Full wwPDB X-ray Structure Validation Report (i)

Sep 17, 2023 – 07:26 PM EDT

PDB ID	:	4ZKT
Title	:	Crystal structure of the progenitor M complex of Clostridium botulinum type E neurotoxin
Authors	:	Eswaramoorthy, S.; Swaminathan, S.
Deposited on	:	2015-04-30
Resolution	:	3.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

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

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

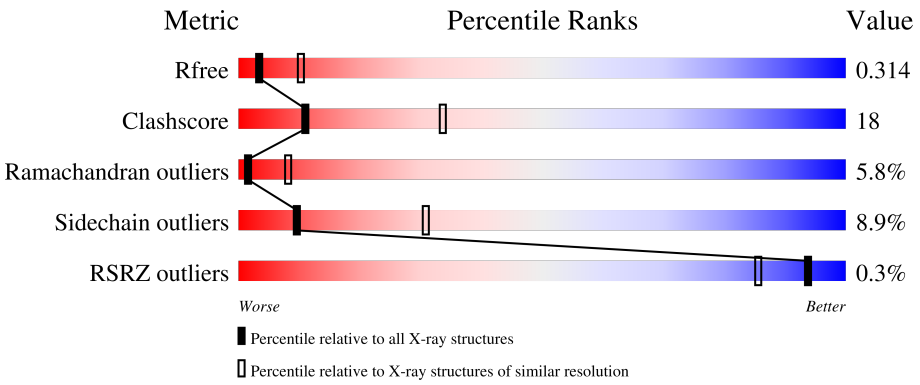
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.05 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	1252	59% 32% 7% •
1	C	1252	60% 32% 7% •
1	E	1252	59% 32% 7% •
2	B	1163	54% 35% 6% • •
2	D	1163	55% 34% 6% •

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Mol	Chain	Length	Quality of chain
2	F	1163	% 55% 34% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 56952 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 Bontoxilysin A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1235	9978	6351	1665	1940	22	0	0	0
1	C	1235	9978	6351	1665	1940	22	0	0	0
1	E	1235	9978	6351	1665	1940	22	0	0	0

- Molecule 2 is a protein called Botulinum neurotoxin type E, nontoxic-nonhemagglutinin component, NTNH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1114	9005	5804	1451	1726	24	0	0	0
2	D	1114	9005	5804	1451	1726	24	0	0	0
2	F	1114	9005	5804	1451	1726	24	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

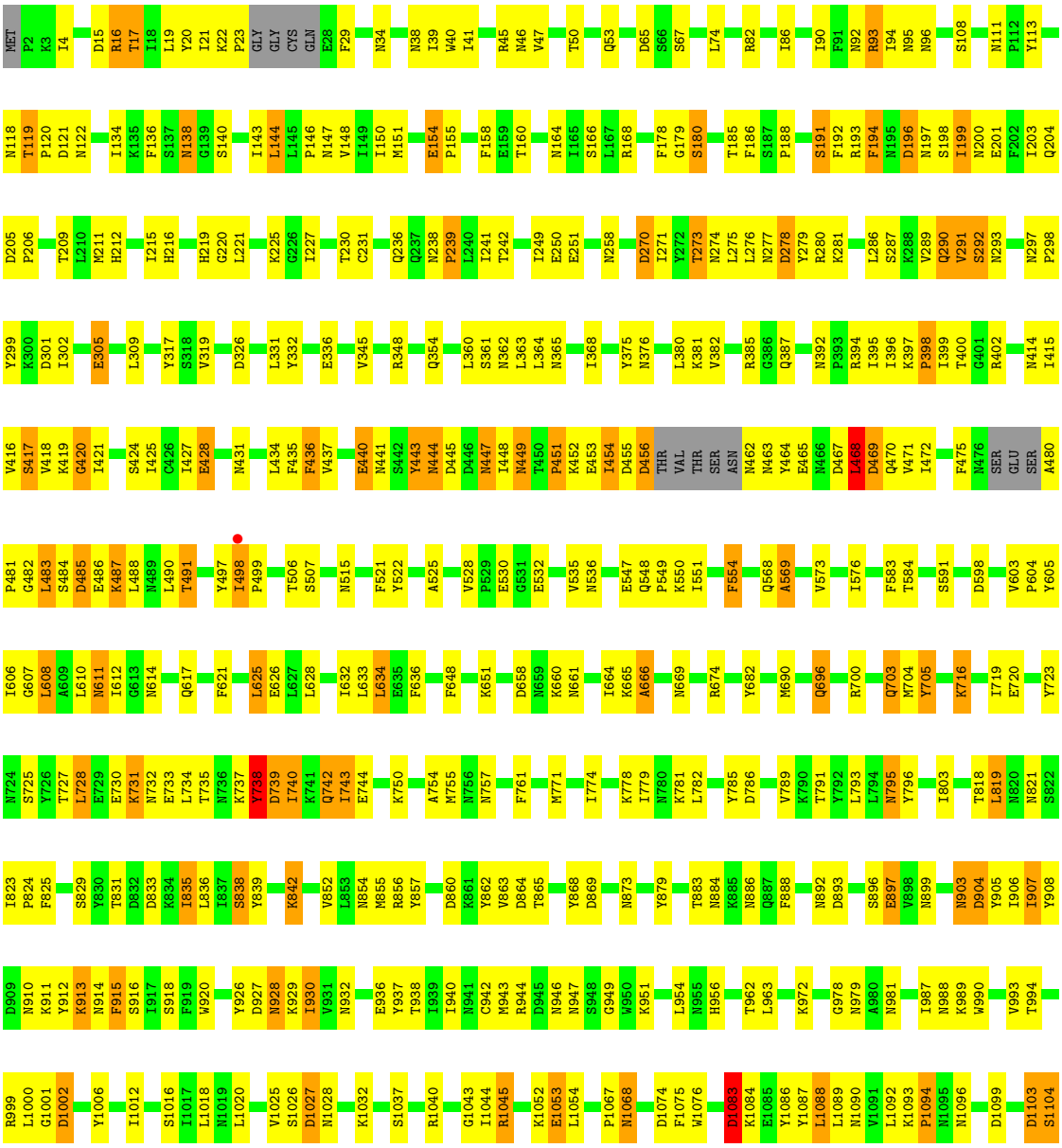
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	1	1	0	0
3	C	1	1	1	0	0
3	E	1	1	1	0	0

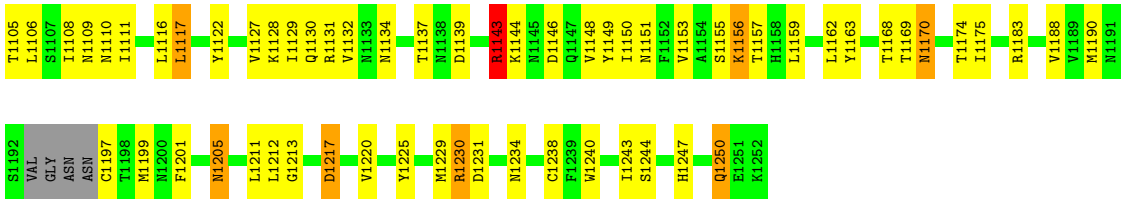
3 Residue-property plots (i)

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: Bontoxilysin A

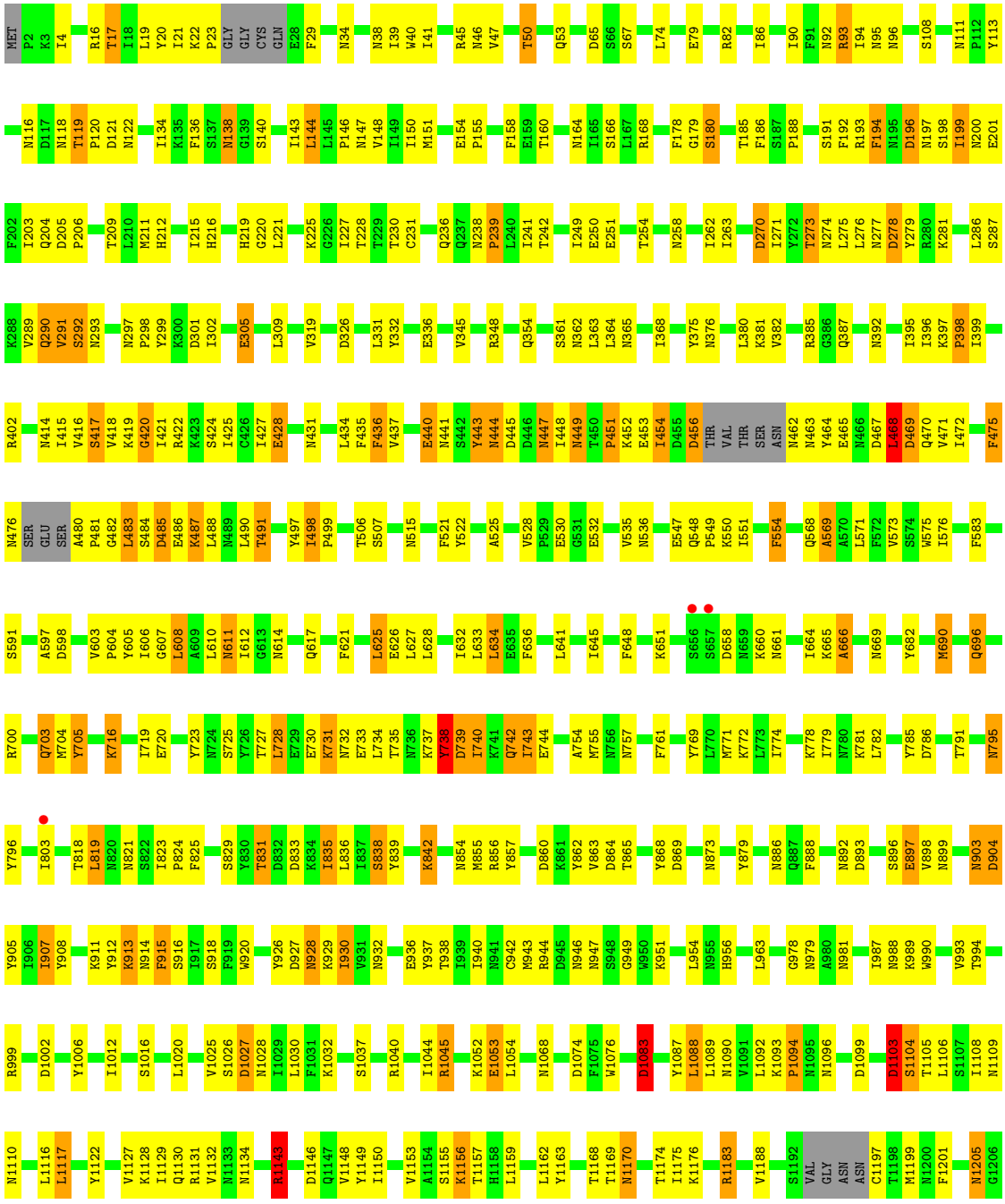
Chain A: 59% 32% 7%

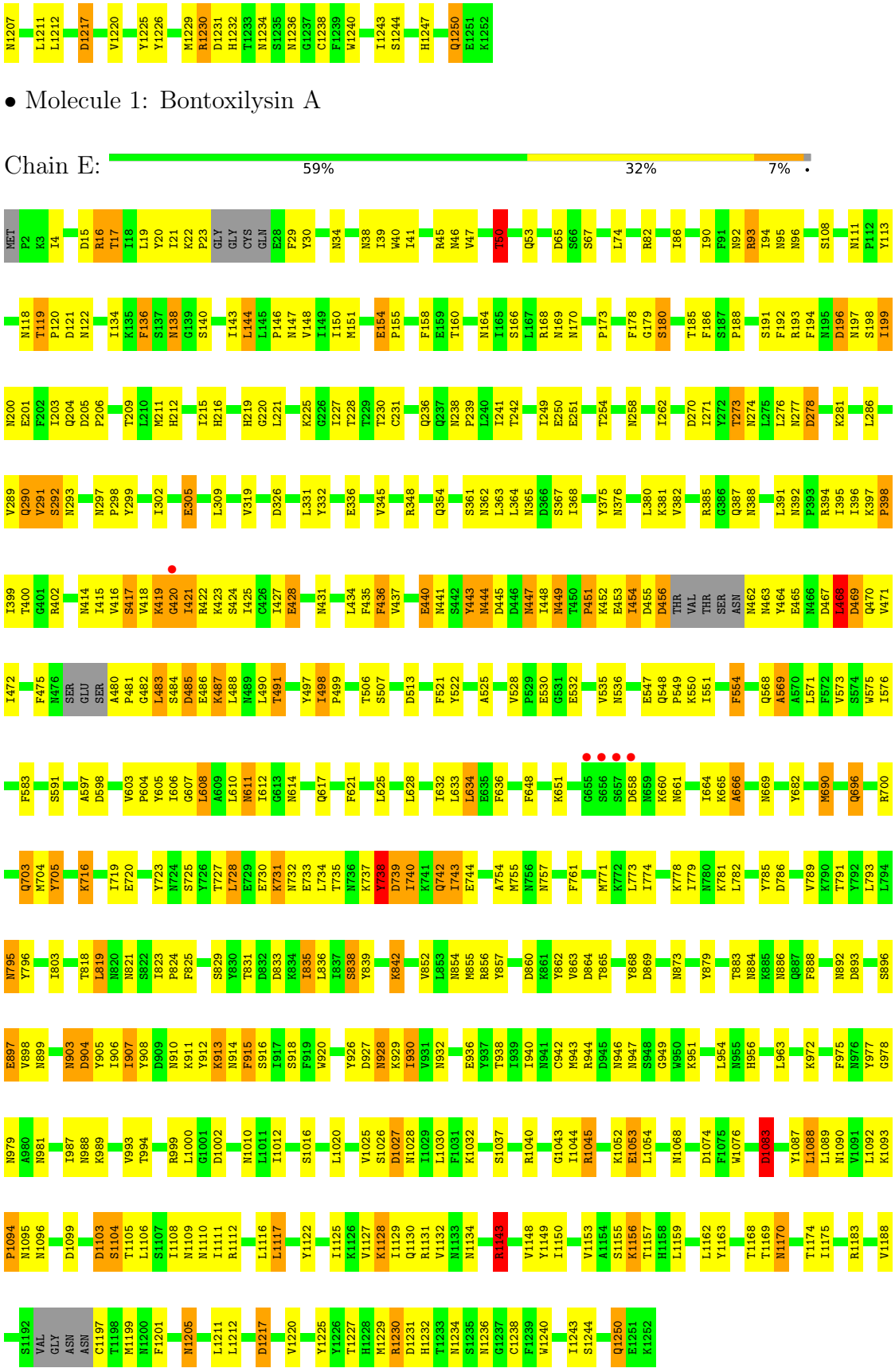




- Molecule 1: Bontoxilysin A

Chain C: 60% 32% 7% •




N1207 L1211 L1212 D1217 V1220 Y1225 Y1226 M1229 R1230 D1231 H1232 T1233 N1234 S1235 N1236 G1237 C1238 F1239 W1240 I1243 S1244 H1247 Q1250 E1251 K1252
• Molecule 1: Bontoxilysin A
Chain E:
59%
32%
7%
• Molecule 2: Botulinum neurotoxin type E, nontoxic-nonhemagglutinin component, NTNH

Chain B: 54% 35% 6%

MET K2 I9 D10 S11 P12 V13 D14 N15 K16 A19 I20 V21 R22 S23 R24 LYS SER D27 V28 F29 V35 A36 P37 W40 I41 V42 P43 E44 R45 Y46 Y47 L51 F59 I63 Y64 D65 S66 N67 F68 L69 S70 T71 E74 K75 D76 D77 F78 A81 T82 I83

K84 R88 N92 V93 L98 L101 I102 A105 I106 P107 F108 P109 N113 T114 E115 D116 Y117 R118 N121 K126 N127 N128 GLU HIS TYR TYR THR ALA ASN L136 V137 I138 P141 G142 I146 I151 Y152 Y153 K154 K155 E156 Y157 M162 M165 L166 E167 I168

W169 F173 D179 D184 P185 A186 L187 E188 C192 K195 S196 L197 I203 K204 P205 N206 D207 N208 L209 N210 I211 Y224 S225 E226 L227 D228 M229 I230 D231 F232 L233 I234 D239 Y240 K241 L242 T245 N246 P247 Y248 I251 D252 K253 Y254 T258 F262 K266

N267 D268 Y269 E270 I271 K272 I273 K274 N275 N276 N277 Y278 I279 A280 N281 L285 Y286 L287 E288 Q289 K290 F291 K292 I293 N294 V295 K296 D297 I298 W299 E300 L301 N302 L303 S304 Y305 F310 Y318 N319 K328 E329 Y330 I333 D334 Y335 Y339 G347 T351 Y358 I363

L372 I373 N374 GLN ASN N377 T378 V379 L380 M381 G392 T393 VAL ASP N396 N400 Y401 I402 I403 P404 Y405 N406 LEU ASN TYR GLU H411 S412 I413 N414 Y415 S416 Y417 L418 D419 N420 V421 N422 I423 E424 E425 I426 E427 K428 I429 P430 N433 D434 E435 D436 I437 Y438 P439 K442

N452 I453 T454 LYS ALA K457 T461 L465 P466 Y469 L470 Q471 I475 N478 D479 I480 N481 L482 S483 S484 S491 SER LYS GLY S495 L496 V497 Y498 S499 F500 L501 N502 N503 T504 M505 D506 K515 P516 I517 D518 W526 A529 I530 F531 Y534 D537 I538 T539 E540

T541 Q542 E543 I544 S545 N546 GLN PHE GLY D550 T551 K552 I553 I554 P555 W556 I557 G558 R559 N562 T566 N567 N568 S569 F570 V571 E572 E573 F574 K575 P579 I580 S581 L582 I583 K586 E587 N588 I589 K593 I594 K595 ILE ASP GLU I599 P600 S601 S602 M603 L604 N605 PHE SER F608

K609 D610 L611 S612 L615 C620 K621 K622 N623 F624 Y625 L626 I629 Y630 Y631 L634 W638 Y641 Y642 S643 Q644 Y645 F646 D647 K654 S655 V656 L657 A658 L662 E676 N677 S678 N679 I680 S681 N684 L687 N694 R697 A706 N709 I710 D711 K712

F713 N716 A717 V721 F722 I726 Y727 P728 K729 F730 M734 C737 I738 I741 N742 T745 N754 I755 N756 E759 K760 L763 Q766 N767 I779 N787 S788 Y789 T790 E791 L792 L793 I794 K795 S799 P800 L803 S804 L805 Y806 Q811 V815 I816

G817 D818 T819 S820 G821 K822 N823 T824 L825 V826 E827 Y828 P829 K830 L845 T846 G847 A848 I852 T855 N856 D857 Y858 F859 E860 N861 G862 L863 T864 N865 N866 F867 S868 I869 Y870 F871 W872 L876 K877 Q878 N879 I880 I881 L885 I886 G887 S888 W895 E896 F899 V905

D910 G913 N914 N917 I918 N922 I923 S924 N925 W928 I931 V932 I933 S934 I935 L943 I944 F945 I946 D947 L950 V951 A952 N953 E954 D955 I956 K957 E958 N961 I962 D966 I967 I968 S969 S972 D973 N974 N975 Y978 I979 E980 S983 V984 L985 N986 K987 T988

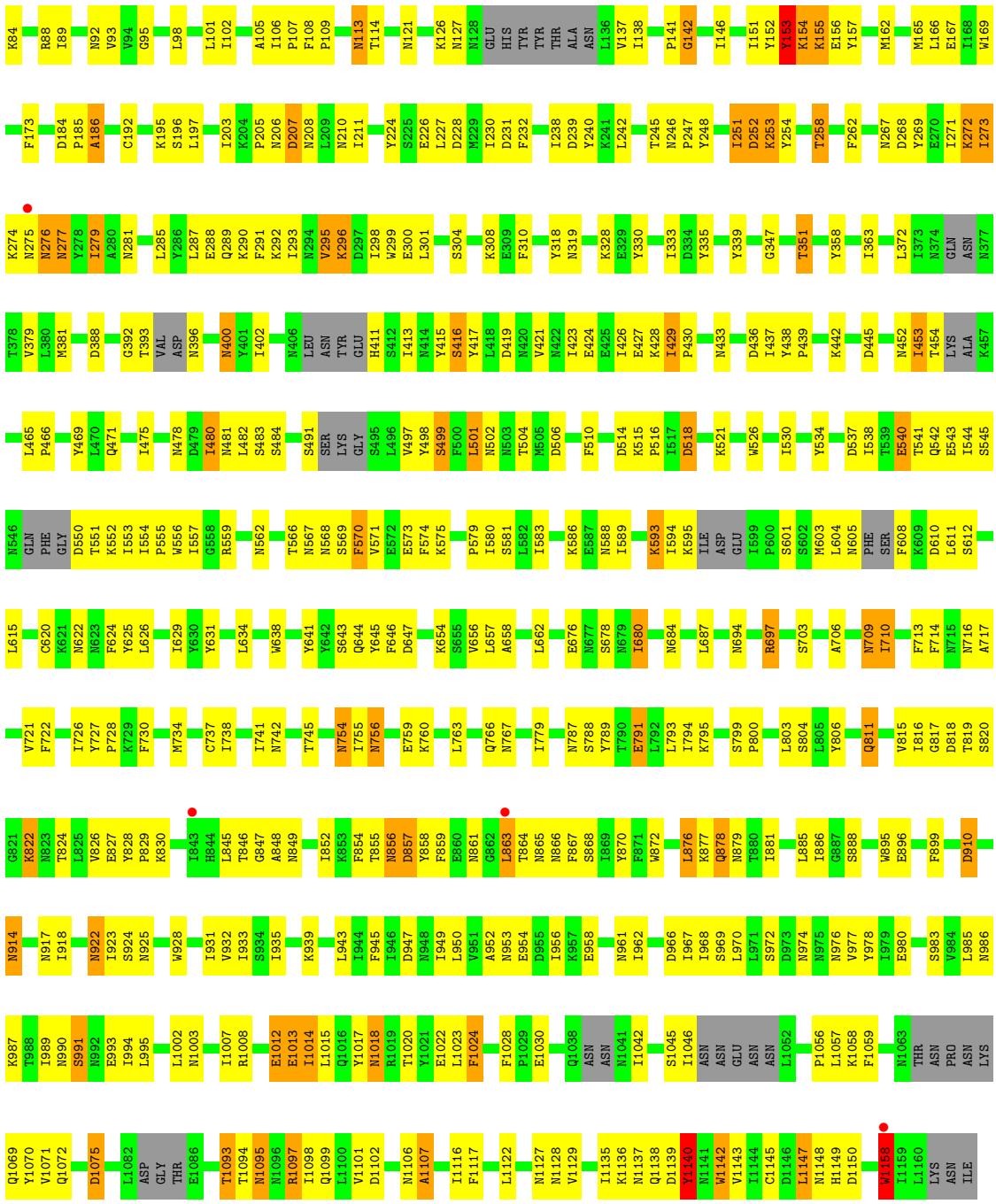
I989 N990 S991 N992 E993 I994 L995 L1002 N1003 I1007 R1008 E1012 E1013 I1014 L1015 Q1016 Y1017 N1018 R1019 T1020 Y1021 E1022 L1023 F1024 E1030 Q1038 ASN ASN N1041 I1042 S1045 I1046 ASN ASN GLU ASN ASN L1052 P1056 L1057 K1058 F1059 N1063 THR ASN PRO ASN LYS Q1069 Y1070 V1071 Q1072

D1075 L1082 ASP GLY THR E1086 T1093 T1094 N1095 N1096 R1097 I1098 Q1099 L1100 V1101 D1102 A1107 Q1108 I1109 I1116 F1117 L1122 N1127 N1128 V1129 I1135 K1136 N1137 Q1138 D1139 Y1140 N1141 W1142 V1143 I1144 C1145 D1146 L1147 N1148 H1149 D1150 W1158 I1159 L1160 LYS ASN ILE

• Molecule 2: Botulinum neurotoxin type E, nontoxic-nonhemagglutinin component, NTNH

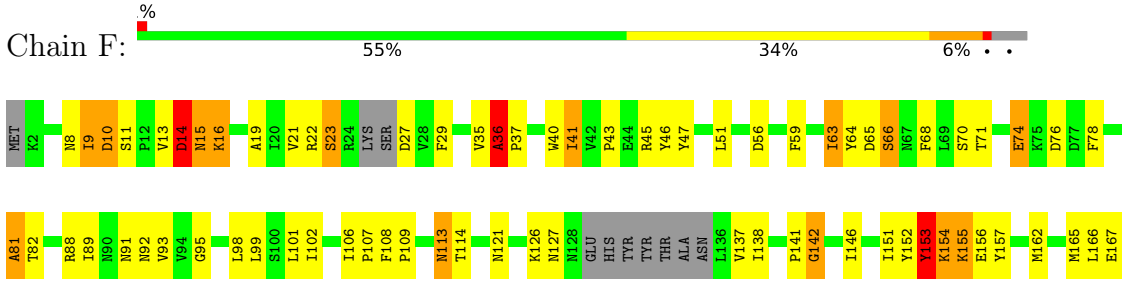
Chain D: 55% 34% 6%

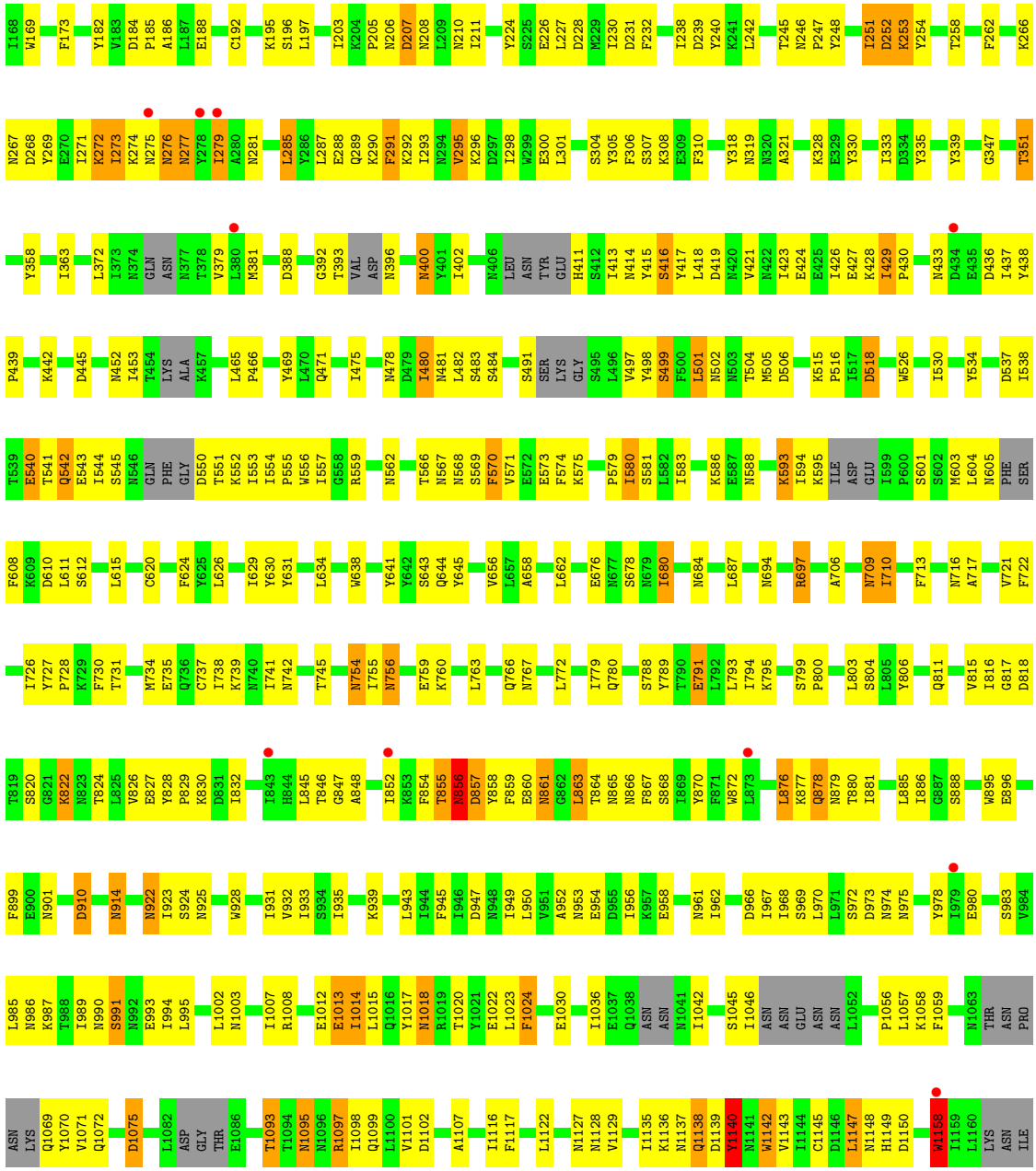
MET K2 I9 D10 S11 P12 V13 D14 N15 K16 A19 I20 V21 R22 S23 R24 LYS SER D27 V28 F29 V35 A36 P37 W40 I41 V42 P43 E44 R45 Y46 Y47 L51 F59 I63 Y64 D65 S66 N67 F68 L69 S70 T71 E74 K75 D76 D77 F78 A81 T82 I83



