



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 04:06 AM GMT

PDB ID : 2GER
Title : Crystal Structure and Oxidative Mechanism of Human Pyrroline-5-carboxylate Reductase
Authors : Meng, Z.; Lou, Z.; Liu, Z.; Rao, Z.
Deposited on : 2006-03-20
Resolution : 3.10 Å (reported)

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

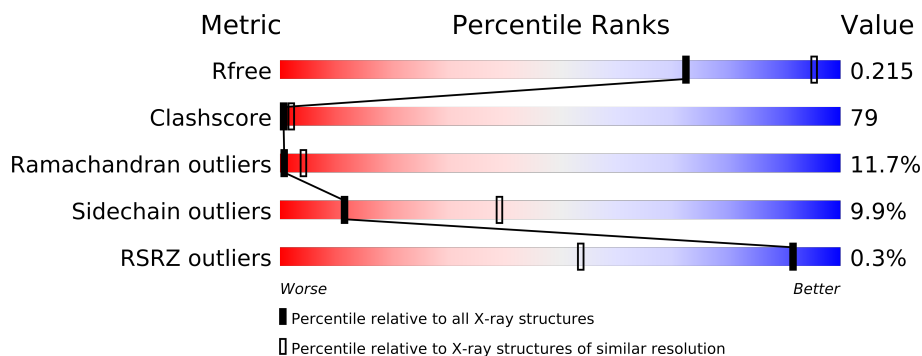
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

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

Mol	Chain	Length	Quality of chain
1	A	321	
1	B	321	
1	C	321	
1	D	321	
1	E	321	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10768 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called Pyrroline-5-carboxylatereductase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	0	0
			2038	1279	363	383	13			
1	B	276	Total	C	N	O	S	0	0	0
			2025	1271	359	382	13			
1	C	277	Total	C	N	O	S	0	0	0
			2032	1276	360	383	13			
1	D	277	Total	C	N	O	S	0	0	0
			2038	1279	363	383	13			
1	E	277	Total	C	N	O	S	0	0	0
			2038	1279	363	383	13			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ARG	-	CLONING ARTIFACT	UNP P32322
A	0	ALA	-	CLONING ARTIFACT	UNP P32322
B	-1	ARG	-	CLONING ARTIFACT	UNP P32322
B	0	ALA	-	CLONING ARTIFACT	UNP P32322
C	-1	ARG	-	CLONING ARTIFACT	UNP P32322
C	0	ALA	-	CLONING ARTIFACT	UNP P32322
D	-1	ARG	-	CLONING ARTIFACT	UNP P32322
D	0	ALA	-	CLONING ARTIFACT	UNP P32322
E	-1	ARG	-	CLONING ARTIFACT	UNP P32322
E	0	ALA	-	CLONING ARTIFACT	UNP P32322

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	106	Total	O	0	0
			106	106		
2	B	118	Total	O	0	0
			118	118		

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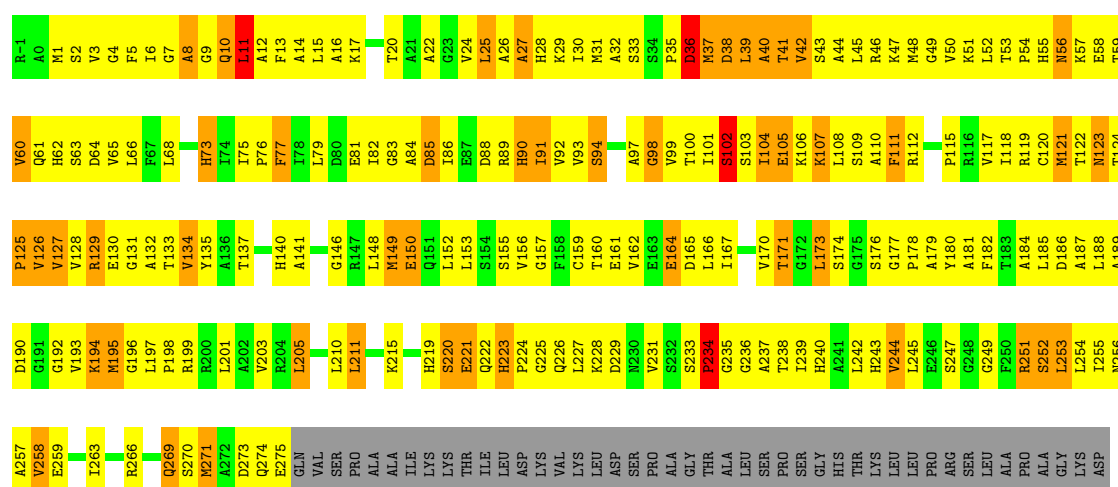
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	119	Total 119	O 119	0	0
2	D	126	Total 126	O 126	0	0
2	E	128	Total 128	O 128	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

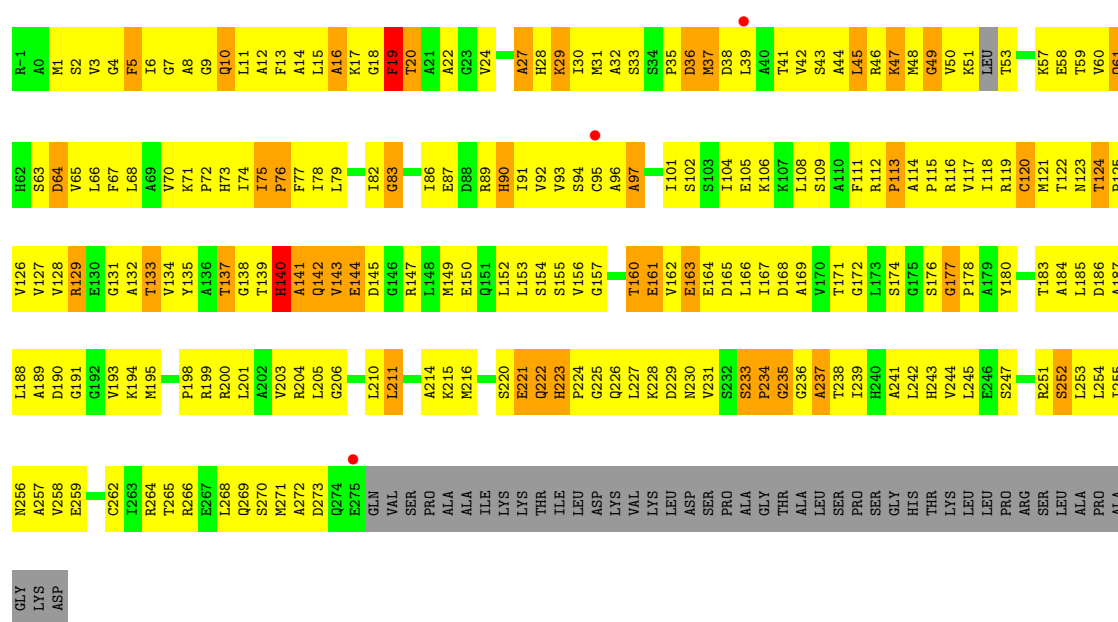
• Molecule 1: Pyrroline-5-carboxylatereductase 1

Chain A:



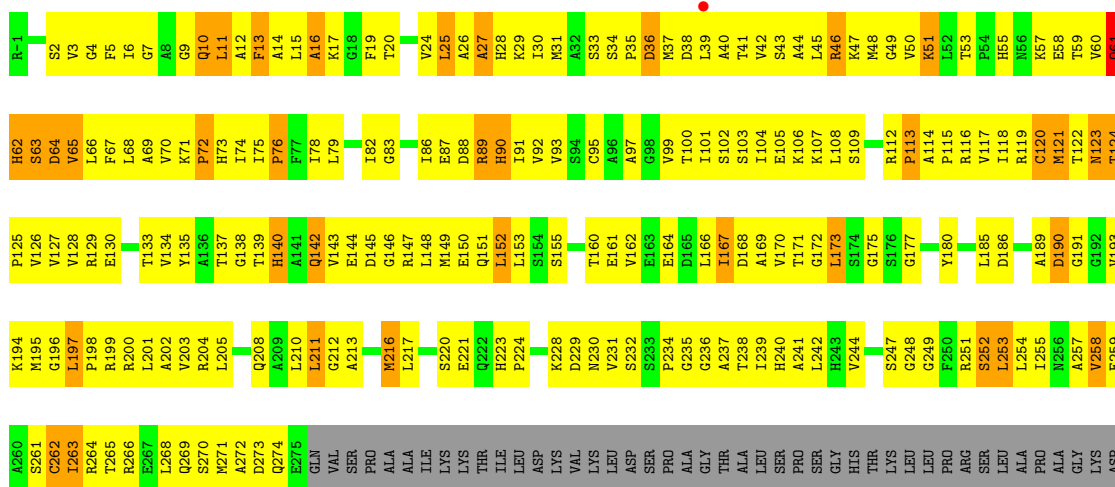
• Molecule 1: Pyrroline-5-carboxylatereductase 1

Chain B:



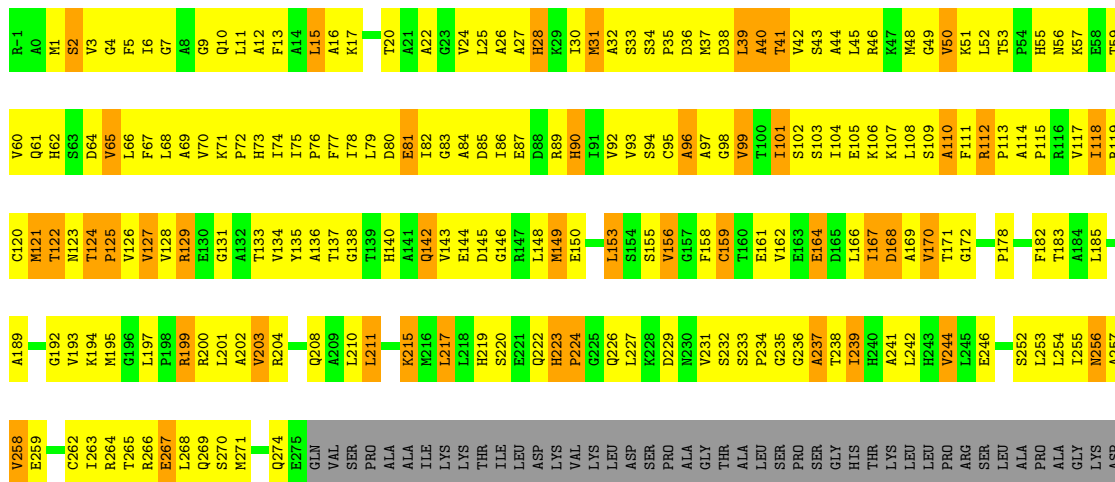
- Molecule 1: Pyrroline-5-carboxylatereductase 1

Chain C:



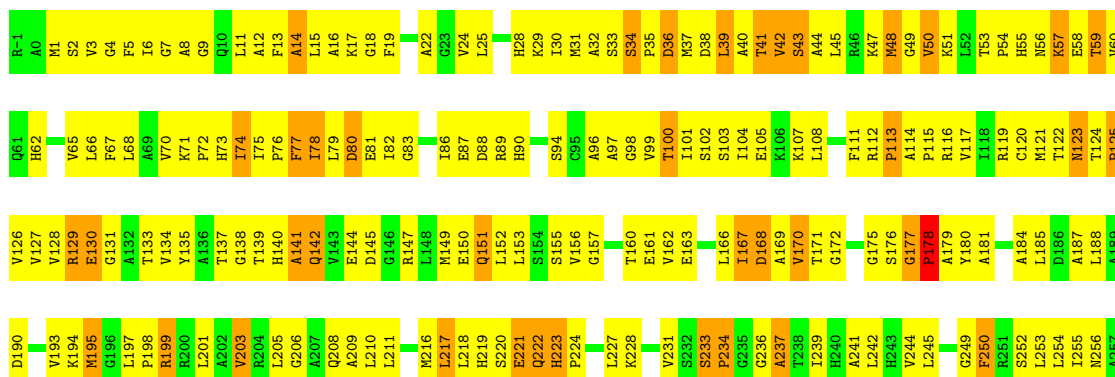
- Molecule 1: Pyrroline-5-carboxylatereductase 1

Chain D:



- Molecule 1: Pyrroline-5-carboxylatereductase 1

Chain E:



V268		S261	C262	I263	T264	R265	<u>E267</u>	L268	Q269	S270		Q274	E275	GLN	VAL	GLY	SER	PRO	ALA	ALA	LYS	LYS	LYS	LYS	LYS	LEU	ASP	LEU	LEU	LEU	LEU	LEU	PRO	PRO	PRO	GLY	THR	THR	THR	LYS	LYS	ARG	SER	LEU	ALA	ALA	PRO	PRO	GLY	GLY	LYS	LYS	ASP
------	--	------	------	------	------	------	-------------	------	------	------	--	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	207.61Å 123.81Å 120.79Å 90.00° 121.76° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 28.79 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.10) 98.7 (28.79-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.82 (at 3.11Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.233 , 0.261 0.222 , 0.215	Depositor DCC
R_{free} test set	2326 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	67.3	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 88.4	EDS
Estimated twinning fraction	0.028 for -1/2*h+1/2*k+l,1/2*h-1/2*k+l,1/2*h+1/2*k 0.036 for -1/2*h-1/2*k+l,-1/2*h-1/2*k-l,1/2*h-1/2*k	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	1 of 47010 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10768	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.68	0/2069	0.90	0/2800
1	B	0.58	0/2055	0.85	2/2781 (0.1%)
1	C	0.62	0/2063	0.86	2/2793 (0.1%)
1	D	0.68	0/2069	0.88	0/2800
1	E	0.65	0/2069	0.89	1/2800 (0.0%)
All	All	0.64	0/10325	0.88	5/13974 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	191	GLY	N-CA-C	-6.07	97.94	113.10
1	C	120	CYS	CA-CB-SG	5.82	124.48	114.00
1	B	45	LEU	CA-CB-CG	5.27	127.43	115.30
1	E	39	LEU	N-CA-C	-5.04	97.39	111.00
1	B	49	GLY	N-CA-C	-5.02	100.55	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2038	0	2082	320	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2025	0	2063	352	0
1	C	2032	0	2071	359	0
1	D	2038	0	2082	291	0
1	E	2038	0	2082	311	0
2	A	106	0	0	48	0
2	B	118	0	0	54	0
2	C	119	0	0	55	0
2	D	126	0	0	49	0
2	E	128	0	0	60	0
All	All	10768	0	10380	1614	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 79.

All (1614) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:239:ILE:H	1:D:239:ILE:HD12	1.08	1.16
1:C:75:ILE:HD12	1:C:99:VAL:HG21	1.27	1.16
1:B:75:ILE:HB	1:B:76:PRO:HD3	1.22	1.14
1:E:101:ILE:HD11	1:E:138:GLY:HA2	1.28	1.14
1:C:86:ILE:HD11	1:C:108:LEU:HD22	1.34	1.09
1:B:9:GLY:H	1:B:12:ALA:HB3	1.17	1.08
1:D:37:MET:HG2	1:D:42:VAL:HG11	1.35	1.06
1:B:74:ILE:HA	1:B:78:ILE:HD12	1.06	1.06
1:A:86:ILE:HD12	1:A:108:LEU:HD11	1.35	1.06
1:C:122:THR:HB	1:C:133:THR:HG22	1.38	1.06
1:C:270:SER:O	1:C:274:GLN:HB2	1.55	1.06
1:B:160:THR:HG22	1:B:161:GLU:H	1.17	1.06
1:B:6:ILE:HA	1:B:33:SER:HB3	1.35	1.04
1:D:31:MET:HG2	1:D:59:THR:HA	1.37	1.04
1:C:112:ARG:HH11	1:C:113:PRO:HD2	1.20	1.03
1:A:133:THR:HG21	1:A:153:LEU:HD13	1.41	1.02
1:E:75:ILE:HA	1:E:78:ILE:HD12	1.42	1.01
1:A:234:PRO:HB3	1:C:196:GLY:O	1.62	1.00
1:B:5:PHE:HZ	1:B:15:LEU:HB2	1.25	1.00
1:D:9:GLY:H	1:D:41:THR:HG21	1.27	1.00
1:D:239:ILE:H	1:D:239:ILE:CD1	1.73	0.99
1:B:142:GLN:HG2	1:B:143:VAL:H	1.26	0.99
1:E:180:TYR:HA	2:E:381:HOH:O	1.63	0.97
1:B:200:ARG:HH11	1:B:204:ARG:HH21	1.11	0.97
1:E:241:ALA:O	1:E:244:VAL:HG12	1.65	0.97
1:C:126:VAL:HA	2:C:334:HOH:O	1.64	0.96

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:135:TYR:CE1	1:C:161:GLU:HB3	2.00	0.96
1:C:236:GLY:HA2	1:C:239:ILE:HG22	1.48	0.96
1:A:123:ASN:HD21	1:A:132:ALA:H	1.07	0.95
1:D:122:THR:HG23	1:D:133:THR:HB	1.49	0.94
1:D:121:MET:CE	1:D:171:THR:HG23	1.97	0.94
1:A:75:ILE:HG22	1:A:76:PRO:HD3	1.47	0.94
1:A:153:LEU:HB2	1:A:159:CYS:SG	2.08	0.94
1:B:74:ILE:HA	1:B:78:ILE:CD1	1.98	0.93
1:A:258:VAL:HA	2:A:419:HOH:O	1.66	0.93
1:A:91:ILE:H	1:A:91:ILE:HD12	1.34	0.93
1:D:239:ILE:N	1:D:239:ILE:HD12	1.86	0.91
1:D:122:THR:CG2	1:D:133:THR:HB	2.00	0.91
1:E:228:LYS:HE3	1:E:242:LEU:HD13	1.50	0.91
1:C:112:ARG:HG3	1:C:113:PRO:HD2	1.51	0.91
1:B:7:GLY:O	1:B:12:ALA:HB2	1.70	0.90
1:E:101:ILE:CD1	1:E:138:GLY:HA2	2.00	0.90
1:B:143:VAL:HG12	1:B:144:GLU:H	1.36	0.90
1:D:178:PRO:HD3	2:D:416:HOH:O	1.68	0.90
1:D:97:ALA:HB1	1:D:265:THR:HG23	1.51	0.90
1:B:71:LYS:HB3	1:B:72:PRO:HD2	1.55	0.89
1:B:121:MET:O	1:B:133:THR:HB	1.72	0.89
1:B:63:SER:HB2	1:B:89:ARG:HH12	1.36	0.89
1:A:6:ILE:HG23	1:A:56:ASN:HB2	1.55	0.88
1:B:160:THR:HG22	1:B:161:GLU:N	1.87	0.88
1:A:121:MET:HG2	1:A:171:THR:HG23	1.55	0.88
1:E:236:GLY:HA2	1:E:239:ILE:HG22	1.56	0.88
1:C:31:MET:HB3	1:C:59:THR:HG23	1.56	0.87
1:B:3:VAL:H	1:B:30:ILE:HG23	1.37	0.87
1:E:53:THR:HG22	1:E:55:HIS:H	1.37	0.87
1:E:122:THR:HG22	1:E:133:THR:HB	1.57	0.87
1:E:86:ILE:HD11	1:E:108:LEU:HD22	1.54	0.86
1:A:79:LEU:HD11	1:A:104:ILE:CD1	2.05	0.86
1:C:258:VAL:O	1:C:258:VAL:HG12	1.75	0.86
1:C:252:SER:O	1:C:254:LEU:N	2.08	0.86
1:E:220:SER:HB2	1:E:222:GLN:HG2	1.56	0.86
1:B:243:HIS:HB3	2:B:400:HOH:O	1.75	0.86
1:D:83:GLY:O	1:D:86:ILE:HG22	1.75	0.86
1:E:221:GLU:O	1:E:223:HIS:N	2.07	0.86
1:B:5:PHE:CZ	1:B:15:LEU:HB2	2.10	0.86
1:B:79:LEU:HD13	1:B:104:ILE:HG23	1.57	0.86
1:A:33:SER:OG	1:A:56:ASN:HB3	1.76	0.85
1:B:185:LEU:HD21	1:B:210:LEU:HD12	1.58	0.85

