



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 02:01 am BST

PDB ID : 2QZP
Title : Crystal structure of mutation of an acylptide hydrolase/esterase from *Aeropyrum 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 ⓘ symbol.

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

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

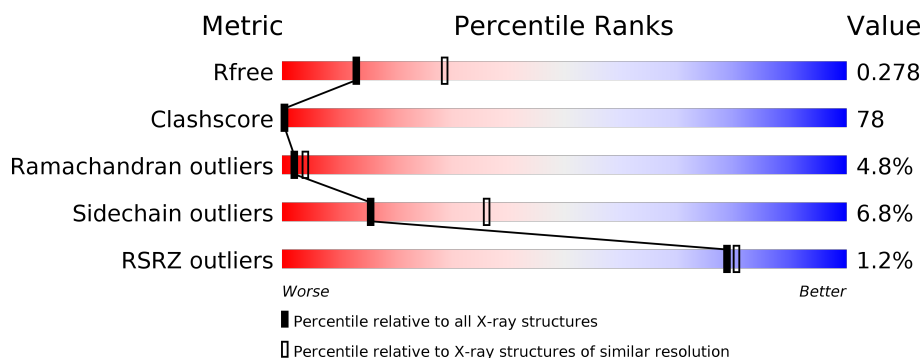
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
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 on 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	562	<div> <div> <div></div> <div>22%</div> <div>70%</div> <div>7%</div> </div> <div> <div></div> <div>22%</div> <div>70%</div> <div>7%</div> </div> </div>
1	B	562	<div> <div> <div></div> <div>20%</div> <div>72%</div> <div>8%</div> </div> <div> <div></div> <div>20%</div> <div>72%</div> <div>8%</div> </div> </div>

2 Entry composition

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	Atoms					ZeroOcc	AltConf	Trace
1	A	560	Total	C	N	O	S	0	0	0
			4255	2685	750	808	12			
1	B	561	Total	C	N	O	S	0	0	0
			4260	2688	751	809	12			

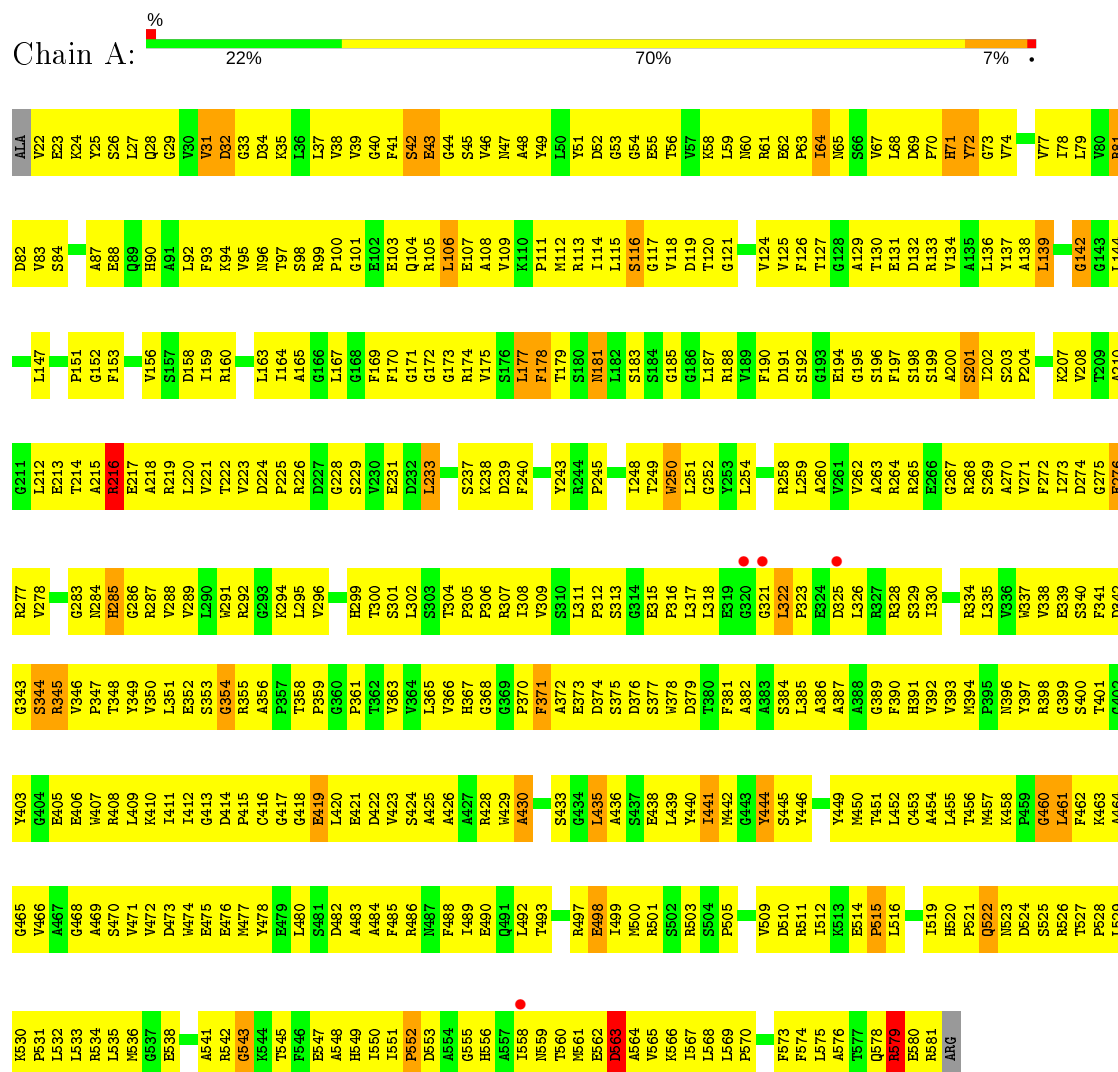
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	154	Total	O	0	0
			154	154		
2	B	212	Total	O	0	0
			212	212		

