Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2023 – 02:18 AM EDT

PDB ID	:	1RYZ
Title	:	Uridine Phosphorylase from Salmonella typhimurium. Crystal Structure at 2.9 A Resolution
Authors	:	Dontsova, M.V.; Gabdoulkhakov, A.G.; Lyashenko, A.V.; Nikonov, S.V.; Ealick, S.E.; Mikhailov, A.M.
Deposited on	:	2003-12-23
Resolution	:	2.90 Å(reported)

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

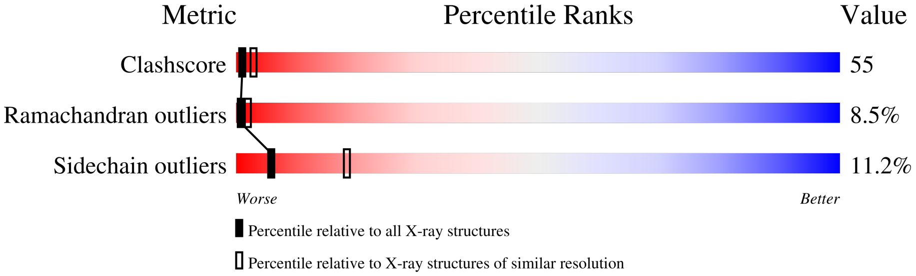
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.90 Å.

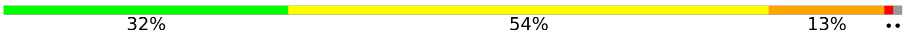
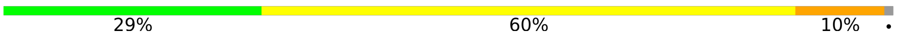
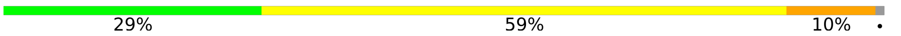
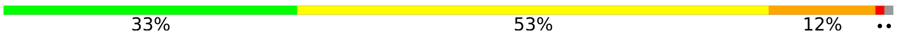
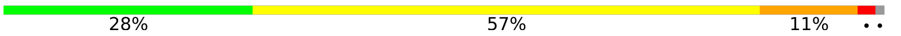
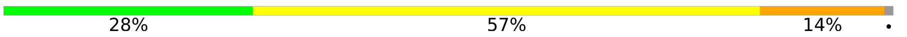
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	253	
1	B	253	
1	C	253	
1	D	253	
1	E	253	
1	F	253	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACY	B	254	-	-	X	-

2 Entry composition ⓘ

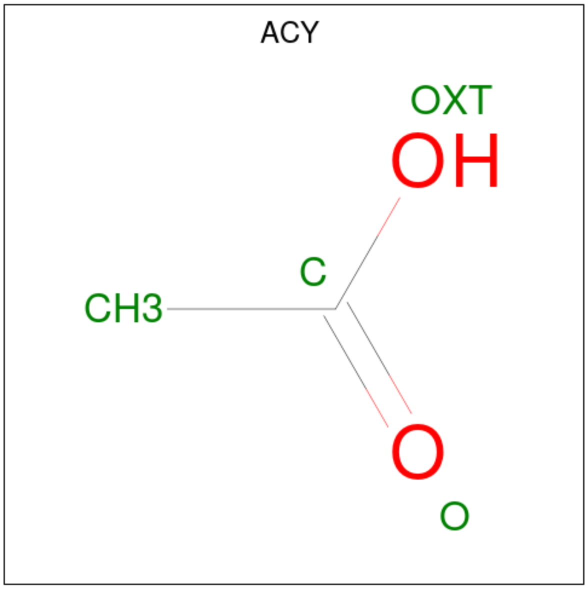
There are 2 unique types of molecules in this entry. The entry contains 11270 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Uridine phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	250	1877	1174	330	361	12	0	0	0
1	B	250	1877	1174	330	361	12	0	0	0
1	C	250	1877	1174	330	361	12	0	0	0
1	D	250	1877	1174	330	361	12	0	0	0
1	E	250	1877	1174	330	361	12	0	0	0
1	F	250	1877	1174	330	361	12	0	0	0

- Molecule 2 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



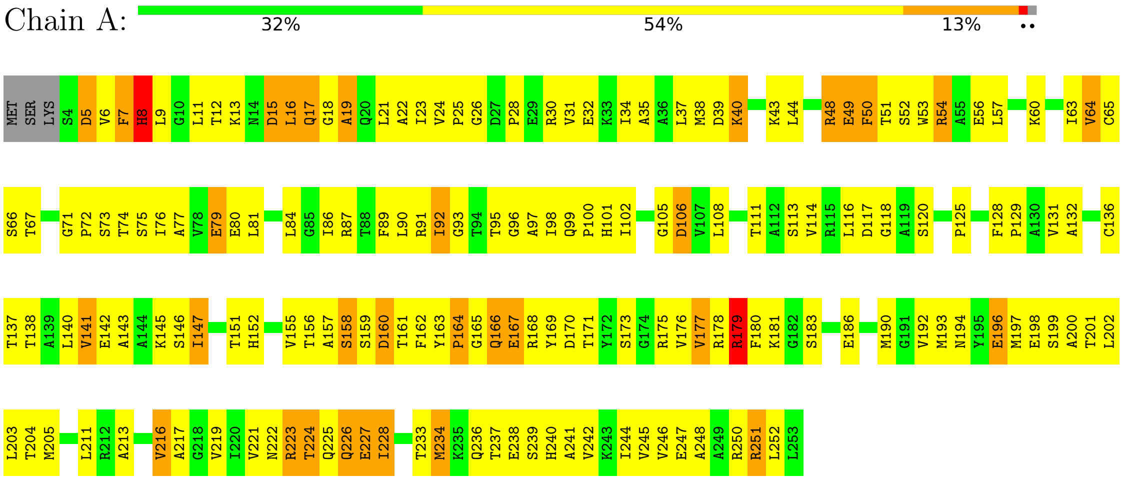
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0

3 Residue-property plots ⓘ

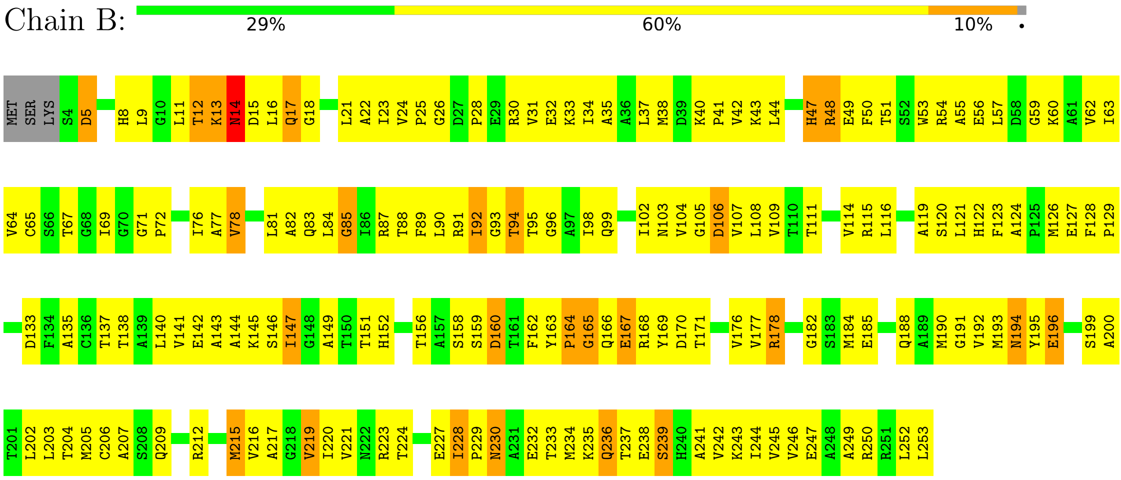
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

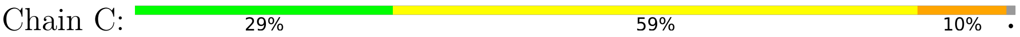
- Molecule 1: Uridine phosphorylase

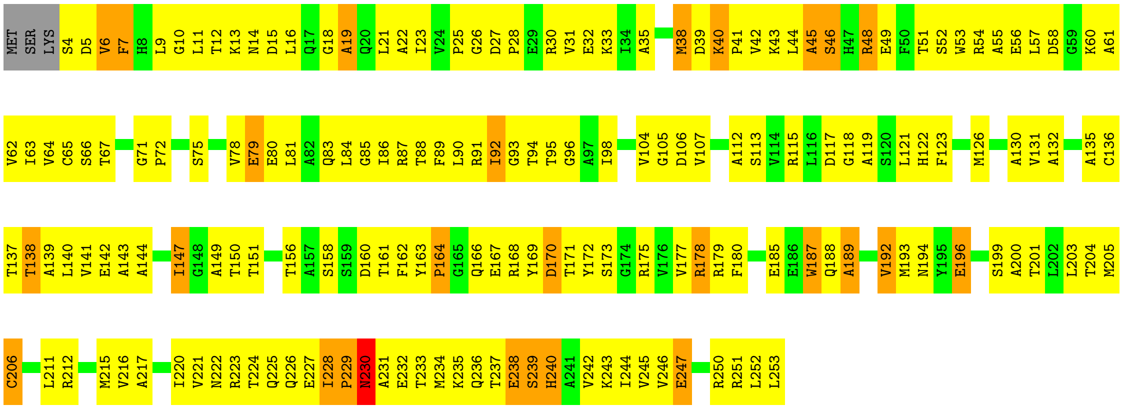


- Molecule 1: Uridine phosphorylase



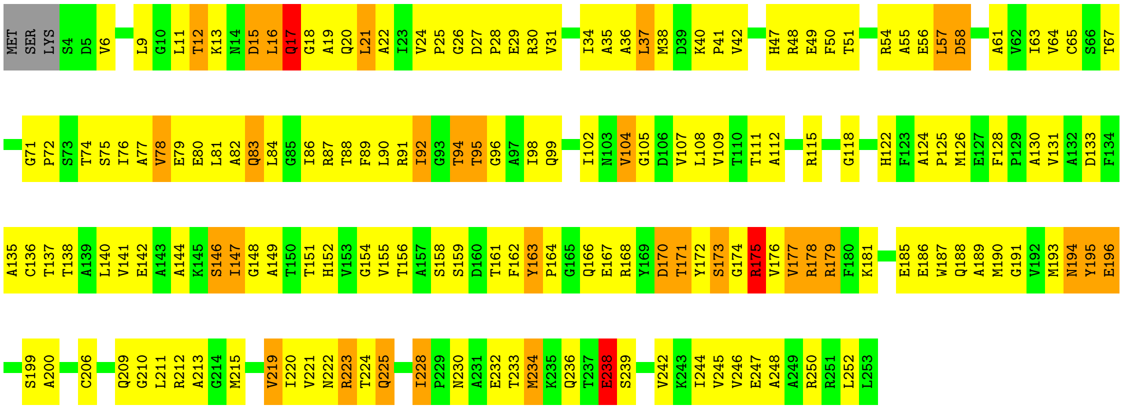
- Molecule 1: Uridine phosphorylase





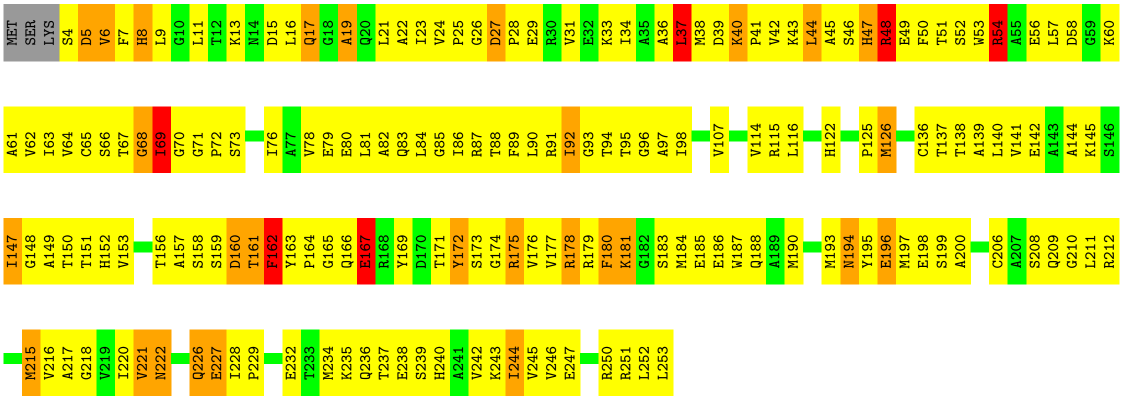
- Molecule 1: Uridine phosphorylase

Chain D:



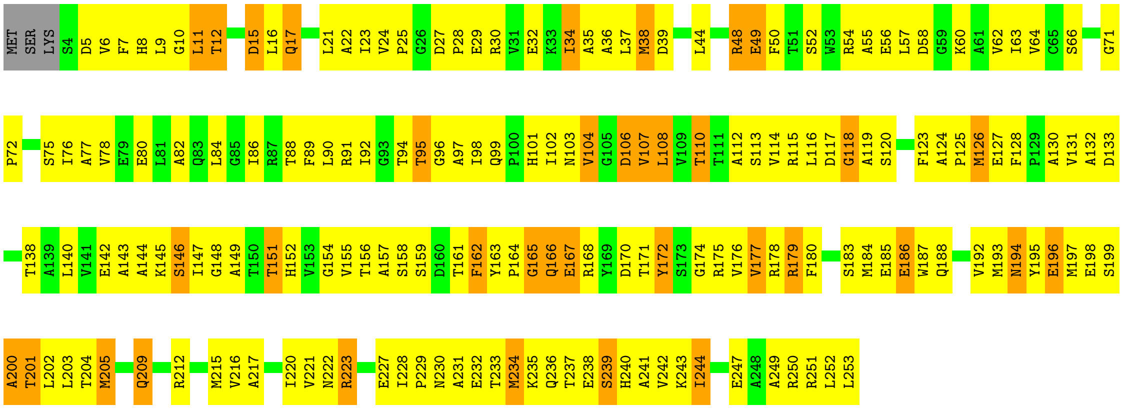
- Molecule 1: Uridine phosphorylase

Chain E:



- Molecule 1: Uridine phosphorylase

Chain F:


MET
SER
LYS
S4
D5
V6
F7
H8
L9
G10
L11
T12
D15
L16
Q17
L21
A22
I23
V24
P25
G26
D27
P28
E29
R30
V31
E32
K33
I34
A35
A36
L37
M38
D39
L44
R48
E49
F50
T51
S52
W53
R54
A55
E56
L57
D58
G59
K60
A61
V62
I63
V64
C65
S66
G71
P72
S75
I76
A77
V78
E79
E80
L81
A82
Q83
L84
G85
I86
R87
T88
F89
L90
R91
I92
G93
T94
T95
G96
A97
I98
Q99
P100
H101
I102
N103
V104
G105
D106
V107
L108
V109
T110
T111
A112
S113
V114
R115
L116
D117
G118
A119
S120
F123
A124
P125
M126
E127
F128
P129
A130
V131
A132
D133
T138
A139
L140
V141
E142
A143
A144
K145
S146
I147
G148
A149
T150
T151
H152
V153
G154
V155
T156
A157
S158
S159
D160
T161
F162
Y163
P164
G165
Q166
E167
R168
Y169
D170
T171
Y172
S173
G174
R175
V176
V177
R178
R179
F180
S183
M184
E185
E186
W187
Q188
V192
M193
N194
Y195
E196
M197
E198
S199
A200
T201
L202
L203
T204
M205
Q209
R212
M215
V216
A217
I220
V221
N222
R223
E227
I228
P229
N230
A231
E232
T233
M234
K235
Q236
T237
E238
S239
H240
A241
V242
K243
I244
E247
A248
A249
R250
R251
L252
L253

4 Data and refinement statistics ⓘ

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

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	92.26Å 92.26Å 267.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.46 – 2.90	Depositor
% Data completeness (in resolution range)	93.9 (29.46-2.90)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	0.18	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.212 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11270	wwPDB-VP
Average B, all atoms ($Å^2$)	18.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ACY

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	0.42	0/1907	0.74	0/2584
1	B	0.40	0/1907	0.72	0/2584
1	C	0.41	0/1907	0.70	0/2584
1	D	0.40	0/1907	0.67	0/2584
1	E	0.41	0/1907	0.74	2/2584 (0.1%)
1	F	0.40	0/1907	0.73	0/2584
All	All	0.41	0/11442	0.72	2/15504 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	6	VAL	N-CA-C	-6.19	94.29	111.00
1	E	47	HIS	N-CA-C	5.18	124.98	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	1877	0	1887	184	0
1	B	1877	0	1887	230	0
1	C	1877	0	1887	195	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1877	0	1887	202	0
1	E	1877	0	1887	251	0
1	F	1877	0	1887	239	0
2	B	8	0	6	5	0
All	All	11270	0	11328	1237	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 55.

