

Full wwPDB X-ray Structure Validation Report (i)

Aug 16, 2023 – 07:49 PM EDT

PDB ID	:	2F1Z
Title	:	Crystal structure of HAUSP
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Deposited on	:	2005-11-15
Resolution	:	3.20 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 3.20 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	Similar resolution (#Entries, resolution range(Å))		
	(#Entries)	$(\#$ Entries, resolution range(\mathbf{A}))		
Clashscore	141614	1253 (3.20-3.20)		
Ramachandran outliers	138981	1234 (3.20-3.20)		
Sidechain outliers	138945	1233 (3.20-3.20)		

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain					
1	А	522	22%	52%	15% • 10%			
1	В	522	29%	48%	14% • 8%			



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8015 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	470	Total	С	N	0	S	0	0	0
			3842	2442	652	726	22	-		
1	В	/81	Total	\mathbf{C}	Ν	0	\mathbf{S}	0	0	0
1	I D	401	3933	2500	668	743	22	0		

• Molecule 1 is a protein called Ubiquitin carboxyl-terminal hydrolase 7.

There are 8	discrepancies	between	the modelled	and	reference	sequences:
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Chain	Residue	Modelled	Actual	Comment	Reference
А	39	GLY	-	cloning artifact	UNP Q93009
А	40	SER	-	cloning artifact	UNP Q93009
А	41	HIS	-	cloning artifact	UNP Q93009
А	42	MET	-	cloning artifact	UNP Q93009
В	39	GLY	-	cloning artifact	UNP Q93009
В	40	SER	-	cloning artifact	UNP Q93009
В	41	HIS	-	cloning artifact	UNP Q93009
В	42	MET	-	cloning artifact	UNP Q93009

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	118	Total O 118 118	0	0
2	В	122	Total O 122 122	0	0



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.

Note EDS was not executed.

• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 7









4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	C 2 2 21	Depositor	
Cell constants	97.62Å 219.86Å 130.55Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	20.00 - 3.20	Depositor	
% Data completeness	(Not available) $(20.00-3.20)$	Depositor	
(in resolution range)	(1101 available) (20.00 9.20)		
R_{merge}	(Not available)	Depositor	
R_{sym}	(Not available)	Depositor	
Refinement program	CNS	Depositor	
R, R_{free}	0.265 , 0.316	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	8015	wwPDB-VP	
Average B, all atoms $(Å^2)$	56.0	wwPDB-VP	



5 Model quality (i)

5.1 Standard geometry (i)

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

Mol Chain		Bo	nd lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.46	0/3935	0.74	1/5312~(0.0%)	
1	В	0.50	2/4032~(0.0%)	0.81	9/5449~(0.2%)	
All	All	0.48	2/7967~(0.0%)	0.78	10/10761~(0.1%)	

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	В	104	ARG	CZ-NH1	5.37	1.40	1.33
1	В	104	ARG	CB-CG	5.26	1.66	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	104	ARG	NE-CZ-NH2	-9.38	115.61	120.30
1	В	414	GLN	N-CA-C	-9.00	86.71	111.00
1	В	104	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	В	105	PHE	N-CA-C	7.61	131.54	111.00
1	В	387	GLN	CB-CA-C	-6.44	97.52	110.40
1	В	412	ASP	C-N-CA	-6.03	96.66	122.00
1	В	412	ASP	N-CA-C	-5.68	95.66	111.00
1	В	413	PRO	N-CA-C	5.44	126.24	112.10
1	В	90	CYS	N-CA-C	-5.26	96.80	111.00
1	А	470	ASN	N-CA-C	-5.03	97.41	111.00

There are no chirality outliers.



All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	448	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	3842	0	3710	428	1
1	В	3933	0	3794	406	0
2	А	118	0	0	44	0
2	В	122	0	0	41	0
All	All	8015	0	7504	821	1

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 54.

All (821) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:109:ARG:HE	1:B:110:PRO:HD2	1.21	1.04
1:B:491:GLU:HA	1:B:495:GLU:HG3	1.39	1.03
1:A:501:HIS:HB3	1:B:413:PRO:HG3	1.38	1.01
1:B:214:VAL:HG22	1:B:215:GLY:H	1.27	1.00
1:A:294:HIS:HB3	1:A:298:GLU:HG3	1.47	0.97
1:A:257:PRO:HG2	1:A:310:LYS:HG3	1.47	0.96
1:B:380:ASP:O	1:B:386:LEU:HA	1.65	0.96
1:B:237:GLN:HE21	1:B:527:VAL:HA	1.29	0.95
1:A:239:ARG:O	1:A:242:VAL:HG12	1.66	0.95
1:B:526:GLU:O	1:B:529:GLN:HG3	1.68	0.94
1:A:489:THR:HG22	1:A:492:GLU:OE2	1.68	0.92
1:A:256:VAL:HG22	1:A:282:SER:HB3	1.53	0.89
1:A:370:VAL:HG23	1:B:344:ARG:O	1.72	0.88
1:A:225:MET:HG3	1:A:299:LEU:HD21	1.58	0.86
1:A:448:TYR:HB3	1:A:518:TYR:HB3	1.58	0.86
1:A:302:VAL:O	1:A:306:ASN:HB2	1.76	0.86
1:B:92:VAL:HB	1:B:97:TRP:NE1	1.89	0.86



	lo ao pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:445:PRO:HB2	2:A:626:HOH:O	1.76	0.85
1:B:327:LYS:HB2	1:B:397:THR:HG23	1.57	0.84
1:B:382:GLY:HA3	2:B:659:HOH:O	1.76	0.84
1:A:412:ASP:HA	1:B:386:LEU:HD21	1.59	0.84
1:A:494:ILE:HG22	1:A:495:GLU:N	1.91	0.84
1:B:142:ASN:HD21	1:B:182:GLY:HA3	1.41	0.84
1:B:262:ARG:NH1	1:B:278:LYS:HD3	1.92	0.83
1:B:109:ARG:NE	1:B:110:PRO:HD2	1.93	0.83
1:B:142:ASN:ND2	1:B:182:GLY:HA3	1.93	0.83
1:A:354:ILE:HD13	1:A:355:LYS:N	1.93	0.82
1:A:135:GLN:HB2	1:A:196:GLN:HB2	1.61	0.82
1:B:184:ILE:HD11	1:B:187:ASP:HA	1.61	0.81
1:B:242:VAL:HG13	1:B:245:MET:HE2	1.60	0.81
1:A:266:GLU:HG2	1:A:270:SER:HB2	1.62	0.81
1:B:489:THR:OG1	1:B:492:GLU:HG3	1.80	0.81
1:A:323:LEU:O	1:A:400:PRO:HD2	1.80	0.81
1:A:210:HIS:H	1:A:210:HIS:CD2	1.99	0.80
1:A:239:ARG:NH2	1:A:531:VAL:HG11	1.97	0.80
1:B:448:TYR:HB3	1:B:518:TYR:HB3	1.64	0.79
1:A:115:VAL:HG21	1:A:176:VAL:HG11	1.64	0.79
1:A:429:GLU:H	1:B:293:GLN:NE2	1.79	0.79
1:A:415:THR:O	1:A:416:ASP:HB3	1.82	0.78
1:A:434:ASP:HB3	1:A:446:ALA:HB3	1.63	0.78
1:A:333:GLN:HE22	1:A:340:ARG:HD2	1.49	0.78
1:B:332:ILE:HG12	1:B:391:LYS:CB	2.13	0.78
1:A:412:ASP:HB3	1:A:415:THR:CG2	2.13	0.78
1:A:153:ARG:HD3	1:A:153:ARG:H	1.49	0.77
1:B:331:TYR:CD2	1:B:342:ASP:HB3	2.19	0.77
1:A:371:GLU:HB2	2:B:672:HOH:O	1.84	0.77
1:B:203:VAL:HG23	1:B:204:ALA:H	1.49	0.77
1:A:413:PRO:HG3	1:B:386:LEU:O	1.85	0.77
1:A:431:LEU:HG	1:A:433:LEU:HD13	1.65	0.77
1:B:221:ALA:HB1	1:B:288:LEU:HA	1.67	0.77
1:A:96:PRO:HG2	1:A:122:ASN:HA	1.68	0.76
1:A:529:GLN:HB2	2:A:673:HOH:O	1.85	0.76
1:B:119:LEU:CD1	1:B:193:VAL:HG11	2.15	0.76
1:B:324:PHE:HZ	2:B:585:HOH:O	1.66	0.76
1:B:217:LYS:HE2	1:B:275:GLY:HA2	1.67	0.76
1:B:332:ILE:HG12	1:B:391:LYS:HB3	1.68	0.76
1:B:350:ILE:HB	1:B:404:LEU:HD23	1.65	0.76
1:B:117:PHE:CE2	1:B:138:LEU:HB3	2.20	0.76