3 Residue-property plots

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



R526	R527	R528	R529	K530	P531	L532	L533	R534	L535	M536	G537	E538	L539	L540	A541	R542	G543	D544	A545	T546	F546	E547	A548	H549	I550	I551	P552	D553	A554	G555	H556	A557	I558	N559	T560	M561	E562	D563	A564	V565	K566	I567	L568	L569	P570	A571	V572	F573	F574	T577	Q578	R579	E580	R581	ARG	G465	V466	A467	G468	A469	S470	V471	V472	D473	D474	V475	E476	M477	Y478	E479	L480	S481	D482	A483	A484	F485	R486	M487	F488	I489	E490	Q491	L492	G493	G494	G495	S496	R497	E498	I499	M500	R501	S502	R503	S504	P505	I506	N507	H508	V509	D510	R511	I512	K513	E514	P515	L516	A517	L518	I519	H520	P521	Q522	N523	G402	G403	S404	T401	F402	A464	L461	G460	P459	K458	T457	L455	T456	M455	M456	M457	K458	P459	V459	C453	L452	L451	M450	Y449	G448	Y446	S445	G443	M442	I441	Y440	L439	E438	D376	S375	D374	E373	A372	F371	L365	V364	T363	P362	P361	G360	L295	T358	P357	A356	R355	G354	V291	R292	G293	K294	L296	V296	V295	E234	D232	E231	V230	D227	P226	D224	V223	T222	N284	G283	V221	L220	R219	K218	E213	E212	G211	A210	T209	V208	L139	A138	Y137	M136	L135	V134	R133	S201	A200	S198	F197	G195	V189	E188	L187	G185	T120	D119	V118	G117	S116	L115	I114	R113	M112	P111	K110	V109	A108	G107	G101	P100	R99	N96	R160	I159	D158	S157	V156	F153	H90	Q89	R88	A87	G86	R85	S84	V80	G29	Q28	L27	S26	A21	V83	D82	R81	L79	I78	V77	R76	G75	V74	G73	Y72	H71	P70	D69	L68	V67	S66	N65	V125	F126	T127	E122	R121	L120	K58	D119	V118	T56	E55	G54	G53	D52	R114	T119	F178	L177	M112	P111	K110	V109	A108	G107	L106	R105	Q104	E103	E102	G40	V39	L163	D162	G161	R160	I159	D158	S157	V156	F153	H90	Q89	R88	A87	G86	R85	S84	V80	G29	Q28	L27	S26	A21	V83	D82	R81	L79	I78	V77	R76	G75	V74	G73	Y72	H71	P70	D69	L68	V67	S66	N65	V125	F126	T127	E122	R121	L120	K58	D119	V118	T56	E55	G54	G53	D52	R114	T119	F178	L177	M112	P111	K110	V109	A108	G107	L106	R105	Q104	E103	E102	G40	V39	L163	D162	G161	R160	I159	D158	S157	V156	F153	H90	Q89	R88	A87	G86	R85	S84	V80	G29	Q28	L27	S26	A21	V83	D82	R81	L79	I78	V77	R76	G75	V74	G73	Y72	H71	P70	D69	L68	V67	S66	N65	V125	F126	T127	E122	R121	L120	K58	D119	V118	T56	E55	G54	G53	D52	R114	T119	F178	L177	M112	P111	K110	V109	A108	G107	L106	R105	Q104	E103	E102	G40	V39	L163	D162	G161	R160	I159	D158	S157	V156	F153	H90	Q89	R88	A87	G86	R85	S84	V80	G29	Q28	L27	S26	A21	V83	D82	R81	L79	I78	V77	R76	G75	V74	G73	Y72	H71	P70	D69	L68	V67	S66	N65	V125	F126	T127	E122	R121	L120	K58	D119	V118	T56	E55	G54	G53	D52	R114	T119	F178	L177	M112	P111	K110	V109	A108	G107	L106	R105	Q104	E103	E102	G40	V39	L163	D162	G161	R160	I159	D158	S157	V156	F153	H90	Q89	R88	A87	G86	R85	S84	V80	G29	Q28	L27	S26	A21	V83	D82	R81	L79	I78	V77	R76	G75	V74	G73	Y72	H71	P70	D69	L68	V67	S66	N65	V125	F126	T127	E122	R121	L120	K58	D119	V118	T56	E55	G54	G53	D52	R114	T119	F178	L177	M112	P111	K110	V109	A108	G107	L106	R105	Q104	E103	E102	G40	V39	L163	D162	G161	R160	I159	D158	S157	V156	F153	H90	Q89	R88	A87	G86	R85	S84	V80	G29	Q28	L27	S26	A21	V83	D82	R81	L79	I78	V77	R76	G75	V74	G73	Y72	H71	P70	D69	L68	V67	S66	N65	V125	F126	T127	E122	R121	L120	K58	D119	V118	T56	E55	G54	G53	D52	R114	T119	F178	L177	M112	P111	K110	V109	A108	G107	L106	R105	Q104	E103	E102	G40	V39	L163	D162	G161	R160	I159	D158	S157	V156	F153	H90	Q89	R88	A87	G86	R85	S84	V80	G29	Q28	L27	S26	A21	V83	D82	R81	L79	I78	V77	R76	G75	V74	G73	Y72	H71	P70	D69	L68	V67	S66	N65	V125	F126	T127	E122	R121	L120	K58	D119	V118	T56	E55	G54	G53	D52	R114	T119	F178	L177	M112	P111	K110	V109	A108	G107	L106	R105	Q104	E103	E102	G40	V39	L163	D162	G161	R160	I159	D158	S157	V156	F153	H90	Q89	R88	A87	G86	R85	S84	V80	G29	Q28	L27	S26	A21	V83	D82	R81	L79	I78	V77	R76	G75	V74	G73	Y72	H71	P70	D69	L68	V67	S66	N65	V125	F126	T127	E122	R121	L120	K58	D119	V118	T56	E55	G54	G53	D52	R114	T119	F178	L177	M112	P111	K110	V109	A108	G107	L106	R105	Q104	E103	E102	G40	V39	L163	D162	G161	R160	I159	D158	S157	V156	F153	H90	Q89	R88	A87	G86	R85	S84	V80	G29	Q28	L27	S26	A21	V83	D82	R81	L79	I78	V77	R76	G75	V74	G73	Y72	H71	P70	D69	L68	V67	S66	N65	V125	F126	T127	E122	R121	L120	K58	D119	V118	T56	