Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 02:46 AM EDT

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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

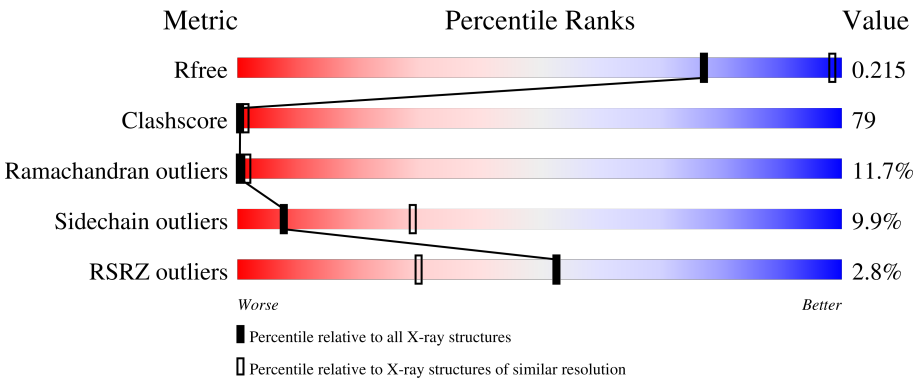
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	321	% 21% 49% 15% • 14%
1	B	321	5% 19% 54% 13% • 14%
1	C	321	5% 20% 55% 11% 14%
1	D	321	22% 50% 14% 14%
1	E	321	% 22% 51% 12% 14%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10768 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 Pyrroline-5-carboxylate reductase 1.

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

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
			Total	O		
2	A	106	106	106	0	0
2	B	118	118	118	0	0

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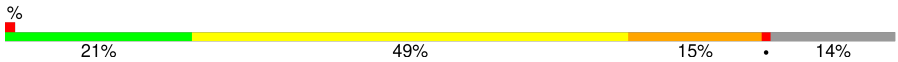
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	C	119	119	119	0	0
			Total	O		
2	D	126	126	126	0	0
			Total	O		
2	E	128	128	128	0	0

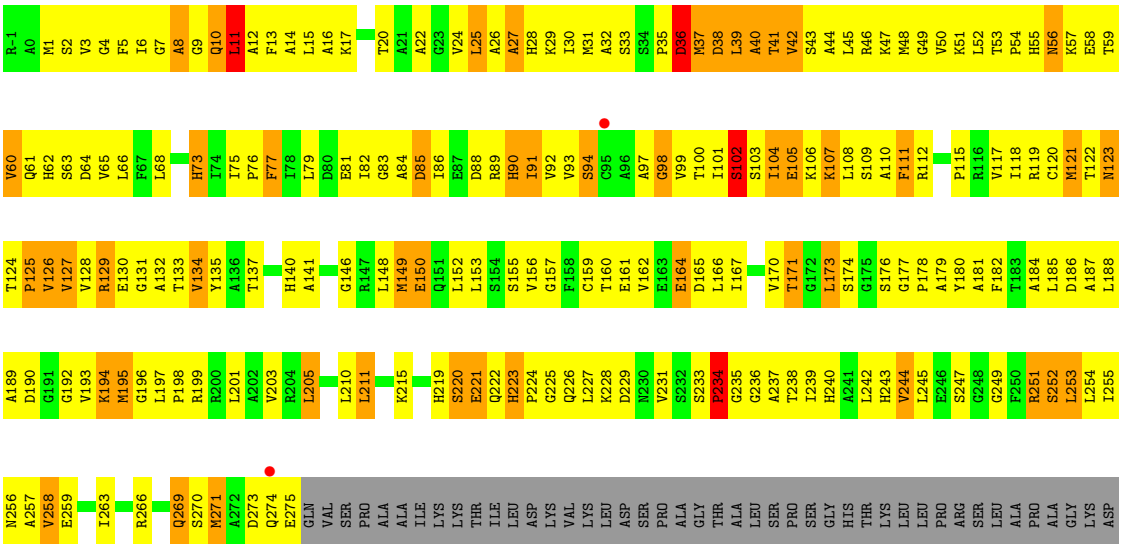
3 Residue-property plots (i)

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

• Molecule 1: Pyrroline-5-carboxylate reductase 1

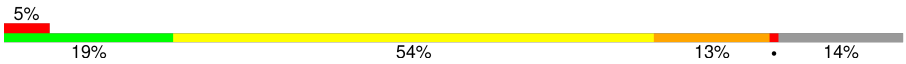
Chain A:

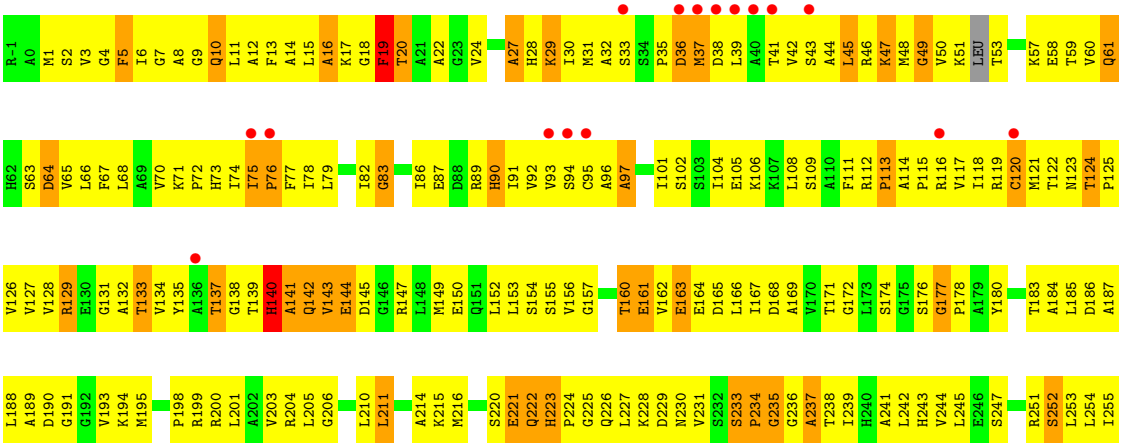


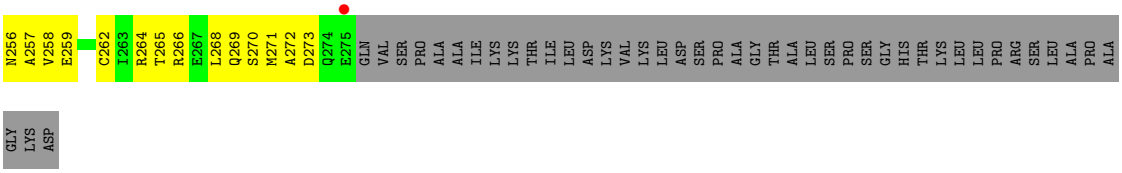


• Molecule 1: Pyrroline-5-carboxylate reductase 1

Chain B:

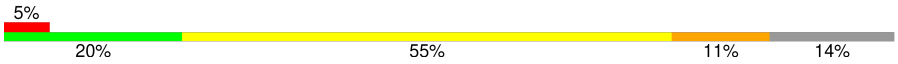


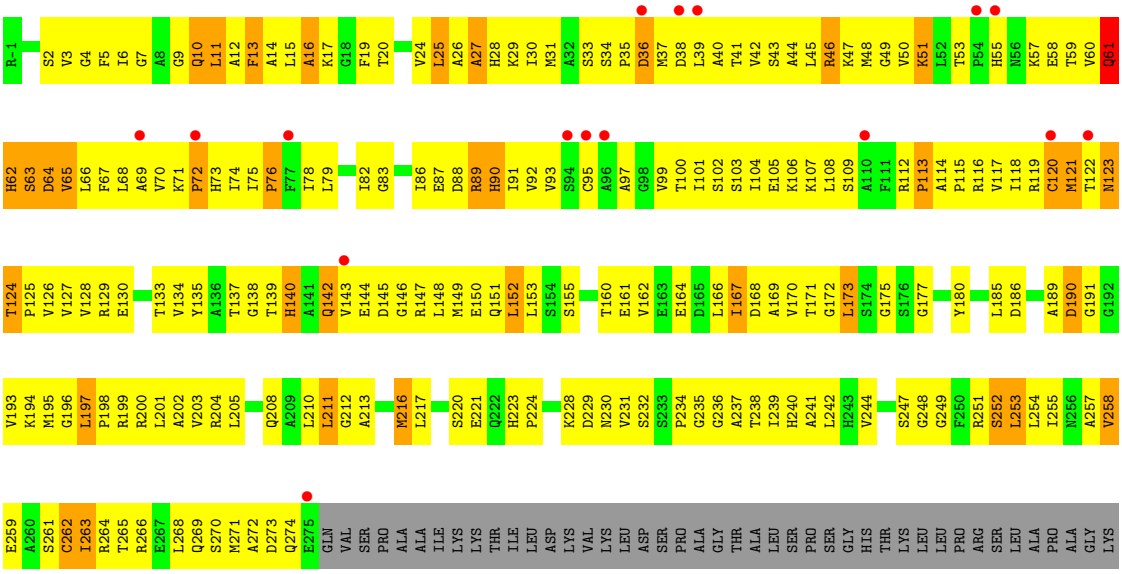




- Molecule 1: Pyrroline-5-carboxylate reductase 1

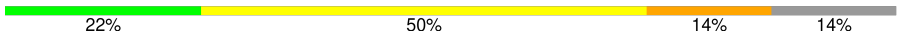
Chain C:

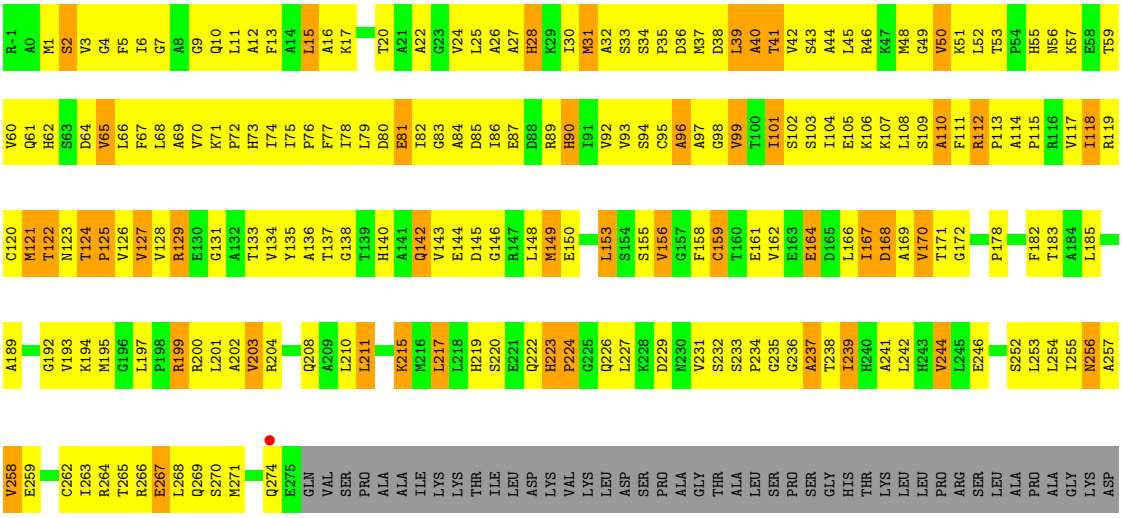




- Molecule 1: Pyrroline-5-carboxylate reductase 1

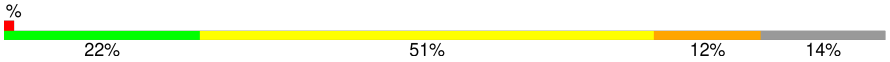
Chain D:

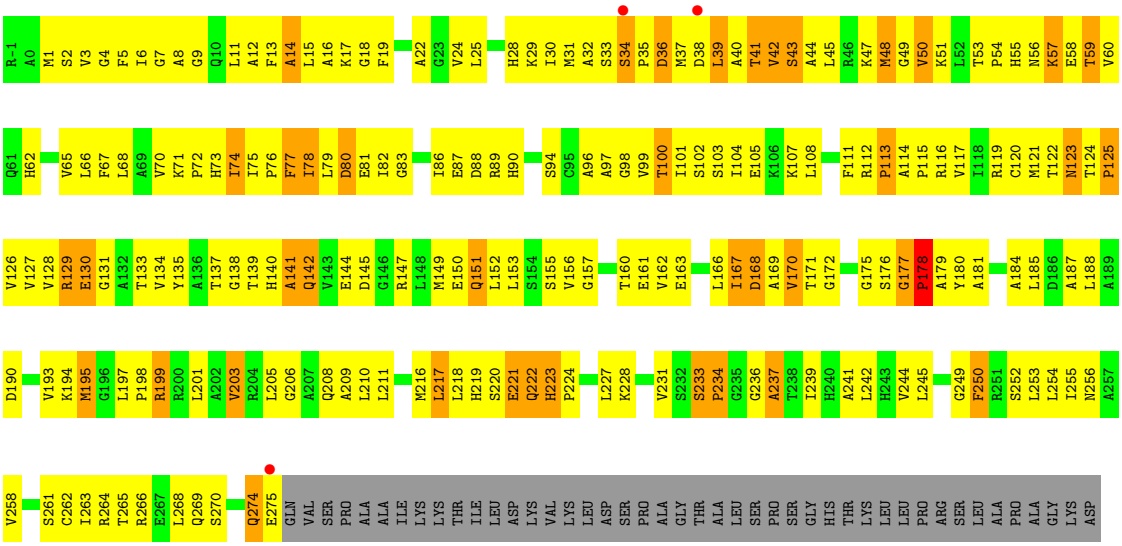




- Molecule 1: Pyrroline-5-carboxylate reductase 1

Chain E:


%
22%
51%
12%
14%


R-1 A0 M1 S2 V3 G4 F5 I6 G7 A8 G9 Q10 L11 A12 F13 A14 L15 A16 K17 G18 F19 A22 G23 V24 L25 H28 K29 I30 M31 A32 S33 S34 P35 D36 M37 D38 L39 A40 T41 V42 S43 A44 L45 R46 K47 M48 G49 V50 K51 L52 T53 P54 H55 N56 K57 E58 T59 V60
Q61 H62 V65 L66 F67 L68 A69 V70 K71 P72 H73 I74 I75 P76 F77 I78 L79 D80 E81 I82 G83 I86 E87 D88 R89 H90 S94 C95 A96 A97 G98 V99 T100 I101 S102 S103 I104 E105 K106 K107 L108 F111 R112 P113 A114 P115 R116 V117 I118 R119 C120 M121 T122 N123 T124 P125
V126 V127 V128 R129 E130 G131 A132 T133 V134 Y135 A136 T137 G138 T139 H140 A141 Q142 V143 E144 D145 G146 R147 L148 M149 E150 Q151 L152 L153 S154 S155 V156 G157 T160 E161 V162 E163 L166 I167 D168 A169 V170 T171 G172 G175 S176 G177 P178 A179 Y180 A181 A184 L185 D186 A187 L188 A189
D190 V193 K194 M195 G196 L197 P198 R199 R200 L201 A202 V203 R204 L205 G206 A207 Q208 A209 L210 L211 M216 L217 L218 H219 S220 E221 Q222 H223 P224 L227 K228 V231 S232 S233 P234 G235 G236 A237 T238 I239 H240 A241 L242 H243 V244 L245 G249 F250 R251 S252 L253 L254 I255 N256 A257
V258 S261 C262 I263 R264 T265 R266 E267 L268 Q269 S270 Q274 E275 GLN VAL SER PRO ALA ALA ILE LYS LYS THR ILE LEU ASP LYS VAL LYS LEU ASP SER PRO ALA GLY THR ALA LEU SER PRO SER GLY HIS THR LYS LEU LEU PRO ARG SER LEU ALA PRO ALA GLY LYS ASP

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	3.82 (at 3.11Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.233 , 0.261 0.221 , 0.215	Depositor DCC
R_{free} test set	2346 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	67.3	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 123.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
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
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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.68	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(^{o})	Ideal(^{o})
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 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	2038	0	2082	320	0
1	B	2025	0	2063	352	0
1	C	2032	0	2071	359	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 79.

