:PHE:O	1:B:329:PHE:CG	2.71	0.42
1:B:24:SER:OG	1:B:495:HIS:HA	2.19	0.42
1:A:240:LEU:O	1:A:242:MET:N	2.53	0.42
1:A:309:ILE:O	1:A:342:VAL:HG22	2.19	0.42
1:B:164:ILE:N	1:B:167:PRO:HD2	2.35	0.42
1:B:362:GLY:C	1:B:364:ASN:H	2.22	0.42
1:A:128:ILE:O	1:A:132:ILE:HG22	2.20	0.42
1:A:164:ILE:C	1:A:167:PRO:HD2	2.40	0.42
1:A:229:ASN:N	1:A:230:PRO:HD3	2.35	0.42
1:A:280:SER:O	1:A:281:HIS:HB2	2.20	0.42
1:A:32:TYR:OH	1:A:249:SER:HA	2.20	0.42
1:A:365:MET:CA	1:A:437:ILE:HD11	2.45	0.42
1:A:68:ASP:CB	1:A:69:GLY:HA2	2.48	0.42
1:A:98:GLN:O	1:A:98:GLN:HG2	2.20	0.42
1:B:283:ALA:CB	1:B:284:PRO:HA	2.32	0.42
1:B:311:GLY:O	1:B:313:SER:N	2.53	0.42
1:B:464:TYR:CE2	1:B:468:ASP:C	2.93	0.42
1:A:207:PHE:O	1:A:208:VAL:C	2.58	0.42
1:A:372:ALA:O	1:A:375:VAL:HB	2.19	0.42
1:A:54:PHE:CG	1:A:214:TYR:CD1	3.08	0.42
1:B:75:VAL:HA	1:B:78:TRP:CE3	2.54	0.42
1:A:161:PHE:CE2	1:A:493:PHE:CE1	3.06	0.42
1:B:229:ASN:O	1:B:230:PRO:C	2.59	0.42
1:A:413:LEU:O	1:A:414:VAL:C	2.58	0.42
1:B:92:ILE:HG23	1:B:316:MET:SD	2.60	0.42
1:B:110:VAL:CG1	1:B:137:ILE:HD13	2.42	0.41
1:B:242:MET:O	1:B:246:ILE:HG13	2.20	0.41
1:B:51:ILE:HD13	1:B:242:MET:SD	2.60	0.41
1:B:244:ALA:C	1:B:246:ILE:N	2.73	0.41
1:B:323:ASN:O	1:B:324:LEU:C	2.58	0.41
1:B:54:PHE:CE2	1:B:242:MET:HB2	2.55	0.41
1:A:64:MET:HB3	1:A:64:MET:HE2	1.88	0.41
1:B:240:LEU:HD23	1:B:243:VAL:CG1	2.50	0.41
1:B:22:THR:C	1:B:24:SER:N	2.66	0.41
1:B:260:ILE:HB	1:B:261:PRO:HD3	2.02	0.41
1:B:29:VAL:O	1:B:30:TYR:C	2.58	0.41
1:B:447:GLU:O	1:B:451:VAL:HG23	2.20	0.41
1:A:230:PRO:O	1:A:231:GLY:C	2.58	0.41
1:A:436:ASN:HD22	1:A:436:ASN:C	2.17	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:PRO:HB3	1:B:262:GLY:HA2	2.02	0.41
1:B:48:LEU:CD2	1:B:52:LEU:HD12	2.51	0.41
1:A:244:ALA:C	1:A:246:ILE:N	2.74	0.41
1:A:279:MET:HG3	1:A:283:ALA:HB2	2.02	0.41
1:A:456:VAL:O	1:A:459:LEU:N	2.46	0.41
1:A:68:ASP:HB2	1:A:69:GLY:CA	2.50	0.41
1:B:330:ALA:O	1:B:331:LYS:HB2	2.19	0.41
1:B:434:PRO:O	1:B:443:ASP:OD2	2.37	0.41
1:A:419:GLY:O	1:A:420:LEU:C	2.59	0.41
1:A:52:LEU:O	1:A:56:PRO:HG2	2.21	0.41
1:B:295:ALA:O	1:B:298:LEU:HB3	2.21	0.41
1:B:376:VAL:CG2	1:B:453:PHE:HD1	2.32	0.41
1:A:317:TYR:C	1:A:319:THR:N	2.72	0.41
1:B:318:VAL:O	1:B:322:LYS:HB2	2.20	0.41
1:A:272:MET:O	1:A:276:THR:HG23	2.20	0.41
1:A:67:VAL:CG1	1:A:401:ARG:H	2.30	0.41
1:A:52:LEU:HB3	1:A:422:THR:CG2	2.44	0.41
1:A:68:ASP:CB	1:A:69:GLY:CA	2.98	0.41
1:B:54:PHE:CD1	1:B:214:TYR:HD1	2.38	0.41
1:B:25:MET:HB3	1:B:495:HIS:CE1	2.56	0.41
1:B:106:MET:HE3	1:B:305:ILE:HG12	2.01	0.41
1:A:154:ARG:HA	1:A:157:LYS:HB2	2.03	0.41
1:A:255:SER:O	1:A:256:ILE:C	2.58	0.41
1:B:299:LEU:HD23	1:B:299:LEU:HA	1.78	0.41
1:B:348:ILE:HG22	1:B:349:THR:N	2.36	0.41
1:B:387:ILE:O	1:B:390:ILE:HG12	2.21	0.41
1:A:102:GLY:HA2	1:A:374:THR:OG1	2.20	0.41
1:A:44:PHE:HA	1:A:47:LEU:HD12	2.02	0.41
1:A:495:HIS:CD2	1:A:497:ARG:H	2.39	0.41
1:A:62:ALA:O	1:A:64:MET:N	2.54	0.41
1:B:345:GLN:HG3	1:B:345:GLN:O	2.20	0.41
1:B:351:ILE:HG22	1:B:355:ILE:CD1	2.51	0.41
1:B:459:LEU:CB	1:B:460:PRO:HD3	2.51	0.41
1:A:273:GLN:O	1:A:277:VAL:HG22	2.21	0.41
1:B:166:LEU:O	1:B:167:PRO:C	2.56	0.41
1:B:384:MET:O	1:B:385:LEU:C	2.60	0.41
1:B:94:PHE:C	1:B:96:TYR:N	2.74	0.41
1:A:131:THR:HG22	1:A:357:THR:CG2	2.50	0.40
1:A:171:LEU:HD13	1:A:275:PHE:CE1	2.56	0.40
1:A:282:VAL:O	1:A:282:VAL:HG12	2.21	0.40
1:A:317:TYR:O	1:A:320:ALA:N	2.54	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:GLY:HA3	1:A:337:VAL:CB	2.23	0.40
1:B:230:PRO:HB2	1:B:231:GLY:H	1.72	0.40
1:B:254:LEU:CA	1:B:257:ALA:HB3	2.36	0.40
1:B:347:VAL:O	1:B:351:ILE:HG12	2.21	0.40
1:B:459:LEU:HA	1:B:459:LEU:HD13	1.61	0.40
1:B:88:GLY:O	1:B:91:ALA:HB3	2.20	0.40
1:A:96:TYR:O	1:A:99:ILE:HB	2.20	0.40
1:B:167:PRO:HB2	1:B:297:LEU:HD21	2.02	0.40
1:B:93:SER:HB3	1:B:460:PRO:HG3	2.02	0.40
1:B:49:GLY:O	1:B:53:TRP:HB3	2.22	0.40
1:A:99:ILE:HG22	1:A:100:ALA:N	2.36	0.40
1:A:288:TRP:C	1:A:290:VAL:N	2.74	0.40
1:A:30:TYR:CZ	1:A:301:VAL:CG2	3.05	0.40
1:A:491:HIS:CE1	1:A:492:PHE:HE2	2.39	0.40
1:B:19:PHE:CG	1:B:19:PHE:O	2.75	0.40
1:B:339:VAL:O	1:B:340:THR:O	2.40	0.40
1:B:361:GLY:O	1:B:440:ASP:HB3	2.21	0.40
1:A:167:PRO:CB	1:A:297:LEU:HD21	2.52	0.40
1:A:33:PRO:HG3	1:A:267:LEU:O	2.22	0.40
1:A:55:ILE:HB	1:A:56:PRO:HD3	2.03	0.40
1:B:107:LEU:HB3	1:B:134:ALA:HB1	2.03	0.40
1:B:259:VAL:O	1:B:260:ILE:HG12	2.22	0.40
1:B:70:TRP:N	1:B:70:TRP:CD2	2.75	0.40
1:A:401:ARG:HB3	1:A:403:PHE:O	2.22	0.40
1:B:415:VAL:HG12	1:B:416:ALA:N	2.35	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	443/511 (87%)	307 (69%)	82 (18%)	54 (12%)	<b>0</b> <b>1</b>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	443/511 (87%)	304 (69%)	84 (19%)	55 (12%)	0	1
All	All	886/1022 (87%)	611 (69%)	166 (19%)	109 (12%)	0	1