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:160:THR:HG21	2:C:421:HOH:O	1.76	0.85
1:E:217:LEU:HD21	1:E:224:PRO:HG3	1.58	0.85
1:C:112:ARG:HH11	1:C:113:PRO:CD	1.89	0.85
1:E:68:LEU:HG	2:E:358:HOH:O	1.76	0.84
1:B:58:GLU:O	1:B:61:GLN:HG3	1.77	0.84
1:E:68:LEU:HB2	1:E:94:SER:HA	1.60	0.84
1:B:74:ILE:CA	1:B:78:ILE:HD12	2.00	0.84
1:C:123:ASN:HB2	1:C:125:PRO:HD2	1.60	0.84
1:B:160:THR:CG2	1:B:161:GLU:H	1.91	0.84
1:E:114:ALA:HB1	1:E:140:HIS:CG	2.13	0.84
1:E:203:VAL:HG23	2:E:422:HOH:O	1.76	0.83
1:D:32:ALA:HB3	1:D:52:LEU:HD23	1.60	0.83
1:D:129:ARG:HD3	1:D:155:SER:O	1.77	0.83
1:E:9:GLY:H	1:E:41:THR:HG21	1.42	0.82
1:E:101:ILE:HD11	1:E:138:GLY:CA	2.09	0.82
1:D:162:VAL:HG13	1:D:166:LEU:HD12	1.60	0.82
1:A:124:THR:O	1:A:127:VAL:HG23	1.79	0.82
1:D:170:VAL:HG12	1:D:170:VAL:O	1.76	0.82
1:A:88:ASP:CB	1:A:112:ARG:HH21	1.92	0.82
1:A:123:ASN:HD21	1:A:132:ALA:N	1.77	0.82
1:D:98:GLY:HA3	1:D:269:GLN:HB2	1.60	0.82
1:B:71:LYS:HB2	1:B:73:HIS:CE1	2.14	0.81
1:D:262:CYS:HA	2:D:364:HOH:O	1.81	0.81
1:A:123:ASN:ND2	1:A:132:ALA:H	1.79	0.81
1:B:75:ILE:HB	1:B:76:PRO:CD	2.07	0.81
1:D:101:ILE:HD13	1:D:138:GLY:HA2	1.63	0.81
1:B:29:LYS:O	1:B:30:ILE:HG13	1.80	0.81
1:C:24:VAL:O	1:C:25:LEU:HB2	1.81	0.81
1:E:199:ARG:HG3	2:E:422:HOH:O	1.81	0.81
1:E:147:ARG:O	1:E:151:GLN:HB2	1.81	0.81
1:E:194:LYS:HA	2:E:363:HOH:O	1.81	0.81
1:A:9:GLY:H	1:A:41:THR:HG21	1.45	0.80
1:C:172:GLY:HA2	1:C:261:SER:OG	1.81	0.80
1:C:122:THR:HG22	1:C:133:THR:HB	1.63	0.80
1:B:60:VAL:HG12	1:B:89:ARG:NH2	1.96	0.80
1:C:45:LEU:O	1:C:48:MET:HB3	1.81	0.80
1:C:223:HIS:ND1	1:C:224:PRO:HD2	1.96	0.80
1:C:122:THR:CB	1:C:133:THR:HG22	2.11	0.79
1:E:162:VAL:HG13	1:E:166:LEU:HD12	1.62	0.79
1:E:205:LEU:HA	2:E:408:HOH:O	1.81	0.79
1:A:3:VAL:HG12	1:A:4:GLY:H	1.47	0.79
1:A:244:VAL:HG23	2:A:387:HOH:O	1.83	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:3:VAL:HG22	1:D:65:VAL:HG13	1.62	0.79
1:A:9:GLY:N	1:A:41:THR:HG21	1.98	0.79
1:E:124:THR:O	1:E:127:VAL:HG23	1.83	0.79
1:A:115:PRO:HG3	2:A:354:HOH:O	1.83	0.79
1:C:71:LYS:HD3	1:C:71:LYS:H	1.48	0.78
1:A:123:ASN:H	1:A:123:ASN:HD22	1.31	0.78
1:E:53:THR:HG21	1:E:58:GLU:HB2	1.66	0.78
1:A:239:ILE:HD11	1:C:190:ASP:O	1.83	0.78
1:D:32:ALA:HB3	1:D:52:LEU:CD2	2.13	0.78
1:D:67:PHE:C	1:D:68:LEU:HD23	2.04	0.78
1:C:201:LEU:HA	2:C:337:HOH:O	1.83	0.78
1:D:133:THR:HG21	1:D:153:LEU:HB3	1.64	0.78
1:B:14:ALA:HA	1:B:127:VAL:HG22	1.66	0.78
1:B:79:LEU:HD11	1:B:104:ILE:HG12	1.66	0.78
1:C:101:ILE:CD1	1:C:138:GLY:HA3	2.14	0.78
1:E:25:LEU:H	1:E:25:LEU:HD23	1.49	0.77
1:B:82:ILE:HG22	1:B:86:ILE:HD11	1.65	0.77
1:C:101:ILE:O	1:C:105:GLU:HG3	1.85	0.77
1:B:78:ILE:O	1:B:82:ILE:HG13	1.84	0.77
1:B:8:ALA:HA	1:B:12:ALA:CB	2.13	0.77
1:D:30:ILE:HB	1:D:50:VAL:HG22	1.67	0.77
1:D:166:LEU:O	1:D:168:ASP:N	2.18	0.77
1:A:166:LEU:O	1:A:170:VAL:HG23	1.83	0.77
1:E:123:ASN:O	1:E:126:VAL:HG23	1.83	0.77
1:A:239:ILE:HG21	2:C:344:HOH:O	1.84	0.77
1:B:60:VAL:O	1:B:89:ARG:NH2	2.16	0.77
1:B:139:THR:HG22	2:B:393:HOH:O	1.85	0.77
1:A:115:PRO:O	1:A:140:HIS:HB2	1.85	0.77
1:B:128:VAL:HB	2:B:340:HOH:O	1.85	0.77
1:A:79:LEU:HD11	1:A:104:ILE:HD12	1.67	0.77
1:E:4:GLY:O	1:E:66:LEU:HD12	1.84	0.76
1:E:172:GLY:HA2	1:E:261:SER:OG	1.84	0.76
1:C:122:THR:HB	1:C:133:THR:CG2	2.15	0.76
1:A:73:HIS:O	1:A:76:PRO:HD2	1.86	0.76
1:B:122:THR:HG22	1:B:133:THR:HB	1.66	0.76
1:E:122:THR:HB	1:E:133:THR:HG22	1.67	0.76
1:C:79:LEU:HD22	1:C:108:LEU:HD11	1.66	0.76
1:C:6:ILE:H	1:C:66:LEU:HD21	1.51	0.76
1:A:201:LEU:O	1:A:205:LEU:HG	1.86	0.76
1:A:3:VAL:HG12	1:A:4:GLY:N	2.00	0.76
1:D:80:ASP:O	1:D:82:ILE:N	2.18	0.76
1:C:72:PRO:HG2	1:C:97:ALA:O	1.86	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:116:ARG:HA	1:C:140:HIS:HB2	1.67	0.75
1:D:9:GLY:N	1:D:41:THR:HG21	2.00	0.75
1:D:169:ALA:C	1:D:171:THR:H	1.89	0.75
1:B:264:ARG:O	1:B:268:LEU:HG	1.86	0.75
1:D:124:THR:O	1:D:127:VAL:HG23	1.86	0.75
1:E:129:ARG:HG2	1:E:130:GLU:N	2.02	0.75
1:C:202:ALA:HB2	2:C:371:HOH:O	1.85	0.75
1:D:92:VAL:HA	2:D:420:HOH:O	1.86	0.75
1:B:191:GLY:O	1:B:194:LYS:HB3	1.87	0.75
1:C:128:VAL:HG12	1:C:129:ARG:N	2.01	0.75
1:B:135:TYR:CE1	1:B:161:GLU:HB3	2.22	0.75
1:E:60:VAL:HG21	1:E:82:ILE:HD13	1.69	0.75
1:A:28:HIS:CE1	1:A:29:LYS:HG3	2.21	0.74
1:C:75:ILE:CD1	1:C:99:VAL:HG21	2.14	0.74
1:B:259:GLU:N	2:B:336:HOH:O	2.19	0.74
1:A:225:GLY:O	1:A:228:LYS:HB3	1.87	0.74
1:B:142:GLN:HG2	1:B:143:VAL:N	2.01	0.74
1:B:29:LYS:C	1:B:30:ILE:HG13	2.08	0.74
1:A:118:ILE:HD12	1:A:149:MET:SD	2.27	0.74
1:B:141:ALA:O	1:B:145:ASP:HB3	1.87	0.74
1:E:274:GLN:HG3	1:E:275:GLU:H	1.52	0.74
1:B:9:GLY:H	1:B:12:ALA:CB	1.96	0.73
1:A:253:LEU:C	2:A:390:HOH:O	2.26	0.73
1:E:55:HIS:HB3	1:E:57:LYS:HG2	1.70	0.73
1:C:114:ALA:HB1	1:C:140:HIS:ND1	2.04	0.73
1:A:107:LYS:HB3	2:A:357:HOH:O	1.89	0.73
1:E:122:THR:HG22	1:E:133:THR:CB	2.17	0.73
1:A:6:ILE:HD11	1:A:66:LEU:HD21	1.71	0.73
1:B:200:ARG:O	1:B:204:ARG:HG2	1.89	0.73
1:A:14:ALA:HA	1:A:127:VAL:HG22	1.69	0.73
1:E:195:MET:CE	1:E:195:MET:HA	2.19	0.73
1:E:55:HIS:HB3	1:E:57:LYS:HE2	1.70	0.73
1:B:93:VAL:HA	1:B:118:ILE:O	1.87	0.73
1:B:162:VAL:HB	1:B:166:LEU:HD12	1.70	0.73
1:C:89:ARG:HD2	1:C:90:HIS:N	2.04	0.73
1:A:88:ASP:HB2	1:A:112:ARG:HH21	1.54	0.73
1:B:176:SER:HA	2:B:410:HOH:O	1.89	0.73
1:D:93:VAL:HG12	1:D:118:ILE:HG13	1.71	0.73
1:B:82:ILE:O	1:B:86:ILE:HG13	1.89	0.72
1:D:70:VAL:HG12	1:D:74:ILE:HB	1.69	0.72
1:D:227:LEU:O	1:D:231:VAL:HG23	1.89	0.72
1:B:70:VAL:HG12	1:B:71:LYS:H	1.54	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:27:ALA:HB1	1:B:49:GLY:O	1.89	0.72
1:C:4:GLY:C	1:C:66:LEU:HG	2.09	0.72
1:A:93:VAL:HG23	2:A:368:HOH:O	1.89	0.72
1:B:186:ASP:HB3	2:B:388:HOH:O	1.89	0.72
1:D:3:VAL:HG22	1:D:65:VAL:CG1	2.19	0.72
1:A:275:GLU:HB2	2:A:353:HOH:O	1.89	0.72
1:C:68:LEU:HD21	2:C:332:HOH:O	1.88	0.72
1:C:95:CYS:HB2	2:C:412:HOH:O	1.88	0.72
1:D:75:ILE:HB	1:D:76:PRO:HD3	1.72	0.71
1:E:125:PRO:HG2	2:E:325:HOH:O	1.89	0.71
1:A:121:MET:HG2	1:A:171:THR:CG2	2.21	0.71
1:A:91:ILE:N	1:A:91:ILE:HD12	2.06	0.71
1:A:43:SER:HA	1:A:46:ARG:HG3	1.72	0.71
1:C:121:MET:HE3	2:C:370:HOH:O	1.91	0.71
1:B:2:SER:HA	1:B:30:ILE:HG12	1.71	0.71
1:B:251:ARG:O	1:B:254:LEU:N	2.24	0.71
1:E:83:GLY:HA2	1:E:86:ILE:CD1	2.19	0.71
1:C:124:THR:N	1:C:125:PRO:HD2	2.05	0.71
1:B:29:LYS:HD3	2:B:333:HOH:O	1.89	0.71
1:E:169:ALA:O	1:E:171:THR:N	2.24	0.71
1:B:198:PRO:HG2	1:B:201:LEU:HB3	1.71	0.71
1:E:72:PRO:HG3	1:E:96:ALA:HB1	1.73	0.71
1:B:124:THR:O	1:B:127:VAL:HG23	1.90	0.71
1:C:249:GLY:O	1:C:253:LEU:HD13	1.91	0.71
1:C:185:LEU:HD21	1:C:210:LEU:HD12	1.70	0.71
1:C:51:LYS:H	1:C:51:LYS:HD3	1.55	0.71
1:A:26:ALA:HB3	1:A:29:LYS:HE2	1.70	0.71
1:A:211:LEU:HB2	2:A:328:HOH:O	1.90	0.71
1:D:170:VAL:HG23	2:D:393:HOH:O	1.90	0.71
1:A:79:LEU:HD11	1:A:104:ILE:HD13	1.71	0.71
1:B:236:GLY:HA2	1:B:239:ILE:HG22	1.71	0.71
1:D:185:LEU:HD21	1:D:210:LEU:HD12	1.70	0.71
1:D:211:LEU:HD12	1:D:211:LEU:O	1.91	0.71
1:C:269:GLN:HG3	1:C:270:SER:H	1.56	0.70
1:A:196:GLY:O	1:E:234:PRO:HB3	1.90	0.70
1:C:53:THR:HG22	1:C:55:HIS:H	1.57	0.70
1:B:70:VAL:HG11	1:B:78:ILE:HD11	1.74	0.70
1:B:228:LYS:HA	2:B:339:HOH:O	1.91	0.70
1:D:258:VAL:HG12	1:D:259:GLU:N	2.07	0.70
1:B:5:PHE:CE1	1:B:12:ALA:HA	2.26	0.70
1:E:3:VAL:HG22	1:E:65:VAL:HB	1.73	0.70
1:E:180:TYR:HB2	2:E:391:HOH:O	1.91	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:262:CYS:O	1:C:265:THR:N	2.24	0.70
1:A:128:VAL:HG12	1:A:129:ARG:N	2.07	0.69
1:D:122:THR:HG23	1:D:133:THR:CB	2.21	0.69
1:B:105:GLU:OE2	1:B:139:THR:HB	1.92	0.69
1:D:185:LEU:HD21	1:D:210:LEU:CD1	2.22	0.69
1:A:171:THR:HA	2:A:410:HOH:O	1.93	0.69
1:E:126:VAL:HB	2:E:376:HOH:O	1.91	0.69
1:B:19:PHE:HA	1:B:22:ALA:HB3	1.72	0.69
1:C:101:ILE:HB	1:C:164:GLU:OE1	1.92	0.69
1:C:4:GLY:O	1:C:66:LEU:HG	1.92	0.69
1:C:177:GLY:HA2	1:C:180:TYR:CD1	2.28	0.69
1:E:77:PHE:HD1	1:E:77:PHE:H	1.40	0.69
1:B:33:SER:HB2	1:B:59:THR:OG1	1.92	0.69
1:E:169:ALA:C	1:E:171:THR:H	1.94	0.69
1:E:31:MET:HG2	1:E:51:LYS:HB2	1.74	0.69
1:E:3:VAL:HG13	1:E:65:VAL:O	1.92	0.69
1:D:6:ILE:N	2:D:344:HOH:O	2.26	0.69
1:C:5:PHE:HE2	1:C:15:LEU:HD12	1.58	0.69
1:A:3:VAL:HG13	1:A:65:VAL:O	1.93	0.69
1:D:7:GLY:H	1:D:33:SER:HB2	1.57	0.69
1:A:215:LYS:HD2	1:A:219:HIS:CE1	2.28	0.69
1:A:233:SER:O	1:A:235:GLY:N	2.26	0.69
1:C:82:ILE:O	1:C:86:ILE:HG13	1.93	0.69
1:B:123:ASN:HB2	1:B:125:PRO:HD2	1.75	0.69
1:C:204:ARG:HB2	2:C:337:HOH:O	1.92	0.69
1:C:241:ALA:O	1:C:244:VAL:HG12	1.93	0.69
1:E:34:SER:HB3	1:E:54:PRO:HA	1.72	0.69
1:B:222:GLN:O	1:B:223:HIS:HB2	1.92	0.69
1:E:57:LYS:HD3	1:E:57:LYS:H	1.58	0.69
1:A:222:GLN:HB3	2:A:340:HOH:O	1.93	0.69
1:C:51:LYS:HE2	2:C:355:HOH:O	1.92	0.68
1:C:240:HIS:CE1	1:D:194:LYS:HE2	2.28	0.68
1:C:92:VAL:HA	2:C:420:HOH:O	1.93	0.68
1:B:3:VAL:N	1:B:30:ILE:HG23	2.06	0.68
1:D:79:LEU:HD21	1:D:104:ILE:HA	1.76	0.68
1:A:190:ASP:OD1	1:A:199:ARG:NH1	2.26	0.68
1:C:271:MET:HA	1:C:274:GLN:HB3	1.76	0.68
1:B:200:ARG:NH1	1:B:204:ARG:HH21	1.89	0.68
1:E:53:THR:HG22	1:E:55:HIS:N	2.09	0.68
1:B:258:VAL:HG13	1:B:259:GLU:N	2.09	0.68
1:B:13:PHE:HB2	1:B:41:THR:HG21	1.76	0.68
1:B:164:GLU:HG3	1:B:167:ILE:HD12	1.76	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:43:SER:O	1:C:46:ARG:HB2	1.94	0.68
1:B:109:SER:OG	1:B:115:PRO:HD2	1.93	0.67
1:C:13:PHE:HE2	1:C:17:LYS:HE3	1.58	0.67
1:D:238:THR:HB	1:D:239:ILE:HD12	1.76	0.67
1:C:53:THR:HG21	1:C:58:GLU:HB2	1.76	0.67
1:D:22:ALA:HB3	1:D:24:VAL:HG23	1.77	0.67
1:D:121:MET:HE3	1:D:171:THR:HG23	1.77	0.67
1:D:123:ASN:HB2	1:D:125:PRO:HD2	1.76	0.67
1:A:266:ARG:HG2	1:A:266:ARG:HH11	1.60	0.67
1:E:220:SER:CB	1:E:222:GLN:HG2	2.24	0.67
1:D:118:ILE:HG22	1:D:137:THR:HA	1.76	0.67
1:C:35:PRO:O	1:C:36:ASP:HB2	1.95	0.67
1:D:171:THR:HB	2:D:364:HOH:O	1.95	0.67
1:B:221:GLU:O	1:B:223:HIS:N	2.27	0.67
1:C:251:ARG:O	1:C:252:SER:O	2.13	0.67
1:D:64:ASP:O	1:D:90:HIS:HA	1.94	0.67
1:A:141:ALA:HA	2:A:350:HOH:O	1.95	0.67
1:E:198:PRO:HG2	1:E:201:LEU:HB3	1.77	0.67
1:A:88:ASP:HB3	1:A:112:ARG:HH21	1.59	0.67
1:D:72:PRO:HG3	1:D:96:ALA:HB1	1.77	0.67
1:E:266:ARG:HD2	2:E:388:HOH:O	1.94	0.67
1:E:68:LEU:HA	2:E:322:HOH:O	1.95	0.67
1:E:17:LYS:HB2	2:E:412:HOH:O	1.95	0.67
1:B:78:ILE:HG22	1:B:82:ILE:HD11	1.75	0.66
1:E:9:GLY:N	1:E:41:THR:HG21	2.10	0.66
1:E:3:VAL:HG12	1:E:4:GLY:N	2.08	0.66
1:C:173:LEU:HD12	1:C:258:VAL:HG21	1.77	0.66
1:C:41:THR:O	1:C:45:LEU:HB2	1.95	0.66
1:A:160:THR:HG22	1:A:161:GLU:O	1.95	0.66
1:C:134:VAL:HG11	1:C:162:VAL:HG22	1.77	0.66
1:B:101:ILE:HD12	1:B:138:GLY:HA2	1.78	0.66
1:A:270:SER:HA	1:A:273:ASP:OD2	1.96	0.66
1:B:124:THR:N	1:B:125:PRO:HD2	2.11	0.66
1:C:266:ARG:HD2	2:C:361:HOH:O	1.96	0.66
1:C:29:LYS:C	1:C:30:ILE:HG13	2.15	0.66
1:C:7:GLY:HA2	1:C:70:VAL:HG22	1.77	0.66
1:D:37:MET:HA	1:D:42:VAL:HG21	1.76	0.66
1:D:169:ALA:O	1:D:171:THR:N	2.29	0.66
1:E:195:MET:HE2	1:E:195:MET:HA	1.76	0.66
1:A:86:ILE:HD12	1:A:108:LEU:CD1	2.20	0.66
1:E:86:ILE:CD1	1:E:108:LEU:HD22	2.25	0.66
1:B:105:GLU:HG2	1:B:139:THR:OG1	1.94	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:15:LEU:HG	1:D:126:VAL:HG11	1.77	0.66
1:C:166:LEU:O	1:C:169:ALA:N	2.29	0.66
1:B:67:PHE:CD2	1:B:93:VAL:HB	2.31	0.66
1:E:39:LEU:H	1:E:39:LEU:HD23	1.61	0.66
1:A:156:VAL:O	1:A:156:VAL:HG12	1.95	0.66
1:B:185:LEU:HD21	1:B:210:LEU:CD1	2.26	0.66
1:C:108:LEU:HB2	2:C:377:HOH:O	1.96	0.65
1:B:108:LEU:HB2	2:B:331:HOH:O	1.94	0.65
1:A:252:SER:O	1:A:254:LEU:N	2.29	0.65
1:D:66:LEU:HB3	2:D:420:HOH:O	1.97	0.65
1:D:93:VAL:CG1	1:D:118:ILE:HG13	2.26	0.65
1:B:198:PRO:HD2	1:B:201:LEU:HD23	1.78	0.65
1:E:179:ALA:HB1	2:E:333:HOH:O	1.96	0.65
1:D:105:GLU:O	1:D:107:LYS:N	2.21	0.65
1:C:71:LYS:HE2	1:C:73:HIS:HE1	1.61	0.65
1:B:9:GLY:N	1:B:12:ALA:HB3	2.02	0.65
1:B:236:GLY:O	1:B:238:THR:N	2.29	0.65
1:A:5:PHE:O	1:A:32:ALA:HA	1.96	0.65
1:B:233:SER:O	1:B:235:GLY:N	2.29	0.65
1:E:75:ILE:HG21	1:E:104:ILE:HD11	1.78	0.65
1:D:68:LEU:N	1:D:68:LEU:HD23	2.07	0.65
1:B:22:ALA:HB2	2:B:323:HOH:O	1.97	0.65
1:E:197:LEU:HD23	1:E:201:LEU:HD23	1.78	0.65
1:C:199:ARG:HD3	2:C:349:HOH:O	1.96	0.65
1:A:61:GLN:O	1:A:89:ARG:NH2	2.30	0.65
1:D:124:THR:HG23	2:D:425:HOH:O	1.97	0.65
1:B:122:THR:HG22	1:B:133:THR:CB	2.27	0.65
1:D:271:MET:HE2	2:D:395:HOH:O	1.96	0.65
1:C:198:PRO:HG2	1:C:201:LEU:HB3	1.79	0.65
1:B:176:SER:HB2	2:B:341:HOH:O	1.97	0.65
1:D:53:THR:HG22	1:D:55:HIS:H	1.61	0.65
1:B:75:ILE:CB	1:B:76:PRO:HD3	2.13	0.65
1:C:134:VAL:HG13	1:C:160:THR:O	1.97	0.65
1:E:122:THR:CB	1:E:133:THR:HG22	2.26	0.65
1:E:124:THR:N	1:E:125:PRO:HD2	2.12	0.65
1:E:3:VAL:CG1	1:E:4:GLY:N	2.59	0.65
1:A:3:VAL:HG22	2:A:365:HOH:O	1.97	0.65
1:E:220:SER:O	1:E:221:GLU:HB2	1.97	0.65
1:B:256:ASN:C	2:B:336:HOH:O	2.35	0.65
1:D:13:PHE:HZ	1:D:17:LYS:HZ1	1.44	0.65
1:C:221:GLU:OE2	1:C:221:GLU:HA	1.97	0.65
1:C:100:THR:HB	1:C:103:SER:HB2	1.78	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:3:VAL:HB	1:C:30:ILE:HG12	1.79	0.64
1:A:128:VAL:HB	2:A:331:HOH:O	1.96	0.64
1:E:172:GLY:HA2	1:E:261:SER:CB	2.26	0.64
1:C:101:ILE:HD11	1:C:138:GLY:HA3	1.78	0.64
1:D:70:VAL:CG1	1:D:74:ILE:HB	2.27	0.64
1:A:65:VAL:HG22	1:A:91:ILE:HD13	1.79	0.64
1:A:256:ASN:HB2	2:A:390:HOH:O	1.97	0.64
1:D:192:GLY:O	1:D:197:LEU:HB2	1.96	0.64
1:C:152:LEU:O	1:C:152:LEU:HD12	1.97	0.64
1:D:182:PHE:HA	2:D:351:HOH:O	1.96	0.64
1:B:15:LEU:O	1:B:19:PHE:CE1	2.51	0.64
1:B:264:ARG:O	1:B:264:ARG:HD2	1.99	0.64
1:C:89:ARG:NE	1:C:90:HIS:CD2	2.66	0.63
1:C:118:ILE:HG22	1:C:137:THR:HA	1.79	0.63
1:C:269:GLN:HG3	1:C:270:SER:N	2.13	0.63
1:A:115:PRO:HD2	1:A:140:HIS:CD2	2.32	0.63
1:C:186:ASP:O	1:C:190:ASP:HB2	1.98	0.63
1:A:123:ASN:H	1:A:123:ASN:ND2	1.95	0.63
1:B:195:MET:HA	1:B:195:MET:CE	2.29	0.63
1:D:204:ARG:HB3	2:D:383:HOH:O	1.97	0.63
1:E:3:VAL:O	1:E:30:ILE:HA	1.98	0.63
1:A:33:SER:O	1:A:35:PRO:HD3	1.98	0.63
1:B:143:VAL:HG12	1:B:144:GLU:N	2.11	0.63
1:A:126:VAL:HG13	1:A:156:VAL:HG11	1.79	0.63
1:C:65:VAL:HG23	1:C:91:ILE:O	1.98	0.63
1:B:70:VAL:HG12	1:B:71:LYS:N	2.13	0.63
1:E:222:GLN:O	1:E:223:HIS:HB3	1.98	0.63
1:B:114:ALA:HB1	2:B:393:HOH:O	1.98	0.63
1:B:194:LYS:HG3	2:D:331:HOH:O	1.99	0.63
1:A:68:LEU:HB2	1:A:94:SER:HA	1.79	0.63
1:D:39:LEU:O	1:D:43:SER:HB3	1.98	0.63
1:B:125:PRO:HG2	1:B:131:GLY:HA2	1.80	0.63
1:C:128:VAL:HG12	1:C:129:ARG:H	1.62	0.63
1:C:262:CYS:O	1:C:265:THR:HG22	1.99	0.63
1:A:269:GLN:HG2	1:A:270:SER:N	2.13	0.63
1:B:15:LEU:HB3	1:B:19:PHE:CZ	2.33	0.63
1:A:86:ILE:CD1	1:A:108:LEU:HD11	2.20	0.63
1:A:45:LEU:HD21	2:A:333:HOH:O	1.99	0.63
1:D:114:ALA:HB1	1:D:140:HIS:CG	2.34	0.63
1:E:101:ILE:CG2	1:E:102:SER:N	2.62	0.63
1:A:153:LEU:CB	1:A:159:CYS:SG	2.84	0.63
1:A:189:ALA:O	1:A:193:VAL:HG23	1.97	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:231:VAL:HG12	2:D:357:HOH:O	1.99	0.63
1:C:79:LEU:HD11	1:C:104:ILE:HG13	1.81	0.63
1:E:79:LEU:O	1:E:81:GLU:N	2.28	0.63
1:A:135:TYR:CE1	1:A:161:GLU:HG2	2.34	0.63
1:B:101:ILE:HB	2:B:405:HOH:O	1.98	0.63
1:E:56:ASN:O	1:E:60:VAL:HG23	1.97	0.63
1:A:198:PRO:HG2	1:A:201:LEU:CB	2.29	0.62
1:E:217:LEU:C	1:E:219:HIS:H	2.01	0.62
1:D:60:VAL:HG21	1:D:82:ILE:HG21	1.81	0.62
1:D:89:ARG:HG3	1:D:90:HIS:H	1.63	0.62
1:E:128:VAL:O	1:E:128:VAL:HG12	1.99	0.62
1:D:239:ILE:N	2:D:435:HOH:O	2.32	0.62
1:D:189:ALA:O	1:D:193:VAL:HG23	1.99	0.62
1:A:20:THR:HG21	1:A:48:MET:HE2	1.81	0.62
1:C:101:ILE:HD13	1:C:138:GLY:HA3	1.81	0.62
1:D:128:VAL:O	1:D:129:ARG:HB2	1.99	0.62
1:E:231:VAL:HG12	2:E:339:HOH:O	1.99	0.62
1:D:232:SER:HB3	1:D:239:ILE:HG13	1.81	0.62
1:E:128:VAL:O	1:E:129:ARG:HB3	1.99	0.62
1:E:25:LEU:HD23	1:E:25:LEU:N	2.12	0.62
1:E:126:VAL:HA	1:E:129:ARG:O	2.00	0.62
1:E:227:LEU:HD23	2:E:442:HOH:O	1.99	0.62
1:C:6:ILE:HG13	1:C:66:LEU:HD11	1.80	0.62
1:A:15:LEU:HD23	1:A:126:VAL:HG11	1.82	0.62
1:D:170:VAL:CG1	1:D:170:VAL:O	2.46	0.62
1:B:198:PRO:HG2	1:B:201:LEU:CB	2.28	0.62
1:D:143:VAL:HB	2:D:349:HOH:O	2.00	0.62
1:E:75:ILE:HA	1:E:78:ILE:CD1	2.26	0.62
1:E:96:ALA:HB2	2:E:362:HOH:O	1.98	0.62
1:B:11:LEU:O	1:B:15:LEU:HD12	1.99	0.62
1:C:266:ARG:NH2	2:C:381:HOH:O	2.32	0.62
1:A:198:PRO:HG2	1:A:201:LEU:HB3	1.81	0.62
1:E:47:LYS:HG3	2:E:350:HOH:O	1.98	0.62
1:A:35:PRO:O	1:A:36:ASP:HB2	1.98	0.62
1:B:51:LYS:HG2	2:B:320:HOH:O	2.00	0.62
1:E:6:ILE:HD12	1:E:68:LEU:HD21	1.81	0.62
1:B:165:ASP:OD1	1:B:166:LEU:N	2.32	0.62
1:B:74:ILE:O	1:B:78:ILE:HB	1.99	0.61
1:A:223:HIS:ND1	1:A:224:PRO:HD2	2.14	0.61
1:A:123:ASN:HB2	1:A:178:PRO:HG2	1.81	0.61
1:A:6:ILE:HG23	1:A:56:ASN:CB	2.29	0.61
1:E:126:VAL:HG23	2:E:325:HOH:O	1.99	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:227:LEU:O	1:E:231:VAL:HG23	2.00	0.61
1:E:68:LEU:HB2	1:E:94:SER:CA	2.29	0.61
1:A:129:ARG:HG2	1:A:129:ARG:O	2.00	0.61
1:B:101:ILE:HD12	1:B:138:GLY:CA	2.30	0.61
1:E:36:ASP:OD1	1:E:37:MET:N	2.34	0.61
