



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:14 PM GMT

PDB ID : 1M1C  
Title : Structure of the L-A virus  
Authors : Naitow, H.; Tang, J.; Canady, M.; Wickner, R.B.; Johnson, J.E.  
Deposited on : 2002-06-18  
Resolution : 3.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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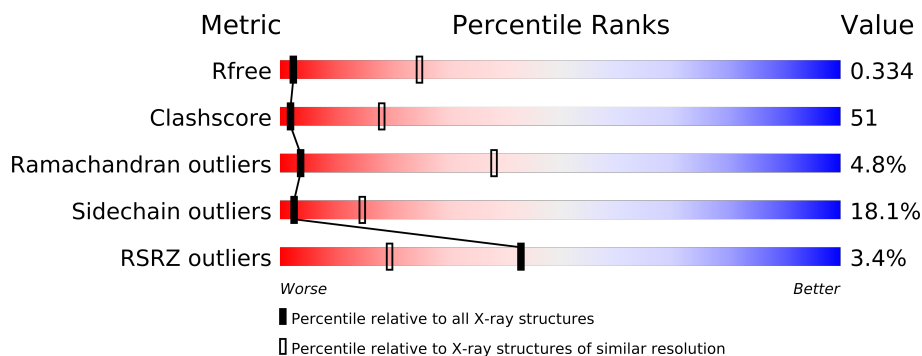
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.50 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))
$R_{free}$	66092	1243 (3.70-3.30)
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	680	
1	B	680	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10302 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Major coat protein.

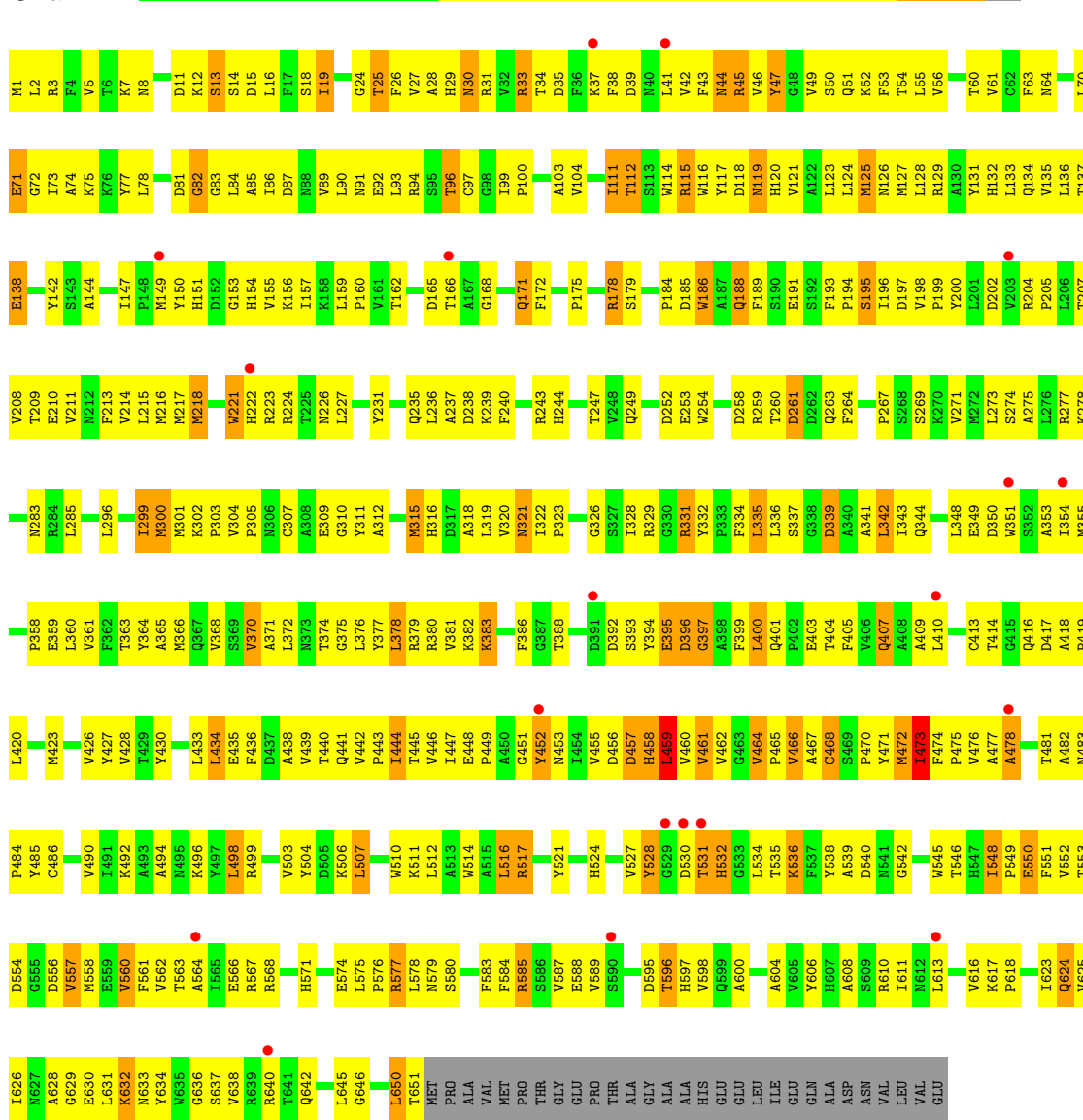
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	651	Total	C	N	O	S	0	0	0
			5151	3302	871	955	23			
1	B	651	Total	C	N	O	S	0	0	0
			5151	3302	871	955	23			

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Major coat protein

Chain A:



- Molecule 1: Major coat protein

Chain B:

[illegible]

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	407.00Å 403.20Å 572.00Å 90.00° 90.46° 90.00°	Depositor
Resolution (Å)	30.00 – 3.50 47.85 – 3.28	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.50) 22.6 (47.85-3.28)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.31 (at 3.25Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.266 , 0.268 0.335 , 0.334	Depositor DCC
$R_{free}$ test set	65500 reflections (11.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.0	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , -20.0	EDS
Estimated twinning fraction	0.064 for k,h,-l 0.065 for -k,-h,-l 0.067 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 969926 reflections	Xtriage
$F_o, F_c$ correlation	0.58	EDS
Total number of atoms	10302	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.29	0/5289	0.57	4/7212 (0.1%)
1	B	0.29	0/5289	0.60	4/7212 (0.1%)
All	All	0.29	0/10578	0.59	8/14424 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	532	HIS	N-CA-C	-8.36	88.42	111.00
1	A	452	TYR	N-CA-C	-7.01	92.06	111.00
1	B	492	LYS	N-CA-C	-5.83	95.27	111.00
1	B	474	PHE	N-CA-C	5.65	126.25	111.00
1	B	613	LEU	N-CA-C	5.56	126.02	111.00
1	B	447	ILE	N-CA-C	-5.13	97.14	111.00
1	A	459	LEU	CA-CB-CG	5.12	127.09	115.30
1	A	557	VAL	N-CA-C	-5.10	97.22	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5151	0	5012	470	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5151	0	5012	579	0
All	All	10302	0	10024	1036	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 51.

All (1036) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:16:LEU:HB2	1:B:363:THR:HG21	1.23	1.14
1:B:445:THR:HG23	1:B:446:VAL:H	1.05	1.14
1:A:15:ASP:HB2	1:A:608:ALA:HB1	1.25	1.13
1:A:144:ALA:HB3	1:A:165:ASP:HA	1.26	1.10
1:B:376:LEU:HB3	1:B:464:VAL:HG21	1.31	1.10
1:A:506:LYS:HE3	1:A:552:VAL:HG23	1.31	1.08
1:B:109:TYR:HA	1:B:113:SER:HB2	1.35	1.08
1:A:310:GLY:HA2	1:A:465:PRO:HB2	1.35	1.08
1:B:502:ALA:HB1	1:B:562:VAL:H	1.13	1.07
1:B:506:LYS:HB3	1:B:552:VAL:HG13	1.37	1.07
1:A:154:HIS:HA	1:A:448:GLU:HG3	1.38	1.05
1:B:445:THR:HG23	1:B:446:VAL:N	1.71	1.05
1:B:198:VAL:HG22	1:B:199:PRO:HD2	1.33	1.05
1:A:154:HIS:HA	1:A:448:GLU:CG	1.88	1.04
1:B:390:ILE:HD12	1:B:390:ILE:H	1.21	1.01
1:B:310:GLY:HA2	1:B:465:PRO:HB2	1.43	1.01
1:A:506:LYS:HD2	1:A:558:MET:HA	1.41	1.00
1:B:10:GLN:C	1:B:12:LYS:H	1.64	0.98
1:B:14:SER:O	1:B:610:ARG:HA	1.63	0.97
1:B:450:ALA:O	1:B:452:TYR:N	1.97	0.97
1:B:299:ILE:HG22	1:B:428:VAL:HG21	1.44	0.96
1:B:154:HIS:HA	1:B:447:ILE:CG2	1.96	0.96
1:A:198:VAL:CG1	1:A:240:PHE:HA	1.95	0.94
1:B:451:GLY:HA2	1:B:532:HIS:O	1.69	0.93
1:B:99:ILE:HG21	1:B:104:VAL:HA	1.51	0.92
1:B:280:VAL:HA	1:B:285:LEU:HD12	1.48	0.92
1:B:613:LEU:O	1:B:616:VAL:HG12	1.69	0.91
1:A:15:ASP:HB3	1:A:610:ARG:CZ	2.00	0.91
1:B:99:ILE:HG21	1:B:104:VAL:CA	2.01	0.91
1:B:509:ALA:HB2	1:B:560:VAL:HG11	1.51	0.91
1:A:395:GLU:HG3	1:A:396:ASP:N	1.84	0.90
1:B:154:HIS:HA	1:B:447:ILE:HG21	1.52	0.89
1:B:394:TYR:O	1:B:644:GLY:HA3	1.72	0.89
1:A:123:LEU:HD13	1:A:218:MET:HE3	1.53	0.89