All (1237) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:GLU:HG2	1:B:236:GLN:HB2	1.27	1.16
1:E:167:GLU:HG3	1:E:183:SER:H	1.15	1.10
1:C:228:ILE:HB	1:C:229:PRO:HD2	1.37	1.06
1:C:104:VAL:HG11	1:C:229:PRO:HB3	1.34	1.06
1:E:22:ALA:HB2	1:E:86:ILE:HD13	1.36	1.05
1:C:222:ASN:HB3	1:C:225:GLN:HE21	1.21	1.05
1:C:16:LEU:HB3	1:C:19:ALA:HB3	1.40	1.03
1:C:21:LEU:HD23	1:C:22:ALA:H	1.19	1.01
1:B:21:LEU:HD23	1:B:22:ALA:N	1.75	1.01
1:F:54:ARG:HH11	1:F:54:ARG:HB3	1.23	0.99
1:D:171:THR:HG22	1:D:172:TYR:H	1.21	0.99
1:F:30:ARG:CZ	1:F:238:GLU:HG2	1.92	0.99
1:F:194:ASN:N	1:F:194:ASN:HD22	1.61	0.98
1:B:60:LYS:HD2	1:B:253:LEU:HB3	1.46	0.97
1:E:194:ASN:HD22	1:E:194:ASN:H	1.06	0.96
1:E:17:GLN:HE21	1:E:17:GLN:HA	1.29	0.96
1:A:16:LEU:HB3	1:A:63:ILE:HD11	1.45	0.95
1:B:33:LYS:HA	1:B:33:LYS:HE2	1.46	0.95
1:B:21:LEU:HD23	1:B:22:ALA:H	1.31	0.95
1:C:67:THR:HG21	1:C:91:ARG:HH12	1.31	0.95
1:D:16:LEU:HB3	1:D:63:ILE:HD11	1.49	0.93
1:D:21:LEU:HD12	1:D:88:THR:HB	1.50	0.93
1:D:147:ILE:HD11	1:D:149:ALA:HB2	1.51	0.93
1:E:242:VAL:O	1:E:246:VAL:HG23	1.69	0.92
1:E:31:VAL:HG13	1:E:64:VAL:HG12	1.52	0.92
1:C:54:ARG:HH11	1:C:54:ARG:HB3	1.33	0.91
1:F:57:LEU:HD11	1:F:250:ARG:NH1	1.85	0.90
1:E:90:LEU:HD11	1:E:252:LEU:HD12	1.54	0.90
1:B:94:THR:HG22	1:B:220:ILE:HG21	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:ASN:H	1:D:194:ASN:HD22	1.18	0.90
1:E:240:HIS:O	1:E:244:ILE:HG12	1.72	0.89
1:E:17:GLN:HG3	1:E:54:ARG:HH21	1.35	0.89
1:F:38:MET:HB2	1:F:55:ALA:HB1	1.53	0.89
1:B:16:LEU:HD12	1:B:63:ILE:HG13	1.54	0.89
1:F:143:ALA:N	1:F:251:ARG:HH12	1.70	0.88
1:A:17:GLN:HG2	1:A:54:ARG:HE	1.36	0.88
1:C:21:LEU:HD23	1:C:22:ALA:N	1.86	0.88
1:E:11:LEU:HD22	1:E:44:LEU:HD22	1.55	0.88
1:E:87:ARG:HH11	1:E:87:ARG:HG3	1.39	0.88
1:B:9:LEU:HD11	1:B:81:LEU:HD23	1.55	0.87
1:B:126:MET:HE1	1:F:127:GLU:HG3	1.54	0.87
1:A:242:VAL:O	1:A:246:VAL:HG23	1.74	0.87
1:A:117:ASP:HA	1:A:160:ASP:OD1	1.75	0.87
1:B:194:ASN:HD22	1:B:194:ASN:H	1.24	0.86
1:F:163:TYR:HA	1:F:168:ARG:HD2	1.57	0.85
2:B:254:ACY:H2	1:D:48:ARG:HH12	1.41	0.85
1:E:44:LEU:HD12	1:E:54:ARG:HB2	1.57	0.84
1:A:186:GLU:O	1:A:190:MET:HG3	1.76	0.84
1:D:30:ARG:O	1:D:34:ILE:HG12	1.77	0.84
1:A:105:GLY:HA2	1:A:237:THR:HG23	1.58	0.84
1:C:107:VAL:HG21	1:C:244:ILE:HD12	1.58	0.84
1:B:163:TYR:HA	1:B:168:ARG:HD2	1.59	0.84
1:D:31:VAL:HG13	1:D:64:VAL:HG12	1.58	0.84
1:D:76:ILE:HG22	1:D:80:GLU:HG3	1.59	0.84
1:B:158:SER:HB3	1:B:200:ALA:HB2	1.58	0.83
1:C:67:THR:HG21	1:C:91:ARG:NH1	1.93	0.83
1:A:108:LEU:HD13	1:A:193:MET:HG3	1.59	0.83
1:A:179:ARG:HD2	1:A:180:PHE:CE1	2.12	0.83
1:F:194:ASN:HD22	1:F:194:ASN:H	1.23	0.83
1:A:156:THR:HG22	1:A:157:ALA:H	1.41	0.83
1:F:187:TRP:HB3	1:F:192:VAL:HG21	1.61	0.83
1:F:249:ALA:O	1:F:253:LEU:HG	1.79	0.82
1:A:6:VAL:HB	1:A:80:GLU:OE2	1.79	0.82
1:D:171:THR:HG22	1:D:172:TYR:N	1.96	0.81
1:F:240:HIS:O	1:F:244:ILE:HG12	1.80	0.81
1:B:25:PRO:HD2	1:B:65:CYS:O	1.79	0.81
1:E:15:ASP:O	1:E:44:LEU:HD11	1.81	0.81
1:E:57:LEU:HD21	1:E:250:ARG:HG2	1.62	0.81
1:F:44:LEU:HD11	1:F:54:ARG:HB2	1.60	0.81
1:A:91:ARG:O	1:A:91:ARG:HG3	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:ASN:HD22	1:B:194:ASN:N	1.78	0.80
1:F:30:ARG:NH2	1:F:238:GLU:HG2	1.96	0.80
1:E:194:ASN:HD22	1:E:194:ASN:N	1.79	0.80
1:D:179:ARG:HH11	1:D:179:ARG:HB2	1.45	0.79
1:F:89:PHE:O	1:F:90:LEU:HG	1.82	0.79
1:C:201:THR:HG22	1:C:205:MET:HE2	1.62	0.79
1:E:169:TYR:OH	1:E:181:LYS:HG3	1.82	0.79
1:A:16:LEU:HB3	1:A:63:ILE:CD1	2.13	0.79
1:A:196:GLU:CD	1:A:199:SER:H	1.86	0.79
1:B:69:ILE:HD12	1:B:69:ILE:H	1.46	0.79
1:D:133:ASP:CG	1:D:212:ARG:HG2	2.03	0.79
1:C:38:MET:HG3	1:C:57:LEU:HD13	1.63	0.79
1:C:231:ALA:O	1:C:234:MET:HB2	1.83	0.79
1:D:177:VAL:HG22	1:D:179:ARG:H	1.48	0.79
1:F:21:LEU:HD13	1:F:253:LEU:HD23	1.65	0.79
1:B:17:GLN:HG2	1:B:54:ARG:NH1	1.98	0.78
1:C:96:GLY:O	1:C:194:ASN:HB2	1.83	0.78
1:C:117:ASP:HA	1:C:160:ASP:HB2	1.64	0.78
1:C:44:LEU:HD11	1:C:54:ARG:HB2	1.64	0.78
1:F:54:ARG:HH11	1:F:54:ARG:CB	1.96	0.78
1:E:194:ASN:H	1:E:194:ASN:ND2	1.81	0.77
1:E:161:THR:OG1	1:E:165:GLY:HA3	1.84	0.77
1:F:114:VAL:HG11	1:F:187:TRP:CZ3	2.19	0.77
1:C:222:ASN:HB3	1:C:225:GLN:NE2	1.98	0.77
1:D:34:ILE:HD12	1:D:242:VAL:HG13	1.67	0.77
1:B:5:ASP:HB2	1:B:12:THR:HA	1.65	0.77
1:C:58:ASP:O	1:C:60:LYS:HG2	1.85	0.77
1:C:16:LEU:HD22	1:C:63:ILE:CD1	2.15	0.77
1:C:91:ARG:HB3	1:C:215:MET:HG3	1.67	0.77
1:F:236:GLN:HA	1:F:239:SER:OG	1.85	0.77
1:E:156:THR:HG23	1:E:194:ASN:ND2	1.99	0.76
1:D:161:THR:OG1	1:D:164:PRO:HG2	1.86	0.76
1:C:49:GLU:OE1	1:E:48:ARG:O	2.04	0.76
1:D:17:GLN:HE21	1:D:17:GLN:HA	1.50	0.76
1:D:247:GLU:O	1:D:250:ARG:HB2	1.86	0.76
1:B:137:THR:O	1:B:141:VAL:HG23	1.85	0.76
1:F:8:HIS:HB2	1:F:80:GLU:OE2	1.86	0.76
1:C:4:SER:N	1:C:12:THR:HG22	2.01	0.75
1:E:8:HIS:HB3	1:E:50:PHE:CE1	2.21	0.75
1:C:222:ASN:O	1:C:225:GLN:HB3	1.85	0.75
1:F:138:THR:O	1:F:142:GLU:HG3	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:GLY:HA3	2:B:254:ACY:H1	1.69	0.74
1:E:138:THR:O	1:E:142:GLU:HG3	1.87	0.74
1:C:21:LEU:HD21	1:C:90:LEU:HD12	1.69	0.74
1:F:142:GLU:HB2	1:F:251:ARG:NH1	2.03	0.74
1:A:156:THR:HG22	1:A:157:ALA:N	2.03	0.74
1:C:144:ALA:O	1:C:147:ILE:HD13	1.88	0.74
1:D:89:PHE:O	1:D:213:ALA:HA	1.87	0.74
1:B:230:ASN:HB2	1:B:233:THR:OG1	1.89	0.73
1:D:22:ALA:HA	1:D:63:ILE:O	1.87	0.73
1:F:6:VAL:HG21	1:F:9:LEU:HB2	1.70	0.73
1:D:34:ILE:HD12	1:D:242:VAL:CG1	2.18	0.73
1:E:22:ALA:CB	1:E:86:ILE:HD13	2.17	0.72
1:E:76:ILE:HA	1:E:79:GLU:OE1	1.88	0.72
1:E:86:ILE:O	1:E:87:ARG:HG3	1.88	0.72
1:A:48:ARG:HH11	1:A:48:ARG:HB3	1.52	0.72
1:F:229:PRO:HG2	1:F:234:MET:SD	2.29	0.72
1:E:115:ARG:NH1	1:E:126:MET:HA	2.04	0.72
1:F:22:ALA:HB2	1:F:86:ILE:HD12	1.69	0.72
1:F:220:ILE:O	1:F:229:PRO:HG3	1.88	0.72
1:F:104:VAL:HG21	1:F:227:GLU:OE1	1.90	0.72
1:C:54:ARG:HH11	1:C:54:ARG:CB	2.03	0.72
1:E:57:LEU:HD23	1:E:253:LEU:HD11	1.71	0.72
1:E:91:ARG:HG3	1:E:92:ILE:N	2.02	0.72
1:E:186:GLU:HG3	1:E:190:MET:HE1	1.71	0.72
1:B:158:SER:CB	1:B:200:ALA:HB2	2.20	0.72
1:F:163:TYR:HA	1:F:168:ARG:CD	2.20	0.72
1:F:11:LEU:HD21	1:F:52:SER:OG	1.90	0.71
1:E:17:GLN:HG2	1:E:54:ARG:HE	1.54	0.71
1:B:149:ALA:CB	1:B:244:ILE:HD11	2.21	0.71
1:A:17:GLN:HG3	1:A:54:ARG:HH21	1.56	0.71
1:C:28:PRO:HG3	1:C:49:GLU:OE2	1.90	0.71
1:F:147:ILE:HD11	1:F:244:ILE:HD11	1.70	0.71
1:C:104:VAL:CG1	1:C:229:PRO:HB3	2.15	0.71
1:F:230:ASN:ND2	1:F:232:GLU:H	1.87	0.71
1:E:184:MET:O	1:E:188:GLN:HG3	1.91	0.71
1:B:71:GLY:N	1:B:72:PRO:HD3	2.06	0.71
1:D:175:ARG:NH1	1:D:177:VAL:HA	2.06	0.71
1:F:112:ALA:HB2	1:F:131:VAL:HA	1.70	0.71
1:B:126:MET:CE	1:F:127:GLU:HG3	2.21	0.71
1:C:107:VAL:HG21	1:C:244:ILE:CD1	2.19	0.70
1:F:99:GLN:HB2	1:F:102:ILE:HG12	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:LYS:HB2	1:A:53:TRP:CZ2	2.26	0.70
1:F:238:GLU:OE1	1:F:238:GLU:N	2.24	0.70
1:D:96:GLY:HA2	1:D:221:VAL:O	1.90	0.70
1:A:12:THR:O	1:A:84:LEU:HD22	1.91	0.70
1:A:67:THR:HG21	1:A:74:THR:HG23	1.74	0.70
1:B:94:THR:HG22	1:B:220:ILE:HD13	1.73	0.70
1:F:196:GLU:OE2	1:F:198:GLU:N	2.24	0.70
1:B:151:THR:O	1:B:152:HIS:HD2	1.75	0.70
1:F:140:LEU:HD13	1:F:216:VAL:HB	1.74	0.70
1:C:25:PRO:HD2	1:C:65:CYS:O	1.92	0.70
1:E:93:GLY:O	1:E:217:ALA:HA	1.92	0.70
1:F:112:ALA:HA	1:F:130:ALA:O	1.92	0.69
1:C:54:ARG:HB3	1:C:54:ARG:NH1	2.07	0.69
1:D:171:THR:CG2	1:D:172:TYR:H	2.03	0.69
1:F:177:VAL:HG22	1:F:178:ARG:H	1.57	0.69
1:C:54:ARG:HG3	1:C:62:VAL:O	1.92	0.69
1:F:54:ARG:HB3	1:F:54:ARG:NH1	2.02	0.69
1:C:26:GLY:HA2	1:C:67:THR:OG1	1.92	0.69
1:D:72:PRO:O	1:D:75:SER:HB3	1.92	0.69
1:A:37:LEU:N	1:A:37:LEU:HD22	2.08	0.69
1:E:8:HIS:HB3	1:E:50:PHE:CD1	2.28	0.69
1:D:63:ILE:HD12	1:D:86:ILE:HD11	1.74	0.68
1:D:98:ILE:HG12	1:D:193:MET:O	1.93	0.68
1:E:21:LEU:HD23	1:E:22:ALA:N	2.07	0.68
1:E:27:ASP:OD2	1:E:29:GLU:HB2	1.93	0.68
1:E:38:MET:O	1:F:145:LYS:HE3	1.93	0.68
1:B:17:GLN:HA	1:B:17:GLN:HE21	1.58	0.68
1:C:79:GLU:O	1:C:83:GLN:HG3	1.92	0.68
1:B:108:LEU:HB3	1:B:193:MET:HE2	1.75	0.68
1:D:136:CYS:SG	1:D:212:ARG:HB3	2.34	0.68
1:A:137:THR:O	1:A:141:VAL:HG23	1.94	0.68
1:D:87:ARG:HH21	1:D:212:ARG:HH22	1.40	0.68
1:F:108:LEU:HD13	1:F:193:MET:HB3	1.76	0.68
1:C:49:GLU:OE2	1:C:49:GLU:HA	1.93	0.68
1:C:201:THR:HG22	1:C:205:MET:CE	2.23	0.68
1:D:228:ILE:N	1:D:228:ILE:HD13	2.08	0.68
1:B:232:GLU:HG3	1:B:235:LYS:HD3	1.76	0.68
1:B:104:VAL:HA	1:B:219:VAL:HG12	1.76	0.67
1:E:15:ASP:HB3	1:E:44:LEU:HD21	1.75	0.67
1:D:111:THR:O	1:D:131:VAL:HG23	1.94	0.67
1:E:17:GLN:HG3	1:E:54:ARG:NH2	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:94:THR:O	1:E:95:THR:HB	1.94	0.67
1:A:251:ARG:H	1:A:251:ARG:HD2	1.59	0.67
1:B:212:ARG:NH2	1:B:252:LEU:HD22	2.08	0.67
1:A:159:SER:OG	1:A:165:GLY:HA3	1.94	0.67
1:B:127:GLU:N	1:F:126:MET:HE1	2.09	0.67
1:E:161:THR:CB	1:E:165:GLY:HA3	2.25	0.67
1:C:175:ARG:NH2	1:E:208:SER:HB2	2.09	0.67
1:D:112:ALA:O	1:D:155:VAL:HG13	1.95	0.67
1:E:76:ILE:O	1:E:79:GLU:HG2	1.94	0.67
1:C:98:ILE:HG12	1:C:193:MET:O	1.95	0.67
1:C:228:ILE:HB	1:C:229:PRO:CD	2.21	0.67
1:D:194:ASN:HD22	1:D:194:ASN:N	1.89	0.67
1:F:126:MET:O	1:F:126:MET:SD	2.54	0.67
1:F:194:ASN:N	1:F:194:ASN:ND2	2.34	0.67
1:A:17:GLN:HG2	1:A:54:ARG:NE	2.09	0.66
1:E:159:SER:O	1:E:197:MET:HG2	1.95	0.66
1:F:25:PRO:O	1:F:66:SER:HA	1.95	0.66
1:A:11:LEU:HD21	1:A:52:SER:OG	1.96	0.66
1:E:44:LEU:H	1:E:53:TRP:HA	1.61	0.66
1:F:57:LEU:HD11	1:F:250:ARG:HH11	1.59	0.66
1:E:196:GLU:CD	1:E:199:SER:H	1.99	0.66
1:A:15:ASP:HB3	1:A:16:LEU:HD23	1.76	0.66
1:B:124:ALA:HA	1:D:175:ARG:HE	1.61	0.66
1:E:186:GLU:HG3	1:E:190:MET:CE	2.25	0.66
1:D:12:THR:HB	1:D:15:ASP:OD2	1.96	0.65
1:E:167:GLU:CG	1:E:183:SER:H	2.01	0.65
1:C:242:VAL:O	1:C:246:VAL:HG23	1.96	0.65
1:F:6:VAL:HB	1:F:80:GLU:OE1	1.95	0.65
1:B:159:SER:HB3	1:B:166:GLN:HE21	1.61	0.65
1:F:104:VAL:HG22	1:F:222:ASN:HB2	1.77	0.65
1:B:144:ALA:O	1:B:149:ALA:HB3	1.96	0.65
1:B:194:ASN:N	1:B:194:ASN:ND2	2.44	0.65
1:D:178:ARG:NH2	1:D:181:LYS:NZ	2.44	0.65
1:C:201:THR:O	1:C:205:MET:HE2	1.97	0.65
1:B:164:PRO:C	1:B:166:GLN:H	2.00	0.65
1:D:87:ARG:HH21	1:D:212:ARG:NH2	1.95	0.65
1:B:115:ARG:NH2	1:B:121:LEU:HD23	2.12	0.65
1:B:164:PRO:HG2	1:B:165:GLY:H	1.61	0.65
1:E:69:ILE:HD13	1:E:69:ILE:N	2.11	0.65
1:E:239:SER:HA	1:E:242:VAL:HG23	1.78	0.65
1:A:162:PHE:HB2	1:A:197:MET:SD	2.37	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:ILE:HD12	1:B:69:ILE:N	2.12	0.65
1:B:98:ILE:HD11	1:B:192:VAL:O	1.97	0.65
1:D:104:VAL:O	1:D:233:THR:HG21	1.96	0.65
1:B:15:ASP:O	1:B:54:ARG:HD3	1.96	0.64
1:F:38:MET:CB	1:F:55:ALA:HB1	2.27	0.64
1:F:184:MET:O	1:F:188:GLN:HB2	1.97	0.64
1:B:89:PHE:O	1:B:90:LEU:HD12	1.97	0.64
1:D:151:THR:HG22	1:D:152:HIS:N	2.11	0.64
1:D:67:THR:HG22	1:D:77:ALA:CB	2.27	0.64
1:A:86:ILE:O	1:A:87:ARG:HG2	1.98	0.64
1:C:13:LYS:HE3	1:C:84:LEU:O	1.97	0.64
1:A:136:CYS:O	1:A:140:LEU:HG	1.97	0.64
1:D:91:ARG:HB3	1:D:215:MET:HG2	1.80	0.64
1:F:196:GLU:OE2	1:F:199:SER:N	2.26	0.64
1:B:71:GLY:N	1:B:72:PRO:CD	2.61	0.64
1:B:168:ARG:CZ	1:B:223:ARG:HH22	2.11	0.64
1:C:21:LEU:HD21	1:C:90:LEU:CD1	2.28	0.63
1:D:163:TYR:N	1:D:164:PRO:HD2	2.13	0.63
1:E:237:THR:HA	1:E:240:HIS:CD2	2.33	0.63
1:F:132:ALA:HB2	1:F:203:LEU:HD22	1.80	0.63
1:F:161:THR:HB	1:F:164:PRO:HG2	1.79	0.63
1:F:162:PHE:O	1:F:168:ARG:HD2	1.98	0.63
1:A:117:ASP:CA	1:A:160:ASP:OD1	2.45	0.63
1:F:196:GLU:CD	1:F:199:SER:H	2.00	0.63
1:E:57:LEU:HD11	1:E:250:ARG:HG2	1.81	0.63
1:D:40:LYS:O	1:D:42:VAL:HG23	1.98	0.63
1:D:87:ARG:HA	1:D:211:LEU:HD22	1.80	0.63
1:F:34:ILE:HD13	1:F:242:VAL:HG13	1.80	0.63
1:F:163:TYR:CG	1:F:168:ARG:HD3	2.33	0.63
1:B:62:VAL:HG22	1:B:253:LEU:HD11	1.81	0.63
1:B:169:TYR:O	1:B:171:THR:N	2.29	0.63
1:E:76:ILE:O	1:E:80:GLU:HG2	1.99	0.63
1:F:144:ALA:HA	1:F:244:ILE:HD12	1.80	0.63
1:A:177:VAL:O	1:A:181:LYS:HG3	1.99	0.63
1:B:94:THR:CG2	1:B:220:ILE:HD13	2.28	0.63
1:C:158:SER:HB3	1:C:200:ALA:HB2	1.79	0.63
1:D:175:ARG:CZ	1:D:177:VAL:HA	2.28	0.63
1:A:131:VAL:HG22	1:A:132:ALA:N	2.14	0.62
1:A:201:THR:O	1:A:205:MET:HB3	1.99	0.62
1:A:241:ALA:HA	1:A:244:ILE:HD12	1.81	0.62
1:B:138:THR:O	1:B:142:GLU:HG3	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:ALA:HA	1:C:203:LEU:HD22	1.82	0.62
1:F:176:VAL:HG12	1:F:177:VAL:H	1.65	0.62
1:E:196:GLU:O	1:E:197:MET:HG3	1.97	0.62
