

Full wwPDB X-ray Structure Validation Report (i)

Oct 19, 2023 – 04:50 AM EDT

PDB ID	:	2QZP
Title	:	Crystal structure of mutation of an acylptide hydrolase/esterase from Aeropy-
		rum pernix K1
Authors	:	Zhang, H.F.; Zheng, B.S.; Rao, Z.
Deposited on	:	2007-08-17
Resolution	:	2.70 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)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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.



Motria	Whole archive	Similar resolution
	$(\# {\rm Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length		Quality of chain	
1	А	562	22%	70%	7% •
1	В	562	20%	72%	8%



2QZP

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8881 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

• Molecule 1 is a protein called Acylamino-acid-releasing enzyme.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	560	Total 4255	C 2685	N 750	O 808	S 12	0	0	0
1	В	561	Total 4260	C 2688	N 751	O 809	S 12	0	0	0

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	154	Total O 154 154	0	0
2	В	212	Total O 212 212	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 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: Acylamino-acid-releasing enzyme





A21	U U U	520 L27	<mark>Q</mark> 28	G29 V30	V31	D32	633 D24	K35	L36	L37	V38	V39 CAO	F41	S42	E43	644 c / c	046 V46	N47	A48	Y49	L50 Y51	D52	<mark>G53</mark>	G54	E55 TE6	V57	K58	L59	N60	10X	P63	164	N65	V67	L68	D69	P70 H71		G73	V74	G75	R76	178 178	L79	V80	R81 Dec	V83
S84	K85	A87	E88	089 H90	A91	L92	F93 V04	V95	N96		R99	P100	E102	E103	Q104	4105 1406	E107	A108	V109	K110	M112	R113	I114	L115	S116	V118	D119	T120	G121	E1 22 A1 02	V124	V125	F126	1711	T130	E131	D132 D132	V134	A135	L136	Y137	A138	L139 D140	G141	G142	G143	L144 R145
E146	L147	R149	L150	F153		V156	S157	1159 1159	R160	G161	D162	L163 T164		G168	F169	F1/0	6172	G173	R174	V175	1177 L177	F178	T179	S180	N181 1 182	7017	G185	G186	L187	K188 V100		G195	S196	5198	<mark>S199</mark>	A200	5201 1202	1202 S203	P204	G205	M206	K207	V208 T209	A210	G211	L212 E212	0123
A218	R219	V221	T222	V223 D224	P225	R226	D227	V230	E231	D232	L233	E234	P236		D239	F'240	S242	Y243	R244	P245	1240 A247	1248	T249	W250	L251 C252	Y253	L254	P255	D256	6297 D760	L259	A260	V261	V262 A263	R264	R265	E266	R268	S269	A270	V271	F272	1273 D274	G275	E276	R277	V2/0 E279
A280	281	1283	V284	1285 1286	3287	1288	7289	1291	3292	1293	{294	1295 1796	000	1299	1300	1053	303	r304	2305	2306	1308	/309	3310	.311	2312	1314 1314	3315	2316	1317	1318 1910	1010	.322	2323	1325 0325	1326	3327	1328	1330	A331	332	3333	1334 201	-335 /336	1337	<mark>/338</mark>	1339	5341
342	343	1345 (345 (1) (1) (1) (1) (1) (1) (1) (1) (1) (1)	346	347	350	351	352 252	354	1355	356	357	358	360	361 1	362	363	365	366	[367	368	370	371	372	373	0374	376	377	1378	0379 1960	380	382	383	1384 1901	386	387	388	000000000000000000000000000000000000000	391	392	(<u>393</u>	[394 201	395	396	1398	399	400	401
F03	04 01	106 R	LO7	F08	10 V	11 L		115 C	16 R	L17 A	18 P		121 121	122 P	123 I			128 V	t29 H	130 130	132 132	F 1	134 A	E35	136 137		39 S	140 W	141 100	1		145 A	146 17		49 A	E50		53 H	454 V	155 V	156 M		59 Y	LEO R	61 G	62 62	103 164 0
65 Y.	99 67	ын 89 89	00 Mr	70 R ^v 71	72 K	73 I.	74 75	76 P.	77 C	78 G ⁷	-20 	E E	函 82 82	83 D ²	84 V ⁷	85 86	87	88 R/	89 M ⁴	90 A4	92 92	03 03	94 G	95	96 A4	98 80	66	۸ ^۰	01		04 V	05 S ¹	00 V		λ ²	10 	11 13	13 13 07 13	14 A	15 L	16 15	17 M	18 19 19	20	21 L4	22 23	23 A
G4	N4	64 G4	A4	S4 V4	V4	D4	M4 EA	E4 E4	M4	Y4	E4	L4 C4	D4	A4	A4	14 14	EN N4	F4	14	E4	μ4 1.4	T4	G4	G4	S4 B4	E4	14	M5	R5	CS BE	S5 S5	P5	IS	H5	V5	DS	R5 TE	KE	ES	P5		A5		HE	P5		
R526	T527	L529	K530	P531 1.532	L533	R534	L535 ME26	G537	E538	L539	L540	А541 ведо	G543	K544	T545	F546 FE47	A548	H549	1550	1551 7570	P553	A554	G555	H556	A557 TEE8	N559	T560	M561	E562	D563	V565	K566	1567 1567	L569	P570	A571	V572 E573	F574		T577	Q578	R579	E580 R581	ARG			



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	63.12Å 102.18Å 163.59Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	48.11 - 2.70	Depositor
Resolution (A)	48.11 - 2.50	EDS
% Data completeness	92.0 (48.11-2.70)	Depositor
(in resolution range)	90.3 (48.11-2.50)	EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.58 (at 2.51 \text{\AA})$	Xtriage
Refinement program	CNS	Depositor
P. P.	0.226 , 0.277	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.226 , 0.277	DCC
R_{free} test set	1393 reflections (3.96%)	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.33, 81.0	EDS
L-test for twinning ²	$ < L >=0.38, < L^2>=0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	8881	wwPDB-VP
Average B, all atoms $(Å^2)$	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

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).

Mal	Chain	Bond	lengths	Bond angles					
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5				
1	А	0.47	0/4346	0.76	0/5892				
1	В	0.46	0/4351	0.75	1/5899~(0.0%)				
All	All	0.46	0/8697	0.75	1/11791~(0.0%)				

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	374	ASP	N-CA-C	-5.06	97.33	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	4255	0	4219	642	0
1	В	4260	0	4224	704	0
2	А	154	0	0	93	0
2	В	212	0	0	137	0
All	All	8881	0	8443	1329	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 78.

All (1329) 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:497:ARG:HH11	1:B:497:ARG:HB2	0.94	1.11
1:A:552:PRO:HD3	1:B:547:GLU:HB2	1.30	1.11
1:A:346:VAL:HG21	1:A:422:ASP:HB3	1.32	1.09
1:B:334:ARG:HH21	1:B:350:VAL:HG11	1.03	1.09
1:A:547:GLU:HB3	1:B:552:PRO:HD3	1.18	1.07
1:B:92:LEU:HD12	1:B:109:VAL:HG21	1.34	1.03
1:B:90:HIS:HB2	1:B:114:ILE:HD13	1.42	1.00
1:A:530:LYS:HB3	1:A:531:PRO:HD3	1.41	1.00
1:B:376:ASP:HA	2:B:791:HOH:O	1.60	1.00
1:B:323:PRO:HB2	1:B:326:LEU:HB2	1.42	0.99
1:B:497:ARG:HB2	1:B:497:ARG:NH1	1.79	0.98
1:B:347:PRO:O	1:B:396:ASN:HB2	1.63	0.98
1:B:212:LEU:HD23	1:B:219:ARG:HH12	1.26	0.96
1:B:201:SER:HB3	2:B:767:HOH:O	1.65	0.96
1:A:558:ILE:HD12	1:A:563:ASP:HB3	1.45	0.95
1:B:322:LEU:HD12	1:B:323:PRO:HD2	1.49	0.94
1:B:567:ILE:HD12	1:B:568:LEU:N	1.82	0.94
1:B:497:ARG:HH11	1:B:497:ARG:CB	1.81	0.93
1:A:522:GLN:HA	1:A:529:LEU:HD22	1.45	0.93
1:A:471:VAL:HG12	2:A:657:HOH:O	1.68	0.92
1:A:558:ILE:HG23	1:A:563:ASP:HB2	1.51	0.92
1:B:212:LEU:HD23	1:B:219:ARG:NH1	1.85	0.91
1:A:529:LEU:HD11	1:A:550:ILE:HD12	1.51	0.90
1:B:530:LYS:HB3	1:B:531:PRO:HD3	1.51	0.90
1:B:42:SER:HA	1:B:561:MET:SD	2.12	0.90
1:B:88:GLU:HG2	1:B:113:ARG:NH1	1.85	0.90
1:B:363:VAL:HG22	1:B:440:TYR:HB2	1.52	0.89
1:A:449:TYR:HA	2:A:709:HOH:O	1.71	0.88
1:A:69:ASP:HB2	1:A:118:VAL:HG22	1.56	0.88
1:A:68:LEU:HD12	1:A:78:ILE:HG21	1.52	0.88
1:B:325:ASP:HA	1:B:328:ARG:HB2	1.56	0.88
1:A:65:ASN:HD21	1:A:82:ASP:HB2	1.37	0.88
1:A:547:GLU:CB	1:B:552:PRO:HD3	2.03	0.88
1:B:334:ARG:NH2	1:B:350:VAL:HG11	1.87	0.88
1:B:509:VAL:HA	1:B:512:ILE:HD13	1.56	0.87
1:A:574:PHE:HA	2:A:602:HOH:O	1.74	0.87
1:A:127:THR:HB	2:A:677:HOH:O	1.73	0.87
1:B:208:VAL:HB	1:B:223:VAL:HB	1.56	0.87
1:B:528:PRO:HG3	2:B:756:HOH:O	1.75	0.86
1:A:545:THR:HB	2:A:613:HOH:O	1.73	0.86
1:A:457:MET:HB2	2:A:696:HOH:O	1.75	0.86
1:B:49:TYR:HA	1:B:57:VAL:O	1.74	0.86
		Continue	ed on next page



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:505:PRO:HG2	2:B:731:HOH:O	1.76	0.86
1:B:520:HIS:HD2	1:B:521:PRO:HD2	1.40	0.86
1:B:539:LEU:HB2	2:B:678:HOH:O	1.75	0.86
1:A:515:PRO:HA	2:A:613:HOH:O	1.76	0.85
1:B:303:SER:O	1:B:304:THR:HG23	1.74	0.85
1:B:26:SER:HB3	1:B:39:VAL:HB	1.58	0.85
1:A:569:LEU:HB3	1:A:570:PRO:HD3	1.57	0.85
1:A:412:ILE:HB	2:A:721:HOH:O	1.77	0.84
1:B:127:THR:HG23	1:B:156:VAL:HG23	1.59	0.84
1:B:278:VAL:HG11	1:B:295:LEU:HD12	1.56	0.84
1:A:215:ALA:HB1	1:A:406:GLU:HB2	1.57	0.84
1:A:558:ILE:HG22	1:A:560:THR:O	1.78	0.84
1:A:547:GLU:HB3	1:B:552:PRO:CD	2.07	0.84
1:A:273:ILE:O	1:A:276:GLU:HB2	1.77	0.83
1:B:561:MET:HA	2:B:589:HOH:O	1.76	0.83
1:B:338:VAL:HG11	1:B:425:ALA:O	1.78	0.83
1:B:484:ALA:HB3	2:B:604:HOH:O	1.79	0.83
1:A:194:GLU:HB2	1:A:212:LEU:HD21	1.60	0.83
1:A:548:ALA:HB3	1:B:550:ILE:HD13	1.58	0.83
1:B:463:LYS:HB2	2:B:658:HOH:O	1.77	0.82
1:B:458:LYS:HE3	2:B:778:HOH:O	1.79	0.82
1:A:116:SER:N	2:A:677:HOH:O	2.13	0.82
1:A:452:LEU:HD22	2:A:709:HOH:O	1.78	0.82
1:A:532:LEU:HD13	1:A:532:LEU:O	1.79	0.82
1:B:70:PRO:HB2	1:B:74:VAL:HG21	1.61	0.82
1:A:94:LYS:O	1:A:94:LYS:HG3	1.79	0.82
1:B:420:LEU:HD21	1:B:458:LYS:HD3	1.59	0.82
1:B:284:ASN:HD22	1:B:376:ASP:C	1.83	0.81
1:B:302:LEU:HG	2:B:600:HOH:O	1.79	0.81
1:A:177:LEU:HD21	1:A:208:VAL:HG11	1.62	0.81
1:A:138:ALA:HB2	1:A:147:LEU:HD21	1.63	0.81
1:A:458:LYS:HD3	1:A:461:LEU:HD13	1.63	0.80
1:B:102:GLU:HA	2:B:621:HOH:O	1.79	0.80
1:A:322:LEU:HD23	1:A:323:PRO:HD2	1.63	0.80
1:A:23:GLU:HA	2:A:730:HOH:O	1.80	0.80
1:B:158:ASP:O	1:B:159:ILE:HD13	1.80	0.80
1:B:374:ASP:CG	1:B:394:MET:HB3	2.01	0.80
1:B:406:GLU:HG2	1:B:410:LYS:HE2	1.64	0.80
1:A:545:THR:HG23	1:B:553:ASP:OD1	1.80	0.80
1:B:570:PRO:HD2	2:B:594:HOH:O	1.82	0.79
1:B:44:GLY:O	1:B:560:THR:HG22	1.83	0.79