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:310:GLY:HA2	1:B:465:PRO:CB	2.04	0.88
1:A:260:THR:HG23	1:A:263:GLN:H	1.38	0.88
1:B:72:GLY:HA3	1:B:329:ARG:HH12	1.39	0.87
1:A:473:ILE:O	1:A:476:VAL:HG22	1.74	0.87
1:A:15:ASP:HB2	1:A:608:ALA:CB	2.06	0.86
1:B:630:GLU:HG2	1:B:632:LYS:H	1.40	0.86
1:A:332:TYR:HB2	1:A:335:LEU:HD13	1.57	0.86
1:B:507:LEU:H	1:B:507:LEU:HD22	1.40	0.86
1:B:573:VAL:HG12	1:B:574:GLU:H	1.40	0.85
1:A:396:ASP:OD2	1:B:277:ARG:HD3	1.75	0.85
1:B:526:LYS:O	1:B:561:PHE:HB2	1.77	0.85
1:B:498:LEU:H	1:B:501:GLY:HA2	1.40	0.84
1:B:420:LEU:HD13	1:B:637:SER:HA	1.58	0.83
1:B:531:THR:HG22	1:B:534:LEU:HB2	1.57	0.83
1:B:474:PHE:C	1:B:476:VAL:H	1.82	0.83
1:A:440:THR:HB	1:A:461:VAL:HG23	1.60	0.83
1:B:570:ARG:HG2	1:B:570:ARG:HH11	1.43	0.83
1:B:22:ASP:HB2	1:B:601:GLY:HA2	1.60	0.82
1:A:200:TYR:HB2	1:A:331:ARG:HG2	1.62	0.82
1:B:445:THR:CG2	1:B:446:VAL:N	2.40	0.82
1:A:73:ILE:HB	1:A:78:LEU:HD21	1.62	0.82
1:A:236:LEU:H	1:A:236:LEU:HD22	1.43	0.82
1:A:52:LYS:HG3	1:A:304:VAL:HB	1.61	0.81
1:A:147:ILE:HG21	1:A:159:LEU:HB2	1.63	0.81
1:B:72:GLY:HA3	1:B:329:ARG:NH1	1.95	0.81
1:B:128:LEU:HD22	1:B:296:LEU:HD23	1.62	0.81
1:A:198:VAL:HG11	1:A:240:PHE:HA	1.64	0.80
1:B:446:VAL:O	1:B:447:ILE:HG12	1.81	0.80
1:B:496:LYS:HG2	1:B:503:VAL:HG11	1.63	0.80
1:B:199:PRO:HG2	1:B:240:PHE:HB3	1.63	0.80
1:B:22:ASP:HB2	1:B:601:GLY:CA	2.11	0.80
1:B:277:ARG:HA	1:B:351:TRP:HH2	1.48	0.78
1:A:312:ALA:HB2	1:A:461:VAL:HG21	1.65	0.78
1:B:126:ASN:HA	1:B:129:ARG:HD3	1.65	0.78
1:B:353:ALA:HA	1:B:616:VAL:CG2	2.14	0.78
1:B:418:ALA:HB3	1:B:638:VAL:HG12	1.66	0.78
1:B:5:VAL:HG11	1:B:360:LEU:HD11	1.63	0.78
1:A:577:ARG:HD2	1:A:579:ASN:OD1	1.84	0.77
1:A:285:LEU:HD21	1:A:329:ARG:HD2	1.67	0.77
1:A:506:LYS:CE	1:A:552:VAL:HG23	2.14	0.77
1:B:1:MET:HE3	1:B:361:VAL:HA	1.66	0.77
1:A:260:THR:CG2	1:A:263:GLN:H	1.98	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:471:TYR:HA	1:B:474:PHE:HB2	1.68	0.77
1:A:381:VAL:HG22	1:A:553:THR:HG22	1.67	0.76
1:B:121:VAL:HG13	1:B:292:ALA:HB2	1.65	0.76
1:B:153:GLY:O	1:B:447:ILE:HG21	1.84	0.76
1:B:502:ALA:HB1	1:B:562:VAL:N	1.97	0.76
1:B:496:LYS:O	1:B:503:VAL:HB	1.86	0.75
1:A:202:ASP:OD2	1:A:204:ARG:HD3	1.86	0.75
1:B:318:ALA:HB2	1:B:430:TYR:CZ	2.22	0.75
1:A:443:PRO:HA	1:A:458:HIS:HB3	1.69	0.74
1:B:156:LYS:HG3	1:B:445:THR:HG21	1.69	0.74
1:B:144:ALA:HB3	1:B:165:ASP:HA	1.69	0.74
1:A:393:SER:OG	1:A:395:GLU:HG2	1.88	0.74
1:A:137:THR:HG21	1:A:172:PHE:H	1.52	0.74
1:B:14:SER:HB2	1:B:611:ILE:O	1.87	0.74
1:B:14:SER:O	1:B:610:ARG:CA	2.36	0.74
1:B:223:ARG:NH1	1:B:231:TYR:HA	2.01	0.74
1:B:423:MET:HB2	1:B:426:VAL:HG21	1.70	0.74
1:B:150:TYR:CE2	1:B:308:ALA:HB2	2.23	0.73
1:A:249:GLN:O	1:A:253:GLU:HG3	1.88	0.73
1:A:70:LEU:HD22	1:A:328:ILE:HD11	1.68	0.73
1:A:267:PRO:HB2	1:A:271:VAL:CG1	2.18	0.73
1:A:576:PRO:O	1:A:578:LEU:HG	1.88	0.73
1:B:526:LYS:HA	1:B:526:LYS:HZ3	1.51	0.73
1:B:630:GLU:HG2	1:B:632:LYS:N	2.03	0.73
1:B:22:ASP:CB	1:B:601:GLY:HA2	2.18	0.73
1:A:574:GLU:O	1:A:575:LEU:HD23	1.87	0.73
1:B:65:GLU:HG3	1:B:117:TYR:CE1	2.23	0.73
1:B:526:LYS:HZ2	1:B:527:VAL:H	1.37	0.73
1:A:55:LEU:HB2	1:A:227:LEU:HD12	1.70	0.73
1:B:120:HIS:O	1:B:124:LEU:HG	1.88	0.72
1:B:283:ASN:O	1:B:284:ARG:HB2	1.90	0.72
1:B:284:ARG:HD3	1:B:340:ALA:HB2	1.71	0.72
1:A:75:LYS:HG2	1:A:341:ALA:HB2	1.71	0.72
1:A:632:LYS:HG3	1:B:334:PHE:HB2	1.71	0.72
1:A:198:VAL:HG13	1:A:199:PRO:HD2	1.72	0.72
1:A:155:VAL:HA	1:A:447:ILE:HG12	1.70	0.71
1:B:390:ILE:CD1	1:B:390:ILE:H	1.94	0.71
1:A:444:ILE:HD13	1:A:457:ASP:O	1.90	0.71
1:A:531:THR:O	1:A:531:THR:HG23	1.89	0.71
1:A:423:MET:HB3	1:A:426:VAL:HG21	1.72	0.71
1:B:328:ILE:HG22	1:B:328:ILE:O	1.89	0.71
1:B:469:SER:HB2	1:B:470:PRO:HD2	1.72	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:189:PHE:CZ	1:A:191:GLU:HB2	2.26	0.71
1:B:493:ALA:HB2	1:B:584:PHE:CD1	2.26	0.71
1:B:368:VAL:HG13	1:B:410:LEU:HD21	1.72	0.71
1:B:410:LEU:O	1:B:414:THR:HG22	1.91	0.71
1:B:348:LEU:HD12	1:B:618:PRO:HB3	1.71	0.70
1:A:299:ILE:HG22	1:A:428:VAL:HG11	1.74	0.70
1:A:549:PRO:O	1:A:552:VAL:HG12	1.91	0.70
1:A:557:VAL:O	1:A:557:VAL:HG13	1.91	0.70
1:A:395:GLU:CB	1:A:436:PHE:HE1	2.04	0.70
1:A:15:ASP:HB3	1:A:610:ARG:NH2	2.06	0.70
1:A:157:ILE:HG22	1:A:444:ILE:HA	1.74	0.70
1:B:548:ILE:HD12	1:B:548:ILE:H	1.57	0.70
1:A:150:TYR:HB3	1:A:157:ILE:HG13	1.72	0.70
1:A:267:PRO:HB2	1:A:271:VAL:HG11	1.74	0.70
1:B:259:ARG:HG3	1:B:263:GLN:OE1	1.91	0.70
1:A:5:VAL:HG11	1:A:360:LEU:HD11	1.74	0.69
1:B:630:GLU:HG2	1:B:631:LEU:N	2.06	0.69
1:A:441:GLN:HE22	1:A:460:VAL:HG12	1.57	0.69
1:B:380:ARG:HA	1:B:436:PHE:CD2	2.27	0.69
1:B:156:LYS:HE3	1:B:445:THR:HB	1.75	0.69
1:B:91:ASN:HA	1:B:94:ARG:HD2	1.74	0.69
1:B:55:LEU:HA	1:B:301:MET:HB2	1.75	0.69
1:A:199:PRO:HG2	1:A:240:PHE:HB3	1.74	0.69
1:A:260:THR:HG22	1:A:263:GLN:HB2	1.74	0.69
1:A:3:ARG:O	1:A:7:LYS:HG2	1.93	0.69
1:B:131:TYR:O	1:B:135:VAL:HG23	1.92	0.69
1:A:154:HIS:HA	1:A:448:GLU:HG2	1.71	0.69
1:B:526:LYS:HA	1:B:526:LYS:NZ	2.07	0.69
1:A:629:GLY:H	1:A:650:LEU:HD11	1.58	0.69
1:B:523:THR:HB	1:B:565:ILE:HG22	1.74	0.69
1:B:299:ILE:HG22	1:B:428:VAL:CG2	2.22	0.69
1:A:378:LEU:HG	1:A:478:ALA:HB1	1.75	0.69
1:B:70:LEU:O	1:B:73:ILE:HG23	1.93	0.68
1:B:198:VAL:CG2	1:B:199:PRO:HD2	2.19	0.68
1:B:175:PRO:O	1:B:222:HIS:HB2	1.94	0.68
1:A:452:TYR:HB3	1:A:459:LEU:HD22	1.74	0.68
1:B:277:ARG:HA	1:B:351:TRP:CH2	2.28	0.68
1:A:494:ALA:HB2	1:A:504:TYR:CZ	2.27	0.68
1:A:472:MET:HE3	1:A:472:MET:HA	1.76	0.68
1:B:598:VAL:O	1:B:606:TYR:HB2	1.93	0.68
1:A:320:VAL:HG12	1:A:428:VAL:HG22	1.73	0.68
1:B:474:PHE:O	1:B:476:VAL:HG23	1.93	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:10:GLN:C	1:B:12:LYS:N	2.39	0.68
1:B:211:VAL:O	1:B:215:LEU:HD12	1.94	0.68
1:A:395:GLU:HB2	1:A:436:PHE:CE1	2.30	0.67
1:A:576:PRO:HG2	1:A:578:LEU:HD21	1.74	0.67
1:B:137:THR:HG23	1:B:171:GLN:HA	1.76	0.67
1:A:342:LEU:N	1:A:342:LEU:HD23	2.09	0.67
1:A:532:HIS:O	1:A:532:HIS:ND1	2.27	0.67
1:B:602:ALA:O	1:B:603:HIS:HB3	1.93	0.67
1:A:210:GLU:HG2	1:A:275:ALA:HB2	1.76	0.67
1:A:73:ILE:HG23	1:A:335:LEU:O	1.94	0.67
1:A:379:ARG:NH2	1:A:395:GLU:O	2.22	0.67
1:B:499:ARG:HB2	1:B:500:LYS:HD2	1.77	0.67
1:A:49:VAL:HA	1:A:542:GLY:O	1.95	0.67
1:B:154:HIS:HD2	1:B:448:GLU:HG3	1.59	0.67
1:A:277:ARG:HB2	1:A:355:MET:HE1	1.75	0.67
1:B:525:PHE:HB2	1:B:561:PHE:O	1.94	0.67
1:A:254:TRP:HA	1:A:259:ARG:HB3	1.77	0.67
1:A:94:ARG:HE	1:A:104:VAL:HG21	1.60	0.67
1:A:496:LYS:HB3	1:A:503:VAL:HG22	1.77	0.67
1:B:22:ASP:CG	1:B:601:GLY:HA2	2.16	0.66
1:A:490:VAL:HG22	1:A:588:GLU:HB2	1.76	0.66
1:B:513:ALA:HA	1:B:523:THR:HG21	1.77	0.66
1:A:37:LYS:HA	1:A:41:LEU:O	1.95	0.66
1:A:70:LEU:HB3	1:A:73:ILE:HD12	1.76	0.66
1:A:482:ALA:O	1:A:511:LYS:HD2	1.95	0.66
1:A:184:PRO:HB3	1:A:237:ALA:O	1.95	0.66
1:B:291:THR:HG21	1:B:423:MET:CG	2.27	0.65
1:A:375:GLY:HA2	1:A:413:CYS:HB2	1.78	0.65
1:B:490:VAL:HG22	1:B:491:ILE:N	2.12	0.65
1:B:1:MET:CE	1:B:361:VAL:HA	2.26	0.65
1:A:472:MET:HA	1:A:472:MET:CE	2.27	0.65
1:A:35:ASP:O	1:A:589:VAL:HA	1.96	0.65
1:A:383:LYS:O	1:A:383:LYS:HG2	1.97	0.65
1:A:535:THR:O	1:A:536:LYS:CB	2.44	0.65
1:B:526:LYS:HD3	1:B:527:VAL:N	2.12	0.65
1:A:354:ILE:HD13	1:A:360:LEU:HB3	1.77	0.65
1:A:348:LEU:HD11	1:A:623:ILE:HG21	1.79	0.65
1:A:535:THR:O	1:A:536:LYS:HB2	1.95	0.64
1:B:254:TRP:HE1	1:B:261:ASP:HA	1.59	0.64
1:A:403:GLU:HG3	1:A:634:TYR:CZ	2.33	0.64
1:B:117:TYR:O	1:B:118:ASP:O	2.14	0.64
1:B:10:GLN:O	1:B:12:LYS:N	2.28	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:351:TRP:O	1:B:355:MET:HB2	1.98	0.64
1:A:395:GLU:CB	1:A:436:PHE:CE1	2.81	0.64
1:B:291:THR:HG21	1:B:423:MET:HG2	1.78	0.64
1:B:565:ILE:H	1:B:565:ILE:HD13	1.61	0.64
1:B:400:LEU:HD23	1:B:434:LEU:HD11	1.78	0.64
1:B:527:VAL:CG1	1:B:531:THR:HG23	2.28	0.64
1:B:407:GLN:HB3	1:B:638:VAL:HG12	1.79	0.64
1:B:57:GLY:O	1:B:59:PRO:HD3	1.97	0.64
1:A:149:MET:SD	1:A:151:HIS:HB3	2.38	0.64
1:B:379:ARG:CZ	1:B:436:PHE:HB3	2.28	0.64
1:B:123:LEU:HD13	1:B:218:MET:HE2	1.80	0.63
1:B:284:ARG:NH2	1:B:336:LEU:O	2.31	0.63
1:A:358:PRO:HD2	1:A:359:GLU:OE2	1.98	0.63
1:B:531:THR:HG22	1:B:534:LEU:CB	2.25	0.63
1:B:593:ILE:H	1:B:593:ILE:HD12	1.64	0.63
1:A:420:LEU:HG	1:A:636:GLY:O	1.99	0.63
1:B:375:GLY:HA3	1:B:409:ALA:O	1.98	0.63
1:A:379:ARG:HD2	1:A:399:PHE:CE1	2.33	0.63
1:A:82:GLY:HA3	1:B:95:SER:HB3	1.80	0.63
1:A:186:TRP:HD1	1:A:215:LEU:HD12	1.64	0.63
1:B:476:VAL:O	1:B:477:ALA:HB3	1.99	0.63
1:A:307:CYS:HB2	1:A:309:GLU:OE1	1.98	0.63
1:B:353:ALA:HA	1:B:616:VAL:HG21	1.79	0.62
1:B:72:GLY:H	1:B:329:ARG:HH22	1.45	0.62
1:B:438:ALA:O	1:B:463:GLY:N	2.33	0.62
1:B:150:TYR:HB2	1:B:311:TYR:CE1	2.35	0.62
1:B:156:LYS:HG3	1:B:445:THR:CG2	2.29	0.62
1:A:377:TYR:CE1	1:A:466:VAL:HG22	2.34	0.62
1:B:327:SER:O	1:B:328:ILE:HD12	2.00	0.62
1:A:218:MET:HE2	1:A:218:MET:HA	1.81	0.62
1:A:8:ASN:O	1:A:475:PRO:HG2	2.00	0.62
1:B:22:ASP:HB2	1:B:601:GLY:N	2.15	0.62
1:A:650:LEU:CD1	1:A:651:THR:H	2.13	0.62
1:B:418:ALA:HB3	1:B:638:VAL:CG1	2.29	0.62
1:A:29:HIS:HB2	1:A:597:HIS:CE1	2.35	0.62
1:B:294:GLN:HE22	1:B:419:PRO:HB2	1.65	0.62
1:B:75:LYS:HA	1:B:341:ALA:HB2	1.81	0.62
1:B:117:TYR:O	1:B:117:TYR:CD1	2.53	0.61
1:B:332:TYR:HB2	1:B:335:LEU:HD13	1.82	0.61
1:A:126:ASN:HB3	1:A:217:MET:CE	2.30	0.61
1:A:483:ASN:O	1:A:486:CYS:HB2	1.99	0.61
1:A:371:ALA:HB3	1:A:410:LEU:HD23	1.82	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:235:GLN:HE21	1:A:238:ASP:HA	1.64	0.61
1:B:506:LYS:CB	1:B:552:VAL:HG13	2.22	0.61
1:B:73:ILE:HG13	1:B:74:ALA:N	2.16	0.61
1:B:453:ASN:O	1:B:453:ASN:OD1	2.18	0.61
1:B:493:ALA:HB2	1:B:584:PHE:CE1	2.34	0.61
1:A:186:TRP:CD1	1:A:215:LEU:HD12	2.35	0.61
1:B:155:VAL:N	1:B:447:ILE:HB	2.15	0.61
1:A:379:ARG:HG3	1:A:394:TYR:HB3	1.81	0.61
1:A:28:ALA:O	1:A:50:SER:HA	2.00	0.61
1:B:348:LEU:HD12	1:B:618:PRO:CB	2.30	0.61
1:A:439:VAL:HG12	1:A:462:VAL:HG22	1.83	0.61
1:B:359:GLU:O	1:B:363:THR:HG23	2.01	0.61
1:B:109:TYR:O	1:B:114:TRP:HD1	1.84	0.61
1:B:283:ASN:HA	1:B:336:LEU:HD13	1.83	0.61
1:A:310:GLY:HA2	1:A:465:PRO:CB	2.21	0.61
1:B:476:VAL:HG12	1:B:477:ALA:N	2.16	0.61
1:B:358:PRO:HD2	1:B:359:GLU:OE2	2.01	0.60
1:B:112:THR:CG2	1:B:197:ASP:HA	2.31	0.60
1:B:7:LYS:HD2	1:B:10:GLN:NE2	2.15	0.60
1:A:194:PRO:HD3	1:A:331:ARG:O	2.01	0.60
1:A:204:ARG:HD2	1:A:243:ARG:HG2	1.82	0.60
1:B:381:VAL:HG22	1:B:553:THR:CG2	2.31	0.60
1:A:506:LYS:HE3	1:A:552:VAL:CG2	2.21	0.60
1:B:15:ASP:HB3	1:B:610:ARG:HG2	1.82	0.60
1:A:401:GLN:HB3	1:A:404:THR:OG1	2.01	0.60
1:B:455:VAL:HG12	1:B:456:ASP:OD1	2.02	0.60
1:A:8:ASN:O	1:A:475:PRO:CG	2.50	0.60
1:A:524:HIS:HB2	1:A:563:THR:O	2.01	0.60
1:A:75:LYS:HD3	1:A:624:GLN:NE2	2.16	0.60
1:A:37:LYS:HG2	1:A:42:VAL:HG22	1.84	0.60
1:B:277:ARG:HB2	1:B:355:MET:SD	2.42	0.60
1:A:56:VAL:HA	1:A:227:LEU:HA	1.82	0.60
1:B:509:ALA:CB	1:B:560:VAL:HG11	2.27	0.60
1:B:58:ASN:O	1:B:317:ASP:HB3	2.01	0.60
1:A:129:ARG:O	1:A:133:LEU:HD23	2.00	0.60
1:A:35:ASP:OD2	1:A:44:ASN:HB3	2.02	0.60
1:B:68:SER:HB2	1:B:117:TYR:O	2.02	0.60
1:A:100:PRO:HG2	1:A:103:ALA:HB2	1.83	0.60
1:B:341:ALA:HA	1:B:624:GLN:HB3	1.81	0.60
1:A:549:PRO:O	1:A:552:VAL:CG1	2.50	0.59