E55	G54	G53	D52	R114	T119	F178	L177	M112	P111	K110	V109	A108	G107	L106	R105	Q104	E103	E102	G40	V39	L163	D162	G161	R160	I159	D158	S157	V156	F153	H90	Q89	R88	A87	G86	R85	S84	V80	G29	Q28	L27	S26	A21	V83	D82	R81	L79	I78	V77	R76	G75	V74	G73	Y72	H71	P70	D69	L68	V67	S66	N65	V125	F126	T127	E122	R121	L120	K58	D119	V118	T56	E55	G54	G53	D52	R114	T119	F178	L177	M112	P111	K110	V109	A108	G107	L106	R105	Q104	E103	E102	G40	V39	L163	D162	G161	R160	I159	D158	S157	V156	F153	H90	Q89	R88	A87	G86	R85	S84	V80	G29	Q28	L27	S26	A21	V83	D82	R81	L79	I78	V77	R76	G75	V74	G73	Y72	H71	P70	D69	L68	V67	S66	N65	V125	F126	T127	E122	R121	L120	K58	D119	V118	T56	E55	G54	G53	D52	R114	T119	F178	L177	M112	P111	K110	V109	A108	G107	L106	R105	Q104	E103	E102	G40	V39	L163	D162	G161	R160	I159	D158	S157	V156	F153	H90	Q89	R88	A87	G86	R85	S84	V80	G29	Q28	L27	S26	A21	V83	D82	R81	L79	I78	V77	R76	G75	V74	G73	Y72	H71	P70	D69	L68	V67	S66	N65	V125	F126	T127	E122	R121	L120	K58	D119	V118	T56	E55	G54	G53	D52	R114	T119	F178	L177	M112	P111	K110	V109	A108	G107	L106	R105	Q104	E103	E102	G40	V39	L163	D162	G161	R160	I159	D158	S157	V156	F153	H90	Q89	R88	A87	G86	R85	S84	V80	G29	Q28	L27	S26	A21	V83	D82	R81	L79	I78	V77	R76	G75	V74	G73	Y72	H71	P70	D69	L68	V67	S66	N65	V125	F126	T127	E122	R121	L120	K58	D119	V118	T56	E55	G54	G53	D52	R114	T119	F178	L177	M112	P111	K110	V109	A108	G107	L106	R105	Q104	E103	E102	G40	V39	L163	D162	G161	R160	I159	D158	S157	V156	F153	H90	Q89	R88	A87	G86	R85	S84	V80	G29	Q28	L27	S26	A21	V83	D82	R81	L79	I78	V77	R76	G75	V74	G73	Y72	H71	P70	D69	L68	V67	S66	N65	V125	F126	T127	E122	R121	L120	K58	D119	V118	T56	E55	G54	G53	D52	R114	T119	F178	L177	M112	P111	K110	V109	A108	G107	L106	R105	Q104	E103	E102	G40	V39	L163	D162	G161	R160	I159	D158	S157	V156	F153	H90	Q89	R88	A87	G86	R85	S84	V80	G29	Q28	L27	S26	A21	V83	D82	R81	L79	I78	V77	R76	G75	V74	G73	Y72	H71	P70	D69	L68	V67	S66	N65	V125	F126	T127	E122	R121	L120	K58	D119	V118	T56	E55	G54	G53	D52	R114	T119	F178	L177	M112	P111	K110	V109	A108	G107	L106	R105	Q104	E103	E102	G40	V39	L163	D162	G161	R160	I159	D158	S157	V156	F153	H90	Q89	R88	A87	G86	R85	S84	V80	G29	Q28	L27	S26	A21	V83	D82	R81	L79	I78	V77	R76	G75	V74	G73	Y72	H71	P70	D69	L68	V67	S66	N65	V125	F126	T127	E122	R121	L120	K58	D119	V118	T56	E55	G54	G53	D52	R114	T119	F178	L177	M112	P111	K110	V109	A108	G107	L106	R105	Q104	E103	E102	G40	V39	L163	D162	G161	R160	I159	D158	S157	V156	F153	H90	Q89	R88	A87	G86	R85	S84	V80	G29	Q28	L27	S26	A21	V83	D82	R81	L79	I78	V77	R76	G75	V74	G73	Y72	H71	P70	D69	L68	V67	S66	N65	V125	F126	T127	E122	R121	L120	K58	D119	V118	T56	E55	G54	G53	D52	R114	T119	F178	L177	M112	P111	K110	V109	A108	G107	L106	R105	Q104	E103	E102	G40	V39	L163	D162	G161	R160	I159	D158	S157	V156	F153	H90	Q89	R88	A87	G86	R85	S84	V80	G29	Q28	L27	S26	A21	V83	D82	R81	L79	I78	V77	R76	G75	V74	G73	Y72	H71	P70	D69	L68	V67	S66	N65	V125	F126	T127	E122	R121	L120	K58	D119	V118	T56	E55	G54	G53	D52	R114	T119	F178	L177	M112	P111	K110	V109	A108	G107	L106	R105	Q104	E103	E102	G40	V39	L163	D162	G161	R160	I159	D158	S157	V156	F153	H90	Q89	R88	A87	G86	R85	S84	V80	G29	Q28	L27	S26	A21	V83	D82	R81	L79	I78	V77	R76	G75	V74	G73	Y72	H71	P70	D69	L68	V67	S66	N65	V125	F126	T127	E122	R121	L120	K58	D119	V118	T56	E55	G54	G53	D52	R114	T119	F178	L177	M112	P111	K110	V109	A108	G107	L106	R105	Q104	E103	E102	G40	V39	L163	D162	G161	R160	I159	D158	S157	V156	F153	H90	Q89	R88	A87	G86	R85	S84	V80	G29	Q28	L27	S26	A21	V83	D82	R81	L79	I78	V77	R76	G75	V74	G73	Y72	H71	P70	D69	L68	V67	S66	N65	V125	F126	T127
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.12Å 102.18Å 163.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.11 – 2.70 48.11 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.0 (48.11-2.70) 90.3 (48.11-2.50)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.226 , 0.277 0.226 , 0.278	Depositor 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/Å ³), B_{sol} (Å ²)	0.33 , 81.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	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.*