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:78:ILE:HD13	1:B:124:VAL:HG13	1.63	0.79
1:A:38:VAL:HG12	1:A:39:VAL:N	1.97	0.79
1:B:281:PRO:O	1:B:285:HIS:HE1	1.66	0.78
1:A:238:LYS:HG2	2:A:614:HOH:O	1.84	0.78
1:B:376:ASP:HB2	2:B:616:HOH:O	1.82	0.78
1:A:558:ILE:HG23	1:A:563:ASP:CB	2.14	0.78
1:A:32:ASP:HB2	1:A:35:LYS:HB2	1.64	0.78
1:A:44:GLY:HA2	1:A:561:MET:H	1.49	0.78
1:B:353:SER:HB3	1:B:356:ALA:HB3	1.66	0.78
1:A:406:GLU:O	1:A:410:LYS:HG3	1.85	0.77
1:A:469:ALA:O	1:A:527:THR:HG21	1.84	0.77
1:B:522:GLN:HA	1:B:529:LEU:HD22	1.64	0.77
1:B:569:LEU:HB3	1:B:570:PRO:HD3	1.66	0.77
1:B:574:PHE:HA	2:B:784:HOH:O	1.84	0.77
1:A:83:VAL:HA	2:A:717:HOH:O	1.84	0.77
1:B:406:GLU:O	1:B:410:LYS:HG3	1.85	0.77
1:A:138:ALA:CB	1:A:147:LEU:HD21	2.13	0.77
1:A:562:GLU:O	1:A:564:ALA:N	2.17	0.77
1:B:268:ARG:HA	2:B:614:HOH:O	1.83	0.77
1:A:61:ARG:NH1	1:A:101:GLY:HA3	1.99	0.77
1:A:519:ILE:HA	1:A:549:HIS:HB2	1.66	0.77
1:A:523:ASN:ND2	1:A:553:ASP:HA	1.99	0.77
1:A:417:GLY:N	1:A:419:GLU:OE2	2.18	0.77
1:B:323:PRO:HG2	1:B:326:LEU:HD12	1.67	0.77
1:B:387:ALA:HB2	2:B:643:HOH:O	1.83	0.77
1:A:334:ARG:HH21	1:A:350:VAL:HG11	1.50	0.76
1:A:90:HIS:HD2	1:A:114:ILE:H	1.32	0.76
1:A:215:ALA:N	1:A:405:GLU:HB3	2.01	0.75
1:A:420:LEU:HD21	2:A:696:HOH:O	1.84	0.75
1:B:567:ILE:HD11	1:B:568:LEU:HD22	1.69	0.75
1:B:520:HIS:ND1	1:B:532:LEU:HG	2.01	0.75
1:A:552:PRO:CD	1:B:547:GLU:HB2	2.14	0.75
1:A:411:ILE:HD11	1:A:446:TYR:OH	1.87	0.74
1:A:194:GLU:HB3	1:A:214:THR:CG2	2.16	0.74
1:B:139:LEU:HD13	1:B:144:LEU:HB2	1.69	0.74
1:B:542:ARG:HG3	1:B:542:ARG:HH11	1.49	0.74
1:A:428:ARG:HG3	2:A:622:HOH:O	1.87	0.74
1:B:480:LEU:HB2	2:B:756:HOH:O	1.88	0.74
1:A:534:ARG:O	1:A:538:GLU:HG2	1.88	0.74
1:A:309:VAL:HA	1:A:316:PRO:HA	1.68	0.73
1:B:59:LEU:O	1:B:95:VAL:HG11	1.87	0.73



	lo ao pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:311:LEU:HG	2:A:670:HOH:O	1.87	0.73
1:B:239:ASP:HB2	1:B:275:GLY:O	1.87	0.73
1:B:579:ARG:C	1:B:581:ARG:H	1.91	0.73
1:A:136:LEU:HD21	1:A:164:ILE:HG21	1.70	0.73
1:A:526:ARG:HH11	1:A:556:HIS:HD2	1.34	0.73
1:B:265:ARG:HB3	2:B:696:HOH:O	1.87	0.73
1:A:194:GLU:HB3	1:A:214:THR:HG21	1.70	0.73
1:B:428:ARG:HG2	2:B:592:HOH:O	1.88	0.73
1:B:445:SER:H	1:B:469:ALA:HB3	1.54	0.73
1:A:529:LEU:HD23	1:B:540:LEU:HD13	1.70	0.72
1:A:65:ASN:ND2	1:A:82:ASP:HB2	2.04	0.72
1:B:90:HIS:CB	1:B:114:ILE:HD13	2.20	0.72
1:B:477:MET:HG3	1:B:528:PRO:HD2	1.72	0.72
1:B:485:PHE:HA	1:B:488:PHE:HB3	1.72	0.72
1:B:503:ARG:O	1:B:505:PRO:HD3	1.89	0.72
1:B:133:ARG:HD3	1:B:149:ARG:HE	1.54	0.72
1:B:177:LEU:CD2	1:B:223:VAL:HG21	2.19	0.72
1:B:496:SER:HB3	2:B:619:HOH:O	1.89	0.72
1:A:251:LEU:HD13	1:A:259:LEU:HD11	1.71	0.71
1:B:71:HIS:O	1:B:74:VAL:HG13	1.89	0.71
1:B:519:ILE:HD13	2:B:594:HOH:O	1.90	0.71
1:A:271:VAL:HB	1:A:278:VAL:HB	1.71	0.71
1:A:419:GLU:HG3	2:A:643:HOH:O	1.90	0.71
1:B:95:VAL:HA	2:B:742:HOH:O	1.90	0.71
1:B:347:PRO:O	1:B:396:ASN:CB	2.38	0.71
1:B:573:PHE:HB2	2:B:653:HOH:O	1.90	0.71
1:A:549:HIS:CE1	1:A:570:PRO:HB3	2.26	0.71
1:A:361:PRO:HA	1:A:438:GLU:CG	2.21	0.71
1:B:374:ASP:OD2	1:B:394:MET:HB3	1.90	0.71
1:B:381:PHE:CZ	1:B:567:ILE:HD13	2.25	0.71
1:B:417:GLY:O	1:B:421:GLU:HG2	1.89	0.71
1:A:350:VAL:O	1:A:351:LEU:HD23	1.89	0.71
1:B:364:VAL:HG22	2:B:775:HOH:O	1.91	0.71
1:B:472:VAL:HG12	1:B:506:ILE:HB	1.71	0.71
1:B:475:GLU:O	1:B:479:GLU:HG3	1.88	0.71
1:B:451:THR:CG2	1:B:467:ALA:HB2	2.21	0.71
1:B:577:THR:HB	2:B:784:HOH:O	1.89	0.71
1:B:160:ARG:HB3	1:B:202:ILE:HG21	1.74	0.70
1:A:338:VAL:O	1:A:345:ARG:HA	1.91	0.70
1:A:308:ILE:HB	1:A:318:LEU:HB2	1.73	0.70
1:B:45:SER:HA	1:B:560:THR:HA	1.72	0.70



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:71:HIS:O	1:A:74:VAL:HG23	1.91	0.70
1:A:363:VAL:HG12	2:A:693:HOH:O	1.92	0.70
1:A:284:ASN:ND2	1:A:377:SER:OG	2.25	0.70
1:A:309:VAL:HG12	1:A:316:PRO:HA	1.73	0.70
1:B:30:VAL:HG23	1:B:289:VAL:CG1	2.21	0.70
1:B:356:ALA:HB2	1:B:389:GLY:O	1.92	0.70
1:B:362:THR:HG22	1:B:363:VAL:N	2.06	0.70
1:B:564:ALA:O	1:B:567:ILE:HD11	1.92	0.70
1:A:129:ALA:CB	1:A:134:VAL:HG22	2.21	0.70
1:B:164:ILE:HB	1:B:180:SER:HB3	1.74	0.70
1:B:373:GLU:OE2	1:B:396:ASN:HB3	1.91	0.70
1:B:331:ALA:HB3	1:B:352:GLU:HB3	1.73	0.69
1:A:335:LEU:HD12	1:A:348:THR:O	1.93	0.69
1:B:51:TYR:HE2	1:B:317:LEU:HB3	1.58	0.69
1:B:79:LEU:HD11	1:B:95:VAL:HG21	1.74	0.69
1:A:346:VAL:HG13	1:A:407:TRP:HZ2	1.58	0.69
1:A:90:HIS:HB2	1:A:114:ILE:HD13	1.75	0.69
1:B:565:VAL:C	1:B:567:ILE:H	1.93	0.69
1:A:441:ILE:HD13	1:A:442:MET:N	2.06	0.69
1:A:439:LEU:N	2:A:729:HOH:O	2.24	0.69
1:A:511:ARG:O	2:A:630:HOH:O	2.10	0.69
1:B:178:PHE:HB3	2:B:706:HOH:O	1.93	0.69
1:B:208:VAL:HG23	1:B:223:VAL:O	1.93	0.69
1:A:528:PRO:HD3	2:A:644:HOH:O	1.91	0.69
1:B:245:PRO:HA	2:B:696:HOH:O	1.93	0.69
1:B:324:GLU:O	1:B:327:ARG:HB3	1.92	0.69
1:A:130:THR:OG1	1:A:132:ASP:OD1	2.10	0.68
1:B:327:ARG:O	2:B:720:HOH:O	2.11	0.68
1:A:174:ARG:HE	1:A:409:LEU:HD11	1.59	0.68
1:B:35:LYS:HG2	1:B:52:ASP:OD1	1.93	0.68
1:A:200:ALA:HB3	2:A:639:HOH:O	1.92	0.68
1:A:405:GLU:OE1	1:A:409:LEU:HG	1.93	0.68
1:A:163:LEU:C	1:A:164:ILE:HD12	2.13	0.68
1:A:474:TRP:HB2	1:A:500:MET:HB3	1.75	0.68
1:A:175:VAL:HG23	1:A:196:SER:HB3	1.76	0.68
1:B:169:PHE:CZ	1:B:175:VAL:HG22	2.28	0.68
1:B:329:SER:HB2	1:B:387:ALA:HA	1.76	0.68
1:A:352:GLU:HA	1:A:391:HIS:ND1	2.09	0.68
1:A:361:PRO:HA	1:A:438:GLU:HG2	1.76	0.68
1:A:27:LEU:HD21	1:A:289:VAL:HG22	1.76	0.68
1:B:92:LEU:O	1:B:106:LEU:HD12	1.94	0.68



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:477:MET:HA	2:B:756:HOH:O	1.93	0.68
1:B:526:ARG:NH2	1:B:557:ALA:HB2	2.08	0.68
1:B:218:ALA:HB1	1:B:248:ILE:HD11	1.76	0.67
1:B:526:ARG:HA	2:B:680:HOH:O	1.94	0.67
1:A:42:SER:HB2	2:A:649:HOH:O	1.94	0.67
1:B:222:THR:O	1:B:230:VAL:HG13	1.95	0.67
1:B:59:LEU:HD13	1:B:77:VAL:HG21	1.76	0.67
1:B:218:ALA:HB1	1:B:248:ILE:CD1	2.25	0.67
1:A:27:LEU:HD23	1:A:287:ARG:O	1.93	0.67
1:A:368:GLY:HA2	2:A:686:HOH:O	1.95	0.67
1:B:295:LEU:O	1:B:311:LEU:HG	1.95	0.67
1:B:485:PHE:O	1:B:489:ILE:HG12	1.95	0.67
1:B:91:ALA:HB3	1:B:93:PHE:CZ	2.30	0.66
1:B:440:TYR:OH	1:B:463:LYS:HD3	1.94	0.66
1:B:221:VAL:HB	1:B:230:VAL:HG12	1.77	0.66
1:A:90:HIS:O	1:A:111:PRO:HA	1.96	0.66
1:A:386:ALA:HA	1:A:390:PHE:O	1.95	0.66
1:B:438:GLU:HA	2:B:714:HOH:O	1.95	0.66
1:B:449:TYR:HB2	2:B:685:HOH:O	1.94	0.66
1:A:498:GLU:HA	1:A:501:ARG:HD2	1.77	0.66
1:B:559:ASN:O	1:B:560:THR:HG23	1.95	0.66
1:A:58:LYS:O	1:A:100:PRO:HB3	1.96	0.66
1:A:81:ARG:HB2	1:A:81:ARG:HH11	1.61	0.66
1:A:423:VAL:HA	2:A:651:HOH:O	1.95	0.66
1:A:353:SER:O	1:A:356:ALA:N	2.29	0.66
1:A:529:LEU:HD11	1:A:550:ILE:CD1	2.25	0.66
1:B:159:ILE:HD12	1:B:164:ILE:HG23	1.78	0.66
1:A:322:LEU:HD23	1:A:323:PRO:CD	2.25	0.66
1:A:548:ALA:O	1:B:549:HIS:HA	1.95	0.66
1:A:551:ILE:HG23	1:A:552:PRO:HD2	1.77	0.66
1:B:421:GLU:OE2	1:B:421:GLU:HA	1.96	0.66
1:B:574:PHE:O	1:B:577:THR:HB	1.96	0.66
1:A:480:LEU:HD21	1:A:530:LYS:HD2	1.78	0.66
1:A:567:ILE:HG13	1:A:567:ILE:O	1.95	0.66
1:B:424:SER:HB3	1:B:428:ARG:NH1	2.11	0.66
1:A:45:SER:HB2	1:A:63:PRO:HB3	1.76	0.65
1:A:125:VAL:HA	1:A:137:TYR:O	1.96	0.65
1:A:392:VAL:HG22	2:A:720:HOH:O	1.95	0.65
1:B:153:PHE:HE1	1:B:488:PHE:HB2	1.61	0.65
1:A:308:ILE:O	1:A:318:LEU:N	2.23	0.65
1:B:171:GLY:O	1:B:173:GLY:N	2.30	0.65



	ti a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:90:HIS:N	1:A:112:MET:O	2.21	0.65
1:A:555:GLY:HA3	2:A:663:HOH:O	1.96	0.65
1:B:99:ARG:HB2	1:B:102:GLU:OE2	1.96	0.65
1:B:410:LYS:HG2	2:B:695:HOH:O	1.95	0.65
1:A:302:LEU:HD13	1:A:351:LEU:HD21	1.78	0.65
1:B:523:ASN:ND2	1:B:553:ASP:HA	2.11	0.65
1:A:579:ARG:NH1	1:A:579:ARG:HB2	2.12	0.65
1:B:103:GLU:HB2	2:B:687:HOH:O	1.97	0.65
1:B:458:LYS:HB3	1:B:461:LEU:HD22	1.79	0.65
1:B:532:LEU:O	1:B:536:MET:HG3	1.97	0.65
1:B:469:ALA:HB1	1:B:556:HIS:CE1	2.31	0.65
1:A:563:ASP:HA	1:A:566:LYS:CG	2.27	0.65
1:A:63:PRO:HA	2:A:595:HOH:O	1.97	0.65
1:B:278:VAL:HG11	1:B:295:LEU:CD1	2.27	0.64
1:B:29:GLY:CA	1:B:289:VAL:HG21	2.28	0.64
1:B:136:LEU:O	1:B:147:LEU:N	2.31	0.64
1:A:353:SER:O	1:A:355:ARG:N	2.30	0.64
1:B:100:PRO:O	1:B:102:GLU:HG3	1.96	0.64
1:B:133:ARG:HA	1:B:483:ALA:CB	2.27	0.64
1:B:137:TYR:HA	1:B:146:GLU:HA	1.80	0.64
1:B:362:THR:CG2	1:B:363:VAL:N	2.60	0.64
1:A:88:GLU:HG3	1:A:113:ARG:HH12	1.61	0.64
1:A:223:VAL:HA	1:A:229:SER:O	1.98	0.64
1:A:263:ALA:O	1:A:269:SER:HB2	1.97	0.64
1:A:325:ASP:HA	1:A:328:ARG:HB3	1.79	0.64
1:A:337:TRP:CZ3	1:A:347:PRO:HB3	2.33	0.64
1:B:69:ASP:O	1:B:118:VAL:HG13	1.97	0.64
1:B:201:SER:N	2:B:652:HOH:O	2.30	0.64
1:A:61:ARG:HH12	1:A:101:GLY:HA3	1.62	0.64
1:A:438:GLU:HB2	2:A:729:HOH:O	1.96	0.64
1:A:525:SER:C	2:A:644:HOH:O	2.35	0.64
1:A:526:ARG:HD2	1:A:556:HIS:CD2	2.32	0.64
1:B:181:ASN:HB2	1:B:185:GLY:O	1.97	0.64
1:A:38:VAL:CG1	1:A:39:VAL:N	2.61	0.64
1:A:272:PHE:CE2	1:A:277:ARG:HD3	2.33	0.64
1:A:415:PRO:O	1:A:503:ARG:HD2	1.98	0.64
1:B:46:VAL:HG23	2:B:764:HOH:O	1.98	0.64
1:A:172:GLY:O	1:A:409:LEU:HD22	1.98	0.64
1:B:90:HIS:HB2	1:B:114:ILE:CD1	2.23	0.64
1:B:201:SER:CB	1:B:252:GLY:HA2	2.28	0.64
1:B:251:LEU:HG	2:B:652:HOH:O	1.97	0.64



