Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2023 – 10:05 AM EDT

PDB ID	:	4K1N
Title	:	Crystal structure of full-length mouse alphaE-catenin
Authors	:	Ishiyama, N.; Ikura, M.
Deposited on	:	2013-04-05
Resolution	:	6.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The 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:

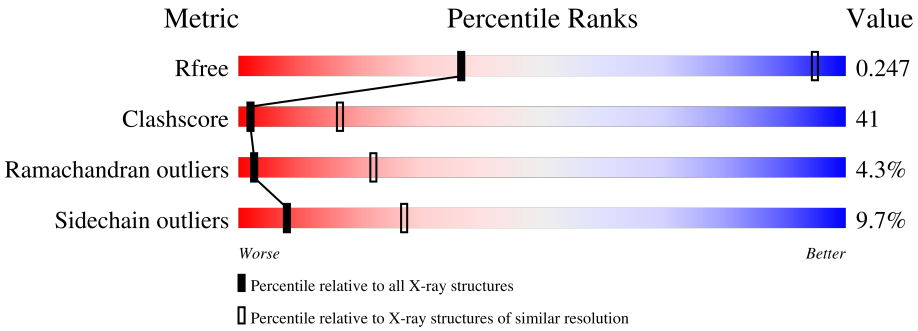
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 6.50 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	1000 (9.00-3.90)
Clashscore	141614	1064 (9.00-3.90)
Ramachandran outliers	138981	1012 (9.00-3.88)
Sidechain outliers	138945	1010 (9.00-3.84)

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

Mol	Chain	Length	Quality of chain
1	A	912	25% 28% • • 43%
1	B	912	25% 28% • • 43%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8020 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 Catenin alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	520	Total	C	N	O	S	0	0	0
			4010	2486	713	789	22			
1	B	520	Total	C	N	O	S	0	0	0
			4010	2486	713	789	22			

There are 12 discrepancies between the modelled and reference sequences:

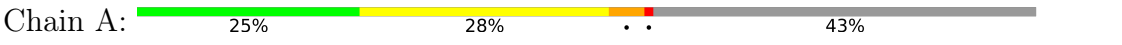
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP P26231
A	-4	SER	-	expression tag	UNP P26231
A	-3	HIS	-	expression tag	UNP P26231
A	-2	MET	-	expression tag	UNP P26231
A	-1	ALA	-	expression tag	UNP P26231
A	0	SER	-	expression tag	UNP P26231
B	-5	GLY	-	expression tag	UNP P26231
B	-4	SER	-	expression tag	UNP P26231
B	-3	HIS	-	expression tag	UNP P26231
B	-2	MET	-	expression tag	UNP P26231
B	-1	ALA	-	expression tag	UNP P26231
B	0	SER	-	expression tag	UNP P26231

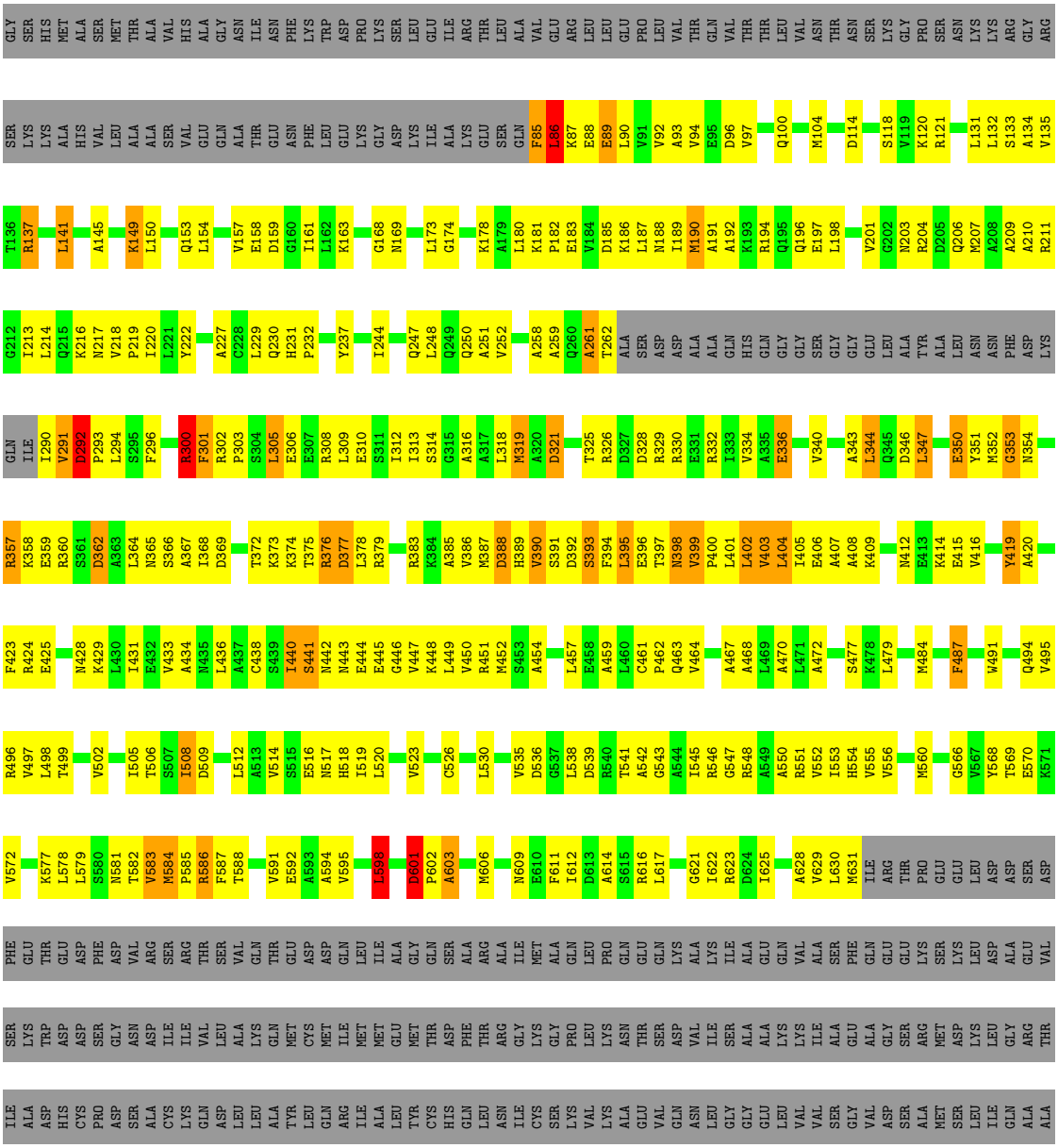
3 Residue-property plots (i)

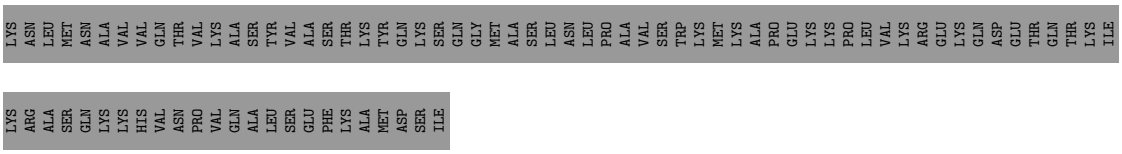
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: Catenin alpha-1

Chain A:

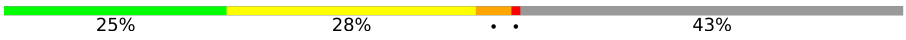


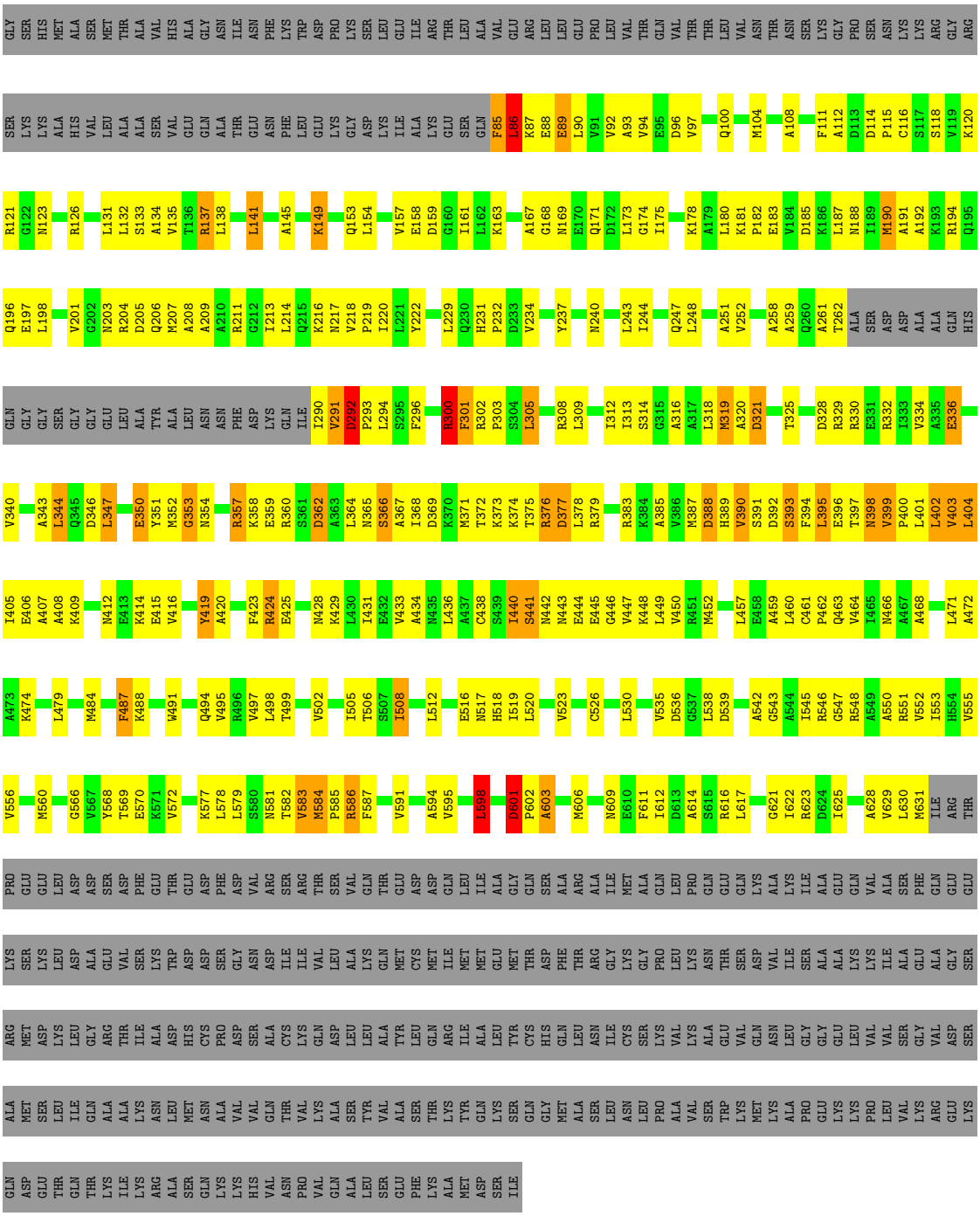




• Molecule 1: Catenin alpha-1

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	144.68Å 144.68Å 136.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 6.50 47.36 – 6.40	Depositor EDS
% Data completeness (in resolution range)	94.6 (50.00-6.50) 94.2 (47.36-6.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	4.84 (at 6.67Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.247 0.224 , 0.247	Depositor DCC
R_{free} test set	716 reflections (10.90%)	wwPDB-VP
Wilson B-factor (Å^2)	439.2	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 357.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.032 for -h,-k,l 0.051 for h,-h-k,-l 0.023 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	8020	wwPDB-VP
Average B, all atoms (Å^2)	354.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.22	0/4048	0.46	0/5464
1	B	0.22	0/4048	0.46	0/5464
All	All	0.22	0/8096	0.46	0/10928

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4010	0	4051	336	0
1	B	4010	0	4051	346	0
All	All	8020	0	8102	666	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 41.