• Molecule 2: Botulinum neurotoxin type E, nontoxic-nonhemagglutinin component, NTNH

Chain F:




I168 W169 F173 Y182 V183 D184 P185 A186 L187 E188 C192 K195 S196 L197 I203 K204 P205 N206 D207 N208 L209 N210 I211 Y224 S225 E226 L227 D228 M229 I230 D231 F232 I238 D239 Y240 K241 L242 T245 N246 P247 Y248 I251 D252 K253 Y254 T258 F262 K266
N267 D268 Y269 E270 I271 K272 I273 K274 N275 N276 N277 Y278 I279 A280 N281 L285 Y286 L287 E288 Q289 K290 F291 K292 I293 N294 V295 K296 D297 I298 W299 E300 L301 S304 Y305 F306 S307 K308 E309 F310 Y318 N319 N320 A321 K328 E329 Y330 I333 D334 Y335 Y339 G347 T351
Y358 I363 L372 I373 N374 GLN ASN N377 T378 V379 L380 M381 D388 G392 T393 VAL ASP N396 N400 Y401 I402 N406 LEU ASN TYR GLU H411 S412 I413 N414 Y415 S416 Y417 L418 D419 N420 V421 N422 I423 E424 E425 I426 E427 K428 I429 P430 N433 D434 E435 D436 I437 Y438
P439 K442 D445 N452 I453 T454 LYS ALA K457 L465 P466 Y469 L470 Q471 I475 N478 D479 I480 N481 L482 S483 S484 S491 SER LYS GLY S495 L496 V497 Y498 S499 F500 L501 N502 N503 T504 M505 D506 K515 P516 I517 D518 W526 I530 Y534 D537 I538
T539 E540 T541 Q542 E543 I544 S545 N546 GLN PHE GLY D550 T551 K552 I553 I554 P555 W556 I557 G558 R559 N562 T566 N567 N568 S569 F570 V571 E572 E573 F574 K575 P579 I580 S581 L582 I583 K586 E587 N588 K593 I594 K595 ILE ASP GLU I599 P600 S601 S602 M603 L604 N605 PHE SER
F608 K609 D610 L611 S612 L615 C620 F624 Y625 L626 I629 Y630 Y631 L634 W638 Y641 Y642 S643 Q644 Y645 V656 L657 A658 L662 E676 N677 S678 N679 I680 N684 L687 N694 R697 A706 N709 I710 F713 N716 A717 V721 F722
I726 Y727 P728 K729 F730 T731 M734 E735 Q736 C737 I738 K739 N740 I741 N742 T745 N754 I755 N766 E759 K760 L763 Q766 N767 L772 I779 Q780 S788 Y789 I790 E791 L792 L793 I794 K795 S799 P800 L803 S804 L805 Y806 Q811 V815 I816 G817 D818
T819 S820 G821 K822 N823 T824 L825 V826 E827 Y828 P829 K830 D831 I832 I843 H844 L845 T846 G847 A848 I852 K853 F854 T855 N856 D857 Y858 F859 E860 N861 G862 L863 T864 N865 N866 F867 S868 I869 Y870 F871 W872 L873 L876 K877 Q878 N879 T880 I881 L885 I886 G887 S888 W895 E896
F899 E900 N901 D910 N914 N922 I923 S924 N925 W928 I931 V932 I933 S934 I935 K939 L943 I944 F945 I946 D947 N948 I949 L950 V951 A952 N953 E954 D955 I956 K957 E958 N961 I962 D966 I967 I968 S969 L970 L971 S972 D973 N974 N975 Y978 I979 E980 S983 V984
L985 N986 K987 T988 I989 N990 S991 N992 E993 I994 L995 L1002 N1003 I1007 R1008 E1012 E1013 I1014 L1015 Q1016 Y1017 N1018 R1019 T1020 Y1021 E1022 L1023 F1024 E1030 I1036 E1037 Q1038 ASN ASN N1041 I1042 S1045 I1046 ASN ASN GLU ASN ASN L1052 P1056 L1057 K1058 F1059 M1063 THR ASN PRO
ASN LYS Q1069 Y1070 V1071 Q1072 D1075 L1082 ASP GLY THR E1086 T1093 T1094 N1095 N1096 R1097 I1098 Q1099 L1100 V1101 D1102 A1107 I1116 F1117 L1122 N1127 N1128 V1129 I1135 K1136 N1137 Q1138 D1139 Y1140 N1141 W1142 V1143 I1144 C1145 D1146 L1147 N1148 H1149 D1150 W1158 I1159 L1160 LYS ASN ILE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	192.60Å 192.60Å 286.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.30 – 3.05 49.25 – 3.05	Depositor EDS
% Data completeness (in resolution range)	59.7 (49.30-3.05) 59.8 (49.25-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.243 , 0.321 0.247 , 0.314	Depositor DCC
R_{free} test set	1334 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å^2)	110.6	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 110.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	0.135 for -h,-k,l 0.196 for h,-h-k,-l 0.137 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	56952	wwPDB-VP
Average B, all atoms (Å^2)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% 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)

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

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	0.58	0/10176	0.74	2/13800 (0.0%)
1	C	0.56	0/10176	0.73	1/13800 (0.0%)
1	E	0.54	0/10176	0.72	2/13800 (0.0%)
2	B	0.64	2/9182 (0.0%)	0.75	0/12454
2	D	0.60	1/9182 (0.0%)	0.74	0/12454
2	F	0.58	1/9182 (0.0%)	0.73	0/12454
All	All	0.58	4/58074 (0.0%)	0.73	5/78762 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	D	0	1
2	F	0	2
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1158	TRP	CB-CG	-7.00	1.37	1.50
2	D	1158	TRP	CB-CG	-5.84	1.39	1.50
2	F	1158	TRP	CB-CG	-5.69	1.40	1.50
2	B	116	ASP	C-O	5.60	1.33	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1143	ARG	NE-CZ-NH2	7.34	123.97	120.30
1	E	1143	ARG	NE-CZ-NH2	7.21	123.90	120.30
1	A	394	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	C	1143	ARG	NE-CZ-NH2	6.28	123.44	120.30
1	E	394	ARG	NE-CZ-NH2	-5.63	117.48	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	36	ALA	Peptide
2	D	36	ALA	Peptide
2	F	1138	GLN	Peptide
2	F	36	ALA	Peptide

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	9978	0	9735	338	1
1	C	9978	0	9735	348	1
1	E	9978	0	9735	352	0
2	B	9005	0	8666	361	0
2	D	9005	0	8666	344	0
2	F	9005	0	8666	356	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
All	All	56952	0	55203	2034	1

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 18.