1:E:142:GLN:HB2	1:E:145:ASP:OD2	1.99	0.61
1:C:105:GLU:HA	2:C:377:HOH:O	1.99	0.61
1:D:1:MET:HG2	1:D:2:SER:N	2.16	0.61
1:C:3:VAL:HG13	1:C:65:VAL:O	2.00	0.61
1:C:3:VAL:HG12	1:C:4:GLY:N	2.16	0.61
1:A:184:ALA:O	1:A:187:ALA:HB3	1.99	0.61
1:E:129:ARG:O	1:E:131:GLY:N	2.34	0.61
1:C:69:ALA:HB2	2:C:412:HOH:O	2.00	0.61
1:B:70:VAL:HG22	2:B:364:HOH:O	2.01	0.61
1:D:162:VAL:CG1	1:D:166:LEU:HB2	2.30	0.61
1:E:220:SER:HB2	1:E:222:GLN:CG	2.30	0.61
1:C:93:VAL:HG12	1:C:118:ILE:HG13	1.82	0.61
1:C:217:LEU:O	1:C:220:SER:HB3	2.01	0.61
1:B:141:ALA:HB1	1:B:145:ASP:OD2	2.01	0.61
1:D:153:LEU:HB2	1:D:159:CYS:SG	2.40	0.61
1:A:109:SER:C	1:A:111:PHE:H	2.05	0.61
1:D:269:GLN:C	1:D:271:MET:H	2.04	0.60
1:C:160:THR:HG22	1:C:161:GLU:N	2.16	0.60
1:B:225:GLY:O	1:B:228:LYS:HB3	2.01	0.60
1:A:89:ARG:HG3	1:A:90:HIS:N	2.16	0.60
1:C:112:ARG:NH1	1:C:113:PRO:HD2	2.04	0.60
1:C:170:VAL:HB	2:C:401:HOH:O	2.00	0.60
1:E:121:MET:HA	1:E:121:MET:HE3	1.83	0.60
1:E:129:ARG:HG2	1:E:130:GLU:H	1.66	0.60
1:D:215:LYS:HG3	1:D:219:HIS:CE1	2.36	0.60
1:E:45:LEU:O	1:E:49:GLY:O	2.18	0.60
1:B:211:LEU:HD12	1:B:211:LEU:O	2.02	0.60
1:C:11:LEU:HD12	1:C:14:ALA:HB3	1.82	0.60
1:D:133:THR:HG22	1:D:158:PHE:O	2.00	0.60
1:A:75:ILE:HG22	1:A:76:PRO:CD	2.28	0.60
1:B:2:SER:HA	1:B:30:ILE:CG1	2.30	0.60
1:A:130:GLU:HB2	2:A:331:HOH:O	2.00	0.60
1:D:87:GLU:HB3	2:D:380:HOH:O	2.02	0.60
1:D:60:VAL:O	1:D:90:HIS:NE2	2.33	0.60
1:C:115:PRO:HD2	2:C:379:HOH:O	2.02	0.60
1:B:66:LEU:HB2	1:B:92:VAL:HG22	1.83	0.60
1:C:89:ARG:HE	1:C:90:HIS:CD2	2.17	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:3:VAL:HA	1:C:65:VAL:O	2.02	0.60
1:C:51:LYS:HB2	2:C:324:HOH:O	2.01	0.60
1:C:199:ARG:O	1:C:203:VAL:HG23	2.01	0.60
1:C:100:THR:HG22	1:C:101:ILE:N	2.16	0.60
1:D:263:ILE:O	1:D:267:GLU:HG3	2.00	0.60
1:D:44:ALA:HB3	2:D:413:HOH:O	2.02	0.60
1:D:122:THR:HG22	1:D:133:THR:HB	1.81	0.59
1:E:115:PRO:O	1:E:140:HIS:HB2	2.01	0.59
1:E:123:ASN:HB2	1:E:178:PRO:HG2	1.82	0.59
1:A:77:PHE:CD1	1:A:77:PHE:N	2.70	0.59
1:D:202:ALA:HB1	2:D:350:HOH:O	2.02	0.59
1:C:105:GLU:HB2	2:C:366:HOH:O	2.01	0.59
1:E:79:LEU:HD11	1:E:104:ILE:HG12	1.82	0.59
1:B:152:LEU:HD12	1:B:152:LEU:O	2.03	0.59
1:D:126:VAL:HG13	1:D:156:VAL:HG11	1.84	0.59
1:E:134:VAL:CG1	1:E:162:VAL:HB	2.32	0.59
1:C:87:GLU:H	1:C:90:HIS:HE1	1.49	0.59
1:D:59:THR:O	1:D:62:HIS:N	2.33	0.59
1:A:3:VAL:CG1	1:A:4:GLY:H	2.15	0.59
1:D:1:MET:HG2	1:D:2:SER:H	1.68	0.59
1:C:33:SER:HB2	1:C:59:THR:OG1	2.02	0.59
1:D:75:ILE:HD12	1:D:99:VAL:HG21	1.83	0.59
1:A:221:GLU:O	1:A:223:HIS:N	2.33	0.59
1:B:48:MET:O	1:B:50:VAL:HG23	2.03	0.59
1:A:38:ASP:O	1:A:39:LEU:C	2.40	0.59
1:E:223:HIS:ND1	1:E:224:PRO:HD2	2.18	0.59
1:A:222:GLN:O	1:A:223:HIS:CB	2.49	0.59
1:D:109:SER:C	1:D:111:PHE:H	2.05	0.59
1:E:68:LEU:N	2:E:358:HOH:O	2.35	0.59
1:E:73:HIS:O	1:E:74:ILE:HG13	2.02	0.59
1:E:79:LEU:HD12	1:E:107:LYS:HD2	1.85	0.59
1:C:128:VAL:HG23	2:C:417:HOH:O	2.03	0.59
1:C:171:THR:HB	2:C:360:HOH:O	2.02	0.59
1:D:60:VAL:HG21	1:D:82:ILE:HD13	1.85	0.59
1:B:118:ILE:HG21	1:B:149:MET:SD	2.42	0.59
1:B:251:ARG:O	1:B:253:LEU:N	2.36	0.59
1:E:59:THR:O	1:E:62:HIS:HB3	2.03	0.59
1:C:231:VAL:O	1:C:231:VAL:HG12	2.03	0.59
1:A:194:LYS:HG2	1:E:239:ILE:HG23	1.85	0.59
1:A:194:LYS:O	1:A:195:MET:SD	2.61	0.59
1:D:197:LEU:HD22	1:D:201:LEU:HD23	1.84	0.59
1:C:127:VAL:O	1:C:127:VAL:HG12	2.03	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:169:ALA:HB3	2:D:393:HOH:O	2.03	0.59
1:D:264:ARG:O	1:D:268:LEU:HB2	2.03	0.59
1:C:147:ARG:O	1:C:151:GLN:HG3	2.03	0.59
1:E:122:THR:HG22	1:E:133:THR:CG2	2.33	0.58
1:B:189:ALA:HB2	1:B:203:VAL:HA	1.85	0.58
1:B:71:LYS:HB3	1:B:72:PRO:CD	2.31	0.58
1:B:4:GLY:HA3	1:B:66:LEU:HD23	1.84	0.58
1:B:89:ARG:HD2	1:B:89:ARG:O	2.02	0.58
1:A:64:ASP:O	1:A:90:HIS:HB3	2.03	0.58
1:A:57:LYS:HA	1:A:60:VAL:HG23	1.84	0.58
1:C:236:GLY:O	1:C:237:ALA:HB3	2.03	0.58
1:C:28:HIS:ND1	1:C:51:LYS:HE3	2.17	0.58
1:D:258:VAL:CG1	1:D:259:GLU:N	2.65	0.58
1:A:77:PHE:HD1	1:A:77:PHE:N	2.00	0.58
1:C:155:SER:HB3	2:C:358:HOH:O	2.02	0.58
1:E:187:ALA:HB3	2:E:402:HOH:O	2.03	0.58
1:E:111:PHE:HB3	2:E:386:HOH:O	2.04	0.58
1:D:117:VAL:O	1:D:138:GLY:HA3	2.04	0.58
1:E:80:ASP:HA	2:E:327:HOH:O	2.03	0.58
1:B:41:THR:HA	1:B:44:ALA:HB3	1.85	0.58
1:A:121:MET:CE	1:A:171:THR:HG22	2.33	0.58
1:B:83:GLY:HA3	1:B:111:PHE:CD2	2.38	0.58
1:B:8:ALA:HA	1:B:12:ALA:HB2	1.85	0.58
1:A:122:THR:CG2	1:A:123:ASN:N	2.66	0.58
1:B:206:GLY:O	1:B:210:LEU:HG	2.04	0.58
1:E:170:VAL:HG12	1:E:170:VAL:O	2.04	0.58
1:B:82:ILE:CG2	1:B:86:ILE:HD11	2.32	0.58
1:B:269:GLN:C	1:B:271:MET:H	2.06	0.58
1:E:38:ASP:HB3	1:E:40:ALA:HB3	1.86	0.58
1:A:152:LEU:O	1:A:155:SER:HB3	2.03	0.58
1:A:101:ILE:HG22	1:A:105:GLU:HG3	1.85	0.58
1:D:53:THR:HG22	1:D:55:HIS:N	2.17	0.58
1:A:121:MET:CG	1:A:171:THR:HG23	2.33	0.58
1:B:119:ARG:HB3	2:B:337:HOH:O	2.02	0.58
1:C:86:ILE:HD11	1:C:108:LEU:CD2	2.22	0.57
1:B:72:PRO:HB3	1:B:97:ALA:CB	2.34	0.57
1:B:160:THR:CG2	1:B:161:GLU:N	2.56	0.57
1:C:39:LEU:HA	1:C:43:SER:HB2	1.84	0.57
1:D:125:PRO:HB2	1:D:131:GLY:HA2	1.86	0.57
1:D:135:TYR:CE1	1:D:161:GLU:HB2	2.39	0.57
1:E:68:LEU:HD12	1:E:94:SER:HB2	1.85	0.57
1:A:37:MET:HA	1:A:42:VAL:HG21	1.85	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:121:MET:SD	1:A:171:THR:HG22	2.44	0.57
1:C:249:GLY:O	1:C:252:SER:HB2	2.04	0.57
1:E:180:TYR:O	2:E:372:HOH:O	2.17	0.57
1:A:201:LEU:HG	1:A:205:LEU:HD11	1.85	0.57
1:B:2:SER:O	1:B:3:VAL:HG23	2.04	0.57
1:C:149:MET:C	1:C:151:GLN:H	2.08	0.57
1:B:45:LEU:O	1:B:48:MET:HB2	2.05	0.57
1:A:55:HIS:C	1:A:57:LYS:H	2.07	0.57
1:D:164:GLU:HA	1:D:167:ILE:CG1	2.35	0.57
1:E:193:VAL:HG21	1:E:199:ARG:HD2	1.86	0.57
1:A:25:LEU:HG	1:A:26:ALA:H	1.70	0.57
1:A:29:LYS:HG2	2:A:396:HOH:O	2.05	0.57
1:B:258:VAL:CG1	1:B:259:GLU:N	2.68	0.57
1:B:72:PRO:HA	2:B:361:HOH:O	2.05	0.57
1:B:94:SER:HA	2:B:324:HOH:O	2.04	0.57
1:D:39:LEU:HA	1:D:43:SER:HB3	1.87	0.57
1:C:31:MET:HB2	1:C:62:HIS:CE1	2.39	0.57
1:E:101:ILE:HG23	1:E:102:SER:N	2.19	0.57
1:E:45:LEU:HA	1:E:48:MET:HE3	1.85	0.57
1:D:129:ARG:CD	1:D:155:SER:O	2.51	0.57
1:D:118:ILE:CG2	1:D:137:THR:HA	2.34	0.57
1:D:115:PRO:O	1:D:140:HIS:HB2	2.05	0.57
1:D:146:GLY:O	1:D:149:MET:HB3	2.04	0.57
1:E:233:SER:HB2	2:E:320:HOH:O	2.03	0.57
1:B:227:LEU:O	1:B:231:VAL:HG23	2.05	0.57
1:B:199:ARG:HD3	2:D:442:HOH:O	2.04	0.57
1:E:166:LEU:O	1:E:168:ASP:N	2.38	0.57
1:D:156:VAL:O	1:D:156:VAL:HG12	2.05	0.56
1:B:186:ASP:HA	2:B:358:HOH:O	2.03	0.56
1:B:57:LYS:HG3	1:B:58:GLU:N	2.20	0.56
1:A:238:THR:N	2:A:369:HOH:O	2.36	0.56
1:C:127:VAL:HA	2:C:418:HOH:O	2.05	0.56
1:B:63:SER:HB2	1:B:89:ARG:NH1	2.13	0.56
1:D:146:GLY:O	1:D:149:MET:N	2.38	0.56
1:E:119:ARG:HA	2:E:445:HOH:O	2.04	0.56
1:E:35:PRO:HG2	2:E:401:HOH:O	2.05	0.56
1:B:11:LEU:HA	1:B:14:ALA:HB3	1.87	0.56
1:A:93:VAL:HG22	1:A:118:ILE:HD11	1.88	0.56
1:D:6:ILE:HG13	1:D:66:LEU:HD11	1.86	0.56
1:A:146:GLY:O	1:A:150:GLU:HB2	2.05	0.56
1:C:135:TYR:HE1	1:C:161:GLU:HB3	1.68	0.56
1:B:185:LEU:O	1:B:186:ASP:C	2.43	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:134:VAL:HG13	1:E:162:VAL:HB	1.86	0.56
1:E:14:ALA:HB2	2:E:324:HOH:O	2.04	0.56
1:A:253:LEU:HD23	1:A:253:LEU:N	2.18	0.56
1:E:264:ARG:CZ	1:E:268:LEU:HD21	2.35	0.56
1:E:19:PHE:O	1:E:24:VAL:HG23	2.04	0.56
1:A:242:LEU:O	1:A:243:HIS:C	2.44	0.56
1:B:147:ARG:NH1	1:B:150:GLU:OE2	2.38	0.56
1:E:121:MET:HE2	1:E:122:THR:H	1.71	0.56
1:D:211:LEU:HD12	1:D:211:LEU:C	2.25	0.56
1:A:64:ASP:O	1:A:90:HIS:CB	2.54	0.56
1:B:112:ARG:HB2	2:B:419:HOH:O	2.04	0.56
1:B:134:VAL:HG12	1:B:135:TYR:N	2.21	0.56
1:C:19:PHE:CE2	1:C:152:LEU:HD11	2.40	0.56
1:E:236:GLY:O	1:E:237:ALA:HB3	2.05	0.56
1:B:60:VAL:HG12	1:B:89:ARG:HH22	1.71	0.56
1:E:222:GLN:O	1:E:223:HIS:CB	2.53	0.56
1:D:57:LYS:O	1:D:61:GLN:HG3	2.06	0.56
1:E:126:VAL:O	1:E:156:VAL:HG12	2.05	0.56
1:E:38:ASP:O	1:E:42:VAL:HB	2.05	0.56
1:B:74:ILE:HG23	1:B:78:ILE:HG21	1.86	0.56
1:C:124:THR:O	1:C:127:VAL:HG23	2.05	0.56
1:A:122:THR:HG22	1:A:123:ASN:N	2.20	0.56
1:E:129:ARG:HG3	1:E:157:GLY:N	2.20	0.56
1:B:211:LEU:HD12	1:B:211:LEU:C	2.26	0.56
1:B:112:ARG:HG3	1:B:113:PRO:HD2	1.86	0.56
1:B:153:LEU:C	1:B:155:SER:H	2.09	0.56
1:B:216:MET:HA	2:B:372:HOH:O	2.05	0.56
1:D:94:SER:HA	2:D:422:HOH:O	2.06	0.56
1:E:185:LEU:HD21	1:E:210:LEU:HD12	1.87	0.56
1:A:82:ILE:O	1:A:82:ILE:HG22	2.05	0.56
1:A:40:ALA:O	1:A:44:ALA:HB2	2.06	0.56
1:B:239:ILE:N	2:B:338:HOH:O	2.38	0.56
1:B:119:ARG:HD3	1:B:167:ILE:CD1	2.36	0.56
1:B:129:ARG:O	1:B:129:ARG:HD3	2.05	0.56
1:B:258:VAL:CG1	1:B:259:GLU:H	2.19	0.56
1:D:192:GLY:HA3	2:D:350:HOH:O	2.05	0.56
1:D:232:SER:HB3	1:D:239:ILE:CG1	2.36	0.56
1:C:71:LYS:HE2	1:C:73:HIS:CE1	2.41	0.56
1:C:122:THR:HG22	1:C:133:THR:CB	2.35	0.56
1:D:93:VAL:HA	1:D:118:ILE:O	2.06	0.56
1:C:45:LEU:CD2	1:C:50:VAL:HB	2.36	0.55
1:C:25:LEU:HD21	1:C:30:ILE:HD11	1.88	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:6:ILE:HD12	1:E:68:LEU:CD2	2.36	0.55
1:B:37:MET:HE3	2:B:355:HOH:O	2.06	0.55
1:A:82:ILE:HG23	1:A:85:ASP:HB2	1.88	0.55
1:C:152:LEU:C	1:C:152:LEU:HD12	2.26	0.55
1:C:162:VAL:HB	1:C:166:LEU:HD12	1.87	0.55
1:E:188:LEU:N	2:E:402:HOH:O	2.39	0.55
1:D:34:SER:HB2	1:D:36:ASP:O	2.07	0.55
1:B:123:ASN:O	1:B:126:VAL:HG23	2.07	0.55
1:A:228:LYS:HZ1	1:C:199:ARG:HH12	1.53	0.55
1:D:33:SER:O	1:D:35:PRO:HD2	2.06	0.55
1:C:31:MET:HB3	1:C:59:THR:CG2	2.32	0.55
1:A:33:SER:CB	1:A:56:ASN:HB3	2.36	0.55
1:D:128:VAL:O	1:D:129:ARG:CB	2.53	0.55
1:A:101:ILE:O	1:A:102:SER:C	2.44	0.55
1:E:14:ALA:HB1	2:E:376:HOH:O	2.06	0.55
1:B:37:MET:SD	1:B:46:ARG:NH2	2.73	0.55
1:A:119:ARG:HD3	1:A:164:GLU:HG3	1.87	0.55
1:C:45:LEU:HD23	1:C:50:VAL:HB	1.88	0.55
1:D:38:ASP:O	1:D:39:LEU:C	2.44	0.55
1:E:75:ILE:CA	1:E:78:ILE:HD12	2.29	0.55
1:C:123:ASN:O	1:C:126:VAL:HG13	2.07	0.55
1:C:128:VAL:CG1	1:C:129:ARG:N	2.69	0.55
1:D:5:PHE:CD2	1:D:67:PHE:HB2	2.42	0.55
1:E:126:VAL:HG22	1:E:131:GLY:HA3	1.89	0.55
1:D:107:LYS:HD2	2:D:329:HOH:O	2.07	0.55
1:D:111:PHE:O	1:D:112:ARG:C	2.45	0.55
1:D:57:LYS:HE2	1:D:85:ASP:OD2	2.07	0.55
1:B:239:ILE:HG21	2:E:363:HOH:O	2.05	0.55
1:B:139:THR:HG22	1:B:139:THR:O	2.07	0.55
1:C:88:ASP:N	2:C:352:HOH:O	2.39	0.54
1:B:13:PHE:HB2	1:B:41:THR:CG2	2.37	0.54
1:B:199:ARG:NH2	2:B:358:HOH:O	2.39	0.54
1:E:5:PHE:O	1:E:32:ALA:HA	2.07	0.54
1:A:274:GLN:HB2	2:A:353:HOH:O	2.07	0.54
1:C:83:GLY:HA2	1:C:86:ILE:CD1	2.37	0.54
1:E:6:ILE:O	1:E:70:VAL:HG22	2.07	0.54
1:B:123:ASN:CB	1:B:125:PRO:HD2	2.37	0.54
1:D:89:ARG:NH2	2:D:370:HOH:O	2.40	0.54
1:C:11:LEU:CD1	1:C:124:THR:HA	2.37	0.54
1:A:126:VAL:O	1:A:128:VAL:N	2.40	0.54
1:D:217:LEU:O	1:D:217:LEU:HD12	2.07	0.54
1:E:137:THR:HG23	2:E:330:HOH:O	2.05	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:109:SER:HA	1:C:115:PRO:CD	2.37	0.54
1:C:15:LEU:O	1:C:19:PHE:CD1	2.61	0.54
1:D:125:PRO:O	1:D:128:VAL:HG12	2.07	0.54
1:E:205:LEU:HD23	2:E:408:HOH:O	2.08	0.54
1:E:97:ALA:HB1	1:E:265:THR:HG23	1.89	0.54
1:C:119:ARG:HG3	2:C:351:HOH:O	2.08	0.54
1:D:241:ALA:O	1:D:244:VAL:N	2.38	0.54
1:C:78:ILE:HD11	2:C:380:HOH:O	2.07	0.54
1:A:149:MET:CE	1:A:149:MET:HA	2.37	0.54
1:B:239:ILE:HD11	1:E:190:ASP:O	2.08	0.54
1:A:88:ASP:HB2	1:A:112:ARG:NH2	2.22	0.54
1:C:194:LYS:HA	2:C:344:HOH:O	2.08	0.54
1:E:1:MET:HG2	1:E:2:SER:N	2.23	0.54
1:B:241:ALA:O	1:B:242:LEU:C	2.44	0.54
1:C:255:ILE:C	1:C:257:ALA:H	2.11	0.54
1:B:180:TYR:CD2	1:B:180:TYR:N	2.75	0.54
1:D:26:ALA:HB3	1:D:28:HIS:CD2	2.42	0.54
1:C:236:GLY:HA3	1:C:240:HIS:HD2	1.73	0.54
1:A:30:ILE:HG22	1:A:31:MET:N	2.23	0.54
1:D:227:LEU:HB2	2:D:419:HOH:O	2.08	0.54
1:C:65:VAL:HG13	1:C:65:VAL:O	2.08	0.54
1:B:75:ILE:CD1	1:B:272:ALA:HA	2.38	0.54
1:C:262:CYS:HA	2:C:360:HOH:O	2.08	0.54
1:E:55:HIS:CB	1:E:57:LYS:HE2	2.34	0.54
1:C:252:SER:HB3	2:C:321:HOH:O	2.07	0.54
1:A:112:ARG:HG3	2:A:407:HOH:O	2.08	0.54
1:E:126:VAL:N	2:E:325:HOH:O	2.41	0.54
1:D:107:LYS:HB3	2:D:329:HOH:O	2.07	0.54
1:D:226:GLN:O	1:D:229:ASP:HB2	2.08	0.54
1:D:143:VAL:C	1:D:145:ASP:H	2.10	0.54
1:E:80:ASP:OD2	1:E:107:LYS:NZ	2.35	0.54
1:B:12:ALA:O	1:B:16:ALA:HB2	2.08	0.54
1:D:6:ILE:HG21	1:D:78:ILE:HG21	1.88	0.54
1:C:266:ARG:HA	2:C:323:HOH:O	2.08	0.54
1:E:217:LEU:O	1:E:219:HIS:N	2.40	0.54
1:B:105:GLU:HG2	2:B:417:HOH:O	2.08	0.54
1:C:78:ILE:O	1:C:82:ILE:HG13	2.07	0.53
1:E:102:SER:O	1:E:103:SER:C	2.43	0.53
1:B:126:VAL:HA	2:B:328:HOH:O	2.08	0.53
1:D:98:GLY:HA2	2:D:336:HOH:O	2.07	0.53
1:C:129:ARG:HG2	1:C:129:ARG:O	2.08	0.53
1:A:68:LEU:HD12	1:A:94:SER:HB2	1.90	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:3:VAL:HG22	1:C:65:VAL:HG13	1.90	0.53
1:C:66:LEU:N	2:C:420:HOH:O	2.40	0.53
1:A:123:ASN:HD22	1:A:123:ASN:N	1.94	0.53
1:D:265:THR:HG22	2:D:377:HOH:O	2.07	0.53
1:E:86:ILE:O	1:E:112:ARG:HD3	2.08	0.53
1:A:88:ASP:HB2	1:A:112:ARG:HE	1.73	0.53
1:A:88:ASP:CB	1:A:112:ARG:NH2	2.68	0.53
1:E:13:PHE:O	1:E:16:ALA:HB3	2.09	0.53
1:D:210:LEU:O	1:D:211:LEU:C	2.46	0.53
1:E:11:LEU:O	1:E:15:LEU:HD12	2.07	0.53
1:C:104:ILE:HG22	1:C:117:VAL:HG21	1.90	0.53
1:D:30:ILE:HB	1:D:50:VAL:CG2	2.38	0.53
1:C:171:THR:O	1:C:175:GLY:HA3	2.09	0.53
1:C:223:HIS:ND1	1:C:224:PRO:CD	2.70	0.53
1:A:226:GLN:HB3	2:A:340:HOH:O	2.08	0.53
1:B:17:LYS:C	1:B:20:THR:HG23	2.28	0.53
1:D:98:GLY:HA3	1:D:269:GLN:CB	2.37	0.53
1:B:1:MET:SD	1:B:2:SER:O	2.67	0.53
1:B:2:SER:CA	1:B:30:ILE:HG12	2.39	0.53
1:E:55:HIS:HB3	1:E:57:LYS:CG	2.37	0.53
1:D:82:ILE:HG23	1:D:85:ASP:HB2	1.89	0.53
1:D:222:GLN:O	1:D:223:HIS:HB3	2.08	0.53
1:E:253:LEU:O	1:E:256:ASN:HB2	2.08	0.53
1:C:29:LYS:O	1:C:30:ILE:HG13	2.09	0.53
1:C:75:ILE:N	1:C:76:PRO:CD	2.71	0.53
1:B:75:ILE:HD11	1:B:272:ALA:HA	1.91	0.53
1:D:89:ARG:HG3	1:D:90:HIS:N	2.22	0.53
1:D:119:ARG:HB3	1:D:136:ALA:HB3	1.90	0.53
1:B:255:ILE:O	1:B:255:ILE:HG22	2.09	0.53
1:A:124:THR:N	1:A:125:PRO:HD2	2.24	0.53
1:B:63:SER:CB	1:B:89:ARG:HH12	2.15	0.53
1:C:173:LEU:HA	1:C:258:VAL:HG22	1.91	0.53
1:E:33:SER:O	1:E:35:PRO:HD2	2.09	0.53
1:A:167:ILE:HG22	1:A:167:ILE:O	2.09	0.53
1:D:236:GLY:C	2:D:435:HOH:O	2.47	0.53
1:C:34:SER:O	1:C:36:ASP:N	2.41	0.53
1:B:12:ALA:O	1:B:16:ALA:N	2.41	0.53
1:C:14:ALA:HB1	1:C:126:VAL:HG23	1.91	0.53
1:E:113:PRO:HD2	2:E:342:HOH:O	2.07	0.53
1:C:33:SER:HA	1:C:53:THR:O	2.09	0.53
1:A:193:VAL:HG13	1:E:234:PRO:HA	1.91	0.53
1:D:13:PHE:CZ	1:D:17:LYS:NZ	2.77	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:257:ALA:HA	2:B:418:HOH:O	2.08	0.53
1:C:53:THR:HG23	1:C:58:GLU:OE2	2.09	0.53
1:C:57:LYS:O	1:C:60:VAL:HG23	2.07	0.53
1:E:117:VAL:O	1:E:138:GLY:HA3	2.09	0.53
1:C:51:LYS:N	1:C:51:LYS:HD3	2.23	0.53
1:B:176:SER:O	1:B:177:GLY:C	2.47	0.53
1:D:77:PHE:HD1	1:D:77:PHE:N	2.06	0.53
1:E:75:ILE:CG2	1:E:104:ILE:HD11	2.38	0.53
1:B:2:SER:OG	1:B:30:ILE:HA	2.09	0.53
1:E:28:HIS:HB3	2:E:407:HOH:O	2.09	0.52
1:A:185:LEU:HD23	1:A:185:LEU:N	2.23	0.52
1:A:190:ASP:O	1:E:239:ILE:HD11	2.09	0.52
1:C:234:PRO:O	1:C:235:GLY:C	2.47	0.52
1:B:143:VAL:C	1:B:145:ASP:H	2.11	0.52
1:D:121:MET:HE2	2:D:376:HOH:O	2.09	0.52
1:E:162:VAL:HG12	1:E:163:GLU:O	2.09	0.52
1:C:61:GLN:N	1:C:61:GLN:OE1	2.42	0.52
1:C:3:VAL:O	1:C:30:ILE:HA	2.08	0.52
1:E:83:GLY:C	1:E:111:PHE:CD2	2.82	0.52
1:D:82:ILE:C	1:D:84:ALA:N	2.63	0.52
1:B:93:VAL:HG12	1:B:95:CYS:SG	2.50	0.52
1:A:227:LEU:N	2:A:340:HOH:O	2.41	0.52
1:E:264:ARG:NE	1:E:268:LEU:HD21	2.24	0.52
1:E:74:ILE:C	1:E:76:PRO:HD2	2.30	0.52
1:B:123:ASN:HA	2:B:398:HOH:O	2.08	0.52
1:B:42:VAL:C	1:B:44:ALA:H	2.12	0.52
1:A:93:VAL:HG22	1:A:118:ILE:CD1	2.39	0.52
1:E:177:GLY:O	1:E:180:TYR:N	2.42	0.52
1:E:208:GLN:HB3	2:E:408:HOH:O	2.10	0.52
1:B:147:ARG:HG3	1:B:147:ARG:O	2.08	0.52
1:D:123:ASN:O	1:D:126:VAL:HG23	2.10	0.52
1:D:13:PHE:CE1	1:D:17:LYS:HE3	2.43	0.52
1:D:233:SER:O	1:D:235:GLY:N	2.42	0.52
1:D:103:SER:HA	2:D:342:HOH:O	2.10	0.52
1:D:129:ARG:HA	1:D:156:VAL:HG13	1.92	0.52
1:D:164:GLU:HA	1:D:167:ILE:HG12	1.91	0.52
1:E:123:ASN:HB2	1:E:125:PRO:HD2	1.91	0.52
1:C:112:ARG:CG	1:C:113:PRO:HD2	2.33	0.52
1:E:70:VAL:O	1:E:71:LYS:HB2	2.10	0.52
1:B:45:LEU:HD22	1:B:48:MET:SD	2.50	0.52
1:A:82:ILE:O	1:A:83:GLY:C	2.48	0.52
1:A:75:ILE:CG2	1:A:76:PRO:HD3	2.32	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:79:LEU:CD1	1:A:104:ILE:HA	2.39	0.52
1:B:79:LEU:CD1	1:B:104:ILE:HG23	2.36	0.52
1:A:256:ASN:N	2:A:390:HOH:O	2.43	0.52
1:D:77:PHE:N	1:D:77:PHE:CD1	2.77	0.52
1:B:50:VAL:HB	2:B:350:HOH:O	2.08	0.52
1:C:160:THR:CG2	1:C:161:GLU:N	2.73	0.52
1:A:121:MET:CG	1:A:171:THR:CG2	2.88	0.52
1:D:133:THR:CG2	1:D:158:PHE:O	2.58	0.52
1:B:258:VAL:HG13	1:B:259:GLU:H	1.75	0.52
1:C:124:THR:C	1:C:126:VAL:H	2.13	0.52
1:A:177:GLY:O	1:A:178:PRO:C	2.47	0.52
1:D:169:ALA:C	1:D:171:THR:N	2.56	0.52
1:A:258:VAL:HG12	1:A:259:GLU:N	2.25	0.52
1:D:105:GLU:C	1:D:107:LYS:H	2.10	0.52
1:C:4:GLY:HA2	1:C:30:ILE:HG23	1.92	0.52