	louo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:411:ILE:CD1	1:B:419:GLU:HG2	2.27	0.64
1:A:129:ALA:HB2	1:A:134:VAL:HG22	1.80	0.64
1:A:200:ALA:CB	2:A:639:HOH:O	2.46	0.64
1:A:214:THR:C	1:A:405:GLU:HB3	2.18	0.64
1:B:361:PRO:HA	1:B:438:GLU:HG2	1.80	0.64
1:B:373:GLU:OE1	1:B:396:ASN:ND2	2.31	0.64
1:A:164:ILE:HD13	1:A:181:ASN:C	2.18	0.63
1:A:370:PRO:O	1:A:372:ALA:N	2.29	0.63
1:A:511:ARG:HG2	2:A:630:HOH:O	1.98	0.63
1:B:137:TYR:CD2	1:B:146:GLU:HG3	2.32	0.63
1:A:493:THR:O	1:A:499:ILE:HD12	1.97	0.63
1:B:90:HIS:HD2	1:B:114:ILE:H	1.47	0.63
1:B:92:LEU:HD12	1:B:109:VAL:CG2	2.22	0.63
1:B:180:SER:HA	2:B:750:HOH:O	1.98	0.63
1:B:104:GLN:HG2	2:B:620:HOH:O	1.98	0.63
1:B:428:ARG:O	1:B:431:ARG:HB2	1.98	0.63
1:B:471:VAL:HG11	1:B:474:TRP:CH2	2.33	0.63
1:A:93:PHE:C	2:A:589:HOH:O	2.36	0.63
1:A:133:ARG:HA	1:A:483:ALA:CB	2.28	0.63
1:B:411:ILE:HD11	1:B:446:TYR:OH	1.99	0.63
1:B:441:ILE:HG21	2:B:615:HOH:O	1.96	0.63
1:A:62:GLU:HB2	1:A:81:ARG:HH21	1.64	0.63
1:B:186:GLY:O	1:B:187:LEU:HB2	1.98	0.63
1:B:171:GLY:C	1:B:173:GLY:H	2.00	0.63
1:B:472:VAL:CG1	1:B:506:ILE:HB	2.29	0.63
1:B:542:ARG:HG3	1:B:542:ARG:NH1	2.14	0.63
1:B:61:ARG:HB2	1:B:103:GLU:OE1	1.99	0.62
1:B:278:VAL:HG13	1:B:312:PRO:HB3	1.80	0.62
1:B:340:SER:HB3	2:B:722:HOH:O	1.98	0.62
1:A:109:VAL:HG12	2:A:594:HOH:O	1.99	0.62
1:A:475:GLU:HB3	2:A:627:HOH:O	2.00	0.62
1:B:99:ARG:NH2	1:B:102:GLU:HB3	2.13	0.62
1:B:264:ARG:O	1:B:264:ARG:HG3	1.97	0.62
1:B:78:ILE:HD13	1:B:124:VAL:CG1	2.30	0.62
1:A:523:ASN:HD21	1:A:553:ASP:HA	1.61	0.62
1:B:91:ALA:HB1	1:B:105:ARG:HE	1.65	0.62
1:B:116:SER:C	2:B:596:HOH:O	2.38	0.62
1:A:45:SER:OG	1:A:47:ASN:ND2	2.30	0.62
1:B:523:ASN:HB2	1:B:554:ALA:O	1.99	0.62
1:A:58:LYS:HE2	1:A:60:ASN:O	1.99	0.62
1:B:68:LEU:O	1:B:70:PRO:HD3	2.00	0.62



	lo uo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:345:ARG:HD2	2:B:684:HOH:O	2.00	0.62
1:B:539:LEU:HD13	1:B:546:PHE:CG	2.34	0.62
1:A:328:ARG:HG2	1:A:328:ARG:HH11	1.64	0.62
1:B:29:GLY:HA2	1:B:289:VAL:HG21	1.82	0.62
1:B:420:LEU:CD2	1:B:458:LYS:HD3	2.29	0.62
1:A:90:HIS:HB2	1:A:114:ILE:CD1	2.30	0.62
1:B:133:ARG:NH1	1:B:146:GLU:OE2	2.32	0.62
1:A:45:SER:HB2	2:A:595:HOH:O	1.99	0.61
1:A:251:LEU:HD12	1:A:252:GLY:N	2.13	0.61
1:A:283:GLY:HA2	1:A:376:ASP:OD2	2.00	0.61
1:A:470:SER:O	1:A:527:THR:HB	2.00	0.61
1:B:115:LEU:HB2	1:B:127:THR:OG1	2.00	0.61
1:A:341:PHE:CD2	1:A:421:GLU:HB3	2.35	0.61
1:A:346:VAL:HG22	1:A:407:TRP:CH2	2.36	0.61
1:B:373:GLU:OE1	1:B:373:GLU:HA	1.99	0.61
1:A:273:ILE:HG13	1:A:295:LEU:HD11	1.82	0.61
1:A:499:ILE:HD11	2:A:732:HOH:O	2.01	0.61
1:B:160:ARG:NH2	2:B:715:HOH:O	2.33	0.61
1:A:419:GLU:CD	1:A:420:LEU:H	2.03	0.61
1:B:370:PRO:O	1:B:372:ALA:N	2.33	0.61
1:A:340:SER:HB2	1:A:344:SER:O	1.99	0.61
1:B:31:VAL:HG12	1:B:32:ASP:N	2.15	0.61
1:B:559:ASN:HB2	2:B:762:HOH:O	2.00	0.61
1:A:547:GLU:OE2	1:A:574:PHE:HB2	2.00	0.61
1:A:558:ILE:HG12	2:A:583:HOH:O	2.01	0.61
1:A:533:LEU:CD1	1:B:536:MET:HB3	2.30	0.61
1:B:323:PRO:CG	1:B:326:LEU:HD12	2.31	0.61
1:A:497:ARG:O	1:A:499:ILE:N	2.34	0.61
1:B:55:GLU:C	2:B:735:HOH:O	2.38	0.61
1:B:399:GLY:HA2	1:B:408:ARG:O	2.01	0.61
1:A:533:LEU:HD11	1:B:536:MET:HB3	1.81	0.61
1:B:45:SER:HB2	1:B:63:PRO:HB3	1.83	0.60
1:B:127:THR:HG23	1:B:156:VAL:CG2	2.29	0.60
1:B:347:PRO:HG2	1:B:396:ASN:HB2	1.83	0.60
1:B:282:GLN:HB3	2:B:700:HOH:O	1.99	0.60
1:B:567:ILE:CD1	1:B:568:LEU:HD22	2.32	0.60
1:A:264:ARG:NH2	1:A:373:GLU:OE2	2.33	0.60
1:A:562:GLU:C	1:A:564:ALA:H	2.05	0.60
1:B:26:SER:O	1:B:308:ILE:HD11	2.01	0.60
1:B:30:VAL:H	1:B:289:VAL:HG11	1.64	0.60
1:A:296:VAL:HG13	1:A:309:VAL:O	2.02	0.60



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:41:PHE:CE2	1:A:561:MET:HA	2.37	0.60
1:A:160:ARG:N	1:A:202:ILE:HD12	2.16	0.60
1:B:90:HIS:CD2	1:B:114:ILE:HD13	2.35	0.60
1:A:533:LEU:HD21	1:B:536:MET:SD	2.42	0.60
1:A:41:PHE:CZ	1:A:561:MET:HA	2.35	0.60
1:A:309:VAL:HG12	1:A:316:PRO:CA	2.32	0.60
1:A:468:GLY:HA2	1:A:519:ILE:O	2.02	0.60
1:B:135:ALA:HB3	1:B:137:TYR:CZ	2.37	0.60
1:B:517:ALA:HB2	1:B:574:PHE:CD1	2.37	0.60
1:B:530:LYS:HB3	1:B:531:PRO:CD	2.27	0.60
1:A:334:ARG:HG3	2:A:694:HOH:O	2.01	0.60
1:B:330:ILE:HD12	2:B:720:HOH:O	2.02	0.60
1:A:385:LEU:HD13	2:A:720:HOH:O	2.00	0.60
1:B:361:PRO:O	1:B:390:PHE:HA	2.02	0.59
1:B:325:ASP:CA	1:B:328:ARG:HB2	2.30	0.59
1:B:410:LYS:HE3	2:B:786:HOH:O	2.02	0.59
1:A:171:GLY:O	1:A:174:ARG:HB2	2.02	0.59
1:B:175:VAL:HB	1:B:196:SER:HB3	1.84	0.59
1:A:55:GLU:HA	2:A:604:HOH:O	2.03	0.59
1:A:267:GLY:HA2	1:A:375:SER:HB2	1.83	0.59
1:A:356:ALA:HB2	1:A:389:GLY:O	2.01	0.59
1:B:451:THR:HG21	1:B:467:ALA:HB2	1.85	0.59
1:A:558:ILE:CG2	1:A:560:THR:O	2.51	0.59
1:B:361:PRO:HG3	1:B:438:GLU:CD	2.23	0.59
1:B:471:VAL:HG11	1:B:474:TRP:CZ3	2.37	0.59
1:A:37:LEU:HD23	1:A:70:PRO:HG3	1.85	0.59
1:A:480:LEU:HD21	1:A:530:LYS:CD	2.32	0.59
1:A:530:LYS:CB	1:A:531:PRO:HD3	2.24	0.59
1:A:109:VAL:HG12	1:A:109:VAL:O	2.02	0.59
1:A:306:PRO:HD3	1:A:378:TRP:HB3	1.83	0.59
1:B:565:VAL:C	1:B:567:ILE:N	2.56	0.59
1:A:526:ARG:HH11	1:A:556:HIS:CD2	2.18	0.59
1:B:145:ARG:HG3	2:B:748:HOH:O	2.01	0.58
1:B:302:LEU:HD13	1:B:351:LEU:CD1	2.33	0.58
1:B:46:VAL:HB	1:B:64:ILE:O	2.03	0.58
1:B:246:THR:HG22	1:B:264:ARG:O	2.03	0.58
1:B:251:LEU:CD1	1:B:259:LEU:HD11	2.33	0.58
1:B:456:THR:CG2	1:B:512:ILE:HD11	2.32	0.58
1:A:475:GLU:HA	1:A:500:MET:HE2	1.85	0.58
1:B:414:ASP:HA	1:B:503:ARG:HH12	1.66	0.58
1:B:210:ALA:HA	1:B:251:LEU:HD23	1.84	0.58



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:307:ARG:NH2	2:B:595:HOH:O	2.33	0.58
1:A:165:ALA:CB	2:A:653:HOH:O	2.51	0.58
1:A:455:LEU:HD23	2:A:682:HOH:O	2.03	0.58
1:A:465:GLY:O	1:A:516:LEU:HA	2.04	0.58
1:B:28:GLN:HG3	1:B:67:VAL:CG2	2.33	0.58
1:B:61:ARG:HB2	1:B:103:GLU:CD	2.24	0.58
1:B:250:TRP:HZ3	1:B:260:ALA:HB3	1.67	0.58
1:B:324:GLU:OE2	1:B:327:ARG:NH1	2.33	0.58
1:B:390:PHE:CE1	1:B:579:ARG:NH2	2.72	0.58
1:A:177:LEU:HB3	1:A:190:PHE:HB2	1.86	0.58
1:B:248:ILE:HD12	1:B:248:ILE:H	1.69	0.58
1:A:40:GLY:C	1:A:42:SER:H	2.07	0.58
1:B:27:LEU:CD1	1:B:38:VAL:HG12	2.33	0.58
1:B:284:ASN:ND2	1:B:376:ASP:C	2.54	0.58
1:B:528:PRO:O	1:B:532:LEU:HD23	2.03	0.58
1:A:159:ILE:HG23	1:A:163:LEU:O	2.03	0.58
1:A:38:VAL:CG1	1:A:39:VAL:H	2.17	0.58
1:A:160:ARG:HD3	1:A:202:ILE:HG22	1.85	0.58
1:B:133:ARG:HA	1:B:483:ALA:HB2	1.85	0.58
1:B:497:ARG:O	1:B:500:MET:N	2.37	0.58
1:A:120:THR:HB	2:A:617:HOH:O	2.04	0.57
1:A:403:TYR:HD1	2:A:618:HOH:O	1.87	0.57
1:B:60:ASN:O	1:B:101:GLY:HA2	2.05	0.57
1:B:201:SER:HB2	1:B:252:GLY:HA2	1.86	0.57
1:A:217:GLU:HG2	1:A:245:PRO:O	2.05	0.57
1:B:295:LEU:HB2	1:B:311:LEU:HB2	1.85	0.57
1:B:343:GLY:N	2:B:722:HOH:O	2.37	0.57
1:A:44:GLY:HA2	1:A:561:MET:CB	2.34	0.57
1:A:51:TYR:CZ	1:A:53:GLY:HA2	2.39	0.57
1:B:266:GLU:HG2	1:B:337:TRP:HZ2	1.69	0.57
1:B:477:MET:HB3	2:B:642:HOH:O	2.05	0.57
1:B:477:MET:CE	1:B:489:ILE:HD11	2.34	0.57
1:B:326:LEU:HA	1:B:355:ARG:HH11	1.67	0.57
1:A:187:LEU:HD12	1:A:188:ARG:H	1.68	0.57
1:A:412:ILE:HD13	1:A:492:LEU:HD12	1.86	0.57
1:B:233:LEU:HD23	1:B:234:GLU:N	2.20	0.57
1:A:38:VAL:HG12	1:A:39:VAL:H	1.65	0.57
1:A:187:LEU:HD12	1:A:188:ARG:N	2.20	0.57
1:A:267:GLY:HA2	1:A:375:SER:CB	2.34	0.57
1:A:372:ALA:O	1:A:401:THR:N	2.34	0.57
1:B:271:VAL:O	1:B:277:ARG:HA	2.03	0.57