1:A:197:ASP:HA	1:A:331:ARG:HH12	1.67	0.59
1:A:123:LEU:HB2	1:A:218:MET:HE3	1.82	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:236:LEU:H	1:A:236:LEU:CD2	2.15	0.59
1:B:470:PRO:O	1:B:473:ILE:HD13	2.01	0.59
1:A:150:TYR:HB2	1:A:311:TYR:CZ	2.37	0.59
1:A:227:LEU:HD22	1:A:227:LEU:H	1.66	0.59
1:A:223:ARG:HE	1:A:231:TYR:HA	1.67	0.59
1:A:366:MET:O	1:A:370:VAL:HG12	2.02	0.59
1:B:444:ILE:HG22	1:B:445:THR:N	2.17	0.59
1:B:55:LEU:H	1:B:55:LEU:HD12	1.67	0.59
1:B:577:ARG:HG3	1:B:579:ASN:OD1	2.02	0.59
1:B:394:TYR:CE1	1:B:644:GLY:HA2	2.37	0.59
1:A:55:LEU:HD22	1:A:55:LEU:H	1.67	0.59
1:A:74:ALA:HB2	1:A:337:SER:O	2.02	0.59
1:B:38:PHE:O	1:B:39:ASP:HB2	2.02	0.59
1:B:381:VAL:HG11	1:B:386:PHE:CZ	2.38	0.59
1:A:111:ILE:HG23	1:A:111:ILE:O	2.00	0.59
1:B:17:PHE:O	1:B:359:GLU:HB3	2.03	0.59
1:B:199:PRO:HG2	1:B:240:PHE:CB	2.32	0.59
1:A:441:GLN:NE2	1:A:460:VAL:HG12	2.18	0.59
1:A:417:ASP:HB3	1:A:637:SER:OG	2.03	0.59
1:B:52:LYS:HB2	1:B:304:VAL:HB	1.82	0.59
1:A:443:PRO:CA	1:A:458:HIS:HB3	2.33	0.59
1:B:474:PHE:O	1:B:476:VAL:N	2.36	0.58
1:A:150:TYR:HB3	1:A:157:ILE:CG1	2.33	0.58
1:A:126:ASN:HB3	1:A:217:MET:HE3	1.84	0.58
1:B:235:GLN:HE21	1:B:238:ASP:HA	1.68	0.58
1:A:56:VAL:HG13	1:A:226:ASN:HB3	1.85	0.58
1:B:174:TRP:CE3	1:B:216:MET:HE2	2.38	0.58
1:A:198:VAL:HG13	1:A:240:PHE:HA	1.83	0.58
1:A:27:VAL:HG23	1:A:51:GLN:C	2.23	0.58
1:A:33:ARG:HB2	1:A:46:VAL:HG12	1.84	0.58
1:B:364:TYR:O	1:B:368:VAL:HG23	2.04	0.58
1:A:610:ARG:HH11	1:A:610:ARG:HG2	1.68	0.58
1:B:13:SER:O	1:B:14:SER:OG	2.12	0.58
1:A:414:THR:HB	1:A:416:GLN:HE21	1.69	0.58
1:B:376:LEU:HD23	1:B:464:VAL:HG11	1.86	0.58
1:B:23:ARG:HH11	1:B:23:ARG:HB2	1.69	0.58
1:B:68:SER:HB2	1:B:117:TYR:C	2.24	0.58
1:A:199:PRO:O	1:A:240:PHE:HB2	2.03	0.58
1:A:323:PRO:HD3	1:A:426:VAL:HG12	1.86	0.58
1:B:201:LEU:N	1:B:201:LEU:HD23	2.19	0.58
1:B:59:PRO:HD2	1:B:223:ARG:HH22	1.66	0.58
1:A:632:LYS:HG3	1:B:334:PHE:CB	2.33	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:277:ARG:HD3	1:A:355:MET:HE2	1.85	0.58
1:B:15:ASP:HB2	1:B:608:ALA:HB1	1.85	0.58
1:A:119:ASN:HD21	1:A:323:PRO:HG2	1.69	0.58
1:A:650:LEU:HD12	1:A:651:THR:H	1.69	0.58
1:B:154:HIS:HA	1:B:447:ILE:CB	2.34	0.57
1:A:371:ALA:CB	1:A:410:LEU:HD23	2.34	0.57
1:A:149:MET:SD	1:A:156:LYS:HG3	2.45	0.57
1:B:476:VAL:O	1:B:477:ALA:CB	2.51	0.57
1:B:498:LEU:N	1:B:501:GLY:HA2	2.17	0.57
1:B:491:ILE:O	1:B:586:SER:HB2	2.04	0.57
1:A:483:ASN:HB2	1:A:484:PRO:HD2	1.86	0.57
1:B:117:TYR:CD2	1:B:326:GLY:HA3	2.40	0.57
1:B:15:ASP:HB2	1:B:608:ALA:CB	2.34	0.57
1:B:249:GLN:O	1:B:253:GLU:HG3	2.04	0.57
1:A:386:PHE:CE2	1:A:507:LEU:HG	2.39	0.57
1:B:207:THR:O	1:B:211:VAL:HG23	2.05	0.57
1:A:120:HIS:O	1:A:124:LEU:HG	2.04	0.57
1:A:92:GLU:O	1:A:96:THR:HG22	2.03	0.57
1:B:517:ARG:NE	1:B:539:ALA:HB3	2.19	0.57
1:A:218:MET:HG2	1:A:240:PHE:CE2	2.40	0.57
1:A:577:ARG:NH2	1:A:580:SER:HB2	2.19	0.57
1:B:125:MET:HE1	1:B:292:ALA:HA	1.86	0.57
1:A:178:ARG:HG3	1:A:254:TRP:CH2	2.39	0.57
1:B:380:ARG:HG3	1:B:380:ARG:NH1	2.19	0.57
1:B:483:ASN:HB2	1:B:484:PRO:CD	2.35	0.57
1:B:490:VAL:HG22	1:B:491:ILE:H	1.69	0.56
1:B:506:LYS:HE2	1:B:552:VAL:O	2.05	0.56
1:B:126:ASN:HA	1:B:129:ARG:CD	2.34	0.56
1:B:381:VAL:HG22	1:B:553:THR:HG23	1.85	0.56
1:A:375:GLY:HA3	1:A:409:ALA:O	2.04	0.56
1:A:440:THR:HB	1:A:461:VAL:CG2	2.32	0.56
1:B:155:VAL:HG13	1:B:444:ILE:HG23	1.87	0.56
1:B:305:PRO:HA	1:B:467:ALA:O	2.05	0.56
1:A:645:LEU:HD23	1:A:645:LEU:H	1.70	0.56
1:B:117:TYR:CG	1:B:117:TYR:O	2.58	0.56
1:B:552:VAL:O	1:B:552:VAL:HG12	2.05	0.56
1:B:423:MET:HB2	1:B:426:VAL:CG2	2.35	0.56
1:B:428:VAL:HG13	1:B:428:VAL:O	2.04	0.56
1:A:442:VAL:O	1:A:458:HIS:CB	2.53	0.56
1:B:283:ASN:O	1:B:284:ARG:CB	2.53	0.56
1:B:253:GLU:CB	1:B:259:ARG:HB2	2.36	0.56
1:B:380:ARG:HH11	1:B:380:ARG:HG3	1.69	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:69:TYR:HB2	1:B:288:GLN:HE21	1.71	0.56
1:B:355:MET:HA	1:B:355:MET:CE	2.36	0.56
1:B:473:ILE:O	1:B:473:ILE:HG12	2.05	0.56
1:A:403:GLU:HG3	1:A:634:TYR:CE2	2.40	0.56
1:B:453:ASN:C	1:B:453:ASN:OD1	2.43	0.56
1:B:473:ILE:H	1:B:473:ILE:HD13	1.71	0.56
1:B:150:TYR:O	1:B:156:LYS:HA	2.05	0.56
1:A:476:VAL:O	1:A:485:TYR:O	2.24	0.56
1:A:133:LEU:HB3	1:A:172:PHE:CD1	2.40	0.56
1:A:131:TYR:O	1:A:135:VAL:HG23	2.06	0.56
1:B:19:ILE:HB	1:B:136:LEU:HD11	1.88	0.56
1:A:305:PRO:HG2	1:A:311:TYR:CD1	2.41	0.55
1:B:55:LEU:N	1:B:55:LEU:HD12	2.22	0.55
1:A:470:PRO:HG2	1:A:545:TRP:CH2	2.40	0.55
1:A:484:PRO:HD2	1:A:510:TRP:CZ3	2.41	0.55
1:A:254:TRP:HE1	1:A:261:ASP:HA	1.71	0.55
1:A:423:MET:HB3	1:A:426:VAL:CG2	2.35	0.55
1:B:328:ILE:CG2	1:B:328:ILE:O	2.55	0.55
1:A:557:VAL:O	1:A:557:VAL:CG1	2.55	0.55
1:A:123:LEU:CD1	1:A:218:MET:HE3	2.33	0.55
1:B:510:TRP:CE2	1:B:548:ILE:HG13	2.42	0.55
1:B:2:LEU:HD23	1:B:360:LEU:HD22	1.89	0.55
1:B:150:TYR:CE2	1:B:152:ASP:HB3	2.40	0.55
1:B:628:ALA:HA	1:B:651:THR:O	2.07	0.55
1:B:16:LEU:HD13	1:B:359:GLU:HB2	1.88	0.55
1:B:151:HIS:ND1	1:B:156:LYS:HB3	2.21	0.55
1:B:283:ASN:N	1:B:283:ASN:HD22	2.03	0.55
1:A:386:PHE:CE1	1:A:552:VAL:HG21	2.41	0.55
1:A:419:PRO:HA	1:A:637:SER:HB3	1.87	0.55
1:B:14:SER:O	1:B:611:ILE:N	2.39	0.55
1:B:446:VAL:HG22	1:B:447:ILE:N	2.21	0.55
1:B:295:LEU:O	1:B:299:ILE:HG23	2.07	0.55
1:A:577:ARG:HH21	1:A:580:SER:HB2	1.72	0.55
1:B:93:LEU:HA	1:B:96:THR:OG1	2.06	0.55
1:A:259:ARG:HD2	1:A:263:GLN:HB3	1.88	0.54
1:B:514:TRP:O	1:B:518:VAL:HG23	2.06	0.54
1:B:483:ASN:HB2	1:B:484:PRO:HD2	1.88	0.54
1:A:516:LEU:CD1	1:A:521:TYR:HB2	2.37	0.54
1:B:507:LEU:HD22	1:B:507:LEU:N	2.18	0.54
1:A:55:LEU:HD22	1:A:55:LEU:N	2.22	0.54
1:A:7:LYS:HD3	1:A:11:ASP:OD1	2.07	0.54
1:B:104:VAL:HG22	1:B:105:ALA:N	2.23	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:277:ARG:HB2	1:A:355:MET:CE	2.37	0.54
1:B:57:GLY:O	1:B:228:ALA:HA	2.06	0.54
1:A:188:GLN:HG2	1:A:247:THR:OG1	2.07	0.54
1:A:638:VAL:HG23	1:A:646:GLY:C	2.28	0.54
1:A:604:ALA:HB1	1:A:606:TYR:CE1	2.42	0.54
1:B:442:VAL:HG23	1:B:459:LEU:O	2.07	0.54
1:A:70:LEU:CD2	1:A:328:ILE:HD11	2.38	0.54
1:A:55:LEU:CB	1:A:227:LEU:HD12	2.37	0.54
1:B:210:GLU:O	1:B:214:VAL:HG23	2.08	0.54
1:B:611:ILE:HG23	1:B:611:ILE:O	2.07	0.54
1:B:527:VAL:HG13	1:B:531:THR:HG23	1.90	0.54
1:A:477:ALA:HA	1:A:485:TYR:HB3	1.89	0.54
1:A:442:VAL:C	1:A:458:HIS:HB3	2.28	0.54
1:A:61:VAL:HA	1:A:320:VAL:HG22	1.90	0.54
1:A:300:MET:HE3	1:A:365:ALA:CB	2.37	0.54
1:B:454:ILE:HD12	1:B:454:ILE:N	2.22	0.54
1:B:571:HIS:CE1	1:B:573:VAL:O	2.61	0.53
1:B:204:ARG:HG3	1:B:243:ARG:O	2.08	0.53
1:A:200:TYR:CD1	1:A:331:ARG:HD3	2.43	0.53
1:B:603:HIS:O	1:B:604:ALA:HB3	2.07	0.53
1:B:126:ASN:HA	1:B:129:ARG:HG2	1.91	0.53
1:B:260:THR:OG1	1:B:263:GLN:HG3	2.07	0.53
1:B:544:THR:O	1:B:544:THR:HG22	2.09	0.53
1:B:71:GLU:HG2	1:B:287:ASN:HD22	1.73	0.53
1:B:521:TYR:HA	1:B:568:ARG:HG3	1.90	0.53
1:B:99:ILE:CG2	1:B:104:VAL:HB	2.38	0.53
1:B:99:ILE:HB	1:B:104:VAL:HB	1.90	0.53
1:A:260:THR:HG22	1:A:263:GLN:CB	2.37	0.53
1:A:490:VAL:HG22	1:A:588:GLU:CB	2.37	0.53
1:A:86:ILE:HG13	1:B:100:PRO:HB3	1.91	0.53
1:B:469:SER:CB	1:B:470:PRO:HD2	2.39	0.53
1:B:500:LYS:HD2	1:B:500:LYS:N	2.23	0.53
1:A:368:VAL:HG13	1:A:410:LEU:HD11	1.91	0.53
1:A:512:LEU:O	1:A:516:LEU:HB2	2.08	0.53
1:B:402:PRO:CB	1:B:429:THR:HG21	2.39	0.53
1:A:178:ARG:HG3	1:A:254:TRP:CZ2	2.43	0.53
1:B:130:ALA:C	1:B:272:MET:HE1	2.29	0.53
1:B:513:ALA:HA	1:B:523:THR:CG2	2.38	0.53
1:B:382:LYS:HB3	1:B:394:TYR:CZ	2.44	0.53
1:B:307:CYS:HB3	1:B:538:TYR:CE2	2.43	0.53
1:B:147:ILE:HD12	1:B:147:ILE:H	1.74	0.53
1:B:113:SER:O	1:B:116:TRP:NE1	2.42	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:459:LEU:C	1:A:459:LEU:HD12	2.29	0.53
1:B:490:VAL:HG23	1:B:587:VAL:O	2.09	0.53
1:B:493:ALA:HB1	1:B:497:TYR:OH	2.08	0.52
1:B:56:VAL:HG22	1:B:145:GLY:HA3	1.91	0.52
1:B:630:GLU:HG2	1:B:631:LEU:H	1.71	0.52
1:A:64:ASN:O	1:A:323:PRO:HA	2.10	0.52
1:A:207:THR:HG22	1:A:210:GLU:CG	2.39	0.52
1:B:622:GLY:O	1:B:623:ILE:HG13	2.09	0.52
1:B:310:GLY:CA	1:B:465:PRO:HB2	2.28	0.52
1:B:614:ASP:HB3	1:B:617:LYS:HE3	1.90	0.52
1:B:254:TRP:HA	1:B:259:ARG:HB3	1.91	0.52
1:A:364:TYR:O	1:A:368:VAL:HG23	2.10	0.52
1:A:312:ALA:CB	1:A:461:VAL:HG21	2.37	0.52
1:B:283:ASN:HA	1:B:336:LEU:CD1	2.40	0.52
1:B:568:ARG:HH11	1:B:568:ARG:HB3	1.74	0.52
1:B:406:VAL:O	1:B:410:LEU:HD13	2.10	0.52
1:B:155:VAL:CG1	1:B:444:ILE:HG23	2.40	0.52
1:B:442:VAL:O	1:B:458:HIS:HA	2.09	0.52
1:A:375:GLY:CA	1:A:413:CYS:HB2	2.38	0.52
1:A:227:LEU:N	1:A:227:LEU:HD22	2.24	0.52
1:A:16:LEU:HA	1:A:363:THR:HG21	1.92	0.52
1:A:483:ASN:ND2	1:A:486:CYS:SG	2.82	0.52
1:B:17:PHE:H	1:B:363:THR:CG2	2.22	0.52
1:B:175:PRO:HB2	1:B:221:TRP:HA	1.91	0.52
1:A:638:VAL:HG23	1:A:646:GLY:O	2.10	0.52
1:A:111:ILE:CG2	1:A:111:ILE:O	2.58	0.52
1:A:527:VAL:HG12	1:A:560:VAL:HA	1.90	0.52
1:B:149:MET:HE2	1:B:156:LYS:HD3	1.91	0.52
1:B:280:VAL:HB	1:B:351:TRP:CH2	2.45	0.52
1:A:441:GLN:HE22	1:A:460:VAL:CG1	2.21	0.52
1:B:570:ARG:NH1	1:B:570:ARG:HG2	2.14	0.52
1:B:601:GLY:O	1:B:602:ALA:HB2	2.09	0.52
1:B:493:ALA:HB2	1:B:584:PHE:CG	2.44	0.52
1:A:342:LEU:H	1:A:342:LEU:HD23	1.74	0.52
1:B:573:VAL:HG12	1:B:574:GLU:N	2.19	0.52
1:A:459:LEU:O	1:A:459:LEU:HD12	2.10	0.52
1:A:273:LEU:HD23	1:A:277:ARG:NH1	2.25	0.52
1:A:610:ARG:HG2	1:A:610:ARG:NH1	2.25	0.52
1:A:154:HIS:HB3	1:A:448:GLU:HB2	1.91	0.52
1:B:394:TYR:HA	1:B:643:GLN:O	2.09	0.52
1:B:134:GLN:HG3	1:B:272:MET:SD	2.50	0.52
1:B:650:LEU:HD23	1:B:650:LEU:H	1.76	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:386:PHE:CD1	1:A:552:VAL:HG21	2.46	0.51
1:A:377:TYR:HD1	1:A:464:VAL:O	1.93	0.51
1:A:575:LEU:HB3	1:A:576:PRO:CD	2.40	0.51
1:B:156:LYS:H	1:B:445:THR:HG22	1.74	0.51
1:B:61:VAL:HG11	1:B:231:TYR:HD1	1.75	0.51
1:B:402:PRO:HB3	1:B:429:THR:HG21	1.92	0.51
1:B:629:GLY:O	1:B:630:GLU:O	2.29	0.51
1:B:593:ILE:N	1:B:593:ILE:HD12	2.25	0.51
1:A:41:LEU:HB3	1:A:43:PHE:HE2	1.75	0.51
1:B:184:PRO:HG3	1:B:235:GLN:HB2	1.92	0.51
1:B:147:ILE:HD12	1:B:147:ILE:N	2.26	0.51
1:A:115:ARG:H	1:A:115:ARG:HD2	1.75	0.51
1:B:116:TRP:HE3	1:B:328:ILE:HG12	1.75	0.51
1:B:218:MET:SD	1:B:236:LEU:HD12	2.51	0.51
1:A:218:MET:HG2	1:A:240:PHE:CZ	2.45	0.51
1:B:285:LEU:O	1:B:288:GLN:N	2.43	0.51
1:A:457:ASP:OD1	1:A:457:ASP:N	2.44	0.51
1:A:29:HIS:HA	1:A:49:VAL:O	2.11	0.51
1:B:161:VAL:HG22	1:B:226:ASN:CG	2.30	0.51
1:B:10:GLN:O	1:B:11:ASP:CG	2.49	0.51
1:A:81:ASP:HB2	1:B:95:SER:OG	2.11	0.51
1:B:318:ALA:HB2	1:B:430:TYR:CE1	2.46	0.51
1:B:99:ILE:HG21	1:B:104:VAL:CB	2.41	0.51
1:B:498:LEU:H	1:B:501:GLY:CA	2.20	0.51
1:B:254:TRP:CA	1:B:259:ARG:HB3	2.41	0.51
1:B:78:LEU:HD12	1:B:342:LEU:HD12	1.93	0.51
1:B:112:THR:HG23	1:B:197:ASP:HA	1.93	0.51
1:B:353:ALA:CA	1:B:616:VAL:CG2	2.89	0.51
1:B:407:GLN:HB3	1:B:638:VAL:CG1	2.39	0.51
1:B:61:VAL:HB	1:B:320:VAL:HG13	1.93	0.51
1:A:407:GLN:HG3	1:A:420:LEU:CD2	2.40	0.51
1:A:123:LEU:O	1:A:127:MET:HG3	2.10	0.51
1:A:137:THR:CG2	1:A:171:GLN:HA	2.41	0.51
1:A:532:HIS:C	1:A:532:HIS:ND1	2.65	0.51
1:A:16:LEU:HD13	1:A:359:GLU:HB2	1.93	0.51
1:B:251:ALA:O	1:B:255:ILE:HG12	2.11	0.51
1:A:399:PHE:HB3	1:A:405:PHE:CD1	2.46	0.50
1:A:640:ARG:HA	1:A:645:LEU:HA	1.93	0.50
1:B:185:ASP:HB3	1:B:239:LYS:HG3	1.93	0.50