1:C:3:VAL:HG12	1:C:4:GLY:H	1.75	0.52
1:A:199:ARG:O	1:A:203:VAL:HG23	2.10	0.52
1:B:28:HIS:HA	2:B:320:HOH:O	2.09	0.52
1:C:173:LEU:CD1	1:C:258:VAL:HG21	2.40	0.52
1:C:27:ALA:HB1	1:C:50:VAL:HG22	1.92	0.52
1:E:162:VAL:CG1	1:E:166:LEU:HB2	2.39	0.52
1:E:166:LEU:O	1:E:167:ILE:C	2.49	0.51
1:D:67:PHE:CE2	1:D:93:VAL:HG21	2.45	0.51
1:B:70:VAL:HG11	1:B:78:ILE:CD1	2.39	0.51
1:C:251:ARG:C	1:C:252:SER:O	2.45	0.51
1:B:101:ILE:O	1:B:105:GLU:HB2	2.10	0.51
1:C:35:PRO:O	1:C:36:ASP:CB	2.59	0.51
1:A:33:SER:HA	1:A:53:THR:O	2.09	0.51
1:B:1:MET:HG3	1:B:2:SER:N	2.25	0.51
1:B:119:ARG:HG2	1:B:120:CYS:N	2.25	0.51
1:E:8:ALA:HB1	1:E:41:THR:CG2	2.41	0.51
1:A:269:GLN:C	1:A:271:MET:H	2.13	0.51
1:D:183:THR:N	2:D:415:HOH:O	2.43	0.51
1:A:55:HIS:HA	2:A:374:HOH:O	2.11	0.51
1:D:153:LEU:HD23	1:D:153:LEU:N	2.25	0.51
1:E:57:LYS:H	1:E:57:LYS:CD	2.18	0.51
1:E:121:MET:HE2	1:E:122:THR:N	2.26	0.51
1:D:252:SER:O	1:D:255:ILE:N	2.43	0.51
1:D:81:GLU:HG2	1:D:81:GLU:O	2.09	0.51
1:B:4:GLY:HA3	1:B:66:LEU:CD2	2.40	0.51
1:D:50:VAL:HG13	1:D:51:LYS:N	2.26	0.51
1:B:87:GLU:C	1:B:89:ARG:H	2.13	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:126:VAL:O	1:E:156:VAL:CG1	2.59	0.51
1:E:264:ARG:NH2	1:E:268:LEU:HD21	2.25	0.51
1:B:124:THR:N	1:B:125:PRO:CD	2.73	0.51
1:E:134:VAL:HG21	1:E:170:VAL:HG11	1.91	0.51
1:E:4:GLY:HA2	1:E:31:MET:O	2.11	0.51
1:E:114:ALA:HB1	1:E:140:HIS:ND1	2.25	0.51
1:A:233:SER:C	1:A:235:GLY:H	2.14	0.51
1:C:149:MET:O	1:C:151:GLN:N	2.41	0.51
1:E:264:ARG:O	1:E:268:LEU:HG	2.11	0.51
1:C:50:VAL:HG13	2:C:343:HOH:O	2.10	0.51
1:B:266:ARG:O	1:B:269:GLN:HG2	2.11	0.51
1:E:119:ARG:NE	2:E:349:HOH:O	2.44	0.51
1:D:142:GLN:HB3	2:D:375:HOH:O	2.11	0.51
1:B:39:LEU:HA	1:B:43:SER:HB2	1.93	0.51
1:B:13:PHE:O	1:B:16:ALA:HB3	2.11	0.51
1:A:135:TYR:OH	1:A:150:GLU:CG	2.59	0.51
1:C:258:VAL:CG1	1:C:258:VAL:O	2.47	0.51
1:D:82:ILE:O	1:D:85:ASP:N	2.44	0.51
1:E:8:ALA:HB1	1:E:41:THR:HG21	1.92	0.51
1:C:61:GLN:C	1:C:63:SER:H	2.14	0.51
1:C:13:PHE:O	1:C:16:ALA:HB3	2.11	0.51
1:E:233:SER:N	2:E:320:HOH:O	2.43	0.51
1:A:176:SER:O	1:A:179:ALA:N	2.40	0.51
1:E:250:PHE:N	2:E:341:HOH:O	2.44	0.51
1:C:208:GLN:HB2	2:C:354:HOH:O	2.11	0.51
1:C:105:GLU:O	1:C:109:SER:HB2	2.11	0.51
1:E:135:TYR:CZ	1:E:161:GLU:HB3	2.46	0.51
1:E:99:VAL:O	1:E:99:VAL:HG12	2.11	0.50
1:A:6:ILE:HB	2:A:322:HOH:O	2.10	0.50
1:B:6:ILE:HB	2:B:325:HOH:O	2.11	0.50
1:A:4:GLY:HA2	1:A:31:MET:O	2.10	0.50
1:A:105:GLU:O	1:A:107:LYS:N	2.42	0.50
1:E:15:LEU:HB3	1:E:19:PHE:CE1	2.46	0.50
1:A:24:VAL:HG21	1:A:155:SER:OG	2.11	0.50
1:B:184:ALA:O	1:B:188:LEU:HG	2.10	0.50
1:B:72:PRO:HB3	1:B:97:ALA:HB2	1.92	0.50
1:E:45:LEU:O	1:E:50:VAL:HB	2.11	0.50
1:B:19:PHE:CD2	1:B:152:LEU:HD11	2.47	0.50
1:B:161:GLU:O	1:B:162:VAL:CG2	2.59	0.50
2:B:400:HOH:O	1:E:194:LYS:HE3	2.11	0.50
1:E:60:VAL:CG2	1:E:82:ILE:HD13	2.39	0.50
1:E:42:VAL:O	1:E:43:SER:C	2.49	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:93:VAL:HG22	1:A:118:ILE:HG13	1.94	0.50
1:A:125:PRO:HG2	1:A:131:GLY:HA2	1.92	0.50
1:B:121:MET:O	1:B:133:THR:CB	2.54	0.50
1:B:101:ILE:HG12	1:B:164:GLU:OE1	2.11	0.50
1:A:57:LYS:HA	1:A:60:VAL:CG2	2.41	0.50
1:B:121:MET:SD	1:B:122:THR:N	2.83	0.50
1:E:124:THR:O	1:E:126:VAL:N	2.44	0.50
1:E:249:GLY:O	1:E:252:SER:HB3	2.12	0.50
1:E:49:GLY:O	1:E:50:VAL:O	2.30	0.50
1:C:269:GLN:O	1:C:272:ALA:N	2.45	0.50
1:B:222:GLN:O	1:B:223:HIS:CB	2.58	0.50
1:E:89:ARG:O	1:E:116:ARG:NH2	2.42	0.50
1:C:124:THR:N	1:C:125:PRO:CD	2.74	0.50
1:A:123:ASN:N	1:A:123:ASN:ND2	2.50	0.50
1:E:18:GLY:HA3	1:E:156:VAL:HG11	1.94	0.50
1:A:1:MET:HG2	1:A:2:SER:N	2.27	0.50
1:C:25:LEU:HD21	1:C:30:ILE:CD1	2.42	0.50
1:C:262:CYS:SG	1:C:263:ILE:N	2.85	0.50
1:B:121:MET:HE3	2:B:406:HOH:O	2.12	0.50
1:E:122:THR:CG2	1:E:133:THR:CG2	2.89	0.50
1:B:105:GLU:OE2	1:B:117:VAL:HB	2.11	0.50
1:B:220:SER:O	1:B:221:GLU:HB2	2.12	0.50
1:C:255:ILE:C	1:C:257:ALA:N	2.65	0.50
1:E:29:LYS:C	1:E:30:ILE:HG13	2.32	0.49
1:D:15:LEU:HA	1:D:126:VAL:HG11	1.93	0.49
1:D:143:VAL:C	1:D:145:ASP:N	2.65	0.49
1:C:71:LYS:NZ	1:C:74:ILE:HD12	2.26	0.49
1:B:73:HIS:C	1:B:75:ILE:H	2.15	0.49
1:B:45:LEU:HB3	2:B:350:HOH:O	2.11	0.49
1:A:8:ALA:HA	1:A:12:ALA:CB	2.42	0.49
1:E:25:LEU:CD2	1:E:25:LEU:N	2.75	0.49
1:B:172:GLY:O	1:B:258:VAL:HA	2.12	0.49
1:D:258:VAL:HG12	1:D:259:GLU:H	1.76	0.49
1:C:198:PRO:HG2	1:C:201:LEU:CB	2.42	0.49
1:B:228:LYS:HE2	1:B:229:ASP:OD1	2.12	0.49
1:C:86:ILE:HB	1:C:112:ARG:HB2	1.93	0.49
1:B:71:LYS:H	1:B:71:LYS:HD2	1.77	0.49
1:D:189:ALA:CB	1:D:203:VAL:HG23	2.42	0.49
1:B:193:VAL:N	2:B:382:HOH:O	2.44	0.49
1:C:3:VAL:C	1:C:30:ILE:HG23	2.33	0.49
1:C:271:MET:HA	1:C:274:GLN:CB	2.41	0.49
1:B:134:VAL:HG22	2:B:334:HOH:O	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:194:LYS:O	1:D:194:LYS:HG2	2.12	0.49
1:A:186:ASP:HA	2:A:424:HOH:O	2.12	0.49
1:D:134:VAL:HA	2:D:384:HOH:O	2.11	0.49
1:D:166:LEU:O	1:D:167:ILE:C	2.51	0.49
1:B:236:GLY:O	1:B:237:ALA:HB3	2.12	0.49
1:E:172:GLY:HA2	1:E:261:SER:HB3	1.93	0.49
1:D:204:ARG:HD3	2:D:404:HOH:O	2.11	0.49
1:E:149:MET:O	1:E:152:LEU:HB3	2.12	0.49
1:B:216:MET:HG3	2:B:372:HOH:O	2.12	0.49
1:B:262:CYS:HA	2:B:343:HOH:O	2.13	0.49
1:C:152:LEU:HG	1:C:153:LEU:HG	1.95	0.49
1:A:197:LEU:HD22	1:A:201:LEU:HD23	1.94	0.49
1:E:22:ALA:HB3	1:E:24:VAL:HG23	1.94	0.49
1:B:168:ASP:HB2	2:B:375:HOH:O	2.12	0.49
1:D:199:ARG:O	1:D:200:ARG:C	2.49	0.49
1:C:3:VAL:O	1:C:30:ILE:HG23	2.13	0.49
1:C:266:ARG:HG2	1:C:266:ARG:HH11	1.77	0.49
1:C:239:ILE:HD13	1:D:193:VAL:HG12	1.94	0.49
1:A:199:ARG:NH2	2:A:424:HOH:O	2.45	0.49
1:D:124:THR:O	1:D:126:VAL:N	2.46	0.49
1:A:65:VAL:HB	2:A:365:HOH:O	2.12	0.49
1:D:3:VAL:HG11	1:D:67:PHE:CE1	2.47	0.49
1:B:195:MET:HA	1:B:195:MET:HE2	1.92	0.49
1:A:100:THR:HG23	1:A:164:GLU:OE1	2.13	0.49
1:C:46:ARG:O	1:C:48:MET:N	2.46	0.49
1:E:68:LEU:HB2	1:E:94:SER:CB	2.43	0.49
1:A:39:LEU:O	1:A:40:ALA:C	2.51	0.49
1:A:60:VAL:CG2	1:A:82:ILE:HD13	2.43	0.49
1:A:185:LEU:HA	1:A:188:LEU:HD12	1.94	0.49
1:A:239:ILE:N	2:A:369:HOH:O	2.46	0.49
1:B:251:ARG:O	1:B:252:SER:C	2.50	0.49
1:E:34:SER:HB3	1:E:54:PRO:CA	2.41	0.49
1:D:38:ASP:OD2	1:D:40:ALA:HB3	2.13	0.49
1:C:7:GLY:HA3	1:C:69:ALA:O	2.13	0.49
1:D:69:ALA:N	2:D:344:HOH:O	2.25	0.49
1:A:13:PHE:HA	2:A:333:HOH:O	2.13	0.49
1:E:227:LEU:HA	2:E:442:HOH:O	2.13	0.49
1:C:112:ARG:HG3	1:C:112:ARG:HH11	1.77	0.48
1:B:75:ILE:HD11	1:B:272:ALA:CB	2.43	0.48
1:B:71:LYS:CB	1:B:73:HIS:CE1	2.91	0.48
1:B:18:GLY:O	1:B:19:PHE:C	2.52	0.48
1:B:41:THR:HG22	2:B:367:HOH:O	2.12	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:82:ILE:O	1:A:86:ILE:HG13	2.13	0.48
1:C:269:GLN:C	1:C:271:MET:N	2.67	0.48
1:D:74:ILE:HG22	1:D:78:ILE:HG13	1.94	0.48
1:D:168:ASP:HB2	2:D:423:HOH:O	2.12	0.48
1:A:101:ILE:O	1:A:104:ILE:N	2.45	0.48
1:C:148:LEU:HA	1:C:151:GLN:OE1	2.13	0.48
1:B:38:ASP:HB3	1:B:42:VAL:HB	1.94	0.48
1:B:41:THR:CA	1:B:44:ALA:HB3	2.43	0.48
1:A:36:ASP:O	1:A:37:MET:CB	2.60	0.48
1:D:70:VAL:HG21	1:D:78:ILE:CD1	2.43	0.48
1:C:128:VAL:CG1	1:C:129:ARG:H	2.26	0.48
1:D:264:ARG:NE	2:D:321:HOH:O	2.29	0.48
1:E:217:LEU:C	1:E:219:HIS:N	2.67	0.48
1:B:94:SER:O	1:B:94:SER:OG	2.22	0.48
1:D:222:GLN:HG3	1:D:227:LEU:HD21	1.96	0.48
1:C:13:PHE:HE1	1:C:44:ALA:HB3	1.78	0.48
1:E:144:GLU:HB3	2:E:352:HOH:O	2.13	0.48
1:E:77:PHE:N	1:E:77:PHE:CD1	2.80	0.48
1:A:178:PRO:O	1:A:181:ALA:HB3	2.14	0.48
1:A:100:THR:HG22	1:A:101:ILE:N	2.28	0.48
1:B:119:ARG:HD2	1:B:164:GLU:OE2	2.13	0.48
1:D:102:SER:HA	2:D:337:HOH:O	2.12	0.48
1:C:67:PHE:HA	1:C:93:VAL:HG23	1.95	0.48
1:E:141:ALA:O	1:E:142:GLN:O	2.31	0.48
1:B:3:VAL:HG13	1:B:65:VAL:O	2.14	0.48
1:E:122:THR:CG2	1:E:133:THR:HG22	2.43	0.48
1:C:173:LEU:HB3	2:C:437:HOH:O	2.12	0.48
1:A:176:SER:HB3	1:A:180:TYR:CE2	2.48	0.48
1:C:102:SER:HB3	1:C:106:LYS:HG3	1.94	0.48
1:B:166:LEU:O	1:B:169:ALA:N	2.44	0.48
1:C:11:LEU:HD12	1:C:14:ALA:CB	2.44	0.48
1:B:105:GLU:OE1	1:B:117:VAL:HG21	2.13	0.48
1:B:183:THR:HA	2:B:388:HOH:O	2.12	0.48
1:A:26:ALA:CB	1:A:29:LYS:HE2	2.40	0.48
1:A:98:GLY:O	1:A:269:GLN:OE1	2.31	0.48
1:B:233:SER:C	1:B:235:GLY:N	2.65	0.48
1:E:185:LEU:HD21	1:E:210:LEU:CD1	2.44	0.48
1:E:96:ALA:HA	2:E:447:HOH:O	2.14	0.48
1:A:10:GLN:O	1:A:12:ALA:N	2.46	0.48
1:A:127:VAL:HG12	1:A:127:VAL:O	2.14	0.48
1:D:162:VAL:CG1	1:D:166:LEU:HD12	2.38	0.48
1:C:26:ALA:O	1:C:28:HIS:N	2.46	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:219:HIS:O	1:A:220:SER:HB3	2.13	0.48
1:D:238:THR:O	1:D:241:ALA:HB3	2.13	0.48
1:C:112:ARG:HG3	1:C:113:PRO:CD	2.35	0.48
1:C:7:GLY:HA3	1:C:69:ALA:C	2.34	0.48
1:C:79:LEU:HG	2:C:332:HOH:O	2.14	0.48
1:A:135:TYR:CD1	1:A:135:TYR:C	2.86	0.48
1:B:184:ALA:O	1:B:187:ALA:HB3	2.13	0.48
1:E:134:VAL:CG2	1:E:170:VAL:HG11	2.43	0.48
1:A:165:ASP:OD2	1:A:166:LEU:N	2.47	0.48
1:A:266:ARG:NH1	1:A:266:ARG:HG2	2.28	0.48
1:A:173:LEU:HB3	1:A:174:SER:H	1.44	0.48
1:E:206:GLY:O	1:E:209:ALA:HB3	2.13	0.48
1:B:156:VAL:HG12	1:B:156:VAL:O	2.14	0.48
1:E:211:LEU:HD13	1:E:211:LEU:C	2.34	0.48
1:E:269:GLN:HG3	2:E:373:HOH:O	2.13	0.48
1:D:123:ASN:CB	1:D:125:PRO:HD2	2.43	0.48
1:E:220:SER:O	1:E:222:GLN:N	2.47	0.48
1:A:26:ALA:O	1:A:29:LYS:N	2.46	0.48
1:B:118:ILE:HD13	1:B:149:MET:SD	2.54	0.48
1:C:211:LEU:C	1:C:211:LEU:CD1	2.82	0.48
1:C:68:LEU:HD11	1:C:78:ILE:HG21	1.95	0.48
1:C:86:ILE:CD1	1:C:108:LEU:HB3	2.44	0.48
1:B:135:TYR:HE1	1:B:161:GLU:OE1	1.97	0.48
1:A:129:ARG:O	1:A:157:GLY:HA2	2.14	0.48
1:E:129:ARG:O	1:E:130:GLU:C	2.52	0.48
1:A:236:GLY:O	1:A:237:ALA:HB3	2.14	0.48
1:B:82:ILE:HG22	1:B:86:ILE:CD1	2.39	0.48
1:A:30:ILE:HB	1:A:50:VAL:HG13	1.96	0.48
1:E:169:ALA:C	1:E:171:THR:N	2.64	0.48
1:D:33:SER:HB3	1:D:56:ASN:OD1	2.13	0.48
1:B:220:SER:O	1:B:221:GLU:CB	2.62	0.48
1:B:233:SER:C	1:B:235:GLY:H	2.17	0.48
1:D:242:LEU:O	1:D:246:GLU:HB2	2.14	0.48
1:E:70:VAL:O	1:E:74:ILE:HD12	2.14	0.47
1:A:86:ILE:HG22	1:A:86:ILE:O	2.13	0.47
1:E:181:ALA:O	1:E:184:ALA:N	2.45	0.47
1:C:123:ASN:O	1:C:126:VAL:HG22	2.14	0.47
1:D:264:ARG:NH2	2:D:321:HOH:O	2.46	0.47
1:E:121:MET:CE	1:E:122:THR:H	2.26	0.47
1:B:234:PRO:HB3	1:E:197:LEU:O	2.13	0.47
1:C:43:SER:O	1:C:46:ARG:N	2.46	0.47
1:C:51:LYS:NZ	2:C:324:HOH:O	2.44	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:60:VAL:HG12	1:E:90:HIS:NE2	2.29	0.47
1:E:137:THR:O	1:E:137:THR:HG23	2.15	0.47
1:A:135:TYR:HE1	1:A:161:GLU:HG2	1.77	0.47
1:C:11:LEU:O	1:C:15:LEU:HG	2.14	0.47
1:E:57:LYS:HD3	1:E:57:LYS:N	2.26	0.47
1:A:92:VAL:HG12	1:A:117:VAL:HG23	1.96	0.47
1:B:94:SER:OG	1:B:119:ARG:HG3	2.14	0.47
1:C:230:ASN:HA	2:C:328:HOH:O	2.14	0.47
1:B:42:VAL:HA	1:B:45:LEU:HG	1.97	0.47
1:B:143:VAL:O	1:B:145:ASP:N	2.42	0.47
1:B:68:LEU:HA	2:B:325:HOH:O	2.14	0.47
1:C:128:VAL:C	1:C:130:GLU:H	2.17	0.47
1:B:119:ARG:HD3	1:B:167:ILE:HD12	1.95	0.47
1:C:64:ASP:O	1:C:65:VAL:HB	2.15	0.47
1:C:123:ASN:C	1:C:125:PRO:HD2	2.34	0.47
1:A:17:LYS:HB3	1:A:127:VAL:HG13	1.97	0.47
1:A:188:LEU:O	1:A:192:GLY:N	2.45	0.47
1:A:57:LYS:HE3	2:A:374:HOH:O	2.14	0.47
1:A:124:THR:C	1:A:126:VAL:H	2.17	0.47
1:A:194:LYS:C	2:E:356:HOH:O	2.53	0.47
1:B:89:ARG:HD2	1:B:89:ARG:C	2.35	0.47
1:D:137:THR:O	1:D:137:THR:HG23	2.14	0.47
1:E:17:LYS:CB	2:E:412:HOH:O	2.56	0.47
1:D:222:GLN:O	1:D:223:HIS:CB	2.62	0.47
1:D:33:SER:O	1:D:35:PRO:CD	2.62	0.47
1:D:1:MET:HE2	1:D:25:LEU:HD21	1.97	0.47
1:B:47:LYS:NZ	1:B:47:LYS:HB3	2.28	0.47
1:C:100:THR:HG22	1:C:101:ILE:H	1.77	0.47
1:E:45:LEU:HD23	1:E:48:MET:CE	2.45	0.47
1:B:123:ASN:C	1:B:125:PRO:HD2	2.35	0.47
1:B:17:LYS:HA	1:B:20:THR:HG21	1.97	0.47
1:B:41:THR:O	1:B:45:LEU:HG	2.14	0.47
1:B:91:ILE:HD11	1:B:145:ASP:OD1	2.14	0.47
1:C:166:LEU:O	1:C:168:ASP:N	2.48	0.47
1:B:31:MET:HG3	1:B:51:LYS:CB	2.45	0.47
1:E:83:GLY:HA2	1:E:86:ILE:HD11	1.95	0.47
1:D:60:VAL:HG21	1:D:82:ILE:CG2	2.45	0.47
1:C:61:GLN:C	1:C:63:SER:N	2.66	0.47
1:E:171:THR:HA	1:E:175:GLY:HA3	1.96	0.47
1:C:93:VAL:HG12	1:C:118:ILE:CD1	2.44	0.47
1:E:43:SER:HB2	2:E:380:HOH:O	2.14	0.47
1:E:19:PHE:CE2	1:E:152:LEU:HG	2.50	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:10:GLN:O	1:C:12:ALA:N	2.48	0.47
1:A:36:ASP:O	1:A:37:MET:HB2	2.15	0.47
1:D:6:ILE:CD1	1:D:66:LEU:HD21	2.45	0.47
1:A:133:THR:HG22	1:A:134:VAL:N	2.28	0.47
1:A:160:THR:HG22	1:A:161:GLU:N	2.30	0.47
1:C:262:CYS:O	1:C:263:ILE:C	2.54	0.47
1:A:198:PRO:HG2	1:A:201:LEU:HB2	1.96	0.47
1:D:89:ARG:CG	1:D:90:HIS:H	2.28	0.47
1:B:46:ARG:HB2	2:B:345:HOH:O	2.15	0.47
1:C:169:ALA:O	1:C:170:VAL:C	2.51	0.47
1:A:13:PHE:N	2:A:333:HOH:O	2.48	0.47
1:A:181:ALA:O	1:A:184:ALA:HB3	2.13	0.47
1:A:198:PRO:HD2	1:A:201:LEU:HD23	1.97	0.47
1:E:55:HIS:ND1	1:E:57:LYS:HE2	2.29	0.47
1:C:46:ARG:O	1:C:49:GLY:N	2.45	0.47
1:C:6:ILE:HD11	1:C:60:VAL:HG22	1.97	0.47
1:B:5:PHE:HZ	1:B:15:LEU:CB	2.10	0.47
1:D:75:ILE:CG2	1:D:79:LEU:HD22	2.45	0.47
1:D:167:ILE:HG22	2:D:397:HOH:O	2.14	0.47
1:D:60:VAL:CG2	1:D:82:ILE:HD13	2.44	0.47
1:D:3:VAL:HG11	1:D:67:PHE:HE1	1.80	0.47
1:D:217:LEU:HD13	2:D:323:HOH:O	2.14	0.47
1:D:258:VAL:O	1:D:259:GLU:C	2.51	0.47
1:C:70:VAL:HG21	1:C:78:ILE:HD12	1.96	0.46
1:B:76:PRO:O	1:B:78:ILE:N	2.47	0.46
1:A:193:VAL:C	1:A:195:MET:H	2.17	0.46
1:E:228:LYS:HE3	1:E:242:LEU:CD1	2.35	0.46
1:E:112:ARG:HG3	2:E:342:HOH:O	2.13	0.46
1:B:239:ILE:HD13	1:E:194:LYS:N	2.30	0.46
1:C:211:LEU:C	1:C:211:LEU:HD13	2.36	0.46
1:C:171:THR:HG21	2:C:423:HOH:O	2.14	0.46
1:A:10:GLN:O	1:A:13:PHE:N	2.49	0.46
1:A:102:SER:O	1:A:103:SER:C	2.54	0.46
1:B:79:LEU:CD1	1:B:104:ILE:HG12	2.42	0.46
1:A:228:LYS:NZ	1:C:199:ARG:HH12	2.12	0.46
1:E:255:ILE:O	1:E:256:ASN:C	2.53	0.46
1:C:9:GLY:O	1:C:10:GLN:C	2.53	0.46
1:C:55:HIS:C	1:C:57:LYS:H	2.19	0.46
1:C:66:LEU:HD23	1:C:66:LEU:C	2.36	0.46
1:D:4:GLY:HA2	1:D:31:MET:O	2.16	0.46
1:D:164:GLU:HA	1:D:167:ILE:HG13	1.97	0.46
1:B:129:ARG:O	1:B:157:GLY:HA2	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:27:ALA:CB	1:B:49:GLY:O	2.60	0.46
1:D:150:GLU:O	1:D:150:GLU:HG2	2.15	0.46
1:B:35:PRO:O	1:B:36:ASP:HB2	2.15	0.46
1:D:98:GLY:O	1:D:99:VAL:C	2.54	0.46
1:A:11:LEU:O	1:A:14:ALA:HB3	2.15	0.46
1:D:134:VAL:HG21	1:D:162:VAL:HG21	1.98	0.46
1:A:30:ILE:O	1:A:51:LYS:HB2	2.15	0.46
1:A:31:MET:HA	1:A:51:LYS:O	2.14	0.46
1:D:101:ILE:HG13	1:D:119:ARG:HB2	1.97	0.46
1:B:74:ILE:HD11	1:B:96:ALA:HB3	1.98	0.46
1:E:67:PHE:O	1:E:68:LEU:HD23	2.16	0.46
1:B:45:LEU:O	1:B:46:ARG:C	2.53	0.46
1:A:33:SER:HB3	1:A:56:ASN:HA	1.96	0.46
1:A:126:VAL:C	1:A:128:VAL:H	2.18	0.46
1:B:1:MET:CG	1:B:2:SER:N	2.77	0.46
1:E:125:PRO:C	1:E:127:VAL:N	2.67	0.46
1:A:252:SER:C	1:A:254:LEU:H	2.18	0.46
1:C:93:VAL:HG23	1:C:93:VAL:O	2.16	0.46
1:A:55:HIS:HB2	1:A:58:GLU:HG3	1.98	0.46
1:B:3:VAL:O	1:B:30:ILE:HG23	2.16	0.46
1:B:188:LEU:C	1:B:190:ASP:H	2.19	0.46
1:D:172:GLY:C	1:D:258:VAL:HG22	2.36	0.46
1:B:73:HIS:C	1:B:75:ILE:N	2.67	0.46
1:C:269:GLN:C	1:C:271:MET:H	2.18	0.46
1:D:30:ILE:O	1:D:51:LYS:HB2	2.16	0.46
1:A:135:TYR:OH	1:A:150:GLU:HG3	2.16	0.46
1:B:60:VAL:O	1:B:63:SER:HB2	2.16	0.46
1:E:98:GLY:HA2	2:E:400:HOH:O	2.16	0.46
1:B:8:ALA:HA	1:B:12:ALA:HB1	1.93	0.46
1:B:161:GLU:O	1:B:162:VAL:HG22	2.16	0.46
1:B:3:VAL:O	1:B:30:ILE:CG2	2.64	0.46
1:C:172:GLY:O	1:C:258:VAL:HG22	2.15	0.46
1:B:128:VAL:O	1:B:129:ARG:HB2	2.16	0.46
1:C:210:LEU:O	1:C:211:LEU:C	2.54	0.46
1:D:252:SER:O	1:D:254:LEU:N	2.49	0.46
1:D:16:ALA:C	1:D:48:MET:HE1	2.37	0.46
1:D:121:MET:HE2	1:D:171:THR:HG23	1.94	0.46
1:B:189:ALA:C	2:B:382:HOH:O	2.54	0.46
1:C:61:GLN:O	1:C:89:ARG:NH2	2.46	0.46
1:A:20:THR:HG21	1:A:48:MET:CE	2.45	0.46
1:C:83:GLY:HA2	1:C:108:LEU:HD22	1.98	0.46
1:B:76:PRO:C	1:B:78:ILE:H	2.19	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:70:VAL:O	1:E:71:LYS:CB	2.63	0.46
1:A:159:CYS:O	1:A:160:THR:OG1	2.29	0.46
1:E:176:SER:O	1:E:177:GLY:C	2.55	0.46
1:A:79:LEU:HD21	1:A:104:ILE:HG23	1.97	0.46
1:E:13:PHE:O	1:E:14:ALA:C	2.54	0.46
1:C:9:GLY:O	1:C:12:ALA:CB	2.63	0.46
1:C:264:ARG:O	1:C:268:LEU:HG	2.15	0.46
1:E:153:LEU:C	1:E:155:SER:N	2.69	0.46
1:C:104:ILE:HG21	1:C:117:VAL:HG11	1.98	0.45
1:B:5:PHE:HA	2:B:371:HOH:O	2.14	0.45
1:D:74:ILE:O	1:D:75:ILE:C	2.54	0.45
1:B:239:ILE:HD12	1:E:193:VAL:HG12	1.98	0.45
1:B:79:LEU:O	1:B:108:LEU:CD2	2.64	0.45
1:C:185:LEU:HD22	2:C:434:HOH:O	2.15	0.45
1:C:6:ILE:HG21	1:C:78:ILE:HG21	1.97	0.45
1:A:93:VAL:HG22	1:A:118:ILE:CG1	2.47	0.45
1:B:140:HIS:O	1:B:141:ALA:HB2	2.16	0.45
1:D:70:VAL:HG11	1:D:78:ILE:CD1	2.46	0.45
1:E:236:GLY:HA2	1:E:239:ILE:CG2	2.39	0.45
1:B:234:PRO:HA	1:E:193:VAL:HG13	1.98	0.45
1:C:61:GLN:O	1:C:63:SER:N	2.49	0.45
1:D:224:PRO:HA	2:D:419:HOH:O	2.15	0.45
1:B:112:ARG:O	1:B:113:PRO:O	2.34	0.45
1:D:255:ILE:O	1:D:256:ASN:C	2.55	0.45
1:E:75:ILE:O	1:E:78:ILE:HB	2.16	0.45
1:D:99:VAL:HG12	1:D:104:ILE:HD11	1.98	0.45
1:A:101:ILE:O	1:A:104:ILE:HB	2.17	0.45
1:A:92:VAL:CG1	1:A:117:VAL:HG23	2.46	0.45
1:B:119:ARG:HD3	1:B:167:ILE:HD13	1.98	0.45