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:47:ASN:HA	2:B:679:HOH:O	2.04	0.57
1:B:198:SER:HB3	1:B:213:GLU:OE2	2.04	0.57
1:B:551:ILE:HB	1:B:554:ALA:HB2	1.87	0.57
1:A:251:LEU:HD12	1:A:251:LEU:C	2.24	0.57
1:A:323:PRO:HD2	1:A:326:LEU:HD12	1.86	0.57
1:A:569:LEU:HG	1:A:573:PHE:HE2	1.70	0.57
1:B:329:SER:HB3	1:B:355:ARG:HE	1.69	0.57
1:B:464:ALA:CB	1:B:578:GLN:HG3	2.35	0.57
1:A:169:PHE:HE2	1:A:371:PHE:CD1	2.22	0.57
1:A:449:TYR:HB2	1:A:471:VAL:HG23	1.86	0.57
1:A:113:ARG:NH2	1:A:525:SER:OG	2.38	0.56
1:A:446:TYR:HB3	2:A:686:HOH:O	2.05	0.56
1:B:68:LEU:HG	1:B:78:ILE:HB	1.87	0.56
1:A:174:ARG:HH21	1:A:405:GLU:CD	2.08	0.56
1:A:342:ASP:CG	1:A:398:ARG:HH22	2.08	0.56
1:A:419:GLU:O	1:A:423:VAL:HG23	2.06	0.56
1:A:473:ASP:N	2:A:657:HOH:O	2.38	0.56
1:A:526:ARG:HD2	1:A:556:HIS:CG	2.40	0.56
1:B:127:THR:HA	1:B:135:ALA:O	2.06	0.56
1:B:304:THR:O	1:B:378:TRP:HB2	2.06	0.56
1:A:363:VAL:HA	1:A:440:TYR:O	2.05	0.56
1:B:420:LEU:HD22	1:B:453:CYS:SG	2.46	0.56
1:A:305:PRO:HA	1:A:378:TRP:CG	2.41	0.56
1:A:429:TRP:CD1	1:A:433:SER:HB2	2.40	0.56
1:B:240:PHE:HE1	1:B:263:ALA:HB2	1.70	0.56
1:B:361:PRO:HA	1:B:438:GLU:CG	2.34	0.56
1:B:516:LEU:HD12	1:B:517:ALA:H	1.70	0.56
1:A:519:ILE:HG12	1:A:549:HIS:CD2	2.40	0.56
1:B:99:ARG:CZ	1:B:102:GLU:HB3	2.36	0.56
1:B:198:SER:HB3	1:B:213:GLU:CD	2.26	0.56
1:B:455:LEU:HD22	1:B:514:GLU:HB2	1.88	0.56
1:A:393:VAL:HG11	1:A:426:ALA:HB1	1.88	0.56
1:A:441:ILE:HB	1:A:462:PHE:CD1	2.41	0.56
1:A:486:ARG:HH11	1:A:486:ARG:HG3	1.71	0.56
1:B:90:HIS:O	1:B:111:PRO:HA	2.05	0.56
1:B:517:ALA:HB2	1:B:574:PHE:CE1	2.41	0.56
1:A:305:PRO:HD3	1:A:322:LEU:HD12	1.88	0.56
1:B:456:THR:HG23	1:B:512:ILE:HD11	1.87	0.56
1:A:46:VAL:N	2:A:595:HOH:O	2.38	0.56
1:A:106:LEU:HA	2:A:698:HOH:O	2.04	0.56
1:A:164:ILE:O	1:A:179:THR:HA	2.06	0.56



	A L C	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:347:PRO:HG3	1:A:403:TYR:CD2	2.41	0.56
1:A:458:LYS:O	1:A:460:GLY:N	2.39	0.56
1:B:271:VAL:O	1:B:277:ARG:HD2	2.06	0.56
1:B:331:ALA:HB3	1:B:352:GLU:CB	2.36	0.56
1:A:550:ILE:O	1:B:547:GLU:HA	2.06	0.55
1:A:219:ARG:HG3	1:A:219:ARG:HH11	1.71	0.55
1:A:445:SER:HA	1:A:469:ALA:O	2.06	0.55
1:A:520:HIS:O	1:A:550:ILE:HA	2.06	0.55
1:B:350:VAL:HG21	1:B:429:TRP:CH2	2.41	0.55
1:B:453:CYS:HB2	2:B:731:HOH:O	2.07	0.55
1:A:92:LEU:O	1:A:106:LEU:HG	2.04	0.55
1:A:178:PHE:CD1	1:A:178:PHE:C	2.80	0.55
1:A:563:ASP:OD2	2:A:585:HOH:O	2.18	0.55
1:B:471:VAL:HG23	2:B:685:HOH:O	2.05	0.55
1:A:25:TYR:HB3	1:A:38:VAL:HG11	1.88	0.55
1:A:426:ALA:HB2	2:A:651:HOH:O	2.06	0.55
1:B:123:ALA:HA	1:B:139:LEU:O	2.06	0.55
1:B:268:ARG:NH1	1:B:282:GLN:CD	2.60	0.55
1:B:326:LEU:HB3	2:B:794:HOH:O	2.05	0.55
1:B:455:LEU:CD2	1:B:514:GLU:HB2	2.37	0.55
1:A:399:GLY:O	1:A:408:ARG:HG3	2.06	0.55
1:A:478:TYR:HE1	1:A:486:ARG:O	1.90	0.55
1:A:499:ILE:HG23	1:A:503:ARG:HG3	1.89	0.55
1:A:532:LEU:HD13	1:A:532:LEU:C	2.26	0.55
1:A:541:ALA:C	1:A:543:GLY:H	2.09	0.55
1:B:51:TYR:CZ	1:B:53:GLY:HA2	2.42	0.55
1:A:379:ASP:OD1	1:A:381:PHE:N	2.38	0.55
1:A:474:TRP:CD1	1:A:500:MET:HA	2.42	0.55
1:B:59:LEU:HD22	2:B:727:HOH:O	2.07	0.55
1:B:255:PRO:O	1:B:257:GLY:N	2.39	0.55
1:B:496:SER:CB	2:B:619:HOH:O	2.52	0.55
1:A:579:ARG:HG2	1:A:580:GLU:HG3	1.88	0.55
1:B:169:PHE:CE2	1:B:175:VAL:HG22	2.40	0.55
1:B:246:THR:CG2	1:B:402:GLY:O	2.55	0.55
1:B:259:LEU:HD11	2:B:767:HOH:O	2.06	0.55
1:A:169:PHE:HE2	1:A:371:PHE:HD1	1.54	0.55
1:A:215:ALA:CB	1:A:406:GLU:HB2	2.35	0.55
1:A:418:GLY:O	1:A:421:GLU:HB2	2.07	0.55
1:A:550:ILE:HB	1:B:548:ALA:H	1.71	0.55
1:B:219:ARG:HG3	1:B:220:LEU:N	2.22	0.55
1:A:237:SER:HB3	1:A:276:GLU:N	2.21	0.55



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:510:ASP:CG	1:A:542:ARG:HE	2.10	0.55
1:B:373:GLU:HB3	2:B:739:HOH:O	2.05	0.55
1:B:451:THR:HG21	1:B:466:VAL:C	2.27	0.55
1:A:173:GLY:O	1:A:408:ARG:NH1	2.38	0.55
1:A:449:TYR:HB2	1:A:471:VAL:CG2	2.36	0.55
1:A:472:VAL:HG21	1:A:535:LEU:HD13	1.88	0.55
1:A:159:ILE:HD12	1:A:164:ILE:HG13	1.89	0.54
1:A:269:SER:OG	1:A:285:HIS:CD2	2.60	0.54
1:A:563:ASP:HA	1:A:566:LYS:HB2	1.88	0.54
1:B:220:LEU:HG	1:B:240:PHE:CE2	2.43	0.54
1:B:250:TRP:CD2	1:B:287:ARG:HA	2.42	0.54
1:B:355:ARG:HG3	1:B:387:ALA:HA	1.88	0.54
1:B:406:GLU:HA	2:B:763:HOH:O	2.07	0.54
1:A:284:ASN:HB2	1:A:300:THR:HG23	1.89	0.54
1:A:519:ILE:HG22	1:A:567:ILE:HG22	1.89	0.54
1:B:90:HIS:CD2	1:B:114:ILE:H	2.25	0.54
1:B:300:THR:O	1:B:301:SER:HB2	2.06	0.54
1:B:357:PRO:O	1:B:360:GLY:HA3	2.07	0.54
1:B:359:PRO:HB3	1:B:434:GLY:O	2.07	0.54
1:B:458:LYS:O	1:B:461:LEU:HB2	2.07	0.54
1:A:322:LEU:HD22	1:A:323:PRO:O	2.07	0.54
1:B:35:LYS:HE2	1:B:52:ASP:OD2	2.07	0.54
1:B:52:ASP:C	1:B:54:GLY:H	2.11	0.54
1:B:411:ILE:HD12	1:B:419:GLU:HG2	1.87	0.54
1:A:307:ARG:HB2	1:A:318:LEU:O	2.08	0.54
1:A:346:VAL:HG13	1:A:407:TRP:CZ2	2.40	0.54
1:A:353:SER:O	1:A:354:GLY:C	2.45	0.54
1:A:220:LEU:HB3	1:A:233:LEU:HD12	1.89	0.54
1:A:549:HIS:HD1	1:B:549:HIS:CE1	2.25	0.54
1:B:91:ALA:HB1	1:B:105:ARG:NE	2.22	0.54
1:B:562:GLU:HG3	2:B:724:HOH:O	2.07	0.54
1:A:24:LYS:O	1:A:40:GLY:HA2	2.08	0.54
1:A:59:LEU:O	1:A:101:GLY:N	2.41	0.54
1:A:249:THR:HG22	1:A:250:TRP:HB3	1.88	0.54
1:A:175:VAL:HB	1:A:197:PHE:H	1.73	0.54
1:A:309:VAL:HG12	1:A:316:PRO:HB3	1.90	0.54
1:A:379:ASP:OD1	1:A:381:PHE:CD1	2.61	0.54
1:B:60:ASN:CG	2:B:679:HOH:O	2.46	0.54
1:B:171:GLY:C	1:B:173:GLY:N	2.61	0.54
1:B:376:ASP:CB	2:B:616:HOH:O	2.46	0.54
1:B:397:TYR:HD1	1:B:419:GLU:HB3	1.71	0.54



	A L C	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:105:ARG:O	1:A:107:GLU:N	2.40	0.54
1:B:245:PRO:HB2	1:B:263:ALA:HB1	1.90	0.54
1:B:323:PRO:CB	1:B:326:LEU:HD12	2.37	0.54
1:A:308:ILE:N	1:A:318:LEU:O	2.33	0.54
1:B:408:ARG:O	1:B:411:ILE:HG22	2.08	0.54
1:B:421:GLU:O	1:B:425:ALA:N	2.39	0.54
1:B:570:PRO:HA	2:B:653:HOH:O	2.07	0.54
1:B:164:ILE:HD11	1:B:182:LEU:HA	1.89	0.54
1:B:565:VAL:O	1:B:568:LEU:N	2.40	0.54
1:A:23:GLU:HG2	2:A:600:HOH:O	2.08	0.53
1:A:536:MET:HE1	1:A:550:ILE:HD11	1.89	0.53
1:A:578:GLN:O	1:A:579:ARG:C	2.46	0.53
1:B:30:VAL:N	1:B:289:VAL:HG11	2.23	0.53
1:B:205:GLY:O	1:B:206:MET:HB2	2.08	0.53
1:A:258:ARG:HD2	1:A:273:ILE:CG2	2.38	0.53
1:B:177:LEU:HD22	1:B:223:VAL:HG21	1.89	0.53
1:B:178:PHE:C	1:B:178:PHE:CD1	2.81	0.53
1:B:490:GLU:O	1:B:495:GLY:N	2.27	0.53
1:B:522:GLN:HB3	1:B:551:ILE:O	2.07	0.53
1:A:96:ASN:HD21	1:A:98:SER:HB2	1.73	0.53
1:A:175:VAL:CG2	1:A:196:SER:HB3	2.38	0.53
1:B:114:ILE:N	1:B:114:ILE:HD12	2.23	0.53
1:B:249:THR:N	1:B:262:VAL:O	2.42	0.53
1:A:37:LEU:HD12	1:A:49:TYR:O	2.08	0.53
1:A:292:ARG:O	1:A:294:LYS:HD2	2.08	0.53
1:A:334:ARG:NH2	1:A:350:VAL:HG11	2.22	0.53
1:A:579:ARG:HG2	1:A:580:GLU:N	2.22	0.53
1:A:46:VAL:O	1:A:64:ILE:HG12	2.09	0.53
1:A:115:LEU:O	1:A:116:SER:HB3	2.07	0.53
1:A:174:ARG:NH2	1:A:405:GLU:OE2	2.41	0.53
1:A:351:LEU:CD1	1:A:382:ALA:HB1	2.38	0.53
1:A:469:ALA:HA	1:A:520:HIS:CE1	2.44	0.53
1:B:92:LEU:C	1:B:106:LEU:HD12	2.29	0.53
1:B:195:GLY:HA3	1:B:213:GLU:O	2.08	0.53
1:A:22:VAL:HG21	1:A:323:PRO:HD3	1.90	0.53
1:A:442:MET:HG3	1:A:466:VAL:HB	1.89	0.53
1:A:456:THR:HG22	1:A:512:ILE:HG12	1.90	0.53
1:A:524:ASP:OD1	1:A:556:HIS:HB2	2.09	0.53
1:B:509:VAL:HA	1:B:512:ILE:CD1	2.35	0.53
1:A:58:LYS:HD3	2:A:736:HOH:O	2.08	0.53
1:A:62:GLU:HB2	1:A:81:ARG:NH2	2.23	0.53



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:A:115:LEU:HB2	2:A:677:HOH:O	2.08	0.53
1:A:379:ASP:OD1	1:A:381:PHE:HD1	1.92	0.53
1:B:423:VAL:HG21	1:B:450:MET:HG2	1.90	0.53
1:A:194:GLU:HB3	1:A:214:THR:HG22	1.91	0.53
1:A:348:THR:HG21	1:A:393:VAL:HG13	1.90	0.53
1:B:31:VAL:CG1	1:B:32:ASP:N	2.71	0.53
1:B:42:SER:OG	1:B:43:GLU:N	2.42	0.53
1:A:151:PRO:HB2	1:A:170:PHE:CD2	2.44	0.53
1:A:169:PHE:CE2	1:A:371:PHE:HD1	2.27	0.53
1:A:497:ARG:C	1:A:499:ILE:H	2.13	0.53
1:A:328:ARG:HG2	1:A:328:ARG:NH1	2.23	0.52
1:A:350:VAL:HA	2:A:652:HOH:O	2.09	0.52
1:A:84:SER:OG	1:A:87:ALA:HB3	2.10	0.52
1:A:125:VAL:HG13	1:A:137:TYR:O	2.09	0.52
1:B:493:THR:O	1:B:494:GLY:C	2.47	0.52
1:B:133:ARG:HD2	1:B:146:GLU:OE2	2.09	0.52
1:B:539:LEU:HD13	1:B:546:PHE:CD1	2.44	0.52
1:A:106:LEU:HD11	2:A:589:HOH:O	2.09	0.52
1:A:551:ILE:N	1:A:551:ILE:HD12	2.25	0.52
1:B:209:THR:O	1:B:210:ALA:HB2	2.09	0.52
1:B:366:VAL:HG12	2:B:588:HOH:O	2.07	0.52
1:A:198:SER:HB3	1:A:213:GLU:OE2	2.09	0.52
1:A:392:VAL:HG12	1:A:393:VAL:N	2.25	0.52
1:A:441:ILE:HB	1:A:462:PHE:CE1	2.45	0.52
1:A:442:MET:HE2	1:A:444:TYR:HE1	1.74	0.52
1:A:463:LYS:HB2	2:A:729:HOH:O	2.09	0.52
1:B:59:LEU:HA	1:B:100:PRO:HB3	1.90	0.52
1:B:325:ASP:HA	1:B:328:ARG:NE	2.24	0.52
1:B:579:ARG:C	1:B:581:ARG:N	2.59	0.52
1:A:132:ASP:O	1:A:133:ARG:HB3	2.09	0.52
1:A:415:PRO:HD3	1:A:492:LEU:O	2.08	0.52
1:B:246:THR:HG21	1:B:402:GLY:O	2.10	0.52
1:A:309:VAL:HG12	1:A:316:PRO:CB	2.39	0.52
1:A:353:SER:HB2	1:A:386:ALA:HA	1.92	0.52
1:B:501:ARG:O	1:B:507:ASN:OD1	2.27	0.52
1:A:304:THR:HG23	2:A:654:HOH:O	2.10	0.52
1:A:339:GLU:OE2	1:A:343:GLY:HA2	2.09	0.52
1:A:463:LYS:O	1:A:514:GLU:HB3	2.09	0.52
1:A:530:LYS:HB3	1:A:531:PRO:CD	2.28	0.52
1:B:159:ILE:CD1	1:B:164:ILE:HG23	2.39	0.52
1:B:472:VAL:HG23	1:B:532:LEU:HD22	1.92	0.52