1:A:101:HIS:CE1	1:A:102:ILE:HG13	2.34	0.62
1:B:235:LYS:HA	1:B:238:GLU:OE1	2.00	0.62
1:F:142:GLU:O	1:F:145:LYS:HB3	1.99	0.62
1:E:22:ALA:HB2	1:E:86:ILE:CD1	2.21	0.62
1:E:49:GLU:HA	1:E:49:GLU:OE2	1.99	0.62
1:E:247:GLU:OE2	1:E:250:ARG:NE	2.33	0.62
1:F:34:ILE:O	1:F:36:ALA:N	2.33	0.62
1:C:25:PRO:O	1:C:67:THR:HG23	2.00	0.61
1:E:17:GLN:CG	1:E:54:ARG:HE	2.13	0.61
1:A:48:ARG:HB3	1:A:48:ARG:NH1	2.15	0.61
1:C:38:MET:HB3	1:C:56:GLU:O	2.00	0.61
1:E:63:ILE:HD12	1:E:86:ILE:HD11	1.82	0.61
1:B:108:LEU:HB3	1:B:193:MET:CE	2.29	0.61
1:E:175:ARG:HD2	1:E:176:VAL:N	2.15	0.61
1:F:120:SER:HB3	1:F:201:THR:HA	1.82	0.61
1:E:63:ILE:HG22	1:E:64:VAL:N	2.14	0.61
1:B:104:VAL:HA	1:B:219:VAL:CG1	2.31	0.61
1:C:143:ALA:O	1:C:147:ILE:HG23	2.01	0.61
1:F:78:VAL:HG11	1:F:205:MET:SD	2.41	0.61
1:A:21:LEU:HD23	1:A:22:ALA:N	2.16	0.61
1:B:190:MET:HE1	1:F:124:ALA:HA	1.82	0.61
1:C:79:GLU:HG3	1:C:83:GLN:HE21	1.64	0.60
1:C:233:THR:HA	1:C:236:GLN:HG3	1.81	0.60
1:E:167:GLU:HG3	1:E:183:SER:N	2.00	0.60
1:A:28:PRO:HB3	1:A:49:GLU:O	2.01	0.60
1:E:141:VAL:O	1:E:145:LYS:HB2	2.01	0.60
1:B:88:THR:HA	1:B:212:ARG:HB2	1.84	0.60
1:C:27:ASP:HA	1:E:48:ARG:NH1	2.15	0.60
1:B:23:ILE:HG22	1:B:24:VAL:N	2.15	0.60
1:A:226:GLN:NE2	1:A:227:GLU:H	1.99	0.60
1:C:220:ILE:HG13	1:C:234:MET:SD	2.40	0.60
1:F:145:LYS:C	1:F:147:ILE:H	2.05	0.60
1:F:184:MET:HA	1:F:195:TYR:OH	2.02	0.60
1:B:8:HIS:HB3	1:B:50:PHE:CE1	2.36	0.60
1:C:123:PHE:HA	1:E:175:ARG:HH21	1.65	0.60
1:A:116:LEU:HB2	1:A:158:SER:O	2.01	0.60
1:E:139:ALA:CB	1:E:252:LEU:HD21	2.31	0.60
1:F:163:TYR:CD2	1:F:168:ARG:HD3	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:GLU:O	1:A:250:ARG:HB2	2.01	0.60
1:B:89:PHE:C	1:B:90:LEU:HD12	2.22	0.60
1:C:137:THR:O	1:C:141:VAL:HG23	2.01	0.60
1:D:87:ARG:NH2	1:D:212:ARG:HH22	2.00	0.60
1:D:90:LEU:HD21	1:D:252:LEU:CD1	2.32	0.60
1:E:96:GLY:HA2	1:E:221:VAL:O	2.02	0.60
1:F:247:GLU:OE2	1:F:250:ARG:NE	2.33	0.60
1:A:132:ALA:HA	1:A:203:LEU:HD22	1.83	0.60
1:B:102:ILE:HG12	1:B:152:HIS:CE1	2.37	0.60
1:B:102:ILE:HG12	1:B:152:HIS:ND1	2.17	0.60
1:F:62:VAL:HG12	1:F:63:ILE:N	2.17	0.60
1:F:227:GLU:O	1:F:228:ILE:HG23	2.02	0.60
1:C:229:PRO:HB2	1:C:233:THR:HB	1.82	0.59
1:B:246:VAL:O	1:B:249:ALA:HB3	2.01	0.59
1:C:78:VAL:HG13	1:C:89:PHE:CZ	2.36	0.59
1:E:216:VAL:HG13	1:E:216:VAL:O	2.01	0.59
1:C:228:ILE:CB	1:C:229:PRO:HD2	2.23	0.59
1:E:92:ILE:HD12	1:E:93:GLY:H	1.66	0.59
1:A:23:ILE:O	1:A:64:VAL:HA	2.02	0.59
1:C:38:MET:HB2	1:C:55:ALA:HB1	1.85	0.59
1:E:25:PRO:O	1:E:66:SER:HA	2.02	0.59
1:E:136:CYS:O	1:E:140:LEU:HG	2.03	0.59
1:F:29:GLU:O	1:F:32:GLU:N	2.34	0.59
1:C:163:TYR:HD2	1:C:171:THR:HG22	1.67	0.59
1:C:30:ARG:HD3	1:C:33:LYS:HG3	1.82	0.59
1:C:172:TYR:HB2	1:E:83:GLN:HG3	1.85	0.59
1:D:162:PHE:HA	1:D:166:GLN:HE21	1.66	0.59
1:E:17:GLN:HA	1:E:17:GLN:NE2	2.11	0.59
1:E:23:ILE:HD13	1:E:90:LEU:HB2	1.83	0.59
1:F:92:ILE:HD11	1:F:241:ALA:HB1	1.84	0.59
1:B:21:LEU:CD2	1:B:22:ALA:N	2.61	0.59
1:D:95:THR:O	1:D:219:VAL:HA	2.03	0.59
1:B:23:ILE:HG22	1:B:24:VAL:H	1.68	0.58
1:B:60:LYS:CD	1:B:253:LEU:HB3	2.27	0.58
1:A:30:ARG:HH11	1:A:30:ARG:HG2	1.68	0.58
1:B:24:VAL:HG23	1:B:24:VAL:O	2.03	0.58
1:D:6:VAL:HB	1:D:80:GLU:OE1	2.02	0.58
1:A:87:ARG:HA	1:A:211:LEU:HD22	1.85	0.58
1:B:105:GLY:HA2	1:B:237:THR:HG23	1.85	0.58
1:B:122:HIS:O	1:D:175:ARG:O	2.22	0.58
1:C:9:LEU:HD11	1:C:81:LEU:HG	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:PHE:HA	1:C:166:GLN:NE2	2.19	0.58
1:D:79:GLU:O	1:D:83:GLN:HB2	2.03	0.58
1:E:39:ASP:O	1:E:40:LYS:HB2	2.03	0.58
1:F:221:VAL:HG22	1:F:223:ARG:N	2.18	0.58
1:B:24:VAL:HA	1:B:65:CYS:O	2.04	0.58
1:E:90:LEU:HD11	1:E:252:LEU:CD1	2.31	0.58
1:C:67:THR:CG2	1:C:91:ARG:HH12	2.13	0.58
1:C:136:CYS:HA	1:C:252:LEU:HD11	1.85	0.58
1:E:11:LEU:CD2	1:E:44:LEU:HD22	2.28	0.58
1:B:35:ALA:HA	1:B:38:MET:CE	2.33	0.58
1:C:94:THR:CG2	1:C:220:ILE:HB	2.34	0.58
1:C:160:ASP:O	1:E:72:PRO:HB3	2.03	0.58
1:E:24:VAL:HA	1:E:65:CYS:O	2.04	0.58
1:A:151:THR:HG22	1:A:152:HIS:N	2.19	0.58
1:A:245:VAL:HA	1:A:248:ALA:HB3	1.86	0.58
1:B:56:GLU:CD	1:B:59:GLY:HA2	2.24	0.58
1:E:40:LYS:N	1:E:41:PRO:CD	2.65	0.58
1:E:147:ILE:C	1:E:147:ILE:HD13	2.24	0.58
1:A:72:PRO:O	1:A:76:ILE:HG12	2.04	0.58
1:E:46:SER:HA	1:E:51:THR:HA	1.85	0.58
1:F:183:SER:O	1:F:186:GLU:HB3	2.02	0.58
1:A:155:VAL:HG23	1:A:192:VAL:HA	1.85	0.58
1:B:31:VAL:HG12	1:B:53:TRP:HB2	1.86	0.58
1:E:216:VAL:HG11	1:E:245:VAL:HB	1.86	0.58
1:F:94:THR:O	1:F:95:THR:HB	2.03	0.58
1:A:95:THR:OG1	1:A:96:GLY:N	2.36	0.57
1:A:221:VAL:HG13	1:A:221:VAL:O	2.02	0.57
1:C:201:THR:O	1:C:205:MET:HG2	2.04	0.57
1:E:158:SER:HB3	1:E:200:ALA:HB2	1.84	0.57
1:B:23:ILE:O	1:B:24:VAL:HG13	2.04	0.57
1:B:228:ILE:HD13	1:B:228:ILE:H	1.69	0.57
1:C:21:LEU:CD2	1:C:22:ALA:N	2.63	0.57
1:C:98:ILE:O	1:C:224:THR:HG21	2.04	0.57
1:F:6:VAL:CG2	1:F:9:LEU:HB2	2.34	0.57
1:A:225:GLN:HG2	1:A:226:GLN:N	2.19	0.57
1:A:239:SER:O	1:A:242:VAL:HB	2.05	0.57
1:B:15:ASP:HB3	1:B:44:LEU:HD22	1.86	0.57
1:E:177:VAL:CG1	1:E:180:PHE:HB2	2.33	0.57
1:A:180:PHE:HA	1:A:183:SER:HB2	1.85	0.57
1:A:240:HIS:O	1:A:244:ILE:HG13	2.04	0.57
1:D:99:GLN:HA	1:D:99:GLN:OE1	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:GLN:CG	1:A:54:ARG:HE	2.11	0.57
1:B:169:TYR:HE2	1:B:176:VAL:HG23	1.70	0.57
1:D:16:LEU:CB	1:D:63:ILE:HD11	2.29	0.57
1:F:220:ILE:HG13	1:F:221:VAL:N	2.19	0.57
1:B:242:VAL:O	1:B:245:VAL:HG12	2.05	0.57
1:E:232:GLU:HG3	1:E:236:GLN:OE1	2.04	0.57
1:C:38:MET:HG3	1:C:57:LEU:HB2	1.85	0.57
1:B:17:GLN:HA	1:B:17:GLN:NE2	2.19	0.57
1:C:147:ILE:HD12	1:C:244:ILE:HG12	1.85	0.57
1:E:87:ARG:HG3	1:E:87:ARG:NH1	2.15	0.57
1:B:43:LYS:HB2	1:B:53:TRP:CZ2	2.40	0.57
1:E:137:THR:O	1:E:141:VAL:HG23	2.04	0.57
1:B:35:ALA:HA	1:B:38:MET:HE3	1.87	0.57
1:F:97:ALA:CB	1:F:102:ILE:HB	2.35	0.57
1:F:21:LEU:HG	1:F:88:THR:HB	1.86	0.56
1:F:29:GLU:O	1:F:30:ARG:C	2.43	0.56
1:B:90:LEU:HD23	1:B:140:LEU:HD21	1.87	0.56
1:B:91:ARG:HB3	1:B:215:MET:HG3	1.86	0.56
1:C:62:VAL:CG1	1:C:63:ILE:N	2.67	0.56
1:C:156:THR:HG23	1:C:194:ASN:O	2.05	0.56
1:D:16:LEU:HD22	1:D:63:ILE:CD1	2.35	0.56
1:D:159:SER:HB2	1:D:195:TYR:HE1	1.70	0.56
1:A:196:GLU:CD	1:A:198:GLU:H	2.08	0.56
1:A:244:ILE:O	1:A:248:ALA:N	2.28	0.56
1:C:229:PRO:O	1:C:230:ASN:HB2	2.04	0.56
1:D:228:ILE:HD13	1:D:228:ILE:H	1.70	0.56
1:E:42:VAL:O	1:E:43:LYS:C	2.43	0.56
1:E:176:VAL:HG12	1:E:180:PHE:HB3	1.85	0.56
1:F:5:ASP:HB2	1:F:12:THR:HA	1.85	0.56
1:B:128:PHE:CD1	1:B:129:PRO:HD2	2.40	0.56
1:C:126:MET:O	1:C:126:MET:HG3	2.05	0.56
1:F:168:ARG:HB3	1:F:170:ASP:OD2	2.05	0.56
1:B:144:ALA:CB	1:B:244:ILE:HD13	2.36	0.56
1:D:82:ALA:HB2	1:D:89:PHE:CZ	2.41	0.56
1:D:242:VAL:O	1:D:246:VAL:HG23	2.05	0.56
1:F:39:ASP:HB2	1:F:56:GLU:HB3	1.87	0.56
1:F:106:ASP:OD1	1:F:106:ASP:N	2.38	0.56
1:F:114:VAL:HG12	1:F:116:LEU:HG	1.88	0.56
1:A:23:ILE:HB	1:A:64:VAL:HG12	1.87	0.56
1:D:232:GLU:HG3	1:D:236:GLN:OE1	2.05	0.56
1:F:56:GLU:HA	1:F:60:LYS:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:GLN:CG	1:A:54:ARG:HH21	2.18	0.56
1:A:151:THR:HG22	1:A:152:HIS:H	1.71	0.56
1:B:12:THR:O	1:B:14:ASN:N	2.33	0.56
1:B:104:VAL:HG13	1:B:219:VAL:O	2.06	0.56
1:A:196:GLU:OE2	1:A:199:SER:N	2.35	0.56
1:C:149:ALA:O	1:C:151:THR:N	2.39	0.56
1:B:13:LYS:HE2	1:B:84:LEU:O	2.06	0.55
1:B:49:GLU:OE2	1:B:49:GLU:HA	2.06	0.55
1:B:114:VAL:HG22	1:F:128:PHE:HA	1.88	0.55
1:D:158:SER:HB3	1:D:200:ALA:HB2	1.88	0.55
1:E:161:THR:HB	1:E:165:GLY:HA3	1.88	0.55
1:F:98:ILE:HD12	1:F:195:TYR:CD2	2.41	0.55
1:A:81:LEU:O	1:A:84:LEU:HB2	2.06	0.55
1:B:228:ILE:HB	1:B:229:PRO:HD2	1.88	0.55
1:C:138:THR:O	1:C:142:GLU:HG3	2.07	0.55
1:D:156:THR:CB	1:D:194:ASN:HD21	2.19	0.55
1:D:187:TRP:HA	1:D:187:TRP:CE3	2.42	0.55
1:A:13:LYS:C	1:A:15:ASP:H	2.10	0.55
1:A:24:VAL:O	1:A:24:VAL:HG23	2.07	0.55
1:A:49:GLU:CG	1:F:49:GLU:HG2	2.37	0.55
1:A:113:SER:OG	1:A:156:THR:HB	2.06	0.55
1:E:177:VAL:HG13	1:E:180:PHE:HB2	1.88	0.55
1:E:239:SER:HA	1:E:242:VAL:CG2	2.36	0.55
1:F:237:THR:HB	1:F:238:GLU:OE1	2.05	0.55
1:B:30:ARG:HH12	1:B:93:GLY:HA2	1.71	0.55
1:B:32:GLU:HG2	1:B:53:TRP:CZ2	2.41	0.55
1:B:34:ILE:HD13	1:B:242:VAL:HG13	1.88	0.55
1:A:56:GLU:HG2	1:A:57:LEU:H	1.71	0.55
1:B:128:PHE:HA	1:F:114:VAL:HG22	1.88	0.55
1:F:63:ILE:CG2	1:F:64:VAL:N	2.69	0.55
1:A:178:ARG:HA	1:A:181:LYS:HE2	1.88	0.55
1:B:57:LEU:HG	1:B:250:ARG:HG2	1.89	0.55
1:B:166:GLN:HG2	1:B:195:TYR:CD1	2.42	0.55
1:D:166:GLN:NE2	1:D:168:ARG:HH22	2.04	0.55
1:E:7:PHE:O	1:E:9:LEU:N	2.40	0.55
1:D:242:VAL:O	1:D:245:VAL:HG12	2.07	0.55
1:E:44:LEU:HB2	1:E:53:TRP:O	2.07	0.55
1:F:62:VAL:CG1	1:F:63:ILE:N	2.70	0.55
1:B:23:ILE:O	1:B:24:VAL:CG1	2.55	0.55
1:A:160:ASP:HB3	1:F:119:ALA:HB2	1.89	0.55
1:F:196:GLU:OE2	1:F:197:MET:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:ILE:C	1:D:147:ILE:HD12	2.28	0.54
1:F:37:LEU:HD22	1:F:242:VAL:HG12	1.88	0.54
1:A:15:ASP:OD1	1:A:44:LEU:HD13	2.07	0.54
1:C:26:GLY:C	1:E:48:ARG:HH12	2.10	0.54
1:C:87:ARG:HA	1:C:211:LEU:HD22	1.88	0.54
1:E:54:ARG:NH1	1:E:54:ARG:HG2	2.23	0.54
1:E:71:GLY:N	1:E:72:PRO:CD	2.70	0.54
1:C:237:THR:C	1:C:239:SER:H	2.11	0.54
1:D:31:VAL:HG13	1:D:64:VAL:CG1	2.35	0.54
1:E:139:ALA:HB2	1:E:252:LEU:HD21	1.89	0.54
1:A:143:ALA:O	1:A:146:SER:HB3	2.08	0.54
1:A:223:ARG:O	1:A:225:GLN:N	2.41	0.54
1:B:106:ASP:O	1:B:219:VAL:HG23	2.07	0.54
1:B:107:VAL:HG11	1:B:149:ALA:HB1	1.89	0.54
1:C:131:VAL:HG22	1:C:132:ALA:O	2.08	0.54
1:D:171:THR:C	1:D:173:SER:H	2.10	0.54
1:E:24:VAL:HG23	1:E:24:VAL:O	2.07	0.54
1:A:167:GLU:O	1:A:167:GLU:HG2	2.07	0.54
1:B:123:PHE:O	1:D:175:ARG:HD3	2.07	0.54
1:B:124:ALA:CA	1:D:175:ARG:HE	2.20	0.54
1:E:92:ILE:HG13	1:E:93:GLY:N	2.21	0.54
1:E:98:ILE:HG12	1:E:193:MET:O	2.07	0.54
1:F:50:PHE:CD2	1:F:50:PHE:N	2.74	0.54
1:F:234:MET:O	1:F:238:GLU:OE2	2.25	0.54
1:B:9:LEU:HD13	1:B:11:LEU:HD12	1.87	0.54
1:C:251:ARG:HG2	1:C:251:ARG:HH11	1.73	0.54
1:F:158:SER:HA	1:F:196:GLU:O	2.08	0.54
1:A:176:VAL:O	1:A:181:LYS:HG2	2.08	0.54
1:B:162:PHE:O	1:B:168:ARG:NE	2.40	0.54
1:B:209:GLN:NE2	1:D:174:GLY:HA2	2.23	0.54
1:C:31:VAL:HG12	1:C:53:TRP:HB2	1.90	0.54
1:D:162:PHE:HA	1:D:166:GLN:NE2	2.23	0.54
1:E:87:ARG:HH11	1:E:87:ARG:CG	2.16	0.54
1:F:15:ASP:HB3	1:F:44:LEU:HD22	1.90	0.54
1:F:145:LYS:O	1:F:147:ILE:N	2.40	0.54
1:A:18:GLY:O	1:A:19:ALA:C	2.45	0.54
1:B:56:GLU:OE1	1:B:59:GLY:HA2	2.08	0.54
1:D:74:THR:O	1:D:78:VAL:HG23	2.07	0.54
1:F:34:ILE:O	1:F:37:LEU:N	2.40	0.54
1:F:157:ALA:O	1:F:195:TYR:HA	2.06	0.54
1:A:132:ALA:CA	1:A:203:LEU:HD22	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:ALA:HB2	1:D:89:PHE:HZ	1.73	0.54
1:E:91:ARG:NH2	1:E:198:GLU:OE1	2.41	0.54
1:F:63:ILE:HG22	1:F:64:VAL:N	2.23	0.54
1:F:132:ALA:HB2	1:F:203:LEU:CD2	2.38	0.54
1:C:38:MET:CB	1:C:55:ALA:HB1	2.38	0.53
1:C:49:GLU:HG2	1:E:49:GLU:OE2	2.07	0.53
1:D:16:LEU:HD11	1:D:84:LEU:HB3	1.90	0.53
1:D:156:THR:HG23	1:D:194:ASN:ND2	2.23	0.53
1:E:28:PRO:HA	1:E:31:VAL:HG23	1.89	0.53
1:E:194:ASN:N	1:E:194:ASN:ND2	2.47	0.53
1:A:28:PRO:HA	1:A:31:VAL:HG23	1.90	0.53
1:A:111:THR:O	1:A:131:VAL:HG23	2.08	0.53
1:A:222:ASN:HB3	1:A:225:GLN:HB3	1.89	0.53
1:D:89:PHE:HE1	1:D:211:LEU:HD13	1.72	0.53
1:A:35:ALA:HA	1:A:38:MET:HE3	1.90	0.53
1:C:35:ALA:HA	1:C:38:MET:HE2	1.89	0.53
1:D:194:ASN:H	1:D:194:ASN:ND2	1.98	0.53
1:D:245:VAL:HG13	1:D:246:VAL:N	2.22	0.53
1:F:92:ILE:HD11	1:F:241:ALA:CB	2.38	0.53
1:B:17:GLN:HE21	1:B:17:GLN:CA	2.20	0.53
1:E:88:THR:HA	1:E:212:ARG:O	2.09	0.53
1:F:82:ALA:HA	1:F:86:ILE:O	2.09	0.53
1:A:95:THR:HG22	1:A:217:ALA:HB1	1.90	0.53
1:B:115:ARG:HH21	1:B:121:LEU:HD23	1.74	0.53
1:D:178:ARG:NH2	1:D:181:LYS:HZ1	2.07	0.53
1:E:142:GLU:OE1	1:E:251:ARG:HD2	2.09	0.53
1:A:53:TRP:HB2	1:A:64:VAL:HG23	1.90	0.53
1:B:71:GLY:H	1:B:72:PRO:HD3	1.73	0.53
1:C:7:PHE:N	1:C:80:GLU:OE2	2.42	0.53
1:D:15:ASP:OD2	1:D:15:ASP:N	2.42	0.53
1:E:34:ILE:HG22	1:E:64:VAL:HG21	1.91	0.53
1:E:216:VAL:HG21	1:E:244:ILE:HG21	1.91	0.53
1:A:128:PHE:CD1	1:A:129:PRO:HD2	2.44	0.53
1:C:19:ALA:HA	1:C:61:ALA:O	2.08	0.53
1:D:89:PHE:CE1	1:D:211:LEU:HD13	2.42	0.53
1:A:196:GLU:OE2	1:A:198:GLU:N	2.41	0.53
1:B:111:THR:OG1	1:F:131:VAL:HG21	2.09	0.53
1:F:233:THR:C	1:F:235:LYS:H	2.11	0.53
1:F:247:GLU:CD	1:F:250:ARG:HH21	2.12	0.53
1:B:81:LEU:HA	1:B:84:LEU:HD12	1.89	0.53
1:D:91:ARG:HG2	1:D:215:MET:SD	2.48	0.53