All (109) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	VAL
1	A	100	ALA
1	A	118	LEU
1	A	152	THR
1	A	223	HIS
1	A	241	LEU
1	A	269	ALA
1	A	280	SER
1	A	281	HIS
1	A	287	GLU
1	A	323	ASN
1	A	328	ALA
1	A	339	VAL
1	A	406	PRO
1	A	407	GLY
1	A	442	THR
1	A	492	PHE
1	A	499	ARG
1	A	500	SER
1	B	23	ALA
1	B	67	VAL
1	B	223	HIS
1	B	230	PRO
1	B	233	ASP
1	B	241	LEU
1	B	259	VAL
1	B	261	PRO
1	B	263	ASN
1	B	275	PHE
1	B	280	SER
1	B	286	ILE
1	B	336	GLY
1	B	337	VAL
1	B	339	VAL
1	B	340	THR
1	B	399	LEU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	401	ARG
1	B	441	SER
1	B	492	PHE
1	B	499	ARG
1	B	500	SER
1	A	21	ILE
1	A	102	GLY
1	A	164	ILE
1	A	226	GLU
1	A	231	GLY
1	A	233	ASP
1	A	244	ALA
1	A	245	ALA
1	A	270	GLY
1	A	282	VAL
1	A	332	MET
1	A	336	GLY
1	A	409	LYS
1	A	441	SER
1	A	445	TYR
1	B	30	TYR
1	B	68	ASP
1	B	100	ALA
1	B	119	LYS
1	B	149	THR
1	B	164	ILE
1	B	205	VAL
1	B	208	VAL
1	B	240	LEU
1	B	245	ALA
1	B	257	ALA
1	B	338	PRO
1	B	367	PHE
1	A	30	TYR
1	A	119	LYS
1	A	194	PHE
1	B	218	GLU
1	B	260	ILE
1	B	326	PRO
1	A	24	SER
1	A	169	PHE
1	A	262	GLY