All (2034) 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)
2:D:885:LEU:HG	2:D:886:ILE:HD12	1.33	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:885:LEU:HG	2:F:886:ILE:HD12	1.32	1.09
2:B:436:ASP:HA	2:B:437:ILE:HB	1.34	1.08
2:B:885:LEU:HG	2:B:886:ILE:HD12	1.29	1.08
2:D:436:ASP:HA	2:D:437:ILE:HB	1.35	1.05
2:F:436:ASP:HA	2:F:437:ILE:HB	1.37	1.03
2:B:818:ASP:OD2	2:B:820:SER:OG	1.79	0.99
2:F:818:ASP:OD2	2:F:820:SER:OG	1.80	0.98
2:D:818:ASP:OD2	2:D:820:SER:OG	1.80	0.98
1:C:1130:GLN:O	1:C:1148:VAL:HG23	1.63	0.98
1:A:1130:GLN:O	1:A:1148:VAL:HG23	1.66	0.96
1:E:1130:GLN:O	1:E:1148:VAL:HG23	1.66	0.95
1:C:628:LEU:HB2	1:E:419:LYS:HE3	1.48	0.95
1:A:289:VAL:HB	1:A:290:GLN:HA	1.49	0.91
2:B:879:ASN:HB3	2:B:881:ILE:HG22	1.54	0.89
1:C:289:VAL:HB	1:C:290:GLN:HA	1.53	0.89
2:D:879:ASN:HB3	2:D:881:ILE:HG22	1.55	0.89
1:E:289:VAL:HB	1:E:290:GLN:HA	1.53	0.88
1:C:227:ILE:HD11	1:C:274:ASN:HB2	1.57	0.86
1:A:289:VAL:HB	1:A:290:GLN:CA	2.06	0.86
2:D:1045:SER:OG	2:D:1046:ILE:N	2.09	0.86
1:C:855:MET:O	1:C:856:ARG:HD3	1.76	0.85
1:E:238:ASN:CG	1:E:239:PRO:HD2	1.96	0.85
2:F:879:ASN:HB3	2:F:881:ILE:HG22	1.58	0.85
1:A:227:ILE:HD11	1:A:274:ASN:HB2	1.59	0.84
1:A:855:MET:O	1:A:856:ARG:HD3	1.77	0.84
1:E:227:ILE:HD11	1:E:274:ASN:HB2	1.58	0.84
1:A:238:ASN:CG	1:A:239:PRO:HD2	1.98	0.84
2:F:1045:SER:OG	2:F:1046:ILE:N	2.07	0.84
1:C:289:VAL:HB	1:C:290:GLN:CA	2.09	0.83
1:E:855:MET:O	1:E:856:ARG:HD3	1.79	0.83
1:E:289:VAL:HB	1:E:290:GLN:CA	2.09	0.83
2:D:1137:ASN:HB3	2:D:1142:TRP:HE1	1.46	0.81
2:B:1045:SER:OG	2:B:1046:ILE:N	2.12	0.81
1:A:1155:SER:O	1:A:1157:THR:N	2.13	0.81
1:A:522:TYR:CE2	1:A:611:ASN:HB2	2.16	0.81
1:A:897:GLU:HG2	1:A:1032:LYS:HB2	1.61	0.81
1:E:1155:SER:O	1:E:1157:THR:N	2.13	0.81
1:E:522:TYR:CE2	1:E:611:ASN:HB2	2.17	0.80
1:C:238:ASN:CG	1:C:239:PRO:HD2	2.03	0.80
1:C:1155:SER:O	1:C:1157:THR:N	2.14	0.80
2:B:1137:ASN:HB3	2:B:1142:TRP:HE1	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:421:ILE:HD11	2:D:510:PHE:CD1	2.17	0.79
1:E:513:ASP:OD1	2:D:521:LYS:NZ	2.16	0.79
1:C:627:LEU:HB3	1:E:419:LYS:HE2	1.65	0.79
1:C:522:TYR:CE2	1:C:611:ASN:HB2	2.17	0.78
1:E:897:GLU:HG2	1:E:1032:LYS:HB2	1.65	0.77
2:F:1137:ASN:HB3	2:F:1142:TRP:HE1	1.48	0.77
2:F:603:MET:O	2:F:605:ASN:N	2.17	0.76
1:A:199:ILE:HA	1:A:705:TYR:HE2	1.50	0.76
1:C:897:GLU:HG2	1:C:1032:LYS:HB2	1.67	0.76
2:B:815:VAL:O	2:B:816:ILE:HG13	1.87	0.74
2:D:526:TRP:CE2	2:D:530:ILE:HD11	2.23	0.74
1:E:728:LEU:HA	1:E:731:LYS:HB2	1.68	0.74
2:F:108:PHE:HB3	2:F:162:MET:HG3	1.70	0.73
2:B:108:PHE:HB3	2:B:162:MET:HG3	1.69	0.73
1:A:836:LEU:HD11	2:B:945:PHE:CD1	2.24	0.73
2:B:603:MET:O	2:B:605:ASN:N	2.22	0.73
2:B:526:TRP:CE2	2:B:530:ILE:HD11	2.24	0.73
1:C:836:LEU:HB2	2:D:995:LEU:HD11	1.69	0.73
1:A:728:LEU:HA	1:A:731:LYS:HB2	1.70	0.73
1:C:728:LEU:HA	1:C:731:LYS:HB2	1.69	0.73
2:D:603:MET:O	2:D:605:ASN:N	2.21	0.73
2:B:1127:ASN:O	2:B:1129:VAL:N	2.22	0.72
2:F:556:TRP:HA	2:F:559:ARG:HD3	1.71	0.72
1:A:227:ILE:HD12	1:A:271:ILE:HA	1.72	0.72
2:D:815:VAL:O	2:D:816:ILE:HG13	1.89	0.72
2:F:436:ASP:HA	2:F:437:ILE:CB	2.16	0.72
2:D:108:PHE:HB3	2:D:162:MET:HG3	1.72	0.72
2:F:815:VAL:O	2:F:816:ILE:HG13	1.90	0.71
1:C:199:ILE:HA	1:C:705:TYR:HE2	1.53	0.71
2:D:469:TYR:CZ	2:D:562:ASN:HB2	2.25	0.71
2:B:59:PHE:HB2	2:B:452:ASN:ND2	2.06	0.71
2:D:63:ILE:HD12	2:D:358:TYR:HB3	1.72	0.71
2:F:469:TYR:CZ	2:F:562:ASN:HB2	2.26	0.71
1:C:118:ASN:HA	1:C:119:THR:HB	1.74	0.70
1:E:738:TYR:HA	1:E:743:ILE:HG13	1.73	0.70
1:A:238:ASN:ND2	1:A:239:PRO:HD2	2.06	0.70
2:F:626:LEU:HA	2:F:629:ILE:HD12	1.74	0.70
2:B:876:LEU:O	2:B:877:LYS:HB2	1.92	0.70
2:B:63:ILE:HD12	2:B:358:TYR:HB3	1.73	0.70
1:E:199:ILE:HA	1:E:705:TYR:HE2	1.56	0.70
2:F:21:VAL:HG13	2:F:121:ASN:HA	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:436:PHE:C	1:C:436:PHE:HD1	1.96	0.69
2:F:526:TRP:CE2	2:F:530:ILE:HD11	2.27	0.69
1:E:238:ASN:ND2	1:E:239:PRO:HD2	2.07	0.69
2:B:556:TRP:HA	2:B:559:ARG:HD3	1.75	0.69
2:D:121:ASN:CB	2:D:127:ASN:HA	2.22	0.69
2:F:59:PHE:HB2	2:F:452:ASN:ND2	2.08	0.69
1:A:118:ASN:HA	1:A:119:THR:HB	1.74	0.69
1:C:944:ARG:HG2	1:C:1026:SER:HA	1.72	0.69
2:F:224:TYR:O	2:F:392:GLY:HA2	1.93	0.69
2:D:867:PHE:HB2	2:D:985:LEU:O	1.93	0.68
1:C:227:ILE:HD12	1:C:271:ILE:HA	1.75	0.68
2:D:224:TYR:O	2:D:392:GLY:HA2	1.93	0.68
2:F:876:LEU:O	2:F:877:LYS:HB2	1.93	0.68
2:B:21:VAL:HG13	2:B:121:ASN:HA	1.75	0.68
1:E:436:PHE:HD1	1:E:436:PHE:C	1.96	0.68
2:D:626:LEU:HA	2:D:629:ILE:HD12	1.76	0.68
2:B:626:LEU:HA	2:B:629:ILE:HD12	1.74	0.68
2:F:63:ILE:HD12	2:F:358:TYR:HB3	1.76	0.68
1:C:449:ASN:O	1:C:451:PRO:HD3	1.94	0.68
2:D:556:TRP:HA	2:D:559:ARG:HD3	1.76	0.68
2:B:469:TYR:CZ	2:B:562:ASN:HB2	2.28	0.68
1:E:944:ARG:HG2	1:E:1026:SER:HA	1.75	0.67
2:D:1149:HIS:CG	2:D:1150:ASP:N	2.62	0.67
1:E:449:ASN:O	1:E:451:PRO:HD3	1.94	0.67
1:E:836:LEU:HB2	2:F:995:LEU:HD11	1.75	0.67
1:E:227:ILE:HD12	1:E:271:ILE:HA	1.76	0.67
1:E:436:PHE:C	1:E:436:PHE:CD1	2.67	0.67
1:A:738:TYR:HA	1:A:743:ILE:HG13	1.76	0.67
1:C:1207:ASN:OD1	2:D:811:GLN:N	2.28	0.67
2:D:876:LEU:O	2:D:877:LYS:HB2	1.94	0.67
2:D:59:PHE:HB2	2:D:452:ASN:ND2	2.08	0.67
2:D:423:ILE:HG23	2:D:423:ILE:O	1.94	0.67
1:A:436:PHE:C	1:A:436:PHE:HD1	1.97	0.67
2:B:1149:HIS:CG	2:B:1150:ASP:N	2.62	0.67
1:C:436:PHE:C	1:C:436:PHE:CD1	2.66	0.67
1:C:738:TYR:HA	1:C:743:ILE:HG13	1.76	0.67
1:A:449:ASN:O	1:A:451:PRO:HD3	1.94	0.67
2:D:1127:ASN:O	2:D:1129:VAL:N	2.27	0.66
1:A:20:TYR:HB3	1:A:29:PHE:HB3	1.77	0.66
1:E:904:ASP:HA	1:E:907:ILE:HD11	1.75	0.66
2:B:393:THR:HG1	2:B:396:ASN:N	1.92	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1127:ASN:O	2:F:1129:VAL:N	2.27	0.66
2:B:295:VAL:O	2:B:298:ILE:N	2.29	0.66
1:A:436:PHE:C	1:A:436:PHE:CD1	2.68	0.66
2:B:436:ASP:HA	2:B:437:ILE:CB	2.12	0.66
2:F:423:ILE:O	2:F:423:ILE:HG23	1.94	0.66
2:F:867:PHE:HB2	2:F:985:LEU:O	1.95	0.66
2:B:423:ILE:HG23	2:B:423:ILE:O	1.93	0.66
1:A:944:ARG:HG2	1:A:1026:SER:HA	1.76	0.66
2:F:1149:HIS:CG	2:F:1150:ASP:N	2.64	0.66
2:B:877:LYS:HB3	2:B:878:GLN:HB3	1.78	0.66
1:E:154:GLU:HB2	1:E:155:PRO:HD2	1.78	0.66
1:C:154:GLU:HB2	1:C:155:PRO:HD2	1.77	0.65
2:D:21:VAL:HG13	2:D:121:ASN:HA	1.77	0.65
2:F:877:LYS:HB3	2:F:878:GLN:HB3	1.78	0.65
1:C:628:LEU:CB	1:E:419:LYS:HE3	2.25	0.65
2:D:877:LYS:HB3	2:D:878:GLN:HB3	1.78	0.65
1:E:118:ASN:HA	1:E:119:THR:HB	1.77	0.65
1:E:928:ASN:HB3	1:E:930:ILE:HG22	1.77	0.65
2:B:867:PHE:HB2	2:B:985:LEU:O	1.97	0.65
2:D:1013:GLU:O	2:D:1014:ILE:HB	1.97	0.65
2:F:121:ASN:CB	2:F:127:ASN:HA	2.27	0.65
1:C:238:ASN:ND2	1:C:239:PRO:HD2	2.11	0.65
2:B:121:ASN:CB	2:B:127:ASN:HA	2.26	0.65
1:E:771:MET:HA	1:E:774:ILE:HG22	1.79	0.64
1:A:928:ASN:HB3	1:A:930:ILE:HG22	1.79	0.64
1:C:415:ILE:HD12	1:C:425:ILE:HD12	1.78	0.64
1:C:836:LEU:HD11	2:D:945:PHE:CD1	2.32	0.64
1:E:236:GLN:HB3	1:E:241:ILE:HD13	1.79	0.64
1:E:926:TYR:HB3	1:E:1250:GLN:CG	2.28	0.64
1:A:216:HIS:NE2	1:A:251:GLU:OE1	2.30	0.64
1:A:289:VAL:CB	1:A:290:GLN:HA	2.23	0.64
1:A:771:MET:HA	1:A:774:ILE:HG22	1.79	0.64
1:A:926:TYR:HB3	1:A:1250:GLN:CG	2.28	0.64
1:E:216:HIS:NE2	1:E:251:GLU:OE1	2.31	0.64
2:B:1013:GLU:O	2:B:1014:ILE:HB	1.97	0.64
1:A:415:ILE:HD12	1:A:425:ILE:HD12	1.79	0.64
1:A:468:LEU:O	1:A:470:GLN:N	2.31	0.64
1:E:836:LEU:HD11	2:F:945:PHE:CD1	2.33	0.64
2:B:1137:ASN:HB3	2:B:1142:TRP:NE1	2.13	0.64
2:D:552:LYS:O	2:D:713:PHE:HD1	1.81	0.64
2:B:35:VAL:HG12	2:B:36:ALA:H	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:35:VAL:HG12	2:D:36:ALA:H	1.63	0.64
2:F:1013:GLU:O	2:F:1014:ILE:HB	1.98	0.64
1:E:415:ILE:HD12	1:E:425:ILE:HD12	1.79	0.64
1:A:705:TYR:CD1	1:A:705:TYR:C	2.72	0.63
1:E:468:LEU:O	1:E:470:GLN:N	2.30	0.63
1:A:904:ASP:HA	1:A:907:ILE:HD11	1.79	0.63
2:B:13:VAL:HG12	2:B:14:ASP:N	2.14	0.63
2:B:1122:LEU:HD21	2:B:1158:TRP:CZ2	2.33	0.63
1:C:365:ASN:O	1:C:368:ILE:HG22	1.97	0.63
2:B:224:TYR:O	2:B:392:GLY:HA2	1.97	0.63
1:E:454:ILE:HD13	1:E:666:ALA:HA	1.79	0.63
2:B:608:PHE:O	2:B:612:SER:N	2.31	0.63
2:D:1122:LEU:HD21	2:D:1158:TRP:CZ2	2.33	0.63
2:D:1137:ASN:HB3	2:D:1142:TRP:NE1	2.12	0.63
2:F:269:TYR:OH	2:F:288:GLU:HB2	1.98	0.63
1:A:154:GLU:HB2	1:A:155:PRO:HD2	1.79	0.63
1:C:926:TYR:HB3	1:C:1250:GLN:CG	2.29	0.63
2:B:856:ASN:HB3	2:B:859:PHE:CE2	2.34	0.63
1:C:857:TYR:CZ	1:C:860:ASP:HA	2.33	0.63
2:D:608:PHE:O	2:D:612:SER:N	2.32	0.63
2:F:1122:LEU:HD21	2:F:1158:TRP:CZ2	2.33	0.63
1:A:926:TYR:HB3	1:A:1250:GLN:HG3	1.80	0.63
1:C:444:ASN:OD1	1:C:445:ASP:N	2.33	0.62
1:C:928:ASN:HB3	1:C:930:ILE:HG22	1.80	0.62
2:F:961:ASN:OD1	2:F:962:ILE:N	2.33	0.62
1:C:754:ALA:O	1:C:757:ASN:HB2	1.99	0.62
2:B:910:ASP:HB3	2:B:914:ASN:HB2	1.81	0.62
2:B:962:ILE:O	2:B:962:ILE:HG22	1.99	0.62
2:D:295:VAL:O	2:D:298:ILE:N	2.31	0.62
2:F:429:ILE:N	2:F:430:PRO:CD	2.63	0.62
1:C:216:HIS:NE2	1:C:251:GLU:OE1	2.33	0.62
1:C:771:MET:HA	1:C:774:ILE:HG22	1.82	0.62
1:E:219:HIS:ND1	1:E:250:GLU:OE2	2.27	0.62
2:B:552:LYS:O	2:B:713:PHE:HD1	1.83	0.62
2:D:269:TYR:OH	2:D:288:GLU:HB2	1.98	0.62
2:F:295:VAL:O	2:F:298:ILE:N	2.32	0.62
1:A:914:ASN:O	1:A:915:PHE:HB3	1.99	0.62
1:C:926:TYR:HB3	1:C:1250:GLN:HG3	1.81	0.62
2:B:268:ASP:HA	2:B:271:ILE:HG22	1.80	0.62
2:B:429:ILE:N	2:B:430:PRO:CD	2.63	0.62
2:D:268:ASP:HA	2:D:271:ILE:HG22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:962:ILE:O	2:F:962:ILE:HG22	2.00	0.62
1:E:926:TYR:HB3	1:E:1250:GLN:HG3	1.80	0.62
2:D:910:ASP:HB3	2:D:914:ASN:HB2	1.82	0.62
2:D:962:ILE:O	2:D:962:ILE:HG22	2.00	0.62
2:F:35:VAL:HG12	2:F:36:ALA:H	1.65	0.62
2:F:608:PHE:O	2:F:612:SER:N	2.32	0.62
1:A:365:ASN:O	1:A:368:ILE:HG22	2.00	0.62
1:E:414:ASN:HA	1:E:424:SER:HA	1.81	0.62
1:A:236:GLN:HB3	1:A:241:ILE:HD13	1.82	0.61
1:C:20:TYR:HB3	1:C:29:PHE:HB3	1.81	0.61
1:C:454:ILE:HD13	1:C:666:ALA:HA	1.81	0.61
1:E:119:THR:H	1:E:120:PRO:CD	2.14	0.61
2:D:1093:THR:HG23	2:D:1095:ASN:H	1.65	0.61
2:F:268:ASP:HA	2:F:271:ILE:HG22	1.82	0.61
1:A:380:LEU:HA	1:A:385:ARG:HB3	1.82	0.61
1:E:857:TYR:CZ	1:E:860:ASP:HA	2.36	0.61
2:B:1149:HIS:CE1	2:B:1150:ASP:HB3	2.35	0.61
2:D:961:ASN:OD1	2:D:962:ILE:N	2.33	0.61
2:F:1023:LEU:HD13	2:F:1158:TRP:HZ3	1.66	0.61
2:F:1137:ASN:HB3	2:F:1142:TRP:NE1	2.14	0.61
1:C:414:ASN:HA	1:C:424:SER:HA	1.82	0.61
2:F:184:ASP:OD1	2:F:185:PRO:HD2	2.01	0.61
2:F:910:ASP:HB3	2:F:914:ASN:HB2	1.83	0.61
1:C:1131:ARG:HD2	1:C:1132:VAL:N	2.16	0.61
2:F:393:THR:HG1	2:F:396:ASN:N	1.99	0.61
1:C:236:GLN:HB3	1:C:241:ILE:HD13	1.83	0.61
1:A:454:ILE:HD13	1:A:666:ALA:HA	1.82	0.61
1:C:468:LEU:O	1:C:470:GLN:N	2.33	0.61
1:C:705:TYR:CD1	1:C:705:TYR:C	2.74	0.61
2:D:552:LYS:HB2	2:D:713:PHE:HE1	1.65	0.61
2:D:956:ILE:HG22	2:D:956:ILE:O	2.00	0.61
1:E:981:ASN:HD21	2:F:414:ASN:HB3	1.64	0.61
2:D:856:ASN:HB3	2:D:859:PHE:CE2	2.36	0.61
1:C:289:VAL:CB	1:C:290:GLN:HA	2.27	0.60
2:B:184:ASP:OD1	2:B:185:PRO:HD2	2.00	0.60
1:A:754:ALA:O	1:A:757:ASN:HB2	1.99	0.60
1:A:854:ASN:HB2	1:A:865:THR:HG22	1.82	0.60
1:A:1131:ARG:HD2	1:A:1132:VAL:N	2.15	0.60
1:C:427:ILE:CD1	1:C:521:PHE:HA	2.31	0.60
2:F:956:ILE:HG22	2:F:956:ILE:O	2.00	0.60
1:C:914:ASN:O	1:C:915:PHE:HB3	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:904:ASP:HA	1:C:907:ILE:HD11	1.82	0.60
1:E:365:ASN:O	1:E:368:ILE:HG22	2.00	0.60
2:F:856:ASN:HB3	2:F:859:PHE:CE2	2.36	0.60
1:C:219:HIS:ND1	1:C:250:GLU:OE2	2.28	0.60
1:E:380:LEU:HA	1:E:385:ARG:HB3	1.84	0.60
2:D:184:ASP:OD1	2:D:185:PRO:HD2	2.02	0.60
1:E:427:ILE:CD1	1:E:521:PHE:HA	2.31	0.60
1:E:914:ASN:O	1:E:915:PHE:HB3	2.01	0.60
2:B:269:TYR:OH	2:B:288:GLU:HB2	2.01	0.60
2:B:552:LYS:HB2	2:B:713:PHE:HE1	1.65	0.60
2:D:13:VAL:HG12	2:D:14:ASP:N	2.16	0.60
2:D:246:ASN:ND2	2:D:413:ILE:O	2.34	0.60
2:D:429:ILE:N	2:D:430:PRO:CD	2.65	0.60
2:D:1023:LEU:HD13	2:D:1158:TRP:HZ3	1.67	0.60
2:F:246:ASN:ND2	2:F:413:ILE:O	2.34	0.60
2:F:465:LEU:HB3	2:F:466:PRO:HD2	1.84	0.60
2:F:465:LEU:HB3	2:F:466:PRO:CD	2.32	0.60
2:F:552:LYS:O	2:F:713:PHE:HD1	1.83	0.60
2:B:605:ASN:HA	2:B:754:ASN:HB2	1.83	0.60
2:F:989:ILE:HG22	2:F:994:ILE:HG13	1.82	0.60
1:C:1211:LEU:HD12	1:C:1225:TYR:HB3	1.83	0.60
1:E:754:ALA:O	1:E:757:ASN:HB2	2.01	0.60
1:A:414:ASN:HA	1:A:424:SER:HA	1.84	0.60
1:C:143:ILE:HD13	1:C:491:THR:HG23	1.83	0.59
1:C:779:ILE:O	1:C:779:ILE:HG22	2.02	0.59
2:B:544:ILE:HD12	2:B:553:ILE:HD12	1.83	0.59
1:A:987:ILE:C	1:A:989:LYS:H	2.06	0.59
2:D:544:ILE:HD12	2:D:553:ILE:HD12	1.82	0.59
1:C:417:SER:OG	1:C:418:VAL:N	2.33	0.59
2:B:411:HIS:HA	2:B:624:PHE:HE1	1.66	0.59
1:A:857:TYR:CZ	1:A:860:ASP:HA	2.36	0.59
1:C:836:LEU:CB	2:D:995:LEU:HD11	2.31	0.59
2:B:498:TYR:OH	2:B:559:ARG:O	2.21	0.59
2:D:989:ILE:HG22	2:D:994:ILE:HG13	1.84	0.59
2:F:544:ILE:HD12	2:F:553:ILE:HD12	1.83	0.59
1:A:417:SER:OG	1:A:418:VAL:N	2.34	0.59
1:E:705:TYR:C	1:E:705:TYR:CD1	2.75	0.59
2:D:605:ASN:HA	2:D:754:ASN:HB2	1.84	0.59
1:A:219:HIS:ND1	1:A:250:GLU:OE2	2.28	0.59
2:B:961:ASN:OD1	2:B:962:ILE:N	2.35	0.59
2:D:552:LYS:O	2:D:713:PHE:CD1	2.55	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:ILE:CD1	1:A:521:PHE:HA	2.33	0.59
1:E:854:ASN:HB2	1:E:865:THR:HG22	1.85	0.59
2:B:543:GLU:HA	2:B:552:LYS:HA	1.83	0.59
2:B:552:LYS:O	2:B:713:PHE:CD1	2.56	0.59
2:B:956:ILE:O	2:B:956:ILE:HG22	2.03	0.59
2:B:1142:TRP:N	2:B:1142:TRP:CD1	2.70	0.59
1:A:368:ILE:HD11	1:A:395:ILE:HA	1.84	0.59
1:A:462:ASN:HB3	1:A:463:ASN:HA	1.85	0.59
2:B:1093:THR:HG23	2:B:1095:ASN:H	1.66	0.59
2:F:9:ILE:HG23	2:F:10:ASP:H	1.67	0.59
1:A:143:ILE:HD13	1:A:491:THR:HG23	1.83	0.59
2:B:579:PRO:C	2:B:581:SER:H	2.06	0.59
2:F:543:GLU:HA	2:F:552:LYS:HA	1.85	0.59
1:A:454:ILE:HD11	1:A:456:ASP:OD1	2.03	0.58
1:E:198:SER:O	1:E:200:ASN:N	2.36	0.58
1:E:444:ASN:OD1	1:E:445:ASP:N	2.36	0.58
2:B:1023:LEU:HD12	2:B:1024:PHE:N	2.17	0.58
2:D:1149:HIS:CE1	2:D:1150:ASP:HB3	2.38	0.58
1:C:854:ASN:HB2	1:C:865:THR:HG22	1.84	0.58
1:E:628:LEU:HD23	1:E:632:ILE:HB	1.85	0.58
2:D:469:TYR:CE2	2:D:562:ASN:HB2	2.38	0.58
2:D:526:TRP:CZ2	2:D:530:ILE:HD11	2.38	0.58
1:A:453:GLU:O	1:A:454:ILE:HG22	2.03	0.58
1:E:453:GLU:O	1:E:454:ILE:HG22	2.04	0.58
1:E:943:MET:HB3	1:E:947:ASN:HA	1.85	0.58
2:B:246:ASN:ND2	2:B:413:ILE:O	2.35	0.58
1:E:454:ILE:HD11	1:E:456:ASP:OD1	2.03	0.58
1:E:779:ILE:O	1:E:779:ILE:HG22	2.03	0.58
2:B:990:ASN:HB3	2:B:993:GLU:CD	2.23	0.58
2:D:245:THR:O	2:D:247:PRO:C	2.42	0.58
2:D:465:LEU:HB3	2:D:466:PRO:HD2	1.86	0.58
2:D:990:ASN:HB3	2:D:993:GLU:CD	2.23	0.58
2:F:804:SER:O	2:F:818:ASP:HA	2.03	0.58
1:A:836:LEU:HB2	2:B:995:LEU:HD11	1.85	0.58
1:A:1211:LEU:HD12	1:A:1225:TYR:HB3	1.84	0.58
1:C:436:PHE:HD1	1:C:437:VAL:N	2.01	0.58
1:E:143:ILE:HD13	1:E:491:THR:HG23	1.83	0.58
1:E:417:SER:OG	1:E:418:VAL:N	2.32	0.58
2:D:436:ASP:HA	2:D:437:ILE:CB	2.14	0.58
2:F:13:VAL:HG12	2:F:14:ASP:N	2.18	0.58
2:B:427:GLU:C	2:B:430:PRO:HD3	2.24	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:ILE:CD1	1:A:456:ASP:OD1	2.51	0.58
1:A:779:ILE:HG22	1:A:779:ILE:O	2.03	0.58
1:C:164:ASN:HB3	1:C:180:SER:OG	2.04	0.58
1:E:1131:ARG:HD2	1:E:1132:VAL:N	2.18	0.58
1:A:164:ASN:HB3	1:A:180:SER:OG	2.03	0.58
1:C:168:ARG:HA	1:C:497:TYR:HB2	1.86	0.58
2:F:469:TYR:CE2	2:F:562:ASN:HB2	2.39	0.58
2:D:427:GLU:C	2:D:430:PRO:HD3	2.24	0.58
1:A:444:ASN:OD1	1:A:445:ASP:N	2.37	0.58
1:C:154:GLU:HB2	1:C:155:PRO:CD	2.34	0.58
2:D:113:ASN:HB3	2:D:279:ILE:CB	2.33	0.58
2:D:465:LEU:HB3	2:D:466:PRO:CD	2.34	0.58
2:F:788:SER:O	2:F:791:GLU:HB3	2.04	0.58
2:F:990:ASN:HB3	2:F:993:GLU:CD	2.24	0.58
1:A:1044:ILE:HG22	1:A:1045:ARG:N	2.19	0.57
1:C:824:PRO:HB3	2:D:952:ALA:HB2	1.86	0.57
2:D:788:SER:O	2:D:791:GLU:HB3	2.04	0.57
2:D:804:SER:O	2:D:818:ASP:HA	2.04	0.57
2:F:227:LEU:HD11	2:F:231:ASP:HB2	1.86	0.57
2:F:411:HIS:HA	2:F:624:PHE:HE1	1.69	0.57
1:A:605:TYR:CD1	1:A:605:TYR:O	2.57	0.57
1:C:1205:ASN:C	1:C:1205:ASN:OD1	2.42	0.57
2:B:856:ASN:HB3	2:B:859:PHE:HE2	1.69	0.57
2:B:989:ILE:HG22	2:B:994:ILE:HG13	1.86	0.57
2:D:1023:LEU:HD12	2:D:1024:PHE:N	2.19	0.57
2:D:498:TYR:OH	2:D:559:ARG:O	2.21	0.57
2:D:756:ASN:OD1	2:D:756:ASN:N	2.37	0.57
2:F:552:LYS:O	2:F:713:PHE:CD1	2.57	0.57
2:F:1142:TRP:CD1	2:F:1142:TRP:N	2.72	0.57
1:E:20:TYR:HB3	1:E:29:PHE:HB3	1.84	0.57
1:E:236:GLN:HB3	1:E:241:ILE:CD1	2.33	0.57
2:B:554:ILE:HG21	2:B:556:TRP:CE2	2.39	0.57
2:B:1023:LEU:HD13	2:B:1158:TRP:HZ3	1.68	0.57
2:D:543:GLU:HA	2:D:552:LYS:HA	1.87	0.57
1:A:168:ARG:HA	1:A:497:TYR:HB2	1.87	0.57
1:C:628:LEU:HD23	1:C:632:ILE:HB	1.86	0.57
1:E:168:ARG:HA	1:E:497:TYR:HB2	1.87	0.57
1:E:368:ILE:HD11	1:E:395:ILE:HA	1.85	0.57
1:E:824:PRO:CB	2:F:952:ALA:HB2	2.35	0.57
2:F:1093:THR:HG23	2:F:1095:ASN:H	1.69	0.57
1:C:416:VAL:HG13	1:C:420:GLY:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:GLU:HB2	1:E:155:PRO:CD	2.35	0.57
1:E:164:ASN:HB3	1:E:180:SER:OG	2.04	0.57
1:E:454:ILE:CD1	1:E:456:ASP:OD1	2.52	0.57
1:C:380:LEU:HA	1:C:385:ARG:HB3	1.86	0.57
1:C:857:TYR:OH	1:C:860:ASP:HA	2.05	0.57
2:D:552:LYS:HB2	2:D:713:PHE:CE1	2.40	0.57
1:A:309:LEU:CD2	1:A:319:VAL:HG12	2.35	0.57
1:C:453:GLU:O	1:C:454:ILE:HG22	2.04	0.57
2:B:166:LEU:HD12	2:B:196:SER:HB2	1.86	0.57
2:D:742:ASN:HA	2:D:745:THR:HG22	1.87	0.57
2:F:552:LYS:HB2	2:F:713:PHE:HE1	1.69	0.57
1:A:289:VAL:HB	1:A:290:GLN:CB	2.35	0.57
1:C:368:ILE:HD11	1:C:395:ILE:HA	1.86	0.57
1:E:436:PHE:HD1	1:E:437:VAL:N	2.01	0.57
1:E:836:LEU:HD13	2:F:991:SER:HA	1.87	0.57
1:C:943:MET:HB3	1:C:947:ASN:HA	1.86	0.57
2:D:9:ILE:HG23	2:D:10:ASP:H	1.69	0.57
2:F:870:TYR:CE2	2:F:983:SER:OG	2.57	0.57
1:A:198:SER:O	1:A:200:ASN:N	2.38	0.56
1:E:742:GLN:O	1:E:744:GLU:N	2.38	0.56
1:E:1205:ASN:C	1:E:1205:ASN:OD1	2.43	0.56
2:F:605:ASN:HA	2:F:754:ASN:HB2	1.87	0.56
2:B:895:TRP:O	2:B:896:GLU:HG2	2.05	0.56
2:F:40:TRP:O	2:F:137:VAL:HA	2.05	0.56
2:F:113:ASN:HB3	2:F:279:ILE:CB	2.34	0.56
2:F:756:ASN:N	2:F:756:ASN:OD1	2.37	0.56
2:F:1023:LEU:HD13	2:F:1158:TRP:CZ3	2.40	0.56
2:F:1149:HIS:CE1	2:F:1150:ASP:HB3	2.40	0.56
1:A:427:ILE:HG22	1:A:428:GLU:N	2.19	0.56
1:E:452:LYS:HB2	1:E:651:LYS:HE2	1.88	0.56
1:E:1149:TYR:CD1	1:E:1183:ARG:HD2	2.40	0.56
2:B:756:ASN:OD1	2:B:756:ASN:N	2.39	0.56
2:B:804:SER:O	2:B:818:ASP:HA	2.04	0.56
2:B:943:LEU:HD23	2:B:953:ASN:HA	1.88	0.56
2:F:245:THR:O	2:F:247:PRO:C	2.42	0.56
1:A:452:LYS:HB2	1:A:651:LYS:HE2	1.87	0.56
1:A:628:LEU:HD23	1:A:632:ILE:HB	1.86	0.56
1:C:481:PRO:HG2	1:C:483:LEU:HD21	1.88	0.56
2:B:526:TRP:CZ2	2:B:530:ILE:HD11	2.40	0.56
1:A:1205:ASN:C	1:A:1205:ASN:OD1	2.43	0.56
1:C:454:ILE:HD11	1:C:456:ASP:OD1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:824:PRO:CB	2:D:952:ALA:HB2	2.36	0.56
2:B:465:LEU:HB3	2:B:466:PRO:CD	2.36	0.56
2:B:788:SER:O	2:B:791:GLU:HB3	2.04	0.56
2:D:227:LEU:HD11	2:D:231:ASP:HB2	1.88	0.56
2:D:393:THR:HG1	2:D:396:ASN:N	2.03	0.56
1:A:289:VAL:HB	1:A:290:GLN:HB3	1.88	0.56
1:A:436:PHE:HD1	1:A:437:VAL:N	2.03	0.56
1:A:1150:ILE:HG22	1:A:1162:LEU:HD12	1.86	0.56
1:C:1163:TYR:O	1:C:1175:ILE:HG23	2.05	0.56
2:B:113:ASN:HB3	2:B:279:ILE:CB	2.36	0.56
2:B:465:LEU:HB3	2:B:466:PRO:HD2	1.87	0.56
2:B:822:LYS:O	2:B:824:THR:N	2.39	0.56
2:D:856:ASN:HB3	2:D:859:PHE:HE2	1.71	0.56
1:A:38:ASN:HD21	1:A:484:SER:CB	2.19	0.56
1:C:1083:ASP:N	1:C:1129:ILE:O	2.33	0.56
1:E:462:ASN:HB3	1:E:463:ASN:HA	1.87	0.56
2:F:98:LEU:O	2:F:101:LEU:HB3	2.06	0.56
1:C:198:SER:O	1:C:200:ASN:N	2.39	0.56
1:C:454:ILE:CD1	1:C:456:ASP:OD1	2.53	0.56
1:E:416:VAL:HG13	1:E:420:GLY:N	2.21	0.56
2:B:552:LYS:HB2	2:B:713:PHE:CE1	2.40	0.56
2:F:429:ILE:HG22	2:F:429:ILE:O	2.06	0.56
1:A:154:GLU:HB2	1:A:155:PRO:CD	2.35	0.56
1:C:857:TYR:HA	1:C:862:TYR:HA	1.88	0.56
1:C:899:ASN:OD1	1:C:1028:ASN:HB3	2.05	0.56
1:C:1044:ILE:HG22	1:C:1045:ARG:N	2.20	0.56
1:E:289:VAL:CB	1:E:290:GLN:HA	2.27	0.56
2:B:269:TYR:CE1	2:B:287:LEU:HB3	2.41	0.56
2:B:742:ASN:HA	2:B:745:THR:HG22	1.88	0.56
2:D:870:TYR:CE2	2:D:983:SER:OG	2.59	0.56
2:F:554:ILE:HG21	2:F:556:TRP:CE2	2.41	0.56
1:C:119:THR:H	1:C:120:PRO:CD	2.18	0.55
1:E:1163:TYR:O	1:E:1175:ILE:HG23	2.06	0.55
1:E:1211:LEU:HD12	1:E:1225:TYR:HB3	1.86	0.55
2:F:427:GLU:C	2:F:430:PRO:HD3	2.26	0.55
1:C:448:ILE:O	1:C:449:ASN:C	2.44	0.55
2:B:40:TRP:O	2:B:137:VAL:HA	2.06	0.55
2:B:1015:LEU:HB2	2:B:1071:VAL:HB	1.89	0.55
2:D:943:LEU:HD23	2:D:953:ASN:HA	1.88	0.55
2:F:545:SER:HA	2:F:550:ASP:N	2.21	0.55
1:E:376:ASN:HB3	1:E:381:LYS:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:92:ASN:HB3	2:D:310:PHE:CZ	2.42	0.55
2:D:545:SER:HA	2:D:550:ASP:N	2.21	0.55
2:D:554:ILE:HG21	2:D:556:TRP:CE2	2.41	0.55
2:D:1023:LEU:HD13	2:D:1158:TRP:CZ3	2.41	0.55
2:F:269:TYR:CE1	2:F:287:LEU:HB3	2.41	0.55
1:A:67:SER:HA	1:A:158:PHE:CD2	2.41	0.55
1:C:452:LYS:HB2	1:C:651:LYS:HE2	1.87	0.55
1:C:1092:LEU:O	1:C:1094:PRO:HD3	2.06	0.55
2:F:498:TYR:OH	2:F:559:ARG:O	2.23	0.55
2:F:943:LEU:HD23	2:F:953:ASN:HA	1.89	0.55
1:A:705:TYR:C	1:A:705:TYR:HD1	2.09	0.55
1:A:742:GLN:O	1:A:744:GLU:N	2.40	0.55
1:C:427:ILE:HG22	1:C:428:GLU:N	2.22	0.55
2:B:92:ASN:HB3	2:B:310:PHE:CZ	2.42	0.55
2:B:1023:LEU:HD13	2:B:1158:TRP:CZ3	2.42	0.55
2:D:895:TRP:O	2:D:896:GLU:HG2	2.05	0.55
2:F:1023:LEU:HD12	2:F:1024:PHE:N	2.22	0.55
1:A:1092:LEU:O	1:A:1094:PRO:HD3	2.07	0.55
1:C:462:ASN:HB3	1:C:463:ASN:HA	1.88	0.55
1:C:627:LEU:O	1:E:420:GLY:N	2.40	0.55
1:C:738:TYR:O	1:C:739:ASP:C	2.45	0.55
1:E:111:ASN:HA	1:E:147:ASN:OD1	2.07	0.55
2:B:9:ILE:HG23	2:B:10:ASP:H	1.71	0.55
2:B:98:LEU:O	2:B:101:LEU:HB3	2.07	0.55
2:B:469:TYR:CE2	2:B:562:ASN:HB2	2.41	0.55
2:D:23:SER:OG	2:D:29:PHE:HB2	2.07	0.55
1:A:737:LYS:O	1:A:738:TYR:O	2.24	0.55
2:B:502:ASN:O	2:B:506:ASP:HB2	2.06	0.55
2:F:579:PRO:C	2:F:581:SER:H	2.08	0.55
1:A:119:THR:H	1:A:120:PRO:CD	2.19	0.55
1:A:1025:VAL:HG12	1:A:1026:SER:N	2.22	0.55
1:C:742:GLN:O	1:C:744:GLU:N	2.40	0.55
2:F:727:TYR:N	2:F:728:PRO:HD2	2.22	0.55
1:E:392:ASN:O	1:E:395:ILE:HG12	2.07	0.55
2:B:1149:HIS:NE2	2:B:1150:ASP:HB3	2.22	0.55
2:F:1072:GLN:O	2:F:1075:ASP:HB2	2.07	0.55
1:A:943:MET:HB3	1:A:947:ASN:HA	1.88	0.54
1:C:606:ILE:HD13	1:C:761:PHE:CE2	2.42	0.54
1:E:1044:ILE:HG22	1:E:1045:ARG:N	2.22	0.54
2:B:23:SER:OG	2:B:29:PHE:HB2	2.08	0.54
2:B:544:ILE:HD13	2:B:575:LYS:HG2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:98:LEU:O	2:D:101:LEU:HB3	2.07	0.54
1:C:67:SER:HA	1:C:158:PHE:CD2	2.43	0.54
1:C:467:ASP:OD1	1:C:468:LEU:N	2.40	0.54
1:C:1053:GLU:HG3	1:C:1053:GLU:O	2.07	0.54
1:E:606:ILE:HD13	1:E:761:PHE:CE2	2.42	0.54
1:E:824:PRO:HB3	2:F:952:ALA:HB2	1.89	0.54
2:B:88:ARG:NE	2:B:339:TYR:OH	2.41	0.54
2:B:870:TYR:CE2	2:B:983:SER:OG	2.59	0.54
2:D:579:PRO:C	2:D:581:SER:H	2.10	0.54
2:D:1142:TRP:N	2:D:1142:TRP:CD1	2.75	0.54
2:F:583:ILE:O	2:F:586:LYS:HE3	2.08	0.54
1:A:448:ILE:O	1:A:449:ASN:C	2.45	0.54
1:C:1150:ILE:HG22	1:C:1162:LEU:HD12	1.88	0.54
1:E:480:ALA:N	1:E:481:PRO:HD3	2.23	0.54
2:B:545:SER:HA	2:B:550:ASP:N	2.21	0.54
2:B:1072:GLN:O	2:B:1075:ASP:HB2	2.07	0.54
2:F:269:TYR:CE2	2:F:288:GLU:HA	2.43	0.54
1:A:236:GLN:HB3	1:A:241:ILE:CD1	2.37	0.54
1:A:1131:ARG:HD2	1:A:1131:ARG:C	2.27	0.54
1:A:1163:TYR:O	1:A:1175:ILE:HG23	2.06	0.54
1:E:1150:ILE:HG22	1:E:1162:LEU:HD12	1.88	0.54
2:D:429:ILE:O	2:D:429:ILE:HG22	2.08	0.54
1:C:309:LEU:CD2	1:C:319:VAL:HG12	2.37	0.54
1:C:1131:ARG:HD2	1:C:1131:ARG:C	2.28	0.54
1:E:448:ILE:O	1:E:449:ASN:C	2.45	0.54
1:E:899:ASN:OD1	1:E:1028:ASN:HB3	2.07	0.54
1:A:416:VAL:HG13	1:A:420:GLY:N	2.23	0.54
1:E:309:LEU:CD2	1:E:319:VAL:HG12	2.36	0.54
1:E:427:ILE:HG22	1:E:428:GLU:N	2.23	0.54
1:E:987:ILE:C	1:E:989:LYS:H	2.10	0.54
2:B:429:ILE:O	2:B:429:ILE:HG22	2.07	0.54
1:A:227:ILE:CD1	1:A:271:ILE:HA	2.38	0.54
1:A:278:ASP:N	1:A:278:ASP:OD1	2.40	0.54
1:A:892:ASN:N	1:A:892:ASN:OD1	2.40	0.54
1:C:568:GLN:O	1:C:569:ALA:CB	2.56	0.54
1:C:737:LYS:O	1:C:738:TYR:O	2.24	0.54
1:E:737:LYS:O	1:E:738:TYR:O	2.25	0.54
2:F:502:ASN:O	2:F:506:ASP:N	2.38	0.54
1:A:1155:SER:O	1:A:1156:LYS:C	2.47	0.54
1:C:242:THR:HG22	1:C:435:PHE:O	2.08	0.54
2:B:14:ASP:OD1	2:B:16:LYS:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:574:PHE:C	2:B:574:PHE:CD2	2.81	0.54
2:B:615:LEU:HB3	2:B:767:ASN:ND2	2.23	0.54
2:D:239:ASP:OD2	2:D:318:TYR:N	2.41	0.54
2:D:755:ILE:CG2	2:D:759:GLU:HB2	2.37	0.54
2:F:526:TRP:CZ2	2:F:530:ILE:HD11	2.42	0.54
2:F:742:ASN:HA	2:F:745:THR:HG22	1.90	0.54
1:A:443:TYR:CD1	1:A:444:ASN:N	2.75	0.54
1:A:857:TYR:OH	1:A:860:ASP:HA	2.08	0.54
1:E:857:TYR:OH	1:E:860:ASP:HA	2.07	0.54
2:B:727:TYR:N	2:B:728:PRO:HD2	2.23	0.54
2:B:863:LEU:HD23	2:B:864:THR:HG23	1.90	0.54
2:F:856:ASN:HB3	2:F:859:PHE:HE2	1.72	0.54
1:A:111:ASN:HA	1:A:147:ASN:OD1	2.08	0.54
2:D:1015:LEU:HB2	2:D:1071:VAL:HB	1.90	0.54
2:F:502:ASN:O	2:F:506:ASP:HB2	2.08	0.54
1:A:610:LEU:HD11	1:A:704:MET:HE2	1.90	0.53
1:C:86:ILE:HG13	1:C:364:LEU:HD21	1.90	0.53
1:C:297:ASN:N	1:C:298:PRO:CD	2.71	0.53
1:E:605:TYR:O	1:E:605:TYR:CD1	2.61	0.53
2:B:153:TYR:HD2	2:B:165:MET:HB2	1.73	0.53
2:B:245:THR:O	2:B:247:PRO:C	2.46	0.53
2:D:273:ILE:O	2:D:276:ASN:HB3	2.08	0.53
1:A:738:TYR:O	1:A:739:ASP:C	2.44	0.53
1:C:289:VAL:HB	1:C:290:GLN:CB	2.38	0.53
1:C:480:ALA:N	1:C:481:PRO:HD3	2.23	0.53
2:B:859:PHE:CD1	2:B:968:ILE:HD12	2.43	0.53
2:D:817:GLY:HA2	2:D:826:VAL:HG21	1.91	0.53
2:F:23:SER:OG	2:F:29:PHE:HB2	2.07	0.53
2:F:254:TYR:O	2:F:258:THR:HG22	2.08	0.53
2:F:755:ILE:CG2	2:F:759:GLU:HB2	2.37	0.53
1:E:38:ASN:HD21	1:E:484:SER:CB	2.20	0.53
1:E:289:VAL:HB	1:E:290:GLN:CB	2.37	0.53
1:E:1083:ASP:N	1:E:1129:ILE:O	2.32	0.53
2:D:101:LEU:HD11	2:D:293:ILE:HD12	1.90	0.53
1:A:45:ARG:HG3	1:A:74:LEU:HD23	1.89	0.53
1:A:547:GLU:HB2	1:A:550:LYS:HG3	1.90	0.53
1:A:606:ILE:HD13	1:A:761:PHE:CE2	2.43	0.53
1:A:836:LEU:HD11	2:B:945:PHE:CE1	2.44	0.53
1:A:1149:TYR:CD1	1:A:1183:ARG:HD2	2.43	0.53
1:C:236:GLN:HB3	1:C:241:ILE:CD1	2.37	0.53
1:C:447:ASN:N	1:C:447:ASN:OD1	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:45:ARG:HG3	1:E:74:LEU:HD23	1.89	0.53
1:E:597:ALA:HB2	2:F:939:LYS:HB3	1.90	0.53
2:B:755:ILE:CG2	2:B:759:GLU:HB2	2.37	0.53
2:F:694:ASN:O	2:F:697:ARG:HD2	2.08	0.53
1:A:297:ASN:N	1:A:298:PRO:CD	2.70	0.53
1:C:111:ASN:HA	1:C:147:ASN:OD1	2.09	0.53
1:E:382:VAL:O	1:E:382:VAL:HG13	2.08	0.53
2:D:206:ASN:ND2	2:D:208:ASN:HB2	2.23	0.53
2:D:269:TYR:CE1	2:D:287:LEU:HB3	2.44	0.53
2:D:574:PHE:C	2:D:574:PHE:CD2	2.81	0.53
2:F:817:GLY:HA2	2:F:826:VAL:HG21	1.91	0.53
2:F:859:PHE:CD1	2:F:968:ILE:HD12	2.43	0.53
1:A:1012:ILE:O	2:B:779:ILE:HD12	2.09	0.53
1:C:227:ILE:CD1	1:C:271:ILE:HA	2.39	0.53
2:D:277:ASN:HB3	2:D:281:ASN:CB	2.39	0.53
2:D:1072:GLN:O	2:D:1075:ASP:HB2	2.09	0.53
2:F:544:ILE:HD13	2:F:575:LYS:HG2	1.91	0.53
2:F:895:TRP:O	2:F:896:GLU:HG2	2.08	0.53
1:A:1083:ASP:N	1:A:1129:ILE:O	2.32	0.53
1:C:382:VAL:O	1:C:382:VAL:HG13	2.08	0.53
2:B:254:TYR:O	2:B:258:THR:HG22	2.08	0.53
2:B:554:ILE:CG2	2:B:556:TRP:CE2	2.92	0.53
2:D:166:LEU:HD12	2:D:196:SER:HB2	1.89	0.53
2:D:694:ASN:O	2:D:697:ARG:HD2	2.09	0.53
2:D:1149:HIS:NE2	2:D:1150:ASP:HB3	2.24	0.53
2:F:14:ASP:O	2:F:15:ASN:HB2	2.09	0.53
2:F:206:ASN:ND2	2:F:208:ASN:HB2	2.24	0.53
1:A:568:GLN:O	1:A:569:ALA:CB	2.56	0.53
1:C:1149:TYR:CD1	1:C:1183:ARG:HD2	2.44	0.53
1:C:1174:THR:HA	1:C:1220:VAL:HG12	1.90	0.53
2:B:273:ILE:O	2:B:276:ASN:HB3	2.08	0.53
1:C:605:TYR:O	1:C:605:TYR:CD1	2.61	0.53
1:E:738:TYR:O	1:E:739:ASP:C	2.47	0.53
2:B:227:LEU:HD11	2:B:231:ASP:HB2	1.91	0.53
2:B:239:ASP:OD2	2:B:318:TYR:N	2.41	0.53
2:B:428:LYS:C	2:B:430:PRO:HD2	2.29	0.53
2:B:534:TYR:CE1	2:B:538:ILE:HD12	2.44	0.53
2:D:551:THR:HG21	2:D:716:ASN:HB3	1.91	0.53
2:D:822:LYS:O	2:D:824:THR:N	2.41	0.53
2:D:990:ASN:O	2:D:991:SER:C	2.47	0.53
2:F:273:ILE:O	2:F:276:ASN:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1017:TYR:O	2:F:1018:ASN:CB	2.57	0.53
1:A:274:ASN:HA	1:A:277:ASN:ND2	2.25	0.53
1:A:823:ILE:HG23	1:A:824:PRO:HD2	1.91	0.53
1:C:45:ARG:HG3	1:C:74:LEU:HD23	1.90	0.53
1:E:467:ASP:OD1	1:E:468:LEU:N	2.42	0.53
2:B:583:ILE:O	2:B:586:LYS:HE3	2.09	0.53
2:D:863:LEU:HD23	2:D:864:THR:HG23	1.91	0.53
2:D:1093:THR:HG22	2:D:1097:ARG:O	2.08	0.53
1:A:467:ASP:OD1	1:A:468:LEU:N	2.42	0.52
1:A:1108:ILE:O	1:A:1110:ASN:N	2.42	0.52
1:C:682:TYR:CE2	1:C:825:PHE:HA	2.45	0.52
1:E:1053:GLU:HG3	1:E:1053:GLU:O	2.07	0.52
2:B:101:LEU:HD11	2:B:293:ILE:HD12	1.90	0.52
2:F:1015:LEU:HB2	2:F:1071:VAL:HB	1.90	0.52
1:A:38:ASN:HD21	1:A:484:SER:HB2	1.74	0.52
1:A:209:THR:O	1:A:212:HIS:HB3	2.09	0.52
1:C:38:ASN:HD21	1:C:484:SER:CB	2.23	0.52
1:C:273:THR:O	1:C:276:LEU:N	2.42	0.52
1:E:34:ASN:HB2	1:E:40:TRP:CH2	2.44	0.52
1:E:289:VAL:HB	1:E:290:GLN:HB3	1.90	0.52
2:B:858:TYR:OH	2:B:866:ASN:O	2.27	0.52
2:D:21:VAL:CG1	2:D:22:ARG:N	2.72	0.52
2:D:583:ILE:O	2:D:586:LYS:HE3	2.08	0.52
1:C:443:TYR:CD1	1:C:444:ASN:N	2.76	0.52
1:C:1108:ILE:O	1:C:1110:ASN:N	2.43	0.52
1:E:1174:THR:HA	1:E:1220:VAL:HG12	1.92	0.52
2:B:81:ALA:O	2:B:82:THR:C	2.47	0.52
2:D:40:TRP:O	2:D:137:VAL:HA	2.09	0.52
2:D:254:TYR:O	2:D:258:THR:HG22	2.09	0.52
2:F:568:ASN:OD1	2:F:569:SER:N	2.42	0.52
1:A:382:VAL:HG13	1:A:382:VAL:O	2.09	0.52
1:A:632:ILE:HG23	1:A:633:LEU:N	2.24	0.52
1:A:818:THR:O	1:A:819:LEU:HG	2.09	0.52
1:A:1053:GLU:HG3	1:A:1053:GLU:O	2.09	0.52
1:E:443:TYR:CD1	1:E:444:ASN:N	2.77	0.52
1:E:480:ALA:N	1:E:481:PRO:CD	2.73	0.52
1:E:1092:LEU:O	1:E:1094:PRO:HD3	2.08	0.52
2:B:421:VAL:O	2:B:421:VAL:HG12	2.09	0.52
2:D:502:ASN:O	2:D:506:ASP:HB2	2.09	0.52
2:F:14:ASP:OD1	2:F:16:LYS:N	2.42	0.52
2:F:166:LEU:HD12	2:F:196:SER:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:552:LYS:HB2	2:F:713:PHE:CE1	2.44	0.52
2:F:574:PHE:C	2:F:574:PHE:CD2	2.82	0.52
1:A:462:ASN:CB	1:A:463:ASN:HA	2.38	0.52
1:E:242:THR:HG22	1:E:435:PHE:O	2.10	0.52
1:A:86:ILE:HG13	1:A:364:LEU:HD21	1.92	0.52
1:A:273:THR:O	1:A:276:LEU:N	2.42	0.52
1:C:289:VAL:HB	1:C:290:GLN:HB3	1.90	0.52
1:E:836:LEU:CB	2:F:995:LEU:HD11	2.40	0.52
1:C:944:ARG:CG	1:C:1026:SER:HA	2.39	0.52
1:E:705:TYR:C	1:E:705:TYR:HD1	2.13	0.52
1:E:738:TYR:HA	1:E:743:ILE:CG1	2.38	0.52
2:D:727:TYR:N	2:D:728:PRO:HD2	2.25	0.52
2:F:21:VAL:CG1	2:F:121:ASN:HA	2.39	0.52
2:F:1137:ASN:CB	2:F:1142:TRP:HE1	2.22	0.52
1:A:205:ASP:OD1	1:A:206:PRO:HD2	2.10	0.52
1:A:899:ASN:OD1	1:A:1028:ASN:HB3	2.09	0.52
1:A:1174:THR:HA	1:A:1220:VAL:HG12	1.90	0.52
1:E:1131:ARG:HD2	1:E:1131:ARG:C	2.30	0.52