All (1614) 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:D:239:ILE:HD12	1:D:239:ILE:H	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:A:86:ILE:HD12	1:A:108:LEU:HD11	1.35	1.06
1:B:74:ILE:HA	1:B:78:ILE:HD12	1.06	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	Interatomic distance (Å)	Clash overlap (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:HD12	1:A:91:ILE:H	1.34	0.93
1:D:122:THR:CG2	1:D:133:THR:HB	2.00	0.91
1:D:239:ILE:HD12	1:D:239:ILE:N	1.86	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:A:121:MET:HG2	1:A:171:THR:HG23	1.55	0.88
1:B:160:THR:HG22	1:B:161:GLU:N	1.87	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:HG12	1:C:258:VAL:O	1.75	0.86
1:C:252:SER:O	1:C:254:LEU:N	2.08	0.86
1:B:243:HIS:HB3	2:B:400:HOH:O	1.75	0.86
1:E:220:SER:HB2	1:E:222:GLN:HG2	1.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:LEU:HD21	1:B:210:LEU:HD12	1.58	0.85
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:D:162:VAL:HG13	1:D:166:LEU:HD12	1.60	0.82
1:E:101:ILE:HD11	1:E:138:GLY:CA	2.09	0.82
1:A:124:THR:O	1:A:127:VAL:HG23	1.79	0.82
1:A:88:ASP:CB	1:A:112:ARG:HH21	1.92	0.82
1:D:170:VAL:HG12	1:D:170:VAL:O	1.76	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: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:122:THR:HG22	1:C:133:THR:HB	1.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:H	1:C:71:LYS:HD3	1.48	0.78
1:A:123:ASN:H	1:A:123:ASN:HD22	1.31	0.78
1:A:239:ILE:HD11	1:C:190:ASP:O	1.83	0.78
1:E:53:THR:HG21	1:E:58:GLU:HB2	1.66	0.78
1:D:32:ALA:HB3	1:D:52:LEU:CD2	2.13	0.78
1:C:201:LEU:HA	2:C:337:HOH:O	1.83	0.78
1:D:67:PHE:C	1:D:68:LEU:HD23	2.04	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:HD23	1:E:25:LEU:H	1.49	0.77
1:B:82:ILE:HG22	1:B:86:ILE:HD11	1.65	0.77
1:B:8:ALA:HA	1:B:12:ALA:CB	2.13	0.77
1:B:78:ILE:O	1:B:82:ILE:HG13	1.84	0.77
1:C:101:ILE:O	1:C:105:GLU:HG3	1.85	0.77
1:D:30:ILE:HB	1:D:50:VAL:HG22	1.67	0.77
1:A:166:LEU:O	1:A:170:VAL:HG23	1.83	0.77
1:D:166:LEU:O	1:D:168:ASP:N	2.18	0.77
1:A:239:ILE:HG21	2:C:344:HOH:O	1.84	0.77
1:E:123:ASN:O	1:E:126:VAL:HG23	1.83	0.77
1:A:115:PRO:O	1:A:140:HIS:HB2	1.85	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: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:6:ILE:H	1:C:66:LEU:HD21	1.51	0.76
1:C:79:LEU:HD22	1:C:108:LEU:HD11	1.66	0.76
1:A:3:VAL:HG12	1:A:4:GLY:N	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:LEU:O	1:A:205:LEU:HG	1.86	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
1:B:264:ARG:O	1:B:268:LEU:HG	1.86	0.75
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:C:202:ALA:HB2	2:C:371:HOH:O	1.85	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: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:A:225:GLY:O	1:A:228:LYS:HB3	1.87	0.74
1:B:259:GLU:N	2:B:336:HOH:O	2.19	0.74
1:C:75:ILE:CD1	1:C:99:VAL:HG21	2.14	0.74
1:B:29:LYS:C	1:B:30:ILE:HG13	2.08	0.74
1:B:142:GLN:HG2	1:B:143:VAL:N	2.01	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:A:253:LEU:C	2:A:390:HOH:O	2.26	0.73
1:B:9:GLY:H	1:B:12:ALA:CB	1.96	0.73
1:E:55:HIS:HB3	1:E:57:LYS:HG2	1.70	0.73
1:A:107:LYS:HB3	2:A:357:HOH:O	1.89	0.73
1:C:114:ALA:HB1	1:C:140:HIS:ND1	2.04	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:A:14:ALA:HA	1:A:127:VAL:HG22	1.69	0.73
1:B:200:ARG:O	1:B:204:ARG:HG2	1.89	0.73
1:E:195:MET:HA	1:E:195:MET:CE	2.19	0.73
1:B:93:VAL:HA	1:B:118:ILE:O	1.87	0.73
1:E:55:HIS:HB3	1:E:57:LYS:HE2	1.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:91:ILE:HD12	1:A:91:ILE:N	2.06	0.71
1:A:121:MET:HG2	1:A:171:THR:CG2	2.21	0.71
1:A:43:SER:HA	1:A:46:ARG:HG3	1.72	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:C:121:MET:HE3	2:C:370:HOH:O	1.91	0.71
1:E:83:GLY:HA2	1:E:86:ILE:CD1	2.19	0.71
1:B:29:LYS:HD3	2:B:333:HOH:O	1.89	0.71
1:B:198:PRO:HG2	1:B:201:LEU:HB3	1.71	0.71
1:C:124:THR:N	1:C:125:PRO:HD2	2.05	0.71
1:E:169:ALA:O	1:E:171:THR:N	2.24	0.71
1:B:124:THR:O	1:B:127:VAL:HG23	1.90	0.71
1:C:185:LEU:HD21	1:C:210:LEU:HD12	1.70	0.71
1:C:249:GLY:O	1:C:253:LEU:HD13	1.91	0.71
1:E:72:PRO:HG3	1:E:96:ALA:HB1	1.73	0.71
1:A:26:ALA:HB3	1:A:29:LYS:HE2	1.70	0.71
1:C:51:LYS:H	1:C:51:LYS:HD3	1.55	0.71
1:A:211:LEU:HB2	2:A:328: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:170:VAL:HG23	2:D:393:HOH:O	1.90	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:A:196:GLY:O	1:E:234:PRO:HB3	1.90	0.70
1:C:269:GLN:HG3	1:C:270:SER:H	1.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:THR:HG22	1:C:55:HIS:H	1.57	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
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:B:105:GLU:OE2	1:B:139:THR:HB	1.92	0.69
1:D:122:THR:HG23	1:D:133:THR:CB	2.21	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:4:GLY:O	1:C:66:LEU:HG	1.92	0.69
1:C:101:ILE:HB	1:C:164:GLU:OE1	1.92	0.69
1:C:177:GLY:HA2	1:C:180:TYR:CD1	2.28	0.69
1:B:33:SER:HB2	1:B:59:THR:OG1	1.92	0.69
1:E:77:PHE:HD1	1:E:77:PHE:H	1.40	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:D:6:ILE:N	2:D:344:HOH:O	2.26	0.69
1:E:3:VAL:HG13	1:E:65:VAL:O	1.92	0.69
1:A:3:VAL:HG13	1:A:65:VAL:O	1.93	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:5:PHE:HE2	1:C:15:LEU:HD12	1.58	0.69
1:D:7:GLY:H	1:D:33:SER:HB2	1.57	0.69
1:B:123:ASN:HB2	1:B:125:PRO:HD2	1.75	0.69
1:B:222:GLN:O	1:B:223:HIS:HB2	1.92	0.69
1:C:82:ILE:O	1:C:86:ILE:HG13	1.93	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:A:222:GLN:HB3	2:A:340:HOH:O	1.93	0.69
1:E:57:LYS:H	1:E:57:LYS:HD3	1.58	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:A:190:ASP:OD1	1:A:199:ARG:NH1	2.26	0.68
1:D:79:LEU:HD21	1:D:104:ILE:HA	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:ARG:NH1	1:B:204:ARG:HH21	1.89	0.68
1:B:258:VAL:HG13	1:B:259:GLU:N	2.09	0.68
1:C:271:MET:HA	1:C:274:GLN:HB3	1.76	0.68
1:E:53:THR:HG22	1:E:55:HIS: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
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: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:238:THR:HB	1:D:239:ILE:HD12	1.76	0.67
1:A:266:ARG:HG2	1:A:266:ARG:HH11	1.60	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:D:118:ILE:HG22	1:D:137:THR:HA	1.76	0.67
1:E:220:SER:CB	1:E:222:GLN:HG2	2.24	0.67
1:C:35:PRO:O	1:C:36:ASP:HB2	1.95	0.67
1:B:221:GLU:O	1:B:223:HIS:N	2.27	0.67
1:D:171:THR:HB	2:D:364:HOH:O	1.95	0.67
1:A:141:ALA:HA	2:A:350:HOH:O	1.95	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: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:198:PRO:HG2	1:E:201:LEU:HB3	1.77	0.67
1:E:266:ARG:HD2	2:E:388:HOH:O	1.94	0.67
1:E:17:LYS:HB2	2:E:412:HOH:O	1.95	0.67
1:E:68:LEU:HA	2:E:322: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:C:41:THR:O	1:C:45:LEU:HB2	1.95	0.66
1:C:173:LEU:HD12	1:C:258:VAL:HG21	1.77	0.66
1:E:3:VAL:HG12	1:E:4:GLY:N	2.08	0.66
1:A:160:THR:HG22	1:A:161:GLU:O	1.95	0.66
1:A:270:SER:HA	1:A:273:ASP:OD2	1.96	0.66
1:B:101:ILE:HD12	1:B:138:GLY:HA2	1.78	0.66
1:C:134:VAL:HG11	1:C:162:VAL:HG22	1.77	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:7:GLY:HA2	1:C:70:VAL:HG22	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:LYS:C	1:C:30:ILE:HG13	2.15	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:HA	1:E:195:MET:HE2	1.76	0.66
1:A:86:ILE:HD12	1:A:108:LEU:CD1	2.20	0.66
1:B:105:GLU:HG2	1:B:139:THR:OG1	1.94	0.66
1:E:86:ILE:CD1	1:E:108:LEU:HD22	2.25	0.66
1:D:15:LEU:HG	1:D:126:VAL:HG11	1.77	0.66
1:B:67:PHE:CD2	1:B:93:VAL:HB	2.31	0.66
1:C:166:LEU:O	1:C:169:ALA:N	2.29	0.66
1:E:39:LEU:HD23	1:E:39:LEU:H	1.61	0.66
1:A:156:VAL:HG12	1:A:156:VAL:O	1.95	0.66
1:B:185:LEU:HD21	1:B:210:LEU:CD1	2.26	0.66
1:A:252:SER:O	1:A:254:LEU:N	2.29	0.65
1:B:108:LEU:HB2	2:B:331:HOH:O	1.94	0.65
1:C:108:LEU:HB2	2:C:377:HOH:O	1.96	0.65
1:B:198:PRO:HD2	1:B:201:LEU:HD23	1.78	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:D:105:GLU:O	1:D:107:LYS:N	2.21	0.65
1:E:179:ALA:HB1	2:E:333:HOH:O	1.96	0.65
1:B:9:GLY:N	1:B:12:ALA:HB3	2.02	0.65
1:C:71:LYS:HE2	1:C:73:HIS:HE1	1.61	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:B:236:GLY:O	1:B:238:THR:N	2.29	0.65
1:D:68:LEU:HD23	1:D:68:LEU:N	2.07	0.65
1:E:75:ILE:HG21	1:E:104:ILE:HD11	1.78	0.65
1:A:61:GLN:O	1:A:89:ARG:NH2	2.30	0.65
1:B:22:ALA:HB2	2:B:323:HOH:O	1.97	0.65
1:C:199:ARG:HD3	2:C:349:HOH:O	1.96	0.65
1:E:197:LEU:HD23	1:E:201:LEU:HD23	1.78	0.65
1:B:122:THR:HG22	1:B:133:THR:CB	2.27	0.65
1:D:124:THR:HG23	2:D:425:HOH:O	1.97	0.65
1:B:176:SER:HB2	2:B:341:HOH:O	1.97	0.65
1:C:198:PRO:HG2	1:C:201:LEU:HB3	1.79	0.65
1:D:53:THR:HG22	1:D:55:HIS:H	1.61	0.65
1:D:271:MET:HE2	2:D:395:HOH:O	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:124:THR:N	1:E:125:PRO:HD2	2.12	0.65
1:A:3:VAL:HG22	2:A:365:HOH:O	1.97	0.65
1:B:256:ASN:C	2:B:336:HOH:O	2.35	0.65
1:C:221:GLU:OE2	1:C:221:GLU:HA	1.97	0.65
1:D:13:PHE:HZ	1:D:17:LYS:HZ1	1.44	0.65
1:E:3:VAL:CG1	1:E:4:GLY:N	2.59	0.65
1:E:220:SER:O	1:E:221:GLU:HB2	1.97	0.65
1:A:128:VAL:HB	2:A:331:HOH:O	1.96	0.64
1:C:3:VAL:HB	1:C:30:ILE:HG12	1.79	0.64
1:C:100:THR:HB	1:C:103:SER:HB2	1.78	0.64
1:E:172:GLY:HA2	1:E:261:SER:CB	2.26	0.64
1:A:65:VAL:HG22	1:A:91:ILE:HD13	1.79	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: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:HD12	1:C:152:LEU:O	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: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:C:269:GLN:HG3	1:C:270:SER:N	2.13	0.63
1:A:123:ASN:ND2	1:A:123:ASN:H	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:A:33:SER:O	1:A:35:PRO:HD3	1.98	0.63
1:A:126:VAL:HG13	1:A:156:VAL:HG11	1.79	0.63
1:B:143:VAL:HG12	1:B:144:GLU:N	2.11	0.63
1:E:3:VAL:O	1:E:30:ILE:HA	1.98	0.63
1:A:68:LEU:HB2	1:A:94:SER:HA	1.79	0.63
1:B:70:VAL:HG12	1:B:71:LYS:N	2.13	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:C:65:VAL:HG23	1:C:91:ILE:O	1.98	0.63
1:D:39:LEU:O	1:D:43:SER:HB3	1.98	0.63
1:E:222:GLN:O	1:E:223:HIS:HB3	1.98	0.63
1:A:269:GLN:HG2	1:A:270:SER:N	2.13	0.63
1:B:125:PRO:HG2	1:B:131:GLY:HA2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:45:LEU:HD21	2:A:333:HOH:O	1.99	0.63
1:A:86:ILE:CD1	1:A:108:LEU:HD11	2.20	0.63
1:B:15:LEU:HB3	1:B:19:PHE:CZ	2.33	0.63
1:D:114:ALA:HB1	1:D:140:HIS:CG	2.34	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
1:D:231:VAL:HG12	2:D:357:HOH:O	1.99	0.63
1:E:101:ILE:CG2	1:E:102:SER:N	2.62	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:C:79:LEU:HD11	1:C:104:ILE:HG13	1.81	0.63
1:E:56:ASN:O	1:E:60:VAL:HG23	1.97	0.63
1:E:79:LEU:O	1:E:81:GLU:N	2.28	0.63
1:A:198:PRO:HG2	1:A:201:LEU:CB	2.29	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:HG12	1:E:128:VAL:O	1.99	0.62
1:E:217:LEU:C	1:E:219:HIS:H	2.01	0.62
1:A:20:THR:HG21	1:A:48:MET:HE2	1.81	0.62
1:D:189:ALA:O	1:D:193:VAL:HG23	1.99	0.62
1:D:239:ILE:N	2:D:435:HOH:O	2.32	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:25:LEU:HD23	1:E:25:LEU:N	2.12	0.62