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	329	PHE
1	A	399	LEU
1	A	425	MET
1	A	497	ARG
1	B	21	ILE
1	B	195	PHE
1	B	199	SER
1	B	244	ALA
1	B	276	THR
1	B	285	GLU
1	B	409	LYS
1	A	168	ALA
1	A	240	LEU
1	A	337	VAL
1	A	401	ARG
1	B	32	TYR
1	B	85	PRO
1	B	118	LEU
1	B	287	GLU
1	B	322	LYS
1	B	361	GLY
1	A	208	VAL
1	A	58	GLY
1	A	408	GLY
1	B	282	VAL
1	A	271	VAL
1	B	33	PRO
1	A	95	GLY
1	A	361	GLY
1	B	95	GLY
1	B	246	ILE

### 5.3.2 Protein sidechains [i](#)

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

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	365/414 (88%)	274 (75%)	91 (25%)	0	2
1	B	368/414 (89%)	287 (78%)	81 (22%)	1	4
All	All	733/828 (88%)	561 (76%)	172 (24%)	1	3

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	21	ILE
1	A	22	THR
1	A	30	TYR
1	A	34	THR
1	A	43	VAL
1	A	47	LEU
1	A	48	LEU
1	A	66	THR
1	A	70	TRP
1	A	83	LEU
1	A	92	ILE
1	A	98	GLN
1	A	103	PHE
1	A	107	LEU
1	A	115	SER
1	A	119	LYS
1	A	125	GLU
1	A	131	THR
1	A	132	ILE
1	A	135	LEU
1	A	143	LEU
1	A	144	THR
1	A	149	THR
1	A	151	TYR
1	A	152	THR
1	A	164	ILE
1	A	197	ASP
1	A	198	PHE
1	A	208	VAL
1	A	211	ILE
1	A	217	VAL