¹Intensities estimated from amplitudes.

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.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.47	0/4346	0.76	0/5892
1	B	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(°)	Ideal(°)
1	B	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	A	4255	0	4219	642	0
1	B	4260	0	4224	704	0
2	A	154	0	0	93	0
2	B	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 distance (Å)	Clash 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:B:334:ARG:NH2	1:B:350:VAL:HG11	1.87	0.88
1:A:547:GLU:CB	1:B:552:PRO:HD3	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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: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:477:MET:HG3	1:B:528:PRO:HD2	1.72	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:519:ILE:HD13	2:B:594:HOH:O	1.90	0.71
1:B:71:HIS:O	1:B:74:VAL:HG13	1.89	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: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:B:95:VAL:HA	2:B:742: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:381:PHE:CZ	1:B:567:ILE:HD13	2.25	0.71
1:B:374:ASP:OD2	1:B:394:MET:HB3	1.90	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:475:GLU:O	1:B:479:GLU:HG3	1.88	0.71
1:B:472:VAL:HG12	1:B:506:ILE:HB	1.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:VAL:HG12	2:A:693:HOH:O	1.92	0.70
1:A:71:HIS:O	1:A:74:VAL:HG23	1.91	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:362:THR:HG22	1:B:363:VAL:N	2.06	0.70
1:B:356:ALA:HB2	1:B:389:GLY:O	1.92	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:511:ARG:O	2:A:630:HOH:O	2.10	0.69
1:A:439:LEU:N	2:A:729:HOH:O	2.24	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:477:MET:HA	2:B:756:HOH:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:LEU:O	1:B:106:LEU:HD12	1.94	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:440:TYR:OH	1:B:463:LYS:HD3	1.94	0.66
1:B:91:ALA:HB3	1:B:93:PHE:CZ	2.30	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:423:VAL:HA	2:A:651:HOH:O	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: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:HA	1:B:421:GLU:OE2	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: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:A:45:SER:HB2	1:A:63:PRO:HB3	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:HB2	1:A:579:ARG:NH1	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:136:LEU:O	1:B:147:LEU:N	2.31	0.64
1:B:29:GLY:CA	1:B:289:VAL:HG21	2.28	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: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:A:61:ARG:HH12	1:A:101:GLY:HA3	1.62	0.64
1:B:181:ASN:HB2	1:B:185:GLY:O	1.97	0.64
1:A:272:PHE:CE2	1:A:277:ARG:HD3	2.33	0.64
1:A:38:VAL:CG1	1:A:39:VAL:N	2.61	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:251:LEU:HG	2:B:652:HOH:O	1.97	0.64
1:B:201:SER:CB	1:B:252:GLY:HA2	2.28	0.64
1:B:411:ILE:CD1	1:B:419:GLU:HG2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:HIS:HB2	1:B:114:ILE:CD1	2.23	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:180:SER:HA	2:B:750:HOH:O	1.98	0.63
1:B:92:LEU:HD12	1:B:109:VAL:CG2	2.22	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:133:ARG:HA	1:A:483:ALA:CB	2.28	0.63
1:A:93:PHE:C	2:A:589:HOH:O	2.36	0.63
1:B:441:ILE:HG21	2:B:615:HOH:O	1.96	0.63
1:B:411:ILE:HD11	1:B:446:TYR:OH	1.99	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: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:B:61:ARG:HB2	1:B:103:GLU:OE1	1.99	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:345:ARG:HD2	2:B:684:HOH:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:539:LEU:HD13	1:B:546:PHE:CG	2.34	0.62
1:B:68:LEU:O	1:B:70:PRO:HD3	2.00	0.62
1:A:328:ARG:HH11	1:A:328:ARG:HG2	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: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:45:SER:HB2	2:A:595:HOH:O	1.99	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:346:VAL:HG22	1:A:407:TRP:CH2	2.36	0.61
1:A:341:PHE:CD2	1:A:421:GLU:HB3	2.35	0.61
1:B:373:GLU:HA	1:B:373:GLU:OE1	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:558:ILE:HG12	2:A:583:HOH:O	2.01	0.61
1:A:547:GLU:OE2	1:A:574:PHE:HB2	2.00	0.61
1:B:323:PRO:CG	1:B:326:LEU:HD12	2.31	0.61
1:A:533:LEU:CD1	1:B:536:MET:HB3	2.30	0.61
1:A:497:ARG:O	1:A:499:ILE:N	2.34	0.61
1:B:399:GLY:HA2	1:B:408:ARG:O	2.01	0.61
1:B:55:GLU:C	2:B:735:HOH:O	2.38	0.61
1:A:533:LEU:HD11	1:B:536:MET:HB3	1.81	0.61
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:45:SER:HB2	1:B:63:PRO:HB3	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:30:VAL:H	1:B:289:VAL:HG11	1.64	0.60
1:B:26:SER:O	1:B:308:ILE:HD11	2.01	0.60
1:A:296:VAL:HG13	1:A:309:VAL:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ARG:N	1:A:202:ILE:HD12	2.16	0.60
1:A:41:PHE:CE2	1:A:561:MET:HA	2.37	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: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:A:41:PHE:CZ	1:A:561:MET:HA	2.35	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:356:ALA:HB2	1:A:389:GLY:O	2.01	0.59
1:A:267:GLY:HA2	1:A:375:SER:HB2	1.83	0.59
1:A:55:GLU:HA	2:A:604:HOH:O	2.03	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:480:LEU:HD21	1:A:530:LYS:CD	2.32	0.59
1:A:37:LEU:HD23	1:A:70:PRO:HG3	1.85	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:251:LEU:CD1	1:B:259:LEU:HD11	2.33	0.58
1:B:246:THR:HG22	1:B:264:ARG:O	2.03	0.58
1:B:456:THR:CG2	1:B:512:ILE:HD11	2.32	0.58
1:B:46:VAL:HB	1:B:64:ILE:O	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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: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:B:61:ARG:HB2	1:B:103:GLU:CD	2.24	0.58
1:B:28:GLN:HG3	1:B:67:VAL:CG2	2.33	0.58
1:A:177:LEU:HB3	1:A:190:PHE:HB2	1.86	0.58
1:B:248:ILE:H	1:B:248:ILE:HD12	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:160:ARG:HD3	1:A:202:ILE:HG22	1.85	0.58