1:E:128:VAL:O	1:E:129:ARG:HB3	1.99	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:A:15:LEU:HD23	1:A:126:VAL:HG11	1.82	0.62
1:B:198:PRO:HG2	1:B:201:LEU:CB	2.28	0.62
1:C:6:ILE:HG13	1:C:66:LEU:HD11	1.80	0.62
1:D:143:VAL:HB	2:D:349:HOH:O	2.00	0.62
1:D:170:VAL:O	1:D:170:VAL:CG1	2.46	0.62
1:A:198:PRO:HG2	1:A:201:LEU:HB3	1.81	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:E:47:LYS:HG3	2:E:350:HOH:O	1.98	0.62
1:E:75:ILE:HA	1:E:78:ILE:CD1	2.26	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:96:ALA:HB2	2:E:362: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:B:165:ASP:OD1	1:B:166:LEU:N	2.32	0.62
1:E:6:ILE:HD12	1:E:68:LEU:HD21	1.81	0.62
1:A:223:HIS:ND1	1:A:224:PRO:HD2	2.14	0.61
1:B:74:ILE:O	1:B:78:ILE:HB	1.99	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
1:E:227:LEU:O	1:E:231:VAL:HG23	2.00	0.61
1:A:129:ARG:O	1:A:129:ARG:HG2	2.00	0.61
1:E:68:LEU:HB2	1:E:94:SER:CA	2.29	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:A:184:ALA:O	1:A:187:ALA:HB3	1.99	0.61
1:C:3:VAL:HG12	1:C:4:GLY:N	2.16	0.61
1:C:3:VAL:HG13	1:C:65:VAL:O	2.00	0.61
1:E:129:ARG:O	1:E:131:GLY:N	2.34	0.61
1:B:70:VAL:HG22	2:B:364:HOH:O	2.01	0.61
1:C:69:ALA:HB2	2:C:412:HOH:O	2.00	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: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:A:109:SER:C	1:A:111:PHE:H	2.05	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:C:160:THR:HG22	1:C:161:GLU:N	2.16	0.60
1:D:269:GLN:C	1:D:271:MET:H	2.04	0.60
1:A:89:ARG:HG3	1:A:90:HIS:N	2.16	0.60
1:B:225:GLY:O	1:B:228:LYS:HB3	2.01	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:D:215:LYS:HG3	1:D:219:HIS:CE1	2.36	0.60
1:E:121:MET:HE3	1:E:121:MET:HA	1.83	0.60
1:E:129:ARG:HG2	1:E:130:GLU:H	1.66	0.60
1:B:211:LEU:HD12	1:B:211:LEU:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:45:LEU:O	1:E:49:GLY:O	2.18	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: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: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: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
1:C:115:PRO:HD2	2:C:379:HOH:O	2.02	0.60
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:44:ALA:HB3	2:D:413:HOH:O	2.02	0.60
1:D:263:ILE:O	1:D:267:GLU:HG3	2.00	0.60
1:A:77:PHE:N	1:A:77:PHE:CD1	2.70	0.59
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:D:202:ALA:HB1	2:D:350:HOH:O	2.02	0.59
1:B:152:LEU:HD12	1:B:152:LEU:O	2.03	0.59
1:C:87:GLU:H	1:C:90:HIS:HE1	1.49	0.59
1:C:105:GLU:HB2	2:C:366:HOH:O	2.01	0.59
1:D:126:VAL:HG13	1:D:156:VAL:HG11	1.84	0.59
1:E:79:LEU:HD11	1:E:104:ILE:HG12	1.82	0.59
1:E:134:VAL:CG1	1:E:162:VAL:HB	2.32	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:D:59:THR:O	1:D:62:HIS:N	2.33	0.59
1:A:221:GLU:O	1:A:223:HIS:N	2.33	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:38:ASP:O	1:A:39:LEU:C	2.40	0.59
1:A:222:GLN:O	1:A:223:HIS:CB	2.49	0.59
1:B:48:MET:O	1:B:50:VAL:HG23	2.03	0.59
1:D:109:SER:C	1:D:111:PHE:H	2.05	0.59
1:E:223:HIS:ND1	1:E:224:PRO:HD2	2.18	0.59
1:C:128:VAL:HG23	2:C:417:HOH:O	2.03	0.59
1:E:68:LEU:N	2:E:358:HOH:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:171:THR:HB	2:C:360:HOH:O	2.02	0.59
1:C:231:VAL:HG12	1:C:231:VAL:O	2.03	0.59
1:D:60:VAL:HG21	1:D:82:ILE:HD13	1.85	0.59
1:E:59:THR:O	1:E:62:HIS:HB3	2.03	0.59
1:A:194:LYS:O	1:A:195:MET:SD	2.61	0.59
1:A:194:LYS:HG2	1:E:239:ILE:HG23	1.85	0.59
1:D:197:LEU:HD22	1:D:201:LEU:HD23	1.84	0.59
1:C:127:VAL:HG12	1:C:127:VAL:O	2.03	0.59
1:C:147:ARG:O	1:C:151:GLN:HG3	2.03	0.59
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:B:189:ALA:HB2	1:B:203:VAL:HA	1.85	0.58
1:E:122:THR:HG22	1:E:133:THR:CG2	2.33	0.58
1:B:71:LYS:HB3	1:B:72:PRO:CD	2.31	0.58
1:A:64:ASP:O	1:A:90:HIS:HB3	2.03	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:57:LYS:HA	1:A:60:VAL:HG23	1.84	0.58
1:A:77:PHE:N	1:A:77:PHE:HD1	2.00	0.58
1:C:28:HIS:ND1	1:C:51:LYS:HE3	2.17	0.58
1:C:155:SER:HB3	2:C:358:HOH:O	2.02	0.58
1:C:236:GLY:O	1:C:237:ALA:HB3	2.03	0.58
1:D:258:VAL:CG1	1:D:259:GLU:N	2.65	0.58
1:E:187:ALA:HB3	2:E:402:HOH:O	2.03	0.58
1:D:117:VAL:O	1:D:138:GLY:HA3	2.04	0.58
1:E:111:PHE:HB3	2:E:386:HOH:O	2.04	0.58
1:A:121:MET:CE	1:A:171:THR:HG22	2.33	0.58
1:B:41:THR:HA	1:B:44:ALA:HB3	1.85	0.58
1:B:83:GLY:HA3	1:B:111:PHE:CD2	2.38	0.58
1:E:80:ASP:HA	2:E:327:HOH:O	2.03	0.58
1:A:122:THR:CG2	1:A:123:ASN:N	2.66	0.58
1:B:8:ALA:HA	1:B:12:ALA:HB2	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ILE:HG22	1:A:105:GLU:HG3	1.85	0.58
1:A:152:LEU:O	1:A:155:SER:HB3	2.03	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: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:C:86:ILE:HD11	1:C:108:LEU:CD2	2.22	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:A:37:MET:HA	1:A:42:VAL:HG21	1.85	0.57
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:68:LEU:HD12	1:E:94:SER:HB2	1.85	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:E:180:TYR:O	2:E:372:HOH:O	2.17	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:A:55:HIS:C	1:A:57:LYS:H	2.07	0.57
1:B:45:LEU:O	1:B:48:MET:HB2	2.05	0.57
1:B:258:VAL:CG1	1:B:259:GLU:N	2.68	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: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:B:227:LEU:O	1:B:231:VAL:HG23	2.05	0.57
1:C:31:MET:HB2	1:C:62:HIS:CE1	2.39	0.57
1:D:115:PRO:O	1:D:140:HIS:HB2	2.05	0.57
1:D:118:ILE:CG2	1:D:137:THR:HA	2.34	0.57
1:D:129:ARG:CD	1:D:155:SER:O	2.51	0.57
1:D:146:GLY:O	1:D:149:MET:HB3	2.04	0.57
1:E:45:LEU:HA	1:E:48:MET:HE3	1.85	0.57
1:E:101:ILE:HG23	1:E:102:SER:N	2.19	0.57
1:E:233:SER:HB2	2:E:320:HOH:O	2.03	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:A:238:THR:N	2:A:369:HOH:O	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:LYS:HG3	1:B:58:GLU:N	2.20	0.56
1:B:186:ASP:HA	2:B:358:HOH:O	2.03	0.56
1:D:156:VAL:HG12	1:D:156:VAL:O	2.05	0.56
1:B:63:SER:HB2	1:B:89:ARG:NH1	2.13	0.56
1:C:127:VAL:HA	2:C:418:HOH:O	2.05	0.56
1:D:146:GLY:O	1:D:149:MET:N	2.38	0.56
1:E:35:PRO:HG2	2:E:401:HOH:O	2.05	0.56
1:E:119:ARG:HA	2:E:445:HOH:O	2.04	0.56
1:A:93:VAL:HG22	1:A:118:ILE:HD11	1.88	0.56
1:A:146:GLY:O	1:A:150:GLU:HB2	2.05	0.56
1:A:242:LEU:O	1:A:243:HIS:C	2.44	0.56
1:A:253:LEU:HD23	1:A:253:LEU:N	2.18	0.56
1:B:11:LEU:HA	1:B:14:ALA:HB3	1.87	0.56
1:B:147:ARG:NH1	1:B:150:GLU:OE2	2.38	0.56
1:B:185:LEU:O	1:B:186:ASP:C	2.43	0.56
1:C:135:TYR:HE1	1:C:161:GLU:HB3	1.68	0.56
1:D:6:ILE:HG13	1:D:66:LEU:HD11	1.86	0.56
1:E:14:ALA:HB2	2:E:324:HOH:O	2.04	0.56
1:E:19:PHE:O	1:E:24:VAL:HG23	2.04	0.56
1:E:134:VAL:HG13	1:E:162:VAL:HB	1.86	0.56
1:E:264:ARG:CZ	1:E:268:LEU:HD21	2.35	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:D:211:LEU:HD12	1:D:211:LEU:C	2.25	0.56
1:E:121:MET:HE2	1:E:122:THR:H	1.71	0.56
1:B:60:VAL:HG12	1:B:89:ARG:HH22	1.71	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:D:57:LYS:O	1:D:61:GLN:HG3	2.06	0.56
1:E:38:ASP:O	1:E:42:VAL:HB	2.05	0.56
1:E:126:VAL:O	1:E:156:VAL:HG12	2.05	0.56
1:E:222:GLN:O	1:E:223:HIS:CB	2.53	0.56
1:E:236:GLY:O	1:E:237:ALA:HB3	2.05	0.56
1:A:122:THR:HG22	1:A:123:ASN:N	2.20	0.56
1:B:74:ILE:HG23	1:B:78:ILE:HG21	1.86	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:211:LEU:HD12	1:B:211:LEU:C	2.26	0.56
1:B:216:MET:HA	2:B:372:HOH:O	2.05	0.56
1:C:124:THR:O	1:C:127:VAL:HG23	2.05	0.56
1:E:129:ARG:HG3	1:E:157:GLY:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG22	1:A:82:ILE:O	2.05	0.56
1:A:40:ALA:O	1:A:44:ALA:HB2	2.06	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:239:ILE:N	2:B:338:HOH:O	2.38	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: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:D:232:SER:HB3	1:D:239:ILE:CG1	2.36	0.56
1:C:45:LEU:CD2	1:C:50:VAL:HB	2.36	0.55
1:A:82:ILE:HG23	1:A:85:ASP:HB2	1.88	0.55
1:B:37:MET:HE3	2:B:355:HOH:O	2.06	0.55
1:C:25:LEU:HD21	1:C:30:ILE:HD11	1.88	0.55
1:C:152:LEU:HD12	1:C:152:LEU:C	2.26	0.55
1:C:162:VAL:HB	1:C:166:LEU:HD12	1.87	0.55
1:E:6:ILE:HD12	1:E:68:LEU:CD2	2.36	0.55
1:D:34:SER:HB2	1:D:36:ASP:O	2.07	0.55
1:E:188:LEU:N	2:E:402:HOH:O	2.39	0.55
1:A:228:LYS:HZ1	1:C:199:ARG:HH12	1.53	0.55
1:B:123:ASN:O	1:B:126:VAL:HG23	2.07	0.55
1:D:33:SER:O	1:D:35:PRO:HD2	2.06	0.55
1:A:33:SER:CB	1:A:56:ASN:HB3	2.36	0.55
1:A:101:ILE:O	1:A:102:SER:C	2.44	0.55
1:C:31:MET:HB3	1:C:59:THR:CG2	2.32	0.55
1:D:128:VAL:O	1:D:129:ARG:CB	2.53	0.55
1:E:14:ALA:HB1	2:E:376:HOH:O	2.06	0.55
1:A:119:ARG:HD3	1:A:164:GLU:HG3	1.87	0.55
1:B:37:MET:SD	1:B:46:ARG:NH2	2.73	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:C:123:ASN:O	1:C:126:VAL:HG13	2.07	0.55
1:E:75:ILE:CA	1:E:78:ILE:HD12	2.29	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: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:E:126:VAL:HG22	1:E:131:GLY:HA3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:LYS:HE2	1:D:85:ASP:OD2	2.07	0.55
1:B:139:THR:HG22	1:B:139:THR:O	2.07	0.55
1:B:239:ILE:HG21	2:E:363:HOH:O	2.05	0.55
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:C:88:ASP:N	2:C:352: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:B:123:ASN:CB	1:B:125:PRO:HD2	2.37	0.54
1:C:83:GLY:HA2	1:C:86:ILE:CD1	2.37	0.54
1:D:89:ARG:NH2	2:D:370:HOH:O	2.40	0.54
1:E:6:ILE:O	1:E:70:VAL:HG22	2.07	0.54
1:A:126:VAL:O	1:A:128:VAL:N	2.40	0.54
1:C:11:LEU:CD1	1:C:124:THR:HA	2.37	0.54
1:D:217:LEU:HD12	1:D:217:LEU:O	2.07	0.54
1:E:137:THR:HG23	2:E:330:HOH:O	2.05	0.54
1:C:15:LEU:O	1:C:19:PHE:CD1	2.61	0.54
1:C:109:SER:HA	1:C:115:PRO:CD	2.37	0.54
1:C:119:ARG:HG3	2:C:351:HOH:O	2.08	0.54
1:D:125:PRO:O	1:D:128:VAL:HG12	2.07	0.54
1:E:97:ALA:HB1	1:E:265:THR:HG23	1.89	0.54
1:E:205:LEU:HD23	2:E:408:HOH:O	2.08	0.54
1:A:88:ASP:HB2	1:A:112:ARG:NH2	2.22	0.54
1:A:149:MET:HA	1:A:149:MET:CE	2.37	0.54
1:B:180:TYR:N	1:B:180:TYR:CD2	2.75	0.54
1:B:239:ILE:HD11	1:E:190:ASP:O	2.08	0.54
1:B:241:ALA:O	1:B:242:LEU:C	2.44	0.54
1:C:78:ILE:HD11	2:C:380:HOH:O	2.07	0.54
1:C:194:LYS:HA	2:C:344:HOH:O	2.08	0.54
1:C:255:ILE:C	1:C:257:ALA:H	2.11	0.54
1:D:26:ALA:HB3	1:D:28:HIS:CD2	2.42	0.54
1:D:241:ALA:O	1:D:244:VAL:N	2.38	0.54
1:E:1:MET:HG2	1:E:2:SER:N	2.23	0.54
1:A:30:ILE:HG22	1:A:31:MET:N	2.23	0.54
1:C:236:GLY:HA3	1:C:240:HIS:HD2	1.73	0.54
1:D:227:LEU:HB2	2:D:419:HOH:O	2.08	0.54
1:A:112:ARG:HG3	2:A:407:HOH:O	2.08	0.54
1:B:75:ILE:CD1	1:B:272:ALA:HA	2.38	0.54
1:C:65:VAL:O	1:C:65:VAL:HG13	2.08	0.54
1:C:252:SER:HB3	2:C:321:HOH:O	2.07	0.54
1:C:262:CYS:HA	2:C:360:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:LYS:HB3	2:D:329:HOH:O	2.07	0.54
1:E:55:HIS:CB	1:E:57:LYS:HE2	2.34	0.54
1:E:126:VAL:N	2:E:325:HOH:O	2.41	0.54
1:D:143:VAL:C	1:D:145:ASP:H	2.10	0.54
1:D:226:GLN:O	1:D:229:ASP:HB2	2.08	0.54
1:B:12:ALA:O	1:B:16:ALA:HB2	2.08	0.54
1:B:105:GLU:HG2	2:B:417:HOH:O	2.08	0.54
1:C:266:ARG:HA	2:C:323:HOH:O	2.08	0.54
1:D:6:ILE:HG21	1:D:78:ILE:HG21	1.88	0.54
1:E:80:ASP:OD2	1:E:107:LYS:NZ	2.35	0.54