All (666) 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:369:ASP:O	1:A:373:LYS:HB3	1.65	0.97
1:A:149:LYS:HG2	1:A:190:MET:HE1	1.47	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:MET:HG2	1:A:131:LEU:HD22	1.48	0.96
1:B:86:LEU:HD22	1:B:87:LYS:H	1.31	0.95
1:B:104:MET:HG2	1:B:131:LEU:HD22	1.48	0.93
1:A:451:ARG:HH12	1:B:308:ARG:HG3	1.35	0.92
1:B:149:LYS:HG2	1:B:190:MET:HE1	1.49	0.91
1:B:208:ALA:HB3	1:B:448:LYS:NZ	1.84	0.91
1:A:86:LEU:HD22	1:A:87:LYS:H	1.34	0.90
1:A:519:ILE:HG12	1:A:548:ARG:HD2	1.55	0.86
1:B:519:ILE:HG12	1:B:548:ARG:HD2	1.57	0.85
1:A:399:VAL:HG12	1:A:400:PRO:HD3	1.59	0.85
1:A:291:VAL:HG22	1:A:292:ASP:H	1.41	0.85
1:B:243:LEU:HD12	1:B:466:ASN:HD21	1.40	0.84
1:B:174:GLY:O	1:B:178:LYS:HG3	1.78	0.83
1:A:395:LEU:HD22	1:A:547:GLY:HA2	1.61	0.83
1:B:399:VAL:HG12	1:B:400:PRO:HD3	1.59	0.83
1:A:347:LEU:HB2	1:A:372:THR:OG1	1.80	0.81
1:B:347:LEU:HB2	1:B:372:THR:OG1	1.80	0.81
1:B:369:ASP:O	1:B:373:LYS:HB3	1.80	0.81
1:B:231:HIS:NE2	1:B:479:LEU:HD13	1.96	0.81
1:A:444:GLU:O	1:A:447:VAL:HG12	1.80	0.81
1:B:291:VAL:HG22	1:B:292:ASP:H	1.43	0.81
1:A:174:GLY:O	1:A:178:LYS:HG3	1.81	0.80
1:A:502:VAL:O	1:A:505:ILE:HG22	1.81	0.80
1:B:329:ARG:NH2	1:B:389:HIS:HB2	1.97	0.80
1:B:468:ALA:HA	1:B:484:MET:HE1	1.62	0.80
1:B:502:VAL:O	1:B:505:ILE:HG22	1.81	0.80
1:B:444:GLU:O	1:B:447:VAL:HG12	1.83	0.78
1:A:154:LEU:HD12	1:A:187:LEU:HD21	1.65	0.78
1:A:468:ALA:HA	1:A:484:MET:HE1	1.63	0.78
1:B:154:LEU:HD12	1:B:187:LEU:HD21	1.65	0.78
1:A:354:ASN:HA	1:A:358:LYS:HD2	1.66	0.78
1:A:601:ASP:HB3	1:A:602:PRO:HD2	1.65	0.78
1:B:302:ARG:HE	1:B:309:LEU:HD11	1.48	0.77
1:A:290:ILE:HG13	1:B:308:ARG:NH2	1.99	0.77
1:A:550:ALA:O	1:A:553:ILE:HG13	1.85	0.77
1:A:201:VAL:HA	1:A:204:ARG:HD3	1.68	0.76
1:B:601:ASP:HB3	1:B:602:PRO:HD2	1.65	0.76
1:A:329:ARG:NH2	1:A:389:HIS:HB2	2.00	0.76
1:B:542:ALA:HA	1:B:545:ILE:HD12	1.68	0.76
1:B:354:ASN:HA	1:B:358:LYS:HD2	1.68	0.75
1:B:550:ALA:O	1:B:553:ILE:HG13	1.87	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:GLU:C	1:B:141:LEU:HD11	2.07	0.74
1:A:89:GLU:C	1:A:141:LEU:HD11	2.08	0.74
1:B:208:ALA:HB3	1:B:448:LYS:HZ3	1.53	0.74
1:A:161:ILE:HD13	1:A:180:LEU:HD21	1.70	0.73
1:B:168:GLY:O	1:B:229:LEU:HD22	1.88	0.73
1:A:614:ALA:HA	1:A:617:LEU:HD12	1.69	0.73
1:A:302:ARG:HE	1:A:309:LEU:HD11	1.53	0.73
1:A:542:ALA:HA	1:A:545:ILE:HD12	1.71	0.72
1:B:161:ILE:HD13	1:B:180:LEU:HD21	1.72	0.72
1:B:614:ALA:HA	1:B:617:LEU:HD12	1.71	0.72
1:B:391:SER:HB3	1:B:548:ARG:HG3	1.71	0.72
1:A:347:LEU:HD22	1:A:372:THR:HG23	1.72	0.72
1:B:234:VAL:HG22	1:B:474:LYS:HZ1	1.55	0.71
1:A:89:GLU:HB3	1:A:141:LEU:HG	1.72	0.71
1:A:291:VAL:HB	1:A:442:ASN:HA	1.72	0.71
1:B:86:LEU:CD2	1:B:87:LYS:H	2.05	0.69
1:B:291:VAL:HB	1:B:442:ASN:HA	1.72	0.69
1:B:351:TYR:HB2	1:B:368:ILE:HG12	1.74	0.69
1:A:508:ILE:HD13	1:A:555:VAL:HG12	1.75	0.69
1:B:519:ILE:HD11	1:B:548:ARG:HB3	1.75	0.69
1:A:218:VAL:HB	1:A:219:PRO:HD3	1.75	0.69
1:B:395:LEU:HD22	1:B:547:GLY:HA2	1.74	0.69
1:B:89:GLU:HB3	1:B:141:LEU:HG	1.74	0.69
1:B:198:LEU:HD22	1:B:261:ALA:HB3	1.75	0.69
1:A:395:LEU:HD13	1:A:547:GLY:O	1.92	0.68
1:A:451:ARG:HH12	1:B:308:ARG:CG	2.07	0.68
1:B:508:ILE:HD13	1:B:555:VAL:HG12	1.74	0.68
1:A:86:LEU:CD2	1:A:87:LYS:H	2.07	0.68
1:A:440:ILE:O	1:A:441:SER:HB2	1.94	0.68
1:B:329:ARG:NH1	1:B:389:HIS:N	2.42	0.68
1:B:218:VAL:HB	1:B:219:PRO:HD3	1.74	0.67
1:B:546:ARG:HA	1:B:584:MET:HE2	1.77	0.67
1:A:220:ILE:HG22	1:A:244:ILE:HD13	1.76	0.67
1:B:292:ASP:CG	1:B:293:PRO:HD3	2.15	0.67
1:A:292:ASP:CG	1:A:293:PRO:HD3	2.15	0.67
1:B:194:ARG:O	1:B:198:LEU:HG	1.93	0.67
1:A:291:VAL:HG22	1:A:293:PRO:HD2	1.76	0.67
1:B:201:VAL:HA	1:B:204:ARG:HD3	1.77	0.66
1:B:347:LEU:HD22	1:B:372:THR:HG23	1.77	0.66
1:A:412:ASN:OD1	1:A:414:LYS:HG3	1.96	0.66
1:A:85:PHE:N	1:A:88:GLU:HG3	2.11	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:TYR:HB2	1:A:368:ILE:HG12	1.77	0.66
1:A:391:SER:HB3	1:A:548:ARG:HG3	1.77	0.66
1:B:205:ASP:HA	1:B:448:LYS:NZ	2.10	0.66
1:B:340:VAL:HG21	1:B:378:LEU:CB	2.26	0.66
1:B:628:ALA:O	1:B:631:MET:HE3	1.96	0.66
1:A:350:GLU:C	1:A:368:ILE:HD11	2.16	0.65
1:B:114:ASP:HB3	1:B:120:LYS:HD2	1.78	0.65
1:B:93:ALA:HB2	1:B:141:LEU:HD12	1.77	0.65
1:A:194:ARG:O	1:A:198:LEU:HG	1.96	0.65
1:A:390:VAL:HA	1:A:394:PHE:CD2	2.31	0.65
1:A:379:ARG:O	1:A:383:ARG:HG3	1.96	0.65
1:B:440:ILE:O	1:B:441:SER:HB2	1.94	0.65
1:B:291:VAL:HG22	1:B:293:PRO:HD2	1.77	0.65
1:B:86:LEU:HD12	1:B:86:LEU:H	1.60	0.65
1:B:205:ASP:HA	1:B:448:LYS:HZ2	1.62	0.65
1:B:343:ALA:HB1	1:B:375:THR:HG21	1.79	0.65
1:A:168:GLY:O	1:A:229:LEU:HD22	1.97	0.64
1:B:566:GLY:O	1:B:570:GLU:HG2	1.98	0.64
1:A:340:VAL:HG21	1:A:378:LEU:CB	2.28	0.64
1:B:350:GLU:C	1:B:368:ILE:HD11	2.17	0.64
1:B:302:ARG:CZ	1:B:305:LEU:HD11	2.27	0.64
1:B:412:ASN:OD1	1:B:414:LYS:HG3	1.98	0.64
1:A:93:ALA:HB2	1:A:141:LEU:HD12	1.80	0.64
1:A:93:ALA:HB2	1:A:137:ARG:NH1	2.13	0.64
1:A:198:LEU:HD22	1:A:261:ALA:HB3	1.79	0.63
1:B:93:ALA:HB2	1:B:137:ARG:NH1	2.13	0.63
1:B:351:TYR:N	1:B:368:ILE:HD11	2.13	0.63
1:A:90:LEU:N	1:A:141:LEU:HD11	2.13	0.63
1:B:220:ILE:HG22	1:B:244:ILE:HD13	1.78	0.63
1:A:86:LEU:HD12	1:A:86:LEU:H	1.62	0.63
1:A:290:ILE:HG13	1:B:308:ARG:HH21	1.63	0.63
1:A:625:ILE:O	1:A:629:VAL:HG23	1.99	0.63
1:B:291:VAL:HG11	1:B:294:LEU:HB3	1.81	0.63
1:A:97:VAL:HA	1:A:134:ALA:HB1	1.79	0.63
1:A:114:ASP:HB3	1:A:120:LYS:HD2	1.80	0.63
1:A:227:ALA:HB2	1:A:479:LEU:HD21	1.80	0.63
1:A:463:GLN:HB3	1:A:487:PHE:CZ	2.33	0.63
1:A:90:LEU:O	1:A:94:VAL:HG23	1.99	0.63
1:A:198:LEU:HA	1:A:262:THR:HG22	1.81	0.63
1:A:519:ILE:HD11	1:A:548:ARG:HB3	1.79	0.63
1:B:463:GLN:HB3	1:B:487:PHE:CZ	2.34	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:TYR:N	1:A:368:ILE:HD11	2.14	0.62
1:A:457:LEU:HD13	1:A:494:GLN:HB3	1.81	0.62
1:B:625:ILE:O	1:B:629:VAL:HG23	1.98	0.62
1:A:247:GLN:HE22	1:A:463:GLN:NE2	1.96	0.62
1:A:601:ASP:CB	1:A:602:PRO:HD2	2.29	0.62
1:B:97:VAL:HA	1:B:134:ALA:HB1	1.81	0.62