1:A:38:VAL:CG1	1:A:39:VAL:H	2.17	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: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:A:38:VAL:HG12	1:A:39:VAL:H	1.65	0.57
1:B:271:VAL:O	1:B:277:ARG:HA	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:SER:HB3	1:B:213:GLU:OE2	2.04	0.57
1:B:47:ASN:HA	2:B:679:HOH:O	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:419:GLU:O	1:A:423:VAL:HG23	2.06	0.56
1:A:526:ARG:HD2	1:A:556:HIS:CG	2.40	0.56
1:B:304:THR:O	1:B:378:TRP:HB2	2.06	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:473:ASP:N	2:A:657:HOH:O	2.38	0.56
1:B:127:THR:HA	1:B:135:ALA:O	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:198:SER:HB3	1:B:213:GLU:CD	2.26	0.56
1:B:99:ARG:CZ	1:B:102:GLU:HB3	2.36	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:HG3	1:A:486:ARG:HH11	1.71	0.56
1:B:517:ALA:HB2	1:B:574:PHE:CE1	2.41	0.56
1:B:90:HIS:O	1:B:111:PRO:HA	2.05	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: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
1:A:347:PRO:HG3	1:A:403:TYR:CD2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:LYS:O	1:A:460:GLY:N	2.39	0.56
1:A:46:VAL:N	2:A:595:HOH:O	2.38	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:HH11	1:A:219:ARG:HG3	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: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:B:59:LEU:HD22	2:B:727:HOH:O	2.07	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:259:LEU:HD11	2:B:767:HOH:O	2.06	0.55
1:B:246:THR:CG2	1:B:402:GLY:O	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:411:ILE:HD12	1:B:419:GLU:HG2	1.87	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:A:307:ARG:HB2	1:A:318:LEU:O	2.08	0.54
1:A:353:SER:O	1:A:354:GLY:C	2.45	0.54
1:A:346:VAL:HG13	1:A:407:TRP:CZ2	2.40	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:562:GLU:HG3	2:B:724:HOH:O	2.07	0.54
1:B:91:ALA:HB1	1:B:105:ARG:NE	2.22	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:24:LYS:O	1:A:40:GLY:HA2	2.08	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: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
1:B:60:ASN:CG	2:B:679:HOH:O	2.46	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:205:GLY:O	1:B:206:MET:HB2	2.08	0.53
1:B:30:VAL:N	1:B:289:VAL:HG11	2.23	0.53
1:A:258:ARG:HD2	1:A:273:ILE:CG2	2.38	0.53
1:B:178:PHE:C	1:B:178:PHE:CD1	2.81	0.53
1:B:177:LEU:HD22	1:B:223:VAL:HG21	1.89	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:175:VAL:CG2	1:A:196:SER:HB3	2.38	0.53
1:A:96:ASN:HD21	1:A:98:SER:HB2	1.73	0.53
1:B:114:ILE:HD12	1:B:114:ILE:N	2.23	0.53
1:B:249:THR:N	1:B:262:VAL:O	2.42	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:37:LEU:HD12	1:A:49:TYR:O	2.08	0.53
1:A:579:ARG:HG2	1:A:580:GLU:N	2.22	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:A:46:VAL:O	1:A:64:ILE:HG12	2.09	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:NH1	1:A:328:ARG:HG2	2.23	0.52
1:A:350:VAL:HA	2:A:652:HOH:O	2.09	0.52
1:A:125:VAL:HG13	1:A:137:TYR:O	2.09	0.52
1:A:84:SER:OG	1:A:87:ALA:HB3	2.10	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:442:MET:HE2	1:A:444:TYR:HE1	1.74	0.52
1:A:441:ILE:HB	1:A:462:PHE:CE1	2.45	0.52
1:A:463:LYS:HB2	2:A:729:HOH:O	2.09	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:B:59:LEU:HA	1:B:100:PRO:HB3	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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: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:B:37:LEU:HD23	1:B:70:PRO:HG3	1.91	0.51
1:A:133:ARG:HD2	2:A:609:HOH:O	2.10	0.51
1:A:129:ALA:HB1	1:A:134:VAL:HG22	1.91	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:136:LEU:O	1:B:147:LEU:HB2	2.10	0.51
1:B:72:TYR:CE2	1:B:289:VAL:HG13	2.46	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: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:A:87:ALA:HA	1:A:523:ASN:O	2.11	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:B:78:ILE:HD11	1:B:124:VAL:HG22	1.93	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:385:LEU:HB3	2:A:720:HOH:O	2.11	0.51
1:A:174:ARG:HH21	1:A:405:GLU:CG	2.23	0.51
1:A:474:TRP:CB	1:A:500:MET:HB3	2.40	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:207:LYS:HE2	1:A:224:ASP:HB2	1.93	0.50
1:A:29:GLY:O	1:A:37:LEU:HB3	2.11	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:362:THR:OG1	1:B:391:HIS:HB2	2.11	0.50
1:B:76:ARG:NH2	2:B:725:HOH:O	2.32	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: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: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: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:B:35:LYS:CG	1:B:52:ASP:OD1	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:508:HIS:C	1:B:510:ASP:N	2.64	0.49
1:A:441:ILE:C	1:A:441:ILE:HD13	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:HH11	1:B:431:ARG:HG3	1.77	0.49
1:A:240:PHE:HD1	1:A:272:PHE:CD1	2.31	0.49
1:A:60:ASN:ND2	1:A:62:GLU:O	2.37	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: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:A:71:HIS:HB2	1:A:119:ASP:O	2.11	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:B:49:TYR:CA	1:B:57:VAL:O	2.54	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:A:68:LEU:HB2	1:A:78:ILE:HB	1.94	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:B:153:PHE:CE1	1:B:488:PHE:HB2	2.45	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: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:A:87:ALA:O	1:A:525:SER:OG	2.24	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:209:THR:HG23	1:B:233:LEU:HD12	1.95	0.49
1:B:36:LEU:HD11	1:B:296:VAL:HG11	1.94	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:280:ALA:CB	1:B:285:HIS:CE1	2.96	0.49
1:B:522:GLN:HG3	1:B:523:ASN:N	2.27	0.49
1:B:506:ILE:CD1	1:B:535:LEU:HA	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:ASN:HD21	1:B:82:ASP:HB2	1.77	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:411:ILE:HD13	1:B:419:GLU:HG2	1.94	0.48