1:C:204:ARG:CB	2:C:337:HOH:O	2.59	0.45
1:B:259:GLU:HB3	2:B:336:HOH:O	2.15	0.45
1:C:71:LYS:HB2	1:C:73:HIS:CE1	2.52	0.45
1:D:37:MET:CE	1:D:42:VAL:HG12	2.46	0.45
1:D:31:MET:HA	1:D:51:LYS:O	2.15	0.45
1:A:51:LYS:NZ	2:A:403:HOH:O	2.48	0.45
1:B:104:ILE:C	1:B:106:LYS:H	2.19	0.45
1:C:13:PHE:CE2	1:C:17:LYS:HE3	2.47	0.45
1:C:238:THR:HB	2:C:326:HOH:O	2.17	0.45
1:C:143:VAL:HG12	1:C:143:VAL:O	2.16	0.45
1:A:6:ILE:HG22	1:A:6:ILE:O	2.17	0.45
1:A:84:ALA:C	1:A:86:ILE:H	2.20	0.45
1:D:4:GLY:O	1:D:66:LEU:HD12	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:156:VAL:CG1	1:A:156:VAL:O	2.62	0.45
1:D:266:ARG:O	1:D:268:LEU:N	2.50	0.45
1:E:169:ALA:HA	2:E:335:HOH:O	2.16	0.45
1:A:36:ASP:O	1:A:37:MET:HG3	2.17	0.45
1:A:10:GLN:O	1:A:11:LEU:C	2.55	0.45
1:E:82:ILE:O	1:E:82:ILE:HG22	2.16	0.45
1:C:164:GLU:O	1:C:164:GLU:HG2	2.16	0.45
1:E:48:MET:HE3	1:E:48:MET:HB3	1.86	0.45
1:E:75:ILE:HD11	2:E:362:HOH:O	2.16	0.45
1:B:161:GLU:HA	2:B:330:HOH:O	2.16	0.45
1:D:75:ILE:CD1	1:D:99:VAL:HG11	2.47	0.45
1:C:27:ALA:O	1:C:28:HIS:CG	2.70	0.45
1:D:224:PRO:N	2:D:323:HOH:O	2.49	0.45
1:C:210:LEU:HA	1:C:210:LEU:HD23	1.65	0.45
1:C:122:THR:CG2	1:C:133:THR:CG2	2.95	0.45
1:A:160:THR:CG2	1:A:161:GLU:N	2.79	0.45
1:A:258:VAL:CG2	2:A:419:HOH:O	2.64	0.45
1:A:3:VAL:CG1	1:A:4:GLY:N	2.69	0.45
1:C:253:LEU:HD12	1:C:253:LEU:N	2.32	0.45
1:C:87:GLU:H	1:C:90:HIS:CE1	2.33	0.45
1:C:177:GLY:HA2	1:C:180:TYR:CE1	2.50	0.45
1:C:83:GLY:HA2	1:C:86:ILE:HD11	1.99	0.45
1:E:102:SER:C	1:E:104:ILE:N	2.67	0.45
1:A:135:TYR:CE2	1:A:150:GLU:HG2	2.51	0.45
1:D:134:VAL:HG22	1:D:162:VAL:HB	1.98	0.45
1:E:55:HIS:CG	1:E:57:LYS:HE2	2.52	0.45
1:D:101:ILE:HG22	1:D:102:SER:N	2.32	0.45
1:C:185:LEU:HA	1:C:185:LEU:HD23	1.69	0.45
1:D:6:ILE:O	1:D:70:VAL:CG2	2.65	0.45
1:A:122:THR:CG2	1:A:123:ASN:H	2.30	0.45
1:A:124:THR:O	1:A:126:VAL:N	2.50	0.45
1:A:222:GLN:O	1:A:223:HIS:HB3	2.16	0.45
1:A:57:LYS:CA	1:A:60:VAL:HG23	2.48	0.44
1:D:122:THR:HB	1:D:123:ASN:H	1.38	0.44
1:C:252:SER:O	1:C:253:LEU:C	2.54	0.44
1:B:239:ILE:HD13	1:E:194:LYS:CA	2.48	0.44
1:E:172:GLY:O	1:E:258:VAL:HA	2.16	0.44
1:C:147:ARG:HB2	1:C:147:ARG:HE	1.40	0.44
1:C:93:VAL:HG12	1:C:118:ILE:CG1	2.47	0.44
1:B:269:GLN:O	1:B:271:MET:N	2.48	0.44
1:D:124:THR:N	1:D:125:PRO:CD	2.80	0.44
1:A:108:LEU:O	1:A:108:LEU:HG	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:124:THR:O	1:C:126:VAL:N	2.51	0.44
1:D:121:MET:O	1:D:133:THR:HA	2.18	0.44
1:A:259:GLU:O	1:A:263:ILE:HG13	2.18	0.44
1:B:122:THR:HG22	1:B:133:THR:CG2	2.47	0.44
1:E:188:LEU:HD23	1:E:188:LEU:HA	1.73	0.44
1:B:244:VAL:HG12	1:B:245:LEU:N	2.30	0.44
1:B:28:HIS:C	1:B:30:ILE:H	2.20	0.44
1:E:55:HIS:HB3	1:E:57:LYS:CE	2.43	0.44
1:D:80:ASP:C	1:D:82:ILE:H	2.21	0.44
1:E:172:GLY:O	1:E:258:VAL:HG22	2.18	0.44
1:C:180:TYR:N	1:C:180:TYR:CD2	2.81	0.44
1:D:107:LYS:O	1:D:110:ALA:HB3	2.16	0.44
1:C:242:LEU:HA	1:C:242:LEU:HD23	1.60	0.44
1:C:11:LEU:HD13	1:C:124:THR:HA	2.00	0.44
1:D:126:VAL:HG13	1:D:156:VAL:CG1	2.48	0.44
1:E:178:PRO:N	2:E:404:HOH:O	2.50	0.44
1:E:38:ASP:H	1:E:42:VAL:CG2	2.30	0.44
1:C:10:GLN:NE2	2:C:382:HOH:O	2.50	0.44
1:C:3:VAL:HB	1:C:30:ILE:CG1	2.47	0.44
1:E:177:GLY:HA2	1:E:180:TYR:CD1	2.53	0.44
1:C:265:THR:HG23	2:C:323:HOH:O	2.17	0.44
1:E:242:LEU:O	1:E:245:LEU:N	2.51	0.44
1:B:176:SER:O	1:B:178:PRO:N	2.51	0.44
1:B:254:LEU:HB2	2:B:362:HOH:O	2.16	0.44
1:C:17:LYS:O	1:C:20:THR:HB	2.18	0.44
1:C:167:ILE:HB	2:C:422:HOH:O	2.17	0.44
1:E:83:GLY:HA2	1:E:86:ILE:HD12	1.97	0.44
1:A:249:GLY:O	1:A:252:SER:HB3	2.17	0.44
1:D:38:ASP:O	1:D:40:ALA:N	2.51	0.44
1:C:75:ILE:HB	1:C:76:PRO:HD3	2.00	0.44
1:E:6:ILE:HD11	1:E:66:LEU:HD21	2.00	0.44
1:A:26:ALA:O	1:A:27:ALA:C	2.56	0.44
1:A:227:LEU:HG	2:A:340:HOH:O	2.16	0.44
1:D:26:ALA:CB	1:D:28:HIS:CD2	3.01	0.44
1:E:75:ILE:O	1:E:79:LEU:HG	2.18	0.44
1:A:104:ILE:O	1:A:105:GLU:C	2.56	0.44
1:C:173:LEU:HD13	1:C:258:VAL:HG11	1.99	0.44
1:D:95:CYS:O	1:D:96:ALA:HB2	2.16	0.44
1:C:31:MET:HG2	1:C:53:THR:OG1	2.18	0.43
1:C:88:ASP:OD2	1:C:112:ARG:NH1	2.51	0.43
1:B:86:ILE:HA	1:B:90:HIS:NE2	2.33	0.43
1:E:236:GLY:O	1:E:237:ALA:CB	2.65	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:102:SER:OG	1:A:103:SER:N	2.49	0.43
1:C:17:LYS:HA	1:C:20:THR:OG1	2.18	0.43
1:C:151:GLN:HA	2:C:335:HOH:O	2.17	0.43
1:D:135:TYR:CE1	1:D:161:GLU:CB	3.01	0.43
1:E:77:PHE:O	1:E:78:ILE:C	2.56	0.43
1:B:66:LEU:N	1:B:91:ILE:O	2.51	0.43
1:B:91:ILE:HG12	1:B:116:ARG:CD	2.48	0.43
1:A:185:LEU:O	1:A:186:ASP:C	2.55	0.43
1:C:46:ARG:C	1:C:48:MET:N	2.71	0.43
1:E:205:LEU:HA	1:E:205:LEU:HD23	1.85	0.43
1:A:77:PHE:H	1:A:77:PHE:HD1	1.66	0.43
1:C:144:GLU:C	1:C:146:GLY:H	2.21	0.43
1:C:35:PRO:HD3	2:C:380:HOH:O	2.17	0.43
1:B:71:LYS:HB2	1:B:73:HIS:ND1	2.33	0.43
1:A:199:ARG:HD2	1:A:199:ARG:HA	1.86	0.43
1:B:121:MET:HG2	1:B:171:THR:OG1	2.18	0.43
1:A:79:LEU:HD11	1:A:104:ILE:HA	2.01	0.43
1:E:33:SER:O	1:E:35:PRO:CD	2.66	0.43
1:B:214:ALA:O	1:B:215:LYS:C	2.57	0.43
1:E:49:GLY:CA	2:E:407:HOH:O	2.66	0.43
1:B:140:HIS:CD2	1:B:142:GLN:HB2	2.53	0.43
1:D:31:MET:HE2	1:D:62:HIS:HB2	1.99	0.43
1:A:134:VAL:CG1	1:A:135:TYR:N	2.81	0.43
1:A:121:MET:SD	1:A:122:THR:N	2.91	0.43
1:A:123:ASN:HB2	1:A:125:PRO:HD2	2.00	0.43
1:A:13:PHE:CA	2:A:333:HOH:O	2.66	0.43
1:C:172:GLY:HA2	1:C:261:SER:CB	2.48	0.43
1:B:190:ASP:CG	1:B:199:ARG:HH12	2.21	0.43
1:C:51:LYS:NZ	1:C:51:LYS:HB2	2.33	0.43
1:E:123:ASN:CB	1:E:178:PRO:HG2	2.48	0.43
1:A:134:VAL:HG12	2:A:373:HOH:O	2.18	0.43
1:A:153:LEU:C	1:A:155:SER:N	2.71	0.43
1:A:126:VAL:O	1:A:156:VAL:CG1	2.66	0.43
1:B:132:ALA:O	1:B:133:THR:HG22	2.18	0.43
1:A:257:ALA:N	2:A:390:HOH:O	2.51	0.43
1:C:13:PHE:CE1	1:C:44:ALA:HB3	2.53	0.43
1:C:36:ASP:O	1:C:37:MET:CG	2.67	0.43
1:B:6:ILE:O	1:B:6:ILE:HG22	2.17	0.43
1:A:121:MET:HE1	2:A:386:HOH:O	2.17	0.43
1:E:221:GLU:C	1:E:223:HIS:N	2.71	0.43
1:C:223:HIS:CE1	1:C:224:PRO:HD2	2.52	0.43
1:B:13:PHE:CD1	1:B:41:THR:HG23	2.53	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:171:THR:O	1:C:175:GLY:CA	2.66	0.43
1:B:115:PRO:HG3	2:B:331:HOH:O	2.18	0.43
1:A:233:SER:C	1:A:235:GLY:N	2.69	0.43
1:D:197:LEU:HD23	1:D:197:LEU:HA	1.71	0.43
1:B:32:ALA:O	1:B:53:THR:HB	2.19	0.43
1:A:229:ASP:N	1:A:229:ASP:OD1	2.52	0.43
1:C:2:SER:C	1:C:3:VAL:HG23	2.39	0.43
1:C:31:MET:CG	1:C:53:THR:OG1	2.66	0.43
1:B:134:VAL:CG1	1:B:135:TYR:N	2.82	0.43
1:C:196:GLY:O	1:C:197:LEU:O	2.37	0.43
1:A:126:VAL:C	1:A:128:VAL:N	2.72	0.43
2:A:405:HOH:O	1:E:228:LYS:HE2	2.17	0.43
1:B:101:ILE:HG13	1:B:102:SER:N	2.34	0.43
1:B:190:ASP:N	2:B:382:HOH:O	2.50	0.43
1:E:126:VAL:HG13	1:E:156:VAL:O	2.19	0.43
1:E:12:ALA:O	1:E:13:PHE:C	2.56	0.43
1:C:228:LYS:NZ	1:C:229:ASP:OD1	2.52	0.43
1:D:148:LEU:O	1:D:148:LEU:HD12	2.19	0.43
1:D:236:GLY:HA2	2:D:435:HOH:O	2.18	0.43
1:C:79:LEU:CD1	1:C:104:ILE:HG13	2.47	0.43
1:E:75:ILE:N	1:E:76:PRO:CD	2.82	0.43
1:B:31:MET:HG3	1:B:51:LYS:HB2	2.01	0.43
1:B:105:GLU:O	1:B:109:SER:HB2	2.18	0.43
1:D:185:LEU:CD2	1:D:210:LEU:CD1	2.95	0.43
1:C:59:THR:HA	1:C:62:HIS:HE1	1.84	0.43
1:B:41:THR:O	1:B:45:LEU:N	2.52	0.43
1:C:269:GLN:O	1:C:271:MET:N	2.52	0.43
1:B:134:VAL:HA	2:B:334:HOH:O	2.19	0.43
1:A:133:THR:CG2	1:A:134:VAL:N	2.82	0.43
1:C:123:ASN:HB2	1:C:125:PRO:CD	2.42	0.43
1:C:124:THR:C	1:C:126:VAL:N	2.71	0.43
1:B:194:LYS:HG2	1:B:195:MET:HE3	2.01	0.43
1:E:59:THR:O	1:E:62:HIS:N	2.52	0.43
1:C:213:ALA:O	1:C:216:MET:HB2	2.19	0.43
2:B:390:HOH:O	1:D:239:ILE:CG2	2.67	0.42
1:C:3:VAL:HB	1:C:30:ILE:CD1	2.49	0.42
1:C:274:GLN:HG2	1:C:274:GLN:O	2.18	0.42
1:B:102:SER:HA	1:B:105:GLU:CB	2.49	0.42
1:B:164:GLU:O	1:B:164:GLU:CG	2.67	0.42
1:A:223:HIS:ND1	1:A:224:PRO:CD	2.82	0.42
1:C:13:PHE:HE2	1:C:17:LYS:CE	2.31	0.42
1:D:27:ALA:HB1	1:D:49:GLY:HA3	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:18:GLY:O	1:B:20:THR:N	2.53	0.42
1:B:79:LEU:O	1:B:108:LEU:HD23	2.19	0.42
1:C:189:ALA:HA	1:C:202:ALA:HB1	2.01	0.42
1:D:143:VAL:O	1:D:145:ASP:N	2.52	0.42
1:D:135:TYR:CD1	1:D:135:TYR:C	2.92	0.42
1:B:90:HIS:N	1:B:90:HIS:CD2	2.87	0.42
1:A:41:THR:O	1:A:44:ALA:HB3	2.19	0.42
1:A:41:THR:HG22	1:A:42:VAL:N	2.34	0.42
1:C:126:VAL:C	1:C:128:VAL:N	2.73	0.42
1:A:103:SER:HA	2:A:391:HOH:O	2.20	0.42
1:D:80:ASP:C	1:D:82:ILE:N	2.70	0.42
1:C:45:LEU:O	1:C:45:LEU:HD23	2.20	0.42
1:D:16:ALA:HB3	2:D:365:HOH:O	2.19	0.42
1:C:38:ASP:O	1:C:42:VAL:HB	2.18	0.42
1:A:182:PHE:HB2	2:A:335:HOH:O	2.18	0.42
1:C:68:LEU:CD2	1:C:79:LEU:HD21	2.50	0.42
1:E:203:VAL:CG2	2:E:422:HOH:O	2.52	0.42
1:B:105:GLU:OE1	1:B:117:VAL:CG2	2.67	0.42
1:B:199:ARG:CZ	1:D:229:ASP:OD1	2.68	0.42
1:B:57:LYS:CG	1:B:58:GLU:N	2.82	0.42
1:E:126:VAL:HG12	1:E:156:VAL:CG1	2.50	0.42
1:A:25:LEU:CG	1:A:26:ALA:H	2.30	0.42
1:A:256:ASN:CB	2:A:390:HOH:O	2.60	0.42
1:B:112:ARG:O	1:B:113:PRO:C	2.58	0.42
1:C:99:VAL:CG1	1:C:104:ILE:HD11	2.49	0.42
1:B:125:PRO:C	1:B:127:VAL:N	2.71	0.42
1:A:39:LEU:O	1:A:43:SER:HB3	2.19	0.42
1:D:99:VAL:CG1	1:D:104:ILE:HD11	2.50	0.42
1:C:201:LEU:O	1:C:205:LEU:HB2	2.19	0.42
1:D:220:SER:HB2	1:D:222:GLN:HG2	2.01	0.42
1:A:118:ILE:HG22	1:A:137:THR:HA	2.00	0.42
1:A:55:HIS:O	1:A:57:LYS:N	2.50	0.42
1:D:133:THR:O	1:D:159:CYS:HA	2.19	0.42
1:A:75:ILE:HD13	1:A:99:VAL:HG11	2.01	0.42
1:B:89:ARG:O	1:B:89:ARG:CD	2.67	0.42
1:B:239:ILE:HD12	1:E:193:VAL:CG1	2.50	0.42
1:E:17:LYS:O	1:E:18:GLY:C	2.58	0.42
1:A:162:VAL:HG13	1:A:166:LEU:HD12	2.00	0.42
1:D:7:GLY:HA2	1:D:33:SER:O	2.18	0.42
1:A:227:LEU:O	1:A:231:VAL:HG23	2.19	0.42
1:D:13:PHE:HZ	1:D:17:LYS:NZ	2.12	0.42
1:E:231:VAL:O	1:E:231:VAL:HG12	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:244:VAL:O	1:B:247:SER:HB2	2.20	0.42
1:E:262:CYS:O	1:E:263:ILE:C	2.56	0.42
1:C:68:LEU:HD23	1:C:79:LEU:HD21	2.02	0.42
1:E:80:ASP:C	1:E:81:GLU:HG3	2.40	0.42
1:A:193:VAL:HA	1:A:197:LEU:O	2.20	0.42
1:A:7:GLY:O	1:A:8:ALA:HB2	2.19	0.42
1:E:198:PRO:HG2	1:E:201:LEU:CB	2.48	0.42
1:D:82:ILE:O	1:D:84:ALA:N	2.52	0.42
1:B:79:LEU:HB3	1:B:108:LEU:HG	2.02	0.42
1:D:112:ARG:HA	1:D:113:PRO:HD3	1.93	0.42
1:B:269:GLN:O	1:B:273:ASP:N	2.46	0.42
1:D:45:LEU:O	1:D:46:ARG:C	2.58	0.42
1:C:100:THR:CG2	1:C:101:ILE:N	2.83	0.42
1:A:190:ASP:N	1:A:199:ARG:HH12	2.17	0.42
1:D:82:ILE:O	1:D:83:GLY:C	2.57	0.42
1:A:61:GLN:O	1:A:63:SER:N	2.53	0.42
1:E:105:GLU:OE1	1:E:139:THR:HB	2.20	0.42
1:C:104:ILE:CG2	1:C:117:VAL:HG21	2.49	0.42
1:D:121:MET:HG2	2:D:376:HOH:O	2.19	0.42
1:C:249:GLY:O	1:C:253:LEU:CD1	2.64	0.42
1:D:83:GLY:O	1:D:86:ILE:CG2	2.59	0.42
1:A:245:LEU:HA	2:A:387:HOH:O	2.20	0.42
1:D:109:SER:C	1:D:111:PHE:N	2.73	0.42
1:C:10:GLN:C	1:C:12:ALA:H	2.23	0.42
1:C:212:GLY:O	1:C:216:MET:HB2	2.20	0.42
1:B:70:VAL:CG1	1:B:71:LYS:N	2.83	0.42
1:E:6:ILE:N	2:E:322:HOH:O	2.52	0.42
1:C:266:ARG:HG2	2:C:323:HOH:O	2.19	0.42
1:A:251:ARG:O	1:A:252:SER:C	2.57	0.42
1:D:17:LYS:O	1:D:20:THR:HB	2.20	0.42
1:E:35:PRO:CG	2:E:401:HOH:O	2.65	0.42
1:E:270:SER:HA	2:E:373:HOH:O	2.19	0.42
1:C:142:GLN:HB2	1:C:145:ASP:OD2	2.20	0.42
2:B:390:HOH:O	1:D:239:ILE:HG23	2.20	0.41
1:E:99:VAL:O	1:E:100:THR:C	2.57	0.41
1:A:33:SER:C	1:A:35:PRO:HD3	2.40	0.41
1:A:42:VAL:HG13	1:A:52:LEU:HD13	2.02	0.41
1:E:181:ALA:N	2:E:391:HOH:O	2.52	0.41
1:C:19:PHE:HE2	1:C:153:LEU:HD23	1.85	0.41
1:E:121:MET:O	1:E:133:THR:HA	2.20	0.41
1:E:34:SER:C	1:E:36:ASP:H	2.23	0.41
1:A:47:LYS:O	1:A:48:MET:C	2.59	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:3:VAL:CG1	1:C:4:GLY:N	2.83	0.41
1:B:70:VAL:CG1	1:B:71:LYS:H	2.28	0.41
1:E:75:ILE:HD12	1:E:99:VAL:HG21	2.02	0.41
1:B:11:LEU:HB3	1:B:15:LEU:CD1	2.50	0.41
1:A:149:MET:HE2	1:A:149:MET:HA	2.02	0.41
1:A:66:LEU:N	2:A:368:HOH:O	2.53	0.41
1:A:57:LYS:HE2	1:A:81:GLU:OE1	2.19	0.41
1:B:141:ALA:O	1:B:145:ASP:CB	2.62	0.41
1:C:166:LEU:O	1:C:167:ILE:C	2.59	0.41
1:B:198:PRO:CD	1:B:201:LEU:HD23	2.49	0.41
1:C:13:PHE:HE1	1:C:44:ALA:CB	2.33	0.41
1:E:7:GLY:H	1:E:33:SER:HB2	1.85	0.41
1:D:270:SER:O	1:D:274:GLN:OE1	2.37	0.41
1:D:236:GLY:O	1:D:237:ALA:HB3	2.20	0.41
1:B:68:LEU:HG	1:B:92:VAL:CG1	2.50	0.41
1:C:135:TYR:C	1:C:135:TYR:CD1	2.93	0.41
1:A:97:ALA:O	1:A:99:VAL:N	2.53	0.41
1:B:109:SER:OG	1:B:115:PRO:CD	2.65	0.41
1:B:119:ARG:NE	1:B:167:ILE:HG21	2.34	0.41
1:B:201:LEU:O	1:B:205:LEU:HG	2.20	0.41
1:A:109:SER:C	1:A:111:PHE:N	2.70	0.41
1:C:213:ALA:O	1:C:216:MET:CB	2.68	0.41
1:B:161:GLU:C	1:B:162:VAL:HG23	2.41	0.41
1:A:123:ASN:C	1:A:125:PRO:HD2	2.40	0.41
1:D:266:ARG:HG3	2:D:377:HOH:O	2.20	0.41
1:C:251:ARG:HB2	2:C:340:HOH:O	2.19	0.41
1:E:131:GLY:H	1:E:157:GLY:HA3	1.85	0.41
2:A:422:HOH:O	1:C:199:ARG:HB2	2.18	0.41
1:D:33:SER:CB	1:D:56:ASN:OD1	2.69	0.41
1:B:226:GLN:O	1:B:230:ASN:OD1	2.38	0.41
1:E:150:GLU:O	1:E:152:LEU:N	2.53	0.41
1:E:135:TYR:CE1	1:E:161:GLU:HB3	2.56	0.41
1:A:55:HIS:C	1:A:57:LYS:N	2.73	0.41
1:C:122:THR:CB	1:C:133:THR:CG2	2.88	0.41
1:C:135:TYR:CZ	1:C:161:GLU:HB3	2.52	0.41
1:A:15:LEU:O	1:A:16:ALA:C	2.59	0.41
1:A:244:VAL:CG2	1:A:245:LEU:N	2.84	0.41
1:C:205:LEU:HD23	1:C:205:LEU:HA	1.87	0.41
1:C:17:LYS:HE3	1:C:17:LYS:HB2	1.85	0.41
1:A:59:THR:O	1:A:61:GLN:N	2.53	0.41
1:D:12:ALA:O	1:D:16:ALA:HB2	2.20	0.41
1:D:16:ALA:O	1:D:48:MET:HE1	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:112:ARG:NH1	1:C:113:PRO:CD	2.68	0.41
1:C:2:SER:O	1:C:3:VAL:CG2	2.69	0.41
1:D:134:VAL:HG11	1:D:170:VAL:HG11	2.02	0.41
1:D:134:VAL:CG1	1:D:170:VAL:HG11	2.50	0.41
1:B:75:ILE:HD11	1:B:272:ALA:CA	2.51	0.41
1:E:70:VAL:HB	1:E:78:ILE:HD11	2.03	0.41
1:E:74:ILE:C	1:E:76:PRO:CD	2.89	0.41
1:E:79:LEU:C	1:E:81:GLU:H	2.18	0.41
1:C:121:MET:HE2	1:C:122:THR:H	1.85	0.41
1:C:168:ASP:HB2	1:C:266:ARG:NH1	2.36	0.41
1:A:210:LEU:HA	1:A:210:LEU:HD23	1.79	0.41
1:D:129:ARG:HG2	1:D:156:VAL:HG13	2.03	0.41
1:E:121:MET:CE	2:E:405:HOH:O	2.68	0.41
1:E:87:GLU:O	1:E:89:ARG:N	2.54	0.41
1:D:45:LEU:O	1:D:48:MET:N	2.53	0.41
1:A:56:ASN:O	1:A:82:ILE:HD11	2.21	0.41
1:B:6:ILE:CA	1:B:33:SER:HB3	2.26	0.41
1:A:92:VAL:HB	1:A:117:VAL:HG23	2.03	0.41
1:B:185:LEU:HD23	1:B:185:LEU:HA	1.87	0.41
1:C:48:MET:HB3	1:C:50:VAL:HG23	2.03	0.41
1:E:131:GLY:HA2	2:E:325:HOH:O	2.20	0.41
1:A:240:HIS:CD2	1:C:194:LYS:HG3	2.56	0.41
1:D:33:SER:HA	1:D:53:THR:O	2.21	0.41
1:B:223:HIS:ND1	1:B:224:PRO:HD2	2.35	0.41
1:D:254:LEU:HD23	1:D:254:LEU:HA	1.83	0.41
1:A:180:TYR:N	1:A:180:TYR:CD2	2.86	0.41
1:E:116:ARG:HB2	2:E:396:HOH:O	2.20	0.41
1:E:153:LEU:C	1:E:155:SER:H	2.21	0.41
1:C:114:ALA:HA	2:C:379:HOH:O	2.21	0.41
1:C:66:LEU:HB2	2:C:402:HOH:O	2.20	0.41
1:D:193:VAL:C	1:D:195:MET:H	2.25	0.41
1:D:203:VAL:HA	2:D:388:HOH:O	2.21	0.41
1:A:187:ALA:O	1:A:190:ASP:N	2.53	0.41
1:B:185:LEU:O	1:B:187:ALA:N	2.54	0.41
1:A:27:ALA:HB1	1:A:49:GLY:C	2.42	0.41
1:C:31:MET:CG	1:C:53:THR:HG1	2.34	0.40
1:C:75:ILE:O	1:C:79:LEU:HG	2.21	0.40
1:C:126:VAL:C	1:C:128:VAL:H	2.23	0.40
1:C:126:VAL:O	1:C:128:VAL:O	2.39	0.40
1:C:125:PRO:HB2	1:C:130:GLU:O	2.22	0.40
1:E:111:PHE:O	1:E:112:ARG:C	2.60	0.40
1:A:101:ILE:HG23	1:A:117:VAL:CG1	2.51	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:86:ILE:HD12	1:D:108:LEU:HD13	2.03	0.40
1:B:185:LEU:C	1:B:187:ALA:N	2.74	0.40
1:D:252:SER:HA	1:D:255:ILE:HD12	2.02	0.40
1:C:99:VAL:HG11	1:C:104:ILE:HD11	2.03	0.40
1:C:53:THR:HG22	1:C:55:HIS:O	2.21	0.40
1:E:28:HIS:O	1:E:51:LYS:HE3	2.21	0.40
1:B:132:ALA:C	1:B:133:THR:CG2	2.89	0.40
1:B:185:LEU:CD2	1:B:210:LEU:CD1	2.97	0.40
1:C:93:VAL:HG11	1:C:149:MET:SD	2.61	0.40
1:C:119:ARG:NH2	2:C:339:HOH:O	2.48	0.40
1:A:22:ALA:HA	2:A:379:HOH:O	2.21	0.40
1:E:254:LEU:HD23	1:E:254:LEU:HA	1.83	0.40
1:C:70:VAL:CG1	1:C:74:ILE:HB	2.52	0.40
1:B:17:LYS:HA	1:B:20:THR:CG2	2.52	0.40
1:A:36:ASP:O	1:A:37:MET:CG	2.70	0.40
1:A:65:VAL:N	2:A:365:HOH:O	2.52	0.40
1:D:82:ILE:O	1:D:82:ILE:HG22	2.20	0.40
1:A:252:SER:HA	1:A:255:ILE:HD12	2.03	0.40
1:D:135:TYR:CE2	1:D:150:GLU:HB2	2.57	0.40
1:C:164:GLU:HG2	2:C:416:HOH:O	2.21	0.40
1:C:31:MET:SD	1:C:53:THR:OG1	2.79	0.40
1:B:18:GLY:O	1:B:19:PHE:CD1	2.75	0.40
1:A:54:PRO:HG2	1:A:55:HIS:CD2	2.57	0.40
1:A:185:LEU:HD21	1:A:210:LEU:CD1	2.51	0.40
1:D:101:ILE:O	1:D:102:SER:C	2.60	0.40
1:A:274:GLN:HB2	1:A:275:GLU:H	1.66	0.40
1:D:255:ILE:O	1:D:257:ALA:N	2.53	0.40
1:C:114:ALA:HB1	1:C:140:HIS:CE1	2.55	0.40
1:A:41:THR:O	1:A:42:VAL:C	2.60	0.40
1:D:70:VAL:O	1:D:71:LYS:C	2.59	0.40
1:A:129:ARG:CG	1:A:129:ARG:O	2.68	0.40
1:B:137:THR:HG22	1:B:138:GLY:N	2.37	0.40
1:C:193:VAL:HG12	2:C:344:HOH:O	2.21	0.40
1:A:26:ALA:HB3	1:A:29:LYS:CE	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	275/321 (86%)	182 (66%)	60 (22%)	33 (12%)	1	4
1	B	272/321 (85%)	168 (62%)	68 (25%)	36 (13%)	0	2
1	C	275/321 (86%)	183 (66%)	60 (22%)	32 (12%)	1	4
1	D	275/321 (86%)	183 (66%)	68 (25%)	24 (9%)	1	9
1	E	275/321 (86%)	183 (66%)	57 (21%)	35 (13%)	0	3
All	All	1372/1605 (86%)	899 (66%)	313 (23%)	160 (12%)	1	4