1:B:362:ASP:O	1:B:366:SER:HB2	1.99	0.62
1:B:587:PHE:O	1:B:591:VAL:HG23	1.99	0.62
1:A:291:VAL:HG11	1:A:294:LEU:HB3	1.82	0.62
1:A:329:ARG:NH1	1:A:389:HIS:N	2.48	0.62
1:B:90:LEU:N	1:B:141:LEU:HD11	2.14	0.62
1:B:440:ILE:O	1:B:440:ILE:HD13	1.99	0.62
1:A:214:LEU:O	1:A:218:VAL:HG23	2.00	0.62
1:B:395:LEU:HD13	1:B:547:GLY:O	2.00	0.62
1:A:362:ASP:O	1:A:366:SER:HB2	2.00	0.61
1:A:209:ALA:HB1	1:A:452:MET:CE	2.30	0.61
1:B:302:ARG:HH21	1:B:309:LEU:HG	1.64	0.61
1:A:375:THR:C	1:A:377:ASP:H	2.03	0.61
1:B:214:LEU:O	1:B:218:VAL:HG23	2.01	0.61
1:A:343:ALA:HB1	1:A:375:THR:HG21	1.82	0.61
1:B:379:ARG:O	1:B:383:ARG:HG3	2.01	0.61
1:B:546:ARG:HA	1:B:584:MET:CE	2.30	0.61
1:A:408:ALA:HB1	1:A:472:ALA:N	2.16	0.61
1:B:366:SER:HA	1:B:369:ASP:HB3	1.81	0.60
1:A:344:LEU:HD23	1:A:347:LEU:HD23	1.82	0.60
1:B:198:LEU:HA	1:B:262:THR:HG22	1.83	0.60
1:A:159:ASP:HB3	1:A:163:LYS:HE3	1.84	0.60
1:A:302:ARG:CZ	1:A:305:LEU:HD11	2.32	0.60
1:B:601:ASP:CB	1:B:602:PRO:HD2	2.30	0.60
1:B:208:ALA:HB3	1:B:448:LYS:HZ1	1.64	0.60
1:B:390:VAL:HA	1:B:394:PHE:CD2	2.35	0.60
1:A:302:ARG:HH21	1:A:309:LEU:HG	1.66	0.60
1:A:347:LEU:HD22	1:A:372:THR:CG2	2.32	0.60
1:A:512:LEU:CD1	1:A:629:VAL:HG21	2.32	0.60
1:B:526:CYS:SG	1:B:538:LEU:HD12	2.42	0.60
1:A:366:SER:HA	1:A:369:ASP:HB3	1.82	0.60
1:A:519:ILE:O	1:A:523:VAL:HG23	2.02	0.60
1:A:209:ALA:HB1	1:A:452:MET:HE2	1.84	0.59
1:A:498:LEU:O	1:A:502:VAL:HG23	2.02	0.59
1:B:207:MET:HG2	1:B:258:ALA:CB	2.32	0.59
1:B:302:ARG:HE	1:B:309:LEU:CD1	2.15	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:THR:C	1:B:377:ASP:H	2.03	0.59
1:B:207:MET:O	1:B:211:ARG:HG3	2.03	0.59
1:A:405:ILE:HG22	1:A:409:LYS:HE3	1.84	0.58
1:A:314:SER:O	1:A:318:LEU:HD13	2.03	0.58
1:A:325:THR:HB	1:A:329:ARG:HE	1.67	0.58
1:A:207:MET:HG2	1:A:258:ALA:HB3	1.86	0.58
1:B:344:LEU:HD23	1:B:347:LEU:HD23	1.84	0.58
1:A:207:MET:HG2	1:A:258:ALA:CB	2.33	0.58
1:B:89:GLU:HB3	1:B:141:LEU:CG	2.33	0.58
1:A:159:ASP:O	1:A:163:LYS:HG3	2.03	0.58
1:B:291:VAL:HG13	1:B:292:ASP:N	2.18	0.58
1:A:153:GLN:HG3	1:A:187:LEU:HB2	1.85	0.58
1:B:329:ARG:HH22	1:B:389:HIS:HB2	1.67	0.58
1:B:325:THR:HB	1:B:329:ARG:HE	1.69	0.58
1:B:498:LEU:O	1:B:502:VAL:HG23	2.04	0.57
1:B:530:LEU:HD22	1:B:611:PHE:CG	2.38	0.57
1:B:408:ALA:HB1	1:B:472:ALA:N	2.19	0.57
1:B:601:ASP:HB3	1:B:602:PRO:CD	2.34	0.57
1:A:566:GLY:O	1:A:570:GLU:HG2	2.04	0.57
1:B:512:LEU:CD1	1:B:629:VAL:HG21	2.34	0.57
1:A:89:GLU:HB3	1:A:141:LEU:CG	2.35	0.57
1:A:412:ASN:HD21	1:A:414:LYS:HE3	1.69	0.57
1:A:587:PHE:O	1:A:591:VAL:HG23	2.04	0.57
1:B:207:MET:HG2	1:B:258:ALA:HB3	1.87	0.57
1:A:207:MET:O	1:A:211:ARG:HG3	2.05	0.57
1:A:601:ASP:HB3	1:A:602:PRO:CD	2.34	0.56
1:B:159:ASP:HB3	1:B:163:LYS:HE3	1.87	0.56
1:B:412:ASN:HD21	1:B:414:LYS:HE3	1.70	0.56
1:A:499:THR:HG23	1:A:551:ARG:NH2	2.19	0.56
1:B:468:ALA:CA	1:B:484:MET:HE1	2.34	0.56
1:B:159:ASP:O	1:B:163:LYS:HG3	2.05	0.56
1:A:121:ARG:NH2	1:B:145:ALA:HB1	2.20	0.56
1:A:397:THR:O	1:A:400:PRO:HD2	2.06	0.56
1:B:457:LEU:HD13	1:B:494:GLN:HB3	1.87	0.56
1:A:457:LEU:HD23	1:A:498:LEU:HD22	1.87	0.56
1:B:391:SER:CB	1:B:548:ARG:HG3	2.36	0.56
1:A:491:TRP:O	1:A:495:VAL:HG23	2.06	0.56
1:A:173:LEU:HG	1:A:222:TYR:CE1	2.41	0.56
1:A:291:VAL:HG22	1:A:292:ASP:N	2.16	0.56
1:A:291:VAL:HG13	1:A:292:ASP:N	2.20	0.56
1:A:375:THR:HA	1:A:377:ASP:OD1	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:LEU:O	1:B:94:VAL:HG23	2.06	0.56
1:B:499:THR:HG23	1:B:551:ARG:NH2	2.20	0.56
1:B:519:ILE:O	1:B:523:VAL:HG23	2.06	0.56
1:A:416:VAL:HG21	1:A:472:ALA:HB2	1.87	0.55
1:B:325:THR:CG2	1:B:329:ARG:HE	2.20	0.55
1:B:329:ARG:HH11	1:B:388:ASP:HB2	1.70	0.55
1:B:191:ALA:HB1	1:B:211:ARG:HD2	1.87	0.55
1:B:302:ARG:NE	1:B:309:LEU:HD11	2.18	0.55
1:A:440:ILE:O	1:A:440:ILE:HD13	2.07	0.55
1:A:526:CYS:SG	1:A:538:LEU:HD12	2.46	0.55
1:A:552:VAL:O	1:A:556:VAL:HG23	2.06	0.55
1:B:291:VAL:HG22	1:B:292:ASP:N	2.18	0.55
1:B:347:LEU:HD22	1:B:372:THR:CG2	2.35	0.55
1:B:387:MET:O	1:B:390:VAL:HG23	2.07	0.55
1:B:416:VAL:HG21	1:B:472:ALA:HB2	1.88	0.55
1:B:583:VAL:HG13	1:B:617:LEU:CB	2.36	0.55
1:A:329:ARG:HH22	1:A:389:HIS:HB2	1.72	0.55
1:B:397:THR:O	1:B:400:PRO:HD2	2.06	0.55
1:B:153:GLN:HG3	1:B:187:LEU:HB2	1.88	0.55
1:B:543:GLY:HA2	1:B:546:ARG:NH1	2.22	0.55
1:A:181:LYS:N	1:A:182:PRO:HD2	2.22	0.55
1:A:302:ARG:NE	1:A:309:LEU:HD11	2.22	0.55
1:A:390:VAL:HA	1:A:394:PHE:CE2	2.42	0.55
1:B:403:VAL:HG21	1:B:419:TYR:OH	2.06	0.55
1:B:491:TRP:O	1:B:495:VAL:HG23	2.06	0.55
1:B:85:PHE:N	1:B:88:GLU:HG3	2.22	0.55
1:A:191:ALA:HB1	1:A:211:ARG:HD2	1.88	0.54
1:A:551:ARG:O	1:A:555:VAL:HG23	2.07	0.54
1:B:328:ASP:O	1:B:332:ARG:HG3	2.06	0.54
1:A:325:THR:CG2	1:A:329:ARG:HE	2.20	0.54
1:A:517:ASN:O	1:A:520:LEU:HB3	2.07	0.54
1:B:131:LEU:O	1:B:135:VAL:HG23	2.07	0.54
1:B:181:LYS:N	1:B:182:PRO:HD2	2.22	0.54
1:A:131:LEU:O	1:A:135:VAL:HG23	2.08	0.54
1:B:203:ASN:HA	1:B:206:GLN:NE2	2.23	0.54
1:A:530:LEU:HD22	1:A:611:PHE:CG	2.42	0.54
1:A:203:ASN:HA	1:A:206:GLN:NE2	2.23	0.54
1:A:302:ARG:HE	1:A:309:LEU:CD1	2.20	0.54
1:A:329:ARG:HH11	1:A:388:ASP:HB2	1.73	0.54
1:A:388:ASP:OD2	1:A:388:ASP:N	2.41	0.54
1:B:461:CYS:N	1:B:462:PRO:HD2	2.22	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:CYS:N	1:A:462:PRO:HD2	2.22	0.54
1:A:389:HIS:ND1	1:A:394:PHE:HE1	2.06	0.54
1:B:319:MET:SD	1:B:319:MET:N	2.81	0.54
1:A:194:ARG:HD2	1:A:197:GLU:OE1	2.08	0.54
1:A:319:MET:SD	1:A:319:MET:N	2.81	0.54
1:A:404:LEU:C	1:A:404:LEU:HD13	2.29	0.54
1:A:457:LEU:HD23	1:A:498:LEU:CD2	2.38	0.53
1:B:194:ARG:HD2	1:B:197:GLU:OE1	2.08	0.53
1:B:389:HIS:ND1	1:B:394:PHE:HE1	2.06	0.53
1:A:300:ARG:O	1:A:301:PHE:HB2	2.08	0.53
1:B:388:ASP:OD2	1:B:388:ASP:N	2.40	0.53
1:B:214:LEU:HA	1:B:248:LEU:HD12	1.91	0.53
1:A:94:VAL:HG13	1:B:108:ALA:HB1	1.89	0.53
1:B:209:ALA:HA	1:B:452:MET:SD	2.49	0.53
1:B:375:THR:HA	1:B:377:ASP:OD1	2.09	0.53
1:A:387:MET:O	1:A:390:VAL:HG23	2.09	0.53
1:A:368:ILE:HD12	1:A:368:ILE:N	2.24	0.53
1:B:234:VAL:HG13	1:B:474:LYS:HZ1	1.74	0.53