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:D:16:LEU:HD22	1:D:63:ILE:HD11	1.89	0.52
1:D:24:VAL:HB	1:D:67:THR:HG23	1.91	0.52
1:E:126:MET:O	1:E:126:MET:HG3	2.08	0.52
1:F:165:GLY:O	1:F:167:GLU:N	2.42	0.52
1:A:34:ILE:HA	1:A:37:LEU:HD23	1.90	0.52
1:B:5:ASP:CB	1:B:12:THR:HA	2.36	0.52
1:B:116:LEU:HB2	1:B:158:SER:O	2.10	0.52
1:D:71:GLY:N	1:D:72:PRO:CD	2.72	0.52
1:E:13:LYS:HE3	1:E:84:LEU:O	2.08	0.52
1:E:40:LYS:HE2	1:F:142:GLU:OE2	2.09	0.52
1:E:185:GLU:O	1:E:188:GLN:HB2	2.10	0.52
1:A:161:THR:HG22	1:F:119:ALA:HB1	1.91	0.52
1:B:26:GLY:HA2	1:B:67:THR:OG1	2.09	0.52
1:D:28:PRO:HB3	1:D:51:THR:OG1	2.10	0.52
1:D:115:ARG:NH1	1:D:128:PHE:O	2.41	0.52
1:E:162:PHE:O	1:E:166:GLN:HB2	2.10	0.52
1:F:151:THR:CG2	1:F:152:HIS:N	2.73	0.52
1:A:49:GLU:HG2	1:F:49:GLU:HG2	1.92	0.52
1:B:62:VAL:CG2	1:B:253:LEU:HD11	2.39	0.52
1:C:235:LYS:HA	1:C:238:GLU:OE2	2.09	0.52
1:D:164:PRO:O	1:D:176:VAL:HG13	2.09	0.52
1:C:95:THR:O	1:C:220:ILE:HG22	2.09	0.52
1:F:6:VAL:CG2	1:F:10:GLY:H	2.22	0.52
1:A:156:THR:CG2	1:A:157:ALA:H	2.18	0.52
1:A:163:TYR:HA	1:A:168:ARG:HD2	1.90	0.52
1:B:212:ARG:NH2	1:B:252:LEU:HB3	2.25	0.52
1:D:188:GLN:O	1:D:190:MET:N	2.43	0.52
1:D:219:VAL:HG12	1:D:221:VAL:O	2.10	0.52
1:E:26:GLY:O	1:E:27:ASP:HB2	2.09	0.52
1:E:56:GLU:HA	1:E:60:LYS:O	2.09	0.52
1:F:243:LYS:O	1:F:247:GLU:HB2	2.10	0.52
1:B:43:LYS:HB2	1:B:53:TRP:CH2	2.44	0.52
1:C:169:TYR:C	1:C:171:THR:H	2.12	0.52
1:D:133:ASP:CB	1:D:212:ARG:HG2	2.38	0.52
1:E:206:CYS:HB3	1:E:211:LEU:O	2.08	0.52
1:A:105:GLY:H	1:A:219:VAL:HB	1.75	0.52
1:D:151:THR:CG2	1:D:152:HIS:N	2.72	0.52
1:E:25:PRO:HB3	1:E:92:ILE:HG23	1.92	0.52
1:B:15:ASP:O	1:B:54:ARG:NH1	2.42	0.52
1:D:138:THR:O	1:D:142:GLU:HG3	2.10	0.52
1:F:230:ASN:O	1:F:234:MET:SD	2.68	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:THR:HG23	1:A:194:ASN:CG	2.30	0.52
1:B:69:ILE:H	1:B:69:ILE:CD1	2.22	0.52
1:D:187:TRP:HA	1:D:187:TRP:HE3	1.75	0.52
1:F:17:GLN:HE21	1:F:17:GLN:HA	1.74	0.52
1:F:103:ASN:HB2	1:F:106:ASP:OD1	2.08	0.52
1:A:108:LEU:CD1	1:A:194:ASN:HB3	2.39	0.51
1:B:47:HIS:O	1:B:48:ARG:C	2.48	0.51
1:B:133:ASP:OD2	1:B:135:ALA:HB3	2.09	0.51
1:D:206:CYS:SG	1:D:213:ALA:HB2	2.50	0.51
1:E:161:THR:O	1:E:166:GLN:HG3	2.11	0.51
1:B:81:LEU:HD12	1:B:89:PHE:HE2	1.74	0.51
1:B:92:ILE:CD1	1:B:241:ALA:HB1	2.40	0.51
1:D:36:ALA:O	1:D:37:LEU:HG	2.10	0.51
1:D:162:PHE:O	1:D:166:GLN:HG3	2.10	0.51
1:D:179:ARG:HH11	1:D:179:ARG:CB	2.20	0.51
1:E:81:LEU:HD22	1:E:86:ILE:HD12	1.92	0.51
1:F:145:LYS:C	1:F:147:ILE:N	2.64	0.51
1:C:112:ALA:HA	1:C:130:ALA:O	2.10	0.51
1:B:28:PRO:HG3	1:B:49:GLU:OE1	2.11	0.51
1:E:58:ASP:O	1:E:60:LYS:HG2	2.10	0.51
1:E:158:SER:HB2	1:E:199:SER:HG	1.76	0.51
1:A:162:PHE:O	1:A:166:GLN:HG3	2.10	0.51
1:B:48:ARG:HH22	1:D:26:GLY:C	2.14	0.51
1:B:103:ASN:HB2	1:B:106:ASP:OD1	2.11	0.51
1:D:137:THR:O	1:D:137:THR:HG22	2.11	0.51
1:E:8:HIS:HB3	1:E:50:PHE:HE1	1.70	0.51
1:F:187:TRP:O	1:F:192:VAL:HG23	2.10	0.51
1:A:5:ASP:OD1	1:A:12:THR:HA	2.11	0.51
1:A:8:HIS:H	1:A:8:HIS:HD1	1.53	0.51
1:C:5:ASP:OD1	1:C:12:THR:HA	2.11	0.51
1:D:38:MET:HG2	1:D:57:LEU:HD13	1.93	0.51
1:D:76:ILE:HG22	1:D:80:GLU:CG	2.36	0.51
1:E:29:GLU:O	1:E:33:LYS:HG2	2.11	0.51
1:F:57:LEU:HB3	1:F:253:LEU:HD11	1.92	0.51
1:F:161:THR:O	1:F:166:GLN:HG2	2.11	0.51
1:F:176:VAL:HB	1:F:180:PHE:HB2	1.93	0.51
1:E:21:LEU:HD22	1:E:62:VAL:HG13	1.93	0.51
1:E:54:ARG:HG2	1:E:54:ARG:HH11	1.74	0.51
1:B:28:PRO:HG3	1:B:49:GLU:CD	2.32	0.51
2:B:254:ACY:CH3	1:D:48:ARG:HH12	2.18	0.51
1:F:151:THR:HG23	1:F:152:HIS:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:159:SER:HB3	1:F:166:GLN:NE2	2.25	0.51
1:A:227:GLU:O	1:A:228:ILE:C	2.50	0.50
1:B:57:LEU:CG	1:B:250:ARG:HG2	2.41	0.50
1:B:142:GLU:CD	1:E:42:VAL:HG13	2.32	0.50
1:B:236:GLN:HA	1:B:239:SER:OG	2.11	0.50
1:C:31:VAL:HG21	1:C:51:THR:HB	1.93	0.50
1:F:48:ARG:HG2	1:F:48:ARG:HH11	1.75	0.50
1:D:178:ARG:HG3	1:D:178:ARG:HH11	1.76	0.50
1:E:160:ASP:O	1:E:161:THR:HG23	2.12	0.50
1:A:177:VAL:HG22	1:A:178:ARG:N	2.26	0.50
1:C:158:SER:HB2	1:C:199:SER:OG	2.11	0.50
1:D:170:ASP:O	1:D:171:THR:OG1	2.22	0.50
1:E:97:ALA:O	1:E:222:ASN:ND2	2.44	0.50
1:F:16:LEU:HD22	1:F:63:ILE:HG13	1.92	0.50
1:F:98:ILE:HD12	1:F:195:TYR:CE2	2.47	0.50
1:F:143:ALA:N	1:F:251:ARG:NH1	2.51	0.50
1:A:106:ASP:HB2	1:A:219:VAL:HG21	1.93	0.50
1:B:96:GLY:HA2	1:B:221:VAL:O	2.11	0.50
1:C:177:VAL:O	1:C:178:ARG:C	2.50	0.50
1:D:156:THR:HG23	1:D:194:ASN:HD21	1.77	0.50
1:B:196:GLU:CD	1:B:199:SER:H	2.15	0.50
1:F:113:SER:H	1:F:130:ALA:HB3	1.77	0.50
1:F:199:SER:O	1:F:200:ALA:O	2.30	0.50
1:A:37:LEU:N	1:A:37:LEU:CD2	2.75	0.50
1:A:156:THR:CG2	1:A:157:ALA:N	2.74	0.50
1:C:28:PRO:HB2	1:C:51:THR:OG1	2.12	0.50
1:F:163:TYR:CA	1:F:168:ARG:HD2	2.38	0.50
1:B:142:GLU:OE2	1:E:42:VAL:HG13	2.11	0.50
1:C:22:ALA:HB2	1:C:86:ILE:HD13	1.94	0.50
1:F:21:LEU:HD13	1:F:253:LEU:CD2	2.40	0.50
1:B:124:ALA:HA	1:D:175:ARG:NE	2.24	0.50
1:B:124:ALA:N	1:D:175:ARG:HE	2.09	0.50
1:C:225:GLN:HG2	1:C:226:GLN:N	2.26	0.50
1:D:140:LEU:HD23	1:D:248:ALA:CB	2.42	0.50
1:D:154:GLY:H	1:D:193:MET:HE1	1.77	0.50
1:D:188:GLN:O	1:D:191:GLY:N	2.45	0.50
1:E:81:LEU:HB3	1:E:86:ILE:HD12	1.94	0.50
1:A:13:LYS:C	1:A:15:ASP:N	2.63	0.50
1:A:178:ARG:CA	1:A:181:LYS:HE2	2.42	0.50
1:B:81:LEU:HA	1:B:84:LEU:CD1	2.42	0.50
1:B:169:TYR:CE2	1:B:176:VAL:HG23	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:147:ILE:HD13	1:E:148:GLY:N	2.27	0.50
1:E:25:PRO:HG3	1:E:34:ILE:HD12	1.94	0.49
1:E:57:LEU:O	1:E:60:LYS:HB2	2.11	0.49
1:A:201:THR:O	1:A:205:MET:CB	2.60	0.49
1:B:40:LYS:N	1:B:41:PRO:CD	2.74	0.49
1:B:177:VAL:O	1:B:178:ARG:C	2.51	0.49
1:C:123:PHE:HA	1:E:175:ARG:NH2	2.27	0.49
1:C:140:LEU:HD22	1:C:216:VAL:HB	1.93	0.49
1:E:156:THR:CG2	1:E:194:ASN:ND2	2.74	0.49
1:E:161:THR:HG1	1:E:165:GLY:HA3	1.75	0.49
1:F:49:GLU:C	1:F:50:PHE:HD2	2.16	0.49
1:F:95:THR:OG1	1:F:96:GLY:N	2.45	0.49
1:A:35:ALA:HA	1:A:38:MET:CE	2.41	0.49
1:B:164:PRO:HG2	1:B:165:GLY:N	2.26	0.49
1:E:21:LEU:HD23	1:E:21:LEU:C	2.32	0.49
1:E:94:THR:HG21	1:E:238:GLU:HG2	1.93	0.49
1:F:227:GLU:CG	1:F:228:ILE:N	2.75	0.49
1:A:92:ILE:HD13	1:A:93:GLY:N	2.28	0.49
1:B:95:THR:OG1	1:B:194:ASN:HB2	2.12	0.49
1:B:196:GLU:OE2	1:B:199:SER:N	2.46	0.49
1:C:95:THR:OG1	1:C:96:GLY:N	2.45	0.49
1:D:27:ASP:HB2	1:D:28:PRO:HD2	1.94	0.49
1:E:243:LYS:O	1:E:244:ILE:C	2.50	0.49
1:B:56:GLU:OE2	1:C:43:LYS:NZ	2.46	0.49
1:B:243:LYS:O	1:B:246:VAL:HB	2.13	0.49
1:B:243:LYS:O	1:B:246:VAL:N	2.42	0.49
1:C:172:TYR:CE1	1:E:211:LEU:HD21	2.47	0.49
1:E:15:ASP:C	1:E:16:LEU:HD23	2.33	0.49
1:E:238:GLU:O	1:E:242:VAL:HG23	2.12	0.49
1:F:146:SER:HB3	1:F:251:ARG:HH22	1.77	0.49
1:A:222:ASN:OD1	1:A:225:GLN:HB2	2.12	0.49
1:E:15:ASP:CB	1:E:44:LEU:HD21	2.43	0.49
1:C:92:ILE:C	1:C:92:ILE:HD13	2.33	0.49
1:C:105:GLY:HA3	1:C:236:GLN:NE2	2.28	0.49
1:C:135:ALA:O	1:C:252:LEU:HD21	2.12	0.49
1:C:242:VAL:O	1:C:245:VAL:HG12	2.13	0.49
1:E:16:LEU:HB3	1:E:19:ALA:HB3	1.93	0.49
1:B:232:GLU:O	1:B:236:GLN:N	2.24	0.49
1:C:161:THR:OG1	1:C:164:PRO:HG2	2.12	0.49
1:E:142:GLU:O	1:E:145:LYS:N	2.44	0.49
1:B:31:VAL:CG1	1:B:53:TRP:HB2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:GLN:HA	1:D:17:GLN:NE2	2.21	0.49
1:D:126:MET:HG3	1:D:126:MET:O	2.13	0.49
1:D:176:VAL:O	1:D:177:VAL:C	2.52	0.49
1:C:196:GLU:OE1	1:C:215:MET:SD	2.71	0.49
1:F:163:TYR:N	1:F:164:PRO:HD2	2.28	0.49
1:E:237:THR:HA	1:E:240:HIS:HD2	1.75	0.48
1:F:94:THR:HB	1:F:220:ILE:HG23	1.93	0.48
1:F:144:ALA:HA	1:F:244:ILE:CD1	2.43	0.48
1:A:92:ILE:HG13	1:A:241:ALA:O	2.13	0.48
1:A:140:LEU:HD23	1:A:248:ALA:HB1	1.94	0.48
1:A:142:GLU:O	1:A:145:LYS:HB2	2.13	0.48
1:C:31:VAL:HG13	1:C:64:VAL:HG12	1.96	0.48
1:E:144:ALA:HA	1:E:244:ILE:HD12	1.95	0.48
1:E:163:TYR:HB2	1:E:164:PRO:CD	2.42	0.48
1:E:163:TYR:HB2	1:E:164:PRO:HD3	1.94	0.48
1:B:8:HIS:HB3	1:B:50:PHE:HE1	1.76	0.48
1:B:48:ARG:NH1	1:D:49:GLU:OE1	2.46	0.48
1:B:105:GLY:H	1:B:219:VAL:HB	1.78	0.48
1:C:187:TRP:HB3	1:C:192:VAL:HG21	1.94	0.48
1:C:233:THR:HA	1:C:236:GLN:OE1	2.13	0.48
1:E:78:VAL:HA	1:E:81:LEU:HD12	1.94	0.48
1:A:238:GLU:O	1:A:242:VAL:HG23	2.12	0.48
1:C:39:ASP:O	1:C:40:LYS:C	2.52	0.48
1:F:96:GLY:HA3	1:F:223:ARG:HG2	1.96	0.48
1:B:35:ALA:C	1:B:37:LEU:H	2.17	0.48
1:B:78:VAL:HG21	1:B:205:MET:HE3	1.94	0.48
1:C:25:PRO:O	1:C:66:SER:HA	2.13	0.48
1:E:16:LEU:HD23	1:E:16:LEU:N	2.28	0.48
1:F:158:SER:OG	1:F:200:ALA:HB2	2.12	0.48
1:A:6:VAL:HG23	1:A:6:VAL:O	2.13	0.48
1:A:120:SER:HB2	1:A:204:THR:HG21	1.96	0.48
1:B:5:ASP:HB2	1:B:12:THR:CA	2.41	0.48
1:D:41:PRO:HA	1:D:54:ARG:O	2.14	0.48
1:D:156:THR:CG2	1:D:194:ASN:HD21	2.26	0.48
1:E:91:ARG:HG3	1:E:92:ILE:H	1.74	0.48
1:E:176:VAL:CG1	1:E:180:PHE:HB3	2.43	0.48
1:E:187:TRP:HA	1:E:190:MET:HE3	1.95	0.48
1:F:98:ILE:HD11	1:F:194:ASN:HA	1.96	0.48
1:A:97:ALA:HA	1:A:193:MET:O	2.14	0.48
1:C:121:LEU:O	1:E:177:VAL:HG21	2.14	0.48
1:D:58:ASP:OD2	1:D:58:ASP:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:57:LEU:CD2	1:E:250:ARG:HG2	2.39	0.48
1:E:236:GLN:O	1:E:239:SER:N	2.42	0.48
1:F:183:SER:HB2	1:F:187:TRP:NE1	2.29	0.48
1:A:8:HIS:ND1	1:A:8:HIS:N	2.52	0.48
1:A:177:VAL:HG22	1:A:178:ARG:H	1.79	0.48
1:B:5:ASP:HB2	1:B:11:LEU:O	2.14	0.48
1:B:40:LYS:HD2	1:B:56:GLU:CD	2.34	0.48
1:A:9:LEU:HD23	1:A:50:PHE:HB3	1.95	0.48
1:A:56:GLU:HG2	1:A:57:LEU:N	2.29	0.48
1:A:114:VAL:HG23	1:A:156:THR:O	2.13	0.48
1:A:158:SER:CB	1:A:200:ALA:HB2	2.44	0.48
1:B:236:GLN:OE1	1:B:236:GLN:O	2.32	0.48
1:E:17:GLN:CG	1:E:54:ARG:HH21	2.17	0.48
1:F:27:ASP:OD1	1:F:28:PRO:HD2	2.14	0.48
1:B:144:ALA:HA	1:B:244:ILE:HG12	1.95	0.47
1:B:164:PRO:O	1:B:166:GLN:N	2.46	0.47
1:C:78:VAL:HG13	1:C:89:PHE:CE2	2.48	0.47
1:C:239:SER:O	1:C:243:LYS:HB2	2.13	0.47
1:D:133:ASP:OD2	1:D:135:ALA:N	2.47	0.47
1:E:17:GLN:HE21	1:E:17:GLN:CA	2.10	0.47
1:E:54:ARG:HH11	1:E:54:ARG:CG	2.27	0.47
1:B:78:VAL:HG21	1:B:205:MET:CE	2.43	0.47
1:C:205:MET:HG3	1:C:206:CYS:N	2.28	0.47
1:D:16:LEU:HD11	1:D:84:LEU:CB	2.44	0.47
1:E:91:ARG:HG2	1:E:215:MET:HG2	1.95	0.47
1:E:147:ILE:HD13	1:E:149:ALA:N	2.29	0.47
1:F:57:LEU:HD11	1:F:250:ARG:HH12	1.74	0.47
1:A:143:ALA:HB1	1:A:247:GLU:HG3	1.95	0.47
1:C:172:TYR:HE1	1:E:211:LEU:HD21	1.79	0.47
1:E:114:VAL:HB	1:E:157:ALA:HA	1.96	0.47
1:F:5:ASP:CB	1:F:12:THR:HA	2.44	0.47
1:F:176:VAL:HG12	1:F:177:VAL:N	2.28	0.47
1:B:149:ALA:HB2	1:B:244:ILE:HD11	1.95	0.47
1:C:163:TYR:CD2	1:C:171:THR:HG22	2.48	0.47
1:D:146:SER:O	1:D:148:GLY:N	2.46	0.47
1:F:221:VAL:HG22	1:F:223:ARG:H	1.80	0.47
1:A:93:GLY:O	1:A:217:ALA:HA	2.13	0.47
1:A:178:ARG:HA	1:A:181:LYS:HG3	1.96	0.47
1:C:21:LEU:O	1:C:22:ALA:HB2	2.14	0.47
1:C:132:ALA:HA	1:C:203:LEU:CD2	2.44	0.47
1:D:91:ARG:HG3	1:D:91:ARG:HH11	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:ARG:NH2	1:D:124:ALA:O	2.45	0.47
1:E:63:ILE:CG2	1:E:64:VAL:N	2.78	0.47
1:E:79:GLU:O	1:E:83:GLN:NE2	2.48	0.47
1:F:116:LEU:HD21	1:F:187:TRP:CH2	2.50	0.47
1:F:250:ARG:O	1:F:253:LEU:HB2	2.15	0.47
1:F:91:ARG:O	1:F:216:VAL:HG12	2.14	0.47
1:F:99:GLN:HB3	1:F:101:HIS:ND1	2.30	0.47
1:A:65:CYS:O	1:A:66:SER:C	2.53	0.47
1:E:39:ASP:O	1:E:56:GLU:HB3	2.15	0.47
1:F:9:LEU:HD21	1:F:77:ALA:HA	1.95	0.47
1:F:96:GLY:HA2	1:F:221:VAL:O	2.15	0.47
1:B:119:ALA:O	1:B:122:HIS:HB2	2.15	0.47
1:B:190:MET:HE1	1:F:125:PRO:HD3	1.97	0.47
1:C:163:TYR:HA	1:C:168:ARG:HD2	1.97	0.47
1:D:38:MET:HG2	1:D:57:LEU:CD1	2.45	0.47
1:C:250:ARG:O	1:C:253:LEU:HB2	2.14	0.46
1:E:91:ARG:HB3	1:E:215:MET:HG2	1.97	0.46
1:A:226:GLN:CD	1:A:227:GLU:N	2.69	0.46
1:B:33:LYS:HA	1:B:33:LYS:CE	2.32	0.46