2:B:21:VAL:CG1	2:B:22:ARG:N	2.73	0.52
2:B:1093:THR:HG22	2:B:1097:ARG:O	2.09	0.52
2:D:411:HIS:HA	2:D:624:PHE:HE1	1.74	0.52
2:D:421:VAL:O	2:D:421:VAL:HG12	2.10	0.52
1:A:199:ILE:HA	1:A:705:TYR:CE2	2.39	0.52
1:C:987:ILE:C	1:C:989:LYS:H	2.13	0.52
1:E:481:PRO:HG2	1:E:483:LEU:HD21	1.92	0.52
2:B:251:ILE:O	2:B:252:ASP:CB	2.58	0.52
2:B:1137:ASN:CB	2:B:1142:TRP:HE1	2.20	0.52
2:D:1017:TYR:O	2:D:1018:ASN:CB	2.57	0.52
2:F:863:LEU:HD23	2:F:864:THR:HG23	1.92	0.52
1:A:738:TYR:HA	1:A:743:ILE:CG1	2.40	0.52
1:C:41:ILE:HG22	1:C:150:ILE:HB	1.92	0.52
1:C:209:THR:O	1:C:212:HIS:HB3	2.10	0.52
1:E:209:THR:O	1:E:212:HIS:HB3	2.10	0.52
2:F:277:ASN:HB3	2:F:281:ASN:CB	2.39	0.52
2:F:1093:THR:HG22	2:F:1097:ARG:O	2.09	0.52
1:C:682:TYR:CD2	1:C:825:PHE:HD1	2.28	0.51
1:C:1155:SER:O	1:C:1156:LYS:C	2.49	0.51
1:E:82:ARG:HG3	1:E:364:LEU:HD11	1.92	0.51
1:E:462:ASN:CB	1:E:463:ASN:HA	2.39	0.51
2:D:571:VAL:O	2:D:574:PHE:HB3	2.10	0.51
2:F:41:ILE:HG22	2:F:138:ILE:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:534:TYR:CE1	2:F:538:ILE:HD12	2.45	0.51
2:F:722:PHE:HA	2:F:726:ILE:HD12	1.92	0.51
2:F:822:LYS:O	2:F:824:THR:N	2.42	0.51
1:A:854:ASN:CB	1:A:865:THR:HG22	2.40	0.51
1:A:1143:ARG:HH21	1:A:1143:ARG:CG	2.23	0.51
1:E:297:ASN:N	1:E:298:PRO:CD	2.73	0.51
1:E:568:GLN:O	1:E:569:ALA:CB	2.58	0.51
2:B:151:ILE:HD11	2:B:167:GLU:HB2	1.91	0.51
2:B:1140:TYR:CE2	2:B:1142:TRP:CD2	2.98	0.51
2:D:534:TYR:CE1	2:D:538:ILE:HD12	2.44	0.51
2:F:421:VAL:O	2:F:421:VAL:HG12	2.10	0.51
1:A:392:ASN:O	1:A:395:ILE:HG12	2.10	0.51
1:A:1025:VAL:CG1	1:A:1026:SER:N	2.73	0.51
1:C:205:ASP:OD1	1:C:206:PRO:HD2	2.10	0.51
1:E:1155:SER:O	1:E:1156:LYS:C	2.48	0.51
2:D:14:ASP:OD1	2:D:16:LYS:N	2.43	0.51
2:D:88:ARG:NE	2:D:339:TYR:OH	2.43	0.51
2:D:502:ASN:O	2:D:506:ASP:N	2.41	0.51
2:F:88:ARG:NE	2:F:339:TYR:OH	2.43	0.51
1:A:166:SER:HB3	1:A:498:ILE:HB	1.92	0.51
1:A:376:ASN:HB3	1:A:381:LYS:HA	1.92	0.51
1:C:855:MET:C	1:C:856:ARG:HD3	2.31	0.51
1:E:67:SER:HA	1:E:158:PHE:CD2	2.46	0.51
2:B:923:ILE:O	2:B:925:ASN:N	2.33	0.51
1:C:1025:VAL:HG12	1:C:1026:SER:N	2.25	0.51
1:E:38:ASN:HD21	1:E:484:SER:HB2	1.76	0.51
1:E:227:ILE:CD1	1:E:271:ILE:HA	2.40	0.51
2:B:262:PHE:CZ	2:B:293:ILE:O	2.63	0.51
2:B:1017:TYR:O	2:B:1018:ASN:CB	2.59	0.51
2:B:1042:ILE:O	2:B:1099:GLN:HA	2.11	0.51
1:A:857:TYR:HA	1:A:862:TYR:HA	1.93	0.51
1:C:215:ILE:HG22	1:C:219:HIS:CE1	2.45	0.51
1:C:363:LEU:HD21	1:C:375:TYR:OH	2.10	0.51
1:C:376:ASN:HB3	1:C:381:LYS:HA	1.93	0.51
2:B:277:ASN:HB3	2:B:281:ASN:CB	2.39	0.51
2:B:817:GLY:HA2	2:B:826:VAL:HG21	1.92	0.51
2:F:21:VAL:CG1	2:F:22:ARG:N	2.73	0.51
2:F:858:TYR:OH	2:F:866:ASN:O	2.29	0.51
1:C:220:GLY:CA	1:C:225:LYS:HE3	2.41	0.51
1:C:462:ASN:CB	1:C:463:ASN:HA	2.40	0.51
1:E:273:THR:O	1:E:276:LEU:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:682:TYR:CD2	1:E:825:PHE:HD1	2.29	0.51
1:E:972:LYS:HB2	2:F:772:LEU:HD21	1.93	0.51
2:B:14:ASP:O	2:B:15:ASN:HB2	2.11	0.51
2:D:251:ILE:O	2:D:252:ASP:CB	2.59	0.51
2:D:872:TRP:HB2	2:D:980:GLU:HB3	1.92	0.51
1:A:113:TYR:HB3	1:A:178:PHE:HB3	1.93	0.51
1:C:480:ALA:N	1:C:481:PRO:CD	2.74	0.51
1:E:86:ILE:HG13	1:E:364:LEU:HD21	1.93	0.51
1:E:144:LEU:HA	1:E:487:LYS:HA	1.93	0.51
1:E:823:ILE:HG23	1:E:824:PRO:HD2	1.92	0.51
2:B:22:ARG:HD2	2:B:27:ASP:O	2.11	0.51
2:B:154:LYS:HD3	2:B:157:TYR:CE2	2.45	0.51
2:D:9:ILE:O	2:D:10:ASP:C	2.49	0.51
2:F:482:LEU:HD22	2:F:499:SER:HB3	1.93	0.51
2:F:1022:GLU:HG2	2:F:1023:LEU:N	2.25	0.51
1:A:481:PRO:HG2	1:A:483:LEU:HD21	1.93	0.51
1:C:392:ASN:O	1:C:395:ILE:HG12	2.10	0.51
2:D:859:PHE:CD1	2:D:968:ILE:HD12	2.46	0.51
2:D:1122:LEU:HD21	2:D:1158:TRP:HZ2	1.75	0.51
2:F:428:LYS:C	2:F:430:PRO:HD2	2.31	0.51
2:F:763:LEU:HA	2:F:766:GLN:HB2	1.92	0.51
1:C:47:VAL:O	1:C:47:VAL:HG12	2.11	0.51
1:C:547:GLU:HB2	1:C:550:LYS:HG3	1.92	0.51
1:C:854:ASN:CB	1:C:865:THR:HG22	2.41	0.51
1:E:363:LEU:HD21	1:E:375:TYR:OH	2.11	0.51
2:B:146:ILE:HD13	2:B:330:TYR:CZ	2.46	0.51
2:B:1007:ILE:HG22	2:B:1015:LEU:HD12	1.93	0.51
2:F:81:ALA:O	2:F:82:THR:C	2.48	0.51
1:A:363:LEU:HD21	1:A:375:TYR:OH	2.11	0.50
1:A:1087:TYR:N	1:A:1243:ILE:O	2.45	0.50
1:C:143:ILE:HG22	1:C:144:LEU:N	2.26	0.50
1:C:1093:LYS:HB3	1:C:1096:ASN:HB2	1.91	0.50
1:E:1108:ILE:O	1:E:1110:ASN:N	2.44	0.50
2:B:9:ILE:O	2:B:11:SER:N	2.44	0.50
2:B:153:TYR:CD2	2:B:165:MET:HB2	2.45	0.50
2:B:568:ASN:OD1	2:B:569:SER:N	2.44	0.50
2:B:583:ILE:HG23	2:B:644:GLN:NE2	2.26	0.50
2:D:568:ASN:OD1	2:D:569:SER:N	2.43	0.50
2:F:101:LEU:HD11	2:F:293:ILE:HD12	1.93	0.50
2:F:571:VAL:O	2:F:574:PHE:HB3	2.11	0.50
2:F:824:THR:HA	2:F:856:ASN:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ILE:HG22	1:A:219:HIS:CE1	2.46	0.50
1:C:154:GLU:CB	1:C:155:PRO:HD2	2.41	0.50
1:C:475:PHE:C	2:D:1136:LYS:HE2	2.31	0.50
1:E:143:ILE:HG22	1:E:144:LEU:N	2.26	0.50
1:E:291:VAL:HA	1:E:292:SER:HB2	1.93	0.50
2:B:9:ILE:O	2:B:10:ASP:C	2.49	0.50
2:B:347:GLY:O	2:B:351:THR:HB	2.11	0.50
2:F:9:ILE:O	2:F:10:ASP:C	2.49	0.50
2:F:154:LYS:HD3	2:F:157:TYR:CE2	2.47	0.50
1:A:447:ASN:N	1:A:447:ASN:OD1	2.42	0.50
1:C:632:ILE:HG23	1:C:633:LEU:N	2.26	0.50
1:C:823:ILE:HG23	1:C:824:PRO:HD2	1.92	0.50
1:C:836:LEU:HD21	2:D:945:PHE:HE1	1.75	0.50
2:B:372:LEU:O	2:B:379:VAL:HA	2.11	0.50
2:B:1022:GLU:HG2	2:B:1023:LEU:N	2.26	0.50
2:D:544:ILE:HD13	2:D:575:LYS:HG2	1.92	0.50
2:D:858:TYR:OH	2:D:866:ASN:O	2.30	0.50
2:D:1022:GLU:HG2	2:D:1023:LEU:N	2.26	0.50
1:E:857:TYR:HA	1:E:862:TYR:HA	1.93	0.50
2:B:205:PRO:HD3	2:B:230:ILE:HD11	1.94	0.50
2:B:694:ASN:O	2:B:697:ARG:HD2	2.10	0.50
2:D:269:TYR:CE2	2:D:288:GLU:HA	2.47	0.50
2:D:888:SER:HB3	2:D:968:ILE:HG12	1.94	0.50
2:F:151:ILE:HD11	2:F:167:GLU:HB2	1.94	0.50
2:F:262:PHE:CZ	2:F:293:ILE:O	2.64	0.50
2:F:554:ILE:CG2	2:F:556:TRP:CE2	2.94	0.50
2:F:1149:HIS:NE2	2:F:1150:ASP:HB3	2.26	0.50
1:A:143:ILE:HG22	1:A:144:LEU:N	2.27	0.50
1:A:144:LEU:HA	1:A:487:LYS:HA	1.93	0.50
1:A:154:GLU:CB	1:A:155:PRO:HD2	2.42	0.50
1:C:82:ARG:HG3	1:C:364:LEU:HD11	1.94	0.50
1:E:45:ARG:NH1	1:E:154:GLU:O	2.45	0.50
1:E:447:ASN:OD1	1:E:447:ASN:N	2.43	0.50
1:E:944:ARG:CG	1:E:1026:SER:HA	2.41	0.50
1:E:1093:LYS:HB3	1:E:1096:ASN:HB2	1.93	0.50
2:B:482:LEU:HD22	2:B:499:SER:HB3	1.94	0.50
2:D:277:ASN:HA	2:D:281:ASN:HA	1.92	0.50
2:F:22:ARG:HD2	2:F:27:ASP:O	2.11	0.50
2:F:923:ILE:O	2:F:925:ASN:N	2.37	0.50
1:A:661:ASN:HA	1:A:664:ILE:HG22	1.94	0.50
1:A:829:SER:C	1:A:831:THR:H	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:795:ASN:OD1	1:C:796:TYR:N	2.44	0.50
1:E:278:ASP:OD1	1:E:278:ASP:N	2.43	0.50
2:D:1137:ASN:CB	2:D:1142:TRP:HE1	2.20	0.50
1:A:836:LEU:HD21	2:B:945:PHE:HE1	1.75	0.50
1:C:34:ASN:HB2	1:C:40:TRP:CH2	2.47	0.50
1:C:45:ARG:NH1	1:C:154:GLU:O	2.44	0.50
1:C:1143:ARG:HH21	1:C:1143:ARG:CG	2.24	0.50
1:E:661:ASN:HA	1:E:664:ILE:HG22	1.93	0.50
2:B:9:ILE:HG13	2:B:10:ASP:N	2.27	0.50
2:B:251:ILE:O	2:B:252:ASP:HB2	2.12	0.50
1:A:45:ARG:NH1	1:A:154:GLU:O	2.45	0.50
1:A:90:ILE:O	1:A:93:ARG:HB3	2.12	0.50
1:C:113:TYR:HB3	1:C:178:PHE:HB3	1.93	0.50
1:C:738:TYR:HA	1:C:743:ILE:CG1	2.42	0.50
1:E:818:THR:O	1:E:819:LEU:HG	2.12	0.50
1:E:836:LEU:HD21	2:F:945:PHE:HE1	1.76	0.50
1:E:989:LYS:HG2	1:E:1076:TRP:HA	1.94	0.50
1:E:1025:VAL:HG12	1:E:1026:SER:N	2.27	0.50
2:D:262:PHE:CZ	2:D:293:ILE:O	2.65	0.50
2:F:92:ASN:HB3	2:F:310:PHE:CZ	2.46	0.50
2:F:551:THR:HG21	2:F:716:ASN:HB3	1.94	0.50
2:F:1008:ARG:HA	2:F:1014:ILE:HA	1.94	0.50
1:A:46:ASN:OD1	1:A:151:MET:HG3	2.12	0.50
1:A:82:ARG:HG3	1:A:364:LEU:HD11	1.94	0.50
1:A:242:THR:HG22	1:A:435:PHE:O	2.11	0.50
1:A:573:VAL:HA	1:A:576:ILE:HD12	1.94	0.50
2:B:436:ASP:CA	2:B:437:ILE:HB	2.25	0.50
2:D:658:ALA:O	2:D:662:LEU:HG	2.12	0.50
2:D:1140:TYR:CE2	2:D:1142:TRP:CD2	3.00	0.50
2:F:277:ASN:HA	2:F:281:ASN:HA	1.93	0.50
1:A:607:GLY:HA2	1:A:612:ILE:HG13	1.94	0.49
1:A:897:GLU:HG2	1:A:1032:LYS:CB	2.38	0.49
1:A:897:GLU:CG	1:A:1032:LYS:HD3	2.42	0.49
1:A:1090:ASN:HB2	1:A:1240:TRP:CZ3	2.47	0.49
1:E:41:ILE:HG22	1:E:150:ILE:HB	1.93	0.49
2:B:763:LEU:HA	2:B:766:GLN:HB2	1.94	0.49
2:D:9:ILE:O	2:D:11:SER:N	2.45	0.49
2:D:9:ILE:HG21	2:D:76:ASP:HB2	1.94	0.49
2:D:482:LEU:HD22	2:D:499:SER:HB3	1.93	0.49
2:D:877:LYS:HB3	2:D:878:GLN:CB	2.42	0.49
2:F:990:ASN:O	2:F:991:SER:C	2.50	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:ILE:HG22	2:B:138:ILE:HB	1.94	0.49
2:D:14:ASP:O	2:D:15:ASN:HB2	2.12	0.49
2:D:21:VAL:HG12	2:D:22:ARG:N	2.26	0.49
2:D:388:ASP:OD1	2:D:388:ASP:N	2.42	0.49
2:F:251:ILE:O	2:F:252:ASP:CB	2.60	0.49
2:F:888:SER:HB3	2:F:968:ILE:HG12	1.94	0.49
1:A:836:LEU:HD13	2:B:991:SER:HA	1.94	0.49
1:A:940:ILE:O	1:A:951:LYS:HA	2.13	0.49
1:E:547:GLU:HB2	1:E:550:LYS:HG3	1.94	0.49
2:B:888:SER:HB3	2:B:968:ILE:HG12	1.95	0.49
2:D:554:ILE:CG2	2:D:556:TRP:CE2	2.95	0.49
1:C:705:TYR:C	1:C:705:TYR:HD1	2.12	0.49
1:E:143:ILE:CG2	1:E:144:LEU:N	2.75	0.49
2:B:803:LEU:HD23	2:B:803:LEU:C	2.33	0.49
2:D:290:LYS:O	2:D:290:LYS:HG2	2.13	0.49
2:D:347:GLY:O	2:D:351:THR:HB	2.13	0.49
2:D:824:THR:HA	2:D:856:ASN:HB2	1.94	0.49
2:F:877:LYS:HB3	2:F:878:GLN:CB	2.42	0.49
2:F:1007:ILE:HG22	2:F:1015:LEU:HD12	1.93	0.49
1:A:795:ASN:OD1	1:A:796:TYR:N	2.45	0.49
1:C:38:ASN:HD21	1:C:484:SER:HB2	1.77	0.49
1:C:90:ILE:O	1:C:93:ARG:HB3	2.13	0.49
1:C:1188:VAL:CG1	1:C:1199:MET:HB2	2.43	0.49
1:E:607:GLY:HA2	1:E:612:ILE:CG1	2.42	0.49
2:B:990:ASN:O	2:B:991:SER:C	2.50	0.49
2:D:151:ILE:HD11	2:D:167:GLU:HB2	1.94	0.49
2:D:706:ALA:O	2:D:709:ASN:HB2	2.13	0.49
2:D:827:GLU:O	2:D:852:ILE:HG23	2.12	0.49
1:A:41:ILE:HG22	1:A:150:ILE:HB	1.93	0.49
1:A:1093:LYS:HB3	1:A:1096:ASN:HB2	1.94	0.49
1:C:607:GLY:HA2	1:C:612:ILE:HG13	1.95	0.49
1:E:166:SER:HB3	1:E:498:ILE:HB	1.94	0.49
2:B:717:ALA:O	2:B:721:VAL:HG23	2.12	0.49
2:B:722:PHE:HA	2:B:726:ILE:HD12	1.93	0.49
2:B:755:ILE:HG23	2:B:759:GLU:HB2	1.95	0.49
2:D:755:ILE:HG23	2:D:759:GLU:HB2	1.95	0.49
1:A:607:GLY:HA2	1:A:612:ILE:CG1	2.43	0.49
1:A:989:LYS:HG2	1:A:1076:TRP:HA	1.94	0.49
1:A:1122:TYR:HE1	1:A:1244:SER:O	1.95	0.49
1:C:199:ILE:HA	1:C:705:TYR:CE2	2.42	0.49
1:C:892:ASN:N	1:C:892:ASN:OD1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:113:TYR:HB3	1:E:178:PHE:HB3	1.93	0.49
1:E:607:GLY:HA2	1:E:612:ILE:HG13	1.95	0.49
2:B:64:TYR:HE2	2:B:363:ILE:HD12	1.78	0.49
2:B:1095:ASN:HB2	2:B:1097:ARG:HB2	1.95	0.49
2:D:22:ARG:HD2	2:D:27:ASP:O	2.12	0.49
2:D:41:ILE:HG22	2:D:138:ILE:HB	1.94	0.49
2:D:153:TYR:HD2	2:D:165:MET:HB2	1.77	0.49
2:D:154:LYS:HD3	2:D:157:TYR:CE2	2.47	0.49
2:D:717:ALA:O	2:D:721:VAL:HG23	2.13	0.49
2:F:347:GLY:O	2:F:351:THR:HB	2.12	0.49
2:F:424:GLU:O	2:F:428:LYS:N	2.44	0.49
2:F:518:ASP:O	2:F:680:ILE:HD11	2.12	0.49
1:A:34:ASN:HB2	1:A:40:TRP:CH2	2.48	0.49
1:A:700:ARG:HA	1:A:703:GLN:HB2	1.95	0.49
1:A:854:ASN:HB2	1:A:865:THR:CG2	2.43	0.49
1:E:154:GLU:CB	1:E:155:PRO:HD2	2.40	0.49
1:E:205:ASP:OD1	1:E:206:PRO:HD2	2.13	0.49
2:B:541:THR:O	2:B:542:GLN:CB	2.60	0.49
2:B:806:TYR:O	2:B:806:TYR:CD1	2.65	0.49
2:D:23:SER:HB2	2:D:47:TYR:CZ	2.47	0.49
2:F:203:ILE:HG22	2:F:254:TYR:OH	2.12	0.49
2:F:755:ILE:HG23	2:F:759:GLU:HB2	1.95	0.49
1:C:143:ILE:CG2	1:C:144:LEU:N	2.75	0.49
1:C:331:LEU:HB2	1:C:332:TYR:HD2	1.77	0.49
1:C:940:ILE:O	1:C:951:LYS:HA	2.12	0.49
2:B:393:THR:OG1	2:B:396:ASN:N	2.46	0.49
2:B:872:TRP:HB2	2:B:980:GLU:HB3	1.94	0.49
2:D:763:LEU:HA	2:D:766:GLN:HB2	1.95	0.49
1:A:143:ILE:CG2	1:A:144:LEU:N	2.76	0.49
2:B:277:ASN:HA	2:B:281:ASN:HA	1.94	0.49
2:B:815:VAL:HG12	2:B:816:ILE:N	2.28	0.49
2:F:153:TYR:HD2	2:F:165:MET:HB2	1.77	0.49
1:C:278:ASP:OD1	1:C:278:ASP:N	2.43	0.48
1:C:627:LEU:O	1:E:419:LYS:HG2	2.12	0.48
1:C:854:ASN:HB2	1:C:865:THR:CG2	2.43	0.48
1:C:879:TYR:O	1:C:888:PHE:HA	2.13	0.48
1:C:1025:VAL:CG1	1:C:1026:SER:N	2.76	0.48
1:C:1108:ILE:CG2	1:C:1217:ASP:HA	2.43	0.48
1:E:944:ARG:O	1:E:946:ASN:N	2.46	0.48
2:B:1020:THR:HA	2:B:1059:PHE:O	2.12	0.48
1:E:46:ASN:OD1	1:E:151:MET:HG3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:47:VAL:O	1:E:47:VAL:HG12	2.12	0.48
2:B:877:LYS:HB3	2:B:878:GLN:CB	2.42	0.48
2:D:251:ILE:O	2:D:252:ASP:HB2	2.13	0.48
2:D:428:LYS:C	2:D:430:PRO:HD2	2.33	0.48
2:D:518:ASP:O	2:D:680:ILE:HD11	2.12	0.48
2:F:207:ASP:N	2:F:207:ASP:OD1	2.46	0.48
2:F:658:ALA:O	2:F:662:LEU:HG	2.13	0.48
2:F:803:LEU:HD23	2:F:803:LEU:C	2.33	0.48
1:A:17:THR:HG22	1:A:34:ASN:HB3	1.94	0.48
1:A:220:GLY:CA	1:A:225:LYS:HE3	2.43	0.48
1:A:480:ALA:N	1:A:481:PRO:HD3	2.29	0.48
1:C:548:GLN:HB2	1:C:549:PRO:HD3	1.95	0.48
1:C:818:THR:O	1:C:819:LEU:HG	2.13	0.48
1:C:1087:TYR:N	1:C:1243:ILE:O	2.46	0.48
1:E:940:ILE:O	1:E:951:LYS:HA	2.13	0.48
2:B:206:ASN:ND2	2:B:208:ASN:HB2	2.27	0.48
2:B:424:GLU:O	2:B:428:LYS:N	2.46	0.48
2:D:64:TYR:HE2	2:D:363:ILE:HD12	1.79	0.48
2:F:9:ILE:O	2:F:11:SER:N	2.46	0.48
2:F:21:VAL:HG12	2:F:22:ARG:N	2.28	0.48
2:F:1140:TYR:CE2	2:F:1142:TRP:CD2	3.02	0.48
1:C:573:VAL:HA	1:C:576:ILE:HD12	1.95	0.48
1:C:607:GLY:HA2	1:C:612:ILE:CG1	2.43	0.48
1:C:829:SER:C	1:C:831:THR:H	2.17	0.48
1:E:17:THR:HG22	1:E:34:ASN:HB3	1.95	0.48
1:E:376:ASN:O	1:E:381:LYS:HB3	2.13	0.48
2:B:552:LYS:CB	2:B:713:PHE:HE1	2.26	0.48
2:D:372:LEU:O	2:D:379:VAL:HA	2.14	0.48
2:D:1008:ARG:HA	2:D:1014:ILE:HA	1.96	0.48
1:A:936:GLU:HA	1:A:954:LEU:O	2.14	0.48
1:A:1212:LEU:O	1:A:1238:CYS:HA	2.12	0.48
1:C:46:ASN:OD1	1:C:151:MET:HG3	2.12	0.48
1:E:892:ASN:OD1	1:E:892:ASN:N	2.45	0.48
1:E:972:LYS:CB	2:F:772:LEU:HD11	2.44	0.48
2:B:402:ILE:HG12	2:B:593:LYS:CB	2.44	0.48
2:B:827:GLU:O	2:B:852:ILE:HG23	2.12	0.48
2:D:552:LYS:CB	2:D:713:PHE:HE1	2.26	0.48
2:D:1007:ILE:HG22	2:D:1015:LEU:HD12	1.95	0.48
2:F:615:LEU:HB3	2:F:767:ASN:ND2	2.28	0.48
1:A:47:VAL:O	1:A:47:VAL:HG12	2.13	0.48
1:C:231:CYS:CB	1:C:249:ILE:HD12	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1122:TYR:HE1	1:C:1244:SER:O	1.97	0.48
1:E:440:GLU:O	1:E:443:TYR:CD1	2.67	0.48
1:E:854:ASN:CB	1:E:865:THR:HG22	2.43	0.48
1:E:1122:TYR:HE1	1:E:1244:SER:O	1.97	0.48
2:B:502:ASN:O	2:B:506:ASP:N	2.42	0.48
2:B:570:PHE:O	2:B:573:GLU:HB2	2.13	0.48
2:F:570:PHE:O	2:F:573:GLU:HB2	2.14	0.48
1:E:220:GLY:CA	1:E:225:LYS:HE3	2.44	0.48
1:E:423:LYS:HD2	2:D:510:PHE:CE2	2.48	0.48
1:E:700:ARG:HA	1:E:703:GLN:HB2	1.95	0.48
2:B:518:ASP:O	2:B:680:ILE:HD11	2.13	0.48
2:F:23:SER:HB2	2:F:47:TYR:CZ	2.49	0.48
1:A:291:VAL:HA	1:A:292:SER:HB2	1.95	0.48
1:A:944:ARG:CG	1:A:1026:SER:HA	2.42	0.48
1:E:215:ILE:HG22	1:E:219:HIS:CE1	2.48	0.48
1:E:548:GLN:HB2	1:E:549:PRO:HD3	1.96	0.48
2:B:1122:LEU:HD21	2:B:1158:TRP:HZ2	1.76	0.48
2:D:153:TYR:CD2	2:D:165:MET:HB2	2.48	0.48
2:D:1042:ILE:O	2:D:1099:GLN:HA	2.13	0.48
2:D:1138:GLN:HB3	2:D:1139:ASP:C	2.34	0.48
2:F:232:PHE:CZ	2:F:240:TYR:HA	2.49	0.48
1:A:944:ARG:O	1:A:946:ASN:N	2.47	0.48
1:C:836:LEU:HD13	2:D:991:SER:HA	1.96	0.48
1:E:897:GLU:CG	1:E:1032:LYS:HD3	2.44	0.48
2:B:203:ILE:HG22	2:B:203:ILE:O	2.13	0.48
2:D:146:ILE:HD13	2:D:330:TYR:CZ	2.49	0.48
2:D:615:LEU:HB3	2:D:767:ASN:ND2	2.29	0.48
2:D:684:ASN:O	2:D:687:LEU:N	2.47	0.48
2:F:15:ASN:OD1	2:F:126:LYS:CB	2.62	0.48
2:F:475:ILE:HG21	2:F:497:VAL:HG22	1.95	0.48
2:F:1020:THR:HA	2:F:1059:PHE:O	2.14	0.48
1:C:661:ASN:HA	1:C:664:ILE:HG22	1.95	0.48
1:C:944:ARG:O	1:C:946:ASN:N	2.47	0.48
1:C:1088:LEU:HD23	1:C:1089:LEU:N	2.29	0.48
1:E:1143:ARG:HH21	1:E:1143:ARG:CG	2.26	0.48
2:B:21:VAL:HG12	2:B:22:ARG:N	2.29	0.48
2:B:64:TYR:CD2	2:B:64:TYR:N	2.81	0.48
2:B:571:VAL:O	2:B:574:PHE:HB3	2.14	0.48
2:B:1008:ARG:HA	2:B:1014:ILE:HA	1.96	0.48
2:D:1095:ASN:HB2	2:D:1097:ARG:HB2	1.95	0.48
2:F:1042:ILE:O	2:F:1099:GLN:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:SER:HB3	1:C:498:ILE:HB	1.95	0.47
1:E:90:ILE:O	1:E:93:ARG:HB3	2.14	0.47
2:B:203:ILE:HG22	2:B:254:TYR:OH	2.13	0.47
2:B:232:PHE:CZ	2:B:240:TYR:HA	2.49	0.47
2:F:381:MET:HE3	2:F:471:GLN:HB3	1.95	0.47
2:F:583:ILE:HG23	2:F:644:GLN:NE2	2.29	0.47
2:F:726:ILE:C	2:F:728:PRO:HD2	2.34	0.47
2:F:815:VAL:HG12	2:F:816:ILE:N	2.29	0.47
1:A:929:LYS:HA	1:A:932:ASN:HB2	1.96	0.47
1:E:682:TYR:CE2	1:E:825:PHE:HA	2.49	0.47
1:E:879:TYR:O	1:E:888:PHE:HA	2.13	0.47
2:B:551:THR:HG21	2:B:716:ASN:HB3	1.95	0.47
2:D:205:PRO:HD3	2:D:230:ILE:HD11	1.96	0.47
2:D:945:PHE:CD1	2:D:950:LEU:HA	2.49	0.47
2:D:991:SER:O	2:D:994:ILE:HB	2.13	0.47
2:F:631:TYR:O	2:F:634:LEU:HB2	2.14	0.47
2:F:1122:LEU:HD21	2:F:1158:TRP:HZ2	1.75	0.47
1:A:138:ASN:ND2	1:A:140:SER:OG	2.47	0.47
1:A:270:ASP:O	1:A:273:THR:HG22	2.14	0.47
1:C:936:GLU:HA	1:C:954:LEU:O	2.14	0.47
1:E:854:ASN:HB2	1:E:865:THR:CG2	2.43	0.47
1:E:911:LYS:O	1:E:999:ARG:NE	2.47	0.47
1:E:1025:VAL:CG1	1:E:1026:SER:N	2.78	0.47
2:B:290:LYS:O	2:B:290:LYS:HG2	2.14	0.47
2:B:402:ILE:HG12	2:B:593:LYS:HB2	1.96	0.47
2:B:541:THR:HA	2:B:553:ILE:O	2.14	0.47
2:B:554:ILE:HB	2:B:557:ILE:CD1	2.44	0.47
2:D:1020:THR:HA	2:D:1059:PHE:O	2.14	0.47
2:F:205:PRO:HD3	2:F:230:ILE:HD11	1.96	0.47
2:F:269:TYR:HD1	2:F:287:LEU:HD23	1.79	0.47
2:F:717:ALA:O	2:F:721:VAL:HG23	2.14	0.47
1:A:203:ILE:HD13	1:A:396:ILE:HG21	1.96	0.47
1:A:603:VAL:CG1	1:A:605:TYR:CE2	2.98	0.47
1:C:716:LYS:O	1:C:719:ILE:HG22	2.14	0.47
1:E:231:CYS:HB2	1:E:249:ILE:HD12	1.97	0.47
2:D:192:CYS:O	2:D:195:LYS:HB3	2.14	0.47
2:D:815:VAL:HG12	2:D:816:ILE:N	2.29	0.47
2:F:1095:ASN:HB2	2:F:1097:ARG:HB2	1.96	0.47
1:A:456:ASP:HA	1:A:669:ASN:HD21	1.79	0.47
1:A:528:VAL:HG13	1:A:528:VAL:O	2.15	0.47
1:C:17:THR:HG22	1:C:34:ASN:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:ASN:ND2	1:C:140:SER:OG	2.47	0.47
1:C:949:GLY:O	1:C:963:LEU:HD12	2.15	0.47
1:E:1087:TYR:N	1:E:1243:ILE:O	2.47	0.47
1:E:1108:ILE:CG2	1:E:1217:ASP:HA	2.44	0.47
2:D:794:ILE:O	2:D:795:LYS:C	2.53	0.47
2:F:239:ASP:OD2	2:F:318:TYR:N	2.43	0.47
2:F:402:ILE:HG12	2:F:593:LYS:HB2	1.97	0.47
2:F:827:GLU:O	2:F:852:ILE:HG23	2.14	0.47
1:A:431:ASN:O	1:A:434:LEU:HB2	2.14	0.47
1:A:855:MET:C	1:A:856:ARG:HD3	2.33	0.47
1:A:912:TYR:O	1:A:913:LYS:HB3	2.15	0.47
1:A:1229:MET:O	1:A:1231:ASP:N	2.48	0.47
1:C:897:GLU:CG	1:C:1032:LYS:HD3	2.44	0.47
1:E:186:PHE:CE2	1:E:188:PRO:HB3	2.48	0.47
1:E:1043:GLY:C	1:E:1044:ILE:HG13	2.35	0.47
2:B:706:ALA:O	2:B:709:ASN:HB2	2.13	0.47
2:B:726:ILE:C	2:B:728:PRO:HD2	2.35	0.47
2:B:991:SER:O	2:B:994:ILE:HB	2.15	0.47
2:B:1138:GLN:HB3	2:B:1139:ASP:C	2.34	0.47
2:D:271:ILE:HG23	2:D:272:LYS:N	2.30	0.47
2:D:424:GLU:O	2:D:428:LYS:N	2.47	0.47
2:F:173:PHE:HA	2:F:333:ILE:HB	1.96	0.47
1:A:548:GLN:HB2	1:A:549:PRO:HD3	1.96	0.47
1:A:716:LYS:O	1:A:719:ILE:HG22	2.15	0.47
1:A:778:LYS:HA	1:A:782:LEU:HB2	1.96	0.47
1:C:203:ILE:HD13	1:C:396:ILE:HG21	1.97	0.47
1:C:291:VAL:HA	1:C:292:SER:HB2	1.97	0.47
1:C:376:ASN:O	1:C:381:LYS:HB3	2.15	0.47
1:C:911:LYS:O	1:C:999:ARG:NE	2.47	0.47
1:E:270:ASP:O	1:E:273:THR:HG22	2.15	0.47
1:E:633:LEU:O	1:E:700:ARG:NH2	2.45	0.47
1:E:829:SER:C	1:E:831:THR:H	2.18	0.47
2:B:210:ASN:HB3	2:B:228:ASP:HA	1.97	0.47
2:B:269:TYR:HD1	2:B:287:LEU:HD23	1.79	0.47
2:B:1069:GLN:O	2:B:1070:TYR:CD2	2.68	0.47
2:D:203:ILE:HG22	2:D:254:TYR:OH	2.14	0.47
2:D:541:THR:HA	2:D:553:ILE:O	2.15	0.47
2:D:917:ASN:C	2:D:918:ILE:HG13	2.35	0.47
2:F:9:ILE:HG21	2:F:76:ASP:HB2	1.97	0.47
2:F:290:LYS:HG2	2:F:290:LYS:O	2.15	0.47
2:F:388:ASP:OD1	2:F:388:ASP:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:706:ALA:O	2:F:709:ASN:HB2	2.14	0.47
1:A:231:CYS:HB2	1:A:249:ILE:HD12	1.97	0.47
1:A:286:LEU:O	1:A:287:SER:C	2.52	0.47
1:C:1092:LEU:HD11	1:C:1234:ASN:O	2.15	0.47
1:E:632:ILE:HG23	1:E:633:LEU:N	2.28	0.47
1:E:795:ASN:OD1	1:E:796:TYR:N	2.48	0.47
2:B:13:VAL:HG12	2:B:14:ASP:H	1.77	0.47
2:B:185:PRO:O	2:B:186:ALA:C	2.53	0.47
2:D:868:SER:HA	2:D:933:ILE:O	2.14	0.47
2:F:251:ILE:O	2:F:252:ASP:HB2	2.14	0.47
1:A:911:LYS:O	1:A:999:ARG:NE	2.47	0.47
1:C:857:TYR:HB2	1:C:862:TYR:CE1	2.50	0.47
1:E:331:LEU:HB2	1:E:332:TYR:HD2	1.80	0.47
1:E:1092:LEU:HD11	1:E:1234:ASN:O	2.15	0.47
2:B:15:ASN:OD1	2:B:126:LYS:CB	2.63	0.47
2:B:658:ALA:O	2:B:662:LEU:HG	2.14	0.47
2:B:876:LEU:HD21	2:B:978:TYR:CD2	2.50	0.47
2:D:9:ILE:HG13	2:D:10:ASP:N	2.29	0.47
1:A:942:CYS:SG	1:A:1025:VAL:CG1	3.03	0.47
1:A:949:GLY:O	1:A:963:LEU:HD12	2.15	0.47
1:C:231:CYS:HB2	1:C:249:ILE:HD12	1.97	0.47
1:C:270:ASP:O	1:C:273:THR:HG22	2.15	0.47
2:B:305:TYR:CE1	2:B:418:LEU:CD1	2.97	0.47
2:B:475:ILE:HG21	2:B:497:VAL:HG22	1.96	0.47
2:B:1116:ILE:HG23	2:B:1117:PHE:N	2.29	0.47
2:F:541:THR:HA	2:F:553:ILE:O	2.15	0.47
2:F:876:LEU:HD21	2:F:978:TYR:CD2	2.50	0.47
1:A:480:ALA:N	1:A:481:PRO:CD	2.78	0.46
1:A:1132:VAL:HG23	1:A:1149:TYR:CE2	2.50	0.46
1:A:1188:VAL:CG1	1:A:1199:MET:HB2	2.45	0.46
1:C:535:VAL:HG12	1:C:536:ASN:N	2.30	0.46
1:E:896:SER:C	1:E:897:GLU:HG3	2.35	0.46
2:B:45:ARG:HG3	2:B:141:PRO:O	2.15	0.46
2:B:106:ILE:HG22	2:B:107:PRO:O	2.14	0.46
2:B:155:LYS:O	2:B:156:GLU:C	2.54	0.46
2:F:146:ILE:HD13	2:F:330:TYR:CZ	2.50	0.46
2:F:185:PRO:O	2:F:186:ALA:C	2.53	0.46
1:A:186:PHE:CE2	1:A:188:PRO:HB3	2.51	0.46
1:A:297:ASN:N	1:A:298:PRO:HD3	2.30	0.46
1:C:440:GLU:O	1:C:443:TYR:CD1	2.68	0.46
1:C:470:GLN:HG3	2:D:1028:PHE:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1090:ASN:HB2	1:C:1240:TRP:CZ3	2.50	0.46
1:E:154:GLU:CB	1:E:155:PRO:CD	2.94	0.46
1:E:528:VAL:O	1:E:528:VAL:HG13	2.15	0.46
1:E:824:PRO:HB2	2:F:952:ALA:HB2	1.97	0.46
2:D:81:ALA:O	2:D:82:THR:C	2.53	0.46
2:D:570:PHE:O	2:D:573:GLU:HB2	2.15	0.46
2:D:631:TYR:O	2:D:634:LEU:HB2	2.15	0.46
2:D:722:PHE:HA	2:D:726:ILE:HD12	1.96	0.46
2:D:1093:THR:OG1	2:D:1094:THR:N	2.49	0.46
1:C:528:VAL:O	1:C:528:VAL:HG13	2.15	0.46
1:E:855:MET:C	1:E:856:ARG:HD3	2.36	0.46
1:E:920:TRP:HB2	1:E:1045:ARG:CD	2.45	0.46
1:E:1188:VAL:CG1	1:E:1199:MET:HB2	2.45	0.46
2:B:567:ASN:O	2:B:568:ASN:C	2.53	0.46
2:D:990:ASN:O	2:D:993:GLU:N	2.48	0.46
2:F:45:ARG:HG3	2:F:141:PRO:O	2.15	0.46
1:A:376:ASN:O	1:A:381:LYS:HB3	2.15	0.46
1:A:785:TYR:O	1:A:786:ASP:C	2.53	0.46
1:A:879:TYR:O	1:A:888:PHE:HA	2.16	0.46
1:C:606:ILE:CG2	1:C:621:PHE:CE2	2.98	0.46
1:C:795:ASN:OD1	1:C:795:ASN:C	2.54	0.46
1:E:345:VAL:HG13	1:E:387:GLN:HE22	1.81	0.46
1:E:573:VAL:HA	1:E:576:ILE:HD12	1.97	0.46
1:E:1132:VAL:HG23	1:E:1149:TYR:CE2	2.50	0.46
2:B:23:SER:HB2	2:B:47:TYR:CZ	2.50	0.46
2:D:106:ILE:HG22	2:D:107:PRO:O	2.15	0.46
2:D:846:THR:HG23	2:D:847:GLY:N	2.31	0.46
2:F:153:TYR:CD2	2:F:165:MET:HB2	2.50	0.46
2:F:859:PHE:HD1	2:F:968:ILE:HD12	1.80	0.46
2:F:867:PHE:CZ	2:F:935:ILE:HD12	2.50	0.46
2:F:989:ILE:HG22	2:F:990:ASN:N	2.31	0.46
1:A:22:LYS:CG	1:A:23:PRO:HD2	2.45	0.46
1:A:453:GLU:C	1:A:454:ILE:HG22	2.36	0.46
1:A:1088:LEU:HD23	1:A:1089:LEU:N	2.30	0.46
1:C:22:LYS:CG	1:C:23:PRO:HD2	2.45	0.46
1:C:469:ASP:O	1:C:472:ILE:HB	2.15	0.46
1:C:571:LEU:O	1:C:575:TRP:N	2.42	0.46
2:B:141:PRO:HA	2:B:169:TRP:HB3	1.96	0.46
2:B:192:CYS:O	2:B:195:LYS:HB3	2.15	0.46
2:B:305:TYR:CZ	2:B:418:LEU:CD1	2.99	0.46
2:B:868:SER:HA	2:B:933:ILE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:13:VAL:HG12	2:D:14:ASP:H	1.80	0.46
2:D:610:ASP:OD1	2:D:611:LEU:HD13	2.15	0.46
2:F:14:ASP:O	2:F:15:ASN:CB	2.64	0.46
2:F:872:TRP:HB2	2:F:980:GLU:HB3	1.97	0.46
1:A:179:GLY:HA2	1:A:220:GLY:O	2.15	0.46
1:C:179:GLY:HA2	1:C:220:GLY:O	2.15	0.46
1:C:932:ASN:HA	1:C:956:HIS:CE1	2.51	0.46
1:C:989:LYS:HG2	1:C:1076:TRP:HA	1.97	0.46
1:E:453:GLU:C	1:E:454:ILE:HG22	2.35	0.46
1:E:664:ILE:HG23	1:E:665:LYS:N	2.30	0.46
2:B:269:TYR:CE2	2:B:288:GLU:HA	2.51	0.46
2:B:989:ILE:HG22	2:B:990:ASN:N	2.30	0.46
2:D:203:ILE:HG22	2:D:203:ILE:O	2.16	0.46
2:D:815:VAL:C	2:D:816:ILE:HG13	2.36	0.46
2:D:1003:ASN:HB3	2:D:1116:ILE:CD1	2.46	0.46
2:F:271:ILE:HG23	2:F:272:LYS:N	2.30	0.46
2:F:806:TYR:O	2:F:806:TYR:CD1	2.69	0.46
1:A:231:CYS:CB	1:A:249:ILE:HD12	2.46	0.46
1:A:286:LEU:O	1:A:289:VAL:HG13	2.16	0.46
1:C:942:CYS:SG	1:C:1025:VAL:CG1	3.04	0.46
1:E:873:ASN:N	1:E:899:ASN:O	2.39	0.46
1:E:949:GLY:O	1:E:963:LEU:HD12	2.16	0.46
1:E:981:ASN:ND2	2:F:414:ASN:HB3	2.28	0.46
2:B:207:ASP:OD1	2:B:207:ASP:N	2.48	0.46
2:D:475:ILE:HG21	2:D:497:VAL:HG22	1.96	0.46
2:F:586:LYS:O	2:F:641:TYR:CZ	2.69	0.46
2:F:991:SER:O	2:F:994:ILE:HB	2.16	0.46
1:A:382:VAL:HG11	1:A:868:TYR:CE1	2.51	0.46
1:A:1108:ILE:CG2	1:A:1217:ASP:HA	2.46	0.46
1:E:286:LEU:O	1:E:289:VAL:HG13	2.16	0.46
1:E:456:ASP:HA	1:E:669:ASN:HD21	1.80	0.46
1:E:610:LEU:HD11	1:E:704:MET:HE2	1.98	0.46
2:B:815:VAL:C	2:B:816:ILE:HG13	2.36	0.46
2:B:1007:ILE:CG2	2:B:1015:LEU:HD12	2.46	0.46
2:D:515:LYS:HB3	2:D:516:PRO:HD2	1.97	0.46
2:D:726:ILE:C	2:D:728:PRO:HD2	2.36	0.46
2:D:1003:ASN:HB3	2:D:1116:ILE:HD13	1.97	0.46
2:F:554:ILE:HB	2:F:557:ILE:CD1	2.45	0.46
1:A:468:LEU:HD12	1:A:471:VAL:HG22	1.98	0.46
1:A:937:TYR:CE1	1:A:954:LEU:HB2	2.51	0.46
1:C:297:ASN:N	1:C:298:PRO:HD3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:231:CYS:CB	1:E:249:ILE:HD12	2.45	0.46
1:E:1010:ASN:HB3	2:F:780:GLN:HG3	1.97	0.46
1:E:1212:LEU:O	1:E:1238:CYS:HA	2.16	0.46
2:B:867:PHE:CZ	2:B:935:ILE:HD12	2.51	0.46
2:D:173:PHE:HA	2:D:333:ILE:HB	1.98	0.46
2:F:51:LEU:HB3	2:F:66:SER:HA	1.97	0.46
2:F:402:ILE:HG12	2:F:593:LYS:CB	2.45	0.46
2:F:1003:ASN:HB3	2:F:1116:ILE:CD1	2.46	0.46
2:F:1138:GLN:HB3	2:F:1139:ASP:C	2.36	0.46
1:A:664:ILE:HG23	1:A:665:LYS:N	2.31	0.46
1:A:1127:VAL:HG11	1:A:1150:ILE:HG23	1.97	0.46
1:C:627:LEU:O	1:E:420:GLY:HA3	2.16	0.46
1:C:1168:THR:HG22	1:C:1170:ASN:H	1.80	0.46
2:B:610:ASP:OD1	2:B:611:LEU:HD13	2.16	0.46
2:D:298:ILE:HA	2:D:301:LEU:HD12	1.98	0.46
2:D:806:TYR:CD1	2:D:806:TYR:O	2.69	0.46
2:D:1135:ILE:HG22	2:D:1136:LYS:N	2.31	0.46
2:F:106:ILE:HG22	2:F:107:PRO:O	2.16	0.46
1:A:456:ASP:HA	1:A:669:ASN:ND2	2.31	0.45
1:A:482:GLY:C	1:A:483:LEU:HG	2.36	0.45
1:A:896:SER:C	1:A:897:GLU:HG3	2.36	0.45
1:C:345:VAL:HG13	1:C:387:GLN:HE22	1.81	0.45
1:C:664:ILE:HG23	1:C:665:LYS:N	2.31	0.45
1:C:778:LYS:HA	1:C:782:LEU:HB2	1.98	0.45
1:E:972:LYS:HB2	2:F:772:LEU:HD11	1.98	0.45
1:E:972:LYS:CD	2:F:772:LEU:HD11	2.46	0.45
2:B:21:VAL:CG1	2:B:121:ASN:HA	2.43	0.45
2:B:51:LEU:HB3	2:B:66:SER:HA	1.98	0.45
2:B:846:THR:HG23	2:B:847:GLY:N	2.31	0.45
2:F:298:ILE:HA	2:F:301:LEU:HD12	1.97	0.45
2:F:868:SER:HA	2:F:933:ILE:O	2.16	0.45
1:A:535:VAL:HG12	1:A:536:ASN:N	2.32	0.45
1:A:912:TYR:O	1:A:913:LYS:CB	2.64	0.45
1:C:897:GLU:HG2	1:C:1032:LYS:CB	2.44	0.45
1:E:606:ILE:CG2	1:E:621:PHE:CE2	2.99	0.45
1:E:1168:THR:HG22	1:E:1170:ASN:H	1.80	0.45
2:B:1149:HIS:CE1	2:B:1150:ASP:CB	3.00	0.45
2:D:269:TYR:HD1	2:D:287:LEU:HD23	1.81	0.45
2:F:269:TYR:HE2	2:F:288:GLU:CG	2.29	0.45
2:F:552:LYS:CB	2:F:713:PHE:HE1	2.30	0.45
1:A:94:ILE:HG23	1:A:211:MET:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:ASP:O	1:A:472:ILE:HB	2.15	0.45
1:A:771:MET:HA	1:A:774:ILE:CG2	2.46	0.45
1:C:942:CYS:SG	1:C:1026:SER:HB3	2.56	0.45
1:C:1106:LEU:HD12	1:C:1175:ILE:HB	1.97	0.45
1:E:482:GLY:C	1:E:483:LEU:HG	2.37	0.45
1:E:603:VAL:CG1	1:E:605:TYR:CE2	2.99	0.45
2:B:298:ILE:O	2:B:301:LEU:HB2	2.17	0.45
2:D:15:ASN:OD1	2:D:126:LYS:CB	2.64	0.45
2:D:867:PHE:CB	2:D:985:LEU:O	2.64	0.45
2:F:65:ASP:O	2:F:66:SER:OG	2.31	0.45
2:F:866:ASN:O	2:F:867:PHE:HB3	2.16	0.45
1:A:864:ASP:C	1:A:864:ASP:OD1	2.55	0.45
1:A:1092:LEU:HD11	1:A:1234:ASN:O	2.16	0.45
1:C:21:ILE:HG12	1:C:134:ILE:HG22	1.98	0.45
1:C:448:ILE:O	1:C:449:ASN:O	2.35	0.45
1:C:597:ALA:HB2	2:D:939:LYS:HB3	1.98	0.45
1:E:778:LYS:HA	1:E:782:LEU:HB2	1.97	0.45
1:E:836:LEU:HD11	2:F:945:PHE:CE1	2.52	0.45
1:E:942:CYS:SG	1:E:1026:SER:HB3	2.57	0.45
2:B:374:ASN:C	2:B:374:ASN:OD1	2.54	0.45
2:B:990:ASN:O	2:B:993:GLU:N	2.49	0.45
2:F:594:ILE:CG2	2:F:595:LYS:N	2.79	0.45
2:F:932:VAL:C	2:F:933:ILE:HG13	2.37	0.45
1:A:192:PHE:CE1	1:A:204:GLN:HB3	2.51	0.45
1:A:203:ILE:CD1	1:A:396:ILE:HG21	2.46	0.45
1:A:440:GLU:O	1:A:443:TYR:CD1	2.69	0.45
1:A:606:ILE:CG2	1:A:621:PHE:CE2	3.00	0.45
1:C:160:THR:HA	1:C:185:THR:O	2.17	0.45
1:C:275:LEU:HD11	1:C:279:TYR:CE2	2.51	0.45
1:C:576:ILE:HG12	1:C:719:ILE:HD11	1.97	0.45
1:C:1012:ILE:O	2:D:779:ILE:HD12	2.17	0.45
1:E:199:ILE:HA	1:E:705:TYR:CE2	2.45	0.45
1:E:203:ILE:HD13	1:E:396:ILE:HG21	1.97	0.45
1:E:716:LYS:O	1:E:719:ILE:HG22	2.16	0.45
1:E:1127:VAL:HG11	1:E:1150:ILE:HG23	1.99	0.45
2:B:173:PHE:HA	2:B:333:ILE:HB	1.98	0.45
2:B:1142:TRP:HD1	2:B:1142:TRP:H	1.65	0.45
2:D:932:VAL:C	2:D:933:ILE:HG13	2.36	0.45
2:F:192:CYS:O	2:F:195:LYS:HB3	2.16	0.45
1:A:92:ASN:O	1:A:96:ASN:HB2	2.17	0.45
1:A:857:TYR:HB2	1:A:862:TYR:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:427:ILE:HD12	1:C:521:PHE:CD1	2.52	0.45
1:C:720:GLU:HA	1:C:723:TYR:HB3	1.99	0.45
1:E:981:ASN:HB3	1:E:1117:LEU:HB3	1.99	0.45
2:B:43:PRO:HA	2:B:78:PHE:CE2	2.51	0.45
2:D:402:ILE:HG12	2:D:593:LYS:CB	2.46	0.45
2:F:203:ILE:HG22	2:F:203:ILE:O	2.15	0.45
1:A:275:LEU:HD11	1:A:279:TYR:CE2	2.51	0.45
1:A:345:VAL:HG13	1:A:387:GLN:HE22	1.80	0.45
1:C:453:GLU:C	1:C:454:ILE:HG22	2.37	0.45
1:C:456:ASP:HA	1:C:669:ASN:HD21	1.81	0.45
1:C:484:SER:O	1:C:485:ASP:CB	2.64	0.45
2:B:541:THR:O	2:B:542:GLN:HB3	2.16	0.45
2:B:727:TYR:N	2:B:728:PRO:CD	2.80	0.45
2:B:738:ILE:HA	2:B:741:ILE:HD12	1.99	0.45
2:D:102:ILE:HG12	2:D:197:LEU:HD11	1.98	0.45
2:F:684:ASN:O	2:F:687:LEU:N	2.50	0.45
2:F:734:MET:HA	2:F:737:CYS:SG	2.57	0.45
1:A:427:ILE:CG2	1:A:428:GLU:N	2.79	0.45
1:A:634:LEU:HD23	1:A:696:GLN:CD	2.37	0.45
1:A:1168:THR:HG22	1:A:1170:ASN:H	1.82	0.45
1:C:92:ASN:O	1:C:96:ASN:HB2	2.16	0.45
1:C:416:VAL:CG1	1:C:420:GLY:N	2.80	0.45
2:B:9:ILE:HG21	2:B:76:ASP:HB2	1.98	0.45
2:B:631:TYR:O	2:B:634:LEU:HB2	2.16	0.45
2:B:730:PHE:O	2:B:734:MET:HG2	2.17	0.45
2:D:43:PRO:HA	2:D:78:PHE:CE2	2.52	0.45
2:D:583:ILE:HG23	2:D:644:GLN:NE2	2.32	0.45
2:D:730:PHE:O	2:D:734:MET:HG2	2.17	0.45
2:F:1003:ASN:HB3	2:F:1116:ILE:HD13	1.98	0.45
1:A:206:PRO:O	1:A:209:THR:N	2.50	0.45
1:C:144:LEU:HA	1:C:487:LYS:HA	1.99	0.45
1:C:194:PHE:N	1:C:194:PHE:CD1	2.85	0.45
1:C:203:ILE:CD1	1:C:396:ILE:HG21	2.47	0.45
1:C:610:LEU:HD11	1:C:704:MET:HE2	1.98	0.45
1:E:94:ILE:HG23	1:E:211:MET:HE3	1.99	0.45
1:E:416:VAL:CG1	1:E:420:GLY:N	2.80	0.45
1:E:576:ILE:HG12	1:E:719:ILE:HD11	1.98	0.45
1:E:852:VAL:HG11	1:E:906:ILE:HG23	1.99	0.45
2:B:684:ASN:O	2:B:687:LEU:N	2.49	0.45
2:B:867:PHE:CD1	2:B:867:PHE:C	2.91	0.45
2:D:64:TYR:CD2	2:D:64:TYR:N	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:232:PHE:CZ	2:D:240:TYR:HA	2.52	0.45