1:A:390:VAL:HA	1:A:394:PHE:CG	2.43	0.53
1:A:398:ASN:O	1:A:402:LEU:HD22	2.08	0.52
1:A:546:ARG:HA	1:A:584:MET:HE2	1.91	0.52
1:B:173:LEU:HG	1:B:222:TYR:CE1	2.44	0.52
1:B:243:LEU:HD13	1:B:462:PRO:HB2	1.90	0.52
1:B:314:SER:O	1:B:318:LEU:HD13	2.09	0.52
1:B:357:ARG:NH1	1:B:358:LYS:HE3	2.23	0.52
1:B:373:LYS:HA	1:B:376:ARG:NE	2.24	0.52
1:A:375:THR:C	1:A:377:ASP:N	2.62	0.52
1:B:390:VAL:HA	1:B:394:PHE:CG	2.45	0.52
1:B:457:LEU:HD13	1:B:494:GLN:HG3	1.91	0.52
1:A:87:LYS:NZ	1:B:116:CYS:HA	2.25	0.52
1:A:96:ASP:O	1:A:100:GLN:HG2	2.09	0.52
1:A:350:GLU:HB3	1:A:368:ILE:CD1	2.39	0.52
1:A:387:MET:HE2	1:A:506:THR:HB	1.91	0.52
1:A:357:ARG:NH1	1:A:358:LYS:HE3	2.25	0.52
1:A:395:LEU:HD22	1:A:547:GLY:CA	2.38	0.52
1:B:158:GLU:HG2	1:B:252:VAL:HG11	1.91	0.52
1:B:375:THR:C	1:B:377:ASP:N	2.63	0.52
1:A:628:ALA:O	1:A:631:MET:HG3	2.10	0.52
1:B:350:GLU:HB3	1:B:368:ILE:CD1	2.40	0.52
1:A:214:LEU:HA	1:A:248:LEU:HD12	1.91	0.51
1:A:395:LEU:C	1:A:397:THR:H	2.13	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ASN:HB2	1:B:248:LEU:HD13	1.92	0.51
1:A:546:ARG:HA	1:A:584:MET:CE	2.40	0.51
1:B:457:LEU:HD21	1:B:495:VAL:HA	1.93	0.51
1:A:583:VAL:HG13	1:A:617:LEU:CB	2.41	0.51
1:B:88:GLU:O	1:B:92:VAL:HG23	2.11	0.51
1:B:398:ASN:O	1:B:402:LEU:HD22	2.11	0.51
1:A:375:THR:O	1:A:377:ASP:N	2.43	0.51
1:B:300:ARG:O	1:B:301:PHE:HB2	2.11	0.51
1:B:517:ASN:O	1:B:520:LEU:HB3	2.11	0.51
1:A:543:GLY:HA2	1:A:546:ARG:NH1	2.26	0.51
1:B:518:HIS:HB3	1:B:548:ARG:CZ	2.40	0.51
1:A:451:ARG:NH1	1:B:308:ARG:HG3	2.16	0.51
1:A:512:LEU:HD21	1:A:556:VAL:CG2	2.41	0.51
1:B:343:ALA:CB	1:B:375:THR:HG21	2.41	0.51
1:A:433:VAL:HA	1:A:436:LEU:HD12	1.92	0.50
1:B:86:LEU:HD22	1:B:87:LYS:N	2.14	0.50
1:A:468:ALA:CA	1:A:484:MET:HE1	2.38	0.50
1:A:594:ALA:HA	1:A:606:MET:SD	2.52	0.50
1:B:389:HIS:HE2	1:B:429:LYS:HE2	1.75	0.50
1:B:390:VAL:HA	1:B:394:PHE:CE2	2.45	0.50
1:B:395:LEU:C	1:B:397:THR:H	2.14	0.50
1:B:463:GLN:HB3	1:B:487:PHE:CE1	2.47	0.50
1:B:404:LEU:HD13	1:B:404:LEU:C	2.32	0.50
1:A:343:ALA:CB	1:A:375:THR:HG21	2.40	0.50
1:A:425:GLU:O	1:A:428:ASN:OD1	2.29	0.50
1:A:530:LEU:HD22	1:A:611:PHE:CD1	2.46	0.50
1:B:350:GLU:HB3	1:B:368:ILE:HD11	1.94	0.50
1:A:463:GLN:HB3	1:A:487:PHE:CE1	2.46	0.50
1:B:194:ARG:NH2	1:B:259:ALA:O	2.44	0.50
1:A:457:LEU:HD21	1:A:495:VAL:HA	1.93	0.50
1:A:291:VAL:HB	1:A:442:ASN:CA	2.39	0.50
1:A:374:LYS:O	1:A:377:ASP:OD1	2.29	0.50
1:A:328:ASP:O	1:A:332:ARG:HG3	2.11	0.50
1:A:518:HIS:HB3	1:A:548:ARG:CZ	2.42	0.50
1:B:90:LEU:HA	1:B:141:LEU:CD1	2.42	0.50
1:B:394:PHE:HD2	1:B:551:ARG:HH21	1.59	0.50
1:B:171:GLN:O	1:B:175:ILE:HG13	2.12	0.49
1:B:400:PRO:HB2	1:B:423:PHE:HA	1.94	0.49
1:B:512:LEU:HD21	1:B:556:VAL:CG2	2.41	0.49
1:A:153:GLN:NE2	1:A:183:GLU:HA	2.28	0.49
1:B:291:VAL:HB	1:B:442:ASN:CA	2.39	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:ILE:N	1:B:368:ILE:HD12	2.27	0.49
1:B:375:THR:O	1:B:377:ASP:N	2.45	0.49
1:B:628:ALA:O	1:B:631:MET:HG3	2.12	0.49
1:A:213:ILE:HG23	1:A:217:ASN:ND2	2.27	0.49
1:A:346:ASP:O	1:A:350:GLU:HB2	2.11	0.49
1:A:443:ASN:OD1	1:A:446:GLY:N	2.39	0.49
1:B:247:GLN:OE1	1:B:459:ALA:HB1	2.11	0.49
1:A:389:HIS:HE2	1:A:429:LYS:HE2	1.77	0.49
1:A:400:PRO:HB2	1:A:423:PHE:HA	1.94	0.49
1:B:346:ASP:O	1:B:350:GLU:HB2	2.12	0.49
1:A:290:ILE:N	1:B:308:ARG:CZ	2.75	0.49
1:B:329:ARG:HH12	1:B:389:HIS:H	1.60	0.49
1:B:457:LEU:HD23	1:B:498:LEU:HD22	1.94	0.49
1:A:90:LEU:HA	1:A:141:LEU:CD1	2.42	0.49
1:A:350:GLU:HB3	1:A:368:ILE:HD11	1.94	0.49
1:A:628:ALA:O	1:A:631:MET:HE3	2.12	0.49
1:A:217:ASN:HB2	1:A:248:LEU:HD13	1.94	0.49
1:A:395:LEU:CD1	1:A:550:ALA:HB3	2.43	0.49
1:B:560:MET:SD	1:B:572:VAL:HG11	2.52	0.49
1:B:457:LEU:CD2	1:B:495:VAL:HA	2.43	0.49
1:A:291:VAL:HG22	1:A:293:PRO:CD	2.43	0.49
1:A:387:MET:CE	1:A:506:THR:HB	2.42	0.49
1:A:403:VAL:HG21	1:A:419:TYR:OH	2.13	0.49
1:A:90:LEU:HA	1:A:141:LEU:HD11	1.95	0.48
1:B:234:VAL:HG13	1:B:474:LYS:NZ	2.27	0.48
1:B:457:LEU:HD23	1:B:498:LEU:CD2	2.43	0.48
1:B:505:ILE:HG23	1:B:506:THR:HG23	1.94	0.48
1:A:373:LYS:O	1:A:373:LYS:HG3	2.13	0.48
1:B:347:LEU:HD13	1:B:368:ILE:HG23	1.95	0.48
1:B:594:ALA:HA	1:B:606:MET:SD	2.53	0.48
1:A:351:TYR:O	1:A:353:GLY:N	2.44	0.48
1:A:373:LYS:HA	1:A:376:ARG:NE	2.27	0.48
1:A:505:ILE:HG23	1:A:506:THR:HG23	1.96	0.48
1:B:329:ARG:NH1	1:B:389:HIS:H	2.11	0.48
1:B:516:GLU:OE1	1:B:623:ARG:HG2	2.14	0.48
1:A:94:VAL:CG1	1:B:108:ALA:HB1	2.44	0.48
1:A:303:PRO:HD3	1:A:359:GLU:OE2	2.14	0.48
1:A:391:SER:CB	1:A:548:ARG:HG3	2.43	0.48
1:A:457:LEU:CD2	1:A:495:VAL:HA	2.44	0.48
1:B:90:LEU:HA	1:B:141:LEU:HD11	1.95	0.48
1:A:394:PHE:HD2	1:A:551:ARG:HH21	1.61	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:CYS:SG	1:A:447:VAL:HG23	2.54	0.48
1:B:96:ASP:O	1:B:100:GLN:HG2	2.13	0.48
1:B:387:MET:HE2	1:B:506:THR:HB	1.94	0.48
1:A:325:THR:HB	1:A:329:ARG:NE	2.29	0.48
1:B:203:ASN:ND2	1:B:261:ALA:HB1	2.29	0.48
1:B:552:VAL:O	1:B:556:VAL:HG23	2.12	0.48
1:A:158:GLU:HG2	1:A:252:VAL:HG11	1.95	0.48
1:A:194:ARG:NH2	1:A:259:ALA:O	2.46	0.48
1:B:234:VAL:CG2	1:B:474:LYS:HZ1	2.25	0.48
1:A:145:ALA:CB	1:B:121:ARG:NH2	2.77	0.48
1:A:330:ARG:O	1:A:334:VAL:HG23	2.13	0.48
1:A:602:PRO:O	1:A:603:ALA:HB2	2.14	0.48
1:B:93:ALA:CB	1:B:138:LEU:HD13	2.44	0.48
1:B:443:ASN:OD1	1:B:446:GLY:N	2.41	0.48
1:A:153:GLN:HE22	1:A:183:GLU:HA	1.79	0.47
1:A:325:THR:CB	1:A:329:ARG:HE	2.27	0.47
1:B:519:ILE:CD1	1:B:548:ARG:HB3	2.43	0.47
1:B:583:VAL:HG13	1:B:617:LEU:HB2	1.96	0.47
1:A:161:ILE:HD12	1:A:248:LEU:CD2	2.44	0.47
1:A:467:ALA:HB2	1:A:487:PHE:HD2	1.80	0.47
1:B:240:ASN:HA	1:B:466:ASN:ND2	2.29	0.47
1:B:551:ARG:O	1:B:555:VAL:HG23	2.14	0.47
1:A:173:LEU:HG	1:A:222:TYR:HE1	1.79	0.47
1:B:157:VAL:O	1:B:161:ILE:HG12	2.14	0.47
1:A:185:ASP:O	1:A:188:ASN:HB3	2.14	0.47
1:A:579:LEU:HA	1:A:583:VAL:HB	1.96	0.47
1:B:457:LEU:HD13	1:B:494:GLN:CG	2.45	0.47
1:A:431:ILE:O	1:A:434:ALA:HB3	2.14	0.47
1:B:329:ARG:CZ	1:B:385:ALA:O	2.62	0.47