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:494:ILE:O	1:A:496:HIS:N	2.19	0.76
1:A:224:TYR:HB3	1:A:465:TYR:CE1	2.22	0.75
1:A:401:VAL:HG11	2:A:638:HOH:O	1.87	0.74
1:A:286:GLU:O	1:A:287:THR:HG22	1.87	0.74
1:B:381:ALA:HB1	2:B:576:HOH:O	1.88	0.74
1:B:308:GLU:OE1	1:B:320:ILE:HB	1.88	0.74
1:B:214:VAL:HG22	1:B:215:GLY:N	2.03	0.74
1:B:327:LYS:HB2	1:B:397:THR:CG2	2.16	0.73
1:B:481:ASP:HB3	1:B:484:VAL:HG23	1.70	0.73
1:B:493:ALA:O	1:B:497:ASN:ND2	2.21	0.73
1:A:182:GLY:O	1:A:184:ILE:N	2.22	0.73
1:A:531:VAL:HG21	2:A:567:HOH:O	1.88	0.73
1:B:79:SER:HA	2:B:662:HOH:O	1.87	0.73
1:B:200:PRO:HG2	1:B:203:VAL:HG21	1.70	0.73
1:A:354:ILE:HG22	2:A:603:HOH:O	1.87	0.73
1:A:153:ARG:HG2	1:A:153:ARG:HH11	1.54	0.73
1:A:429:GLU:H	1:B:293:GLN:HE22	1.34	0.73
1:B:237:GLN:NE2	1:B:527:VAL:HA	2.03	0.73
1:B:481:ASP:O	1:B:482:ASP:HB2	1.89	0.73
1:A:262:ARG:HG3	1:A:544:LEU:HD11	1.71	0.72
1:A:359:ASN:HD21	1:A:362:GLU:HG3	1.53	0.72
1:B:378:LYS:HE2	2:B:638:HOH:O	1.89	0.72
1:A:103:PRO:HD2	2:A:624:HOH:O	1.89	0.72
1:A:449:ILE:HD11	1:A:524:LEU:HD13	1.71	0.71
1:B:239:ARG:HA	2:B:639:HOH:O	1.90	0.71
1:B:308:GLU:HB2	1:B:320:ILE:HD12	1.71	0.71
1:A:247:THR:HG21	1:A:261:GLN:HE22	1.52	0.71
1:A:546:GLU:O	1:A:549:ARG:HG2	1.91	0.71
1:B:287:THR:HG22	1:B:288:LEU:N	2.05	0.71
1:A:367:TYR:HB3	2:A:610:HOH:O	1.89	0.71
1:B:460:ASN:O	1:B:462:GLY:N	2.22	0.71
1:A:353:SER:O	1:A:363:SER:OG	2.09	0.71
1:A:407:MET:HA	2:A:653:HOH:O	1.89	0.71
1:A:89:PRO:HD3	1:A:98:LYS:HE3	1.73	0.71
1:A:361:PHE:O	1:A:365:VAL:HG23	1.90	0.71
1:A:495:GLU:HB3	2:A:591:HOH:O	1.90	0.71
1:B:221:ALA:HB1	1:B:288:LEU:CA	2.20	0.71
1:A:286:GLU:OE1	1:A:286:GLU:HA	1.90	0.71
1:A:316:VAL:O	1:A:316:VAL:HG13	1.90	0.71
1:A:447:ASN:HB2	2:A:626:HOH:O	1.90	0.70
1:B:450:LEU:HD23	1:B:451:HIS:N	2.06	0.70



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:494:ILE:HG22	1:B:495:GLU:N	2.06	0.70
1:A:236:ASN:HB3	2:A:673:HOH:O	1.90	0.70
1:B:103:PRO:HB3	1:B:173:TRP:HZ3	1.55	0.70
1:A:307:VAL:O	1:A:311:MET:HG3	1.90	0.70
1:A:333:GLN:NE2	1:A:340:ARG:HD2	2.06	0.70
1:A:409:PHE:CE1	1:A:420:LYS:HD2	2.27	0.70
1:A:441:ASP:OD2	1:A:444:ASP:HB3	1.92	0.70
1:B:357:LYS:HD2	1:B:362:GLU:HB3	1.72	0.70
1:A:83:GLU:HA	2:A:624:HOH:O	1.91	0.69
1:B:87:SER:HB2	1:B:88:PRO:HD2	1.73	0.69
1:A:234:PHE:HE1	1:A:480:PHE:CE2	2.10	0.69
1:A:247:THR:CG2	1:A:261:GLN:HE22	2.05	0.69
1:A:117:PHE:CE2	1:A:138:LEU:HB3	2.28	0.69
1:B:351:GLN:HG3	2:B:591:HOH:O	1.92	0.69
1:A:93:ARG:NH1	1:A:205:TRP:HH2	1.90	0.69
1:A:247:THR:HG21	1:A:261:GLN:NE2	2.07	0.69
1:B:365:VAL:HG22	2:B:643:HOH:O	1.93	0.69
1:A:223:CYS:HB3	1:A:465:TYR:CE2	2.28	0.69
1:A:333:GLN:NE2	1:A:340:ARG:HB2	2.07	0.69
1:A:201:HIS:HB3	2:A:599:HOH:O	1.93	0.68
1:B:333:GLN:O	1:B:389:ALA:HB1	1.94	0.68
1:B:420:LYS:HE2	1:B:512:ASN:HD21	1.56	0.68
1:A:200:PRO:HG2	1:A:203:VAL:HG11	1.75	0.68
1:A:398:LEU:HG	1:A:437:LEU:HD21	1.76	0.68
1:A:177:THR:HG22	2:A:674:HOH:O	1.94	0.68
1:A:216:LEU:HD11	1:A:230:GLN:HG2	1.75	0.68
1:B:267:LEU:HG	2:B:657:HOH:O	1.93	0.68
1:B:76:GLU:HA	1:B:188:LYS:HG2	1.76	0.68
1:A:160:HIS:NE2	1:A:161:LYS:HG3	2.09	0.67
1:A:91:PHE:HB3	2:A:576:HOH:O	1.93	0.67
1:B:287:THR:CG2	1:B:288:LEU:N	2.57	0.67
1:B:405:GLN:HE21	1:B:515:MET:CE	2.07	0.67
1:B:217:LYS:NZ	1:B:277:LYS:HE3	2.09	0.67
1:B:539:GLN:CD	1:B:539:GLN:H	1.97	0.67
1:B:96:PRO:HG2	1:B:122:ASN:HA	1.77	0.66
1:B:114:SER:HB3	2:B:593:HOH:O	1.94	0.66
1:B:73:PHE:CG	1:B:87:SER:HB3	2.31	0.66
1:B:206:ASP:O	1:B:209:LYS:HG2	1.95	0.66
1:B:235:THR:HG21	2:B:585:HOH:O	1.94	0.66
1:B:328:MET:HE2	2:B:619:HOH:O	1.95	0.66
1:B:364:PHE:HB3	1:B:436:PHE:CZ	2.31	0.66



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:123:ALA:HB3	2:A:575:HOH:O	1.96	0.66
1:A:260:LEU:C	1:A:260:LEU:HD23	2.16	0.66
1:A:331:TYR:O	1:A:332:ILE:HG13	1.95	0.66
1:B:413:PRO:C	1:B:415:THR:H	1.82	0.66
1:B:450:LEU:HD22	1:B:477:TRP:HH2	1.60	0.66
1:A:412:ASP:OD2	1:A:413:PRO:HD3	1.96	0.66
1:A:219:GLN:HE22	1:A:464:HIS:HA	1.59	0.66
1:A:334:CYS:HA	1:A:389:ALA:HB2	1.78	0.66
1:B:228:LEU:HD12	1:B:299:LEU:CD1	2.25	0.66
1:B:297:GLN:HG2	1:B:405:GLN:OE1	1.96	0.66
1:A:489:THR:HG22	1:A:492:GLU:CD	2.16	0.65
1:B:114:SER:HB2	2:B:617:HOH:O	1.95	0.65
1:B:167:PHE:HB2	1:B:170:PHE:HB2	1.79	0.65
1:B:219:GLN:HE22	1:B:465:TYR:N	1.93	0.65
1:A:233:PHE:CG	1:A:267:LEU:HD23	2.31	0.65
1:A:136:ALA:HB3	1:A:154:ILE:CG1	2.27	0.65
1:A:466:VAL:HG12	1:A:467:VAL:H	1.62	0.65
1:B:152:ARG:HA	2:B:572:HOH:O	1.97	0.65
1:A:328:MET:O	1:A:344:ARG:HA	1.97	0.65
1:A:282:SER:HB2	2:A:630:HOH:O	1.96	0.65
1:A:494:ILE:HG22	1:A:495:GLU:H	1.59	0.65
1:A:442:PRO:O	1:A:443:LYS:HB2	1.96	0.64
1:B:260:LEU:HG	1:B:264:PHE:CE2	2.31	0.64
1:A:384:HIS:HB3	1:A:387:GLN:OE1	1.98	0.64
1:A:233:PHE:CD1	1:A:267:LEU:HD23	2.33	0.64
1:A:236:ASN:H	1:A:236:ASN:HD22	1.43	0.64
1:B:355:LYS:CD	1:B:356:GLY:H	2.10	0.64
1:B:470:ASN:O	1:B:470:ASN:ND2	2.30	0.64
1:A:211:THR:HG22	1:A:213:TYR:HB2	1.79	0.64
1:A:263:VAL:HG13	1:A:264:PHE:N	2.13	0.64
1:A:198:ASP:HB3	2:A:642:HOH:O	1.97	0.64
1:A:455:VAL:CG1	1:A:466:VAL:HB	2.27	0.64
1:A:308:GLU:OE1	1:A:318:GLY:HA2	1.97	0.64
1:A:308:GLU:C	1:A:310:LYS:H	1.98	0.64
1:B:350:ILE:HA	2:B:646:HOH:O	1.97	0.64
1:B:217:LYS:HE2	1:B:275:GLY:CA	2.28	0.64
1:B:411:TYR:O	1:B:411:TYR:CD1	2.51	0.64
1:A:355:LYS:NZ	1:B:377:ASN:O	2.27	0.64
1:B:219:GLN:O	1:B:220:GLY:O	2.16	0.64
1:B:247:THR:HA	1:B:250:ASP:OD2	1.98	0.64
1:B:350:ILE:HG22	1:B:352:LEU:HD13	1.80	0.64