1:B:71:HIS:HA	2:B:666:HOH:O	2.13	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:CB	1:A:579:ARG:NH1	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:453:CYS:N	2:B:731:HOH:O	2.46	0.48
1:B:68:LEU:HD12	1:B:78:ILE:CD1	2.43	0.48
1:A:563:ASP:HA	1:A:566:LYS:CB	2.43	0.48
1:B:272:PHE:CE2	1:B:277:ARG:HB2	2.48	0.48
1:B:40:GLY:HA3	1:B:49:TYR:HE1	1.79	0.48
1:B:445:SER:C	1:B:447:GLY:N	2.66	0.48
1:A:384:SER:O	1:A:387:ALA:HB3	2.13	0.48
1:A:361:PRO:HB3	1:A:438:GLU:OE2	2.14	0.48
1:B:68:LEU:HD12	1:B:124:VAL:HG13	1.95	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:26:SER:OG	1:A:28:GLN:NE2	2.46	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: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:B:28:GLN:HG3	1:B:67:VAL:HG21	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:THR: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:SER:OG	2.67	0.48
1:B:457:MET:C	1:B:459:PRO:HD2	2.34	0.48
1:B:442:MET:HG3	1:B:466:VAL:CG1	2.44	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: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:38:VAL:CG1	1:B:308:ILE:HD13	2.44	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: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:A:90:HIS:HD2	1:A:114:ILE:N	2.08	0.47
1:B:325:ASP:C	1:B:328:ARG: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: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:27:LEU:HD12	1:B:38:VAL:HG12	1.94	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:N	1:B:248:ILE:HD12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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: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:B:112:MET:HB2	1:B:130:THR:HG22	1.97	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: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:468:GLY:O	1:A:469:ALA:C	2.53	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: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:495:GLY:O	1:B:496:SER:O	2.33	0.47
1:B:476:GLU:CG	1:B:531:PRO:HG3	2.45	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:519:ILE:CG2	1:A:567:ILE:HG22	2.44	0.47
1:A:62:GLU:HB2	1:A:81:ARG:HE	1.80	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:47:ASN:HB2	2:B:656:HOH:O	2.15	0.47
1:B:495:GLY:O	1:B:496:SER:C	2.54	0.47
1:B:89:GLN:HA	1:B:112:MET:O	2.15	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:160:ARG:NH2	1:A:204:PRO:HG3	2.30	0.46
1:A:45:SER:CB	2:A:595:HOH:O	2.59	0.46
1:B:133:ARG:HD2	2:B:608:HOH:O	2.16	0.46
1:B:567:ILE:C	1:B:567:ILE:HD12	2.32	0.46
1:A:305:PRO:O	1:A:306:PRO:C	2.52	0.46
1:A:302:LEU:HG	1:A:376:ASP:OD1	2.15	0.46
1:A:532:LEU:O	1:A:536:MET:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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: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:A:88:GLU:HG3	1:A:113:ARG:NH1	2.29	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:B:41:PHE:HZ	1:B:558:ILE:HG22	1.80	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:323:PRO:HG2	1:B:326:LEU:CD1	2.43	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: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:464:ALA:HB2	1:B:578:GLN:HG3	1.98	0.46
1:B:448:GLY:HA3	1:B:470:SER:HB3	1.97	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: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:B:75:GLY:O	1:B:96:ASN:OD1	2.34	0.46
1:A:400:SER:C	2:A:618:HOH:O	2.53	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:VAL:CG2	1:A:103:GLU:HG2	2.45	0.45
1:B:251:LEU:HD11	1:B:259:LEU:HD21	1.98	0.45
1:B:235:LEU:HD13	1:B:274:ASP:C	2.37	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:B:48:ALA:O	1:B:58:LYS:HA	2.17	0.45
1:A:178:PHE:O	1:A:178:PHE:CD1	2.70	0.45
1:A:420:LEU:HD11	1:A:454:ALA:HA	1.97	0.45
1:A:47:ASN:HB3	1:A:60:ASN:OD1	2.17	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:61:ARG:N	1:B:103:GLU:OE2	2.50	0.45
1:B:27:LEU:HD13	1:B:38:VAL:HG12	1.98	0.45
1:B:551:ILE:HD11	1:B:567:ILE:HG22	1.98	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: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:44:GLY:CA	1:A:561:MET:H	2.24	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:251:LEU:HA	1:A:260:ALA:O	2.17	0.45
1:A:34:ASP:O	1:A:291:TRP:NE1	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:VAL:HG12	1:A:23:GLU:N	2.32	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:68:LEU:HD12	1:A:78:ILE:CG2	2.35	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:479:GLU:HG2	2:B:617:HOH:O	2.16	0.45
1:B:411:ILE:CG1	1:B:492:LEU:HD11	2.46	0.45
1:B:520:HIS:HB2	2:B:744:HOH:O	2.17	0.45
1:B:520:HIS:HD2	1:B:521:PRO:CD	2.21	0.45
1:A:547:GLU:HB2	1:B:550:ILE: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:448:GLY:HA3	1:B:470:SER:HA	1.99	0.45
1:B:415:PRO:O	1:B:503:ARG:HG3	2.17	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:156:VAL:HG23	2:B:596:HOH:O	2.16	0.44
1:B:38:VAL:HG11	1:B:308:ILE:HD13	1.99	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:221:VAL:HG12	1:B:232:ASP:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:THR:HG22	1:B:408:ARG:HD3	1.97	0.44
1:B:40:GLY:N	1:B:47:ASN:O	2.32	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:219:ARG:NH1	1:A:221:VAL:HG12	2.33	0.44
1:A:31:VAL:HB	1:A:74:VAL:O	2.16	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: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:B:59:LEU:HB3	2:B:727:HOH:O	2.17	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:A:51:TYR:CE2	1:A:53:GLY:HA2	2.53	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: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:A:72:TYR:OH	1:A:289:VAL:HG12	2.18	0.44
1:B:523:ASN:ND2	1:B:553:ASP:CA	2.81	0.44
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:174:ARG:NH2	1:A:405:GLU:HG2	2.33	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:A:61:ARG:NH1	1:A:101:GLY:CA	2.74	0.43