1:B:535:VAL:HA	1:B:538:LEU:HB3	1.96	0.47
1:B:598:LEU:HA	1:B:603:ALA:HA	1.97	0.47
1:A:292:ASP:OD1	1:A:293:PRO:HD3	2.15	0.47
1:B:325:THR:CB	1:B:329:ARG:HE	2.28	0.47
1:A:383:ARG:HG2	1:A:440:ILE:CD1	2.45	0.47
1:A:518:HIS:HB3	1:A:548:ARG:NH1	2.30	0.47
1:B:303:PRO:HD3	1:B:359:GLU:OE2	2.15	0.47
1:A:157:VAL:O	1:A:161:ILE:HG12	2.16	0.46
1:A:582:THR:O	1:A:586:ARG:HG2	2.14	0.46
1:B:425:GLU:O	1:B:428:ASN:OD1	2.33	0.46
1:B:457:LEU:HD13	1:B:494:GLN:CB	2.45	0.46
1:A:351:TYR:CB	1:A:368:ILE:HG12	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:LEU:HD13	1:A:494:GLN:HG3	1.97	0.46
1:A:145:ALA:HB1	1:B:121:ARG:NH2	2.30	0.46
1:A:353:GLY:O	1:A:364:LEU:HD23	2.14	0.46
1:A:512:LEU:HD11	1:A:629:VAL:HG21	1.97	0.46
1:B:213:ILE:HG23	1:B:217:ASN:ND2	2.30	0.46
1:B:325:THR:HB	1:B:329:ARG:NE	2.31	0.46
1:B:584:MET:HB3	1:B:585:PRO:HD3	1.97	0.46
1:B:602:PRO:O	1:B:603:ALA:HB2	2.15	0.46
1:A:203:ASN:ND2	1:A:261:ALA:HB1	2.30	0.46
1:A:568:TYR:O	1:A:572:VAL:HG23	2.15	0.46
1:B:329:ARG:HH11	1:B:388:ASP:CB	2.29	0.46
1:B:399:VAL:HA	1:B:402:LEU:HD21	1.98	0.46
1:B:185:ASP:O	1:B:188:ASN:HB3	2.15	0.46
1:B:387:MET:CE	1:B:506:THR:HB	2.45	0.46
1:B:579:LEU:HA	1:B:583:VAL:HB	1.98	0.46
1:A:447:VAL:CG1	1:A:448:LYS:N	2.79	0.46
1:B:85:PHE:N	1:B:85:PHE:CD1	2.83	0.46
1:B:161:ILE:HD12	1:B:248:LEU:CD2	2.45	0.46
1:B:214:LEU:HB2	1:B:251:ALA:HB1	1.98	0.46
1:A:93:ALA:O	1:A:97:VAL:HG23	2.16	0.46
1:A:373:LYS:HA	1:A:376:ARG:NH2	2.31	0.46
1:A:457:LEU:HD13	1:A:494:GLN:CB	2.44	0.46
1:B:153:GLN:NE2	1:B:183:GLU:HA	2.31	0.46
1:B:383:ARG:C	1:B:385:ALA:H	2.18	0.46
1:B:404:LEU:HD22	1:B:404:LEU:O	2.15	0.46
1:B:412:ASN:OD1	1:B:415:GLU:HG2	2.16	0.46
1:A:86:LEU:HD22	1:A:87:LYS:N	2.16	0.46
1:A:329:ARG:CZ	1:A:385:ALA:O	2.64	0.46
1:A:412:ASN:OD1	1:A:415:GLU:HG2	2.16	0.46
1:B:438:CYS:SG	1:B:447:VAL:HG23	2.56	0.46
1:B:556:VAL:O	1:B:560:MET:HG3	2.15	0.46
1:A:86:LEU:HD13	1:A:87:LYS:N	2.30	0.46
1:A:389:HIS:CB	1:A:433:VAL:HG11	2.46	0.46
1:A:392:ASP:O	1:A:393:SER:HB2	2.16	0.46
1:B:192:ALA:O	1:B:196:GLN:HG3	2.16	0.46
1:B:330:ARG:O	1:B:334:VAL:HG23	2.16	0.46
1:B:446:GLY:O	1:B:450:VAL:HG23	2.16	0.46
1:A:85:PHE:N	1:A:85:PHE:CD1	2.84	0.45
1:A:390:VAL:O	1:A:394:PHE:HB2	2.17	0.45
1:A:583:VAL:HG13	1:A:617:LEU:HB2	1.98	0.45
1:B:350:GLU:CD	1:B:367:ALA:HB1	2.36	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:HIS:CB	1:B:433:VAL:HG11	2.47	0.45
1:B:508:ILE:CD1	1:B:555:VAL:HG12	2.46	0.45
1:A:118:SER:O	1:A:121:ARG:HB3	2.15	0.45
1:B:291:VAL:HG22	1:B:293:PRO:CD	2.45	0.45
1:B:351:TYR:CB	1:B:368:ILE:HG12	2.44	0.45
1:A:577:LYS:HG2	1:A:581:ASN:ND2	2.31	0.45
1:B:579:LEU:HD21	1:B:622:ILE:HD13	1.98	0.45
1:B:173:LEU:HG	1:B:222:TYR:HE1	1.81	0.45
1:B:400:PRO:HB2	1:B:423:PHE:HD1	1.81	0.45
1:B:431:ILE:O	1:B:434:ALA:HB3	2.17	0.45
1:A:393:SER:C	1:A:394:PHE:HD1	2.19	0.45
1:A:412:ASN:O	1:A:416:VAL:HG23	2.17	0.45
1:A:447:VAL:HG13	1:A:448:LYS:N	2.32	0.45
1:B:407:ALA:HB1	1:B:415:GLU:HG3	1.98	0.45
1:B:518:HIS:HB3	1:B:548:ARG:NH1	2.31	0.45
1:A:553:ILE:HD12	1:A:554:HIS:N	2.31	0.45
1:B:86:LEU:H	1:B:86:LEU:CD1	2.28	0.45
1:B:583:VAL:HG13	1:B:617:LEU:HB3	1.98	0.45
1:A:360:ARG:HH11	1:A:360:ARG:HG3	1.82	0.45
1:A:394:PHE:O	1:A:396:GLU:N	2.49	0.45
1:B:394:PHE:O	1:B:396:GLU:N	2.49	0.45
1:A:237:TYR:CZ	1:A:470:ALA:HB1	2.51	0.45
1:A:399:VAL:HA	1:A:402:LEU:HD21	1.98	0.45
1:A:496:ARG:HG3	1:A:497:VAL:N	2.32	0.45
1:A:612:ILE:O	1:A:616:ARG:HG3	2.17	0.45
1:B:392:ASP:O	1:B:393:SER:HB2	2.16	0.45
1:B:582:THR:O	1:B:586:ARG:HG2	2.17	0.45
1:A:344:LEU:HD23	1:A:347:LEU:CD2	2.46	0.45
1:A:373:LYS:HA	1:A:376:ARG:CZ	2.47	0.45
1:A:390:VAL:HG13	1:A:551:ARG:NH2	2.31	0.45
1:B:309:LEU:O	1:B:313:ILE:HG13	2.17	0.45
1:B:530:LEU:HD22	1:B:611:PHE:CD1	2.52	0.45
1:B:542:ALA:CB	1:B:591:VAL:HG11	2.46	0.45
1:B:358:LYS:HB3	1:B:365:ASN:OD1	2.16	0.45
1:B:86:LEU:CG	1:B:87:LYS:H	2.30	0.44
1:B:374:LYS:O	1:B:377:ASP:OD1	2.35	0.44
1:A:88:GLU:O	1:A:92:VAL:HG23	2.17	0.44
1:A:220:ILE:HG22	1:A:244:ILE:CD1	2.46	0.44
1:A:583:VAL:HG12	1:A:584:MET:N	2.32	0.44
1:A:598:LEU:HA	1:A:603:ALA:HA	1.97	0.44
1:B:86:LEU:HD13	1:B:87:LYS:N	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:ALA:HA	1:B:137:ARG:NE	2.32	0.44
1:A:90:LEU:CA	1:A:141:LEU:HD11	2.47	0.44
1:A:601:ASP:CB	1:A:602:PRO:CD	2.95	0.44
1:B:577:LYS:HG2	1:B:581:ASN:ND2	2.32	0.44
1:A:186:LYS:HA	1:A:189:ILE:HD12	2.00	0.44
1:B:420:ALA:O	1:B:424:ARG:HB2	2.18	0.44
1:B:583:VAL:HG12	1:B:584:MET:N	2.32	0.44
1:B:290:ILE:HG22	1:B:291:VAL:N	2.33	0.44
1:B:329:ARG:NH1	1:B:385:ALA:O	2.51	0.44
1:A:209:ALA:HB1	1:A:452:MET:HE1	1.98	0.44
1:B:93:ALA:O	1:B:97:VAL:HG23	2.17	0.44
1:B:423:PHE:CZ	1:B:464:VAL:HG11	2.52	0.44
1:A:290:ILE:HG22	1:A:291:VAL:N	2.33	0.44
1:A:347:LEU:HD13	1:A:368:ILE:HG23	1.98	0.44
1:B:393:SER:C	1:B:394:PHE:HD1	2.21	0.44
1:B:512:LEU:HD11	1:B:629:VAL:HG21	1.99	0.44
1:A:347:LEU:O	1:A:351:TYR:HB2	2.18	0.43
1:A:354:ASN:O	1:A:358:LYS:HB2	2.18	0.43
1:A:586:ARG:HG2	1:A:586:ARG:H	1.54	0.43
1:B:112:ALA:O	1:B:115:PRO:HD3	2.18	0.43
1:B:118:SER:O	1:B:121:ARG:HB3	2.17	0.43
1:B:292:ASP:OD1	1:B:293:PRO:HD3	2.17	0.43
1:B:373:LYS:HA	1:B:376:ARG:CZ	2.48	0.43
1:B:412:ASN:O	1:B:416:VAL:HG23	2.17	0.43
1:B:351:TYR:O	1:B:353:GLY:N	2.48	0.43
1:A:216:LYS:O	1:A:219:PRO:HD2	2.18	0.43
1:A:329:ARG:NH1	1:A:385:ALA:O	2.51	0.43
1:A:497:VAL:HG23	1:A:498:LEU:H	1.82	0.43
1:B:405:ILE:HG22	1:B:409:LYS:HE3	2.00	0.43
1:B:497:VAL:HG23	1:B:498:LEU:H	1.82	0.43
1:B:595:VAL:O	1:B:598:LEU:HD12	2.18	0.43
1:B:601:ASP:CB	1:B:602:PRO:CD	2.96	0.43
1:B:621:GLY:O	1:B:625:ILE:HG13	2.19	0.43
1:A:161:ILE:CD1	1:A:180:LEU:HD21	2.45	0.43
1:A:579:LEU:HD13	1:A:621:GLY:HA3	2.00	0.43
1:B:360:ARG:HG3	1:B:360:ARG:HH11	1.83	0.43
1:A:395:LEU:HD11	1:A:550:ALA:HB3	1.99	0.43
1:A:398:ASN:C	1:A:402:LEU:HD22	2.39	0.43
1:B:90:LEU:CA	1:B:141:LEU:HD11	2.48	0.43
1:B:237:TYR:OH	1:B:479:LEU:HD22	2.18	0.43
1:A:192:ALA:O	1:A:196:GLN:HG3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:GLU:OE1	1:A:623:ARG:HG2	2.18	0.43