1:B:383:LYS:NZ	1:B:392:ASP:HB3	2.26	0.50
1:B:599:GLN:O	1:B:599:GLN:HG3	2.10	0.50
1:B:97:CYS:O	1:B:99:ILE:N	2.41	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:61:VAL:HG11	1:B:231:TYR:CD1	2.47	0.50
1:A:30:ASN:HD22	1:A:596:THR:HB	1.77	0.50
1:A:613:LEU:HD12	1:A:613:LEU:H	1.75	0.50
1:B:218:MET:HA	1:B:236:LEU:HD12	1.93	0.50
1:A:123:LEU:HB2	1:A:218:MET:CE	2.42	0.50
1:A:254:TRP:CD1	1:A:264:PHE:HB3	2.46	0.50
1:B:354:ILE:HG12	1:B:361:VAL:CG2	2.42	0.50
1:B:502:ALA:O	1:B:503:VAL:HG23	2.12	0.50
1:B:15:ASP:HA	1:B:610:ARG:HA	1.93	0.50
1:A:399:PHE:CB	1:A:434:LEU:HD21	2.41	0.50
1:A:96:THR:CG2	1:A:97:CYS:N	2.75	0.50
1:B:63:PHE:HA	1:B:322:ILE:O	2.12	0.50
1:B:152:ASP:C	1:B:154:HIS:H	2.14	0.50
1:B:474:PHE:C	1:B:476:VAL:N	2.54	0.50
1:A:61:VAL:HG13	1:A:320:VAL:CG2	2.42	0.50
1:B:453:ASN:OD1	1:B:460:VAL:HG22	2.12	0.50
1:A:26:PHE:CE2	1:A:53:PHE:HB2	2.47	0.50
1:B:549:PRO:HB2	1:B:551:PHE:CD2	2.47	0.50
1:B:157:ILE:HD11	1:B:308:ALA:HB1	1.92	0.50
1:A:378:LEU:O	1:A:382:LYS:HB2	2.11	0.50
1:A:442:VAL:O	1:A:458:HIS:HB3	2.12	0.50
1:B:307:CYS:HB3	1:B:538:TYR:HE2	1.76	0.50
1:A:194:PRO:HD2	1:A:332:TYR:CE2	2.46	0.50
1:A:453:ASN:HB3	1:A:460:VAL:HG22	1.93	0.50
1:A:49:VAL:HG11	1:A:471:TYR:CD1	2.46	0.50
1:A:496:LYS:HB3	1:A:503:VAL:CG2	2.41	0.50
1:A:483:ASN:HB2	1:A:484:PRO:CD	2.41	0.50
1:B:378:LEU:HD11	1:B:478:ALA:HB1	1.94	0.50
1:B:5:VAL:HG11	1:B:360:LEU:CD1	2.36	0.50
1:A:118:ASP:OD2	1:A:328:ILE:HG12	2.12	0.50
1:A:598:VAL:HG13	1:A:606:TYR:HB2	1.94	0.50
1:B:45:ARG:HG2	1:B:46:VAL:N	2.27	0.50
1:B:218:MET:HG2	1:B:240:PHE:CE2	2.46	0.50
1:A:549:PRO:HB2	1:A:551:PHE:CE2	2.47	0.49
1:A:548:ILE:HD11	1:A:552:VAL:HG11	1.93	0.49
1:A:198:VAL:HG13	1:A:199:PRO:CD	2.40	0.49
1:A:315:MET:HG3	1:A:442:VAL:HG12	1.94	0.49
1:B:208:VAL:HG23	1:B:248:VAL:HG23	1.94	0.49
1:A:350:ASP:O	1:A:354:ILE:HG12	2.12	0.49
1:B:576:PRO:O	1:B:578:LEU:HD23	2.12	0.49
1:B:634:TYR:CD1	1:B:634:TYR:N	2.80	0.49
1:B:6:THR:O	1:B:7:LYS:HB2	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:453:ASN:O	1:A:459:LEU:HB2	2.11	0.49
1:B:27:VAL:HG12	1:B:599:GLN:O	2.12	0.49
1:A:89:VAL:HG13	1:A:334:PHE:CZ	2.48	0.49
1:B:353:ALA:CA	1:B:616:VAL:HG21	2.42	0.49
1:B:22:ASP:O	1:B:23:ARG:HB2	2.13	0.49
1:A:516:LEU:HD12	1:A:521:TYR:HB2	1.94	0.49
1:B:161:VAL:HG22	1:B:226:ASN:OD1	2.13	0.49
1:A:73:ILE:HG13	1:A:329:ARG:HH21	1.76	0.49
1:B:527:VAL:HG13	1:B:531:THR:CG2	2.42	0.49
1:A:299:ILE:HG22	1:A:428:VAL:CG1	2.42	0.49
1:A:207:THR:CG2	1:A:210:GLU:H	2.26	0.49
1:A:45:ARG:C	1:A:45:ARG:HD2	2.33	0.49
1:B:6:THR:O	1:B:7:LYS:CB	2.60	0.49
1:A:531:THR:CG2	1:A:531:THR:O	2.60	0.49
1:A:186:TRP:HE3	1:A:186:TRP:O	1.95	0.49
1:B:378:LEU:HD12	1:B:413:CYS:HA	1.95	0.49
1:A:73:ILE:HB	1:A:78:LEU:CD2	2.39	0.49
1:B:22:ASP:HB2	1:B:601:GLY:H	1.78	0.49
1:B:491:ILE:O	1:B:584:PHE:HZ	1.95	0.49
1:A:305:PRO:HB3	1:A:467:ALA:CB	2.43	0.49
1:A:210:GLU:OE2	1:A:278:LYS:HD2	2.13	0.49
1:A:41:LEU:HB3	1:A:43:PHE:CE2	2.47	0.49
1:B:150:TYR:CD2	1:B:308:ALA:HB2	2.47	0.49
1:A:382:LYS:HB3	1:A:394:TYR:CE2	2.48	0.49
1:A:27:VAL:HA	1:A:52:LYS:HA	1.95	0.49
1:A:64:ASN:HD22	1:A:321:ASN:HD21	1.60	0.49
1:A:37:LYS:O	1:A:587:VAL:HA	2.12	0.49
1:B:37:LYS:HB3	1:B:588:GLU:HB2	1.95	0.49
1:B:99:ILE:HG21	1:B:104:VAL:N	2.28	0.49
1:B:121:VAL:HG12	1:B:125:MET:HE2	1.94	0.49
1:A:571:HIS:CE1	1:A:574:GLU:HA	2.48	0.49
1:A:354:ILE:HD12	1:A:361:VAL:CG2	2.43	0.49
1:B:208:VAL:HG13	1:B:209:THR:N	2.28	0.49
1:A:54:THR:HG22	1:A:302:LYS:O	2.13	0.49
1:B:155:VAL:H	1:B:447:ILE:HB	1.76	0.48
1:A:175:PRO:HB2	1:A:221:TRP:HA	1.95	0.48
1:B:142:TYR:CE1	1:B:172:PHE:HB2	2.48	0.48
1:B:370:VAL:HG23	1:B:468:CYS:SG	2.53	0.48
1:A:332:TYR:CB	1:A:335:LEU:HD13	2.37	0.48
1:A:378:LEU:HG	1:A:478:ALA:CB	2.43	0.48
1:B:126:ASN:HA	1:B:129:ARG:CG	2.43	0.48
1:A:407:GLN:HB2	1:A:638:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:399:PHE:O	1:A:434:LEU:HD21	2.13	0.48
1:A:38:PHE:HB3	1:A:587:VAL:HG22	1.94	0.48
1:B:505:ASP:HB2	1:B:508:GLU:HG2	1.96	0.48
1:A:349:GLU:HA	1:A:618:PRO:HG3	1.96	0.48
1:A:534:LEU:HG	1:A:535:THR:N	2.28	0.48
1:A:213:PHE:O	1:A:217:MET:HG2	2.13	0.48
1:B:429:THR:O	1:B:431:PRO:HD3	2.13	0.48
1:A:613:LEU:N	1:A:613:LEU:HD12	2.29	0.48
1:A:19:ILE:H	1:A:19:ILE:HG13	1.39	0.48
1:B:342:LEU:HA	1:B:626:ILE:HG12	1.94	0.48
1:B:568:ARG:NH1	1:B:568:ARG:HB3	2.29	0.48
1:A:528:TYR:CE2	1:A:557:VAL:HG23	2.49	0.48
1:A:395:GLU:HG3	1:A:396:ASP:H	1.70	0.48
1:B:152:ASP:C	1:B:154:HIS:N	2.67	0.48
1:B:13:SER:OG	1:B:610:ARG:NH1	2.46	0.48
1:B:284:ARG:HD3	1:B:340:ALA:CB	2.40	0.48
1:B:163:ILE:HG23	1:B:226:ASN:ND2	2.29	0.48
1:A:195:SER:C	1:A:196:ILE:HG13	2.34	0.48
1:A:29:HIS:ND1	1:A:50:SER:HB3	2.28	0.48
1:B:174:TRP:CD2	1:B:216:MET:HE2	2.49	0.48
1:A:30:ASN:HA	1:A:595:ASP:O	2.14	0.48
1:A:47:TYR:CD2	1:A:47:TYR:N	2.81	0.48
1:B:149:MET:CE	1:B:156:LYS:HD3	2.43	0.48
1:A:27:VAL:HG13	1:A:29:HIS:NE2	2.29	0.48
1:B:129:ARG:O	1:B:133:LEU:HD22	2.13	0.48
1:B:384:THR:HG23	1:B:386:PHE:H	1.78	0.48
1:B:517:ARG:HE	1:B:539:ALA:HB3	1.78	0.48
1:B:142:TYR:O	1:B:170:THR:HA	2.13	0.48
1:B:639:ARG:HG3	1:B:640:ARG:N	2.28	0.48
1:A:283:ASN:HA	1:A:336:LEU:HD22	1.96	0.48
1:A:82:GLY:CA	1:B:95:SER:HB3	2.43	0.48
1:B:57:GLY:O	1:B:223:ARG:NH2	2.47	0.48
1:A:271:VAL:HA	1:A:274:SER:OG	2.14	0.48
1:B:301:MET:SD	1:B:366:MET:HA	2.53	0.48
1:B:634:TYR:N	1:B:634:TYR:HD1	2.12	0.48
1:B:291:THR:HG21	1:B:423:MET:HG3	1.97	0.47
1:B:493:ALA:CB	1:B:497:TYR:OH	2.62	0.47
1:B:204:ARG:HB2	1:B:205:PRO:HD3	1.95	0.47
1:B:162:THR:O	1:B:162:THR:HG22	2.14	0.47
1:A:550:GLU:C	1:A:550:GLU:CD	2.72	0.47
1:B:390:ILE:HD12	1:B:390:ILE:N	2.06	0.47
1:B:631:LEU:O	1:B:631:LEU:HD13	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1:MET:O	1:B:5:VAL:HG12	2.14	0.47
1:B:1:MET:HG3	1:B:364:TYR:CD1	2.50	0.47
1:A:625:VAL:O	1:A:625:VAL:HG13	2.14	0.47
1:B:220:LYS:HG3	1:B:234:PRO:HA	1.95	0.47
1:B:64:ASN:HA	1:B:324:LYS:NZ	2.30	0.47
1:B:630:GLU:CG	1:B:631:LEU:N	2.71	0.47
1:B:284:ARG:NH2	1:B:338:GLY:O	2.48	0.47
1:B:154:HIS:O	1:B:155:VAL:O	2.33	0.47
1:B:444:ILE:HG22	1:B:445:THR:H	1.79	0.47
1:A:296:LEU:O	1:A:299:ILE:HD13	2.15	0.47
1:A:99:ILE:HG22	1:A:104:VAL:HG13	1.96	0.47
1:B:506:LYS:HG3	1:B:558:MET:O	2.15	0.47
1:A:73:ILE:HG22	1:A:74:ALA:N	2.29	0.47
1:A:400:LEU:CD1	1:B:281:ASN:HB3	2.45	0.47
1:A:399:PHE:HB3	1:A:434:LEU:HD21	1.96	0.47
1:B:353:ALA:HA	1:B:616:VAL:HG23	1.93	0.47
1:B:527:VAL:HG11	1:B:531:THR:HG23	1.96	0.47
1:A:254:TRP:CA	1:A:259:ARG:HB3	2.45	0.47
1:A:29:HIS:HD1	1:A:50:SER:HB3	1.80	0.47
1:B:38:PHE:HB3	1:B:587:VAL:HG22	1.97	0.47
1:A:354:ILE:HD12	1:A:361:VAL:HG23	1.96	0.47
1:A:1:MET:HG3	1:A:364:TYR:CE1	2.50	0.47
1:A:371:ALA:HB3	1:A:410:LEU:CD2	2.45	0.47
1:B:56:VAL:HA	1:B:227:LEU:HA	1.96	0.47
1:B:331:ARG:HB3	1:B:332:TYR:CE1	2.49	0.47
1:B:531:THR:O	1:B:534:LEU:HB2	2.15	0.47
1:A:315:MET:SD	1:A:442:VAL:HG12	2.55	0.47
1:A:236:LEU:HD22	1:A:236:LEU:N	2.23	0.47
1:B:129:ARG:NH2	1:B:231:TYR:O	2.44	0.47
1:B:61:VAL:HA	1:B:320:VAL:HG13	1.96	0.47
1:B:284:ARG:CZ	1:B:336:LEU:O	2.63	0.47
1:A:96:THR:HG23	1:A:97:CYS:N	2.30	0.47
1:B:372:LEU:HD12	1:B:409:ALA:HB3	1.96	0.47
1:A:216:MET:CE	1:A:216:MET:HA	2.44	0.47
1:B:14:SER:HB2	1:B:611:ILE:HG23	1.96	0.47
1:A:61:VAL:HG21	1:A:231:TYR:CG	2.50	0.47
1:A:211:VAL:O	1:A:215:LEU:HD23	2.14	0.47
1:B:650:LEU:HD23	1:B:650:LEU:N	2.30	0.47
1:B:297:ALA:O	1:B:365:ALA:HB1	2.15	0.47
1:B:302:LYS:HE2	1:B:313:TRP:CZ2	2.49	0.47
1:B:116:TRP:CE3	1:B:328:ILE:HG12	2.50	0.46
1:A:283:ASN:HB3	1:A:329:ARG:HD3	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:194:PRO:HB3	1:A:331:ARG:HD2	1.97	0.46
1:A:396:ASP:O	1:A:397:GLY:O	2.34	0.46
1:A:353:ALA:HA	1:A:616:VAL:HG21	1.96	0.46
1:B:378:LEU:CD1	1:B:413:CYS:HA	2.45	0.46
1:A:446:VAL:O	1:A:447:ILE:HD13	2.14	0.46
1:B:253:GLU:HB3	1:B:259:ARG:HB2	1.95	0.46
1:A:414:THR:HB	1:A:416:GLN:NE2	2.30	0.46
1:B:66:GLY:O	1:B:117:TYR:HE1	1.99	0.46
1:B:493:ALA:N	1:B:584:PHE:CZ	2.83	0.46
1:B:490:VAL:HG23	1:B:587:VAL:C	2.36	0.46
1:B:519:ALA:O	1:B:572:PHE:O	2.32	0.46
1:B:7:LYS:HB2	1:B:10:GLN:HG2	1.97	0.46
1:B:344:GLN:HG3	1:B:635:TRP:CZ3	2.51	0.46
1:B:420:LEU:HD13	1:B:637:SER:CA	2.39	0.46
1:A:342:LEU:CD2	1:A:342:LEU:N	2.79	0.46
1:A:210:GLU:O	1:A:214:VAL:HG23	2.15	0.46
1:B:381:VAL:O	1:B:384:THR:N	2.48	0.46
1:A:115:ARG:HD2	1:A:115:ARG:N	2.31	0.46
1:B:331:ARG:HB3	1:B:332:TYR:CD1	2.51	0.46
1:B:59:PRO:CD	1:B:223:ARG:HH22	2.28	0.46
1:B:497:TYR:CG	1:B:581:PRO:HG3	2.50	0.46
1:A:316:HIS:CD2	1:A:433:LEU:HD11	2.50	0.46
1:A:318:ALA:HB2	1:A:430:TYR:CZ	2.50	0.46
1:B:531:THR:HG21	1:B:534:LEU:O	2.16	0.46
1:B:380:ARG:HH11	1:B:380:ARG:CG	2.28	0.46
1:B:64:ASN:O	1:B:323:PRO:HA	2.15	0.46
1:A:584:PHE:C	1:A:585:ARG:HG2	2.36	0.46
1:B:424:SER:O	1:B:425:ASP:HB2	2.16	0.46
1:B:1:MET:HG3	1:B:364:TYR:CE1	2.50	0.46
1:B:363:THR:O	1:B:367:GLN:HG3	2.16	0.46
1:B:611:ILE:HD13	1:B:611:ILE:O	2.15	0.46
1:B:570:ARG:NH1	1:B:570:ARG:CG	2.79	0.46
1:A:355:MET:CE	1:A:355:MET:HA	2.46	0.46
1:A:300:MET:HG2	1:A:301:MET:CE	2.46	0.46
1:B:156:LYS:C	1:B:156:LYS:HD2	2.35	0.46
1:A:154:HIS:C	1:A:447:ILE:HB	2.36	0.46
1:B:32:VAL:HG12	1:B:593:ILE:HG13	1.98	0.46
1:A:204:ARG:HD2	1:A:243:ARG:CD	2.46	0.46
1:B:514:TRP:HD1	1:B:546:THR:H	1.63	0.46
1:B:74:ALA:HB2	1:B:337:SER:O	2.15	0.46
1:A:18:SER:HB3	1:A:359:GLU:CG	2.45	0.46
1:B:650:LEU:CD2	1:B:650:LEU:H	2.29	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:154:HIS:CD2	1:B:448:GLU:HG3	2.46	0.46
1:B:603:HIS:O	1:B:604:ALA:O	2.33	0.46
1:A:133:LEU:HD12	1:A:142:TYR:HE2	1.81	0.46
1:A:445:THR:O	1:A:445:THR:HG22	2.16	0.46
1:B:118:ASP:O	1:B:119:ASN:HB2	2.17	0.45
1:B:319:LEU:O	1:B:319:LEU:HD23	2.17	0.45
1:B:76:LYS:HD2	1:B:77:TYR:CE2	2.51	0.45
1:A:198:VAL:O	1:A:200:TYR:CD1	2.68	0.45
1:B:99:ILE:HG21	1:B:104:VAL:HB	1.99	0.45
1:A:175:PRO:O	1:A:222:HIS:HB2	2.15	0.45
1:A:613:LEU:HA	1:A:616:VAL:HG12	1.98	0.45
1:B:563:THR:O	1:B:564:ALA:HB2	2.16	0.45
1:B:16:LEU:HD13	1:B:359:GLU:CB	2.47	0.45
1:B:616:VAL:O	1:B:617:LYS:C	2.54	0.45
1:A:137:THR:HG23	1:A:171:GLN:HA	1.98	0.45
1:B:283:ASN:N	1:B:283:ASN:ND2	2.64	0.45
1:B:581:PRO:O	1:B:582:ALA:HB3	2.17	0.45
1:B:17:PHE:O	1:B:363:THR:HG22	2.15	0.45
1:B:154:HIS:HA	1:B:447:ILE:HB	1.99	0.45
1:B:294:GLN:NE2	1:B:419:PRO:HB2	2.29	0.45
1:B:454:ILE:HD12	1:B:454:ILE:H	1.80	0.45
1:B:220:LYS:CG	1:B:234:PRO:HA	2.46	0.45
1:A:562:VAL:HG13	1:A:562:VAL:O	2.17	0.45
1:A:376:LEU:HB3	1:A:464:VAL:HG21	1.98	0.45
1:B:476:VAL:HB	1:B:485:TYR:O	2.16	0.45
1:A:312:ALA:HA	1:A:315:MET:HG3	1.97	0.45
1:A:198:VAL:O	1:A:200:TYR:HD1	1.99	0.45
1:B:638:VAL:O	1:B:638:VAL:HG13	2.17	0.45
1:B:59:PRO:HD2	1:B:223:ARG:NH2	2.32	0.45
1:A:300:MET:HB3	1:A:365:ALA:HB1	1.99	0.45
1:A:207:THR:HG23	1:A:210:GLU:H	1.82	0.45
1:A:157:ILE:HG22	1:A:443:PRO:O	2.17	0.45
1:B:499:ARG:HG3	1:B:499:ARG:H	1.42	0.45
1:B:19:ILE:HG23	1:B:362:PHE:CD1	2.52	0.45
1:B:42:VAL:O	1:B:42:VAL:HG13	2.17	0.45
1:A:583:PHE:CD1	1:A:583:PHE:N	2.84	0.45
1:B:99:ILE:CB	1:B:104:VAL:HB	2.46	0.45
1:B:418:ALA:O	1:B:637:SER:HB2	2.17	0.45
1:A:300:MET:HE3	1:A:365:ALA:HB3	1.98	0.45
1:B:163:ILE:HG23	1:B:226:ASN:HD21	1.82	0.45