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:236:ASN:H	1:A:236:ASN:ND2	1.94	0.63
1:B:193:VAL:HG23	2:B:635:HOH:O	1.98	0.63
1:B:318:GLY:O	1:B:321:PRO:HD2	1.97	0.63
1:A:364:PHE:O	1:A:368:VAL:HG22	1.98	0.63
1:B:103:PRO:HB3	1:B:173:TRP:CZ3	2.33	0.63
1:B:354:ILE:HG22	1:B:425:PHE:CE2	2.33	0.63
1:A:294:HIS:CB	1:A:298:GLU:HG3	2.27	0.63
1:B:119:LEU:HD13	1:B:193:VAL:HG11	1.79	0.63
1:B:308:GLU:CB	1:B:320:ILE:HD12	2.28	0.63
1:A:421:ILE:CG2	1:A:423:ASP:OD2	2.47	0.63
1:A:329:VAL:CG2	1:A:396:LEU:HD11	2.28	0.63
1:A:359:ASN:C	1:A:359:ASN:HD22	2.02	0.63
1:A:415:THR:OG1	1:A:417:GLN:HG2	1.98	0.63
1:B:153:ARG:HH11	1:B:153:ARG:HG2	1.62	0.63
1:A:153:ARG:H	1:A:153:ARG:CD	2.11	0.62
1:A:225:MET:HG2	1:A:229:LEU:HD22	1.80	0.62
1:A:156:HIS:ND1	1:A:165:TRP:HB2	2.14	0.62
1:A:237:GLN:HE22	1:A:526:GLU:HG2	1.65	0.62
1:A:295:ASP:O	1:A:298:GLU:HG2	1.99	0.62
1:A:476:LYS:HE3	1:A:476:LYS:HA	1.82	0.62
1:B:365:VAL:HA	1:B:368:VAL:CG2	2.30	0.62
1:A:285:TRP:HA	1:A:290:SER:OG	1.98	0.62
1:B:421:ILE:O	1:B:421:ILE:HG22	2.00	0.62
1:B:78:PHE:CE2	1:B:173:TRP:CH2	2.87	0.62
1:A:360:ILE:HD11	1:A:427:PHE:HB3	1.81	0.62
1:B:105:PHE:HE1	1:B:107:PRO:HB3	1.63	0.62
1:B:228:LEU:HD12	1:B:299:LEU:HD13	1.82	0.62
1:B:318:GLY:C	1:B:321:PRO:HD2	2.19	0.62
1:B:329:VAL:HG22	1:B:344:ARG:HG3	1.81	0.62
1:A:245:MET:CE	1:A:257:PRO:HB3	2.29	0.62
1:A:267:LEU:HD12	1:A:274:VAL:HG21	1.82	0.61
1:B:455:VAL:HG22	1:B:512:ASN:O	2.00	0.61
1:A:71:PHE:CE2	1:A:193:VAL:HB	2.35	0.61
1:B:217:LYS:HZ3	1:B:277:LYS:HE3	1.66	0.61
1:B:308:GLU:OE1	1:B:321:PRO:HD3	2.00	0.61
1:A:136:ALA:HB3	1:A:154:ILE:HG13	1.82	0.61
1:A:227:SER:HB3	1:A:467:VAL:HB	1.82	0.61
1:A:449:ILE:HD11	1:A:524:LEU:CD1	2.30	0.61
1:A:470:ASN:N	1:A:470:ASN:HD22	1.97	0.61
1:B:200:PRO:HG2	1:B:203:VAL:CG2	2.29	0.61
1:B:354:ILE:HD12	1:B:355:LYS:N	2.16	0.61



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:237:GLN:NE2	1:A:526:GLU:HG2	2.15	0.61
1:B:323:LEU:O	1:B:400:PRO:HD2	2.01	0.61
1:B:332:ILE:HG12	1:B:391:LYS:HB2	1.80	0.61
1:B:453:VAL:HG13	1:B:468:TYR:HB2	1.81	0.61
1:A:94:ASN:HA	2:A:576:HOH:O	2.01	0.61
1:A:236:ASN:HD22	1:A:236:ASN:N	1.98	0.61
1:B:92:VAL:HB	1:B:97:TRP:HE1	1.64	0.60
1:A:185:ASP:O	1:A:186:ASP:HB2	1.99	0.60
1:A:283:PHE:HB2	1:A:285:TRP:CD1	2.36	0.60
1:A:526:GLU:O	1:A:529:GLN:HG3	2.00	0.60
1:A:288:LEU:HD13	2:A:593:HOH:O	2.02	0.60
1:A:334:CYS:HA	1:A:389:ALA:CB	2.32	0.60
1:B:371:GLU:OE2	1:B:391:LYS:HE3	2.01	0.60
1:B:203:VAL:HG23	1:B:204:ALA:N	2.14	0.60
1:B:532:THR:C	1:B:534:HIS:H	2.04	0.60
1:B:547:GLU:O	1:B:551:GLU:HG3	2.01	0.60
1:A:494:ILE:C	1:A:496:HIS:H	2.05	0.60
1:B:256:VAL:HG22	1:B:282:SER:HB3	1.82	0.60
1:A:298:GLU:O	1:A:302:VAL:HG23	2.01	0.60
1:A:333:GLN:NE2	1:A:340:ARG:CD	2.65	0.60
1:A:71:PHE:CD1	1:A:90:CYS:HB2	2.37	0.60
1:A:537:PRO:O	1:A:538:GLN:HB2	2.02	0.60
1:B:93:ARG:HG3	1:B:198:ASP:O	2.02	0.60
1:B:184:ILE:HG12	1:B:185:ASP:N	2.17	0.60
1:B:78:PHE:HD1	1:B:189:VAL:HG21	1.67	0.60
1:B:382:GLY:O	1:B:384:HIS:N	2.35	0.60
1:A:431:LEU:CG	1:A:433:LEU:HD13	2.32	0.59
1:A:210:HIS:H	1:A:210:HIS:HD2	1.49	0.59
1:A:263:VAL:O	1:A:267:LEU:HB2	2.01	0.59
1:A:211:THR:HG23	1:A:478:CYS:SG	2.42	0.59
1:B:156:HIS:HD2	2:B:680:HOH:O	1.84	0.59
1:A:160:HIS:CG	1:A:161:LYS:H	2.20	0.59
1:A:217:LYS:HB3	2:A:628:HOH:O	2.02	0.59
1:B:406:LEU:N	1:B:514:TYR:O	2.36	0.59
1:B:295:ASP:O	1:B:296:VAL:C	2.41	0.59
1:B:450:LEU:HD22	1:B:477:TRP:CH2	2.37	0.59
1:B:245:MET:SD	1:B:307:VAL:HG13	2.43	0.59
1:A:232:LEU:HD23	1:A:238:LEU:HD23	1.85	0.58
1:A:470:ASN:HD22	1:A:470:ASN:H	1.50	0.58
1:B:242:VAL:HG13	1:B:245:MET:CE	2.31	0.58
1:B:383:GLU:C	1:B:385:GLY:H	2.05	0.58



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:93:ARG:NE	1:B:198:ASP:O	2.34	0.58
1:B:304:LEU:O	1:B:320:ILE:HD13	2.03	0.58
1:B:383:GLU:C	1:B:385:GLY:N	2.57	0.58
1:B:354:ILE:HD12	1:B:355:LYS:H	1.67	0.58
1:B:405:GLN:HE21	1:B:515:MET:HE3	1.69	0.58
1:A:210:HIS:CD2	1:A:210:HIS:N	2.71	0.58
1:B:78:PHE:O	1:B:79:SER:C	2.41	0.58
1:A:446:ALA:HA	1:A:520:ARG:HE	1.68	0.58
1:A:225:MET:HG3	1:A:299:LEU:CD2	2.32	0.58
1:B:355:LYS:HD3	1:B:356:GLY:H	1.69	0.58
1:B:413:PRO:HB2	1:B:415:THR:HB	1.86	0.58
1:B:171:MET:HG2	1:B:172:ALA:H	1.68	0.58
1:B:307:VAL:O	1:B:310:LYS:HB3	2.04	0.58
1:A:259:ALA:HA	1:A:262:ARG:HH21	1.69	0.58
1:B:337:VAL:HG12	1:B:338:ASP:N	2.18	0.58
1:A:260:LEU:O	1:A:263:VAL:HG12	2.03	0.58
1:A:523:LYS:O	1:A:527:VAL:HG23	2.02	0.58
1:A:421:ILE:HG23	1:A:423:ASP:OD2	2.04	0.57
1:A:434:ASP:HB3	1:A:446:ALA:CB	2.31	0.57
1:A:154:ILE:HG13	1:A:154:ILE:O	2.03	0.57
1:A:332:ILE:HA	1:A:390:GLU:O	2.03	0.57
1:A:368:VAL:HG13	2:A:610:HOH:O	2.04	0.57
1:B:73:PHE:CD2	1:B:87:SER:HB3	2.39	0.57
1:B:103:PRO:CB	1:B:173:TRP:HZ3	2.16	0.57
1:B:295:ASP:O	1:B:297:GLN:N	2.37	0.57
1:A:353:SER:HA	2:A:603:HOH:O	2.02	0.57
1:A:455:VAL:HG12	1:A:466:VAL:HB	1.85	0.57
1:A:501:HIS:CB	1:B:413:PRO:HG3	2.24	0.57
1:A:333:GLN:O	1:A:334:CYS:C	2.42	0.57
1:B:263:VAL:O	1:B:267:LEU:HD13	2.05	0.57
1:B:153:ARG:HG2	1:B:153:ARG:NH1	2.19	0.57
1:A:153:ARG:HG2	1:A:153:ARG:NH1	2.17	0.57
1:A:168:SER:HB3	2:A:645:HOH:O	2.03	0.57
1:B:109:ARG:HD3	2:B:571:HOH:O	2.04	0.57
1:B:169:ASN:HA	2:B:593:HOH:O	2.05	0.57
1:B:243:TYR:OH	1:B:268:GLN:NE2	2.38	0.57
1:A:214:VAL:HG12	1:A:215:GLY:H	1.69	0.57
1:A:308:GLU:C	1:A:310:LYS:N	2.58	0.57
1:A:374:ASP:HA	1:A:378:LYS:HG3	1.86	0.57
1:B:102:MET:SD	1:B:104:ARG:NH1	2.78	0.57
1:B:312:LYS:HG3	1:B:313:GLY:N	2.18	0.57