All (160) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ALA
1	A	10	GLN
1	A	11	LEU
1	A	36	ASP
1	A	37	MET
1	A	39	LEU
1	A	40	ALA
1	A	41	THR
1	A	42	VAL
1	A	85	ASP
1	A	106	LYS
1	A	107	LYS
1	A	173	LEU
1	A	253	LEU
1	B	10	GLN
1	B	36	ASP
1	B	37	MET
1	B	61	GLN
1	B	75	ILE
1	B	77	PHE
1	B	97	ALA
1	B	113	PRO
1	B	129	ARG

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Mol	Chain	Res	Type
1	B	137	THR
1	B	140	HIS
1	B	141	ALA
1	B	142	GLN
1	B	163	GLU
1	B	221	GLU
1	B	222	GLN
1	B	223	HIS
1	C	10	GLN
1	C	11	LEU
1	C	16	ALA
1	C	27	ALA
1	C	36	ASP
1	C	63	SER
1	C	65	VAL
1	C	113	PRO
1	C	142	GLN
1	C	197	LEU
1	C	252	SER
1	C	253	LEU
1	D	40	ALA
1	D	81	GLU
1	D	99	VAL
1	D	106	LYS
1	D	129	ARG
1	D	167	ILE
1	D	170	VAL
1	E	42	VAL
1	E	43	SER
1	E	78	ILE
1	E	130	GLU
1	E	142	GLN
1	E	167	ILE
1	E	170	VAL
1	E	218	LEU
1	E	222	GLN
1	E	274	GLN
1	A	60	VAL
1	A	62	HIS
1	A	98	GLY
1	A	102	SER
1	A	105	GLU