1:B:29:HIS:HE1	1:B:48:GLY:HA3	1.81	0.45
1:A:117:TYR:CD2	1:A:326:GLY:HA3	2.52	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:455:VAL:O	1:B:458:HIS:HB2	2.17	0.45
1:A:448:GLU:HA	1:A:449:PRO:HD3	1.63	0.45
1:A:473:ILE:HD12	1:A:476:VAL:HG21	1.98	0.45
1:B:61:VAL:CB	1:B:320:VAL:HG13	2.47	0.45
1:A:204:ARG:HA	1:A:244:HIS:HA	1.99	0.45
1:A:470:PRO:HG2	1:A:545:TRP:CZ3	2.52	0.45
1:A:185:ASP:HB3	1:A:239:LYS:CG	2.47	0.45
1:A:435:GLU:HB2	1:A:438:ALA:HB2	1.99	0.45
1:A:73:ILE:HG13	1:A:329:ARG:NH2	2.32	0.44
1:A:78:LEU:HD13	1:A:84:LEU:HA	1.98	0.44
1:B:470:PRO:HG2	1:B:471:TYR:H	1.82	0.44
1:A:81:ASP:OD1	1:A:81:ASP:N	2.49	0.44
1:B:344:GLN:HG3	1:B:635:TRP:CH2	2.52	0.44
1:B:223:ARG:HH11	1:B:231:TYR:HA	1.79	0.44
1:A:204:ARG:HD2	1:A:243:ARG:CG	2.46	0.44
1:B:123:LEU:HB2	1:B:236:LEU:HD13	1.98	0.44
1:A:320:VAL:CG1	1:A:428:VAL:HG22	2.43	0.44
1:A:631:LEU:O	1:A:634:TYR:N	2.47	0.44
1:B:442:VAL:O	1:B:444:ILE:HG12	2.17	0.44
1:B:7:LYS:HD2	1:B:10:GLN:CD	2.37	0.44
1:B:23:ARG:NH1	1:B:23:ARG:HB2	2.32	0.44
1:B:130:ALA:HB2	1:B:221:TRP:CH2	2.52	0.44
1:A:137:THR:HA	1:A:142:TYR:HB2	2.00	0.44
1:A:521:TYR:CA	1:A:568:ARG:HG3	2.47	0.44
1:B:30:ASN:OD1	1:B:596:THR:HB	2.17	0.44
1:A:303:PRO:HB2	1:A:468:CYS:HB3	1.99	0.44
1:B:115:ARG:CG	1:B:115:ARG:HH11	2.31	0.44
1:A:207:THR:HG22	1:A:210:GLU:HB2	2.00	0.44
1:A:407:GLN:H	1:A:407:GLN:HG2	1.58	0.44
1:B:435:GLU:O	1:B:438:ALA:N	2.48	0.44
1:A:370:VAL:HA	1:A:468:CYS:SG	2.57	0.44
1:B:115:ARG:HD2	1:B:115:ARG:HA	1.61	0.44
1:B:127:MET:HB2	1:B:276:LEU:HD13	2.00	0.44
1:B:118:ASP:HB2	1:B:328:ILE:HB	2.00	0.44
1:B:126:ASN:O	1:B:129:ARG:HG2	2.18	0.44
1:A:204:ARG:N	1:A:205:PRO:CD	2.81	0.44
1:B:547:HIS:O	1:B:549:PRO:HD3	2.18	0.44
1:A:283:ASN:HD22	1:A:283:ASN:N	2.15	0.44
1:A:328:ILE:HA	1:A:331:ARG:HG3	1.99	0.44
1:A:332:TYR:HB2	1:A:335:LEU:CD1	2.39	0.44
1:B:129:ARG:HG3	1:B:221:TRP:CH2	2.52	0.44
1:B:91:ASN:HD22	1:B:94:ARG:HD2	1.82	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:481:THR:HG22	1:A:482:ALA:N	2.33	0.44
1:A:506:LYS:NZ	1:A:557:VAL:O	2.39	0.44
1:A:399:PHE:HB3	1:A:405:PHE:HD1	1.82	0.44
1:B:380:ARG:HA	1:B:436:PHE:HD2	1.78	0.44
1:A:131:TYR:CE1	1:A:269:SER:HB2	2.53	0.44
1:B:252:ASP:O	1:B:255:ILE:HB	2.18	0.44
1:B:470:PRO:O	1:B:472:MET:N	2.50	0.43
1:B:306:ASN:HD21	1:B:547:HIS:HE1	1.66	0.43
1:B:99:ILE:HA	1:B:100:PRO:HD3	1.77	0.43
1:A:395:GLU:HB3	1:A:436:PHE:HE1	1.80	0.43
1:B:223:ARG:HG3	1:B:230:ASP:O	2.18	0.43
1:B:61:VAL:CA	1:B:320:VAL:HG13	2.48	0.43
1:B:195:SER:C	1:B:196:ILE:HG13	2.39	0.43
1:B:479:PHE:C	1:B:481:THR:H	2.19	0.43
1:B:111:ILE:O	1:B:197:ASP:HB2	2.18	0.43
1:A:442:VAL:HA	1:A:443:PRO:HD3	1.85	0.43
1:B:58:ASN:HA	1:B:223:ARG:NH2	2.34	0.43
1:B:495:ASN:HB2	1:B:496:LYS:HE3	1.99	0.43
1:A:194:PRO:HD2	1:A:332:TYR:CZ	2.52	0.43
1:B:43:PHE:HB3	1:B:573:VAL:HG13	2.00	0.43
1:A:207:THR:HG22	1:A:210:GLU:HG3	1.99	0.43
1:B:312:ALA:O	1:B:315:MET:HG2	2.19	0.43
1:A:354:ILE:HD13	1:A:360:LEU:HD23	2.00	0.43
1:A:207:THR:HG22	1:A:210:GLU:CB	2.49	0.43
1:A:539:ALA:HB2	1:A:546:THR:HA	2.00	0.43
1:A:116:TRP:H	1:B:98:GLY:HA3	1.84	0.43
1:A:283:ASN:HA	1:A:336:LEU:HD13	2.00	0.43
1:A:320:VAL:HA	1:A:427:TYR:O	2.19	0.43
1:B:75:LYS:CA	1:B:341:ALA:HB2	2.47	0.43
1:A:616:VAL:O	1:A:616:VAL:HG22	2.19	0.43
1:A:85:ALA:O	1:A:89:VAL:HG23	2.19	0.43
1:A:24:GLY:C	1:A:25:THR:HG22	2.38	0.43
1:A:434:LEU:HA	1:A:434:LEU:HD22	1.84	0.43
1:B:211:VAL:HG12	1:B:215:LEU:HD11	1.99	0.43
1:A:380:ARG:O	1:A:383:LYS:HE3	2.19	0.43
1:B:71:GLU:OE1	1:B:71:GLU:N	2.51	0.43
1:B:112:THR:O	1:B:114:TRP:N	2.51	0.43
1:B:562:VAL:O	1:B:562:VAL:HG22	2.18	0.43
1:B:14:SER:CB	1:B:611:ILE:HG23	2.48	0.43
1:A:204:ARG:HB2	1:A:205:PRO:HD3	2.01	0.43
1:A:137:THR:CG2	1:A:172:PHE:H	2.27	0.43
1:A:89:VAL:O	1:A:93:LEU:HD13	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:188:GLN:HG2	1:B:247:THR:OG1	2.18	0.43
1:B:309:GLU:H	1:B:309:GLU:CD	2.21	0.43
1:B:112:THR:HG22	1:B:197:ASP:HA	2.01	0.43
1:A:82:GLY:N	1:B:95:SER:HB3	2.34	0.43
1:B:474:PHE:CD2	1:B:593:ILE:HD11	2.54	0.43
1:A:157:ILE:HG21	1:A:444:ILE:HG22	2.01	0.43
1:A:532:HIS:O	1:A:532:HIS:CG	2.72	0.43
1:B:210:GLU:HG2	1:B:275:ALA:HB2	2.00	0.43
1:B:200:TYR:CD1	1:B:241:ALA:HB3	2.54	0.43
1:A:154:HIS:CA	1:A:448:GLU:HG3	2.27	0.43
1:B:186:TRP:HA	1:B:240:PHE:O	2.19	0.43
1:B:510:TRP:NE1	1:B:546:THR:O	2.47	0.43
1:B:372:LEU:HD13	1:B:406:VAL:HG13	2.01	0.42
1:B:507:LEU:N	1:B:507:LEU:HD13	2.34	0.42
1:B:407:GLN:C	1:B:638:VAL:HG11	2.40	0.42
1:B:491:ILE:O	1:B:586:SER:HA	2.18	0.42
1:B:25:THR:HA	1:B:53:PHE:O	2.19	0.42
1:A:134:GLN:O	1:A:138:GLU:HB2	2.19	0.42
1:B:150:TYR:CZ	1:B:152:ASP:HB3	2.54	0.42
1:A:155:VAL:CG2	1:A:156:LYS:N	2.81	0.42
1:A:376:LEU:C	1:A:464:VAL:HG21	2.39	0.42
1:A:443:PRO:N	1:A:458:HIS:HB3	2.34	0.42
1:A:617:LYS:HA	1:A:618:PRO:HD3	1.87	0.42
1:B:112:THR:HB	1:B:331:ARG:CZ	2.49	0.42
1:A:74:ALA:O	1:A:78:LEU:HD23	2.19	0.42
1:A:396:ASP:OD2	1:B:277:ARG:CD	2.60	0.42
1:B:229:ILE:HB	1:B:296:LEU:HD11	2.01	0.42
1:B:202:ASP:OD1	1:B:204:ARG:HD3	2.18	0.42
1:A:93:LEU:HD21	1:A:193:PHE:HB3	2.01	0.42
1:A:344:GLN:OE1	1:A:626:ILE:HD11	2.19	0.42
1:B:372:LEU:HD12	1:B:409:ALA:CB	2.49	0.42
1:B:156:LYS:CG	1:B:445:THR:HG21	2.46	0.42
1:B:119:ASN:N	1:B:326:GLY:O	2.51	0.42
1:A:575:LEU:HB3	1:A:576:PRO:HD2	2.00	0.42
1:A:517:ARG:O	1:A:517:ARG:HD3	2.20	0.42
1:B:560:VAL:HG22	1:B:561:PHE:N	2.34	0.42
1:B:43:PHE:N	1:B:43:PHE:CD1	2.87	0.42
1:A:150:TYR:HB2	1:A:311:TYR:CE1	2.54	0.42
1:B:342:LEU:H	1:B:624:GLN:HG2	1.85	0.42
1:B:93:LEU:H	1:B:93:LEU:HG	1.53	0.42
1:B:403:GLU:HB2	1:B:634:TYR:HE2	1.83	0.42
1:B:64:ASN:HA	1:B:324:LYS:HG3	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:16:LEU:HD22	1:B:360:LEU:HA	2.01	0.42
1:B:305:PRO:HB2	1:B:311:TYR:CD1	2.54	0.42
1:B:504:TYR:O	1:B:560:VAL:HG12	2.20	0.42
1:A:159:LEU:HA	1:A:160:PRO:HD3	1.88	0.42
1:B:19:ILE:HG12	1:B:132:HIS:HD2	1.85	0.42
1:B:442:VAL:HB	1:B:459:LEU:HB3	2.01	0.42
1:A:610:ARG:HD3	1:A:610:ARG:HA	1.89	0.42
1:B:32:VAL:HG12	1:B:593:ILE:HA	2.01	0.42
1:B:33:ARG:NH1	1:B:594:TYR:HE1	2.18	0.42
1:A:498:LEU:HD11	1:A:561:PHE:CZ	2.55	0.42
1:A:208:VAL:HG13	1:A:209:THR:N	2.33	0.42
1:B:504:TYR:HB2	1:B:560:VAL:CG1	2.50	0.42
1:B:526:LYS:HB3	1:B:561:PHE:CD2	2.54	0.42
1:B:217:MET:CE	1:B:217:MET:HA	2.50	0.42
1:A:554:ASP:O	1:A:557:VAL:HG12	2.20	0.42
1:B:562:VAL:O	1:B:562:VAL:HG13	2.20	0.42
1:B:611:ILE:HD13	1:B:611:ILE:C	2.41	0.42
1:B:641:THR:HB	1:B:643:GLN:OE1	2.20	0.42
1:A:178:ARG:NH1	1:A:254:TRP:O	2.53	0.42
1:A:91:ASN:HA	1:A:94:ARG:NH1	2.35	0.42
1:A:470:PRO:O	1:A:474:PHE:HA	2.20	0.42
1:A:33:ARG:HG2	1:A:34:THR:N	2.35	0.42
1:A:128:LEU:O	1:A:131:TYR:HB3	2.20	0.42
1:A:435:GLU:OE2	1:B:278:LYS:HE3	2.19	0.42
1:B:643:GLN:HE21	1:B:643:GLN:HB2	1.69	0.41
1:B:474:PHE:HB3	1:B:475:PRO:HD3	2.01	0.41
1:A:442:VAL:O	1:A:444:ILE:HG23	2.20	0.41
1:A:451:GLY:C	1:A:452:TYR:HD1	2.23	0.41
1:B:188:GLN:O	1:B:188:GLN:HG3	2.19	0.41
1:A:121:VAL:O	1:A:125:MET:HB2	2.20	0.41
1:A:63:PHE:HA	1:A:322:ILE:O	2.20	0.41
1:B:218:MET:HG2	1:B:240:PHE:CZ	2.55	0.41
1:B:12:LYS:HB3	1:B:12:LYS:HE2	1.91	0.41
1:A:413:CYS:SG	1:A:478:ALA:HB2	2.61	0.41
1:A:61:VAL:HG13	1:A:320:VAL:HG23	2.02	0.41
1:A:354:ILE:CD1	1:A:360:LEU:HD23	2.51	0.41
1:A:343:ILE:CG2	1:A:348:LEU:HG	2.50	0.41
1:B:403:GLU:HG3	1:B:427:TYR:HD2	1.85	0.41
1:B:526:LYS:HB3	1:B:561:PHE:HD2	1.85	0.41
1:A:442:VAL:C	1:A:458:HIS:CB	2.88	0.41
1:B:19:ILE:HG12	1:B:132:HIS:CD2	2.56	0.41
1:B:505:ASP:O	1:B:508:GLU:N	2.52	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:514:TRP:HA	1:A:546:THR:CB	2.51	0.41
1:A:71:GLU:HG2	1:A:71:GLU:H	1.58	0.41
1:B:437:ASP:O	1:B:437:ASP:CG	2.59	0.41
1:A:528:TYR:CZ	1:A:557:VAL:HG23	2.55	0.41
1:B:394:TYR:CD1	1:B:644:GLY:HA2	2.54	0.41
1:A:426:VAL:HG23	1:A:426:VAL:O	2.20	0.41
1:A:512:LEU:C	1:A:512:LEU:HD23	2.41	0.41
1:A:600:ALA:O	1:A:604:ALA:HB3	2.19	0.41
1:A:132:HIS:O	1:A:136:LEU:HD23	2.20	0.41
1:B:488:ASN:HA	1:B:589:VAL:O	2.20	0.41
1:B:2:LEU:HD23	1:B:360:LEU:CD2	2.50	0.41
1:B:446:VAL:C	1:B:447:ILE:HG12	2.41	0.41
1:A:78:LEU:HD12	1:A:82:GLY:O	2.20	0.41
1:B:294:GLN:O	1:B:298:GLN:HG3	2.20	0.41
1:B:139:GLN:HB3	1:B:141:GLN:NE2	2.35	0.41
1:B:117:TYR:O	1:B:118:ASP:C	2.57	0.41
1:A:77:TYR:C	1:A:78:LEU:HD22	2.40	0.41
1:B:213:PHE:CE2	1:B:272:MET:HE3	2.56	0.41
1:A:423:MET:N	1:A:633:ASN:O	2.54	0.41
1:A:407:GLN:HB2	1:A:638:VAL:CG1	2.50	0.41
1:B:159:LEU:HA	1:B:160:PRO:HD3	1.79	0.41
1:B:54:THR:O	1:B:54:THR:HG23	2.20	0.41
1:B:354:ILE:HG13	1:B:360:LEU:HD23	2.02	0.41
1:A:372:LEU:O	1:A:376:LEU:HG	2.20	0.41
1:A:374:THR:O	1:A:378:LEU:HD23	2.21	0.41
1:A:123:LEU:HD13	1:A:218:MET:CE	2.39	0.41
1:B:470:PRO:HG3	1:B:545:TRP:CZ2	2.56	0.41
1:A:305:PRO:HB3	1:A:467:ALA:HB1	2.03	0.41
1:B:493:ALA:HB1	1:B:494:ALA:H	1.61	0.41
1:A:221:TRP:HZ3	1:A:223:ARG:HA	1.86	0.41
1:A:99:ILE:CG2	1:A:104:VAL:HG13	2.51	0.41
1:A:589:VAL:HG23	1:A:589:VAL:O	2.20	0.41
1:A:403:GLU:CD	1:A:403:GLU:H	2.23	0.41
1:B:4:PHE:HB2	1:B:419:PRO:HG3	2.03	0.41
1:B:172:PHE:O	1:B:266:PRO:HG2	2.20	0.41
1:B:203:VAL:HB	1:B:206:LEU:HD12	2.03	0.41
1:B:273:LEU:HD11	1:B:358:PRO:HG3	2.03	0.41
1:B:150:TYR:HB2	1:B:311:TYR:CZ	2.56	0.41
1:B:442:VAL:HA	1:B:443:PRO:HD3	1.95	0.41
1:A:386:PHE:C	1:A:388:THR:H	2.24	0.41
1:B:525:PHE:CB	1:B:561:PHE:O	2.65	0.41
1:B:630:GLU:OE1	1:B:635:TRP:HD1	2.04	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:130:ALA:O	1:B:272:MET:HE1	2.21	0.41
1:B:61:VAL:HG23	1:B:320:VAL:HG22	2.02	0.41
1:A:100:PRO:HG2	1:A:103:ALA:CB	2.48	0.41
1:B:577:ARG:HH11	1:B:577:ARG:HG2	1.86	0.41
1:A:645:LEU:CD2	1:A:645:LEU:H	2.34	0.41
1:B:33:ARG:HA	1:B:45:ARG:O	2.20	0.41
1:A:12:LYS:HB3	1:A:12:LYS:HE2	1.87	0.41
1:B:597:HIS:HD2	1:B:605:VAL:HG12	1.86	0.41
1:A:388:THR:HG23	1:A:388:THR:O	2.20	0.41
1:A:376:LEU:O	1:A:379:ARG:HB3	2.20	0.41
1:A:434:LEU:O	1:A:434:LEU:HD13	2.21	0.41
1:A:442:VAL:HG22	1:A:459:LEU:O	2.20	0.41
1:A:632:LYS:HB3	1:A:632:LYS:HE3	1.86	0.41
1:B:491:ILE:HG22	1:B:584:PHE:HE1	1.86	0.41
1:A:538:TYR:OH	1:A:540:ASP:HB2	2.21	0.41
1:B:299:ILE:HD12	1:B:299:ILE:C	2.41	0.40
1:B:277:ARG:O	1:B:281:ASN:HB2	2.21	0.40
1:B:59:PRO:HD2	1:B:223:ARG:HH12	1.86	0.40
1:B:473:ILE:HD13	1:B:473:ILE:N	2.36	0.40
1:A:142:TYR:CE2	1:A:172:PHE:HB2	2.56	0.40
1:B:89:VAL:HG13	1:B:334:PHE:CZ	2.56	0.40
1:B:483:ASN:CB	1:B:484:PRO:CD	2.98	0.40
1:B:64:ASN:HA	1:B:324:LYS:HZ2	1.87	0.40
1:B:87:ASP:O	1:B:91:ASN:HB2	2.21	0.40
1:A:474:PHE:N	1:A:475:PRO:CD	2.84	0.40
1:B:315:MET:HG2	1:B:315:MET:H	1.58	0.40
1:A:626:ILE:HD13	1:A:628:ALA:O	2.22	0.40
1:A:315:MET:CG	1:A:442:VAL:HG12	2.51	0.40
1:A:7:LYS:HA	1:A:7:LYS:HD3	1.87	0.40
1:A:74:ALA:HA	1:A:339:ASP:O	2.21	0.40
1:A:86:ILE:HG22	1:A:90:LEU:HD11	2.04	0.40
1:B:526:LYS:NZ	1:B:527:VAL:H	2.13	0.40
1:A:64:ASN:HB3	1:B:190:SER:CB	2.52	0.40
1:A:273:LEU:HD11	1:A:358:PRO:HG3	2.03	0.40
1:A:418:ALA:HA	1:A:419:PRO:HD2	1.87	0.40
1:B:201:LEU:H	1:B:201:LEU:HD23	1.83	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	649/680 (95%)	597 (92%)	36 (6%)	16 (2%)	9	57
1	B	649/680 (95%)	540 (83%)	63 (10%)	46 (7%)	2	25
All	All	1298/1360 (95%)	1137 (88%)	99 (8%)	62 (5%)	4	38