1:B:118:VAL:HG21	1:B:159:ILE:HG12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:ARG:HA	1:B:269:SER:HA	2.00	0.43
1:B:48:ALA:N	2:B:679:HOH:O	2.50	0.43
1:A:62:GLU:CB	1:A:81:ARG:HH21	2.31	0.43
1:B:170:PHE:HD1	1:B:189:VAL:HG11	1.83	0.43
1:B:169:PHE:CZ	1:B:175:VAL:CG2	2.99	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:B:86:GLY:CA	1:B:555:GLY:HA3	2.48	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:A:79:LEU:HD11	1:A:95:VAL:HG21	1.99	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:198:SER:HB2	1:B:248:ILE:O	2.18	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: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:40:GLY:C	1:A:42:SER:N	2.72	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: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:42:SER:HA	1:B:561:MET:CE	2.48	0.43
1:B:493:THR:HA	2:B:629:HOH:O	2.18	0.43
1:B:79:LEU:HD11	1:B:95:VAL:CG2	2.45	0.43
1:A:74:VAL:HG11	1:A:121:GLY:HA3	2.00	0.43
1:A:33:GLY:H	1:A:73:GLY:HA2	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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: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:472:VAL:O	1:B:505:PRO:HD2	2.18	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: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:A:77:VAL:HG23	1:A:97:THR:CG2	2.49	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:167:LEU:CD2	1:A:197:PHE:HB2	2.49	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: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:B:73:GLY:O	1:B:74:VAL:C	2.57	0.43
1:B:59:LEU:CD1	1:B:77:VAL:HG21	2.46	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:HH11	1:A:188:ARG:HG3	1.84	0.42
1:A:350:VAL:HG22	2:A:652:HOH:O	2.19	0.42
1:B:203:SER:O	1:B:206:MET:N	2.46	0.42
1:B:31:VAL:HG21	1:B:37:LEU:HD22	2.00	0.42
1:B:324:GLU:HA	1:B:324:GLU:OE1	2.19	0.42
1:A:120:THR:O	1:A:120:THR:HG22	2.19	0.42
1:A:32:ASP:CB	1:A:35:LYS:HD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:ALA:HB1	1:B:248:ILE:HD12	1.97	0.42
1:B:26:SER:OG	1:B:28:GLN:NE2	2.51	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:B:50:LEU:CD1	1:B:59:LEU:HD21	2.48	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: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:B:84:SER:HB3	1:B:89:GLN:HB2	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:OD1	1:A:342:ASP:N	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:196:SER:OG	1:A:405:GLU:OE2	2.36	0.42
1:A:96:ASN:HD22	1:A:99:ARG:HG3	1.84	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:501:ARG:NH1	2:B:749:HOH:O	2.52	0.42
1:B:70:PRO:HB2	1:B:74:VAL:CG2	2.41	0.42
1:A:152:GLY:O	1:A:153:PHE:C	2.57	0.42
1:A:29:GLY:HA2	1:A:289:VAL:HG11	2.02	0.42
1:A:393:VAL:CG1	1:A:426:ALA:HB1	2.49	0.42
1:A:359:PRO:HA	1:A:435:LEU:HA	2.02	0.42
1:A:48:ALA:HB2	1:A:67:VAL:HG21	2.01	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:A:98:SER:C	1:A:100:PRO:HD3	2.39	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:315:GLU:OE1	1:A:315:GLU:HA	2.18	0.42
1:A:44:GLY:HA2	1:A:561:MET:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:ALA:HB1	1:A:556:HIS:HD1	1.85	0.42
1:A:84:SER:CB	1:A:87:ALA:HB3	2.50	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:B:79:LEU:N	1:B:93:PHE:O	2.43	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: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:B:76:ARG:HA	1:B:96:ASN:HA	2.01	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: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:B:71:HIS:O	1:B:72:TYR:C	2.58	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:HG2	1:B:264:ARG:HH11	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:219:ARG:NH1	1:A:221:VAL:CG1	2.84	0.41
1:A:169:PHE:CE2	1:A:371:PHE:CD1	3.04	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:86:GLY:O	1:B:555:GLY:HA3	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:HG13	1:B:411:ILE:O	2.21	0.41
1:B:456:THR:HG22	1:B:512:ILE:HD11	2.00	0.41
1:A:226:ARG:HD3	1:A:226:ARG:HA	1.93	0.41
1:A:25:TYR:HA	1:A:39:VAL:O	2.20	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:393:VAL:HA	2:A:652:HOH:O	2.21	0.41
1:A:367:HIS:CE1	1:A:396:ASN:HA	2.56	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:514:GLU:HA	1:B:515:PRO:HD3	1.90	0.41
1:B:476:GLU:CD	1:B:531:PRO:HG3	2.41	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:358:THR:HA	1:A:359:PRO:C	2.39	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: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:A:158:ASP:CB	1:A:201:SER:HA	2.50	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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: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:B:77:VAL:O	1:B:94:LYS:HA	2.20	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: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:B:93:PHE:CD1	1:B:93:PHE:N	2.89	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:A:95:VAL:O	1:A:95:VAL:HG12	2.22	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:B:95:VAL:HB	2:B:727:HOH:O	2.20	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:NH1	1:A:219:ARG:HG3	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:188:ARG:CG	1:A:188:ARG:HH11	2.35	0.40
1:A:23:GLU:HG3	1:A:23:GLU:H	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:LEU:O	1:A:424:SER:N	2.54	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:B:60:ASN:O	1:B:61:ARG:HG2	2.21	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:N	1:A:444:TYR:CD1	2.90	0.40
1:A:575:LEU:HD23	1:A:575:LEU:HA	1.93	0.40
1:B:131:GLU:O	1:B:131:GLU:OE2	2.40	0.40
1:B:133:ARG:CD	2:B:608:HOH:O	2.70	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:266:GLU:HA	1:B:403:TYR:CE2	2.57	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	A	558/562 (99%)	445 (80%)	90 (16%)	23 (4%)	3	6
1	B	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	A	43	GLU
1	A	72	TYR