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:564:ALA:HB2	2:B:729:HOH:O	2.10	0.52
1:B:246:THR:HG22	1:B:265:ARG:HA	1.91	0.52
1:A:202:ILE:HG13	2:A:653:HOH:O	2.09	0.51
1:B:37:LEU:HD23	1:B:70:PRO:HG3	1.91	0.51
1:B:145:ARG:HD3	2:B:664:HOH:O	2.09	0.51
1:B:281:PRO:HG3	2:B:595:HOH:O	2.09	0.51
1:A:129:ALA:HB1	1:A:134:VAL:HG22	1.91	0.51
1:A:133:ARG:HD2	2:A:609:HOH:O	2.10	0.51
1:A:341:PHE:C	1:A:343:GLY:H	2.13	0.51
1:A:497:ARG:O	1:A:500:MET:N	2.43	0.51
1:A:471:VAL:HG11	1:A:474:TRP:CZ3	2.46	0.51
1:B:397:TYR:CD1	1:B:419:GLU:HB3	2.45	0.51
1:B:497:ARG:N	2:B:648:HOH:O	2.42	0.51
1:A:482:ASP:OD1	1:A:485:PHE:HD1	1.93	0.51
1:A:172:GLY:C	1:A:174:ARG:N	2.63	0.51
1:A:181:ASN:HB3	1:A:185:GLY:H	1.75	0.51
1:A:299:HIS:CG	1:A:300:THR:N	2.77	0.51
1:B:72:TYR:CE2	1:B:289:VAL:HG13	2.46	0.51
1:B:136:LEU:O	1:B:147:LEU:HB2	2.10	0.51
1:B:463:LYS:O	2:B:689:HOH:O	2.19	0.51
1:B:579:ARG:O	1:B:581:ARG:N	2.43	0.51
1:A:87:ALA:HA	1:A:523:ASN:O	2.11	0.51
1:A:202:ILE:HG22	1:A:203:SER:N	2.26	0.51
1:A:284:ASN:ND2	1:A:376:ASP:O	2.43	0.51
1:B:78:ILE:HD11	1:B:124:VAL:HG22	1.93	0.51
1:B:139:LEU:HD12	1:B:143:GLY:C	2.31	0.51
1:B:411:ILE:HD12	1:B:419:GLU:CG	2.41	0.51
1:B:487:ASN:O	1:B:491:GLN:HG3	2.10	0.51
1:A:27:LEU:HB3	2:A:605:HOH:O	2.10	0.51
1:A:286:GLY:O	1:A:287:ARG:C	2.48	0.51
1:B:225:PRO:HB2	2:B:738:HOH:O	2.11	0.51
1:A:399:GLY:HA2	1:A:408:ARG:O	2.10	0.51
1:A:350:VAL:HG12	1:A:351:LEU:N	2.26	0.51
1:B:344:SER:N	2:B:722:HOH:O	2.43	0.51
1:A:63:PRO:HB3	2:A:595:HOH:O	2.11	0.51
1:A:81:ARG:O	1:A:90:HIS:HA	2.11	0.51
1:A:174:ARG:HH21	1:A:405:GLU:CG	2.23	0.51
1:A:385:LEU:HB3	2:A:720:HOH:O	2.11	0.51
1:A:474:TRP:CB	1:A:500:MET:HB3	2.40	0.51
1:B:362:THR:CG2	1:B:363:VAL:H	2.23	0.51
1:B:401:THR:HG22	1:B:408:ARG:CD	2.41	0.51



	A i a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:477:MET:HE1	1:B:489:ILE:HD11	1.91	0.51
1:B:82:ASP:OD1	1:B:84:SER:OG	2.22	0.50
1:A:371:PHE:N	1:A:371:PHE:CD2	2.78	0.50
1:B:139:LEU:HD12	1:B:143:GLY:O	2.11	0.50
1:B:430:ALA:O	1:B:436:ALA:N	2.38	0.50
1:A:202:ILE:CG1	2:A:653:HOH:O	2.58	0.50
1:A:415:PRO:O	1:A:416:CYS:HB3	2.11	0.50
1:A:472:VAL:HG21	1:A:535:LEU:HD22	1.93	0.50
1:A:551:ILE:CG2	1:A:552:PRO:HD2	2.41	0.50
1:B:451:THR:O	2:B:615:HOH:O	2.18	0.50
1:B:476:GLU:HA	1:B:479:GLU:CD	2.31	0.50
1:B:482:ASP:HB2	2:B:604:HOH:O	2.12	0.50
1:A:29:GLY:O	1:A:37:LEU:HB3	2.11	0.50
1:A:207:LYS:HE2	1:A:224:ASP:HB2	1.93	0.50
1:A:569:LEU:O	1:A:573:PHE:CD2	2.65	0.50
1:B:109:VAL:CG2	1:B:139:LEU:HD22	2.41	0.50
1:B:314:GLY:HA3	2:B:595:HOH:O	2.09	0.50
1:B:353:SER:HB3	1:B:356:ALA:CB	2.38	0.50
1:A:160:ARG:NH1	1:A:203:SER:HA	2.27	0.50
1:A:268:ARG:HA	1:A:283:GLY:O	2.11	0.50
1:B:76:ARG:NH2	2:B:725:HOH:O	2.32	0.50
1:B:362:THR:OG1	1:B:391:HIS:HB2	2.11	0.50
1:B:35:LYS:HB2	1:B:50:LEU:HD22	1.93	0.50
1:B:56:THR:N	2:B:735:HOH:O	2.43	0.50
1:B:81:ARG:HB3	1:B:93:PHE:CE1	2.47	0.50
1:B:393:VAL:HB	2:B:775:HOH:O	2.11	0.50
1:B:476:GLU:O	1:B:480:LEU:HG	2.12	0.50
1:A:365:LEU:HB2	2:A:693:HOH:O	2.12	0.50
1:A:399:GLY:N	1:A:407:TRP:O	2.45	0.50
1:B:35:LYS:CG	1:B:52:ASP:OD1	2.60	0.50
1:B:250:TRP:CZ3	1:B:260:ALA:HB3	2.46	0.50
1:B:371:PHE:CE2	1:B:408:ARG:NH1	2.79	0.50
1:A:249:THR:HG22	1:A:250:TRP:N	2.25	0.50
1:A:294:LYS:O	1:A:296:VAL:HG23	2.12	0.50
1:A:366:VAL:HG12	1:A:367:HIS:O	2.12	0.50
1:B:34:ASP:O	1:B:35:LYS:HG2	2.10	0.50
1:B:455:LEU:CD1	1:B:516:LEU:HD13	2.42	0.50
1:A:94:LYS:HB3	1:A:106:LEU:HD21	1.94	0.50
1:A:413:GLY:HA2	1:A:493:THR:HA	1.93	0.50
1:A:308:ILE:O	1:A:317:LEU:N	2.44	0.49
1:A:536:MET:CE	1:A:550:ILE:HD11	2.41	0.49



	ti a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:508:HIS:C	1:B:510:ASP:N	2.64	0.49
1:A:441:ILE:HD13	1:A:441:ILE:C	2.31	0.49
1:A:529:LEU:CD1	1:A:550:ILE:HD12	2.33	0.49
1:B:268:ARG:HH12	1:B:282:GLN:CD	2.15	0.49
1:B:431:ARG:HG3	1:B:431:ARG:HH11	1.77	0.49
1:A:60:ASN:ND2	1:A:62:GLU:O	2.37	0.49
1:A:240:PHE:HD1	1:A:272:PHE:CD1	2.31	0.49
1:B:251:LEU:HD11	1:B:259:LEU:HD11	1.93	0.49
1:B:543:GLY:O	1:B:544:LYS:C	2.50	0.49
1:A:71:HIS:HB2	1:A:119:ASP:O	2.11	0.49
1:A:468:GLY:C	1:A:470:SER:N	2.61	0.49
1:A:522:GLN:HG2	1:A:552:PRO:HA	1.94	0.49
1:B:49:TYR:CA	1:B:57:VAL:O	2.54	0.49
1:B:405:GLU:HG3	1:B:409:LEU:HG	1.95	0.49
1:B:451:THR:HG21	1:B:466:VAL:O	2.12	0.49
1:A:68:LEU:HB2	1:A:78:ILE:HB	1.94	0.49
1:A:408:ARG:O	1:A:411:ILE:HG22	2.13	0.49
1:A:416:CYS:SG	1:A:416:CYS:O	2.70	0.49
1:B:153:PHE:CE1	1:B:488:PHE:HB2	2.45	0.49
1:B:311:LEU:HB3	1:B:312:PRO:HA	1.95	0.49
1:B:486:ARG:O	1:B:490:GLU:HG3	2.12	0.49
1:A:44:GLY:HA2	1:A:561:MET:N	2.22	0.49
1:B:243:TYR:CZ	1:B:270:ALA:HB2	2.47	0.49
1:B:431:ARG:HG3	1:B:431:ARG:NH1	2.28	0.49
1:A:87:ALA:O	1:A:525:SER:OG	2.24	0.49
1:A:160:ARG:HH22	1:A:204:PRO:HG3	1.78	0.49
1:A:309:VAL:HA	1:A:317:LEU:H	1.77	0.49
1:B:242:SER:C	1:B:244:ARG:H	2.15	0.49
1:B:365:LEU:HD23	1:B:394:MET:HG2	1.94	0.49
1:A:142:GLY:HA3	2:A:636:HOH:O	2.11	0.49
1:B:90:HIS:CG	1:B:114:ILE:HD13	2.46	0.49
1:A:174:ARG:NE	1:A:409:LEU:HD11	2.25	0.49
1:A:489:ILE:O	1:A:490:GLU:C	2.50	0.49
1:B:36:LEU:HD11	1:B:296:VAL:HG11	1.94	0.49
1:B:209:THR:HG23	1:B:233:LEU:HD12	1.95	0.49
1:A:124:VAL:N	1:A:139:LEU:O	2.38	0.49
1:A:224:ASP:OD1	1:A:225:PRO:HD2	2.12	0.49
1:A:475:GLU:OE1	1:A:497:ARG:HG3	2.13	0.49
1:B:65:ASN:HD21	1:B:82:ASP:HB2	1.77	0.49
1:B:280:ALA:CB	1:B:285:HIS:CE1	2.96	0.49
1:B:506:ILE:CD1	1:B:535:LEU:HA	2.43	0.49



	ti a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:522:GLN:HG3	1:B:523:ASN:N	2.27	0.49
1:A:74:VAL:HG11	1:A:121:GLY:CA	2.43	0.48
1:A:240:PHE:CE1	1:A:245:PRO:HG3	2.47	0.48
1:A:305:PRO:HD2	2:A:654:HOH:O	2.11	0.48
1:B:71:HIS:HA	2:B:666:HOH:O	2.13	0.48
1:B:411:ILE:HD13	1:B:419:GLU:HG2	1.94	0.48
1:A:194:GLU:CB	1:A:212:LEU:HD21	2.38	0.48
1:A:277:ARG:HD2	1:A:278:VAL:H	1.77	0.48
1:B:239:ASP:HA	1:B:242:SER:OG	2.13	0.48
1:A:341:PHE:CG	1:A:342:ASP:N	2.82	0.48
1:A:579:ARG:NH1	1:A:579:ARG:CB	2.75	0.48
1:B:379:ASP:HB3	1:B:382:ALA:CB	2.43	0.48
1:B:459:PRO:HG3	2:B:605:HOH:O	2.13	0.48
1:B:516:LEU:HD21	1:B:518:LEU:HD21	1.94	0.48
1:A:136:LEU:HD11	1:A:156:VAL:HG22	1.96	0.48
1:A:194:GLU:OE2	1:A:219:ARG:NH2	2.47	0.48
1:A:274:ASP:C	1:A:276:GLU:H	2.17	0.48
1:B:68:LEU:HD12	1:B:78:ILE:CD1	2.43	0.48
1:B:453:CYS:N	2:B:731:HOH:O	2.46	0.48
1:A:563:ASP:HA	1:A:566:LYS:CB	2.43	0.48
1:B:40:GLY:HA3	1:B:49:TYR:HE1	1.79	0.48
1:B:272:PHE:CE2	1:B:277:ARG:HB2	2.48	0.48
1:B:445:SER:C	1:B:447:GLY:N	2.66	0.48
1:A:361:PRO:HB3	1:A:438:GLU:OE2	2.14	0.48
1:A:384:SER:O	1:A:387:ALA:HB3	2.13	0.48
1:B:68:LEU:HD12	1:B:124:VAL:HG13	1.95	0.48
1:A:26:SER:OG	1:A:28:GLN:NE2	2.46	0.48
1:A:192:SER:HB3	1:A:195:GLY:O	2.13	0.48
1:A:258:ARG:HB3	1:A:273:ILE:HG23	1.96	0.48
1:A:264:ARG:NE	1:A:373:GLU:OE2	2.45	0.48
1:A:374:ASP:N	1:A:396:ASN:OD1	2.35	0.48
1:B:376:ASP:HA	2:B:600:HOH:O	2.12	0.48
1:A:129:ALA:CB	1:A:484:ALA:HB2	2.43	0.48
1:A:330:ILE:HD12	1:A:330:ILE:N	2.29	0.48
1:A:452:LEU:HB3	1:A:505:PRO:HG2	1.95	0.48
1:A:549:HIS:ND1	1:A:570:PRO:HB3	2.29	0.48
1:B:28:GLN:HG3	1:B:67:VAL:HG21	1.96	0.48
1:B:449:TYR:N	2:B:685:HOH:O	2.47	0.48
1:B:519:ILE:HD13	1:B:567:ILE:O	2.13	0.48
1:A:173:GLY:O	1:A:408:ARG:NH2	2.47	0.48
1:A:174:ARG:NH2	1:A:195:GLY:HA2	2.29	0.48