1:E:217:LEU:O	1:E:219:HIS:N	2.40	0.54
1:A:68:LEU:HD12	1:A:94:SER:HB2	1.90	0.53
1:B:126:VAL:HA	2:B:328:HOH:O	2.08	0.53
1:C:78:ILE:O	1:C:82:ILE:HG13	2.07	0.53
1:C:129:ARG:O	1:C:129:ARG:HG2	2.08	0.53
1:D:98:GLY:HA2	2:D:336:HOH:O	2.07	0.53
1:E:102:SER:O	1:E:103:SER:C	2.43	0.53
1:A:88:ASP:CB	1:A:112:ARG:NH2	2.68	0.53
1:A:88:ASP:HB2	1:A:112:ARG:HE	1.73	0.53
1:A:123:ASN:HD22	1:A:123:ASN:N	1.94	0.53
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:D:210:LEU:O	1:D:211:LEU:C	2.46	0.53
1:D:265:THR:HG22	2:D:377:HOH:O	2.07	0.53
1:E:11:LEU:O	1:E:15:LEU:HD12	2.07	0.53
1:E:13:PHE:O	1:E:16:ALA:HB3	2.09	0.53
1:E:86:ILE:O	1:E:112:ARG:HD3	2.08	0.53
1:A:226:GLN:HB3	2:A:340:HOH:O	2.08	0.53
1:C:104:ILE:HG22	1:C:117:VAL:HG21	1.90	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:D:30:ILE:HB	1:D:50:VAL:CG2	2.38	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:B:17:LYS:C	1:B:20:THR:HG23	2.28	0.53
1:D:82:ILE:HG23	1:D:85:ASP:HB2	1.89	0.53
1:D:98:GLY:HA3	1:D:269:GLN:CB	2.37	0.53
1:D:222:GLN:O	1:D:223:HIS:HB3	2.08	0.53
1:E:55:HIS:HB3	1:E:57:LYS:CG	2.37	0.53
1:E:253:LEU:O	1:E:256:ASN:HB2	2.08	0.53
1:B:75:ILE:HD11	1:B:272:ALA:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:ILE:HG22	1:B:255:ILE:O	2.09	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: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:A:124:THR:N	1:A:125:PRO:HD2	2.24	0.53
1:A:167:ILE:O	1:A:167:ILE:HG22	2.09	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: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:C:34:SER:O	1:C:36:ASP:N	2.41	0.53
1:D:236:GLY:C	2:D:435:HOH:O	2.47	0.53
1:E:113:PRO:HD2	2:E:342:HOH:O	2.07	0.53
1:A:193:VAL:HG13	1:E:234:PRO:HA	1.91	0.53
1:B:257:ALA:HA	2:B:418:HOH:O	2.08	0.53
1:C:33:SER:HA	1:C:53:THR:O	2.09	0.53
1:D:13:PHE:CZ	1:D:17:LYS:NZ	2.77	0.53
1:B:176:SER:O	1:B:177:GLY:C	2.47	0.53
1:C:51:LYS:HD3	1:C:51:LYS:N	2.23	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:D:77:PHE:HD1	1:D:77:PHE:N	2.06	0.53
1:E:117:VAL:O	1:E:138:GLY:HA3	2.09	0.53
1:B:2:SER:OG	1:B:30:ILE:HA	2.09	0.53
1:E:75:ILE:CG2	1:E:104:ILE:HD11	2.38	0.53
1:A:185:LEU:N	1:A:185:LEU:HD23	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:E:28:HIS:HB3	2:E:407:HOH:O	2.09	0.52
1:B:143:VAL:C	1:B:145:ASP:H	2.11	0.52
1:C:61:GLN:N	1:C:61:GLN:OE1	2.42	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:A:227:LEU:N	2:A:340:HOH:O	2.41	0.52
1:B:93:VAL:HG12	1:B:95:CYS:SG	2.50	0.52
1:C:3:VAL:O	1:C:30:ILE:HA	2.08	0.52
1:D:82:ILE:C	1:D:84:ALA:N	2.63	0.52
1:E:83:GLY:C	1:E:111:PHE:CD2	2.82	0.52
1:E:264:ARG:NE	1:E:268:LEU:HD21	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:VAL:HG22	1:A:118:ILE:CD1	2.39	0.52
1:B:42:VAL:C	1:B:44:ALA:H	2.12	0.52
1:B:123:ASN:HA	2:B:398:HOH:O	2.08	0.52
1:B:147:ARG:O	1:B:147:ARG:HG3	2.08	0.52
1:E:74:ILE:C	1:E:76:PRO:HD2	2.30	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:D:13:PHE:CE1	1:D:17:LYS:HE3	2.43	0.52
1:D:103:SER:HA	2:D:342:HOH:O	2.10	0.52
1:D:123:ASN:O	1:D:126:VAL:HG23	2.10	0.52
1:D:233:SER:O	1:D:235:GLY:N	2.42	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:A:75:ILE:CG2	1:A:76:PRO:HD3	2.32	0.52
1:A:79:LEU:CD1	1:A:104:ILE:HA	2.39	0.52
1:A:82:ILE:O	1:A:83:GLY:C	2.48	0.52
1:A:256:ASN:N	2:A:390:HOH:O	2.43	0.52
1:B:45:LEU:HD22	1:B:48:MET:SD	2.50	0.52
1:B:79:LEU:CD1	1:B:104:ILE:HG23	2.36	0.52
1:C:112:ARG:CG	1:C:113:PRO:HD2	2.33	0.52
1:D:77:PHE:N	1:D:77:PHE:CD1	2.77	0.52
1:E:70:VAL:O	1:E:71:LYS:HB2	2.10	0.52
1:A:121:MET:CG	1:A:171:THR:CG2	2.88	0.52
1:B:50:VAL:HB	2:B:350:HOH:O	2.08	0.52
1:B:258:VAL:HG13	1:B:259:GLU:H	1.75	0.52
1:C:160:THR:CG2	1:C:161:GLU:N	2.73	0.52
1:D:133:THR:CG2	1:D:158:PHE:O	2.58	0.52
1:A:177:GLY:O	1:A:178:PRO:C	2.47	0.52
1:A:258:VAL:HG12	1:A:259:GLU:N	2.25	0.52
1:C:124:THR:C	1:C:126:VAL:H	2.13	0.52
1:D:105:GLU:C	1:D:107:LYS:H	2.10	0.52
1:D:169:ALA:C	1:D:171:THR:N	2.56	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:3:VAL:HG12	1:C:4:GLY:H	1.75	0.52
1:C:4:GLY:HA2	1:C:30:ILE:HG23	1.92	0.52
1:C:27:ALA:HB1	1:C:50:VAL:HG22	1.92	0.52
1:C:173:LEU:CD1	1:C:258:VAL:HG21	2.40	0.52
1:E:162:VAL:CG1	1:E:166:LEU:HB2	2.39	0.52
1:D:67:PHE:CE2	1:D:93:VAL:HG21	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:166:LEU:O	1:E:167:ILE:C	2.49	0.51
1:B:70:VAL:HG11	1:B:78:ILE:CD1	2.39	0.51
1:B:101:ILE:O	1:B:105:GLU:HB2	2.10	0.51
1:C:251:ARG:C	1:C:252:SER:O	2.45	0.51
1:A:33:SER:HA	1:A:53:THR:O	2.09	0.51
1:A:269:GLN:C	1:A:271:MET:H	2.13	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:C:35:PRO:O	1:C:36:ASP:CB	2.59	0.51
1:D:183:THR:N	2:D:415:HOH:O	2.43	0.51
1:E:8:ALA:HB1	1:E:41:THR:CG2	2.41	0.51
1:A:55:HIS:HA	2:A:374:HOH:O	2.11	0.51
1:D:81:GLU:O	1:D:81:GLU:HG2	2.09	0.51
1:D:153:LEU:N	1:D:153:LEU:HD23	2.25	0.51
1:D:252:SER:O	1:D:255:ILE:N	2.43	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:B:4:GLY:HA3	1:B:66:LEU:CD2	2.40	0.51
1:B:87:GLU:C	1:B:89:ARG:H	2.13	0.51
1:D:50:VAL:HG13	1:D:51:LYS:N	2.26	0.51
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: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: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:E:264:ARG:O	1:E:268:LEU:HG	2.11	0.51
1:B:39:LEU:HA	1:B:43:SER:HB2	1.93	0.51
1:B:266:ARG:O	1:B:269:GLN:HG2	2.11	0.51
1:C:50:VAL:HG13	2:C:343:HOH:O	2.10	0.51
1:D:142:GLN:HB3	2:D:375:HOH:O	2.11	0.51
1:E:119:ARG:NE	2:E:349:HOH:O	2.44	0.51
1:A:135:TYR:OH	1:A:150:GLU:CG	2.59	0.51
1:A:176:SER:O	1:A:179:ALA:N	2.40	0.51
1:B:13:PHE:O	1:B:16:ALA:HB3	2.11	0.51
1:C:13:PHE:O	1:C:16:ALA:HB3	2.11	0.51
1:C:61:GLN:C	1:C:63:SER:H	2.14	0.51
1:C:208:GLN:HB2	2:C:354:HOH:O	2.11	0.51
1:C:258:VAL:O	1:C:258:VAL:CG1	2.47	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:233:SER:N	2:E:320:HOH:O	2.43	0.51
1:E:250:PHE:N	2:E:341:HOH:O	2.44	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:A:4:GLY:HA2	1:A:31:MET:O	2.10	0.50
1:A:6:ILE:HB	2:A:322:HOH:O	2.10	0.50
1:A:105:GLU:O	1:A:107:LYS:N	2.42	0.50
1:B:6:ILE:HB	2:B:325:HOH:O	2.11	0.50
1:E:15:LEU:HB3	1:E:19:PHE:CE1	2.46	0.50
1:E:99:VAL:HG12	1:E:99:VAL:O	2.11	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:19:PHE:CD2	1:B:152:LEU:HD11	2.47	0.50
1:B:72:PRO:HB3	1:B:97:ALA:HB2	1.92	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:42:VAL:O	1:E:43:SER:C	2.49	0.50
1:E:45:LEU:O	1:E:50:VAL:HB	2.11	0.50
1:E:60:VAL:CG2	1:E:82:ILE:HD13	2.39	0.50
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:101:ILE:HG12	1:B:164:GLU:OE1	2.11	0.50
1:B:121:MET:O	1:B:133:THR:CB	2.54	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:B:222:GLN:O	1:B:223:HIS:CB	2.58	0.50
1:C:269:GLN:O	1:C:272:ALA:N	2.45	0.50
1:E:49:GLY:O	1:E:50:VAL:O	2.30	0.50
1:E:89:ARG:O	1:E:116:ARG:NH2	2.42	0.50
1:A:1:MET:HG2	1:A:2:SER:N	2.27	0.50
1:A:123:ASN:ND2	1:A:123:ASN:N	2.50	0.50
1:C:124:THR:N	1:C:125:PRO:CD	2.74	0.50
1:E:18:GLY:HA3	1:E:156:VAL:HG11	1.94	0.50
1:B:121:MET:HE3	2:B:406:HOH:O	2.12	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:105:GLU:OE2	1:B:117:VAL:HB	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:122:THR:CG2	1:E:133:THR:CG2	2.89	0.50
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:E:29:LYS:C	1:E:30:ILE:HG13	2.32	0.49
1:A:8:ALA:HA	1:A:12:ALA:CB	2.42	0.49
1:B:45:LEU:HB3	2:B:350:HOH:O	2.11	0.49
1:B:73:HIS:C	1:B:75:ILE:H	2.15	0.49
1:B:172:GLY:O	1:B:258:VAL:HA	2.12	0.49
1:C:71:LYS:NZ	1:C:74:ILE:HD12	2.26	0.49
1:D:258:VAL:HG12	1:D:259:GLU:H	1.76	0.49
1:E:25:LEU:N	1:E:25:LEU:CD2	2.75	0.49
1:B:228:LYS:HE2	1:B:229:ASP:OD1	2.12	0.49
1:C:198:PRO:HG2	1:C:201:LEU:CB	2.42	0.49
1:B:71:LYS:H	1:B:71:LYS:HD2	1.77	0.49
1:B:193:VAL:N	2:B:382:HOH:O	2.44	0.49
1:C:86:ILE:HB	1:C:112:ARG:HB2	1.93	0.49
1:D:189:ALA:CB	1:D:203:VAL:HG23	2.42	0.49
1:A:186:ASP:HA	2:A:424:HOH:O	2.12	0.49
1:B:134:VAL:HG22	2:B:334:HOH:O	2.12	0.49
1:B:216:MET:HG3	2:B:372:HOH:O	2.12	0.49
1:B:236:GLY:O	1:B:237:ALA:HB3	2.12	0.49
1:B:262:CYS:HA	2:B:343:HOH:O	2.13	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: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:D:194:LYS:HG2	1:D:194:LYS:O	2.12	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:E:172:GLY:HA2	1:E:261:SER:HB3	1.93	0.49
1:A:197:LEU:HD22	1:A:201:LEU:HD23	1.94	0.49
1:B:168:ASP:HB2	2:B:375:HOH:O	2.12	0.49
1:C:152:LEU:HG	1:C:153:LEU:HG	1.95	0.49
1:D:199:ARG:O	1:D:200:ARG:C	2.49	0.49
1:E:22:ALA:HB3	1:E:24:VAL:HG23	1.94	0.49
1:A:65:VAL:HB	2:A:365:HOH:O	2.12	0.49
1:A:199:ARG:NH2	2:A:424:HOH:O	2.45	0.49
1:B:195:MET:HA	1:B:195:MET:HE2	1.92	0.49
1:C:3:VAL:O	1:C:30:ILE:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:ILE:HD13	1:D:193:VAL:HG12	1.94	0.49
1:C:266:ARG:HG2	1:C:266:ARG:HH11	1.77	0.49
1:D:3:VAL:HG11	1:D:67:PHE:CE1	2.47	0.49
1:D:124:THR:O	1:D:126:VAL:N	2.46	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: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:D:38:ASP:OD2	1:D:40:ALA:HB3	2.13	0.49
1:E:34:SER:HB3	1:E:54:PRO:CA	2.41	0.49
1:E:68:LEU:HB2	1:E:94:SER:CB	2.43	0.49
1:A:13:PHE:HA	2:A:333:HOH:O	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:E:227:LEU:HA	2:E:442:HOH:O	2.13	0.49
1:A:82:ILE:O	1:A:86:ILE:HG13	2.13	0.48
1:A:101:ILE:O	1:A:104:ILE:N	2.45	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
1:B:71:LYS:CB	1:B:73:HIS:CE1	2.91	0.48
1:B:75:ILE:HD11	1:B:272:ALA:CB	2.43	0.48
1:C:112:ARG:HH11	1:C:112:ARG:HG3	1.77	0.48
1:C:148:LEU:HA	1:C:151:GLN:OE1	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:36:ASP:O	1:A:37:MET:CB	2.60	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:B:94:SER:O	1:B:94:SER:OG	2.22	0.48
1:C:13:PHE:HE1	1:C:44:ALA:HB3	1.78	0.48
1:C:128:VAL:CG1	1:C:129:ARG:H	2.26	0.48
1:D:70:VAL:HG21	1:D:78:ILE:CD1	2.43	0.48
1:D:222:GLN:HG3	1:D:227:LEU:HD21	1.96	0.48
1:D:264:ARG:NE	2:D:321:HOH:O	2.29	0.48
1:E:144:GLU:HB3	2:E:352:HOH:O	2.13	0.48
1:E:217:LEU:C	1:E:219:HIS:N	2.67	0.48
1:A:100:THR:HG22	1:A:101:ILE:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:PRO:O	1:A:181:ALA:HB3	2.14	0.48
1:B:119:ARG:HD2	1:B:164:GLU:OE2	2.13	0.48
1:C:67:PHE:HA	1:C:93:VAL:HG23	1.95	0.48
1:D:102:SER:HA	2:D:337:HOH:O	2.12	0.48
1:E:77:PHE:N	1:E:77:PHE:CD1	2.80	0.48
1:E:141:ALA:O	1:E:142:GLN:O	2.31	0.48
1:A:176:SER:HB3	1:A:180:TYR:CE2	2.48	0.48
1:B:3:VAL:HG13	1:B:65:VAL:O	2.14	0.48
1:C:102:SER:HB3	1:C:106:LYS:HG3	1.94	0.48
1:C:173:LEU:HB3	2:C:437:HOH:O	2.12	0.48
1:E:122:THR:CG2	1:E:133:THR:HG22	2.43	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:105:GLU:OE1	1:B:117:VAL:HG21	2.13	0.48
1:B:166:LEU:O	1:B:169:ALA:N	2.44	0.48
1:B:183:THR:HA	2:B:388:HOH:O	2.12	0.48
1:B:233:SER:C	1:B:235:GLY:N	2.65	0.48
1:C:11:LEU:HD12	1:C:14:ALA:CB	2.44	0.48
1:E:185:LEU:HD21	1:E:210:LEU:CD1	2.44	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:A:219:HIS:O	1:A:220:SER:HB3	2.13	0.48
1:C:26:ALA:O	1:C:28:HIS:N	2.46	0.48
1:D:162:VAL:CG1	1:D:166:LEU:HD12	2.38	0.48