	lo ao pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:354:ILE:HG22	1:B:425:PHE:CD2	2.39	0.57
1:A:420:LYS:HE2	1:A:422:ASN:OD1	2.05	0.57
1:A:467:VAL:O	1:A:467:VAL:HG13	2.03	0.57
1:B:78:PHE:HD1	1:B:189:VAL:CG2	2.18	0.57
1:B:99:ILE:HG12	1:B:193:VAL:HG21	1.87	0.57
1:B:287:THR:CG2	1:B:288:LEU:H	2.18	0.57
1:B:452:ALA:CB	1:B:469:LEU:HG	2.35	0.57
1:A:76:GLU:HA	1:A:188:LYS:HG2	1.86	0.56
1:B:308:GLU:CD	1:B:321:PRO:HD3	2.25	0.56
1:A:248:GLU:O	1:A:250:ASP:N	2.37	0.56
1:A:333:GLN:O	1:A:334:CYS:O	2.24	0.56
1:A:406:LEU:HD12	1:A:406:LEU:N	2.20	0.56
1:A:519:ILE:HD13	1:A:527:VAL:HG11	1.87	0.56
1:B:156:HIS:CD2	1:B:157:LEU:H	2.23	0.56
1:B:365:VAL:O	1:B:369:ALA:N	2.38	0.56
1:B:495:GLU:HA	1:B:498:TYR:CD1	2.41	0.56
1:A:224:TYR:HB3	1:A:465:TYR:CD1	2.40	0.56
1:A:288:LEU:HA	1:A:291:PHE:HD2	1.70	0.56
1:B:267:LEU:HD12	1:B:274:VAL:HG21	1.88	0.56
1:A:78:PHE:HD2	2:A:674:HOH:O	1.88	0.56
1:B:150:PHE:HD2	1:B:171:MET:CE	2.18	0.56
1:B:299:LEU:O	1:B:299:LEU:HD22	2.06	0.56
1:B:386:LEU:O	1:B:386:LEU:HG	2.04	0.56
1:A:177:THR:HA	1:A:184:ILE:HD13	1.87	0.56
1:B:427:PHE:H	1:B:498:TYR:HE2	1.53	0.56
1:A:454:LEU:HD12	1:A:454:LEU:N	2.21	0.56
1:A:103:PRO:HB3	1:A:173:TRP:CZ3	2.41	0.56
1:A:406:LEU:N	1:A:406:LEU:CD1	2.69	0.56
1:A:494:ILE:CG2	1:A:495:GLU:N	2.63	0.55
1:A:284:GLY:O	1:A:286:GLU:N	2.40	0.55
1:B:118:PHE:HB3	1:B:164:ASP:OD1	2.07	0.55
1:B:411:TYR:O	1:B:411:TYR:HD1	1.88	0.55
1:B:405:GLN:HE21	1:B:515:MET:HE2	1.72	0.55
1:B:334:CYS:HB2	1:B:339:TYR:O	2.07	0.55
1:A:414:GLN:C	1:A:415:THR:HG22	2.27	0.55
1:A:160:HIS:CG	1:A:161:LYS:N	2.73	0.55
1:A:398:LEU:HD13	1:A:433:LEU:HD23	1.87	0.55
1:A:407:MET:HB2	2:A:603:HOH:O	2.05	0.55
1:A:438:GLN:N	1:A:438:GLN:OE1	2.40	0.55
1:B:412:ASP:HB3	2:B:647:HOH:O	2.06	0.55
1:A:467:VAL:HG22	1:A:469:LEU:HD12	1.88	0.55



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:219:GLN:HE22	1:B:465:TYR:H	1.54	0.55
1:B:214:VAL:O	1:B:485:VAL:HG21	2.06	0.55
1:A:283:PHE:CE2	1:A:303:LEU:HD21	2.42	0.55
1:A:479:LYS:O	1:A:485:VAL:HA	2.07	0.55
1:A:339:TYR:HE2	2:A:623:HOH:O	1.89	0.54
1:A:241:ALA:CB	1:A:316:VAL:HG21	2.36	0.54
1:A:279:LEU:HG	1:A:283:PHE:CZ	2.42	0.54
1:A:408:ARG:NH2	1:A:513:ALA:O	2.41	0.54
1:A:214:VAL:HG21	1:A:270:SER:O	2.07	0.54
1:A:248:GLU:OE2	1:A:543:ARG:HD2	2.07	0.54
1:A:256:VAL:HB	1:A:257:PRO:HD3	1.89	0.54
1:A:242:VAL:CG1	1:A:243:TYR:N	2.71	0.54
1:A:314:THR:HA	2:A:596:HOH:O	2.07	0.54
1:A:458:GLY:C	1:A:460:ASN:H	2.09	0.54
1:B:143:TYR:HD1	1:B:185:ASP:HB2	1.73	0.54
1:B:376:ASP:HA	1:B:379:TYR:CD1	2.42	0.54
1:B:453:VAL:O	1:B:453:VAL:HG22	2.07	0.54
1:B:75:VAL:O	1:B:188:LYS:HA	2.07	0.54
1:B:289:ASP:HA	1:B:292:MET:HB2	1.89	0.54
1:B:308:GLU:HG3	2:B:653:HOH:O	2.07	0.54
1:A:258:LEU:O	1:A:261:GLN:N	2.40	0.54
1:B:383:GLU:O	1:B:385:GLY:N	2.41	0.54
1:B:219:GLN:O	1:B:220:GLY:C	2.47	0.53
1:B:524:LEU:HD22	1:B:528:LEU:HD12	1.90	0.53
1:A:308:GLU:OE2	1:A:321:PRO:HD3	2.08	0.53
1:B:99:ILE:HD13	2:B:635:HOH:O	2.08	0.53
1:A:228:LEU:HD13	1:A:299:LEU:HD23	1.89	0.53
1:A:374:ASP:HA	1:A:378:LYS:CG	2.38	0.53
1:B:78:PHE:N	1:B:187:ASP:O	2.38	0.53
1:B:73:PHE:CG	1:B:87:SER:CB	2.91	0.53
1:A:289:ASP:O	1:A:293:GLN:HB2	2.09	0.53
1:A:329:VAL:HG22	1:A:344:ARG:HG2	1.90	0.53
1:A:515:MET:CG	1:A:516:LEU:N	2.72	0.53
1:B:228:LEU:CD1	1:B:299:LEU:HD13	2.38	0.53
1:B:452:ALA:HB2	1:B:469:LEU:HG	1.90	0.53
1:B:173:TRP:HE1	1:B:177:THR:HG21	1.73	0.53
1:B:222:THR:HB	1:B:225:MET:HE2	1.91	0.53
1:A:234:PHE:HE1	1:A:480:PHE:CZ	2.27	0.52
1:B:365:VAL:HA	1:B:368:VAL:HG23	1.91	0.52
1:A:487:ARG:HD3	2:A:612:HOH:O	2.09	0.52
1:B:204:ALA:C	1:B:206:ASP:H	2.12	0.52