	lo uo pugo	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:222:THR:HB	1:A:231:GLU:CG	2.43	0.48
1:A:414:ASP:CG	1:A:414:ASP:O	2.51	0.48
1:A:553:ASP:OD1	1:B:545:THB:CG2	2.61	0.48
1.B.365.LEU.HD11	1.B.381.PHE.HB3	1.96	0.48
1:B:367:HIS:CE1	1:B:400:SEB:OG	2.67	0.48
1:B:442:MET:HG3	1:B:466:VAL:CG1	2.44	0.48
1:B:457:MET:C	1:B:459:PRO:HD2	2.34	0.48
1:B:468:GLY:HA2	1:B:519:ILE:O	2.13	0.48
1:A:497:ARG:C	1:A:499:ILE:N	2.67	0.48
1:B:38:VAL:CG1	1:B:308:ILE:HD13	2.44	0.48
1:B:282:GLN:NE2	2:B:660:HOH:O	2.46	0.48
1:B:294:LYS:HG2	2:B:705:HOH:O	2.13	0.48
1:B:411:ILE:HG12	1:B:492:LEU:HD11	1.95	0.48
1:B:458:LYS:N	1:B:459:PRO:CD	2.77	0.48
1:B:568:LEU:O	1:B:572:VAL:HG23	2.14	0.48
1:A:90:HIS:HD2	1:A:114:ILE:N	2.08	0.47
1:A:415:PRO:HG3	1:A:493:THR:HG22	1.95	0.47
1·A·474·TRP·HD1	1.A.500.MET.HA	1.79	0.47
1:A:569:LEU:HB3	1:A:570:PRO:CD	2.36	0.47
1·B·325·ASP·C	1.B.328.ABG.H	2.17	0.47
1:B:333:SER:HA	1:B:350:VAL:O	2.14	0.47
1:B:520:HIS:CB	2:B:744:HOH:O	2.62	0.47
1:A:372:ALA:O	1:A:373:GLU:HB3	2.14	0.47
1:A:521:PRO:CB	1:A:555:GLY:O	2.62	0.47
1:A:532:LEU:HD12	1:A:536:MET:HE3	1.96	0.47
1:B:406:GLU:HG2	1:B:410:LYS:CE	2.41	0.47
1:B:451:THR:HA	2:B:615:HOH:O	2.14	0.47
1:B:27:LEU:HD12	1:B:38:VAL:HG12	1.94	0.47
1:B:158:ASP:C	1:B:159:ILE:HD13	2.34	0.47
1:B:322:LEU:O	1:B:323:PRO:O	2.33	0.47
1:B:475:GLU:O	1:B:478:TYR:HB3	2.14	0.47
1:A:224:ASP:O	1:A:228:GLY:HA2	2.14	0.47
1:A:515:PRO:CA	2:A:613:HOH:O	2.47	0.47
1:B:212:LEU:CD2	1:B:219:ARG:HH12	2.12	0.47
1:B:550:ILE:N	1:B:550:ILE:HD12	2.29	0.47
1:A:309:VAL:CA	1:A:316:PRO:HA	2.41	0.47
1:B:70:PRO:HA	1:B:119:ASP:HB3	1.97	0.47
1:B:248:ILE:HD12	1:B:248:ILE:N	2.28	0.47
1:B:504:SER:O	1:B:506:ILE:N	2.48	0.47
1:B:520:HIS:CE1	2:B:618:HOH:O	2.67	0.47
1:B:551:ILE:HB	1:B:554:ALA:CB	2.43	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:385:LEU:O	1:B:390:PHE:N	2.45	0.47
1:B:477:MET:HA	1:B:528:PRO:HG3	1.96	0.47
1:A:104:GLN:NE2	2:A:699:HOH:O	2.47	0.47
1:A:219:ARG:HH12	1:A:221:VAL:CG1	2.27	0.47
1:A:254:LEU:HD11	1:A:295:LEU:HD21	1.96	0.47
1:A:430:ALA:HB1	1:A:436:ALA:HB2	1.97	0.47
1:A:468:GLY:O	1:A:469:ALA:C	2.53	0.47
1:B:112:MET:HB2	1:B:130:THR:HG22	1.97	0.47
1:B:250:TRP:CE3	1:B:287:ARG:HA	2.50	0.47
1:B:309:VAL:HG12	1:B:316:PRO:CA	2.45	0.47
1:B:477:MET:CA	2:B:756:HOH:O	2.58	0.47
1:B:480:LEU:CB	2:B:756:HOH:O	2.52	0.47
1:A:258:ARG:HD2	1:A:273:ILE:HG21	1.97	0.47
1:A:346:VAL:HG22	1:A:407:TRP:CZ2	2.50	0.47
1:A:367:HIS:HE1	1:A:396:ASN:HA	1.80	0.47
1:B:476:GLU:CG	1:B:531:PRO:HG3	2.45	0.47
1:B:495:GLY:O	1:B:496:SER:O	2.33	0.47
1:A:237:SER:O	1:A:275:GLY:HA3	2.14	0.47
1:A:267:GLY:CA	1:A:375:SER:HB2	2.45	0.47
1:A:452:LEU:HB2	2:A:709:HOH:O	2.14	0.47
1:B:445:SER:HA	1:B:469:ALA:O	2.15	0.47
1:B:472:VAL:HG23	2:B:683:HOH:O	2.14	0.47
1:A:62:GLU:HB2	1:A:81:ARG:HE	1.80	0.47
1:A:519:ILE:CG2	1:A:567:ILE:HG22	2.44	0.47
1:B:47:ASN:HB2	2:B:656:HOH:O	2.15	0.47
1:B:89:GLN:HA	1:B:112:MET:O	2.15	0.47
1:B:280:ALA:HB3	1:B:285:HIS:CE1	2.50	0.47
1:B:367:HIS:HD2	1:B:368:GLY:O	1.98	0.47
1:B:441:ILE:HD13	2:B:615:HOH:O	2.15	0.47
1:B:495:GLY:O	1:B:496:SER:C	2.54	0.47
1:A:151:PRO:HD2	1:A:170:PHE:CZ	2.49	0.46
1:A:366:VAL:HG13	1:A:397:TYR:CE2	2.50	0.46
1:B:141:GLY:C	1:B:143:GLY:H	2.18	0.46
1:B:431:ARG:HA	1:B:436:ALA:HB3	1.98	0.46
1:A:45:SER:CB	2:A:595:HOH:O	2.59	0.46
1:A:160:ARG:NH2	1:A:204:PRO:HG3	2.30	0.46
1:B:133:ARG:HD2	2:B:608:HOH:O	2.16	0.46
1:B:567:ILE:HD12	1:B:567:ILE:C	2.32	0.46
1:A:302:LEU:HG	1:A:376:ASP:OD1	2.15	0.46
1:A:305:PRO:O	1:A:306:PRO:C	2.52	0.46
1:A:532:LEU:O	1:A:536:MET:HG3	2.15	0.46



	loue page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:332:GLY:H	1:B:352:GLU:HB2	1.80	0.46
1:B:520:HIS:CD2	1:B:521:PRO:HD2	2.32	0.46
1:A:88:GLU:HG3	1:A:113:ARG:NH1	2.29	0.46
1:A:270:ALA:HB3	2:A:588:HOH:O	2.15	0.46
1:A:399:GLY:CA	1:A:408:ARG:HA	2.46	0.46
1:B:41:PHE:HZ	1:B:558:ILE:HG22	1.80	0.46
1:B:134:VAL:HB	1:B:150:LEU:HB2	1.97	0.46
1:B:178:PHE:HB2	1:B:187:LEU:HD11	1.96	0.46
1:B:251:LEU:HD12	1:B:259:LEU:HD11	1.97	0.46
1:B:458:LYS:O	1:B:461:LEU:CB	2.63	0.46
1:A:172:GLY:C	1:A:174:ARG:H	2.18	0.46
1:A:486:ARG:HG3	1:A:486:ARG:NH1	2.29	0.46
1:A:510:ASP:HB2	2:A:607:HOH:O	2.16	0.46
1:B:160:ARG:HD2	1:B:202:ILE:CG2	2.46	0.46
1:A:93:PHE:HA	1:A:104:GLN:O	2.16	0.46
1:A:272:PHE:HD2	1:A:277:ARG:HA	1.80	0.46
1:A:398:ARG:HD3	1:A:410:LYS:HB3	1.97	0.46
1:B:51:TYR:CE2	1:B:53:GLY:HA2	2.51	0.46
1:B:88:GLU:HG2	1:B:113:ARG:HH12	1.74	0.46
1:B:323:PRO:HG2	1:B:326:LEU:CD1	2.43	0.46
1:A:138:ALA:HB2	1:A:147:LEU:CD2	2.38	0.46
1:A:222:THR:HG22	1:A:222:THR:O	2.16	0.46
1:A:240:PHE:CZ	1:A:245:PRO:HG3	2.51	0.46
1:A:265:ARG:HD3	2:A:598:HOH:O	2.15	0.46
1:A:579:ARG:CB	1:A:579:ARG:HH11	2.28	0.46
1:B:125:VAL:HA	1:B:138:ALA:HA	1.96	0.46
1:B:379:ASP:O	1:B:380:THR:C	2.53	0.46
1:A:277:ARG:HD2	1:A:278:VAL:N	2.31	0.46
1:A:444:TYR:O	1:A:445:SER:HB3	2.16	0.46
1:A:474:TRP:HZ3	1:A:477:MET:HE1	1.80	0.46
1:B:51:TYR:CE2	1:B:317:LEU:HB3	2.43	0.46
1:B:448:GLY:HA3	1:B:470:SER:HB3	1.97	0.46
1:B:464:ALA:HB2	1:B:578:GLN:HG3	1.98	0.46
1:B:577:THR:CB	2:B:784:HOH:O	2.57	0.46
1:A:354:GLY:C	1:A:356:ALA:H	2.18	0.46
1:A:574:PHE:O	1:A:578:GLN:HG2	2.15	0.46
1:B:30:VAL:CG2	1:B:290:LEU:O	2.64	0.46
1:B:75:GLY:O	1:B:96:ASN:OD1	2.34	0.46
1:B:347:PRO:HG2	1:B:396:ASN:CB	2.45	0.46
1:B:458:LYS:HB3	1:B:461:LEU:CD2	2.45	0.46
1:A:95:VAL:CG2	1:A:103:GLU:HG2	2.45	0.45



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Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:400:SER:C	2:A:618:HOH:O	2.53	0.45
1:B:48:ALA:O	1:B:58:LYS:HA	2.17	0.45
1:B:235:LEU:HD13	1:B:274:ASP:C	2.37	0.45
1:B:251:LEU:HD11	1:B:259:LEU:HD21	1.98	0.45
1:B:279:GLU:HB2	1:B:312:PRO:O	2.15	0.45
1:B:334:ARG:NH2	1:B:429:TRP:HH2	2.14	0.45
1:A:47:ASN:HB3	1:A:60:ASN:OD1	2.17	0.45
1:A:178:PHE:CD1	1:A:178:PHE:O	2.70	0.45
1:A:420:LEU:HD11	1:A:454:ALA:HA	1.97	0.45
1:A:558:ILE:HD12	1:A:563:ASP:CB	2.31	0.45
1:B:178:PHE:HD2	2:B:706:HOH:O	1.99	0.45
1:B:307:ARG:HB2	1:B:319:GLU:CB	2.46	0.45
1:A:446:TYR:O	1:A:449:TYR:HB3	2.15	0.45
1:B:255:PRO:C	1:B:257:GLY:H	2.19	0.45
1:B:326:LEU:HD23	1:B:355:ARG:NH1	2.31	0.45
1:A:129:ALA:HA	1:A:134:VAL:HA	1.99	0.45
1:B:327:ARG:NH2	2:B:651:HOH:O	2.48	0.45
1:B:445:SER:C	1:B:447:GLY:H	2.19	0.45
1:B:482:ASP:O	1:B:486:ARG:HG3	2.17	0.45
1:A:475:GLU:HG2	1:A:500:MET:HB2	1.98	0.45
1:B:27:LEU:HD13	1:B:38:VAL:HG12	1.98	0.45
1:B:61:ARG:N	1:B:103:GLU:OE2	2.50	0.45
1:B:91:ALA:CB	1:B:105:ARG:NE	2.79	0.45
1:B:92:LEU:CD1	1:B:109:VAL:HG11	2.46	0.45
1:B:95:VAL:HG13	2:B:742:HOH:O	2.15	0.45
1:B:551:ILE:HD11	1:B:567:ILE:HG22	1.98	0.45
1:A:44:GLY:CA	1:A:561:MET:H	2.24	0.45
1:A:160:ARG:HD3	1:A:202:ILE:CG2	2.46	0.45
1:A:346:VAL:HG22	1:A:407:TRP:HH2	1.81	0.45
1:A:463:LYS:CB	2:A:729:HOH:O	2.63	0.45
1:A:579:ARG:HB2	1:A:579:ARG:CZ	2.46	0.45
1:B:164:ILE:O	1:B:179:THR:HA	2.16	0.45
1:B:233:LEU:HD22	1:B:235:LEU:HG	1.99	0.45
1:B:444:TYR:HA	1:B:468:GLY:O	2.17	0.45
1:A:34:ASP:O	1:A:291:TRP:NE1	2.50	0.45
1:A:251:LEU:HA	1:A:260:ALA:O	2.17	0.45
1:A:440:TYR:HE2	1:A:578:GLN:HB3	1.82	0.45
1:B:219:ARG:HD2	1:B:232:ASP:OD1	2.16	0.45
1:B:376:ASP:C	2:B:600:HOH:O	2.55	0.45
1:B:424:SER:CB	2:B:778:HOH:O	2.65	0.45
1:B:522:GLN:HE21	1:B:523:ASN:CG	2.19	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:22:VAL:HG12	1:A:23:GLU:N	2.32	0.45
1:A:68:LEU:HD12	1:A:78:ILE:CG2	2.35	0.45
1:A:239:ASP:O	1:A:243:TYR:N	2.48	0.45
1:A:370:PRO:HG3	1:A:411:ILE:HD13	1.99	0.45
1:A:421:GLU:OE2	1:A:458:LYS:CE	2.65	0.45
1:A:475:GLU:HA	1:A:500:MET:CE	2.47	0.45
1:A:547:GLU:HB2	1:B:550:ILE:O	2.17	0.45
1:B:29:GLY:HA3	1:B:289:VAL:HG21	1.99	0.45
1:B:398:ARG:NH2	1:B:407:TRP:HZ3	2.13	0.45
1:B:411:ILE:CG1	1:B:492:LEU:HD11	2.46	0.45
1:B:479:GLU:HG2	2:B:617:HOH:O	2.16	0.45
1:B:520:HIS:HD2	1:B:521:PRO:CD	2.21	0.45
1:B:520:HIS:HB2	2:B:744:HOH:O	2.17	0.45
1:A:125:VAL:O	1:A:126:PHE:HB3	2.16	0.45
1:A:262:VAL:O	1:A:262:VAL:HG12	2.17	0.45
1:A:263:ALA:O	1:A:269:SER:CB	2.65	0.45
1:A:335:LEU:HD13	1:A:349:TYR:CE1	2.51	0.45
1:B:226:ARG:NE	2:B:769:HOH:O	2.49	0.45
1:B:476:GLU:HA	1:B:479:GLU:CG	2.47	0.45
1:B:476:GLU:HA	1:B:479:GLU:HG3	1.99	0.45
1:B:565:VAL:O	1:B:567:ILE:N	2.50	0.45
1:B:569:LEU:CB	1:B:570:PRO:HD3	2.42	0.45
1:A:179:THR:H	1:A:187:LEU:CD1	2.30	0.45
1:B:415:PRO:O	1:B:503:ARG:HG3	2.17	0.45
1:B:448:GLY:HA3	1:B:470:SER:HA	1.99	0.45
1:A:163:LEU:HB3	1:A:202:ILE:HD13	1.98	0.44
1:A:417:GLY:H	1:A:419:GLU:CD	2.19	0.44
1:B:38:VAL:HG11	1:B:308:ILE:HD13	1.99	0.44
1:B:156:VAL:HG23	2:B:596:HOH:O	2.16	0.44
1:A:25:TYR:HB3	1:A:38:VAL:CG1	2.46	0.44
1:B:330:ILE:HG23	1:B:351:LEU:HD21	1.99	0.44
1:B:364:VAL:HA	1:B:393:VAL:O	2.17	0.44
1:A:224:ASP:HA	1:A:225:PRO:HD3	1.83	0.44
1:A:520:HIS:N	1:A:549:HIS:O	2.35	0.44
1:B:340:SER:CA	2:B:722:HOH:O	2.65	0.44
1:B:551:ILE:HG23	1:B:566:LYS:HD3	1.98	0.44
1:A:109:VAL:HA	2:A:728:HOH:O	2.17	0.44
1:A:217:GLU:HG2	1:A:218:ALA:H	1.82	0.44
1:A:393:VAL:HG22	2:A:652:HOH:O	2.16	0.44
1:A:424:SER:HB3	1:A:461:LEU:HD21	1.99	0.44
1:B:40:GLY:N	1:B:47:ASN:O	2.32	0.44