1:B:105:GLY:O	1:B:106:ASP:C	2.54	0.46
1:B:151:THR:HG22	1:B:152:HIS:N	2.30	0.46
1:E:149:ALA:O	1:E:151:THR:N	2.49	0.46
1:F:17:GLN:HE21	1:F:17:GLN:CA	2.28	0.46
1:F:110:THR:HA	1:F:154:GLY:O	2.15	0.46
1:C:63:ILE:CG2	1:C:64:VAL:N	2.77	0.46
1:C:180:PHE:HE1	1:E:122:HIS:CG	2.33	0.46
1:E:92:ILE:CG1	1:E:93:GLY:N	2.78	0.46
1:A:73:SER:O	1:A:76:ILE:N	2.49	0.46
1:A:131:VAL:CG2	1:A:132:ALA:N	2.78	0.46
1:B:83:GLN:NE2	1:D:171:THR:HG23	2.30	0.46
1:B:107:VAL:O	1:B:151:THR:HA	2.16	0.46
1:C:44:LEU:HB2	1:C:52:SER:O	2.15	0.46
1:C:113:SER:O	1:C:130:ALA:HB3	2.15	0.46
1:C:233:THR:HA	1:C:236:GLN:CG	2.45	0.46
1:F:156:THR:HG23	1:F:194:ASN:CG	2.36	0.46
1:F:199:SER:O	1:F:200:ALA:C	2.54	0.46
1:A:43:LYS:HB2	1:A:53:TRP:CH2	2.50	0.46
1:C:96:GLY:HA2	1:C:221:VAL:O	2.16	0.46
1:D:79:GLU:OE2	1:D:83:GLN:HG3	2.16	0.46
1:E:39:ASP:O	1:E:40:LYS:CB	2.62	0.46
1:A:178:ARG:O	1:A:180:PHE:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:LEU:HD21	1:C:52:SER:OG	2.15	0.46
1:D:21:LEU:HD21	1:D:90:LEU:HD11	1.98	0.46
1:E:44:LEU:O	1:E:45:ALA:HB2	2.16	0.46
1:F:34:ILE:CD1	1:F:242:VAL:HG22	2.45	0.46
1:A:234:MET:O	1:A:237:THR:HB	2.15	0.46
1:B:69:ILE:HG21	1:D:76:ILE:HD11	1.97	0.46
1:C:62:VAL:HG13	1:C:63:ILE:N	2.31	0.46
1:D:230:ASN:HD22	1:D:232:GLU:HB3	1.81	0.46
1:E:31:VAL:HG13	1:E:64:VAL:CG1	2.36	0.46
1:F:71:GLY:N	1:F:72:PRO:CD	2.79	0.46
1:A:7:PHE:O	1:A:8:HIS:C	2.54	0.46
1:B:54:ARG:HG2	1:B:55:ALA:N	2.31	0.46
1:D:175:ARG:HH12	1:D:178:ARG:H	1.64	0.46
1:D:222:ASN:ND2	1:D:225:GLN:HG2	2.30	0.46
1:E:6:VAL:HG11	1:E:84:LEU:HG	1.96	0.46
1:E:81:LEU:O	1:E:84:LEU:HB2	2.15	0.46
1:F:24:VAL:O	1:F:24:VAL:HG23	2.16	0.46
1:A:75:SER:O	1:A:79:GLU:HB3	2.15	0.46
1:B:44:LEU:HD11	1:B:54:ARG:HB2	1.96	0.46
1:B:156:THR:HG21	1:B:196:GLU:HG2	1.98	0.46
1:C:38:MET:CG	1:C:57:LEU:HD13	2.40	0.46
1:C:233:THR:CA	1:C:236:GLN:HG3	2.46	0.46
1:F:236:GLN:HA	1:F:239:SER:HG	1.77	0.46
1:B:236:GLN:O	1:B:239:SER:N	2.49	0.46
1:D:86:ILE:CD1	1:D:86:ILE:N	2.78	0.46
1:D:86:ILE:N	1:D:86:ILE:HD12	2.31	0.46
1:D:168:ARG:HH11	1:D:223:ARG:NH1	2.13	0.46
1:D:177:VAL:HG22	1:D:179:ARG:N	2.23	0.46
1:E:8:HIS:CB	1:E:50:PHE:CE1	2.96	0.46
1:E:39:ASP:HA	1:F:145:LYS:HE3	1.98	0.46
1:F:107:VAL:HG23	1:F:217:ALA:O	2.16	0.46
1:A:247:GLU:OE1	1:A:250:ARG:HD2	2.16	0.45
1:D:25:PRO:HD2	1:D:65:CYS:O	2.15	0.45
1:D:107:VAL:HG23	1:D:151:THR:HA	1.97	0.45
1:E:161:THR:HB	1:E:165:GLY:H	1.80	0.45
1:A:90:LEU:HD22	1:A:140:LEU:HD21	1.97	0.45
1:B:236:GLN:O	1:B:239:SER:HB2	2.17	0.45
1:C:23:ILE:HA	1:C:90:LEU:O	2.16	0.45
1:C:45:ALA:O	1:C:46:SER:HB2	2.16	0.45
1:D:55:ALA:O	1:D:56:GLU:HG3	2.17	0.45
1:D:245:VAL:CG1	1:D:246:VAL:N	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:VAL:HG12	1:E:116:LEU:HG	1.99	0.45
1:F:196:GLU:OE2	1:F:197:MET:C	2.54	0.45
1:A:24:VAL:HB	1:A:67:THR:HG23	1.98	0.45
1:B:82:ALA:O	1:B:85:GLY:N	2.49	0.45
1:B:98:ILE:HG13	1:B:99:GLN:N	2.30	0.45
1:D:98:ILE:O	1:D:188:GLN:NE2	2.49	0.45
1:D:172:TYR:HD1	1:D:172:TYR:O	1.99	0.45
1:F:117:ASP:CG	1:F:118:GLY:N	2.69	0.45
1:A:242:VAL:O	1:A:245:VAL:HG12	2.16	0.45
1:B:120:SER:HB2	1:B:204:THR:HG21	1.99	0.45
1:B:126:MET:CE	1:F:127:GLU:HA	2.47	0.45
1:D:6:VAL:HG22	1:D:11:LEU:O	2.17	0.45
1:D:89:PHE:N	1:D:212:ARG:O	2.48	0.45
1:D:158:SER:CB	1:D:200:ALA:HB2	2.46	0.45
1:B:164:PRO:C	1:B:166:GLN:N	2.68	0.45
1:D:136:CYS:HA	1:D:252:LEU:HD11	1.98	0.45
1:E:19:ALA:HB2	1:E:61:ALA:HB1	1.99	0.45
1:F:200:ALA:O	1:F:201:THR:C	2.55	0.45
1:A:233:THR:O	1:A:234:MET:HB2	2.17	0.45
1:A:49:GLU:O	1:A:51:THR:N	2.50	0.45
1:B:28:PRO:O	1:B:31:VAL:HG23	2.17	0.45
1:B:34:ILE:HB	1:B:64:VAL:HG11	1.99	0.45
1:C:9:LEU:CD1	1:C:81:LEU:HG	2.45	0.45
1:C:143:ALA:HB1	1:C:247:GLU:HB3	1.99	0.45
1:E:210:GLY:O	1:E:211:LEU:HD23	2.15	0.45
1:F:159:SER:CB	1:F:166:GLN:NE2	2.79	0.45
1:B:128:PHE:CD1	1:B:129:PRO:N	2.85	0.45
1:B:142:GLU:O	1:B:145:LYS:N	2.49	0.45
1:C:44:LEU:CD1	1:C:54:ARG:HB2	2.41	0.45
1:F:80:GLU:O	1:F:84:LEU:HG	2.17	0.45
1:A:247:GLU:O	1:A:250:ARG:CB	2.65	0.45
1:C:13:LYS:HG3	1:C:84:LEU:O	2.17	0.45
1:C:139:ALA:O	1:C:142:GLU:N	2.50	0.45
1:C:216:VAL:HG22	1:C:217:ALA:N	2.32	0.45
1:D:56:GLU:HG2	1:D:61:ALA:HA	1.98	0.45
1:D:230:ASN:C	1:D:234:MET:HE1	2.37	0.45
1:E:245:VAL:HG13	1:E:246:VAL:N	2.32	0.45
1:E:250:ARG:HA	1:E:253:LEU:HD12	1.97	0.45
1:B:99:GLN:NE2	1:B:191:GLY:HA2	2.32	0.45
1:D:17:GLN:NE2	1:D:17:GLN:CA	2.80	0.45
1:D:118:GLY:O	1:D:122:HIS:CD2	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:GLU:OE2	1:D:199:SER:OG	2.30	0.45
1:D:228:ILE:N	1:D:228:ILE:CD1	2.76	0.45
1:D:228:ILE:H	1:D:228:ILE:CD1	2.30	0.45
1:A:56:GLU:HG2	1:A:60:LYS:O	2.16	0.44
1:B:60:LYS:CB	1:B:253:LEU:HD22	2.46	0.44
1:B:162:PHE:O	1:B:162:PHE:CD1	2.70	0.44
1:B:184:MET:CE	1:B:188:GLN:NE2	2.80	0.44
1:D:112:ALA:HA	1:D:130:ALA:O	2.17	0.44
1:F:23:ILE:O	1:F:64:VAL:HA	2.16	0.44
1:F:28:PRO:HA	1:F:66:SER:HB3	1.98	0.44
1:F:149:ALA:O	1:F:151:THR:N	2.47	0.44
1:F:177:VAL:HG22	1:F:178:ARG:N	2.27	0.44
1:C:31:VAL:HG11	1:C:51:THR:HG22	1.99	0.44
1:C:92:ILE:HD13	1:C:93:GLY:N	2.32	0.44
1:C:223:ARG:O	1:C:225:GLN:O	2.35	0.44
1:D:91:ARG:HG3	1:D:91:ARG:NH1	2.32	0.44
1:E:4:SER:O	1:E:5:ASP:CG	2.56	0.44
1:E:79:GLU:C	1:E:83:GLN:NE2	2.71	0.44
1:F:37:LEU:HD22	1:F:242:VAL:CG1	2.47	0.44
1:F:236:GLN:O	1:F:237:THR:C	2.55	0.44
1:A:173:SER:OG	1:F:209:GLN:NE2	2.49	0.44
1:B:152:HIS:HB2	1:B:193:MET:HE3	1.99	0.44
1:C:91:ARG:HG3	1:C:91:ARG:HH11	1.82	0.44
1:D:78:VAL:O	1:D:81:LEU:N	2.50	0.44
1:E:21:LEU:HA	1:E:86:ILE:HG23	1.98	0.44
1:F:120:SER:HB2	1:F:204:THR:HG21	1.99	0.44
1:A:71:GLY:N	1:A:72:PRO:CD	2.80	0.44
1:A:147:ILE:HD12	1:A:147:ILE:O	2.17	0.44
1:A:173:SER:HB3	1:F:209:GLN:HG3	1.98	0.44
1:B:56:GLU:HA	1:B:60:LYS:O	2.17	0.44
1:C:75:SER:O	1:C:79:GLU:HB3	2.16	0.44
1:D:178:ARG:HG3	1:D:178:ARG:NH1	2.32	0.44
1:E:140:LEU:HD13	1:E:216:VAL:HB	1.98	0.44
1:F:183:SER:HB2	1:F:187:TRP:HE1	1.81	0.44
1:B:182:GLY:O	1:B:185:GLU:HB3	2.17	0.44
1:B:190:MET:CE	1:F:125:PRO:HD3	2.47	0.44
1:C:38:MET:HA	1:C:57:LEU:HD13	2.00	0.44
1:C:94:THR:HG22	1:C:220:ILE:HB	1.98	0.44
1:C:187:TRP:HA	1:C:187:TRP:CE3	2.52	0.44
1:E:91:ARG:CG	1:E:92:ILE:N	2.77	0.44
1:A:16:LEU:HD13	1:A:63:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:GLU:C	1:B:234:MET:H	2.21	0.44
1:C:91:ARG:NH1	1:C:91:ARG:HG3	2.33	0.44
1:C:173:SER:CB	1:E:209:GLN:HE21	2.30	0.44
1:D:206:CYS:O	1:D:209:GLN:N	2.49	0.44
1:D:210:GLY:O	1:D:211:LEU:HD23	2.18	0.44
1:F:107:VAL:C	1:F:108:LEU:HD23	2.38	0.44
1:F:144:ALA:CA	1:F:244:ILE:HD12	2.48	0.44
1:A:225:GLN:HG2	1:A:226:GLN:H	1.83	0.44
1:B:40:LYS:N	1:B:41:PRO:HD3	2.32	0.44
1:B:108:LEU:HD11	1:B:219:VAL:HG22	2.00	0.44
1:C:38:MET:HB2	1:C:55:ALA:CB	2.47	0.44
1:C:163:TYR:O	1:C:168:ARG:HB2	2.18	0.44
1:D:94:THR:CG2	1:D:220:ILE:HG23	2.47	0.44
1:E:162:PHE:HB3	1:E:163:TYR:H	1.72	0.44
1:E:177:VAL:O	1:E:178:ARG:C	2.56	0.44
1:B:143:ALA:HB1	1:B:247:GLU:HB3	2.00	0.44
1:B:236:GLN:C	1:B:238:GLU:N	2.66	0.44
1:E:161:THR:HB	1:E:165:GLY:N	2.33	0.44
1:F:8:HIS:CG	1:F:76:ILE:HG21	2.52	0.44
1:A:180:PHE:O	1:A:183:SER:N	2.46	0.44
1:A:236:GLN:HA	1:A:239:SER:OG	2.17	0.44
1:B:35:ALA:C	1:B:37:LEU:N	2.71	0.44
1:B:126:MET:HE1	1:F:127:GLU:HA	1.99	0.44
1:B:160:ASP:O	1:D:72:PRO:HB3	2.17	0.44
1:C:88:THR:OG1	1:C:212:ARG:HB2	2.18	0.44
1:C:122:HIS:O	1:E:175:ARG:NH2	2.51	0.44
1:C:187:TRP:HA	1:C:187:TRP:HE3	1.82	0.44
1:D:19:ALA:HB2	1:D:61:ALA:CB	2.48	0.44
1:D:24:VAL:HB	1:D:67:THR:CG2	2.48	0.44
1:D:222:ASN:ND2	1:D:225:GLN:OE1	2.51	0.44
1:E:169:TYR:HH	1:E:181:LYS:HG3	1.82	0.44
1:E:247:GLU:OE2	1:E:250:ARG:CZ	2.65	0.44
1:F:57:LEU:HD23	1:F:253:LEU:HD11	1.99	0.44
1:F:142:GLU:O	1:F:146:SER:N	2.43	0.44
1:C:187:TRP:O	1:C:189:ALA:N	2.39	0.43
1:E:8:HIS:HB3	1:E:50:PHE:HD1	1.82	0.43
1:E:177:VAL:HG12	1:E:180:PHE:HB2	1.99	0.43
1:A:63:ILE:HG22	1:A:64:VAL:N	2.32	0.43
1:A:73:SER:O	1:A:74:THR:C	2.56	0.43
1:A:96:GLY:HA2	1:A:221:VAL:O	2.18	0.43
1:D:47:HIS:O	1:D:48:ARG:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:ALA:HA	1:E:61:ALA:HB3	2.01	0.43
1:E:93:GLY:O	1:E:217:ALA:CA	2.64	0.43
1:F:250:ARG:HA	1:F:253:LEU:HD12	1.98	0.43
1:B:40:LYS:HD2	1:B:56:GLU:CB	2.48	0.43
1:B:91:ARG:HH22	2:B:254:ACY:C	2.30	0.43
1:C:71:GLY:N	1:C:72:PRO:CD	2.81	0.43
1:E:37:LEU:HD22	1:E:37:LEU:HA	1.84	0.43
1:E:115:ARG:HH12	1:E:126:MET:HA	1.80	0.43
1:A:48:ARG:O	1:A:49:GLU:HG2	2.18	0.43
1:A:99:GLN:HB3	1:A:101:HIS:ND1	2.33	0.43
1:B:238:GLU:O	1:B:239:SER:C	2.57	0.43
1:D:178:ARG:NH1	1:D:181:LYS:HD2	2.34	0.43
1:E:58:ASP:OD2	1:E:250:ARG:HD3	2.18	0.43
1:E:76:ILE:HG22	1:E:80:GLU:HG3	1.99	0.43
1:E:175:ARG:C	1:E:175:ARG:HH11	2.21	0.43
1:A:34:ILE:CA	1:A:37:LEU:HD23	2.49	0.43
1:A:160:ASP:O	1:F:72:PRO:HB3	2.18	0.43
1:B:77:ALA:O	1:B:81:LEU:HG	2.19	0.43
1:B:94:THR:OG1	2:B:254:ACY:O	2.32	0.43
1:D:34:ILE:O	1:D:38:MET:HE3	2.18	0.43
1:F:97:ALA:HB1	1:F:102:ILE:HB	2.01	0.43
1:F:113:SER:HA	1:F:155:VAL:HG13	2.01	0.43
1:A:175:ARG:NH1	1:A:175:ARG:HG2	2.34	0.43
1:C:187:TRP:C	1:C:189:ALA:H	2.20	0.43
1:D:102:ILE:HD13	1:D:108:LEU:HD21	2.00	0.43
1:E:161:THR:HB	1:E:165:GLY:CA	2.48	0.43
1:F:220:ILE:HG13	1:F:221:VAL:H	1.81	0.43
1:B:146:SER:O	1:B:147:ILE:HG13	2.18	0.43
1:C:115:ARG:NH2	1:C:121:LEU:HD23	2.34	0.43
1:F:57:LEU:HB3	1:F:253:LEU:CD1	2.49	0.43
1:F:156:THR:OG1	1:F:194:ASN:ND2	2.47	0.43
1:C:6:VAL:HG21	1:C:10:GLY:N	2.34	0.43
1:C:173:SER:HB3	1:E:209:GLN:HE21	1.84	0.43
1:D:168:ARG:HG3	1:D:223:ARG:HH12	1.84	0.43
1:D:238:GLU:C	1:D:238:GLU:OE2	2.57	0.43
1:A:169:TYR:O	1:A:171:THR:N	2.51	0.43
1:B:76:ILE:HD11	1:D:162:PHE:CE2	2.54	0.43
1:C:12:THR:O	1:C:15:ASP:HB2	2.19	0.43
1:C:35:ALA:O	1:C:41:PRO:HB3	2.19	0.43
1:C:237:THR:O	1:C:242:VAL:HG23	2.19	0.43
1:D:102:ILE:HG12	1:D:152:HIS:NE2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:ILE:HD11	1:D:149:ALA:CB	2.36	0.43
1:F:147:ILE:O	1:F:147:ILE:HG13	2.18	0.43
1:B:16:LEU:N	1:B:16:LEU:HD22	2.34	0.43
1:D:151:THR:CG2	1:D:152:HIS:H	2.32	0.43
1:D:188:GLN:C	1:D:190:MET:N	2.73	0.43
1:E:8:HIS:ND1	1:E:8:HIS:N	2.66	0.43
1:E:39:ASP:HA	1:F:145:LYS:CE	2.49	0.43
1:E:40:LYS:H	1:E:41:PRO:CD	2.32	0.43
1:E:167:GLU:HB2	1:E:183:SER:OG	2.18	0.43
1:F:163:TYR:N	1:F:164:PRO:CD	2.82	0.43
1:D:230:ASN:ND2	1:D:233:THR:OG1	2.52	0.42
1:E:92:ILE:CD1	1:E:93:GLY:H	2.32	0.42
1:F:34:ILE:HD13	1:F:242:VAL:HG22	2.01	0.42
1:F:183:SER:O	1:F:184:MET:C	2.55	0.42
1:A:30:ARG:HG2	1:A:30:ARG:NH1	2.34	0.42
1:A:39:ASP:O	1:A:40:LYS:C	2.57	0.42
1:A:106:ASP:HB2	1:A:219:VAL:CG2	2.48	0.42
1:C:172:TYR:HB2	1:E:83:GLN:CG	2.49	0.42
1:C:229:PRO:HG2	1:C:230:ASN:H	1.83	0.42
1:D:20:GLN:HA	1:D:86:ILE:HA	2.00	0.42
1:D:92:ILE:CD1	1:D:242:VAL:HA	2.49	0.42
1:E:23:ILE:HA	1:E:90:LEU:O	2.19	0.42
1:E:76:ILE:O	1:E:80:GLU:CG	2.67	0.42
1:E:141:VAL:O	1:E:145:LYS:N	2.51	0.42
1:A:221:VAL:O	1:A:221:VAL:CG1	2.65	0.42
1:B:128:PHE:CD1	1:B:129:PRO:CD	3.02	0.42
1:C:81:LEU:HB3	1:C:86:ILE:HD12	2.00	0.42
1:D:163:TYR:HD2	1:D:168:ARG:HB3	1.84	0.42
1:F:17:GLN:HA	1:F:17:GLN:NE2	2.34	0.42
1:B:40:LYS:O	1:B:55:ALA:HA	2.19	0.42
1:B:162:PHE:O	1:B:168:ARG:HD2	2.18	0.42
1:C:35:ALA:HA	1:C:38:MET:CE	2.49	0.42
1:C:119:ALA:HB3	1:C:201:THR:OG1	2.18	0.42
1:D:144:ALA:HB2	1:D:244:ILE:HD13	2.01	0.42
1:A:79:GLU:OE2	1:F:171:THR:HG21	2.18	0.42
1:C:22:ALA:CB	1:C:86:ILE:HD13	2.50	0.42
1:D:186:GLU:O	1:D:190:MET:HG3	2.19	0.42
1:B:40:LYS:NZ	1:C:43:LYS:HD2	2.35	0.42
1:D:166:GLN:HG2	1:D:195:TYR:CE1	2.54	0.42
1:E:52:SER:HB3	1:E:65:CYS:SG	2.58	0.42
1:A:99:GLN:HA	1:A:100:PRO:HD3	1.78	0.42