1:E:96:ALA:HA	2:E:447:HOH:O	2.14	0.48
1:A:135:TYR:CD1	1:A:135:TYR:C	2.86	0.48
1:A:165:ASP:OD2	1:A:166:LEU:N	2.47	0.48
1:A:173:LEU:HB3	1:A:174:SER:H	1.44	0.48
1:A:266:ARG:HG2	1:A:266:ARG:NH1	2.28	0.48
1:B:156:VAL:HG12	1:B:156:VAL:O	2.14	0.48
1:B:184:ALA:O	1:B:187:ALA:HB3	2.13	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:C:112:ARG:HG3	1:C:113:PRO:CD	2.35	0.48
1:D:238:THR:O	1:D:241:ALA:HB3	2.13	0.48
1:E:134:VAL:CG2	1:E:170:VAL:HG11	2.43	0.48
1:E:206:GLY:O	1:E:209:ALA:HB3	2.13	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:LEU:CD1	1:C:211:LEU:C	2.82	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:129:ARG:O	1:A:157:GLY:HA2	2.14	0.48
1:A:236:GLY:O	1:A:237:ALA:HB3	2.14	0.48
1:B:135:TYR:HE1	1:B:161:GLU:OE1	1.97	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:E:129:ARG:O	1:E:130:GLU:C	2.52	0.48
1:A:30:ILE:HB	1:A:50:VAL:HG13	1.96	0.48
1:B:82:ILE:HG22	1:B:86:ILE:CD1	2.39	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:33:SER:HB3	1:D:56:ASN:OD1	2.13	0.48
1:D:242:LEU:O	1:D:246:GLU:HB2	2.14	0.48
1:E:169:ALA:C	1:E:171:THR:N	2.64	0.48
1:A:86:ILE:O	1:A:86:ILE:HG22	2.13	0.47
1:E:70:VAL:O	1:E:74:ILE:HD12	2.14	0.47
1:E:181:ALA:O	1:E:184:ALA:N	2.45	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
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:60:VAL:HG12	1:E:90:HIS:NE2	2.29	0.47
1:E:121:MET:CE	1:E:122:THR:H	2.26	0.47
1:E:137:THR:HG23	1:E:137:THR:O	2.15	0.47
1:A:92:VAL:HG12	1:A:117:VAL:HG23	1.96	0.47
1:A:135:TYR:HE1	1:A:161:GLU:HG2	1.77	0.47
1:B:94:SER:OG	1:B:119:ARG:HG3	2.14	0.47
1:C:11:LEU:O	1:C:15:LEU:HG	2.14	0.47
1:C:230:ASN:HA	2:C:328:HOH:O	2.14	0.47
1:E:57:LYS:HD3	1:E:57:LYS:N	2.26	0.47
1:B:42:VAL:HA	1:B:45:LEU:HG	1.97	0.47
1:B:68:LEU:HA	2:B:325:HOH:O	2.14	0.47
1:B:119:ARG:HD3	1:B:167:ILE:HD12	1.95	0.47
1:B:143:VAL:O	1:B:145:ASP:N	2.42	0.47
1:C:128:VAL:C	1:C:130:GLU:H	2.17	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:C:64:ASP:O	1:C:65:VAL:HB	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:ASN:C	1:C:125:PRO:HD2	2.34	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:47:LYS:NZ	1:B:47:LYS:HB3	2.28	0.47
1:B:89:ARG:HD2	1:B:89:ARG:C	2.35	0.47
1:D:1:MET:HE2	1:D:25:LEU:HD21	1.97	0.47
1:D:33:SER:O	1:D:35:PRO:CD	2.62	0.47
1:D:137:THR:HG23	1:D:137:THR:O	2.14	0.47
1:D:222:GLN:O	1:D:223:HIS:CB	2.62	0.47
1:E:17:LYS:CB	2:E:412:HOH:O	2.56	0.47
1:B:17:LYS:HA	1:B:20:THR:HG21	1.97	0.47
1:B:31:MET:HG3	1:B:51:LYS:CB	2.45	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:B:123:ASN:C	1:B:125:PRO:HD2	2.35	0.47
1:C:10:GLN:O	1:C:12:ALA:N	2.48	0.47
1:C:61:GLN:C	1:C:63:SER:N	2.66	0.47
1:C:93:VAL:HG12	1:C:118:ILE:CD1	2.44	0.47
1:C:100:THR:HG22	1:C:101:ILE:H	1.77	0.47
1:C:166:LEU:O	1:C:168:ASP:N	2.48	0.47
1:D:60:VAL:HG21	1:D:82:ILE:CG2	2.45	0.47
1:E:19:PHE:CE2	1:E:152:LEU:HG	2.50	0.47
1:E:43:SER:HB2	2:E:380:HOH:O	2.14	0.47
1:E:45:LEU:HD23	1:E:48:MET:CE	2.45	0.47
1:E:83:GLY:HA2	1:E:86:ILE:HD11	1.95	0.47
1:E:171:THR:HA	1:E:175:GLY:HA3	1.96	0.47
1:A:36:ASP:O	1:A:37:MET:HB2	2.15	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:A:198:PRO:HG2	1:A:201:LEU:HB2	1.96	0.47
1:C:262:CYS:O	1:C:263:ILE:C	2.54	0.47
1:D:6:ILE:CD1	1:D:66:LEU:HD21	2.45	0.47
1:D:89:ARG:CG	1:D:90:HIS:H	2.28	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:B:46:ARG:HB2	2:B:345:HOH:O	2.15	0.47
1:C:46:ARG:O	1:C:49:GLY:N	2.45	0.47
1:C:169:ALA:O	1:C:170:VAL:C	2.51	0.47
1:E:55:HIS:ND1	1:E:57:LYS:HE2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:PHE:HZ	1:B:15:LEU:CB	2.10	0.47
1:C:6:ILE:HD11	1:C:60:VAL:HG22	1.97	0.47
1:D:3:VAL:HG11	1:D:67:PHE:HE1	1.80	0.47
1:D:60:VAL:CG2	1:D:82:ILE:HD13	2.44	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: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:A:193:VAL:C	1:A:195:MET:H	2.17	0.46
1:B:76:PRO:O	1:B:78:ILE:N	2.47	0.46
1:B:239:ILE:HD13	1:E:194:LYS:N	2.30	0.46
1:C:70:VAL:HG21	1:C:78:ILE:HD12	1.96	0.46
1:C:211:LEU:C	1:C:211:LEU:HD13	2.36	0.46
1:E:112:ARG:HG3	2:E:342:HOH:O	2.13	0.46
1:E:228:LYS:HE3	1:E:242:LEU:CD1	2.35	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:A:228:LYS:NZ	1:C:199:ARG:HH12	2.12	0.46
1:B:79:LEU:CD1	1:B:104:ILE:HG12	2.42	0.46
1:C:9:GLY:O	1:C:10:GLN:C	2.53	0.46
1:C:171:THR:HG21	2:C:423:HOH:O	2.14	0.46
1:E:255:ILE:O	1:E:256:ASN:C	2.53	0.46
1:B:27:ALA:CB	1:B:49:GLY:O	2.60	0.46
1:B:35:PRO:O	1:B:36:ASP:HB2	2.15	0.46
1:B:129:ARG:O	1:B:157:GLY:HA2	2.15	0.46
1:C:55:HIS:C	1:C:57:LYS:H	2.19	0.46
1:C:66:LEU:C	1:C:66:LEU:HD23	2.36	0.46
1:D:4:GLY:HA2	1:D:31:MET:O	2.16	0.46
1:D:150:GLU:O	1:D:150:GLU:HG2	2.15	0.46
1:D:164:GLU:HA	1:D:167:ILE:HG13	1.97	0.46
1:A:11:LEU:O	1:A:14:ALA:HB3	2.15	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:98:GLY:O	1:D:99:VAL:C	2.54	0.46
1:D:101:ILE:HG13	1:D:119:ARG:HB2	1.97	0.46
1:D:134:VAL:HG21	1:D:162:VAL:HG21	1.98	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:A:252:SER:C	1:A:254:LEU:H	2.18	0.46
1:B:1:MET:CG	1:B:2:SER:N	2.77	0.46
1:B:45:LEU:O	1:B:46:ARG:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ILE:HD11	1:B:96:ALA:HB3	1.98	0.46
1:C:93:VAL:HG23	1:C:93:VAL:O	2.16	0.46
1:E:67:PHE:O	1:E:68:LEU:HD23	2.16	0.46
1:E:125:PRO:C	1:E:127:VAL:N	2.67	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: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: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:E:98:GLY:HA2	2:E:400:HOH:O	2.16	0.46
1:B:3:VAL:O	1:B:30:ILE:CG2	2.64	0.46
1:B:8:ALA:HA	1:B:12:ALA:HB1	1.93	0.46
1:B:128:VAL:O	1:B:129:ARG:HB2	2.16	0.46
1:B:161:GLU:O	1:B:162:VAL:HG22	2.16	0.46
1:C:172:GLY:O	1:C:258:VAL:HG22	2.15	0.46
1:C:210:LEU:O	1:C:211:LEU:C	2.54	0.46
1:D:16:ALA:C	1:D:48:MET:HE1	2.37	0.46
1:D:252:SER:O	1:D:254:LEU:N	2.49	0.46
1:A:20:THR:HG21	1:A:48:MET:CE	2.45	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:D:121:MET:HE2	1:D:171:THR:HG23	1.94	0.46
1:A:79:LEU:HD21	1:A:104:ILE:HG23	1.97	0.46
1:A:159:CYS:O	1:A:160:THR:OG1	2.29	0.46
1:B:76:PRO:C	1:B:78:ILE:H	2.19	0.46
1:C:9:GLY:O	1:C:12:ALA:CB	2.63	0.46
1:C:83:GLY:HA2	1:C:108:LEU:HD22	1.98	0.46
1:C:264:ARG:O	1:C:268:LEU:HG	2.15	0.46
1:E:13:PHE:O	1:E:14:ALA:C	2.54	0.46
1:E:70:VAL:O	1:E:71:LYS:CB	2.63	0.46
1:E:153:LEU:C	1:E:155:SER:N	2.69	0.46
1:E:176:SER:O	1:E:177:GLY:C	2.55	0.46
1:B:5:PHE:HA	2:B:371:HOH:O	2.14	0.45
1:B:79:LEU:O	1:B:108:LEU:CD2	2.64	0.45
1:B:239:ILE:HD12	1:E:193:VAL:HG12	1.98	0.45
1:C:104:ILE:HG21	1:C:117:VAL:HG11	1.98	0.45
1:C:185:LEU:HD22	2:C:434:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:ILE:O	1:D:75:ILE:C	2.54	0.45
1:A:93:VAL:HG22	1:A:118:ILE:CG1	2.47	0.45
1:B:112:ARG:O	1:B:113:PRO:O	2.34	0.45
1:B:140:HIS:O	1:B:141:ALA:HB2	2.16	0.45
1:B:234:PRO:HA	1:E:193:VAL:HG13	1.98	0.45
1:C:6:ILE:HG21	1:C:78:ILE:HG21	1.97	0.45
1:C:61:GLN:O	1:C:63:SER:N	2.49	0.45
1:D:70:VAL:HG11	1:D:78:ILE:CD1	2.46	0.45
1:D:224:PRO:HA	2:D:419:HOH:O	2.15	0.45
1:D:255:ILE:O	1:D:256:ASN:C	2.55	0.45
1:E:236:GLY:HA2	1:E:239:ILE:CG2	2.39	0.45
1:A:92:VAL:CG1	1:A:117:VAL:HG23	2.46	0.45
1:A:101:ILE:O	1:A:104:ILE:HB	2.17	0.45
1:B:119:ARG:HD3	1:B:167:ILE:HD13	1.98	0.45
1:B:259:GLU:HB3	2:B:336:HOH:O	2.15	0.45
1:C:204:ARG:CB	2:C:337:HOH:O	2.59	0.45
1:D:99:VAL:HG12	1:D:104:ILE:HD11	1.98	0.45
1:E:75:ILE:O	1:E:78:ILE:HB	2.16	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:71:LYS:HB2	1:C:73:HIS:CE1	2.52	0.45
1:C:143:VAL:HG12	1:C:143:VAL:O	2.16	0.45
1:C:238:THR:HB	2:C:326:HOH:O	2.17	0.45
1:D:31:MET:HA	1:D:51:LYS:O	2.15	0.45
1:D:37:MET:CE	1:D:42:VAL:HG12	2.46	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:A:156:VAL:O	1:A:156:VAL:CG1	2.62	0.45
1:D:4:GLY:O	1:D:66:LEU:HD12	2.16	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:10:GLN:O	1:A:11:LEU:C	2.55	0.45
1:A:36:ASP:O	1:A:37:MET:HG3	2.17	0.45
1:E:82:ILE:O	1:E:82:ILE:HG22	2.16	0.45
1:B:161:GLU:HA	2:B:330:HOH:O	2.16	0.45
1:C:27:ALA:O	1:C:28:HIS:CG	2.70	0.45
1:C:164:GLU:O	1:C:164:GLU:HG2	2.16	0.45
1:C:210:LEU:HA	1:C:210:LEU:HD23	1.65	0.45
1:D:75:ILE:CD1	1:D:99:VAL:HG11	2.47	0.45
1:D:224:PRO:N	2:D:323:HOH:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:3:VAL:CG1	1:A:4:GLY:N	2.69	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:C:87:GLU:H	1:C:90:HIS:CE1	2.33	0.45
1:C:122:THR:CG2	1:C:133:THR:CG2	2.95	0.45
1:C:177:GLY:HA2	1:C:180:TYR:CE1	2.50	0.45
1:C:253:LEU:HD12	1:C:253:LEU:N	2.32	0.45
1:A:135:TYR:CE2	1:A:150:GLU:HG2	2.51	0.45
1:C:83:GLY:HA2	1:C:86:ILE:HD11	1.99	0.45
1:C:185:LEU:HA	1:C:185:LEU:HD23	1.69	0.45
1:D:101:ILE:HG22	1:D:102:SER:N	2.32	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:E:102:SER:C	1:E:104:ILE:N	2.67	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:D:6:ILE:O	1:D:70:VAL:CG2	2.65	0.45
1:A:57:LYS:CA	1:A:60:VAL:HG23	2.48	0.44
1:B:239:ILE:HD13	1:E:194:LYS:CA	2.48	0.44
1:B:269:GLN:O	1:B:271:MET:N	2.48	0.44
1:C:93:VAL:HG12	1:C:118:ILE:CG1	2.47	0.44
1:C:147:ARG:HE	1:C:147:ARG:HB2	1.40	0.44
1:C:252:SER:O	1:C:253:LEU:C	2.54	0.44
1:D:122:THR:HB	1:D:123:ASN:H	1.38	0.44
1:E:172:GLY:O	1:E:258:VAL:HA	2.16	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
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:B:244:VAL:HG12	1:B:245:LEU:N	2.30	0.44
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:E:188:LEU:HD23	1:E:188:LEU:HA	1.73	0.44
1:B:28:HIS:C	1:B:30:ILE:H	2.20	0.44
1:C:180:TYR:N	1:C:180:TYR:CD2	2.81	0.44
1:C:242:LEU:HA	1:C:242:LEU:HD23	1.60	0.44
1:D:80:ASP:C	1:D:82:ILE:H	2.21	0.44
1:D:107:LYS:O	1:D:110:ALA:HB3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:HIS:HB3	1:E:57:LYS:CE	2.43	0.44
1:E:172:GLY:O	1:E:258:VAL:HG22	2.18	0.44
1:C:10:GLN:NE2	2:C:382:HOH:O	2.50	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:38:ASP:H	1:E:42:VAL:CG2	2.30	0.44
1:E:178:PRO:N	2:E:404:HOH:O	2.50	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:3:VAL:HB	1:C:30:ILE:CG1	2.47	0.44
1:C:17:LYS:O	1:C:20:THR:HB	2.18	0.44
1:C:265:THR:HG23	2:C:323:HOH:O	2.17	0.44
1:E:177:GLY:HA2	1:E:180:TYR:CD1	2.53	0.44
1:E:242:LEU:O	1:E:245:LEU:N	2.51	0.44
1:A:249:GLY:O	1:A:252:SER:HB3	2.17	0.44
1:C:167:ILE:HB	2:C:422:HOH:O	2.17	0.44
1:D:38:ASP:O	1:D:40:ALA:N	2.51	0.44
1:E:83:GLY:HA2	1:E:86:ILE:HD12	1.97	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:C:75:ILE:HB	1:C:76:PRO:HD3	2.00	0.44
1:D:26:ALA:CB	1:D:28:HIS:CD2	3.01	0.44
1:E:6:ILE:HD11	1:E:66:LEU:HD21	2.00	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:E:75:ILE:O	1:E:79:LEU:HG	2.18	0.44
1:A:102:SER:OG	1:A:103:SER:N	2.49	0.43
1:B:86:ILE:HA	1:B:90:HIS:NE2	2.33	0.43
1:C:17:LYS:HA	1:C:20:THR:OG1	2.18	0.43
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: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:236:GLY:O	1:E:237:ALA:CB	2.65	0.43
1:A:77:PHE:HD1	1:A:77:PHE:H	1.66	0.43
1:A:185:LEU:O	1:A:186:ASP:C	2.55	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:C:46:ARG:C	1:C:48:MET:N	2.71	0.43