2:D:402:ILE:HG12	2:D:593:LYS:HB2	1.99	0.45
2:F:610:ASP:OD1	2:F:611:LEU:HD13	2.17	0.45
2:F:738:ILE:HA	2:F:741:ILE:HD12	1.98	0.45
1:A:154:GLU:CB	1:A:155:PRO:CD	2.94	0.45
1:A:682:TYR:CE2	1:A:825:PHE:HA	2.52	0.45
1:A:942:CYS:SG	1:A:1026:SER:HB3	2.57	0.45
1:C:896:SER:C	1:C:897:GLU:HG3	2.36	0.45
1:C:920:TRP:HB2	1:C:1045:ARG:CD	2.47	0.45
1:C:1212:LEU:O	1:C:1238:CYS:HA	2.16	0.45
1:E:193:ARG:NH2	1:E:196:ASP:OD1	2.50	0.45
1:E:423:LYS:HD2	2:D:510:PHE:CZ	2.52	0.45
1:E:1088:LEU:HD23	1:E:1089:LEU:N	2.31	0.45
2:B:14:ASP:O	2:B:15:ASN:CB	2.64	0.45
2:B:274:LYS:C	2:B:276:ASN:H	2.19	0.45
2:B:856:ASN:O	2:B:857:ASP:C	2.55	0.45
2:D:210:ASN:HB3	2:D:228:ASP:HA	1.99	0.45
2:D:298:ILE:O	2:D:301:LEU:HB2	2.17	0.45
2:D:803:LEU:HD23	2:D:803:LEU:C	2.37	0.45
2:D:1116:ILE:HG23	2:D:1117:PHE:N	2.32	0.45
2:F:423:ILE:O	2:F:423:ILE:CG2	2.64	0.45
2:F:870:TYR:HA	2:F:931:ILE:O	2.17	0.45
2:F:989:ILE:CG2	2:F:994:ILE:HG13	2.47	0.45
1:A:427:ILE:HD12	1:A:521:PHE:CD1	2.52	0.44
1:A:614:ASN:CB	1:A:617:GLN:OE1	2.66	0.44
1:A:633:LEU:O	1:A:700:ARG:NH2	2.46	0.44
1:C:154:GLU:CB	1:C:155:PRO:CD	2.94	0.44
1:C:738:TYR:C	1:C:740:ILE:N	2.70	0.44
1:C:1229:MET:O	1:C:1231:ASP:N	2.50	0.44
1:E:484:SER:O	1:E:485:ASP:CB	2.65	0.44
1:E:785:TYR:O	1:E:786:ASP:C	2.55	0.44
2:B:677:ASN:CG	2:D:849:ASN:ND2	2.70	0.44
2:B:824:THR:HA	2:B:856:ASN:HB2	1.99	0.44
2:B:870:TYR:HA	2:B:931:ILE:O	2.17	0.44
2:B:1056:PRO:O	2:B:1058:LYS:N	2.50	0.44
2:D:14:ASP:O	2:D:15:ASN:CB	2.65	0.44
2:D:51:LEU:HB3	2:D:66:SER:HA	1.98	0.44
2:D:274:LYS:C	2:D:276:ASN:H	2.20	0.44
2:F:1056:PRO:O	2:F:1058:LYS:N	2.50	0.44
1:A:576:ILE:HG12	1:A:719:ILE:HD11	1.99	0.44
1:A:603:VAL:HG13	1:A:605:TYR:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1076:TRP:HZ3	1:A:1244:SER:HG	1.66	0.44
1:C:1127:VAL:HG11	1:C:1150:ILE:HG23	1.99	0.44
1:E:535:VAL:HG11	1:E:551:ILE:HD12	1.99	0.44
1:E:554:PHE:HB3	1:E:608:LEU:HD12	1.99	0.44
2:B:271:ILE:HG23	2:B:272:LYS:N	2.32	0.44
2:B:866:ASN:O	2:B:867:PHE:HB3	2.18	0.44
2:B:922:ASN:C	2:B:923:ILE:HG13	2.37	0.44
2:D:35:VAL:O	2:D:36:ALA:HB2	2.17	0.44
2:D:415:TYR:O	2:D:416:SER:CB	2.65	0.44
2:D:594:ILE:CG2	2:D:595:LYS:N	2.80	0.44
2:D:859:PHE:HD1	2:D:968:ILE:HD12	1.82	0.44
2:F:64:TYR:HE2	2:F:363:ILE:HD12	1.81	0.44
2:F:155:LYS:O	2:F:156:GLU:C	2.55	0.44
1:A:331:LEU:HB2	1:A:332:TYR:HD2	1.81	0.44
1:A:795:ASN:OD1	1:A:795:ASN:C	2.55	0.44
1:C:94:ILE:HG23	1:C:211:MET:HE3	1.99	0.44
1:C:220:GLY:HA2	1:C:225:LYS:HE3	1.99	0.44
1:C:700:ARG:HA	1:C:703:GLN:HB2	1.98	0.44
1:E:22:LYS:CG	1:E:23:PRO:HD2	2.47	0.44
1:E:448:ILE:O	1:E:449:ASN:O	2.36	0.44
1:E:864:ASP:C	1:E:864:ASP:OD1	2.55	0.44
1:E:912:TYR:O	1:E:913:LYS:CB	2.65	0.44
2:B:27:ASP:N	2:B:27:ASP:OD1	2.50	0.44
2:B:622:ASN:O	2:B:625:TYR:N	2.50	0.44
2:D:45:ARG:HG3	2:D:141:PRO:O	2.18	0.44
2:D:866:ASN:O	2:D:867:PHE:HB3	2.18	0.44
2:F:372:LEU:O	2:F:379:VAL:HA	2.17	0.44
1:A:535:VAL:HG11	1:A:551:ILE:HD12	1.99	0.44
1:A:738:TYR:C	1:A:740:ILE:N	2.71	0.44
1:A:908:TYR:HB3	1:A:1025:VAL:CG2	2.47	0.44
1:C:331:LEU:CB	1:C:332:TYR:CD2	3.01	0.44
1:C:908:TYR:HB3	1:C:1025:VAL:CG2	2.47	0.44
1:E:469:ASP:O	1:E:472:ILE:HB	2.17	0.44
1:E:1090:ASN:HB2	1:E:1240:TRP:CZ3	2.53	0.44
2:B:1122:LEU:HD21	2:B:1158:TRP:CE2	2.53	0.44
2:D:1056:PRO:O	2:D:1058:LYS:N	2.50	0.44
2:F:480:ILE:HG21	2:F:497:VAL:HG23	2.00	0.44
2:F:846:THR:HG23	2:F:847:GLY:N	2.32	0.44
2:F:880:THR:CB	2:F:901:ASN:HA	2.48	0.44
2:F:1036:ILE:HD12	2:F:1045:SER:HB3	1.99	0.44
1:A:522:TYR:O	1:A:525:ALA:HB3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:PHE:HD2	1:A:696:GLN:OE1	2.01	0.44
1:C:186:PHE:CE2	1:C:188:PRO:HB3	2.53	0.44
1:C:286:LEU:O	1:C:289:VAL:HG13	2.17	0.44
1:C:785:TYR:O	1:C:786:ASP:C	2.54	0.44
1:E:21:ILE:HG12	1:E:134:ILE:HG22	2.00	0.44
2:B:211:ILE:O	2:B:226:GLU:HA	2.18	0.44
2:B:932:VAL:C	2:B:933:ILE:HG13	2.37	0.44
2:B:1135:ILE:HG22	2:B:1136:LYS:N	2.32	0.44
2:D:554:ILE:HB	2:D:557:ILE:CD1	2.48	0.44
2:F:1013:GLU:O	2:F:1014:ILE:CB	2.66	0.44
1:A:916:SER:OG	1:A:1054:LEU:HG	2.18	0.44
2:B:102:ILE:HG12	2:B:197:LEU:HD11	1.99	0.44
2:B:298:ILE:HA	2:B:301:LEU:HD12	1.99	0.44
2:D:141:PRO:HA	2:D:169:TRP:HB3	1.99	0.44
2:F:727:TYR:N	2:F:728:PRO:CD	2.80	0.44
2:F:815:VAL:C	2:F:816:ILE:HG13	2.37	0.44
2:F:1007:ILE:CG2	2:F:1015:LEU:HD12	2.47	0.44
1:A:920:TRP:HB2	1:A:1045:ARG:CD	2.48	0.44
1:C:912:TYR:O	1:C:913:LYS:HB3	2.18	0.44
1:C:1044:ILE:CG2	1:C:1045:ARG:N	2.80	0.44
1:E:203:ILE:CD1	1:E:396:ILE:HG21	2.47	0.44
2:B:285:LEU:O	2:B:288:GLU:N	2.51	0.44
2:B:877:LYS:CB	2:B:878:GLN:HB3	2.47	0.44
2:D:990:ASN:HB3	2:D:993:GLU:OE2	2.17	0.44
2:F:8:ASN:O	2:F:9:ILE:C	2.55	0.44
1:A:193:ARG:NH2	1:A:196:ASP:OD1	2.51	0.44
1:A:287:SER:HA	1:A:317:TYR:CD2	2.53	0.44
1:A:395:ILE:HG13	1:A:396:ILE:HG23	2.00	0.44
1:A:484:SER:O	1:A:485:ASP:CB	2.66	0.44
1:A:987:ILE:O	1:A:989:LYS:N	2.51	0.44
1:A:1044:ILE:CG2	1:A:1045:ARG:N	2.80	0.44
1:C:380:LEU:HD23	1:C:385:ARG:HD3	2.00	0.44
1:C:431:ASN:O	1:C:434:LEU:HB2	2.17	0.44
1:C:864:ASP:C	1:C:864:ASP:OD1	2.56	0.44
1:C:916:SER:OG	1:C:1054:LEU:HG	2.18	0.44
1:C:1132:VAL:HG23	1:C:1149:TYR:CE2	2.52	0.44
1:C:1153:VAL:HG23	1:C:1159:LEU:CD2	2.48	0.44
1:E:299:TYR:HA	1:E:302:ILE:HG22	1.99	0.44
2:B:153:TYR:HB2	2:B:165:MET:O	2.18	0.44
2:B:400:ASN:OD1	2:B:400:ASN:N	2.50	0.44
2:F:552:LYS:C	2:F:713:PHE:CE1	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ILE:HG12	1:A:134:ILE:HG22	2.00	0.44
1:A:554:PHE:HB3	1:A:608:LEU:HD12	1.99	0.44
1:C:476:ASN:N	2:D:1136:LYS:CE	2.81	0.44
1:C:482:GLY:C	1:C:483:LEU:HG	2.38	0.44
1:E:92:ASN:O	1:E:96:ASN:HB2	2.18	0.44
1:E:431:ASN:O	1:E:434:LEU:HB2	2.17	0.44
1:E:571:LEU:O	1:E:575:TRP:N	2.42	0.44
1:E:942:CYS:SG	1:E:1025:VAL:CG1	3.06	0.44
1:E:1229:MET:O	1:E:1231:ASP:N	2.51	0.44
2:B:106:ILE:N	2:B:290:LYS:HD3	2.33	0.44
2:B:579:PRO:C	2:B:581:SER:N	2.71	0.44
2:D:867:PHE:CZ	2:D:935:ILE:HD12	2.52	0.44
2:F:108:PHE:HB3	2:F:162:MET:CG	2.46	0.44
2:F:274:LYS:C	2:F:276:ASN:H	2.21	0.44
2:F:945:PHE:CD1	2:F:950:LEU:HA	2.53	0.44
2:F:1142:TRP:H	2:F:1142:TRP:HD1	1.66	0.44
1:A:398:PRO:C	1:A:399:ILE:HG13	2.38	0.43
1:C:427:ILE:CG2	1:C:428:GLU:N	2.81	0.43
1:C:636:PHE:HD2	1:C:696:GLN:OE1	2.00	0.43
1:C:727:THR:O	1:C:728:LEU:CB	2.65	0.43
1:E:535:VAL:HG12	1:E:536:ASN:N	2.31	0.43
2:B:173:PHE:O	2:B:333:ILE:N	2.51	0.43
2:B:1003:ASN:HB3	2:B:1116:ILE:HD13	2.00	0.43
2:D:870:TYR:HA	2:D:931:ILE:O	2.18	0.43
2:F:227:LEU:HD11	2:F:231:ASP:CB	2.48	0.43
2:F:298:ILE:O	2:F:301:LEU:HB2	2.17	0.43
2:F:305:TYR:CE1	2:F:418:LEU:CD1	3.01	0.43
1:A:299:TYR:HA	1:A:302:ILE:HG22	1.99	0.43
1:A:416:VAL:CG1	1:A:420:GLY:N	2.81	0.43
1:C:522:TYR:O	1:C:525:ALA:HB3	2.18	0.43
1:C:554:PHE:HB3	1:C:608:LEU:HD12	2.00	0.43
1:E:361:SER:OG	1:E:397:LYS:HE2	2.17	0.43
1:E:857:TYR:HB2	1:E:862:TYR:CE1	2.53	0.43
2:B:501:LEU:HD22	2:B:537:ASP:HB3	2.00	0.43
2:D:381:MET:HE3	2:D:471:GLN:CD	2.39	0.43
2:D:804:SER:HB3	2:D:819:THR:HG22	1.99	0.43
2:D:962:ILE:O	2:D:962:ILE:CG2	2.66	0.43
2:F:141:PRO:HA	2:F:169:TRP:HB3	2.00	0.43
2:F:415:TYR:O	2:F:416:SER:CB	2.65	0.43
2:F:501:LEU:HD22	2:F:537:ASP:HB3	2.00	0.43
1:A:873:ASN:N	1:A:899:ASN:O	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:TYR:HA	1:C:302:ILE:HG22	2.00	0.43
1:E:522:TYR:O	1:E:525:ALA:HB3	2.18	0.43
1:E:993:VAL:HG12	1:E:994:THR:N	2.33	0.43
2:B:645:TYR:O	2:B:646:PHE:C	2.56	0.43
2:B:799:SER:HB2	2:B:800:PRO:HD2	1.99	0.43
2:B:962:ILE:O	2:B:962:ILE:CG2	2.65	0.43
2:F:540:GLU:HB3	2:F:555:PRO:CD	2.49	0.43
2:F:567:ASN:O	2:F:568:ASN:C	2.57	0.43
2:F:867:PHE:C	2:F:867:PHE:CD1	2.91	0.43
2:F:1135:ILE:HG22	2:F:1136:LYS:N	2.33	0.43
1:A:454:ILE:HD12	1:A:456:ASP:OD1	2.19	0.43
1:A:727:THR:O	1:A:728:LEU:CB	2.66	0.43
1:C:398:PRO:C	1:C:399:ILE:HG13	2.38	0.43
1:C:836:LEU:HD11	2:D:945:PHE:CE1	2.54	0.43
1:C:929:LYS:HA	1:C:932:ASN:HB2	1.99	0.43
1:E:771:MET:HA	1:E:774:ILE:CG2	2.45	0.43
1:E:833:ASP:HB3	1:E:835:ILE:HD12	2.01	0.43
1:E:1095:ASN:O	1:E:1112:ARG:N	2.40	0.43
2:B:515:LYS:HB3	2:B:516:PRO:HD2	1.98	0.43
2:B:794:ILE:O	2:B:795:LYS:C	2.56	0.43
2:B:806:TYR:O	2:B:816:ILE:HA	2.19	0.43
2:D:296:LYS:HA	2:D:299:TRP:HE3	1.84	0.43
2:D:552:LYS:C	2:D:713:PHE:CE1	2.92	0.43
2:F:89:ILE:O	2:F:95:GLY:HA3	2.18	0.43
2:F:645:TYR:OH	2:F:721:VAL:HG21	2.19	0.43
2:F:794:ILE:O	2:F:795:LYS:C	2.56	0.43
1:A:361:SER:OG	1:A:397:LYS:HE2	2.18	0.43
1:A:836:LEU:CB	2:B:995:LEU:HD11	2.47	0.43
1:A:981:ASN:HB3	1:A:1117:LEU:HB3	2.01	0.43
1:E:456:ASP:HA	1:E:669:ASN:ND2	2.34	0.43
1:E:634:LEU:HD23	1:E:696:GLN:CD	2.39	0.43
2:B:105:ALA:HA	2:B:290:LYS:CD	2.48	0.43
2:B:146:ILE:HD13	2:B:330:TYR:CE2	2.54	0.43
2:B:1142:TRP:N	2:B:1142:TRP:HD1	2.16	0.43
2:D:35:VAL:CG1	2:D:36:ALA:H	2.29	0.43
2:D:246:ASN:HA	2:D:247:PRO:HA	1.83	0.43
2:D:567:ASN:O	2:D:568:ASN:C	2.54	0.43
2:D:738:ILE:HA	2:D:741:ILE:HD12	1.99	0.43
2:D:876:LEU:HD21	2:D:978:TYR:CD2	2.53	0.43
1:A:380:LEU:HD23	1:A:385:ARG:HD3	2.01	0.43
1:C:4:ILE:HD11	1:C:95:ASN:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:ARG:NH2	1:C:196:ASP:OD1	2.51	0.43
1:E:179:GLY:HA2	1:E:220:GLY:O	2.17	0.43
1:E:522:TYR:CZ	1:E:611:ASN:HB2	2.53	0.43
1:E:617:GLN:OE1	1:E:617:GLN:N	2.47	0.43
1:E:632:ILE:HG23	1:E:633:LEU:HG	2.01	0.43
1:E:883:THR:HG23	1:E:884:ASN:H	1.84	0.43
2:B:81:ALA:O	2:B:84:LYS:N	2.52	0.43
2:D:21:VAL:CG1	2:D:121:ASN:HA	2.46	0.43
2:D:269:TYR:HE2	2:D:288:GLU:CG	2.31	0.43
2:D:645:TYR:O	2:D:646:PHE:C	2.55	0.43
1:C:456:ASP:HA	1:C:669:ASN:ND2	2.34	0.43
1:C:633:LEU:O	1:C:700:ARG:NH2	2.47	0.43
1:E:863:VAL:HG12	1:E:864:ASP:N	2.33	0.43
1:E:912:TYR:O	1:E:913:LYS:HB3	2.16	0.43
1:E:1106:LEU:HD12	1:E:1175:ILE:HB	1.99	0.43
1:E:1232:HIS:CB	1:E:1236:ASN:HD21	2.32	0.43
2:B:1013:GLU:O	2:B:1014:ILE:CB	2.66	0.43
2:F:856:ASN:O	2:F:857:ASP:C	2.56	0.43
1:A:468:LEU:HD12	1:A:468:LEU:C	2.39	0.43
1:A:660:LYS:CG	1:A:661:ASN:N	2.82	0.43
1:A:824:PRO:HB3	2:B:952:ALA:HB2	2.00	0.43
1:C:627:LEU:HG	1:E:419:LYS:O	2.18	0.43
1:C:863:VAL:HG12	1:C:864:ASP:N	2.34	0.43
1:C:898:VAL:O	1:C:1030:LEU:HA	2.18	0.43
1:C:990:TRP:HZ3	1:C:1044:ILE:HA	1.83	0.43
1:C:994:THR:HB	1:C:1006:TYR:HB2	2.00	0.43
1:E:38:ASN:HB3	1:E:147:ASN:HB2	2.00	0.43
1:E:47:VAL:C	1:E:50:THR:HG1	2.22	0.43
1:E:118:ASN:HA	1:E:119:THR:CB	2.41	0.43
1:E:262:ILE:CD1	1:E:690:MET:HB3	2.49	0.43
1:E:423:LYS:NZ	2:D:514:ASP:OD1	2.41	0.43
1:E:603:VAL:HG13	1:E:605:TYR:CE2	2.54	0.43
1:E:897:GLU:HG2	1:E:1032:LYS:CB	2.42	0.43
2:B:13:VAL:CG1	2:B:14:ASP:N	2.82	0.43
2:B:913:GLY:O	2:B:914:ASN:C	2.57	0.43
2:B:1003:ASN:HB3	2:B:1116:ILE:CD1	2.48	0.43
2:F:43:PRO:HA	2:F:78:PHE:CE2	2.54	0.43
2:F:400:ASN:N	2:F:400:ASN:OD1	2.51	0.43
2:F:990:ASN:O	2:F:993:GLU:N	2.51	0.43
1:A:452:LYS:CB	1:A:651:LYS:HE2	2.49	0.43
1:C:250:GLU:O	1:C:254:THR:N	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:682:TYR:HE2	1:C:825:PHE:HA	1.83	0.43
1:C:943:MET:CE	1:C:947:ASN:HB3	2.49	0.43
1:E:795:ASN:OD1	1:E:795:ASN:C	2.57	0.43
2:B:423:ILE:O	2:B:423:ILE:CG2	2.64	0.43
2:B:859:PHE:HD1	2:B:968:ILE:HD12	1.81	0.43
2:D:13:VAL:HG13	2:D:19:ALA:HA	2.01	0.43
2:D:854:PHE:HE2	2:D:970:LEU:HB2	1.83	0.43
2:D:917:ASN:O	2:D:918:ILE:HG13	2.19	0.43
2:D:1093:THR:HG23	2:D:1095:ASN:N	2.34	0.43
2:F:13:VAL:HG12	2:F:14:ASP:H	1.82	0.43
2:F:306:PHE:O	2:F:307:SER:C	2.57	0.43
2:F:867:PHE:CB	2:F:985:LEU:O	2.65	0.43
1:A:730:GLU:O	1:A:732:ASN:N	2.52	0.43
1:A:994:THR:HB	1:A:1006:TYR:HB2	2.00	0.43
1:C:475:PHE:C	2:D:1136:LYS:CE	2.87	0.43
1:C:632:ILE:HG23	1:C:633:LEU:HG	2.01	0.43
1:C:634:LEU:HD23	1:C:696:GLN:CD	2.38	0.43
1:C:1226:TYR:N	1:C:1226:TYR:CD2	2.87	0.43
1:E:173:PRO:HB2	1:E:178:PHE:HB2	2.01	0.43
1:E:838:SER:O	1:E:842:LYS:HB3	2.19	0.43
1:E:916:SER:OG	1:E:1054:LEU:HG	2.18	0.43
2:B:289:GLN:NE2	2:B:423:ILE:HG22	2.34	0.43
2:B:923:ILE:C	2:B:925:ASN:N	2.72	0.43
2:D:1007:ILE:CG2	2:D:1015:LEU:HD12	2.49	0.43
2:F:289:GLN:NE2	2:F:292:LYS:HE3	2.34	0.43
2:F:429:ILE:N	2:F:430:PRO:HD3	2.34	0.43
2:F:554:ILE:HG21	2:F:556:TRP:CZ2	2.54	0.43
2:F:923:ILE:C	2:F:925:ASN:H	2.21	0.43
1:A:191:SER:HB2	1:A:360:LEU:HD11	2.01	0.42
1:A:448:ILE:O	1:A:449:ASN:O	2.36	0.42
1:A:610:LEU:CD1	1:A:704:MET:HE2	2.48	0.42
1:A:912:TYR:N	1:A:912:TYR:CD1	2.83	0.42
1:A:1106:LEU:HD12	1:A:1175:ILE:HB	2.00	0.42
1:C:196:ASP:OD2	1:C:196:ASP:N	2.52	0.42
1:C:286:LEU:O	1:C:287:SER:C	2.58	0.42
1:C:382:VAL:HG11	1:C:868:TYR:CE1	2.54	0.42
1:E:468:LEU:HD12	1:E:471:VAL:HG22	2.01	0.42
1:E:660:LYS:CG	1:E:661:ASN:N	2.82	0.42
1:E:936:GLU:HA	1:E:954:LEU:O	2.19	0.42
1:E:1153:VAL:HG23	1:E:1159:LEU:CD2	2.48	0.42
2:B:35:VAL:O	2:B:36:ALA:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:586:LYS:O	2:B:641:TYR:CZ	2.72	0.42
2:D:211:ILE:O	2:D:226:GLU:HA	2.19	0.42
2:D:254:TYR:O	2:D:258:THR:HB	2.19	0.42
2:D:989:ILE:HG22	2:D:990:ASN:N	2.34	0.42
2:F:973:ASP:O	2:F:975:ASN:N	2.51	0.42
1:A:453:GLU:HG3	1:A:454:ILE:HB	2.01	0.42
1:E:138:ASN:ND2	1:E:140:SER:OG	2.52	0.42
2:B:296:LYS:HA	2:B:299:TRP:HE3	1.84	0.42
2:B:428:LYS:C	2:B:430:PRO:CD	2.88	0.42
2:B:989:ILE:CG2	2:B:994:ILE:HG13	2.50	0.42
2:D:106:ILE:N	2:D:290:LYS:HD3	2.34	0.42
2:D:976:ASN:C	2:D:977:VAL:HG23	2.40	0.42
2:D:1003:ASN:CG	2:D:1003:ASN:O	2.57	0.42
2:F:9:ILE:HG13	2:F:10:ASP:N	2.34	0.42
2:F:211:ILE:O	2:F:226:GLU:HA	2.19	0.42
1:A:194:PHE:N	1:A:194:PHE:CD1	2.87	0.42
1:C:361:SER:OG	1:C:397:LYS:HE2	2.19	0.42
1:C:912:TYR:O	1:C:913:LYS:CB	2.67	0.42
1:C:1188:VAL:HG22	1:C:1201:PHE:CE1	2.54	0.42
1:E:274:ASN:HA	1:E:277:ASN:ND2	2.34	0.42
2:B:266:LYS:HA	2:B:291:PHE:CE1	2.55	0.42
2:B:381:MET:HE3	2:B:471:GLN:CD	2.38	0.42
2:B:480:ILE:HG21	2:B:497:VAL:HG23	2.01	0.42
2:B:645:TYR:OH	2:B:721:VAL:HG21	2.19	0.42
2:D:238:ILE:O	2:D:239:ASP:C	2.55	0.42
2:D:1098:ILE:HD12	2:D:1143:VAL:CG1	2.50	0.42
2:F:210:ASN:HB3	2:F:228:ASP:HA	1.99	0.42
1:A:160:THR:HA	1:A:185:THR:O	2.19	0.42
1:A:990:TRP:HZ3	1:A:1044:ILE:HA	1.84	0.42
1:C:416:VAL:HG13	1:C:420:GLY:CA	2.50	0.42
1:C:467:ASP:OD1	1:C:467:ASP:C	2.57	0.42
1:C:920:TRP:O	1:C:1044:ILE:HA	2.19	0.42
1:E:297:ASN:N	1:E:298:PRO:HD3	2.33	0.42
1:E:597:ALA:HA	2:F:939:LYS:HD3	2.01	0.42
1:E:1083:ASP:HB2	1:E:1128:LYS:HE3	2.01	0.42
2:B:1122:LEU:C	2:B:1122:LEU:HD12	2.40	0.42
2:D:155:LYS:O	2:D:156:GLU:C	2.57	0.42
2:D:289:GLN:NE2	2:D:423:ILE:HG22	2.35	0.42
2:D:855:THR:HG22	2:D:967:ILE:HG12	2.02	0.42
2:D:877:LYS:CB	2:D:878:GLN:HB3	2.47	0.42
2:F:411:HIS:CA	2:F:624:PHE:HE1	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:877:LYS:CB	2:F:878:GLN:HB3	2.47	0.42
2:F:962:ILE:O	2:F:962:ILE:CG2	2.66	0.42
2:F:1116:ILE:HG23	2:F:1117:PHE:N	2.34	0.42
1:A:1043:GLY:C	1:A:1044:ILE:HG13	2.39	0.42
1:C:194:PHE:N	1:C:194:PHE:HD1	2.18	0.42
1:C:535:VAL:HG11	1:C:551:ILE:HD12	2.00	0.42
1:E:727:THR:O	1:E:728:LEU:CB	2.66	0.42
1:E:987:ILE:O	1:E:989:LYS:N	2.52	0.42
1:E:1012:ILE:O	2:F:779:ILE:HD12	2.19	0.42
1:E:1044:ILE:CG2	1:E:1045:ARG:N	2.82	0.42
2:B:234:ILE:O	2:B:302:ASN:HB2	2.19	0.42
2:B:242:LEU:CD1	2:B:638:TRP:CG	3.03	0.42
2:B:415:TYR:O	2:B:416:SER:CB	2.67	0.42
1:A:287:SER:HB3	1:A:317:TYR:H	1.84	0.42
1:A:720:GLU:HA	1:A:723:TYR:HB3	2.02	0.42
1:A:993:VAL:HG12	1:A:994:THR:N	2.35	0.42
1:A:1002:ASP:N	1:A:1002:ASP:OD1	2.53	0.42
1:C:1127:VAL:CG1	1:C:1128:LYS:N	2.82	0.42
1:E:15:ASP:HA	1:E:16:ARG:HA	1.77	0.42
1:E:427:ILE:CG2	1:E:428:GLU:N	2.82	0.42
1:E:738:TYR:C	1:E:740:ILE:N	2.72	0.42
2:D:727:TYR:N	2:D:728:PRO:CD	2.82	0.42
2:F:242:LEU:CD1	2:F:638:TRP:CG	3.02	0.42
2:F:276:ASN:O	2:F:277:ASN:HB3	2.20	0.42
1:A:617:GLN:OE1	1:A:617:GLN:N	2.47	0.42
1:A:932:ASN:HA	1:A:956:HIS:CE1	2.55	0.42
1:A:1190:MET:HE1	1:A:1199:MET:HB3	2.02	0.42
1:C:926:TYR:HD1	1:C:1247:HIS:O	2.03	0.42
1:E:170:ASN:HD21	2:B:377:ASN:ND2	2.18	0.42
1:E:250:GLU:O	1:E:254:THR:N	2.44	0.42
1:E:730:GLU:O	1:E:732:ASN:N	2.52	0.42
2:B:629:ILE:O	2:B:630:TYR:C	2.58	0.42
2:B:1097:ARG:NE	2:B:1142:TRP:CE3	2.87	0.42
2:D:586:LYS:O	2:D:641:TYR:CZ	2.73	0.42
2:D:923:ILE:O	2:D:925:ASN:N	2.39	0.42
2:F:945:PHE:HA	2:F:949:ILE:O	2.20	0.42
1:A:305:GLU:OE1	1:A:305:GLU:HA	2.20	0.42
1:A:436:PHE:CD1	1:A:437:VAL:N	2.86	0.42
1:C:262:ILE:CD1	1:C:690:MET:HB3	2.50	0.42
1:C:452:LYS:CB	1:C:651:LYS:HE2	2.50	0.42
1:C:617:GLN:OE1	1:C:617:GLN:N	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:660:LYS:CG	1:C:661:ASN:N	2.82	0.42
1:C:981:ASN:HB3	1:C:1117:LEU:HB3	2.02	0.42
1:C:1232:HIS:CB	1:C:1236:ASN:HD21	2.32	0.42
1:E:15:ASP:HA	1:E:136:PHE:HZ	1.85	0.42
2:B:13:VAL:HG13	2:B:19:ALA:HA	2.01	0.42
2:B:755:ILE:HG22	2:B:760:LYS:HG3	2.01	0.42
2:B:905:VAL:HA	2:B:918:ILE:O	2.20	0.42
2:D:153:TYR:HB2	2:D:165:MET:O	2.19	0.42
2:D:922:ASN:C	2:D:923:ILE:HG13	2.40	0.42
2:F:238:ILE:O	2:F:239:ASP:C	2.57	0.42
2:F:738:ILE:O	2:F:739:LYS:C	2.58	0.42
1:A:220:GLY:HA2	1:A:225:LYS:HE3	2.01	0.42
1:A:903:ASN:OD1	1:A:903:ASN:C	2.59	0.42
1:A:1111:ILE:HG23	1:A:1111:ILE:O	2.20	0.42
1:A:1153:VAL:HG23	1:A:1159:LEU:CD2	2.50	0.42
1:C:38:ASN:HB3	1:C:147:ASN:HB2	2.02	0.42
1:C:395:ILE:HG13	1:C:396:ILE:HG23	2.02	0.42
1:C:838:SER:O	1:C:842:LYS:HB3	2.20	0.42
1:E:196:ASP:OD2	1:E:196:ASP:N	2.53	0.42
1:E:398:PRO:C	1:E:399:ILE:HG13	2.40	0.42
2:B:108:PHE:CG	2:B:109:PRO:HD2	2.55	0.42
2:B:276:ASN:O	2:B:277:ASN:HB3	2.20	0.42
2:B:945:PHE:CD1	2:B:950:LEU:HA	2.55	0.42
2:B:1093:THR:HG23	2:B:1095:ASN:N	2.35	0.42
2:D:554:ILE:HG21	2:D:556:TRP:CZ2	2.54	0.42
2:D:1149:HIS:CE1	2:D:1150:ASP:CB	3.02	0.42
2:F:266:LYS:HA	2:F:291:PHE:CE1	2.55	0.42
2:F:515:LYS:HB3	2:F:516:PRO:HD2	2.01	0.42
2:F:709:ASN:O	2:F:713:PHE:HD2	2.02	0.42
2:F:922:ASN:C	2:F:923:ILE:HG13	2.39	0.42
1:A:427:ILE:CD1	1:A:521:PHE:CD1	3.03	0.42
1:A:522:TYR:CZ	1:A:611:ASN:HB2	2.53	0.42
1:C:993:VAL:HG12	1:C:994:THR:N	2.35	0.42
1:C:1103:ASP:OD1	1:C:1103:ASP:N	2.36	0.42
1:E:4:ILE:HD11	1:E:95:ASN:HB2	2.02	0.42
1:E:39:ILE:HG12	1:E:148:VAL:HB	2.02	0.42
1:E:908:TYR:HB3	1:E:1025:VAL:CG2	2.49	0.42
1:E:1227:THR:HG22	2:F:806:TYR:CD2	2.54	0.42
2:B:552:LYS:C	2:B:713:PHE:CE1	2.93	0.42
2:B:734:MET:HA	2:B:737:CYS:SG	2.60	0.42
2:B:990:ASN:HB3	2:B:993:GLU:OE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1093:THR:OG1	2:B:1094:THR:N	2.52	0.42
2:D:27:ASP:N	2:D:27:ASP:OD1	2.52	0.42
2:D:81:ALA:O	2:D:84:LYS:N	2.52	0.42
2:D:308:LYS:HA	2:D:789:TYR:CE2	2.55	0.42
2:D:1122:LEU:HD21	2:D:1158:TRP:CE2	2.55	0.42
2:F:629:ILE:O	2:F:630:TYR:C	2.58	0.42
1:C:427:ILE:CD1	1:C:521:PHE:CD1	3.02	0.41
1:E:636:PHE:HD2	1:E:696:GLN:OE1	2.03	0.41
1:E:943:MET:CE	1:E:947:ASN:HB3	2.50	0.41
2:B:917:ASN:C	2:B:918:ILE:HG13	2.40	0.41
2:B:973:ASP:O	2:B:975:ASN:N	2.50	0.41
2:D:856:ASN:O	2:D:857:ASP:C	2.58	0.41
2:F:71:THR:OG1	2:F:74:GLU:HG2	2.20	0.41
2:F:855:THR:HG22	2:F:967:ILE:HG12	2.02	0.41
2:F:855:THR:HA	2:F:966:ASP:O	2.19	0.41
2:F:1003:ASN:O	2:F:1003:ASN:CG	2.58	0.41
2:F:1122:LEU:HD21	2:F:1158:TRP:CE2	2.54	0.41
1:C:192:PHE:CE1	1:C:204:GLN:HB3	2.55	0.41
1:C:468:LEU:HD12	1:C:471:VAL:HG22	2.02	0.41
1:C:522:TYR:CZ	1:C:611:ASN:HB2	2.54	0.41
1:E:216:HIS:CE1	1:E:250:GLU:HG3	2.54	0.41
1:E:720:GLU:HA	1:E:723:TYR:HB3	2.02	0.41
2:B:71:THR:OG1	2:B:74:GLU:HG2	2.19	0.41
2:B:453:ILE:CG1	2:B:454:THR:H	2.32	0.41
2:B:530:ILE:O	2:B:531:PHE:C	2.59	0.41
2:B:917:ASN:O	2:B:918:ILE:HG13	2.20	0.41
2:B:1122:LEU:HD21	2:B:1158:TRP:NE1	2.35	0.41
2:D:89:ILE:O	2:D:95:GLY:HA3	2.21	0.41
2:D:622:ASN:O	2:D:625:TYR:N	2.53	0.41
2:D:828:TYR:HB2	2:D:829:PRO:HD2	2.02	0.41
2:D:1097:ARG:NE	2:D:1142:TRP:CE3	2.89	0.41
2:F:321:ALA:HB1	2:F:388:ASP:HB3	2.02	0.41
2:F:580:ILE:H	2:F:580:ILE:HG13	1.66	0.41
1:A:22:LYS:HG3	1:A:23:PRO:HD2	2.01	0.41
1:A:987:ILE:C	1:A:989:LYS:N	2.73	0.41
1:A:1143:ARG:HB2	1:A:1146:ASP:OD1	2.20	0.41
1:C:912:TYR:CD1	1:C:912:TYR:N	2.87	0.41
1:C:1232:HIS:HB3	1:C:1236:ASN:HD21	1.85	0.41
1:E:436:PHE:CD1	1:E:437:VAL:N	2.85	0.41
1:E:778:LYS:HA	1:E:782:LEU:HD12	2.02	0.41
1:E:1010:ASN:HB3	2:F:780:GLN:CG	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:245:THR:HB	2:B:631:TYR:CE1	2.55	0.41
2:B:1007:ILE:HG12	2:B:1072:GLN:C	2.41	0.41
2:D:185:PRO:O	2:D:186:ALA:C	2.57	0.41
2:D:308:LYS:HA	2:D:789:TYR:CD2	2.56	0.41
2:D:799:SER:HB2	2:D:800:PRO:HD2	2.02	0.41
2:F:308:LYS:HA	2:F:789:TYR:CE2	2.55	0.41
2:F:502:ASN:O	2:F:505:MET:N	2.54	0.41
2:F:730:PHE:O	2:F:734:MET:HG2	2.20	0.41
1:A:38:ASN:HB3	1:A:147:ASN:HB2	2.03	0.41
1:A:584:THR:HG22	1:A:750:LYS:HD2	2.02	0.41
1:A:789:VAL:HG12	1:A:793:LEU:HD12	2.03	0.41
1:A:838:SER:O	1:A:842:LYS:HB3	2.21	0.41
1:A:852:VAL:HG11	1:A:906:ILE:HG23	2.03	0.41
1:A:1000:LEU:N	1:A:1000:LEU:HD12	2.36	0.41
1:C:249:ILE:HG23	1:C:263:ILE:CD1	2.51	0.41
1:C:903:ASN:C	1:C:903:ASN:OD1	2.59	0.41
1:E:614:ASN:CB	1:E:617:GLN:OE1	2.68	0.41
1:E:1188:VAL:HG22	1:E:1201:PHE:CE1	2.55	0.41
2:B:526:TRP:O	2:B:529:ALA:HB3	2.20	0.41
2:B:540:GLU:HB3	2:B:555:PRO:CD	2.50	0.41
2:B:554:ILE:HG21	2:B:556:TRP:CZ2	2.54	0.41
2:B:860:GLU:O	2:B:861:ASN:HB2	2.20	0.41
2:B:885:LEU:HG	2:B:886:ILE:CD1	2.22	0.41
2:D:46:TYR:HB3	2:D:142:GLY:HA2	2.02	0.41
2:D:71:THR:OG1	2:D:74:GLU:HG2	2.19	0.41
2:D:254:TYR:O	2:D:258:THR:CG2	2.69	0.41
2:D:289:GLN:NE2	2:D:292:LYS:HE3	2.36	0.41
2:D:645:TYR:OH	2:D:721:VAL:HG21	2.21	0.41
2:F:35:VAL:O	2:F:36:ALA:HB2	2.19	0.41
2:F:46:TYR:HB3	2:F:142:GLY:HA2	2.03	0.41
2:F:269:TYR:CZ	2:F:288:GLU:HB2	2.55	0.41
2:F:423:ILE:HG23	2:F:426:ILE:HB	2.02	0.41
2:F:860:GLU:O	2:F:861:ASN:HB2	2.21	0.41
2:F:1069:GLN:O	2:F:1070:TYR:CD2	2.74	0.41
1:A:297:ASN:N	1:A:297:ASN:OD1	2.49	0.41
1:A:1001:GLY:HA2	1:A:1018:LEU:HD21	2.02	0.41
1:C:274:ASN:HA	1:C:277:ASN:ND2	2.36	0.41
1:C:614:ASN:HB2	1:C:617:GLN:HE22	1.85	0.41
1:C:730:GLU:O	1:C:732:ASN:N	2.53	0.41
1:C:835:ILE:HG23	2:D:949:ILE:HA	2.03	0.41
1:E:395:ILE:HG13	1:E:396:ILE:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:456:ASP:OD1	1:E:456:ASP:N	2.52	0.41
1:E:932:ASN:HA	1:E:956:HIS:CE1	2.56	0.41
1:E:1127:VAL:CG1	1:E:1128:LYS:N	2.84	0.41
2:B:594:ILE:CG2	2:B:595:LYS:N	2.83	0.41
2:B:709:ASN:O	2:B:712:LYS:N	2.53	0.41
2:B:730:PHE:CE2	2:B:734:MET:HG3	2.55	0.41
2:D:423:ILE:HG23	2:D:426:ILE:HB	2.01	0.41
2:D:654:LYS:HA	2:D:657:LEU:HD12	2.02	0.41
2:F:88:ARG:O	2:F:91:ASN:HB2	2.20	0.41
2:F:755:ILE:HG22	2:F:760:LYS:HG3	2.03	0.41
2:F:799:SER:HB2	2:F:800:PRO:HD2	2.02	0.41
2:F:1098:ILE:HD12	2:F:1143:VAL:CG1	2.51	0.41
1:A:863:VAL:HG12	1:A:864:ASP:N	2.36	0.41
1:A:883:THR:HG23	1:A:884:ASN:H	1.85	0.41
1:A:1083:ASP:HB2	1:A:1128:LYS:HE3	2.02	0.41
1:A:1127:VAL:CG1	1:A:1128:LYS:N	2.83	0.41
1:C:603:VAL:CG1	1:C:605:TYR:CE2	3.04	0.41
1:E:1111:ILE:HG23	1:E:1111:ILE:O	2.20	0.41
2:B:185:PRO:O	2:B:188:GLU:N	2.53	0.41
2:B:583:ILE:HD11	2:B:645:TYR:CE2	2.55	0.41
2:B:626:LEU:HD22	2:B:734:MET:HE3	2.01	0.41
2:B:709:ASN:O	2:B:713:PHE:HD2	2.03	0.41
2:B:828:TYR:HB2	2:B:829:PRO:HD2	2.02	0.41
2:B:1140:TYR:CE2	2:B:1142:TRP:CE2	3.09	0.41
2:D:501:LEU:HD22	2:D:537:ASP:HB3	2.01	0.41
2:D:755:ILE:HG22	2:D:760:LYS:HG3	2.03	0.41
2:D:945:PHE:HA	2:D:949:ILE:O	2.20	0.41
2:F:553:ILE:CG2	2:F:554:ILE:N	2.83	0.41
2:F:731:THR:O	2:F:735:GLU:HG3	2.21	0.41
2:F:1097:ARG:NE	2:F:1142:TRP:CE3	2.89	0.41
1:A:682:TYR:CD2	1:A:825:PHE:HD1	2.38	0.41
1:C:470:GLN:HG3	2:D:1028:PHE:HE1	1.86	0.41
2:B:11:SER:CB	2:B:12:PRO:HA	2.51	0.41
2:B:35:VAL:CG1	2:B:36:ALA:H	2.30	0.41
2:B:254:TYR:O	2:B:258:THR:HB	2.21	0.41
2:B:423:ILE:HG23	2:B:426:ILE:HB	2.02	0.41
2:F:102:ILE:HG12	2:F:197:LEU:HD11	2.03	0.41
2:F:182:TYR:CE2	2:F:351:THR:HG22	2.56	0.41
2:F:185:PRO:O	2:F:188:GLU:N	2.53	0.41
1:A:15:ASP:HA	1:A:16:ARG:HA	1.75	0.41
1:A:143:ILE:CD1	1:A:491:THR:HG23	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1127:VAL:HG13	1:A:1151:ASN:O	2.21	0.41
1:A:1188:VAL:HG22	1:A:1201:PHE:CE1	2.55	0.41
1:C:436:PHE:CD1	1:C:437:VAL:N	2.83	0.41
1:C:1083:ASP:HB2	1:C:1128:LYS:HE3	2.03	0.41
1:E:416:VAL:HG13	1:E:420:GLY:CA	2.51	0.41
1:E:903:ASN:C	1:E:903:ASN:OD1	2.59	0.41
2:B:381:MET:HE3	2:B:471:GLN:HB3	2.03	0.41
2:B:681:SER:HB3	2:B:684:ASN:HD22	1.85	0.41
2:D:480:ILE:HG21	2:D:497:VAL:HG23	2.02	0.41
2:D:583:ILE:HD11	2:D:645:TYR:CE2	2.55	0.41
2:F:13:VAL:HG13	2:F:19:ALA:HA	2.03	0.41
1:A:962:THR:HA	1:A:972:LYS:HG2	2.03	0.41
1:A:989:LYS:HE2	1:A:1075:PHE:CE2	2.55	0.41
1:A:1137:THR:OG1	2:B:1109:ILE:HG21	2.21	0.41
1:A:1190:MET:CE	1:A:1199:MET:HB3	2.51	0.41
1:C:74:LEU:N	1:C:79:GLU:OE1	2.49	0.41
1:C:116:ASN:OD1	1:C:116:ASN:N	2.54	0.41
1:C:331:LEU:HB2	1:C:332:TYR:CD2	2.55	0.41
1:C:468:LEU:O	1:C:469:ASP:C	2.59	0.41
1:C:468:LEU:HD12	1:C:468:LEU:C	2.41	0.41
1:C:610:LEU:O	1:C:611:ASN:C	2.58	0.41
1:C:627:LEU:O	1:E:419:LYS:CG	2.69	0.41
1:C:641:LEU:HD12	1:E:614:ASN:ND2	2.35	0.41
1:C:645:ILE:HD12	1:C:785:TYR:HB2	2.03	0.41
1:C:769:TYR:O	1:C:772:LYS:HB2	2.21	0.41
1:E:192:PHE:CE1	1:E:204:GLN:HB3	2.56	0.41
1:E:220:GLY:HA2	1:E:225:LYS:HE3	2.03	0.41
1:E:382:VAL:HG11	1:E:868:TYR:CE1	2.56	0.41
1:E:468:LEU:O	1:E:469:ASP:C	2.60	0.41
1:E:773:LEU:O	1:E:774:ILE:C	2.59	0.41
1:E:912:TYR:CD1	1:E:912:TYR:N	2.87	0.41
1:E:929:LYS:HA	1:E:932:ASN:HB2	2.02	0.41
1:E:989:LYS:CG	1:E:1076:TRP:HA	2.50	0.41
2:B:197:LEU:N	2:B:197:LEU:HD12	2.36	0.41
2:B:491:SER:O	2:B:495:SER:N	2.54	0.41
2:B:789:TYR:CE2	2:B:793:LEU:CD1	3.03	0.41
2:B:1147:LEU:HD12	2:B:1147:LEU:N	2.36	0.41
2:D:105:ALA:HA	2:D:290:LYS:CD	2.50	0.41
2:D:108:PHE:CG	2:D:109:PRO:HD2	2.55	0.41
2:D:207:ASP:N	2:D:207:ASP:OD1	2.52	0.41
2:D:242:LEU:CD1	2:D:638:TRP:CG	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:453:ILE:CG1	2:D:454:THR:H	2.33	0.41
2:D:709:ASN:O	2:D:713:PHE:HD2	2.03	0.41
2:D:710:ILE:HG23	2:D:714:PHE:CE2	2.56	0.41
2:D:734:MET:HA	2:D:737:CYS:SG	2.60	0.41
2:D:855:THR:HA	2:D:966:ASP:O	2.20	0.41
2:D:1008:ARG:HD2	2:D:1012:GLU:HB3	2.02	0.41
2:F:27:ASP:N	2:F:27:ASP:OD1	2.54	0.41
2:F:35:VAL:CG1	2:F:36:ALA:H	2.31	0.41
2:F:106:ILE:N	2:F:290:LYS:HD3	2.36	0.41
2:F:146:ILE:HD13	2:F:330:TYR:CE2	2.56	0.41
2:F:552:LYS:C	2:F:713:PHE:HE1	2.24	0.41
2:F:709:ASN:O	2:F:710:ILE:C	2.60	0.41
2:F:832:ILE:H	2:F:832:ILE:HG13	1.75	0.41
1:A:778:LYS:HA	1:A:782:LEU:HD12	2.02	0.41
1:A:1067:PRO:O	1:A:1068:ASN:O	2.38	0.41
1:A:1143:ARG:O	1:A:1144:LYS:C	2.59	0.41
1:C:297:ASN:N	1:C:297:ASN:OD1	2.49	0.41
1:C:625:LEU:O	1:C:626:GLU:C	2.59	0.41
1:E:160:THR:HA	1:E:185:THR:O	2.21	0.41
1:E:452:LYS:CB	1:E:651:LYS:HE2	2.50	0.41
2:B:269:TYR:HE2	2:B:288:GLU:CG	2.34	0.41
2:B:502:ASN:O	2:B:505:MET:N	2.54	0.41
2:B:855:THR:HA	2:B:966:ASP:O	2.21	0.41
2:B:1098:ILE:HD12	2:B:1143:VAL:CG1	2.50	0.41
2:D:276:ASN:O	2:D:277:ASN:HB3	2.21	0.41
2:D:400:ASN:N	2:D:400:ASN:OD1	2.54	0.41
2:D:1069:GLN:O	2:D:1070:TYR:CD2	2.74	0.41
2:F:285:LEU:O	2:F:288:GLU:N	2.54	0.41
1:A:4:ILE:HD11	1:A:95:ASN:HB2	2.02	0.40
1:A:196:ASP:N	1:A:196:ASP:OD2	2.54	0.40
1:A:989:LYS:CG	1:A:1076:TRP:HA	2.50	0.40
1:C:225:LYS:HA	1:C:228:THR:OG1	2.21	0.40
1:E:20:TYR:HA	1:E:30:TYR:O	2.21	0.40
1:E:388:ASN:HB3	1:E:391:LEU:HB3	2.01	0.40
1:E:898:VAL:O	1:E:1030:LEU:HA	2.22	0.40
2:B:554:ILE:CG2	2:B:556:TRP:NE1	2.84	0.40
2:D:108:PHE:HB3	2:D:162:MET:CG	2.47	0.40
2:F:108:PHE:CG	2:F:109:PRO:HD2	2.56	0.40
2:F:254:TYR:O	2:F:258:THR:HB	2.21	0.40
2:F:428:LYS:C	2:F:430:PRO:CD	2.89	0.40
1:C:614:ASN:CB	1:C:617:GLN:OE1	2.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:833:ASP:HB3	1:C:835:ILE:HD12	2.03	0.40
2:B:429:ILE:N	2:B:430:PRO:HD3	2.34	0.40
2:B:470:LEU:HD11	2:B:654:LYS:HB3	2.04	0.40
2:D:497:VAL:HG12	2:D:498:TYR:N	2.35	0.40
2:F:583:ILE:HD11	2:F:645:TYR:CE2	2.56	0.40
2:F:854:PHE:HE2	2:F:970:LEU:HB2	1.87	0.40
2:F:880:THR:HB	2:F:901:ASN:HA	2.03	0.40
2:F:990:ASN:HB3	2:F:993:GLU:OE2	2.20	0.40
1:A:625:LEU:O	1:A:626:GLU:C	2.60	0.40
1:A:632:ILE:HG23	1:A:633:LEU:HG	2.02	0.40
1:A:926:TYR:HD1	1:A:1247:HIS:O	2.04	0.40
1:A:1213:GLY:HA3	1:A:1225:TYR:CE2	2.57	0.40
1:C:39:ILE:HG12	1:C:148:VAL:HB	2.04	0.40
1:C:305:GLU:OE1	1:C:305:GLU:HA	2.20	0.40
1:C:897:GLU:HG2	1:C:1032:LYS:HD3	2.04	0.40
1:C:903:ASN:OD1	1:C:904:ASP:N	2.54	0.40
1:E:1125:ILE:HD12	1:E:1125:ILE:HA	1.93	0.40
2:B:107:PRO:HG2	2:B:118:ARG:CB	2.50	0.40
2:B:553:ILE:CG2	2:B:554:ILE:N	2.83	0.40
2:D:197:LEU:HD12	2:D:197:LEU:N	2.36	0.40
2:D:709:ASN:O	2:D:710:ILE:C	2.60	0.40
2:F:205:PRO:CD	2:F:230:ILE:HD11	2.52	0.40
2:F:246:ASN:HA	2:F:247:PRO:HA	1.84	0.40
2:F:254:TYR:O	2:F:258:THR:CG2	2.69	0.40
2:F:298:ILE:HA	2:F:301:LEU:CD1	2.52	0.40
2:F:469:TYR:CE1	2:F:562:ASN:HB2	2.55	0.40
2:F:541:THR:O	2:F:542:GLN:HB3	2.21	0.40
1:A:467:ASP:OD1	1:A:467:ASP:C	2.58	0.40
1:A:614:ASN:HB2	1:A:617:GLN:HE22	1.86	0.40
1:A:833:ASP:HB3	1:A:835:ILE:HD12	2.03	0.40
1:A:1084:LYS:HB3	1:A:1086:TYR:CE2	2.57	0.40
1:C:824:PRO:HB2	2:D:952:ALA:HB2	2.03	0.40
1:C:937:TYR:CE1	1:C:954:LEU:HB2	2.57	0.40
1:E:216:HIS:CE1	1:E:254:THR:HG1	2.39	0.40
1:E:225:LYS:HA	1:E:228:THR:OG1	2.22	0.40
1:E:305:GLU:OE1	1:E:305:GLU:HA	2.21	0.40
1:E:789:VAL:HG12	1:E:793:LEU:HD12	2.03	0.40
1:E:920:TRP:O	1:E:1044:ILE:HA	2.21	0.40
2:B:589:ILE:HG13	2:B:641:TYR:OH	2.22	0.40
2:B:646:PHE:O	2:B:647:ASP:C	2.59	0.40
2:D:646:PHE:O	2:D:647:ASP:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1106:ASN:O	2:D:1107:ALA:C	2.59	0.40
2:F:99:LEU:C	2:F:101:LEU:N	2.75	0.40
2:F:828:TYR:HB2	2:F:829:PRO:HD2	2.04	0.40
1:A:39:ILE:HG12	1:A:148:VAL:HB	2.04	0.40
1:C:22:LYS:HG3	1:C:23:PRO:HD2	2.02	0.40
1:C:249:ILE:O	1:C:250:GLU:C	2.57	0.40
1:C:873:ASN:N	1:C:899:ASN:O	2.41	0.40
1:C:1163:TYR:CZ	1:C:1176:LYS:HB2	2.56	0.40
1:E:169:ASN:OD1	2:B:461:THR:HA	2.20	0.40
1:E:427:ILE:HD12	1:E:521:PHE:CD1	2.56	0.40
1:E:610:LEU:O	1:E:611:ASN:C	2.60	0.40
1:E:975:PHE:CE2	1:E:977:TYR:HB3	2.57	0.40
1:E:1000:LEU:N	1:E:1000:LEU:HD12	2.36	0.40
2:B:373:ILE:HG22	2:B:379:VAL:HG22	2.04	0.40
2:B:403:ILE:HA	2:B:404:PRO:HD3	1.95	0.40
2:B:654:LYS:HA	2:B:657:LEU:HD12	2.02	0.40
2:D:13:VAL:CG1	2:D:14:ASP:N	2.84	0.40
2:D:245:THR:HB	2:D:631:TYR:CE1	2.56	0.40
2:D:271:ILE:CG2	2:D:272:LYS:N	2.84	0.40
2:D:540:GLU:HB3	2:D:555:PRO:CD	2.52	0.40
2:D:589:ILE:HG13	2:D:641:TYR:OH	2.21	0.40
2:F:92:ASN:O	2:F:95:GLY:N	2.55	0.40
2:F:153:TYR:HB2	2:F:165:MET:O	2.21	0.40
2:F:579:PRO:C	2:F:581:SER:N	2.74	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ARG:NH2	1:C:420:GLY:O[3_564]	2.16	0.04