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	SER
1	A	397	GLY
1	A	473	ILE
1	A	531	THR
1	A	536	LYS
1	B	7	LYS
1	B	118	ASP
1	B	155	VAL
1	B	284	ARG
1	B	300	MET
1	B	451	GLY
1	B	454	ILE
1	B	471	TYR
1	B	476	VAL
1	B	477	ALA
1	B	573	VAL
1	B	602	ALA
1	B	630	GLU
1	A	83	GLY
1	A	168	GLY
1	A	556	ASP
1	A	564	ALA
1	B	12	LYS
1	B	14	SER
1	B	98	GLY
1	B	113	SER
1	B	119	ASN

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Mol	Chain	Res	Type
1	B	329	ARG
1	B	453	ASN
1	B	544	THR
1	B	603	HIS
1	A	72	GLY
1	A	114	TRP
1	B	13	SER
1	B	115	ARG
1	B	117	TYR
1	B	286	TYR
1	B	397	GLY
1	B	470	PRO
1	B	563	THR
1	B	604	ALA
1	B	608	ALA
1	B	634	TYR
1	A	112	THR
1	B	8	ASN
1	B	11	ASP
1	B	263	GLN
1	B	265	ARG
1	B	447	ILE
1	B	448	GLU
1	B	236	LEU
1	B	382	LYS
1	B	493	ALA
1	A	82	GLY
1	A	478	ALA
1	B	475	PRO
1	B	644	GLY
1	A	153	GLY
1	B	328	ILE
1	A	455	VAL
1	B	104	VAL
1	B	503	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	550/573 (96%)	462 (84%)	88 (16%)	3	22
1	B	550/573 (96%)	439 (80%)	111 (20%)	2	11
All	All	1100/1146 (96%)	901 (82%)	199 (18%)	2	15