1:C:144:GLU:C	1:C:146:GLY:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:PHE:O	1:E:78:ILE:C	2.56	0.43
1:E:205:LEU:HA	1:E:205:LEU:HD23	1.85	0.43
1:A:79:LEU:HD11	1:A:104:ILE:HA	2.01	0.43
1:A:199:ARG:HD2	1:A:199:ARG:HA	1.86	0.43
1:B:71:LYS:HB2	1:B:73:HIS:ND1	2.33	0.43
1:B:121:MET:HG2	1:B:171:THR:OG1	2.18	0.43
1:B:214:ALA:O	1:B:215:LYS:C	2.57	0.43
1:C:35:PRO:HD3	2:C:380:HOH:O	2.17	0.43
1:E:33:SER:O	1:E:35:PRO:CD	2.66	0.43
1:A:13:PHE:CA	2:A:333:HOH:O	2.66	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:134:VAL:CG1	1:A:135:TYR:N	2.81	0.43
1:B:140:HIS:CD2	1:B:142:GLN:HB2	2.53	0.43
1:B:190:ASP:CG	1:B:199:ARG:HH12	2.21	0.43
1:C:51:LYS:HB2	1:C:51:LYS:NZ	2.33	0.43
1:C:172:GLY:HA2	1:C:261:SER:CB	2.48	0.43
1:D:31:MET:HE2	1:D:62:HIS:HB2	1.99	0.43
1:E:49:GLY:CA	2:E:407:HOH:O	2.66	0.43
1:E:123:ASN:CB	1:E:178:PRO:HG2	2.48	0.43
1:A:126:VAL:O	1:A:156:VAL:CG1	2.66	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:257:ALA:N	2:A:390:HOH:O	2.51	0.43
1:B:132:ALA:O	1:B:133:THR:HG22	2.18	0.43
1:C:13:PHE:CE1	1:C:44:ALA:HB3	2.53	0.43
1:A:121:MET:HE1	2:A:386:HOH:O	2.17	0.43
1:B:6:ILE:O	1:B:6:ILE:HG22	2.17	0.43
1:C:36:ASP:O	1:C:37:MET:CG	2.67	0.43
1:C:223:HIS:CE1	1:C:224:PRO:HD2	2.52	0.43
1:E:221:GLU:C	1:E:223:HIS:N	2.71	0.43
1:A:229:ASP:OD1	1:A:229:ASP:N	2.52	0.43
1:A:233:SER:C	1:A:235:GLY:N	2.69	0.43
1:B:13:PHE:CD1	1:B:41:THR:HG23	2.53	0.43
1:B:32:ALA:O	1:B:53:THR:HB	2.19	0.43
1:B:115:PRO:HG3	2:B:331:HOH:O	2.18	0.43
1:C:171:THR:O	1:C:175:GLY:CA	2.66	0.43
1:D:197:LEU:HA	1:D:197:LEU:HD23	1.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:VAL:CG1	1:B:135:TYR:N	2.82	0.43
1:B:190:ASP:N	2:B:382:HOH:O	2.50	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:C:196:GLY:O	1:C:197:LEU:O	2.37	0.43
1:C:228:LYS:NZ	1:C:229:ASP:OD1	2.52	0.43
1:D:148:LEU:HD12	1:D:148:LEU:O	2.19	0.43
1:E:12:ALA:O	1:E:13:PHE:C	2.56	0.43
1:E:126:VAL:HG13	1:E:156:VAL:O	2.19	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:C:79:LEU:CD1	1:C:104:ILE:HG13	2.47	0.43
1:D:185:LEU:CD2	1:D:210:LEU:CD1	2.95	0.43
1:D:236:GLY:HA2	2:D:435:HOH:O	2.18	0.43
1:E:75:ILE:N	1:E:76:PRO:CD	2.82	0.43
1:A:133:THR:CG2	1:A:134:VAL:N	2.82	0.43
1:B:41:THR:O	1:B:45:LEU:N	2.52	0.43
1:B:134:VAL:HA	2:B:334:HOH:O	2.19	0.43
1:B:194:LYS:HG2	1:B:195:MET:HE3	2.01	0.43
1:C:59:THR:HA	1:C:62:HIS:HE1	1.84	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:C:213:ALA:O	1:C:216:MET:HB2	2.19	0.43
1:C:269:GLN:O	1:C:271:MET:N	2.52	0.43
1:E:59:THR:O	1:E:62:HIS:N	2.52	0.43
1:A:223:HIS:ND1	1:A:224:PRO:CD	2.82	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
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:13:PHE:HE2	1:C:17:LYS:CE	2.31	0.42
1:C:274:GLN:HG2	1:C:274:GLN:O	2.18	0.42
1:D:27:ALA:HB1	1:D:49:GLY:HA3	2.01	0.42
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:135:TYR:CD1	1:D:135:TYR:C	2.92	0.42
1:D:143:VAL:O	1:D:145:ASP:N	2.52	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:A:103:SER:HA	2:A:391:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:PHE:HB2	2:A:335:HOH:O	2.18	0.42
1:B:90:HIS:CD2	1:B:90:HIS:N	2.87	0.42
1:C:38:ASP:O	1:C:42:VAL:HB	2.18	0.42
1:C:45:LEU:O	1:C:45:LEU:HD23	2.20	0.42
1:C:126:VAL:C	1:C:128:VAL:N	2.73	0.42
1:D:16:ALA:HB3	2:D:365:HOH:O	2.19	0.42
1:D:80:ASP:C	1:D:82:ILE:N	2.70	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:57:LYS:CG	1:B:58:GLU:N	2.82	0.42
1:B:105:GLU:OE1	1:B:117:VAL:CG2	2.67	0.42
1:B:112:ARG:O	1:B:113:PRO:C	2.58	0.42
1:B:199:ARG:CZ	1:D:229:ASP:OD1	2.68	0.42
1:C:68:LEU:CD2	1:C:79:LEU:HD21	2.50	0.42
1:E:126:VAL:HG12	1:E:156:VAL:CG1	2.50	0.42
1:E:203:VAL:CG2	2:E:422:HOH:O	2.52	0.42
1:A:39:LEU:O	1:A:43:SER:HB3	2.19	0.42
1:B:125:PRO:C	1:B:127:VAL:N	2.71	0.42
1:C:99:VAL:CG1	1:C:104:ILE:HD11	2.49	0.42
1:C:201:LEU:O	1:C:205:LEU:HB2	2.19	0.42
1:D:99:VAL:CG1	1:D:104:ILE:HD11	2.50	0.42
1:D:220:SER:HB2	1:D:222:GLN:HG2	2.01	0.42
1:A:55:HIS:O	1:A:57:LYS:N	2.50	0.42
1:A:75:ILE:HD13	1:A:99:VAL:HG11	2.01	0.42
1:A:118:ILE:HG22	1:A:137:THR:HA	2.00	0.42
1:A:162:VAL:HG13	1:A:166:LEU:HD12	2.00	0.42
1:A:227:LEU:O	1:A:231:VAL:HG23	2.19	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:B:244:VAL:O	1:B:247:SER:HB2	2.20	0.42
1:D:7:GLY:HA2	1:D:33:SER:O	2.18	0.42
1:D:13:PHE:HZ	1:D:17:LYS:NZ	2.12	0.42
1:D:133:THR:O	1:D:159:CYS:HA	2.19	0.42
1:E:17:LYS:O	1:E:18:GLY:C	2.58	0.42
1:E:231:VAL:HG12	1:E:231:VAL:O	2.20	0.42
1:E:262:CYS:O	1:E:263:ILE:C	2.56	0.42
1:A:7:GLY:O	1:A:8:ALA:HB2	2.19	0.42
1:A:193:VAL:HA	1:A:197:LEU:O	2.20	0.42
1:B:79:LEU:HB3	1:B:108:LEU:HG	2.02	0.42
1:B:269:GLN:O	1:B:273:ASP:N	2.46	0.42
1:C:68:LEU:HD23	1:C:79:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:LEU:O	1:D:46:ARG:C	2.58	0.42
1:D:82:ILE:O	1:D:84:ALA:N	2.52	0.42
1:D:112:ARG:HA	1:D:113:PRO:HD3	1.93	0.42
1:E:80:ASP:C	1:E:81:GLU:HG3	2.40	0.42
1:E:198:PRO:HG2	1:E:201:LEU:CB	2.48	0.42
1:A:61:GLN:O	1:A:63:SER:N	2.53	0.42
1:A:190:ASP:N	1:A:199:ARG:HH12	2.17	0.42
1:C:100:THR:CG2	1:C:101:ILE:N	2.83	0.42
1:D:82:ILE:O	1:D:83:GLY:C	2.57	0.42
1:E:105:GLU:OE1	1:E:139:THR:HB	2.20	0.42
1:A:245:LEU:HA	2:A:387:HOH:O	2.20	0.42
1:C:10:GLN:C	1:C:12:ALA:H	2.23	0.42
1:C:104:ILE:CG2	1:C:117:VAL:HG21	2.49	0.42
1:C:212:GLY:O	1:C:216:MET:HB2	2.20	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:D:109:SER:C	1:D:111:PHE:N	2.73	0.42
1:D:121:MET:HG2	2:D:376:HOH:O	2.19	0.42
1:A:251:ARG:O	1:A:252:SER:C	2.57	0.42
1:B:70:VAL:CG1	1:B:71:LYS:N	2.83	0.42
1:C:142:GLN:HB2	1:C:145:ASP:OD2	2.20	0.42
1:C:266:ARG:HG2	2:C:323:HOH:O	2.19	0.42
1:D:17:LYS:O	1:D:20:THR:HB	2.20	0.42
1:E:6:ILE:N	2:E:322:HOH:O	2.52	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: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:A:47:LYS:O	1:A:48:MET:C	2.59	0.41
2:B:390:HOH:O	1:D:239:ILE:HG23	2.20	0.41
1:C:19:PHE:HE2	1:C:153:LEU:HD23	1.85	0.41
1:E:34:SER:C	1:E:36:ASP:H	2.23	0.41
1:E:99:VAL:O	1:E:100:THR:C	2.57	0.41
1:E:121:MET:O	1:E:133:THR:HA	2.20	0.41
1:E:181:ALA:N	2:E:391:HOH:O	2.52	0.41
1:A:57:LYS:HE2	1:A:81:GLU:OE1	2.19	0.41
1:A:66:LEU:N	2:A:368:HOH:O	2.53	0.41
1:A:149:MET:HA	1:A:149:MET:HE2	2.02	0.41
1:B:11:LEU:HB3	1:B:15:LEU:CD1	2.50	0.41
1:B:70:VAL:CG1	1:B:71:LYS:H	2.28	0.41
1:B:141:ALA:O	1:B:145:ASP:CB	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:PRO:CD	1:B:201:LEU:HD23	2.49	0.41
1:C:3:VAL:CG1	1:C:4:GLY:N	2.83	0.41
1:C:13:PHE:HE1	1:C:44:ALA:CB	2.33	0.41
1:C:166:LEU:O	1:C:167:ILE:C	2.59	0.41
1:D:270:SER:O	1:D:274:GLN:OE1	2.37	0.41
1:E:7:GLY:H	1:E:33:SER:HB2	1.85	0.41
1:E:75:ILE:HD12	1:E:99:VAL:HG21	2.02	0.41
1:A:97:ALA:O	1:A:99:VAL:N	2.53	0.41
1:A:109:SER:C	1:A:111:PHE:N	2.70	0.41
1:B:68:LEU:HG	1:B:92:VAL:CG1	2.50	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:C:135:TYR:CD1	1:C:135:TYR:C	2.93	0.41
1:C:213:ALA:O	1:C:216:MET:CB	2.68	0.41
1:D:236:GLY:O	1:D:237:ALA:HB3	2.20	0.41
1:A:123:ASN:C	1:A:125:PRO:HD2	2.40	0.41
2:A:422:HOH:O	1:C:199:ARG:HB2	2.18	0.41
1:B:161:GLU:C	1:B:162:VAL:HG23	2.41	0.41
1:B:226:GLN:O	1:B:230:ASN:OD1	2.38	0.41
1:C:251:ARG:HB2	2:C:340:HOH:O	2.19	0.41
1:D:33:SER:CB	1:D:56:ASN:OD1	2.69	0.41
1:D:266:ARG:HG3	2:D:377:HOH:O	2.20	0.41
1:E:131:GLY:H	1:E:157:GLY:HA3	1.85	0.41
1:E:135:TYR:CE1	1:E:161:GLU:HB3	2.56	0.41
1:E:150:GLU:O	1:E:152:LEU:N	2.53	0.41
1:A:15:LEU:O	1:A:16:ALA:C	2.59	0.41
1:A:55:HIS:C	1:A:57:LYS:N	2.73	0.41
1:A:59:THR:O	1:A:61:GLN:N	2.53	0.41
1:A:244:VAL:CG2	1:A:245:LEU:N	2.84	0.41
1:C:17:LYS:HE3	1:C:17:LYS:HB2	1.85	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:C:205:LEU:HD23	1:C:205:LEU:HA	1.87	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
1:C:2:SER:O	1:C:3:VAL:CG2	2.69	0.41
1:C:112:ARG:NH1	1:C:113:PRO:CD	2.68	0.41
1:D:134:VAL:CG1	1:D:170:VAL:HG11	2.50	0.41
1:D:134:VAL:HG11	1:D:170:VAL:HG11	2.02	0.41
1:A:210:LEU:HD23	1:A:210:LEU:HA	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:ILE:HD11	1:B:272:ALA:CA	2.51	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:D:45:LEU:O	1:D:48:MET:N	2.53	0.41
1:D:129:ARG:HG2	1:D:156:VAL:HG13	2.03	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:E:87:GLU:O	1:E:89:ARG:N	2.54	0.41
1:E:121:MET:CE	2:E:405:HOH:O	2.68	0.41
1:A:56:ASN:O	1:A:82:ILE:HD11	2.21	0.41
1:A:92:VAL:HB	1:A:117:VAL:HG23	2.03	0.41
1:A:180:TYR:N	1:A:180:TYR:CD2	2.86	0.41
1:A:240:HIS:CD2	1:C:194:LYS:HG3	2.56	0.41
1:B:6:ILE:CA	1:B:33:SER:HB3	2.26	0.41
1:B:185:LEU:HD23	1:B:185:LEU:HA	1.87	0.41
1:B:223:HIS:ND1	1:B:224:PRO:HD2	2.35	0.41
1:C:48:MET:HB3	1:C:50:VAL:HG23	2.03	0.41
1:D:33:SER:HA	1:D:53:THR:O	2.21	0.41
1:D:254:LEU:HD23	1:D:254:LEU:HA	1.83	0.41
1:E:116:ARG:HB2	2:E:396:HOH:O	2.20	0.41
1:E:131:GLY:HA2	2:E:325:HOH:O	2.20	0.41
1:E:153:LEU:C	1:E:155:SER:H	2.21	0.41
1:A:27:ALA:HB1	1:A:49:GLY:C	2.42	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:C:66:LEU:HB2	2:C:402:HOH:O	2.20	0.41
1:C:114:ALA:HA	2:C:379:HOH:O	2.21	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:101:ILE:HG23	1:A:117:VAL:CG1	2.51	0.40
1:B:185:LEU:C	1:B:187:ALA:N	2.74	0.40
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:125:PRO:HB2	1:C:130:GLU:O	2.22	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:D:86:ILE:HD12	1:D:108:LEU:HD13	2.03	0.40
1:D:252:SER:HA	1:D:255:ILE:HD12	2.02	0.40
1:E:111:PHE:O	1:E:112:ARG:C	2.60	0.40
1:A:22:ALA:HA	2:A:379:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:53:THR:HG22	1:C:55:HIS:O	2.21	0.40
1:C:93:VAL:HG11	1:C:149:MET:SD	2.61	0.40
1:C:99:VAL:HG11	1:C:104:ILE:HD11	2.03	0.40
1:C:119:ARG:NH2	2:C:339:HOH:O	2.48	0.40
1:E:28:HIS:O	1:E:51:LYS:HE3	2.21	0.40
1:E:254:LEU:HD23	1:E:254:LEU:HA	1.83	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:A:252:SER:HA	1:A:255:ILE:HD12	2.03	0.40
1:B:17:LYS:HA	1:B:20:THR:CG2	2.52	0.40
1:C:70:VAL:CG1	1:C:74:ILE:HB	2.52	0.40
1:D:82:ILE:O	1:D:82:ILE:HG22	2.20	0.40
1:D:135:TYR:CE2	1:D:150:GLU:HB2	2.57	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:A:274:GLN:HB2	1:A:275:GLU:H	1.66	0.40
1:B:18:GLY:O	1:B:19:PHE:CD1	2.75	0.40
1:C:31:MET:SD	1:C:53:THR:OG1	2.79	0.40
1:C:164:GLU:HG2	2:C:416:HOH:O	2.21	0.40
1:D:101:ILE:O	1:D:102:SER:C	2.60	0.40
1:D:255:ILE:O	1:D:257:ALA:N	2.53	0.40
1:A:26:ALA:HB3	1:A:29:LYS:CE	2.46	0.40
1:A:41:THR:O	1:A:42:VAL:C	2.60	0.40
1:A:129:ARG:O	1:A:129:ARG:CG	2.68	0.40
1:B:137:THR:HG22	1:B:138:GLY:N	2.37	0.40
1:C:114:ALA:HB1	1:C:140:HIS:CE1	2.55	0.40
1:C:193:VAL:HG12	2:C:344:HOH:O	2.21	0.40
1:D:70:VAL:O	1:D:71:LYS:C	2.59	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	275/321 (86%)	182 (66%)	60 (22%)	33 (12%)	0	1
1	B	272/321 (85%)	168 (62%)	68 (25%)	36 (13%)	0	1
1	C	275/321 (86%)	183 (66%)	60 (22%)	32 (12%)	0	2
1	D	275/321 (86%)	183 (66%)	68 (25%)	24 (9%)	1	4
1	E	275/321 (86%)	183 (66%)	57 (21%)	35 (13%)	0	1
All	All	1372/1605 (86%)	899 (66%)	313 (23%)	160 (12%)	0	1