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	1225/1252 (98%)	999 (82%)	159 (13%)	67 (6%)	2 9
1	C	1225/1252 (98%)	995 (81%)	166 (14%)	64 (5%)	2 10
1	E	1225/1252 (98%)	997 (81%)	162 (13%)	66 (5%)	2 9
2	B	1084/1163 (93%)	832 (77%)	183 (17%)	69 (6%)	1 7
2	D	1084/1163 (93%)	835 (77%)	179 (16%)	70 (6%)	1 6
2	F	1084/1163 (93%)	838 (77%)	177 (16%)	69 (6%)	1 7
All	All	6927/7245 (96%)	5496 (79%)	1026 (15%)	405 (6%)	1 8

All (405) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	THR
1	A	199	ILE
1	A	291	VAL
1	A	419	LYS
1	A	449	ASN
1	A	469	ASP
1	A	483	LEU
1	A	485	ASP
1	A	490	LEU
1	A	499	PRO
1	A	738	TYR
1	A	740	ILE
1	A	743	ILE
1	A	928	ASN
1	A	978	GLY
1	A	979	ASN
1	A	1068	ASN
1	A	1074	ASP
1	A	1103	ASP
1	A	1104	SER
1	A	1109	ASN
1	A	1156	LYS
1	C	119	THR
1	C	199	ILE
1	C	291	VAL
1	C	419	LYS
1	C	449	ASN
1	C	469	ASP