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:260:LEU:HG	1:B:264:PHE:CD2	2.43	0.52
1:A:262:ARG:NH2	1:A:278:LYS:HB3	2.24	0.52
1:A:269:HIS:HD2	2:A:678:HOH:O	1.92	0.52
1:A:180:GLU:O	1:A:180:GLU:HG2	2.09	0.52
1:A:117:PHE:HD2	1:A:170:PHE:CZ	2.27	0.52
1:A:150:PHE:HB3	1:A:171:MET:HE2	1.92	0.52
1:A:211:THR:HG21	1:A:485:VAL:HG12	1.92	0.52
1:A:333:GLN:O	1:A:333:GLN:HG3	2.10	0.52
1:B:364:PHE:HB3	1:B:436:PHE:CE2	2.45	0.52
1:A:152:ARG:NH1	1:A:170:PHE:O	2.42	0.52
1:A:218:ASN:HB3	2:A:590:HOH:O	2.09	0.52
1:A:263:VAL:CG1	1:A:264:PHE:N	2.72	0.52
1:A:295:ASP:HB3	1:A:297:GLN:OE1	2.10	0.52
1:A:295:ASP:H	1:A:298:GLU:CG	2.23	0.52
1:A:455:VAL:HG22	1:A:456:HIS:N	2.25	0.52
1:B:160:HIS:NE2	1:B:161:LYS:HG3	2.25	0.52
1:A:455:VAL:HB	1:A:497:ASN:HD21	1.75	0.52
1:B:67:SER:HA	1:B:93:ARG:CZ	2.40	0.52
1:B:78:PHE:O	1:B:80:ARG:N	2.43	0.52
1:B:235:THR:O	1:B:238:LEU:N	2.38	0.52
1:A:211:THR:CG2	1:A:213:TYR:HB2	2.40	0.52
1:A:335:LYS:NZ	1:B:344:ARG:HH22	2.08	0.52
1:B:232:LEU:HD13	1:B:304:LEU:HD21	1.91	0.52
1:B:255:SER:OG	1:B:257:PRO:HD2	2.09	0.52
1:A:239:ARG:HH22	1:A:531:VAL:HG11	1.75	0.51
1:B:191:PHE:CD1	1:B:191:PHE:N	2.76	0.51
1:B:206:ASP:HB3	1:B:209:LYS:HE3	1.92	0.51
1:B:230:GLN:O	1:B:234:PHE:HD1	1.93	0.51
1:A:157:LEU:HB3	2:A:657:HOH:O	2.10	0.51
1:A:536:ILE:CG2	1:A:540:LEU:HD12	2.40	0.51
1:B:409:PHE:HB3	2:B:628:HOH:O	2.09	0.51
1:A:412:ASP:OD2	1:A:413:PRO:CD	2.58	0.51
1:B:105:PHE:CE1	1:B:107:PRO:HB3	2.46	0.51
1:A:279:LEU:HD12	2:A:630:HOH:O	2.09	0.51
1:B:431:LEU:HG	1:B:433:LEU:HD13	1.91	0.51
1:A:407:MET:HA	1:A:407:MET:HE2	1.92	0.51
1:A:410:MET:HE1	1:B:381:ALA:O	2.11	0.51
1:B:78:PHE:O	1:B:81:LEU:N	2.43	0.51
1:B:466:VAL:HG11	1:B:479:LYS:HE3	1.92	0.51
1:A:140:ILE:HG13	1:A:170:PHE:HE2	1.75	0.51
1:A:333:GLN:HE21	1:A:340:ARG:NE	2.08	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:71:PHE:CD1	1:A:90:CYS:CB	2.94	0.51
1:A:359:ASN:ND2	1:A:362:GLU:HG3	2.23	0.51
1:B:335:LYS:HG2	1:B:390:GLU:OE2	2.11	0.51
1:A:279:LEU:HA	2:A:630:HOH:O	2.10	0.51
1:B:414:GLN:O	1:B:416:ASP:N	2.44	0.51
1:A:102:MET:CE	1:A:104:ARG:HD3	2.40	0.51
1:A:203:VAL:HG13	1:A:203:VAL:O	2.11	0.51
1:A:480:PHE:N	1:A:480:PHE:CD1	2.79	0.51
1:A:495:GLU:HG3	2:A:573:HOH:O	2.09	0.51
1:B:191:PHE:HB3	2:B:635:HOH:O	2.10	0.51
1:B:420:LYS:HE2	1:B:512:ASN:ND2	2.24	0.51
1:A:152:ARG:HD3	1:A:167:PHE:CE1	2.45	0.50
1:A:118:PHE:HB3	1:A:164:ASP:OD1	2.11	0.50
1:A:226:ASN:HD21	1:A:276:THR:HG21	1.76	0.50
1:A:426:GLU:HG2	1:A:498:TYR:CD1	2.47	0.50
1:B:357:LYS:NZ	1:B:366:ASP:HB2	2.25	0.50
1:A:427:PHE:CD2	1:A:427:PHE:N	2.78	0.50
1:A:488:CYS:HB2	1:A:492:GLU:OE1	2.12	0.50
1:B:213:TYR:CZ	1:B:471:PRO:HG2	2.47	0.50
1:B:357:LYS:HE3	1:B:366:ASP:CB	2.40	0.50
1:B:361:PHE:C	1:B:361:PHE:CD2	2.85	0.50
1:B:416:ASP:O	1:B:417:GLN:HB2	2.10	0.50
1:B:429:GLU:CG	1:B:430:GLN:N	2.74	0.50
1:B:335:LYS:NZ	1:B:372:GLN:HE22	2.09	0.50
1:A:256:VAL:O	1:A:257:PRO:C	2.50	0.50
1:A:329:VAL:O	1:A:393:VAL:HA	2.12	0.50
1:B:155:SER:O	1:B:156:HIS:HB2	2.12	0.50
1:B:330:SER:O	1:B:342:ASP:HA	2.11	0.50
1:A:285:TRP:HE3	1:A:291:PHE:CD1	2.30	0.50
1:A:458:GLY:C	1:A:460:ASN:N	2.65	0.50
1:B:239:ARG:HD2	1:B:531:VAL:HG11	1.94	0.50
1:B:277:LYS:H	1:B:277:LYS:HD3	1.76	0.50
1:B:405:GLN:HA	1:B:515:MET:HA	1.93	0.50
1:A:214:VAL:HG12	1:A:215:GLY:N	2.26	0.50
1:A:241:ALA:HB1	1:A:316:VAL:HG21	1.93	0.50
1:A:327:LYS:HE2	1:A:346:ASP:OD1	2.12	0.50
1:B:139:LYS:HB2	1:B:151:SER:HB3	1.93	0.50
1:A:415:THR:O	1:A:416:ASP:CB	2.55	0.49
1:B:413:PRO:HD2	2:B:647:HOH:O	2.11	0.49
1:A:318:GLY:O	1:A:321:PRO:HD2	2.12	0.49
1:A:331:TYR:C	1:A:332:ILE:HG13	2.32	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:B:173:TRP:NE1	1:B:177:THR:HG21	2.27	0.49
1:A:412:ASP:HB3	1:A:415:THR:HG23	1.93	0.49
1:B:347:TYR:OH	1:B:398:LEU:HD23	2.13	0.49
1:A:133:HIS:ND1	1:A:134:ALA:N	2.60	0.49
1:A:160:HIS:CE1	1:A:161:LYS:HG3	2.47	0.49
1:A:314:THR:O	1:A:316:VAL:N	2.46	0.49
1:A:409:PHE:HE1	1:A:420:LYS:HD2	1.73	0.49
1:B:135:GLN:O	1:B:136:ALA:HB2	2.12	0.49
1:B:160:HIS:CG	1:B:161:LYS:N	2.81	0.49
1:B:532:THR:C	1:B:534:HIS:N	2.66	0.49
1:B:454:LEU:HD12	1:B:454:LEU:H	1.78	0.49
1:A:240:LYS:HD3	1:A:529:GLN:NE2	2.28	0.49
1:A:419:ILE:CG2	1:A:420:LYS:N	2.74	0.49
1:B:358:LYS:HB2	1:B:358:LYS:NZ	2.27	0.49
1:B:367:TYR:HD1	1:B:367:TYR:O	1.95	0.49
1:A:359:ASN:C	1:A:359:ASN:ND2	2.67	0.48
1:A:490:LYS:C	1:A:492:GLU:H	2.16	0.48
1:A:450:LEU:HG	1:A:477:TRP:HH2	1.78	0.48
1:B:311:MET:HB2	2:B:653:HOH:O	2.12	0.48
1:A:99:ILE:HG23	1:A:117:PHE:HE1	1.77	0.48
1:B:65:TRP:HH2	1:B:204:ALA:HB3	1.78	0.48
1:B:459:ASP:N	1:B:459:ASP:OD2	2.46	0.48
1:B:308:GLU:CG	2:B:653:HOH:O	2.61	0.48
1:A:177:THR:O	1:A:179:PRO:HD3	2.14	0.48
1:A:322:LYS:O	1:A:400:PRO:HG2	2.14	0.48
1:A:422:ASN:HD21	1:A:459:ASP:HA	1.76	0.48
1:A:476:LYS:HE3	1:A:477:TRP:H	1.77	0.48
1:B:338:ASP:C	1:B:338:ASP:OD1	2.51	0.48
1:B:355:LYS:CG	1:B:356:GLY:N	2.76	0.48
1:B:426:GLU:HA	1:B:498:TYR:CD2	2.48	0.48
1:B:465:TYR:N	1:B:465:TYR:CD1	2.81	0.48
1:A:143:TYR:N	1:A:143:TYR:CD2	2.80	0.48
1:A:344:ARG:HD2	1:A:396:LEU:CD1	2.44	0.48
1:B:228:LEU:HD12	1:B:299:LEU:HD12	1.94	0.48
1:B:425:PHE:HB2	2:B:648:HOH:O	2.14	0.48
1:B:191:PHE:N	1:B:191:PHE:HD1	2.12	0.48
1:B:456:HIS:O	1:B:511:THR:HA	2.14	0.48
1:B:489:THR:HG1	1:B:492:GLU:HG3	1.77	0.48
1:A:461:HIS:H	1:A:461:HIS:CD2	2.30	0.48
1:B:113:LYS:C	1:B:173:TRP:HB2	2.34	0.48
1:B:211:THR:HG21	1:B:485:VAL:HG12	1.96	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:132:CYS:SG	1:A:200:PRO:HB3	2.53	0.48
1:B:364:PHE:O	1:B:368:VAL:HG22	2.14	0.48
1:B:474:ASP:OD1	1:B:476:LYS:HD3	2.14	0.48
1:A:283:PHE:N	1:A:283:PHE:CD2	2.81	0.48
1:A:432:PRO:HA	1:A:447:ASN:OD1	2.14	0.48
1:B:534:HIS:C	1:B:536:ILE:H	2.17	0.48
1:B:256:VAL:N	1:B:257:PRO:CD	2.77	0.47
1:B:528:LEU:O	1:B:529:GLN:C	2.53	0.47
1:B:391:LYS:NZ	2:B:569:HOH:O	2.47	0.47
1:B:413:PRO:CA	1:B:415:THR:H	2.27	0.47
1:B:452:ALA:HB2	1:B:469:LEU:CD2	2.45	0.47
1:A:236:ASN:ND2	1:A:236:ASN:N	2.58	0.47
1:A:374:ASP:O	1:A:377:ASN:N	2.47	0.47
1:A:424:ARG:HA	1:A:499:GLY:HA3	1.96	0.47
1:B:105:PHE:HD1	1:B:107:PRO:N	2.12	0.47
1:B:115:VAL:HG21	1:B:176:VAL:HG11	1.96	0.47
1:B:387:GLN:HG3	2:B:563:HOH:O	2.14	0.47
1:A:87:SER:O	1:A:98:LYS:HE2	2.14	0.47
1:B:416:ASP:C	1:B:416:ASP:OD1	2.53	0.47
1:B:422:ASN:ND2	1:B:510:CYS:SG	2.88	0.47
1:A:481:ASP:O	1:A:482:ASP:HB2	2.14	0.47
1:B:102:MET:O	1:B:116:GLY:N	2.45	0.47
1:B:386:LEU:O	1:B:386:LEU:CG	2.63	0.47
1:A:65:TRP:CD1	1:A:94:ASN:HB2	2.49	0.47
1:A:173:TRP:HA	1:A:176:VAL:HG12	1.96	0.47
1:A:235:THR:HG22	1:A:235:THR:O	2.14	0.47
1:A:405:GLN:HE21	1:A:405:GLN:HB2	1.55	0.47
1:A:434:ASP:CB	1:A:446:ALA:HB3	2.41	0.47
1:A:451:HIS:HA	1:A:470:ASN:HD21	1.80	0.47
1:B:63:THR:OG1	1:B:64:SER:N	2.47	0.47
1:B:214:VAL:CG2	1:B:215:GLY:H	2.11	0.47
1:B:460:ASN:O	1:B:461:HIS:C	2.53	0.47
1:A:211:THR:HG21	1:A:485:VAL:CG1	2.45	0.47
1:A:223:CYS:HB3	1:A:465:TYR:CZ	2.49	0.47
1:B:78:PHE:C	1:B:78:PHE:CD2	2.88	0.47
1:B:225:MET:HE1	1:B:280:THR:HG22	1.97	0.47
1:B:142:ASN:HB3	1:B:145:ASP:O	2.15	0.47
1:A:439:LYS:HZ3	1:A:439:LYS:HB3	1.81	0.46
1:B:454:LEU:HD12	1:B:454:LEU:N	2.29	0.46
1:A:202:GLY:O	1:A:203:VAL:HB	2.15	0.46
1:A:216:LEU:HD21	1:A:267:LEU:HD11	1.96	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:262:ARG:CG	1:A:544:LEU:HD11	2.42	0.46
1:B:308:GLU:O	1:B:311:MET:N	2.47	0.46
1:A:115:VAL:O	1:A:170:PHE:HB3	2.15	0.46
1:A:222:THR:HA	1:A:291:PHE:CD1	2.51	0.46
1:A:262:ARG:HH22	1:A:278:LYS:HB3	1.80	0.46
1:B:308:GLU:C	1:B:310:LYS:N	2.67	0.46
1:A:382:GLY:O	1:A:385:GLY:N	2.45	0.46
1:B:225:MET:C	1:B:227:SER:N	2.68	0.46
1:A:92:VAL:HG21	1:A:195:VAL:HG11	1.97	0.46
1:A:337:VAL:HG12	1:A:387:GLN:HG2	1.98	0.46
1:A:491:GLU:HG3	1:A:495:GLU:HB2	1.97	0.46
1:B:118:PHE:CD1	1:B:118:PHE:N	2.83	0.46
1:B:337:VAL:CG1	1:B:338:ASP:N	2.78	0.46
1:A:242:VAL:HG21	1:A:260:LEU:CD2	2.45	0.46
1:A:332:ILE:O	1:A:340:ARG:HA	2.15	0.46
1:A:408:ARG:O	1:A:420:LYS:HA	2.16	0.46
1:A:531:VAL:HG12	2:A:621:HOH:O	2.15	0.46
1:B:308:GLU:HB2	1:B:320:ILE:CD1	2.43	0.46
1:B:320:ILE:N	1:B:321:PRO:CD	2.78	0.46
1:B:355:LYS:N	1:B:355:LYS:HD3	2.30	0.46
1:A:316:VAL:HG22	1:A:319:THR:OG1	2.15	0.46
1:A:331:TYR:C	1:A:331:TYR:CD1	2.89	0.46
1:B:156:HIS:CD2	1:B:157:LEU:N	2.83	0.46
1:A:442:PRO:C	1:A:444:ASP:H	2.18	0.46
1:A:494:ILE:CG2	1:A:495:GLU:OE1	2.64	0.46
1:B:63:THR:O	1:B:66:ARG:NH2	2.48	0.46
1:B:241:ALA:CB	1:B:319:THR:HG21	2.46	0.46
1:A:71:PHE:CD2	1:A:71:PHE:N	2.83	0.46
1:A:87:SER:HB2	1:A:88:PRO:HD2	1.98	0.46
1:A:117:PHE:CD2	1:A:138:LEU:HB3	2.51	0.46
1:A:494:ILE:C	1:A:496:HIS:N	2.66	0.46
1:B:240:LYS:HD2	1:B:529:GLN:OE1	2.16	0.46
1:B:355:LYS:HG2	1:B:356:GLY:N	2.31	0.46
1:B:443:LYS:C	1:B:445:PRO:HD3	2.36	0.46
1:A:208:LYS:CG	1:A:214:VAL:HG22	2.46	0.46
1:B:450:LEU:HD23	1:B:451:HIS:H	1.77	0.46
1:A:536:ILE:O	1:A:537:PRO:C	2.54	0.45
1:B:224:TYR:CD1	1:B:224:TYR:C	2.90	0.45
1:A:459:ASP:O	1:A:459:ASP:OD2	2.34	0.45
1:B:357:LYS:HE3	1:B:366:ASP:HB2	1.97	0.45
1:B:449:ILE:HD12	1:B:449:ILE:N	2.32	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:475:GLY:O	1:B:477:TRP:HD1	1.98	0.45
1:A:71:PHE:N	1:A:71:PHE:HD2	2.14	0.45
1:A:156:HIS:CD2	1:A:157:LEU:H	2.34	0.45
1:A:206:ASP:O	1:A:209:LYS:HB2	2.17	0.45
1:A:448:TYR:HA	1:A:519:ILE:O	2.16	0.45
1:A:455:VAL:HB	1:A:497:ASN:ND2	2.30	0.45
1:A:176:VAL:HG22	1:A:176:VAL:O	2.16	0.45
1:A:242:VAL:HG13	1:A:243:TYR:N	2.32	0.45
1:A:301:ARG:O	1:A:305:ASP:HB2	2.16	0.45
1:B:79:SER:OG	1:B:187:ASP:OD1	2.28	0.45
1:A:115:VAL:CG2	1:A:176:VAL:HG11	2.39	0.45
1:A:233:PHE:HA	1:A:264:PHE:CZ	2.51	0.45
1:A:416:ASP:C	1:A:416:ASP:OD2	2.55	0.45
1:A:418:ASN:HD22	1:A:418:ASN:HA	1.58	0.45
1:B:257:PRO:O	1:B:261:GLN:HG3	2.17	0.45
1:B:386:LEU:N	1:B:386:LEU:HD23	2.31	0.45
1:B:150:PHE:HD2	1:B:171:MET:HE2	1.81	0.45
1:B:208:LYS:O	1:B:212:GLY:N	2.45	0.45
1:B:448:TYR:C	1:B:449:ILE:HD12	2.37	0.45
1:A:551:GLU:HG2	2:A:648:HOH:O	2.16	0.45
1:B:92:VAL:HB	1:B:97:TRP:CD1	2.50	0.45
1:B:239:ARG:HD3	1:B:268:GLN:NE2	2.32	0.45
1:B:239:ARG:HG2	1:B:243:TYR:CE1	2.51	0.45
1:A:343:ARG:O	1:A:343:ARG:HG3	2.16	0.45
1:A:455:VAL:HG23	1:A:512:ASN:C	2.36	0.45
1:B:217:LYS:O	1:B:218:ASN:O	2.34	0.45
1:A:208:LYS:HE3	1:A:212:GLY:O	2.17	0.45
1:B:81:LEU:HG	1:B:82:SER:H	1.82	0.45
1:B:258:LEU:HD13	1:B:262:ARG:NH2	2.31	0.45
1:B:301:ARG:NH1	1:B:301:ARG:HG2	2.32	0.45
1:A:153:ARG:CD	1:A:153:ARG:N	2.75	0.45
1:A:216:LEU:O	1:A:482:ASP:C	2.54	0.45
1:A:281:LYS:O	1:A:284:GLY:N	2.47	0.45
1:B:529:GLN:HB3	2:B:629:HOH:O	2.16	0.45
1:B:141:ILE:HA	1:B:149:SER:OG	2.17	0.44
1:B:238:LEU:CD2	2:B:585:HOH:O	2.64	0.44
1:B:376:ASP:HA	1:B:379:TYR:CE1	2.51	0.44
1:B:411:TYR:CE1	1:B:413:PRO:HB3	2.51	0.44
1:A:243:TYR:OH	1:A:268:GLN:NE2	2.50	0.44
1:A:316:VAL:O	1:A:316:VAL:CG1	2.62	0.44
1:B:99:ILE:HD11	1:B:193:VAL:HG23	1.99	0.44