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

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Mol	Chain	Res	Type
1	A	430	ALA
1	B	301	SER
1	B	417	GLY
1	A	54	GLY
1	A	64	ILE
1	A	142	GLY
1	A	460	GLY
1	A	515	PRO
1	B	306	PRO
1	B	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	Percentiles	
1	A	448/449 (100%)	418 (93%)	30 (7%)	16	37
1	B	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	A	43	GLU
1	A	56	THR
1	A	71	HIS
1	A	81	ARG
1	A	139	LEU
1	A	177	LEU
1	A	178	PHE
1	A	181	ASN
1	A	183	SER
1	A	191	ASP
1	A	201	SER
1	A	216	ARG
1	A	233	LEU

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

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

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

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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, 95th 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	A	560/562 (99%)	-0.10	4 (0%) 87 89	7, 26, 44, 73	0
1	B	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	B	295	LEU	3.9
1	A	558	ILE	3.9
1	A	325	ASP	2.9
1	B	261	VAL	2.8
1	B	296	VAL	2.7
1	B	558	ILE	2.7
1	B	579	ARG	2.6
1	A	320	GLY	2.6
1	A	321	GLY	2.1
1	B	262	VAL	2.1
1	B	235	LEU	2.1
1	B	26	SER	2.1
1	B	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.