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Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:221:VAL:HG12	1:B:232:ASP:HA	2.00	0.44
1:B:401:THR:HG22	1:B:408:ARG:HD3	1.97	0.44
1:B:571:ALA:HA	2:B:723:HOH:O	2.16	0.44
1:A:304:THR:HA	1:A:305:PRO:HD3	1.82	0.44
1:A:488:PHE:HZ	2:A:672:HOH:O	2.00	0.44
1:A:509:VAL:O	1:A:509:VAL:HG12	2.17	0.44
1:B:226:ARG:HG3	1:B:226:ARG:HH11	1.82	0.44
1:B:240:PHE:CE1	1:B:263:ALA:HB2	2.52	0.44
1:B:340:SER:N	2:B:722:HOH:O	2.43	0.44
1:A:31:VAL:HB	1:A:74:VAL:O	2.16	0.44
1:A:219:ARG:NH1	1:A:221:VAL:HG12	2.33	0.44
1:A:367:HIS:HD2	1:A:372:ALA:HB3	1.81	0.44
1:A:499:ILE:O	1:A:503:ARG:HB2	2.17	0.44
1:A:576:ALA:O	1:A:579:ARG:HB3	2.18	0.44
1:B:135:ALA:HB2	2:B:608:HOH:O	2.17	0.44
1:B:239:ASP:HA	1:B:242:SER:HG	1.82	0.44
1:B:243:TYR:O	1:B:244:ARG:C	2.56	0.44
1:B:456:THR:HG22	1:B:512:ILE:CD1	2.47	0.44
1:A:379:ASP:OD1	1:A:379:ASP:C	2.56	0.44
1:A:451:THR:O	1:A:455:LEU:HG	2.18	0.44
1:B:59:LEU:HB3	2:B:727:HOH:O	2.17	0.44
1:B:301:SER:HA	1:B:376:ASP:O	2.18	0.44
1:B:371:PHE:HD2	1:B:408:ARG:HH11	1.61	0.44
1:A:51:TYR:CE2	1:A:53:GLY:HA2	2.53	0.44
1:A:374:ASP:CG	1:A:394:MET:HB3	2.39	0.44
1:A:442:MET:CE	1:A:444:TYR:HE1	2.31	0.44
1:B:465:GLY:O	1:B:516:LEU:HD12	2.18	0.44
1:B:549:HIS:CE1	2:B:686:HOH:O	2.70	0.44
1:A:72:TYR:OH	1:A:289:VAL:HG12	2.18	0.44
1:A:117:GLY:HA2	1:A:126:PHE:HA	2.00	0.44
1:A:430:ALA:HB3	1:A:439:LEU:HD11	2.00	0.44
1:A:440:TYR:HD2	1:A:464:ALA:HB3	1.82	0.44
1:A:475:GLU:CA	1:A:500:MET:HE2	2.48	0.44
1:B:523:ASN:ND2	1:B:553:ASP:CA	2.81	0.44
1:A:61:ARG:NH1	1:A:101:GLY:CA	2.74	0.43
1:A:174:ARG:NH2	1:A:405:GLU:HG2	2.33	0.43
1:A:195:GLY:HA3	1:A:213:GLU:O	2.18	0.43
1:A:309:VAL:HB	1:A:315:GLU:O	2.18	0.43
1:A:499:ILE:CD1	2:A:732:HOH:O	2.63	0.43
1:A:503:ARG:HA	2:A:601:HOH:O	2.17	0.43
1:B:48:ALA:N	2:B:679:HOH:O	2.50	0.43



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Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:118:VAL:HG21	1:B:159:ILE:HG12	1.99	0.43	
1:B:264:ARG:HA	1:B:269:SER:HA	2.00	0.43	
1:A:62:GLU:CB	1:A:81:ARG:HH21	2.31	0.43	
1:B:86:GLY:CA	1:B:555:GLY:HA3	2.48	0.43	
1:B:169:PHE:CZ	1:B:175:VAL:CG2	2.99	0.43	
1:B:170:PHE:HD1	1:B:189:VAL:HG11	1.83	0.43	
1:B:251:LEU:CD2	2:B:652:HOH:O	2.66	0.43	
1:B:477:MET:HE2	1:B:489:ILE:HD11	2.00	0.43	
1:A:79:LEU:HD11	1:A:95:VAL:HG21	1.99	0.43	
1:A:165:ALA:HB2	2:A:653:HOH:O	2.16	0.43	
1:A:438:GLU:HG3	1:A:440:TYR:HE1	1.83	0.43	
1:A:565:VAL:O	1:A:569:LEU:HB2	2.18	0.43	
1:B:198:SER:HB2	1:B:248:ILE:O	2.18	0.43	
1:B:209:THR:CA	1:B:222:THR:HG22	2.48	0.43	
1:B:210:ALA:O	1:B:211:GLY:C	2.55	0.43	
1:B:270:ALA:HB1	1:B:277:ARG:CZ	2.48	0.43	
1:B:431:ARG:NH2	2:B:714:HOH:O	2.47	0.43	
1:B:472:VAL:CG2	1:B:532:LEU:HD22	2.48	0.43	
1:B:487:ASN:HA	1:B:490:GLU:OE1	2.17	0.43	
1:B:580:GLU:O	1:B:581:ARG:HB2	2.18	0.43	
1:A:40:GLY:C	1:A:42:SER:N	2.72	0.43	
1:A:130:THR:O	1:A:131:GLU:C	2.56	0.43	
1:A:164:ILE:HD13	1:A:181:ASN:CA	2.47	0.43	
1:A:248:ILE:N	1:A:248:ILE:HD12	2.33	0.43	
1:A:469:ALA:HB1	1:A:556:HIS:CE1	2.54	0.43	
1:A:469:ALA:HB1	1:A:556:HIS:ND1	2.32	0.43	
1:B:224:ASP:HB3	1:B:227:ASP:OD1	2.18	0.43	
1:B:487:ASN:O	1:B:487:ASN:OD1	2.37	0.43	
1:A:277:ARG:NH1	1:A:277:ARG:HG2	2.33	0.43	
1:A:366:VAL:HG11	1:A:450:MET:HG3	2.00	0.43	
1:A:578:GLN:O	1:A:581:ARG:N	2.52	0.43	
1:B:42:SER:HA	1:B:561:MET:CE	2.48	0.43	
1:B:79:LEU:HD11	1:B:95:VAL:CG2	2.45	0.43	
1:B:207:LYS:HG2	1:B:222:THR:HB	1.99	0.43	
1:B:371:PHE:HA	1:B:399:GLY:O	2.19	0.43	
1:B:414:ASP:OD2	1:B:418:GLY:N	2.30	0.43	
1:B:493:THR:HA	2:B:629:HOH:O	2.18	0.43	
1:A:33:GLY:H	1:A:73:GLY:HA2	1.83	0.43	
1:A:74:VAL:HG11	1:A:121:GLY:HA3	2.00	0.43	
1:A:421:GLU:O	1:A:424:SER:HB2	2.19	0.43	
1:A:509:VAL:O	1:A:509:VAL:CG1	2.66	0.43	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:331:ALA:HB3	1:B:352:GLU:C	2.38	0.43	
1:B:472:VAL:HG21	1:B:532:LEU:HA	2.01	0.43	
1:B:472:VAL:O	1:B:505:PRO:HD2	2.18	0.43	
1:B:473:ASP:OD1	1:B:475:GLU:N	2.49	0.43	
1:B:494:GLY:O	1:B:496:SER:N	2.51	0.43	
1:B:522:GLN:HB3	1:B:550:ILE:HG22	1.99	0.43	
1:B:523:ASN:HD21	1:B:553:ASP:HA	1.82	0.43	
1:A:106:LEU:CD2	2:A:698:HOH:O	2.66	0.43	
1:A:178:PHE:HB2	1:A:187:LEU:HD11	2.01	0.43	
1:B:240:PHE:O	1:B:245:PRO:CD	2.67	0.43	
1:B:419:GLU:O	1:B:423:VAL:HG23	2.19	0.43	
1:A:77:VAL:HG23	1:A:97:THR:CG2	2.49	0.43	
1:A:197:PHE:HD2	1:A:210:ALA:HB1	1.84	0.43	
1:A:214:THR:C	1:A:216:ARG:N	2.70	0.43	
1:A:381:PHE:O	1:A:385:LEU:HB2	2.18	0.43	
1:A:460:GLY:O	1:A:461:LEU:C	2.57	0.43	
1:B:137:TYR:CD1	1:B:137:TYR:N	2.86	0.43	
1:B:209:THR:OG1	1:B:253:TYR:OH	2.32	0.43	
1:B:246:THR:CG2	1:B:265:ARG:HA	2.49	0.43	
1:B:299:HIS:CG	1:B:300:THR:N	2.86	0.43	
1:B:300:THR:O	1:B:301:SER:CB	2.67	0.43	
1:B:377:SER:N	2:B:600:HOH:O	2.51	0.43	
1:B:520:HIS:CE1	1:B:529:LEU:HA	2.54	0.43	
1:B:30:VAL:HG23	1:B:289:VAL:HG12	1.99	0.43	
1:A:71:HIS:HB2	1:A:120:THR:HA	2.01	0.43	
1:A:78:ILE:HG23	2:A:589:HOH:O	2.19	0.43	
1:A:167:LEU:CD2	1:A:197:PHE:HB2	2.49	0.43	
1:B:59:LEU:CD1	1:B:77:VAL:HG21	2.46	0.43	
1:B:73:GLY:O	1:B:74:VAL:C	2.57	0.43	
1:B:205:GLY:O	1:B:206:MET:CB	2.67	0.43	
1:B:334:ARG:NH2	1:B:429:TRP:CH2	2.87	0.43	
1:B:489:ILE:HG13	2:B:642:HOH:O	2.18	0.43	
1:A:138:ALA:HB3	1:A:147:LEU:HD21	1.98	0.42	
1:A:167:LEU:HD11	1:A:199:SER:HA	2.01	0.42	
1:A:188:ARG:HG3	1:A:188:ARG:HH11	1.84	0.42	
1:A:350:VAL:HG22	2:A:652:HOH:O	2.19	0.42	
1:B:31:VAL:HG21	1:B:37:LEU:HD22	2.00	0.42	
1:B:203:SER:O	1:B:206:MET:N	2.46	0.42	
1:B:324:GLU:HA	1:B:324:GLU:OE1	2.19	0.42	
1:A:32:ASP:CB	1:A:35:LYS:HD2	2.49	0.42	
1:A:120:THR:HG22	1:A:120:THR:O	2.19	0.42	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:26:SER:OG	1:B:28:GLN:NE2	2.51	0.42	
1:B:50:LEU:CD1	1:B:59:LEU:HD21	2.48	0.42	
1:B:218:ALA:HB1	1:B:248:ILE:HD12	1.97	0.42	
1:B:401:THR:HG22	1:B:408:ARG:HD2	2.01	0.42	
1:B:526:ARG:HH21	1:B:557:ALA:HB2	1.81	0.42	
1:A:203:SER:CB	1:A:204:PRO:CD	2.97	0.42	
1:A:288:VAL:CG1	1:A:295:LEU:HD22	2.49	0.42	
1:A:351:LEU:HD12	1:A:382:ALA:HB1	2.00	0.42	
1:B:84:SER:HB3	1:B:89:GLN:HB2	2.01	0.42	
1:B:428:ARG:O	1:B:431:ARG:N	2.49	0.42	
1:B:450:MET:HA	1:B:453:CYS:HB3	2.01	0.42	
1:A:203:SER:HB2	1:A:204:PRO:CD	2.49	0.42	
1:A:312:PRO:O	1:A:313:SER:C	2.58	0.42	
1:A:342:ASP:N	1:A:342:ASP:OD1	2.50	0.42	
1:A:440:TYR:HE2	1:A:578:GLN:CB	2.32	0.42	
1:B:330:ILE:HB	2:B:720:HOH:O	2.19	0.42	
1:B:536:MET:HA	2:B:678:HOH:O	2.19	0.42	
1:A:35:LYS:HG2	1:A:52:ASP:OD2	2.20	0.42	
1:A:96:ASN:HD22	1:A:99:ARG:HG3	1.84	0.42	
1:A:196:SER:OG	1:A:405:GLU:OE2	2.36	0.42	
1:B:123:ALA:CB	1:B:182:LEU:HD11	2.50	0.42	
1:B:359:PRO:O	1:B:437:SER:HB3	2.19	0.42	
1:B:574:PHE:CB	2:B:723:HOH:O	2.67	0.42	
1:A:158:ASP:HB2	1:A:201:SER:HA	2.02	0.42	
1:A:170:PHE:HB2	2:A:662:HOH:O	2.20	0.42	
1:B:70:PRO:HB2	1:B:74:VAL:CG2	2.41	0.42	
1:B:501:ARG:NH1	2:B:749:HOH:O	2.52	0.42	
1:A:29:GLY:HA2	1:A:289:VAL:HG11	2.02	0.42	
1:A:48:ALA:HB2	1:A:67:VAL:HG21	2.01	0.42	
1:A:98:SER:C	1:A:100:PRO:HD3	2.39	0.42	
1:A:152:GLY:O	1:A:153:PHE:C	2.57	0.42	
1:A:359:PRO:HA	1:A:435:LEU:HA	2.02	0.42	
1:A:393:VAL:CG1	1:A:426:ALA:HB1	2.49	0.42	
1:A:532:LEU:CD1	1:A:536:MET:CE	2.98	0.42	
1:A:579:ARG:CG	1:A:580:GLU:N	2.82	0.42	
1:B:476:GLU:OE1	1:B:531:PRO:HA	2.20	0.42	
1:A:371:PHE:CE1	1:A:408:ARG:NH1	2.88	0.42	
1:B:392:VAL:HG12	1:B:394:MET:HG3	2.02	0.42	
1:B:418:GLY:O	1:B:421:GLU:HB2	2.19	0.42	
1:A:44:GLY:HA2	1:A:561:MET:HB3	2.01	0.42	
1:A:84:SER:CB	1:A:87:ALA:HB3	2.50	0.42	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:315:GLU:OE1	1:A:315:GLU:HA	2.18	0.42	
1:A:469:ALA:HB1	1:A:556:HIS:HD1	1.85	0.42	
1:B:79:LEU:N	1:B:93:PHE:O	2.43	0.42	
1:B:209:THR:HA	1:B:222:THR:HG22	2.02	0.42	
1:B:305:PRO:HA	1:B:306:PRO:HD3	1.92	0.42	
1:B:428:ARG:O	1:B:429:TRP:C	2.58	0.42	
1:B:443:GLY:HA2	2:B:601:HOH:O	2.19	0.42	
1:A:212:LEU:HG	1:A:214:THR:HG23	2.01	0.42	
1:A:367:HIS:N	2:A:584:HOH:O	2.53	0.42	
1:B:76:ARG:HA	1:B:96:ASN:HA	2.01	0.42	
1:B:133:ARG:NE	1:B:149:ARG:HH21	2.18	0.42	
1:B:322:LEU:O	1:B:323:PRO:C	2.59	0.42	
1:A:92:LEU:HB3	1:A:106:LEU:HD12	2.02	0.41	
1:B:168:GLY:HA3	2:B:706:HOH:O	2.20	0.41	
1:B:240:PHE:HD1	1:B:272:PHE:CD1	2.37	0.41	
1:B:569:LEU:HD12	1:B:569:LEU:HA	1.83	0.41	
1:A:264:ARG:HA	1:A:269:SER:HA	2.02	0.41	
1:B:71:HIS:O	1:B:72:TYR:C	2.58	0.41	
1:B:176:SER:HA	2:B:746:HOH:O	2.19	0.41	
1:B:300:THR:OG1	1:B:301:SER:N	2.53	0.41	
1:B:302:LEU:HD13	1:B:351:LEU:HD13	2.02	0.41	
1:B:315:GLU:HA	1:B:316:PRO:HD2	1.75	0.41	
1:B:520:HIS:HA	1:B:521:PRO:HD3	1.81	0.41	
1:A:296:VAL:HA	2:A:670:HOH:O	2.20	0.41	
1:A:532:LEU:CD1	1:A:536:MET:HE3	2.50	0.41	
1:B:201:SER:HB3	2:B:652:HOH:O	2.20	0.41	
1:B:227:ASP:OD1	1:B:227:ASP:N	2.42	0.41	
1:B:264:ARG:HH11	1:B:264:ARG:HG2	1.85	0.41	
1:B:419:GLU:OE2	1:B:420:LEU:N	2.45	0.41	
1:A:373:GLU:HB2	1:A:396:ASN:OD1	2.20	0.41	
1:B:457:MET:O	1:B:459:PRO:HD2	2.20	0.41	
1:A:169:PHE:CE2	1:A:371:PHE:CD1	3.04	0.41	
1:A:219:ARG:NH1	1:A:221:VAL:CG1	2.84	0.41	
1:B:86:GLY:O	1:B:555:GLY:HA3	2.21	0.41	
1:B:133:ARG:HE	1:B:133:ARG:HB3	1.50	0.41	
1:B:291:TRP:O	1:B:292:ARG:HB2	2.19	0.41	
1:B:309:VAL:HA	1:B:316:PRO:HA	2.02	0.41	
1:B:397:TYR:CB	1:B:422:ASP:HB2	2.49	0.41	
1:B:567:ILE:HD12	1:B:568:LEU:CA	2.47	0.41	
1:B:569:LEU:HB3	1:B:570:PRO:CD	2.43	0.41	
1:A:108:ALA:O	1:A:144:LEU:HB2	2.21	0.41	