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:A:160:ASP:HB3	1:F:119:ALA:CB	2.49	0.42
1:B:40:LYS:HZ1	1:C:43:LYS:HD2	1.84	0.42
1:D:34:ILE:HG22	1:D:38:MET:CE	2.49	0.42
1:E:7:PHE:O	1:E:8:HIS:C	2.58	0.42
1:E:57:LEU:HD11	1:E:250:ARG:NE	2.35	0.42
1:F:7:PHE:O	1:F:7:PHE:CD1	2.72	0.42
1:F:71:GLY:O	1:F:75:SER:OG	2.31	0.42
1:F:90:LEU:HD11	1:F:252:LEU:HD12	2.02	0.42
1:F:187:TRP:HB3	1:F:192:VAL:CG2	2.41	0.42
1:A:9:LEU:HD12	1:A:80:GLU:HB3	2.02	0.42
1:B:23:ILE:C	1:B:24:VAL:HG13	2.40	0.42
1:B:57:LEU:HD21	1:B:250:ARG:CG	2.49	0.42
1:C:80:GLU:O	1:C:83:GLN:HB2	2.19	0.42
1:D:109:VAL:O	1:D:193:MET:HE1	2.20	0.42
1:D:141:VAL:HG12	1:D:141:VAL:O	2.20	0.42
1:D:172:TYR:O	1:D:173:SER:C	2.57	0.42
1:D:174:GLY:O	1:D:175:ARG:C	2.58	0.42
1:E:70:GLY:O	1:E:73:SER:HB3	2.20	0.42
1:F:117:ASP:OD1	1:F:120:SER:OG	2.34	0.42
1:F:147:ILE:CD1	1:F:244:ILE:HD11	2.45	0.42
1:F:198:GLU:H	1:F:198:GLU:CD	2.23	0.42
1:B:15:ASP:HB3	1:B:44:LEU:CD2	2.49	0.42
1:C:163:TYR:CD1	1:E:79:GLU:OE1	2.72	0.42
1:C:236:GLN:O	1:C:240:HIS:HB2	2.18	0.42
1:E:36:ALA:C	1:E:38:MET:H	2.23	0.42
1:A:108:LEU:O	1:A:216:VAL:HA	2.20	0.42
1:D:34:ILE:O	1:D:35:ALA:C	2.58	0.42
1:D:94:THR:HG21	1:D:220:ILE:HG23	2.02	0.42
1:E:196:GLU:OE2	1:E:199:SER:N	2.52	0.42
1:F:108:LEU:HA	1:F:152:HIS:O	2.20	0.42
1:F:174:GLY:O	1:F:175:ARG:HB3	2.19	0.42
1:F:194:ASN:H	1:F:194:ASN:ND2	2.00	0.42
1:A:50:PHE:CE2	1:A:77:ALA:HB2	2.55	0.41
1:A:226:GLN:HE21	1:A:226:GLN:HB3	1.59	0.41
1:C:18:GLY:O	1:C:19:ALA:C	2.58	0.41
1:C:98:ILE:O	1:C:224:THR:CG2	2.68	0.41
1:C:143:ALA:HA	1:C:247:GLU:OE2	2.19	0.41
1:F:22:ALA:HB2	1:F:86:ILE:CD1	2.45	0.41
1:F:163:TYR:HA	1:F:168:ARG:HB2	2.02	0.41
1:C:41:PRO:O	1:C:42:VAL:HG22	2.20	0.41
1:D:171:THR:C	1:D:173:SER:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:226:GLN:O	1:E:227:GLU:C	2.59	0.41
1:F:6:VAL:HG23	1:F:10:GLY:H	1.84	0.41
1:F:98:ILE:HG23	1:F:184:MET:HG3	2.02	0.41
1:F:133:ASP:CG	1:F:212:ARG:HG2	2.41	0.41
1:A:49:GLU:OE2	1:F:48:ARG:O	2.38	0.41
1:B:40:LYS:HD2	1:B:56:GLU:HB2	2.01	0.41
1:C:147:ILE:CD1	1:C:244:ILE:HG12	2.50	0.41
1:A:163:TYR:O	1:A:168:ARG:HB2	2.20	0.41
1:B:60:LYS:HB3	1:B:253:LEU:HD22	2.03	0.41
1:E:57:LEU:O	1:E:58:ASP:C	2.57	0.41
1:E:172:TYR:C	1:E:172:TYR:CD2	2.94	0.41
1:A:158:SER:OG	1:A:196:GLU:OE2	2.39	0.41
1:B:35:ALA:HA	1:B:38:MET:HE2	2.01	0.41
1:B:126:MET:HE1	1:F:127:GLU:CG	2.39	0.41
1:B:216:VAL:HG22	1:B:217:ALA:N	2.35	0.41
1:C:48:ARG:HB3	1:C:49:GLU:H	1.52	0.41
1:C:49:GLU:CG	1:E:49:GLU:OE2	2.67	0.41
1:C:232:GLU:OE2	1:C:235:LYS:HB3	2.21	0.41
1:C:233:THR:HA	1:C:236:GLN:CD	2.40	0.41
1:E:232:GLU:O	1:E:236:GLN:HG3	2.20	0.41
1:F:161:THR:OG1	1:F:165:GLY:HA3	2.21	0.41
1:A:169:TYR:CE2	1:A:176:VAL:HG23	2.56	0.41
1:D:176:VAL:O	1:D:177:VAL:O	2.38	0.41
1:E:28:PRO:HA	1:E:31:VAL:CG2	2.49	0.41
1:F:179:ARG:HE	1:F:179:ARG:HB2	1.50	0.41
1:A:7:PHE:O	1:A:9:LEU:N	2.54	0.41
1:B:33:LYS:HE2	1:B:33:LYS:CA	2.32	0.41
1:B:92:ILE:HD12	1:B:93:GLY:H	1.86	0.41
1:C:94:THR:HG22	1:C:220:ILE:CG2	2.50	0.41
1:D:9:LEU:CD2	1:D:50:PHE:CD1	3.04	0.41
1:D:17:GLN:HE21	1:D:17:GLN:CA	2.17	0.41
1:D:38:MET:HB2	1:D:55:ALA:HB1	2.03	0.41
1:E:16:LEU:HD22	1:E:63:ILE:HD11	2.02	0.41
1:E:57:LEU:HD11	1:E:250:ARG:CG	2.49	0.41
1:E:232:GLU:OE2	1:E:235:LYS:HD3	2.21	0.41
1:E:234:MET:O	1:E:238:GLU:HB2	2.21	0.41
1:F:179:ARG:HB3	1:F:180:PHE:HD1	1.86	0.41
1:B:23:ILE:CG2	1:B:24:VAL:N	2.83	0.41
1:D:13:LYS:HA	1:D:84:LEU:HD22	2.02	0.41
1:F:48:ARG:HG2	1:F:48:ARG:NH1	2.36	0.41
1:A:159:SER:O	1:A:197:MET:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:TYR:CD2	1:A:171:THR:HG22	2.56	0.41
1:B:49:GLU:HB2	1:D:49:GLU:HG2	2.03	0.41
1:B:87:ARG:O	1:B:212:ARG:HG3	2.21	0.41
1:B:128:PHE:HD1	1:B:129:PRO:N	2.19	0.41
1:B:184:MET:SD	1:B:223:ARG:HD2	2.61	0.41
1:D:38:MET:HB3	1:D:56:GLU:O	2.20	0.41
1:E:26:GLY:HA2	1:E:67:THR:H	1.86	0.41
1:E:57:LEU:O	1:E:60:LYS:N	2.54	0.41
1:E:87:ARG:NH1	1:E:87:ARG:CG	2.77	0.41
1:E:196:GLU:CD	1:E:198:GLU:H	2.24	0.41
1:F:123:PHE:CD1	1:F:123:PHE:N	2.89	0.41
1:F:168:ARG:C	1:F:170:ASP:H	2.24	0.41
1:F:198:GLU:N	1:F:198:GLU:CD	2.74	0.41
1:A:89:PHE:O	1:A:213:ALA:HA	2.21	0.41
1:A:141:VAL:O	1:A:145:LYS:HG3	2.21	0.41
1:B:206:CYS:O	1:B:207:ALA:C	2.59	0.41
1:E:11:LEU:HD21	1:E:45:ALA:HB3	2.02	0.41
1:E:218:GLY:O	1:E:220:ILE:HG23	2.21	0.41
1:F:230:ASN:CG	1:F:231:ALA:N	2.74	0.41
1:A:90:LEU:HD11	1:A:252:LEU:HD12	2.03	0.40
1:A:164:PRO:O	1:A:165:GLY:C	2.59	0.40
1:A:227:GLU:O	1:A:227:GLU:HG3	2.21	0.40
1:E:82:ALA:HB2	1:E:89:PHE:HZ	1.87	0.40
1:C:40:LYS:HD2	1:C:56:GLU:HG3	2.03	0.40
1:C:147:ILE:HD11	1:C:244:ILE:HD11	2.03	0.40
1:D:112:ALA:HA	1:D:131:VAL:HA	2.03	0.40
1:D:163:TYR:N	1:D:164:PRO:CD	2.82	0.40
1:E:21:LEU:HG	1:E:88:THR:HB	2.03	0.40
1:E:68:GLY:O	1:E:69:ILE:O	2.39	0.40
1:F:91:ARG:HG3	1:F:92:ILE:N	2.36	0.40
1:B:28:PRO:HB3	1:B:49:GLU:O	2.22	0.40
1:B:109:VAL:HG23	1:B:151:THR:CG2	2.52	0.40
1:C:247:GLU:O	1:C:247:GLU:OE1	2.39	0.40
1:C:251:ARG:HG2	1:C:251:ARG:NH1	2.35	0.40
1:D:154:GLY:N	1:D:193:MET:HE1	2.36	0.40
1:D:155:VAL:HG12	1:D:156:THR:N	2.35	0.40
1:E:236:GLN:O	1:E:237:THR:C	2.60	0.40
1:F:108:LEU:HD13	1:F:193:MET:CB	2.48	0.40
1:F:183:SER:O	1:F:186:GLU:N	2.55	0.40
1:F:230:ASN:HD21	1:F:232:GLU:H	1.64	0.40
1:A:16:LEU:HD23	1:A:16:LEU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:PHE:O	1:A:183:SER:CB	2.69	0.40
1:B:12:THR:HG23	1:B:15:ASP:OD2	2.21	0.40
1:B:28:PRO:HB2	1:B:51:THR:OG1	2.22	0.40
1:B:48:ARG:HB3	1:B:49:GLU:H	1.60	0.40
1:B:162:PHE:CD1	1:B:162:PHE:C	2.95	0.40
1:C:6:VAL:HB	1:C:80:GLU:OE2	2.21	0.40
1:C:177:VAL:HG13	1:C:179:ARG:HB3	2.04	0.40
1:D:57:LEU:HA	1:D:57:LEU:HD12	1.70	0.40
1:E:8:HIS:CB	1:E:50:PHE:HE1	2.33	0.40
1:E:41:PRO:O	1:E:53:TRP:CZ3	2.75	0.40
1:E:107:VAL:O	1:E:107:VAL:HG23	2.20	0.40
1:E:147:ILE:CD1	1:E:149:ALA:HB2	2.52	0.40
1:F:104:VAL:HG22	1:F:222:ASN:HD22	1.86	0.40
1:A:132:ALA:HB2	1:A:203:LEU:CD2	2.52	0.40
1:A:236:GLN:O	1:A:239:SER:HB2	2.21	0.40
1:E:147:ILE:O	1:E:147:ILE:HG12	2.21	0.40
1:E:151:THR:HG22	1:E:152:HIS:N	2.36	0.40
1:F:103:ASN:CB	1:F:106:ASP:OD1	2.69	0.40
1:F:112:ALA:O	1:F:155:VAL:HG13	2.21	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	248/253 (98%)	172 (69%)	53 (21%)	23 (9%)	0	1
1	B	248/253 (98%)	174 (70%)	55 (22%)	19 (8%)	1	2
1	C	248/253 (98%)	186 (75%)	40 (16%)	22 (9%)	1	1
1	D	248/253 (98%)	174 (70%)	58 (23%)	16 (6%)	1	3
1	E	248/253 (98%)	166 (67%)	57 (23%)	25 (10%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	248/253 (98%)	168 (68%)	59 (24%)	21 (8%)	1	2
All	All	1488/1518 (98%)	1040 (70%)	322 (22%)	126 (8%)	1	2