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Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:245:MET:HA	1:B:246:PRO:HD3	1.59	0.44
1:A:480:PHE:N	1:A:480:PHE:HD1	2.16	0.44
1:B:283:PHE:CE2	1:B:299:LEU:HD23	2.52	0.44
1:B:466:VAL:CG1	1:B:467:VAL:N	2.80	0.44
1:A:153:ARG:HD3	1:A:153:ARG:N	2.20	0.44
1:A:256:VAL:CG2	1:A:282:SER:HB3	2.36	0.44
1:A:373:LEU:HB3	1:A:377:ASN:O	2.17	0.44
1:A:414:GLN:O	1:A:415:THR:CB	2.65	0.44
1:A:528:LEU:O	1:A:529:GLN:O	2.36	0.44
1:B:111:HIS:O	1:B:111:HIS:ND1	2.51	0.44
1:B:361:PHE:C	1:B:361:PHE:HD2	2.20	0.44
1:B:91:PHE:HA	1:B:95:LEU:O	2.17	0.44
1:B:421:ILE:O	1:B:423:ASP:N	2.50	0.44
1:A:245:MET:HE1	1:A:257:PRO:HB3	2.00	0.44
1:B:250:ASP:OD1	1:B:310:LYS:NZ	2.48	0.44
1:A:211:THR:HG22	1:A:213:TYR:CB	2.47	0.44
1:A:300:CYS:O	1:A:304:LEU:HB2	2.18	0.44
1:B:235:THR:O	1:B:236:ASN:C	2.55	0.44
1:B:235:THR:CB	2:B:585:HOH:O	2.65	0.44
1:B:466:VAL:HG12	1:B:467:VAL:N	2.32	0.44
1:B:143:TYR:CD1	1:B:185:ASP:HB2	2.52	0.44
1:B:177:THR:O	1:B:179:PRO:HD3	2.17	0.44
1:B:360:ILE:HD11	1:B:516:LEU:HD12	2.00	0.44
1:A:297:GLN:HG3	1:A:405:GLN:NE2	2.33	0.44
1:A:340:ARG:HD3	1:A:342:ASP:OD1	2.17	0.44
1:A:361:PHE:CG	1:B:298:GLU:HG2	2.52	0.44
1:B:76:GLU:O	1:B:77:ARG:C	2.56	0.44
1:B:157:LEU:HD13	1:B:157:LEU:C	2.39	0.44
1:A:237:GLN:HE21	1:A:527:VAL:HA	1.82	0.43
1:A:466:VAL:HG12	1:A:467:VAL:N	2.32	0.43
1:A:490:LYS:O	1:A:492:GLU:N	2.50	0.43
1:A:258:LEU:O	1:A:260:LEU:N	2.51	0.43
1:B:193:VAL:O	1:B:193:VAL:HG12	2.17	0.43
1:A:70:THR:HG1	1:A:194:PHE:HD1	1.64	0.43
1:A:435:GLU:HB3	1:B:305:ASP:OD2	2.18	0.43
1:B:238:LEU:HD22	2:B:585:HOH:O	2.16	0.43
1:B:413:PRO:C	1:B:415:THR:N	2.54	0.43
1:A:354:ILE:HD13	1:A:355:LYS:CA	2.46	0.43
1:A:470:ASN:N	1:A:470:ASN:ND2	2.66	0.43
1:B:130:TRP:O	1:B:130:TRP:CG	2.71	0.43
1:B:184:ILE:CG1	1:B:185:ASP:N	2.80	0.43