All (199) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	13	SER
1	A	14	SER
1	A	19	ILE
1	A	25	THR
1	A	30	ASN
1	A	31	ARG
1	A	33	ARG
1	A	39	ASP
1	A	44	ASN
1	A	45	ARG
1	A	47	TYR
1	A	60	THR
1	A	71	GLU
1	A	87	ASP
1	A	96	THR
1	A	111	ILE
1	A	112	THR
1	A	115	ARG
1	A	119	ASN
1	A	125	MET
1	A	138	GLU
1	A	162	THR
1	A	166	THR
1	A	171	GLN
1	A	178	ARG
1	A	179	SER
1	A	186	TRP
1	A	188	GLN
1	A	195	SER
1	A	218	MET
1	A	221	TRP
1	A	224	ARG
1	A	252	ASP
1	A	258	ASP

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Mol	Chain	Res	Type
1	A	261	ASP
1	A	299	ILE
1	A	300	MET
1	A	315	MET
1	A	319	LEU
1	A	321	ASN
1	A	331	ARG
1	A	335	LEU
1	A	339	ASP
1	A	342	LEU
1	A	351	TRP
1	A	370	VAL
1	A	378	LEU
1	A	383	LYS
1	A	392	ASP
1	A	395	GLU
1	A	396	ASP
1	A	400	LEU
1	A	407	GLN
1	A	434	LEU
1	A	444	ILE
1	A	456	ASP
1	A	457	ASP
1	A	458	HIS
1	A	459	LEU
1	A	461	VAL
1	A	464	VAL
1	A	466	VAL
1	A	468	CYS
1	A	472	MET
1	A	473	ILE
1	A	492	LYS
1	A	498	LEU
1	A	499	ARG
1	A	507	LEU
1	A	516	LEU
1	A	517	ARG
1	A	528	TYR
1	A	530	ASP
1	A	548	ILE
1	A	550	GLU
1	A	560	VAL