All (126) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	PHE
1	A	17	GLN
1	A	26	GLY
1	A	167	GLU
1	A	223	ARG
1	A	224	THR
1	A	234	MET
1	B	48	ARG
1	B	167	GLU
1	B	227	GLU
1	B	230	ASN
1	C	6	VAL
1	C	167	GLU
1	C	188	GLN
1	C	230	ASN
1	D	37	LEU
1	D	173	SER
1	D	177	VAL
1	E	5	ASP
1	E	8	HIS
1	E	40	LYS
1	E	69	ILE
1	E	173	SER
1	E	226	GLN
1	E	244	ILE
1	F	35	ALA
1	F	166	GLN
1	F	200	ALA
1	A	177	VAL
1	A	179	ARG
1	A	227	GLU
1	B	13	LYS
1	B	14	ASN
1	B	18	GLY
1	B	170	ASP
1	C	19	ALA

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Mol	Chain	Res	Type
1	C	46	SER
1	C	150	THR
1	C	228	ILE
1	C	229	PRO
1	D	78	VAL
1	D	171	THR
1	D	175	ARG
1	D	189	ALA
1	E	19	ALA
1	E	150	THR
1	E	178	ARG
1	E	181	LYS
1	F	11	LEU
1	F	34	ILE
1	F	58	ASP
1	F	95	THR
1	F	115	ARG
1	F	146	SER
1	F	148	GLY
1	F	172	TYR
1	F	201	THR
1	F	223	ARG
1	A	19	ALA
1	A	49	GLU
1	A	50	PHE
1	A	141	VAL
1	B	85	GLY
1	B	164	PRO
1	B	239	SER
1	C	45	ALA
1	C	118	GLY
1	C	238	GLU
1	D	17	GLN
1	D	146	SER
1	E	27	ASP
1	E	54	ARG
1	E	174	GLY
1	E	221	VAL
1	F	165	GLY
1	F	167	GLU
1	F	186	GLU
1	A	8	HIS