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:301:ARG:HG2	1:B:301:ARG:HH11	1.84	0.43
1:A:265:TYR:CE2	1:A:536:ILE:HD13	2.54	0.43
1:B:130:TRP:HA	1:B:201:HIS:O	2.18	0.43
1:B:242:VAL:O	1:B:245:MET:HG3	2.18	0.43
1:A:329:VAL:HG23	1:A:396:LEU:HD11	1.99	0.43
1:A:393:VAL:CG1	1:A:394:LYS:N	2.81	0.43
1:B:464:HIS:CD2	2:B:650:HOH:O	2.72	0.43
1:A:64:SER:N	2:A:632:HOH:O	2.51	0.43
1:A:69:ALA:O	1:A:194:PHE:HD1	2.02	0.43
1:A:242:VAL:O	1:A:245:MET:HG3	2.19	0.43
1:A:285:TRP:HE3	1:A:291:PHE:CE1	2.37	0.43
1:B:459:ASP:O	1:B:460:ASN:HB2	2.17	0.43
1:A:136:ALA:HA	1:A:194:PHE:O	2.18	0.43
1:A:416:ASP:O	1:A:416:ASP:CG	2.57	0.43
1:B:63:THR:HG23	1:B:64:SER:H	1.84	0.43
1:A:133:HIS:O	1:A:134:ALA:HB2	2.19	0.43
1:B:77:ARG:O	1:B:77:ARG:HG2	2.19	0.42
1:B:287:THR:HG23	1:B:288:LEU:H	1.84	0.42
1:A:262:ARG:O	1:A:263:VAL:C	2.57	0.42
1:A:263:VAL:CG1	1:A:264:PHE:H	2.32	0.42
1:B:339:TYR:CE1	1:B:384:HIS:NE2	2.84	0.42
1:A:75:VAL:HA	2:A:574:HOH:O	2.19	0.42
1:A:185:ASP:O	1:A:186:ASP:CB	2.65	0.42
1:A:232:LEU:HD21	1:A:304:LEU:HD21	2.01	0.42
1:B:105:PHE:CD1	1:B:107:PRO:N	2.87	0.42
1:B:484:VAL:HG23	1:B:484:VAL:O	2.19	0.42
1:A:118:PHE:HB3	1:A:165:TRP:O	2.19	0.42
1:A:142:ASN:HB3	1:A:145:ASP:O	2.20	0.42
1:A:542:GLU:O	1:A:545:GLN:HB2	2.20	0.42
1:B:236:ASN:O	1:B:239:ARG:N	2.52	0.42
1:B:472:LYS:HB3	2:B:642:HOH:O	2.19	0.42
1:A:69:ALA:O	1:A:194:PHE:CD1	2.73	0.42
1:A:88:PRO:HA	1:A:89:PRO:HD2	1.87	0.42
1:A:198:ASP:N	1:A:198:ASP:OD2	2.53	0.42
1:B:101:VAL:HG22	1:B:191:PHE:CE2	2.55	0.42
1:B:103:PRO:CB	1:B:173:TRP:CZ3	2.98	0.42
1:B:524:LEU:HA	1:B:524:LEU:HD23	1.83	0.42
1:A:405:GLN:OE1	1:A:515:MET:CE	2.68	0.42
1:A:476:LYS:HG3	2:A:612:HOH:O	2.19	0.42
1:B:73:PHE:CD1	1:B:87:SER:HB2	2.55	0.42
1:B:92:VAL:O	1:B:95:LEU:HB2	2.20	0.42



	lo ao pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:426:GLU:HB3	1:B:498:TYR:CD2	2.55	0.42
1:A:135:GLN:O	1:A:136:ALA:HB2	2.20	0.42
1:A:156:HIS:CD2	2:A:657:HOH:O	2.72	0.42
1:A:239:ARG:CZ	1:A:531:VAL:HG11	2.47	0.42
1:A:242:VAL:HG21	1:A:260:LEU:HD21	2.00	0.42
1:A:403:HIS:HE1	2:A:618:HOH:O	2.02	0.42
1:A:410:MET:O	1:A:419:ILE:N	2.53	0.42
1:B:78:PHE:HE2	1:B:173:TRP:CH2	2.35	0.42
1:B:105:PHE:HD1	1:B:106:TYR:C	2.23	0.42
1:B:106:TYR:CD1	1:B:112:GLN:O	2.72	0.42
1:B:148:LYS:HG2	1:B:148:LYS:O	2.20	0.42
1:B:150:PHE:HD2	1:B:171:MET:HE3	1.85	0.42
1:B:429:GLU:HG3	1:B:430:GLN:N	2.35	0.42
1:B:159:PHE:O	1:B:160:HIS:C	2.57	0.42
1:B:350:ILE:HG22	1:B:352:LEU:CD1	2.50	0.42
1:B:418:ASN:N	1:B:418:ASN:OD1	2.51	0.42
1:A:101:VAL:HG11	1:A:191:PHE:CZ	2.55	0.42
1:B:206:ASP:HB3	1:B:209:LYS:CE	2.50	0.42
1:B:216:LEU:CD1	1:B:226:ASN:HB3	2.50	0.42
1:B:225:MET:C	1:B:227:SER:H	2.23	0.42
1:B:239:ARG:O	1:B:240:LYS:C	2.57	0.42
1:B:308:GLU:C	1:B:310:LYS:H	2.23	0.42
1:B:411:TYR:CZ	1:B:413:PRO:HB3	2.54	0.42
1:A:331:TYR:O	1:A:391:LYS:HA	2.20	0.41
1:B:63:THR:HG23	1:B:64:SER:N	2.35	0.41
1:B:260:LEU:HD12	1:B:260:LEU:HA	1.90	0.41
1:B:296:VAL:HG23	1:B:297:GLN:H	1.85	0.41
1:B:357:LYS:CE	1:B:366:ASP:HB2	2.50	0.41
1:B:443:LYS:O	1:B:445:PRO:HD3	2.19	0.41
1:A:222:THR:N	1:A:288:LEU:HD22	2.35	0.41
1:A:448:TYR:CB	1:A:518:TYR:HB3	2.39	0.41
1:A:474:ASP:OD2	1:A:474:ASP:N	2.43	0.41
1:B:459:ASP:O	1:B:460:ASN:CB	2.68	0.41
1:A:102:MET:HE1	1:A:104:ARG:HD3	2.01	0.41
1:A:234:PHE:CE1	1:A:480:PHE:CZ	3.07	0.41
1:B:77:ARG:HA	1:B:187:ASP:HB3	2.02	0.41
1:B:242:VAL:CG1	1:B:245:MET:HE2	2.40	0.41
1:B:411:TYR:CD1	1:B:411:TYR:C	2.93	0.41
1:A:272:LYS:O	1:A:273:PRO:C	2.59	0.41
1:B:81:LEU:HG	1:B:82:SER:N	2.36	0.41
1:B:233:PHE:CD1	1:B:233:PHE:C	2.93	0.41



	lo uo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:258:LEU:HD13	1:B:262:ARG:HH21	1.85	0.41
1:B:532:THR:HG22	1:B:533:ASP:N	2.35	0.41
1:A:159:PHE:O	1:A:160:HIS:C	2.58	0.41
1:A:224:TYR:CD1	1:A:224:TYR:C	2.94	0.41
1:A:457:SER:HB2	1:A:511:THR:HG23	2.02	0.41
1:B:201:HIS:ND1	1:B:201:HIS:N	2.68	0.41
1:A:92:VAL:HB	1:A:97:TRP:NE1	2.35	0.41
1:A:266:GLU:HB3	1:A:274:VAL:HG13	2.03	0.41
1:A:383:GLU:H	1:A:383:GLU:HG2	1.57	0.41
1:A:393:VAL:HG12	1:A:394:LYS:N	2.34	0.41
1:A:490:LYS:C	1:A:492:GLU:N	2.73	0.41
1:B:388:GLU:HG2	2:B:563:HOH:O	2.20	0.41
1:A:159:PHE:N	1:A:159:PHE:CD2	2.88	0.41
1:A:254:LYS:HB2	2:A:569:HOH:O	2.21	0.41
1:B:78:PHE:C	1:B:78:PHE:HD2	2.24	0.41
1:B:139:LYS:CB	1:B:151:SER:HB3	2.51	0.41
1:B:288:LEU:C	1:B:290:SER:H	2.24	0.41
1:B:495:GLU:HA	1:B:498:TYR:CE1	2.55	0.41
1:A:75:VAL:CG1	2:A:671:HOH:O	2.69	0.41
1:A:102:MET:HE2	1:A:104:ARG:HD3	2.03	0.41
1:A:118:PHE:CD1	1:A:118:PHE:N	2.88	0.41
1:A:245:MET:HA	1:A:246:PRO:HD3	1.88	0.41
1:A:394:LYS:HD3	1:A:394:LYS:HA	1.90	0.41
1:B:78:PHE:CD1	1:B:189:VAL:HG21	2.51	0.41
1:B:106:TYR:HB3	1:B:109:ARG:O	2.20	0.41
1:B:245:MET:HG2	1:B:311:MET:HG2	2.02	0.41
1:B:297:GLN:H	1:B:297:GLN:HG3	1.63	0.41
1:B:301:ARG:O	1:B:305:ASP:CB	2.69	0.41
1:B:414:GLN:C	1:B:416:ASP:N	2.74	0.41
1:B:477:TRP:CZ2	1:B:494:ILE:HD11	2.56	0.41
1:A:103:PRO:O	1:A:104:ARG:HG2	2.20	0.41
1:A:118:PHE:HA	1:A:166:GLY:HA3	2.02	0.41
1:A:398:LEU:HB2	1:A:448:TYR:OH	2.21	0.41
1:A:417:GLN:HB3	1:A:419:ILE:HG12	2.02	0.41
1:B:92:VAL:HG21	1:B:195:VAL:CG1	2.50	0.41
1:A:68:GLU:O	1:A:69:ALA:HB2	2.21	0.40
1:A:217:LYS:HD3	1:A:275:GLY:HA2	2.02	0.40
1:A:360:ILE:CD1	1:A:427:PHE:HB3	2.51	0.40
1:A:405:GLN:OE1	1:A:515:MET:HE1	2.21	0.40
1:B:150:PHE:HZ	1:B:152:ARG:NH2	2.19	0.40
1:B:223:CYS:HB3	1:B:465:TYR:CE1	2.57	0.40