	i ageni	Interatomic	c Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:198:SER:CB	1:A:213:GLU:OE2	2.68	0.41	
1:A:421:GLU:O	1:A:425:ALA:N	2.53	0.41	
1:B:30:VAL:H	1:B:289:VAL:CG1	2.33	0.41	
1:B:31:VAL:HG22	1:B:74:VAL:CG2	2.51	0.41	
1:B:325:ASP:O	1:B:328:ARG:HB2	2.21	0.41	
1:B:411:ILE:O	1:B:411:ILE:HG13	2.21	0.41	
1:B:456:THR:HG22	1:B:512:ILE:HD11	2.00	0.41	
1:A:25:TYR:HA	1:A:39:VAL:O	2.20	0.41	
1:A:226:ARG:HA	1:A:226:ARG:HD3	1.93	0.41	
1:A:569:LEU:H	1:A:570:PRO:CD	2.33	0.41	
1:B:78:ILE:CD1	1:B:124:VAL:HG22	2.50	0.41	
1:B:328:ARG:NH1	2:B:682:HOH:O	2.54	0.41	
1:B:444:TYR:OH	1:B:521:PRO:HG2	2.21	0.41	
1:A:26:SER:HA	2:A:725:HOH:O	2.21	0.41	
1:A:367:HIS:CE1	1:A:396:ASN:HA	2.56	0.41	
1:A:393:VAL:HA	2:A:652:HOH:O	2.21	0.41	
1:A:551:ILE:HD13	1:A:567:ILE:HG22	2.03	0.41	
1:B:125:VAL:HG13	1:B:137:TYR:O	2.20	0.41	
1:B:263:ALA:O	1:B:269:SER:HA	2.21	0.41	
1:B:476:GLU:CD	1:B:531:PRO:HG3	2.41	0.41	
1:B:514:GLU:HA	1:B:515:PRO:HD3	1.90	0.41	
1:A:158:ASP:CB	1:A:201:SER:HA	2.50	0.41	
1:A:190:PHE:CD1	1:A:190:PHE:N	2.88	0.41	
1:A:194:GLU:CB	1:A:214:THR:HG22	2.51	0.41	
1:A:224:ASP:O	1:A:228:GLY:N	2.53	0.41	
1:A:322:LEU:HB2	2:A:697:HOH:O	2.21	0.41	
1:A:329:SER:HB2	1:A:387:ALA:HA	2.02	0.41	
1:A:358:THR:HA	1:A:359:PRO:C	2.39	0.41	
1:A:398:ARG:HB2	1:A:410:LYS:HB2	2.03	0.41	
1:A:451:THR:HG21	1:A:466:VAL:C	2.42	0.41	
1:A:562:GLU:O	1:A:565:VAL:N	2.52	0.41	
1:B:29:GLY:HA2	1:B:289:VAL:HG11	2.03	0.41	
1:B:31:VAL:CG1	1:B:32:ASP:H	2.34	0.41	
1:B:145:ARG:NH1	2:B:624:HOH:O	2.53	0.41	
1:B:272:PHE:HA	1:B:276:GLU:O	2.21	0.41	
1:B:491:GLN:NE2	2:B:747:HOH:O	2.53	0.41	
1:B:504:SER:C	1:B:506:ILE:H	2.24	0.41	
1:B:522:GLN:NE2	2:B:663:HOH:O	2.53	0.41	
1:B:522:GLN:OE1	1:B:552:PRO:HA	2.21	0.41	
1:A:59:LEU:O	1:A:101:GLY:HA2	2.20	0.41	
1:A:119:ASP:OD1	1:A:120:THR:N	2.55	0.41	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:270:ALA:HB1	1:A:277:ARG:NE	2.36	0.41	
1:A:309:VAL:CG1	1:A:316:PRO:HA	2.46	0.41	
1:A:476:GLU:C	1:A:478:TYR:N	2.74	0.41	
1:B:77:VAL:O	1:B:94:LYS:HA	2.20	0.41	
1:B:156:VAL:CG1	1:B:159:ILE:HD11	2.51	0.41	
1:B:280:ALA:HB1	1:B:285:HIS:CE1	2.56	0.41	
1:B:357:PRO:O	1:B:360:GLY:CA	2.69	0.41	
1:B:511:ARG:NH1	2:B:605:HOH:O	2.37	0.41	
1:B:520:HIS:O	1:B:550:ILE:HA	2.21	0.41	
1:B:534:ARG:HD3	1:B:534:ARG:HA	1.80	0.41	
1:B:538:GLU:O	1:B:541:ALA:N	2.54	0.41	
1:A:136:LEU:CD1	1:A:156:VAL:HG22	2.51	0.40	
1:A:413:GLY:H	1:A:492:LEU:C	2.24	0.40	
1:A:474:TRP:CZ3	1:A:477:MET:HE1	2.56	0.40	
1:A:520:HIS:HA	1:A:521:PRO:HD3	1.80	0.40	
1:A:521:PRO:HG2	1:A:555:GLY:O	2.21	0.40	
1:B:93:PHE:CD1	1:B:93:PHE:N	2.89	0.40	
1:B:364:VAL:CG1	1:B:395:PRO:HD3	2.51	0.40	
1:B:453:CYS:CB	2:B:731:HOH:O	2.66	0.40	
1:A:95:VAL:O	1:A:95:VAL:HG12	2.22	0.40	
1:A:163:LEU:HD23	1:A:202:ILE:HD13	2.03	0.40	
1:A:249:THR:HB	1:A:262:VAL:O	2.21	0.40	
1:A:284:ASN:ND2	1:A:376:ASP:C	2.75	0.40	
1:B:95:VAL:HB	2:B:727:HOH:O	2.20	0.40	
1:B:199:SER:OG	1:B:251:LEU:HB3	2.22	0.40	
1:B:210:ALA:HA	1:B:251:LEU:CD2	2.51	0.40	
1:B:278:VAL:CG1	1:B:312:PRO:HB3	2.49	0.40	
1:B:397:TYR:HB2	1:B:422:ASP:HB2	2.03	0.40	
1:B:440:TYR:CZ	1:B:463:LYS:HD3	2.56	0.40	
1:B:567:ILE:HA	2:B:594:HOH:O	2.21	0.40	
1:A:117:GLY:HA3	1:A:126:PHE:CB	2.51	0.40	
1:A:147:LEU:HD22	2:A:695:HOH:O	2.21	0.40	
1:A:219:ARG:HG3	1:A:219:ARG:NH1	2.36	0.40	
1:A:428:ARG:CG	2:A:622:HOH:O	2.58	0.40	
1:A:497:ARG:HD3	1:A:501:ARG:HE	1.85	0.40	
1:B:371:PHE:CD2	1:B:408:ARG:NH1	2.79	0.40	
1:B:379:ASP:HB3	1:B:382:ALA:HB3	2.03	0.40	
1:B:398:ARG:HG2	1:B:419:GLU:HA	2.02	0.40	
1:B:429:TRP:O	1:B:431:ARG:N	2.54	0.40	
1:A:23:GLU:H	1:A:23:GLU:HG3	1.69	0.40	
1:A:188:ARG:HH11	1:A:188:ARG:CG	2.35	0.40	



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:420:LEU:O	1:A:424:SER:N	2.54	0.40
1:B:60:ASN:O	1:B:61:ARG:HG2	2.21	0.40
1:B:432:GLU:HG3	2:B:759:HOH:O	2.21	0.40
1:B:444:TYR:O	1:B:447:GLY:N	2.50	0.40
1:A:98:SER:O	1:A:100:PRO:HD3	2.21	0.40
1:A:305:PRO:CD	1:A:322:LEU:HD12	2.50	0.40
1:A:444:TYR:CD1	1:A:444:TYR:N	2.90	0.40
1:A:575:LEU:HD23	1:A:575:LEU:HA	1.93	0.40
1:B:131:GLU:OE2	1:B:131:GLU:O	2.40	0.40
1:B:133:ARG:CD	2:B:608:HOH:O	2.70	0.40
1:B:266:GLU:HA	1:B:403:TYR:CE2	2.57	0.40
1:B:281:PRO:HB2	1:B:299:HIS:CE1	2.57	0.40
1:B:334:ARG:HD2	2:B:661:HOH:O	2.22	0.40
1:B:385:LEU:HD11	1:B:442:MET:CE	2.51	0.40
1:B:520:HIS:O	1:B:550:ILE:HG23	2.21	0.40
1:B:521:PRO:HA	1:B:554:ALA:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	558/562~(99%)	445 (80%)	90 (16%)	23 (4%)	3 6
1	В	559/562~(100%)	432 (77%)	96 (17%)	31 (6%)	2 3
All	All	1117/1124 (99%)	877 (78%)	186 (17%)	54 (5%)	2 4

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	43	GLU
1	А	72	TYR



Mol	Chain	Res	Type
1	А	563	ASP
1	В	206	MET
1	В	232	ASP
1	В	371	PHE
1	В	496	SER
1	А	106	LEU
1	А	321	GLY
1	А	354	GLY
1	А	371	PHE
1	А	498	GLU
1	А	543	GLY
1	А	568	LEU
1	В	45	SER
1	В	60	ASN
1	В	107	GLU
1	В	172	GLY
1	В	187	LEU
1	В	210	ALA
1	В	211	GLY
1	В	256	ASP
1	В	580	GLU
1	А	42	SER
1	А	216	ARG
1	В	323	PRO
1	В	498	GLU
1	В	505	PRO
1	В	522	GLN
1	В	544	LYS
1	А	116	SER
1	В	61	ARG
1	В	74	VAL
1	В	121	GLY
1	В	122	GLU
1	B	380	THR
1	В	430	ALA
1	В	560	THR
1	В	562	GLU
1	А	31	VAL
1	A	32	ASP
1	А	276	GLU
1	A	579	ARG
1	В	292	ARG



Mol	Chain	Res	Type
1	А	430	ALA
1	В	301	SER
1	В	417	GLY
1	А	54	GLY
1	А	64	ILE
1	А	142	GLY
1	А	460	GLY
1	А	515	PRO
1	В	306	PRO
1	В	472	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	448/449 (100%)	418 (93%)	30 (7%)	16	37
1	В	448/449~(100%)	417~(93%)	31 (7%)	15	35
All	All	896/898~(100%)	835~(93%)	61 (7%)	16	36

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	43	GLU
1	А	56	THR
1	А	71	HIS
1	А	81	ARG
1	А	139	LEU
1	А	177	LEU
1	А	178	PHE
1	А	181	ASN
1	А	183	SER
1	А	191	ASP
1	А	201	SER
1	А	216	ARG
1	А	233	LEU



Mol	Chain	Res	Type
1	А	250	TRP
1	А	285	HIS
1	А	301	SER
1	А	322	LEU
1	А	344	SER
1	А	345	ARG
1	А	419	GLU
1	А	435	LEU
1	А	441	ILE
1	А	444	TYR
1	А	453	CYS
1	А	461	LEU
1	А	522	GLN
1	A	552	PRO
1	А	559	ASN
1	A	563	ASP
1	А	579	ARG
1	В	41	PHE
1	В	56	THR
1	В	83	VAL
1	В	99	ARG
1	В	133	ARG
1	В	137	TYR
1	В	162	ASP
1	В	178	PHE
1	В	219	ARG
1	В	222	THR
1	В	236	PRO
1	В	256	ASP
1	В	304	THR
1	В	315	GLU
1	B	322	LEU
1	В	327	ARG
1	B	328	ARG
1	В	336	VAL
1	В	341	PHE
1	В	358	THR
1	В	384	SER
1	В	411	ILE
1	В	419	GLU
1	В	428	ARG
1	В	445	SER



Continued from previous page...

Mol	Chain	Res	Type
1	В	456	THR
1	В	482	ASP
1	В	497	ARG
1	В	522	GLN
1	В	560	THR
1	В	568	LEU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such side chains are listed below:

Mol	Chain	Res	Type
1	А	28	GLN
1	А	90	HIS
1	А	96	ASN
1	А	104	GLN
1	А	284	ASN
1	А	285	HIS
1	А	523	ASN
1	В	28	GLN
1	В	65	ASN
1	В	90	HIS
1	В	96	ASN
1	В	104	GLN
1	В	284	ASN
1	В	299	HIS
1	В	367	HIS
1	В	396	ASN
1	В	507	ASN
1	В	520	HIS
1	В	522	GLN
1	В	523	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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



5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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^{th} 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	$OWAB(Å^2)$	Q<0.9
1	А	560/562~(99%)	-0.10	4 (0%) 87 89	7, 26, 44, 73	0
1	В	561/562~(99%)	0.13	9 (1%) 72 74	9, 32, 51, 71	0
All	All	1121/1124 (99%)	0.02	13 (1%) 79 80	7, 28, 49, 73	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	295	LEU	3.9
1	А	558	ILE	3.9
1	А	325	ASP	2.9
1	В	261	VAL	2.8
1	В	296	VAL	2.7
1	В	558	ILE	2.7
1	В	579	ARG	2.6
1	А	320	GLY	2.6
1	А	321	GLY	2.1
1	В	262	VAL	2.1
1	В	235	LEU	2.1
1	В	26	SER	2.1
1	В	218	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.



6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