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Mol	Chain	Res	Type
1	A	127	VAL
1	A	129	ARG
1	A	164	GLU
1	A	223	HIS
1	A	234	PRO
1	B	19	PHE
1	B	24	VAL
1	B	29	LYS
1	B	76	PRO
1	B	143	VAL
1	B	177	GLY
1	B	252	SER
1	B	270	SER
1	C	47	LYS
1	C	64	ASP
1	C	72	PRO
1	C	139	THR
1	C	150	GLU
1	C	262	CYS
1	D	39	LEU
1	D	90	HIS
1	D	164	GLU
1	D	199	ARG
1	D	223	HIS
1	E	14	ALA
1	E	50	VAL
1	E	59	THR
1	E	74	ILE
1	E	80	ASP
1	E	88	ASP
1	E	113	PRO
1	E	177	GLY
1	B	16	ALA
1	B	83	GLY
1	B	144	GLU
1	B	154	SER
1	B	160	THR
1	C	25	LEU
1	C	40	ALA
1	C	46	ARG
1	C	62	HIS
1	C	107	LYS

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Mol	Chain	Res	Type
1	C	167	ILE
1	C	173	LEU
1	D	110	ALA
1	D	253	LEU
1	D	256	ASN
1	E	36	ASP
1	E	41	THR
1	E	44	ALA
1	E	129	ARG
1	E	151	GLN
1	E	223	HIS
1	E	237	ALA
1	E	250	PHE
1	A	27	ALA
1	B	20	THR
1	B	64	ASP
1	B	234	PRO
1	B	237	ALA
1	C	61	GLN
1	C	140	HIS
1	C	263	ILE
1	D	41	THR
1	D	96	ALA
1	D	237	ALA
1	D	267	GLU
1	E	100	THR
1	E	125	PRO
1	E	199	ARG
1	A	25	LEU
1	A	111	PHE
1	A	125	PRO
1	A	220	SER
1	B	27	ALA
1	C	248	GLY
1	C	259	GLU
1	D	125	PRO
1	D	224	PRO
1	E	34	SER
1	E	141	ALA
1	E	221	GLU
1	A	56	ASN
1	A	110	ALA