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:409:PHE:HZ	1:B:456:HIS:ND1	2.19	0.40
1:A:218:ASN:HB3	1:A:219:GLN:H	1.35	0.40
1:A:233:PHE:HB2	1:A:267:LEU:HD23	2.03	0.40
1:A:266:GLU:OE2	1:A:274:VAL:HG13	2.21	0.40
1:A:294:HIS:HB3	1:A:298:GLU:CG	2.34	0.40
1:A:398:LEU:HA	1:A:399:PRO:HD3	1.91	0.40
1:A:98:LYS:O	1:A:119:LEU:HD12	2.22	0.40
1:A:99:ILE:HG12	1:A:193:VAL:HG21	2.03	0.40
1:A:236:ASN:O	1:A:239:ARG:HB3	2.21	0.40
1:A:414:GLN:O	1:A:415:THR:HB	2.21	0.40
1:B:159:PHE:CE1	1:B:161:LYS:HB2	2.56	0.40
1:B:315:CYS:SG	1:B:316:VAL:HG13	2.62	0.40
1:B:470:ASN:ND2	1:B:473:GLY:HA2	2.37	0.40
1:A:74:THR:OG1	1:A:190:THR:HG23	2.20	0.40
1:A:358:LYS:NZ	1:B:295:ASP:OD2	2.42	0.40
1:A:407:MET:HG2	2:B:637:HOH:O	2.20	0.40
1:B:67:SER:HB3	1:B:93:ARG:NH2	2.37	0.40
1:B:153:ARG:HG3	2:B:572:HOH:O	2.21	0.40
1:A:78:PHE:O	1:A:79:SER:C	2.59	0.40
1:A:301:ARG:HD3	1:A:301:ARG:HA	1.96	0.40
1:B:109:ARG:HE	1:B:110:PRO:CD	2.10	0.40
1:B:138:LEU:N	1:B:138:LEU:HD12	2.36	0.40
1:B:204:ALA:O	1:B:205:TRP:HB3	2.22	0.40
1:B:350:ILE:HG23	2:B:646:HOH:O	2.20	0.40
1:B:354:ILE:CD1	1:B:355:LYS:N	2.85	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:THR:O	1:A:287:THR:O[4_555]	1.83	0.37

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.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	462/522~(88%)	356~(77%)	71 (15%)	35~(8%)	1 7
1	В	477/522~(91%)	364 (76%)	78 (16%)	35~(7%)	1 7
All	All	939/1044~(90%)	720 (77%)	149 (16%)	70 (8%)	1 7

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

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	127	SER
1	А	183	PHE
1	А	203	VAL
1	А	277	LYS
1	А	334	CYS
1	А	495	GLU
1	А	529	GLN
1	А	537	PRO
1	А	538	GLN
1	В	105	PHE
1	В	111	HIS
1	В	160	HIS
1	В	207	SER
1	В	218	ASN
1	В	220	GLY
1	В	296	VAL
1	В	383	GLU
1	В	415	THR
1	В	461	HIS
1	А	160	HIS
1	А	204	ALA
1	А	236	ASN
1	А	249	GLY
1	А	252	SER
1	A	285	TRP
1	А	315	CYS
1	A	375	GLY
1	А	415	THR
1	А	416	ASP
1	В	79	SER
1	В	183	PHE
1	В	208	LYS
1	В	270	SER



Mol	Chain	Res	Type
1	В	382	GLY
1	B	384	HIS
1	B	422	ASN
1	B	482	ASP
1	B	535	ASP
1	A	259	ALA
1	A	273	PRO
1	A	445	PRO
1	A	491	GLU
1	B	113	LYS
1	B	413	PRO
1	B	423	ASP
1	B	471	PRO
1	В	529	GLN
1	A	211	THR
1	А	223	CYS
1	A	244	MET
1	А	355	LYS
1	В	112	GLN
1	В	178	ASP
1	В	236	ASN
1	А	209	LYS
1	А	413	PRO
1	А	428	PRO
1	А	482	ASP
1	В	108	ASP
1	В	203	VAL
1	В	442	PRO
1	В	460	ASN
1	В	524	LEU
1	А	145	ASP
1	А	200	PRO
1	А	399	PRO
1	А	494	ILE
1	В	246	PRO
1	В	399	PRO
1	В	214	VAL

Continued from previous page...

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	А	428/472 (91%)	355~(83%)	73 (17%)	2 10
1	В	437/472 (93%)	374 (86%)	63 (14%)	3 15
All	All	865/944~(92%)	729 (84%)	136 (16%)	2 12

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	71	PHE
1	А	126	ASP
1	А	153	ARG
1	А	159	PHE
1	А	164	ASP
1	А	168	SER
1	А	186	ASP
1	А	198	ASP
1	А	210	HIS
1	А	227	SER
1	А	229	LEU
1	А	232	LEU
1	А	248	GLU
1	А	260	LEU
1	А	271	ASP
1	А	272	LYS
1	А	283	PHE
1	А	286	GLU
1	А	287	THR
1	А	293	GLN
1	А	296	VAL
1	A	298	GLU
1	A	305	ASP
1	А	306	ASN
1	Α	319	THR
1	А	322	LYS
1	A	323	LEU
1	А	325	ARG
1	А	330	SER
1	A	331	TYR
1	А	333	GLN



Mol	Chain	Res	Type
1	А	342	ASP
1	А	343	ARG
1	А	354	ILE
1	А	357	LYS
1	А	359	ASN
1	А	363	SER
1	А	370	VAL
1	А	371	GLU
1	А	376	ASP
1	А	383	GLU
1	А	386	LEU
1	А	387	GLN
1	А	388	GLU
1	А	402	LEU
1	А	405	GLN
1	А	406	LEU
1	А	407	MET
1	А	415	THR
1	А	416	ASP
1	А	418	ASN
1	А	427	PHE
1	А	428	PRO
1	А	433	LEU
1	А	435	GLU
1	А	438	GLN
1	А	441	ASP
1	А	461	HIS
1	А	469	LEU
1	А	470	ASN
1	А	476	LYS
1	А	478	CYS
1	А	480	PHE
1	А	486	SER
1	А	491	GLU
1	А	496	HIS
1	А	512	ASN
1	А	531	VAL
1	А	537	PRO
1	А	540	LEU
1	А	544	LEU
1	А	547	GLU
		1	



Mol	Chain	Res	Type
1	В	78	PHE
1	В	80	ARG
1	В	105	PHE
1	В	106	TYR
1	В	118	PHE
1	В	186	ASP
1	В	191	PHE
1	В	201	HIS
1	В	206	ASP
1	В	228	LEU
1	В	247	THR
1	В	258	LEU
1	В	277	LYS
1	В	282	SER
1	В	288	LEU
1	В	290	SER
1	В	296	VAL
1	В	299	LEU
1	В	301	ARG
1	В	309	ASN
1	В	312	LYS
1	В	314	THR
1	В	327	LYS
1	В	342	ASP
1	В	350	ILE
1	В	351	GLN
1	В	352	LEU
1	В	355	LYS
1	В	360	ILE
1	В	361	PHE
1	В	364	PHE
1	В	365	VAL
1	В	367	TYR
1	В	376	ASP
1	В	379	TYR
1	В	391	LYS
1	В	397	THR
1	В	403	HIS
1	В	407	MET
1	В	411	TYR
1	В	414	GLN
1	В	416	ASP



Mol	Chain	Res	Type
1	В	418	ASN
1	В	419	ILE
1	В	422	ASN
1	В	426	GLU
1	В	450	LEU
1	В	453	VAL
1	В	459	ASP
1	В	460	ASN
1	В	469	LEU
1	В	471	PRO
1	В	474	ASP
1	В	476	LYS
1	В	495	GLU
1	В	511	THR
1	В	526	GLU
1	В	533	ASP
1	В	534	HIS
1	В	535	ASP
1	В	539	GLN
1	В	540	LEU
1	В	544	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	120	GLN
1	А	210	HIS
1	А	218	ASN
1	А	219	GLN
1	А	226	ASN
1	А	230	GLN
1	А	236	ASN
1	А	237	GLN
1	А	261	GLN
1	А	268	GLN
1	А	333	GLN
1	А	359	ASN
1	А	403	HIS
1	А	418	ASN
1	А	461	HIS
1	А	470	ASN
1	А	497	ASN



Mol	Chain	Res	Type
1	А	512	ASN
1	А	529	GLN
1	А	538	GLN
1	А	545	GLN
1	В	156	HIS
1	В	219	GLN
1	В	237	GLN
1	В	268	GLN
1	В	293	GLN
1	В	297	GLN
1	В	351	GLN
1	В	372	GLN
1	В	387	GLN
1	В	405	GLN
1	В	414	GLN
1	В	417	GLN
1	В	422	ASN
1	В	430	GLN
1	В	464	HIS
1	В	470	ASN
1	В	539	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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