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Mol	Chain	Res	Type
1	C	483	LEU
1	C	485	ASP
1	C	490	LEU
1	C	499	PRO
1	C	738	TYR
1	C	740	ILE
1	C	743	ILE
1	C	928	ASN
1	C	978	GLY
1	C	979	ASN
1	C	1068	ASN
1	C	1074	ASP
1	C	1103	ASP
1	C	1104	SER
1	C	1109	ASN
1	C	1156	LYS
1	E	119	THR
1	E	199	ILE
1	E	291	VAL
1	E	419	LYS
1	E	449	ASN
1	E	469	ASP
1	E	483	LEU
1	E	485	ASP
1	E	490	LEU
1	E	499	PRO
1	E	738	TYR
1	E	740	ILE
1	E	743	ILE
1	E	928	ASN
1	E	978	GLY
1	E	979	ASN
1	E	1068	ASN
1	E	1074	ASP
1	E	1103	ASP
1	E	1104	SER
1	E	1109	ASN
1	E	1156	LYS
2	B	9	ILE
2	B	10	ASP
2	B	36	ALA
2	B	37	PRO

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Mol	Chain	Res	Type
2	B	155	LYS
2	B	252	ASP
2	B	253	LYS
2	B	273	ILE
2	B	277	ASN
2	B	279	ILE
2	B	285	LEU
2	B	416	SER
2	B	439	PRO
2	B	480	ILE
2	B	604	LEU
2	B	709	ASN
2	B	848	ALA
2	B	856	ASN
2	B	861	ASN
2	B	914	ASN
2	B	991	SER
2	B	1057	LEU
2	B	1102	ASP
2	B	1107	ALA
2	B	1128	ASN
2	D	9	ILE
2	D	10	ASP
2	D	36	ALA
2	D	37	PRO
2	D	155	LYS
2	D	252	ASP
2	D	253	LYS
2	D	273	ILE
2	D	277	ASN
2	D	279	ILE
2	D	285	LEU
2	D	416	SER
2	D	439	PRO
2	D	480	ILE
2	D	604	LEU
2	D	709	ASN
2	D	848	ALA
2	D	856	ASN
2	D	861	ASN
2	D	914	ASN
2	D	991	SER