1:B:93:ALA:HB1	1:B:138:LEU:HD13	2.00	0.43
1:B:153:GLN:HE22	1:B:183:GLU:HA	1.83	0.43
1:B:568:TYR:HE1	1:B:628:ALA:O	2.02	0.43
1:A:93:ALA:HA	1:A:137:ARG:NE	2.33	0.43
1:A:423:PHE:CZ	1:A:464:VAL:HG11	2.54	0.43
1:A:579:LEU:HD21	1:A:622:ILE:HD13	2.00	0.43
1:A:591:VAL:O	1:A:595:VAL:HG23	2.18	0.43
1:B:216:LYS:O	1:B:219:PRO:HD2	2.18	0.43
1:B:243:LEU:O	1:B:247:GLN:HG3	2.19	0.43
1:B:401:LEU:HD21	1:B:488:LYS:HG3	2.01	0.43
1:A:214:LEU:O	1:A:214:LEU:HD23	2.19	0.43
1:A:440:ILE:O	1:A:441:SER:CB	2.66	0.43
1:B:591:VAL:O	1:B:595:VAL:HG23	2.18	0.43
1:A:312:ILE:O	1:A:312:ILE:HG22	2.18	0.42
1:A:420:ALA:O	1:A:424:ARG:HB2	2.18	0.42
1:B:214:LEU:O	1:B:214:LEU:HD23	2.19	0.42
1:B:424:ARG:O	1:B:428:ASN:OD1	2.37	0.42
1:A:154:LEU:O	1:A:158:GLU:HG3	2.18	0.42
1:A:154:LEU:CD1	1:A:187:LEU:HD21	2.41	0.42
1:A:214:LEU:HB2	1:A:251:ALA:HB1	2.01	0.42
1:A:383:ARG:C	1:A:385:ALA:H	2.21	0.42
1:B:390:VAL:HG13	1:B:551:ARG:NH2	2.33	0.42
1:A:85:PHE:CG	1:A:86:LEU:N	2.87	0.42
1:A:308:ARG:NH1	1:B:320:ALA:HB3	2.34	0.42
1:B:86:LEU:CD1	1:B:86:LEU:N	2.82	0.42
1:B:154:LEU:CD1	1:B:187:LEU:HD21	2.45	0.42
1:B:231:HIS:N	1:B:232:PRO:HD3	2.34	0.42
1:A:621:GLY:O	1:A:625:ILE:HG13	2.18	0.42
1:A:451:ARG:HH12	1:B:308:ARG:CD	2.31	0.42
1:A:467:ALA:HB2	1:A:487:PHE:CD2	2.53	0.42
1:B:399:VAL:HA	1:B:402:LEU:CD2	2.49	0.42
1:B:538:LEU:HD21	1:B:594:ALA:HB3	2.02	0.42
1:A:424:ARG:O	1:A:428:ASN:OD1	2.37	0.42
1:A:535:VAL:HA	1:A:538:LEU:HB3	2.01	0.42
1:B:329:ARG:HG2	1:B:385:ALA:O	2.20	0.42
1:A:149:LYS:HZ3	1:A:149:LYS:HB3	1.85	0.42
1:A:230:GLN:NE2	1:A:479:LEU:HD12	2.34	0.42
1:A:388:ASP:OD2	1:A:514:VAL:HG11	2.20	0.42
1:B:302:ARG:HH21	1:B:309:LEU:CD2	2.33	0.42
1:B:611:PHE:CD1	1:B:611:PHE:C	2.93	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ILE:HD12	1:A:248:LEU:HD21	2.01	0.42
1:A:568:TYR:HE1	1:A:628:ALA:O	2.03	0.42
1:B:207:MET:HG2	1:B:258:ALA:HB1	2.01	0.42
1:B:302:ARG:HH21	1:B:309:LEU:CG	2.30	0.42
1:A:86:LEU:N	1:A:86:LEU:CD1	2.82	0.42
1:A:231:HIS:N	1:A:232:PRO:HD3	2.35	0.42
1:A:358:LYS:HB3	1:A:365:ASN:OD1	2.20	0.42
1:B:329:ARG:HH12	1:B:389:HIS:N	2.13	0.42
1:B:447:VAL:CG1	1:B:448:LYS:N	2.81	0.42
1:B:612:ILE:O	1:B:616:ARG:HG3	2.19	0.42
1:A:401:LEU:C	1:A:403:VAL:H	2.23	0.42
1:A:584:MET:HB3	1:A:585:PRO:HD3	2.02	0.42
1:B:389:HIS:NE2	1:B:429:LYS:HE2	2.34	0.42
1:A:329:ARG:HG2	1:A:385:ALA:O	2.20	0.41
1:A:395:LEU:O	1:A:397:THR:HG22	2.20	0.41
1:A:538:LEU:HD21	1:A:594:ALA:HB3	2.01	0.41
1:B:154:LEU:O	1:B:158:GLU:HG3	2.20	0.41
1:B:353:GLY:O	1:B:364:LEU:HD23	2.20	0.41
1:B:373:LYS:HA	1:B:376:ARG:HE	1.85	0.41
1:B:460:LEU:O	1:B:464:VAL:HG23	2.20	0.41
1:A:336:GLU:OE1	1:A:336:GLU:HA	2.20	0.41
1:A:404:LEU:HD22	1:A:404:LEU:O	2.20	0.41
1:A:454:ALA:N	1:A:498:LEU:HD13	2.35	0.41
1:B:234:VAL:HG22	1:B:474:LYS:NZ	2.31	0.41
1:A:248:LEU:HD12	1:A:248:LEU:HA	1.89	0.41
1:A:508:ILE:HG23	1:A:509:ASP:H	1.85	0.41
1:A:556:VAL:O	1:A:560:MET:HG3	2.21	0.41
1:B:123:ASN:HA	1:B:126:ARG:HH21	1.84	0.41
1:B:383:ARG:HG2	1:B:440:ILE:CD1	2.50	0.41
1:A:86:LEU:CG	1:A:87:LYS:H	2.30	0.41
1:A:497:VAL:HG23	1:A:498:LEU:N	2.34	0.41
1:B:329:ARG:NH1	1:B:388:ASP:CB	2.83	0.41
1:B:383:ARG:C	1:B:385:ALA:N	2.73	0.41
1:B:441:SER:C	1:B:443:ASN:H	2.23	0.41
1:A:218:VAL:CB	1:A:219:PRO:HD3	2.49	0.41
1:A:247:GLN:O	1:A:250:GLN:HB3	2.21	0.41
1:A:326:ARG:NH2	1:A:518:HIS:CD2	2.88	0.41
1:A:519:ILE:CD1	1:A:548:ARG:HB3	2.46	0.41
1:A:560:MET:SD	1:A:572:VAL:HG11	2.60	0.41
1:B:167:ALA:HB3	1:B:173:LEU:HD13	2.02	0.41
1:B:433:VAL:HA	1:B:436:LEU:HD12	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:VAL:HG21	1:B:491:TRP:CE3	2.55	0.41
1:A:182:PRO:HG2	1:A:183:GLU:H	1.85	0.41
1:A:316:ALA:C	1:A:319:MET:HE1	2.40	0.41
1:B:440:ILE:O	1:B:441:SER:CB	2.66	0.41
1:A:446:GLY:O	1:A:450:VAL:HG23	2.20	0.41
1:B:312:ILE:HG22	1:B:312:ILE:O	2.21	0.41
1:A:90:LEU:HG	1:B:111:PHE:CE2	2.55	0.41
1:A:350:GLU:CD	1:A:367:ALA:HB1	2.41	0.41
1:A:595:VAL:O	1:A:598:LEU:HD12	2.21	0.41
1:B:395:LEU:CD1	1:B:550:ALA:HB3	2.50	0.41
1:A:210:ALA:O	1:A:251:ALA:HB1	2.21	0.41
1:A:296:PHE:CE1	1:A:316:ALA:HB3	2.56	0.41
1:A:329:ARG:NH2	1:A:386:VAL:HA	2.36	0.41
1:A:459:ALA:O	1:A:462:PRO:HD2	2.20	0.41
1:B:296:PHE:HE1	1:B:316:ALA:HB3	1.85	0.41
1:B:296:PHE:CE1	1:B:316:ALA:HB3	2.56	0.41
1:B:391:SER:HB3	1:B:548:ARG:CG	2.47	0.41
1:B:395:LEU:O	1:B:397:THR:HG22	2.20	0.41
1:B:398:ASN:C	1:B:402:LEU:HD22	2.40	0.41
1:B:471:LEU:CD2	1:B:484:MET:HE3	2.51	0.41
1:B:535:VAL:HG11	1:B:598:LEU:HD11	2.03	0.41
1:A:407:ALA:HB1	1:A:415:GLU:HG3	2.03	0.41
1:B:371:MET:O	1:B:375:THR:HG23	2.20	0.41
1:A:97:VAL:HG22	1:A:134:ALA:O	2.21	0.40
1:A:150:LEU:O	1:A:154:LEU:HB2	2.22	0.40
1:B:440:ILE:O	1:B:440:ILE:CD1	2.68	0.40
1:B:568:TYR:O	1:B:572:VAL:HG23	2.20	0.40
1:A:87:LYS:HZ2	1:B:116:CYS:HA	1.86	0.40
1:A:526:CYS:SG	1:A:541:THR:OG1	2.78	0.40
1:B:161:ILE:CD1	1:B:180:LEU:HD21	2.46	0.40
1:B:336:GLU:OE1	1:B:336:GLU:HA	2.22	0.40
1:B:394:PHE:O	1:B:395:LEU:C	2.59	0.40
1:B:395:LEU:C	1:B:397:THR:N	2.74	0.40
1:B:447:VAL:HG13	1:B:448:LYS:N	2.35	0.40
1:B:497:VAL:HG23	1:B:498:LEU:N	2.36	0.40
1:A:186:LYS:O	1:A:190:MET:HG3	2.20	0.40
1:A:302:ARG:HH21	1:A:309:LEU:CG	2.34	0.40
1:A:395:LEU:C	1:A:397:THR:N	2.74	0.40
1:A:405:ILE:CG2	1:A:409:LYS:HE3	2.51	0.40
1:A:414:LYS:HG3	1:A:415:GLU:H	1.86	0.40
1:A:588:THR:O	1:A:592:GLU:HG2	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ILE:HG22	1:B:244:ILE:CD1	2.48	0.40
1:B:460:LEU:HD12	1:B:463:GLN:NE2	2.37	0.40
1:A:313:ILE:HG22	1:A:313:ILE:O	2.22	0.40
1:B:182:PRO:HG2	1:B:183:GLU:H	1.86	0.40
1:A:306:GLU:O	1:A:310:GLU:HB2	2.22	0.40
1:A:415:GLU:O	1:A:419:TYR:HB2	2.21	0.40
1:B:85:PHE:CG	1:B:86:LEU:N	2.90	0.40
1:B:161:ILE:HD12	1:B:248:LEU:HD21	2.03	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	516/912 (57%)	444 (86%)	49 (10%)	23 (4%)	2 22
1	B	516/912 (57%)	447 (87%)	48 (9%)	21 (4%)	3 23
All	All	1032/1824 (57%)	891 (86%)	97 (9%)	44 (4%)	2 22