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Mol	Chain	Res	Type
1	A	566	GLU
1	A	567	ARG
1	A	577	ARG
1	A	585	ARG
1	A	596	THR
1	A	611	ILE
1	A	624	GLN
1	A	630	GLU
1	A	632	LYS
1	A	642	GLN
1	A	650	LEU
1	B	5	VAL
1	B	8	ASN
1	B	11	ASP
1	B	12	LYS
1	B	15	ASP
1	B	19	ILE
1	B	31	ARG
1	B	49	VAL
1	B	50	SER
1	B	64	ASN
1	B	67	SER
1	B	68	SER
1	B	73	ILE
1	B	78	LEU
1	B	84	LEU
1	B	87	ASP
1	B	93	LEU
1	B	104	VAL
1	B	106	SER
1	B	112	THR
1	B	115	ARG
1	B	133	LEU
1	B	134	GLN
1	B	156	LYS
1	B	161	VAL
1	B	164	ASP
1	B	170	THR
1	B	178	ARG
1	B	179	SER
1	B	181	ASP
1	B	188	GLN

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Mol	Chain	Res	Type
1	B	196	ILE
1	B	198	VAL
1	B	201	LEU
1	B	224	ARG
1	B	249	GLN
1	B	250	ASP
1	B	256	GLU
1	B	258	ASP
1	B	263	GLN
1	B	270	LYS
1	B	285	LEU
1	B	301	MET
1	B	311	TYR
1	B	314	LEU
1	B	315	MET
1	B	317	ASP
1	B	319	LEU
1	B	320	VAL
1	B	328	ILE
1	B	329	ARG
1	B	332	TYR
1	B	339	ASP
1	B	348	LEU
1	B	355	MET
1	B	363	THR
1	B	376	LEU
1	B	379	ARG
1	B	380	ARG
1	B	390	ILE
1	B	393	SER
1	B	395	GLU
1	B	407	GLN
1	B	416	GLN
1	B	429	THR
1	B	437	ASP
1	B	445	THR
1	B	453	ASN
1	B	454	ILE
1	B	458	HIS
1	B	464	VAL
1	B	473	ILE
1	B	483	ASN

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Mol	Chain	Res	Type
1	B	486	CYS
1	B	488	ASN
1	B	492	LYS
1	B	499	ARG
1	B	500	LYS
1	B	507	LEU
1	B	521	TYR
1	B	522	ASP
1	B	523	THR
1	B	526	LYS
1	B	527	VAL
1	B	530	ASP
1	B	531	THR
1	B	532	HIS
1	B	536	LYS
1	B	545	TRP
1	B	550	GLU
1	B	558	MET
1	B	561	PHE
1	B	565	ILE
1	B	578	LEU
1	B	585	ARG
1	B	586	SER
1	B	595	ASP
1	B	599	GLN
1	B	605	VAL
1	B	609	SER
1	B	610	ARG
1	B	611	ILE
1	B	613	LEU
1	B	616	VAL
1	B	630	GLU
1	B	631	LEU
1	B	634	TYR
1	B	639	ARG
1	B	641	THR
1	B	642	GLN
1	B	643	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	30	ASN
1	A	51	GLN
1	A	58	ASN
1	A	119	ASN
1	A	212	ASN
1	A	235	GLN
1	A	281	ASN
1	A	283	ASN
1	A	298	GLN
1	A	316	HIS
1	A	321	ASN
1	A	344	GLN
1	A	407	GLN
1	A	416	GLN
1	A	441	GLN
1	A	483	ASN
1	A	571	HIS
1	A	597	HIS
1	A	624	GLN
1	B	8	ASN
1	B	10	GLN
1	B	29	HIS
1	B	58	ASN
1	B	64	ASN
1	B	91	ASN
1	B	102	ASN
1	B	107	HIS
1	B	154	HIS
1	B	235	GLN
1	B	283	ASN
1	B	344	GLN
1	B	416	GLN
1	B	495	ASN
1	B	547	HIS
1	B	597	HIS
1	B	599	GLN
1	B	642	GLN
1	B	643	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.



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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	651/680 (95%)	0.40	19 (2%)	49 23	16, 54, 114, 169	0
1	B	651/680 (95%)	0.43	25 (3%)	38 17	14, 60, 127, 167	0
All	All	1302/1360 (95%)	0.41	44 (3%)	43 19	14, 57, 125, 169	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	531	THR	7.0
1	B	499	ARG	5.5
1	A	222	HIS	4.4
1	B	98	GLY	4.1
1	B	530	ASP	3.9
1	B	506	LYS	3.8
1	B	564	ALA	3.6
1	B	453	ASN	3.5
1	B	502	ALA	3.4
1	B	532	HIS	3.2
1	A	391	ASP	3.2
1	B	528	TYR	3.1
1	A	564	ALA	3.1
1	B	454	ILE	3.0
1	B	501	GLY	2.9
1	B	533	GLY	2.9
1	A	166	THR	2.9
1	B	547	HIS	2.9
1	A	149	MET	2.8
1	B	500	LYS	2.8
1	A	452	TYR	2.7
1	A	529	GLY	2.7
1	B	452	TYR	2.7
1	B	419	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	640	ARG	2.6
1	A	410	LEU	2.6
1	A	354	ILE	2.4
1	B	604	ALA	2.4
1	A	590	SER	2.4
1	B	534	LEU	2.3
1	A	41	LEU	2.3
1	B	46	VAL	2.2
1	A	531	THR	2.2
1	A	37	LYS	2.2
1	A	203	VAL	2.1
1	A	613	LEU	2.1
1	B	527	VAL	2.1
1	A	351	TRP	2.1
1	B	620	SER	2.1
1	B	613	LEU	2.1
1	A	478	ALA	2.1
1	B	156	LYS	2.0
1	A	530	ASP	2.0
1	B	89	VAL	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.