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	218	GLU
1	A	220	SER
1	A	225	ASN
1	A	227	MET
1	A	233	ASP
1	A	236	LEU
1	A	239	LEU
1	A	240	LEU
1	A	241	LEU
1	A	247	CYS
1	A	248	LEU
1	A	258	MET
1	A	264	GLU
1	A	267	LEU
1	A	268	SER
1	A	272	MET
1	A	274	THR
1	A	278	LEU
1	A	279	MET
1	A	281	HIS
1	A	288	TRP
1	A	289	THR
1	A	297	LEU
1	A	298	LEU
1	A	310	VAL
1	A	321	GLN
1	A	329	PHE
1	A	332	MET
1	A	340	THR
1	A	343	ILE
1	A	345	GLN
1	A	349	THR
1	A	353	LEU
1	A	359	THR
1	A	364	ASN
1	A	366	SER
1	A	369	ILE
1	A	371	LEU
1	A	373	LEU
1	A	374	THR
1	A	377	ILE
1	A	378	TYR

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	390	ILE
1	A	392	LEU
1	A	400	LYS
1	A	404	ASN
1	A	424	ILE
1	A	425	MET
1	A	428	ILE
1	A	435	ASP
1	A	436	ASN
1	A	437	ILE
1	A	446	VAL
1	A	447	GLU
1	A	448	LEU
1	A	453	PHE
1	A	454	LEU
1	A	457	LEU
1	A	459	LEU
1	B	13	LEU
1	B	29	VAL
1	B	31	GLU
1	B	34	THR
1	B	40	PHE
1	B	57	VAL
1	B	67	VAL
1	B	70	TRP
1	B	92	ILE
1	B	98	GLN
1	B	101	ILE
1	B	103	PHE
1	B	104	ILE
1	B	107	LEU
1	B	115	SER
1	B	123	LEU
1	B	125	GLU
1	B	131	THR
1	B	132	ILE
1	B	135	LEU
1	B	136	ILE
1	B	149	THR
1	B	151	TYR
1	B	154	ARG
1	B	158	VAL

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	164	ILE
1	B	177	ILE
1	B	178	TYR
1	B	193	THR
1	B	194	PHE
1	B	206	VAL
1	B	211	ILE
1	B	217	VAL
1	B	218	GLU
1	B	222	THR
1	B	229	ASN
1	B	233	ASP
1	B	234	TYR
1	B	239	LEU
1	B	240	LEU
1	B	241	LEU
1	B	248	LEU
1	B	251	VAL
1	B	258	MET
1	B	260	ILE
1	B	267	LEU
1	B	268	SER
1	B	272	MET
1	B	277	VAL
1	B	282	VAL
1	B	288	TRP
1	B	299	LEU
1	B	321	GLN
1	B	323	ASN
1	B	324	LEU
1	B	329	PHE
1	B	331	LYS
1	B	343	ILE
1	B	345	GLN
1	B	348	ILE
1	B	366	SER
1	B	371	LEU
1	B	378	TYR
1	B	384	MET
1	B	390	ILE
1	B	391	VAL
1	B	392	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	400	LYS
1	B	413	LEU
1	B	425	MET
1	B	428	ILE
1	B	435	ASP
1	B	437	ILE
1	B	441	SER
1	B	447	GLU
1	B	452	SER
1	B	453	PHE
1	B	456	VAL
1	B	459	LEU
1	B	464	TYR
1	B	493	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	495	HIS
1	B	12	GLN
1	B	145	GLN
1	B	358	ASN
1	B	364	ASN
1	B	467	HIS
1	B	495	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	451/511 (88%)	-0.15	12 (2%) 54 31	89, 136, 198, 249	0
1	B	453/511 (88%)	-0.14	13 (2%) 51 28	86, 137, 212, 265	0
All	All	904/1022 (88%)	-0.15	25 (2%) 53 30	86, 137, 205, 265	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	226	GLU	4.8
1	B	147	GLY	4.6
1	B	68	ASP	4.1
1	B	213	SER	3.7
1	B	408	GLY	3.7
1	B	146	PHE	3.4
1	A	323	ASN	3.2
1	B	16	LEU	3.0
1	A	193	THR	2.9
1	A	16	LEU	2.8
1	B	28	ALA	2.8
1	B	215	MET	2.7
1	A	282	VAL	2.6
1	B	228	SER	2.5
1	A	82	THR	2.4
1	B	229	ASN	2.4
1	A	281	HIS	2.4
1	B	216	GLY	2.3
1	B	102	GLY	2.3
1	A	123	LEU	2.3
1	A	199	SER	2.2
1	A	331	LYS	2.2
1	A	64	MET	2.1
1	A	81	ASN	2.0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	201	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.