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	LEU
1	A	291	VAL
1	A	292	ASP
1	A	301	PHE
1	A	393	SER
1	A	441	SER
1	A	583	VAL
1	B	86	LEU
1	B	291	VAL
1	B	292	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	301	PHE
1	B	393	SER
1	B	441	SER
1	B	583	VAL
1	A	321	ASP
1	A	395	LEU
1	A	601	ASP
1	A	603	ALA
1	B	321	ASP
1	B	395	LEU
1	B	601	ASP
1	B	603	ALA
1	A	300	ARG
1	A	305	LEU
1	A	352	MET
1	A	376	ARG
1	B	300	ARG
1	B	305	LEU
1	B	376	ARG
1	A	353	GLY
1	A	390	VAL
1	A	477	SER
1	A	609	ASN
1	B	352	MET
1	B	353	GLY
1	B	390	VAL
1	B	609	ASN
1	A	598	LEU
1	A	630	LEU
1	B	598	LEU
1	B	630	LEU
1	A	261	ALA
1	A	403	VAL
1	B	403	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	431/766 (56%)	390 (90%)	41 (10%)	8 28
1	B	431/766 (56%)	388 (90%)	43 (10%)	7 26
All	All	862/1532 (56%)	778 (90%)	84 (10%)	8 27

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	PHE
1	A	86	LEU
1	A	89	GLU
1	A	132	LEU
1	A	133	SER
1	A	137	ARG
1	A	141	LEU
1	A	149	LYS
1	A	169	ASN
1	A	190	MET
1	A	292	ASP
1	A	300	ARG
1	A	319	MET
1	A	321	ASP
1	A	336	GLU
1	A	344	LEU
1	A	347	LEU
1	A	350	GLU
1	A	357	ARG
1	A	362	ASP
1	A	377	ASP
1	A	388	ASP
1	A	398	ASN
1	A	399	VAL
1	A	402	LEU
1	A	404	LEU
1	A	406	GLU
1	A	419	TYR
1	A	440	ILE
1	A	445	GLU
1	A	449	LEU
1	A	487	PHE
1	A	508	ILE
1	A	536	ASP
1	A	539	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	569	THR
1	A	578	LEU
1	A	584	MET
1	A	586	ARG
1	A	598	LEU
1	A	601	ASP
1	B	85	PHE
1	B	86	LEU
1	B	89	GLU
1	B	132	LEU
1	B	133	SER
1	B	137	ARG
1	B	141	LEU
1	B	149	LYS
1	B	169	ASN
1	B	190	MET
1	B	292	ASP
1	B	300	ARG
1	B	319	MET
1	B	321	ASP
1	B	336	GLU
1	B	344	LEU
1	B	347	LEU
1	B	350	GLU
1	B	357	ARG
1	B	362	ASP
1	B	366	SER
1	B	377	ASP
1	B	388	ASP
1	B	398	ASN
1	B	399	VAL
1	B	402	LEU
1	B	404	LEU
1	B	406	GLU
1	B	419	TYR
1	B	424	ARG
1	B	440	ILE
1	B	445	GLU
1	B	449	LEU
1	B	487	PHE
1	B	508	ILE
1	B	536	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	539	ASP
1	B	569	THR
1	B	578	LEU
1	B	584	MET
1	B	586	ARG
1	B	598	LEU
1	B	601	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	GLN
1	A	203	ASN
1	A	206	GLN
1	A	217	ASN
1	A	226	GLN
1	A	230	GLN
1	A	354	ASN
1	A	435	ASN
1	A	456	GLN
1	A	463	GLN
1	B	171	GLN
1	B	203	ASN
1	B	206	GLN
1	B	217	ASN
1	B	226	GLN
1	B	230	GLN
1	B	354	ASN
1	B	435	ASN
1	B	456	GLN
1	B	466	ASN
1	B	494	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.