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Mol	Chain	Res	Type
1	A	202	LEU
1	B	178	ARG
1	B	202	LEU
1	B	224	THR
1	C	85	GLY
1	C	138	THR
1	C	170	ASP
1	C	239	SER
1	D	18	GLY
1	D	105	GLY
1	D	147	ILE
1	E	125	PRO
1	E	162	PHE
1	E	179	ARG
1	E	227	GLU
1	E	229	PRO
1	F	15	ASP
1	F	202	LEU
1	A	118	GLY
1	A	170	ASP
1	A	228	ILE
1	B	147	ILE
1	B	203	LEU
1	C	38	MET
1	C	189	ALA
1	C	204	THR
1	D	125	PRO
1	D	223	ARG
1	D	238	GLU
1	E	37	LEU
1	E	48	ARG
1	E	167	GLU
1	F	118	GLY
1	F	244	ILE
1	A	125	PRO
1	B	78	VAL
1	C	40	LYS
1	C	178	ARG
1	B	165	GLY
1	E	85	GLY
1	A	164	PRO
1	E	68	GLY

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Mol	Chain	Res	Type
1	A	25	PRO
1	F	177	VAL
1	A	40	LYS
1	C	164	PRO
1	D	104	VAL
1	B	219	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	199/202 (98%)	176 (88%)	23 (12%)	5	16
1	B	199/202 (98%)	183 (92%)	16 (8%)	12	33
1	C	199/202 (98%)	181 (91%)	18 (9%)	9	29
1	D	199/202 (98%)	170 (85%)	29 (15%)	3	9
1	E	199/202 (98%)	174 (87%)	25 (13%)	4	13
1	F	199/202 (98%)	176 (88%)	23 (12%)	5	16
All	All	1194/1212 (98%)	1060 (89%)	134 (11%)	6	18

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASP
1	A	8	HIS
1	A	15	ASP
1	A	16	LEU
1	A	32	GLU
1	A	48	ARG
1	A	54	ARG
1	A	64	VAL
1	A	79	GLU
1	A	92	ILE
1	A	98	ILE
1	A	106	ASP

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Mol	Chain	Res	Type
1	A	138	THR
1	A	147	ILE
1	A	158	SER
1	A	160	ASP
1	A	166	GLN
1	A	179	ARG
1	A	196	GLU
1	A	216	VAL
1	A	224	THR
1	A	226	GLN
1	A	251	ARG
1	B	5	ASP
1	B	12	THR
1	B	14	ASN
1	B	17	GLN
1	B	42	VAL
1	B	47	HIS
1	B	92	ILE
1	B	94	THR
1	B	106	ASP
1	B	160	ASP
1	B	167	GLU
1	B	194	ASN
1	B	196	GLU
1	B	215	MET
1	B	228	ILE
1	B	236	GLN
1	C	7	PHE
1	C	14	ASN
1	C	32	GLU
1	C	48	ARG
1	C	79	GLU
1	C	92	ILE
1	C	106	ASP
1	C	147	ILE
1	C	170	ASP
1	C	185	GLU
1	C	187	TRP
1	C	192	VAL
1	C	196	GLU
1	C	206	CYS
1	C	227	GLU

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Mol	Chain	Res	Type
1	C	230	ASN
1	C	240	HIS
1	C	247	GLU
1	D	12	THR
1	D	15	ASP
1	D	16	LEU
1	D	17	GLN
1	D	21	LEU
1	D	29	GLU
1	D	57	LEU
1	D	58	ASP
1	D	83	GLN
1	D	92	ILE
1	D	94	THR
1	D	95	THR
1	D	163	TYR
1	D	167	GLU
1	D	170	ASP
1	D	175	ARG
1	D	178	ARG
1	D	179	ARG
1	D	185	GLU
1	D	194	ASN
1	D	195	TYR
1	D	196	GLU
1	D	219	VAL
1	D	224	THR
1	D	225	GLN
1	D	228	ILE
1	D	234	MET
1	D	238	GLU
1	D	239	SER
1	E	17	GLN
1	E	37	LEU
1	E	44	LEU
1	E	47	HIS
1	E	48	ARG
1	E	54	ARG
1	E	69	ILE
1	E	92	ILE
1	E	126	MET
1	E	147	ILE

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Mol	Chain	Res	Type
1	E	153	VAL
1	E	160	ASP
1	E	161	THR
1	E	162	PHE
1	E	167	GLU
1	E	171	THR
1	E	172	TYR
1	E	175	ARG
1	E	180	PHE
1	E	194	ASN
1	E	195	TYR
1	E	196	GLU
1	E	215	MET
1	E	222	ASN
1	E	228	ILE
1	F	12	THR
1	F	17	GLN
1	F	38	MET
1	F	48	ARG
1	F	49	GLU
1	F	104	VAL
1	F	106	ASP
1	F	107	VAL
1	F	108	LEU
1	F	110	THR
1	F	126	MET
1	F	151	THR
1	F	162	PHE
1	F	172	TYR
1	F	179	ARG
1	F	185	GLU
1	F	194	ASN
1	F	196	GLU
1	F	205	MET
1	F	209	GLN
1	F	215	MET
1	F	234	MET
1	F	239	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	83	GLN
1	A	209	GLN
1	A	226	GLN
1	B	14	ASN
1	B	17	GLN
1	B	152	HIS
1	B	166	GLN
1	B	188	GLN
1	B	194	ASN
1	B	209	GLN
1	C	14	ASN
1	C	17	GLN
1	C	83	GLN
1	C	166	GLN
1	C	188	GLN
1	C	194	ASN
1	C	209	GLN
1	C	225	GLN
1	C	236	GLN
1	D	17	GLN
1	D	166	GLN
1	D	194	ASN
1	D	209	GLN
1	D	222	ASN
1	D	225	GLN
1	D	226	GLN
1	D	230	ASN
1	E	17	GLN
1	E	83	GLN
1	E	194	ASN
1	E	209	GLN
1	E	240	HIS
1	F	17	GLN
1	F	83	GLN
1	F	166	GLN
1	F	194	ASN
1	F	209	GLN
1	F	222	ASN
1	F	230	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ACY	B	254	-	3,3,3	1.42	0	3,3,3	1.38	0
2	ACY	B	255	-	3,3,3	1.57	0	3,3,3	1.30	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	254	ACY	5	0

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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.