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Mol	Chain	Res	Type
1	A	252	SER
1	D	234	PRO
1	E	178	PRO
1	A	104	ILE
1	D	112	ARG
1	E	234	PRO
1	B	235	GLY
1	C	258	VAL
1	C	76	PRO
1	D	156	VAL
1	E	203	VAL

5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	215/250 (86%)	185 (86%)	30 (14%)	5	21
1	B	213/250 (85%)	197 (92%)	16 (8%)	19	58
1	C	214/250 (86%)	196 (92%)	18 (8%)	16	52
1	D	215/250 (86%)	185 (86%)	30 (14%)	5	21
1	E	215/250 (86%)	203 (94%)	12 (6%)	30	70
All	All	1072/1250 (86%)	966 (90%)	106 (10%)	11	39

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	36	ASP
1	A	38	ASP
1	A	73	HIS
1	A	77	PHE
1	A	90	HIS
1	A	91	ILE
1	A	94	SER
1	A	102	SER
1	A	120	CYS

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Mol	Chain	Res	Type
1	A	121	MET
1	A	123	ASN
1	A	126	VAL
1	A	134	VAL
1	A	148	LEU
1	A	149	MET
1	A	150	GLU
1	A	171	THR
1	A	194	LYS
1	A	195	MET
1	A	205	LEU
1	A	211	LEU
1	A	221	GLU
1	A	234	PRO
1	A	244	VAL
1	A	247	SER
1	A	251	ARG
1	A	258	VAL
1	A	269	GLN
1	A	271	MET
1	B	5	PHE
1	B	10	GLN
1	B	19	PHE
1	B	47	LYS
1	B	64	ASP
1	B	90	HIS
1	B	120	CYS
1	B	124	THR
1	B	133	THR
1	B	140	HIS
1	B	161	GLU
1	B	163	GLU
1	B	174	SER
1	B	211	LEU
1	B	233	SER
1	B	265	THR
1	C	13	PHE
1	C	51	LYS
1	C	61	GLN
1	C	89	ARG
1	C	90	HIS
1	C	120	CYS

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Mol	Chain	Res	Type
1	C	121	MET
1	C	123	ASN
1	C	124	THR
1	C	152	LEU
1	C	190	ASP
1	C	195	MET
1	C	200	ARG
1	C	211	LEU
1	C	216	MET
1	C	232	SER
1	C	247	SER
1	C	273	ASP
1	D	2	SER
1	D	10	GLN
1	D	11	LEU
1	D	15	LEU
1	D	28	HIS
1	D	31	MET
1	D	50	VAL
1	D	65	VAL
1	D	73	HIS
1	D	101	ILE
1	D	118	ILE
1	D	120	CYS
1	D	121	MET
1	D	122	THR
1	D	124	THR
1	D	127	VAL
1	D	142	GLN
1	D	144	GLU
1	D	149	MET
1	D	153	LEU
1	D	159	CYS
1	D	168	ASP
1	D	203	VAL
1	D	208	GLN
1	D	211	LEU
1	D	215	LYS
1	D	217	LEU
1	D	239	ILE
1	D	244	VAL
1	D	258	VAL

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Mol	Chain	Res	Type
1	E	48	MET
1	E	57	LYS
1	E	77	PHE
1	E	120	CYS
1	E	123	ASN
1	E	160	THR
1	E	168	ASP
1	E	178	PRO
1	E	195	MET
1	E	216	MET
1	E	217	LEU
1	E	233	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	HIS
1	A	90	HIS
1	A	123	ASN
1	A	140	HIS
1	A	240	HIS
1	B	151	GLN
1	B	240	HIS
1	C	73	HIS
1	C	90	HIS
1	C	240	HIS
1	C	243	HIS
1	D	28	HIS
1	D	140	HIS
1	D	240	HIS
1	E	28	HIS
1	E	226	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	277/321 (86%)	-0.30	0 100 100	27, 79, 115, 154	0
1	B	276/321 (85%)	-0.08	3 (1%) 77 22	26, 120, 172, 187	0
1	C	277/321 (86%)	-0.06	1 (0%) 90 45	23, 117, 169, 183	0
1	D	277/321 (86%)	-0.34	0 100 100	24, 70, 117, 163	0
1	E	277/321 (86%)	-0.32	0 100 100	23, 78, 126, 156	0
All	All	1384/1605 (86%)	-0.22	4 (0%) 91 53	23, 82, 160, 187	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	39	LEU	2.2
1	B	275	GLU	2.1
1	C	39	LEU	2.1
1	B	95	CYS	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.