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
1	B	137	THR
1	B	140	HIS
1	B	141	ALA
1	B	142	GLN
1	B	163	GLU

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Mol	Chain	Res	Type
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
1	A	127	VAL
1	A	129	ARG
1	A	164	GLU
1	A	223	HIS
1	A	234	PRO

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Mol	Chain	Res	Type
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
1	C	167	ILE
1	C	173	LEU
1	D	110	ALA
1	D	253	LEU
1	D	256	ASN

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Mol	Chain	Res	Type
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
1	A	252	SER
1	D	234	PRO
1	E	178	PRO
1	A	104	ILE
1	D	112	ARG

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Mol	Chain	Res	Type
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 (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	215/250 (86%)	185 (86%)	30 (14%)	3 15
1	B	213/250 (85%)	197 (92%)	16 (8%)	13 42
1	C	214/250 (86%)	196 (92%)	18 (8%)	11 38
1	D	215/250 (86%)	185 (86%)	30 (14%)	3 15
1	E	215/250 (86%)	203 (94%)	12 (6%)	21 52
All	All	1072/1250 (86%)	966 (90%)	106 (10%)	8 29

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
1	A	121	MET
1	A	123	ASN
1	A	126	VAL

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Mol	Chain	Res	Type
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
1	C	121	MET
1	C	123	ASN
1	C	124	THR

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Mol	Chain	Res	Type
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
1	E	48	MET
1	E	57	LYS
1	E	77	PHE

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Mol	Chain	Res	Type
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

Sometimes 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 (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.38	2 (0%)	87	75	27, 79, 115, 154	0
1	B	276/321 (85%)	0.01	17 (6%)	20	9	26, 120, 172, 187	0
1	C	277/321 (86%)	0.04	16 (5%)	23	10	23, 117, 169, 183	0
1	D	277/321 (86%)	-0.46	1 (0%)	92	84	24, 70, 117, 163	0
1	E	277/321 (86%)	-0.43	3 (1%)	80	64	23, 78, 126, 156	0
All	All	1384/1605 (86%)	-0.24	39 (2%)	53	30	23, 82, 160, 187	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	95	CYS	3.8
1	B	39	LEU	3.7
1	B	38	ASP	3.7
1	C	96	ALA	3.6
1	C	95	CYS	3.6
1	B	41	THR	3.4
1	C	39	LEU	3.2
1	B	275	GLU	3.2
1	A	95	CYS	2.8
1	B	76	PRO	2.7
1	D	274	GLN	2.7
1	B	75	ILE	2.7
1	B	40	ALA	2.7
1	C	94	SER	2.6
1	C	55	HIS	2.6
1	B	33	SER	2.5
1	C	77	PHE	2.5
1	B	93	VAL	2.5
1	E	275	GLU	2.5
1	C	275	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	38	ASP	2.3
1	C	69	ALA	2.3
1	B	116	ARG	2.3
1	B	43	SER	2.3
1	B	120	CYS	2.2
1	B	36	ASP	2.2
1	C	36	ASP	2.2
1	B	94	SER	2.1
1	E	38	ASP	2.1
1	C	110	ALA	2.1
1	C	72	PRO	2.1
1	C	120	CYS	2.1
1	B	136	ALA	2.1
1	B	37	MET	2.1
1	A	274	GLN	2.1
1	C	54	PRO	2.1
1	E	34	SER	2.1
1	C	143	VAL	2.0
1	C	122	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.