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Mol	Chain	Res	Type
2	D	1057	LEU
2	D	1102	ASP
2	D	1128	ASN
2	F	9	ILE
2	F	10	ASP
2	F	36	ALA
2	F	37	PRO
2	F	155	LYS
2	F	252	ASP
2	F	253	LYS
2	F	273	ILE
2	F	277	ASN
2	F	279	ILE
2	F	285	LEU
2	F	416	SER
2	F	439	PRO
2	F	480	ILE
2	F	604	LEU
2	F	709	ASN
2	F	848	ALA
2	F	856	ASN
2	F	861	ASN
2	F	914	ASN
2	F	991	SER
2	F	1057	LEU
2	F	1102	ASP
2	F	1107	ALA
2	F	1128	ASN
1	A	362	ASN
1	A	417	SER
1	A	420	GLY
1	A	444	ASN
1	A	530	GLU
1	A	569	ALA
1	A	611	ASN
1	A	728	LEU
1	A	731	LYS
1	A	739	ASP
1	A	742	GLN
1	A	819	LEU
1	A	835	ILE
1	A	1116	LEU

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Mol	Chain	Res	Type
1	A	1230	ARG
1	C	362	ASN
1	C	417	SER
1	C	420	GLY
1	C	444	ASN
1	C	530	GLU
1	C	569	ALA
1	C	611	ASN
1	C	728	LEU
1	C	731	LYS
1	C	739	ASP
1	C	742	GLN
1	C	819	LEU
1	C	835	ILE
1	C	1027	ASP
1	C	1116	LEU
1	C	1230	ARG
1	E	362	ASN
1	E	417	SER
1	E	420	GLY
1	E	444	ASN
1	E	530	GLU
1	E	569	ALA
1	E	611	ASN
1	E	728	LEU
1	E	731	LYS
1	E	739	ASP
1	E	742	GLN
1	E	819	LEU
1	E	835	ILE
1	E	1116	LEU
1	E	1230	ARG
2	B	15	ASN
2	B	81	ALA
2	B	114	THR
2	B	419	ASP
2	B	501	LEU
2	B	540	GLU
2	B	676	GLU
2	B	710	ILE
2	B	811	GLN
2	B	822	LYS

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Mol	Chain	Res	Type
2	B	947	ASP
2	B	1012	GLU
2	B	1014	ILE
2	D	15	ASN
2	D	81	ALA
2	D	114	THR
2	D	419	ASP
2	D	501	LEU
2	D	540	GLU
2	D	676	GLU
2	D	710	ILE
2	D	811	GLN
2	D	822	LYS
2	D	947	ASP
2	D	1012	GLU
2	D	1014	ILE
2	D	1107	ALA
2	F	15	ASN
2	F	81	ALA
2	F	114	THR
2	F	419	ASP
2	F	501	LEU
2	F	540	GLU
2	F	676	GLU
2	F	710	ILE
2	F	811	GLN
2	F	822	LYS
2	F	947	ASP
2	F	1012	GLU
2	F	1014	ILE
1	A	138	ASN
1	A	293	ASN
1	A	398	PRO
1	A	451	PRO
1	A	507	SER
1	A	583	PHE
1	A	648	PHE
1	A	666	ALA
1	A	1027	ASP
1	C	138	ASN
1	C	293	ASN
1	C	398	PRO

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Mol	Chain	Res	Type
1	C	451	PRO
1	C	507	SER
1	C	583	PHE
1	C	648	PHE
1	C	666	ALA
1	E	138	ASN
1	E	293	ASN
1	E	398	PRO
1	E	451	PRO
1	E	507	SER
1	E	583	PHE
1	E	648	PHE
1	E	666	ALA
1	E	1027	ASP
1	E	1083	ASP
2	B	16	LYS
2	B	113	ASN
2	B	153	TYR
2	B	154	LYS
2	B	276	ASN
2	B	542	GLN
2	B	857	ASP
2	B	922	ASN
2	B	924	SER
2	B	972	SER
2	B	1018	ASN
2	D	16	LYS
2	D	113	ASN
2	D	153	TYR
2	D	154	LYS
2	D	276	ASN
2	D	296	LYS
2	D	417	TYR
2	D	542	GLN
2	D	922	ASN
2	D	924	SER
2	D	972	SER
2	D	1018	ASN
2	F	16	LYS
2	F	113	ASN
2	F	154	LYS
2	F	276	ASN

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Mol	Chain	Res	Type
2	F	417	TYR
2	F	922	ASN
2	F	924	SER
2	F	972	SER
2	F	1018	ASN
1	A	454	ILE
1	A	488	LEU
1	A	498	ILE
1	A	913	LYS
1	A	915	PHE
1	A	927	ASP
1	A	1083	ASP
1	A	1117	LEU
1	C	454	ILE
1	C	488	LEU
1	C	498	ILE
1	C	913	LYS
1	C	927	ASP
1	C	1083	ASP
1	C	1117	LEU
1	E	468	LEU
1	E	498	ILE
1	E	913	LYS
1	E	927	ASP
1	E	988	ASN
2	B	66	SER
2	B	296	LYS
2	B	417	TYR
2	B	442	LYS
2	B	680	ILE
2	B	1093	THR
2	B	1140	TYR
2	B	1147	LEU
2	D	275	ASN
2	D	295	VAL
2	D	442	LYS
2	D	680	ILE
2	D	857	ASP
2	D	878	GLN
2	D	1093	THR
2	D	1140	TYR
2	D	1147	LEU

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Mol	Chain	Res	Type
2	F	153	TYR
2	F	275	ASN
2	F	295	VAL
2	F	296	LYS
2	F	442	LYS
2	F	542	GLN
2	F	857	ASP
2	F	1140	TYR
2	F	1147	LEU
1	A	146	PRO
1	A	292	SER
1	A	400	THR
1	A	468	LEU
1	A	791	THR
1	A	910	ASN
1	A	988	ASN
1	A	1139	ASP
1	C	50	THR
1	C	146	PRO
1	C	292	SER
1	C	468	LEU
1	C	791	THR
1	C	915	PHE
1	C	988	ASN
1	C	1094	PRO
1	E	146	PRO
1	E	292	SER
1	E	400	THR
1	E	454	ILE
1	E	488	LEU
1	E	791	THR
1	E	910	ASN
1	E	915	PHE
1	E	1094	PRO
1	E	1117	LEU
2	B	275	ASN
2	B	295	VAL
2	B	433	ASN
2	B	478	ASN
2	B	878	GLN
2	D	14	ASP
2	D	66	SER

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Mol	Chain	Res	Type
2	D	328	LYS
2	D	433	ASN
2	D	478	ASN
2	F	66	SER
2	F	433	ASN
2	F	478	ASN
2	F	680	ILE
2	F	878	GLN
2	F	1093	THR
1	A	1094	PRO
1	E	50	THR
2	B	14	ASP
2	B	328	LYS
2	B	429	ILE
2	B	1101	VAL
2	D	186	ALA
2	D	429	ILE
2	D	1101	VAL
2	F	14	ASP
2	F	328	LYS
2	F	1101	VAL
1	C	604	PRO
2	B	251	ILE
2	D	142	GLY
2	D	251	ILE
2	F	142	GLY
2	F	251	ILE
2	F	429	ILE
1	A	604	PRO
1	C	239	PRO
2	B	93	VAL
2	B	142	GLY
2	D	93	VAL
2	F	93	VAL
1	A	154	GLU
1	A	803	ILE
1	C	803	ILE
1	E	604	PRO
1	A	239	PRO
1	E	803	ILE
1	E	154	GLU

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	1125/1155 (97%)	1013 (90%)	112 (10%)	7	25
1	C	1125/1155 (97%)	1011 (90%)	114 (10%)	7	25
1	E	1125/1155 (97%)	1014 (90%)	111 (10%)	8	25
2	B	990/1103 (90%)	915 (92%)	75 (8%)	13	38
2	D	990/1103 (90%)	915 (92%)	75 (8%)	13	38
2	F	990/1103 (90%)	914 (92%)	76 (8%)	13	38
All	All	6345/6774 (94%)	5782 (91%)	563 (9%)	9	31

All (563) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ARG
1	A	17	THR
1	A	19	LEU
1	A	50	THR
1	A	53	GLN
1	A	65	ASP
1	A	93	ARG
1	A	108	SER
1	A	121	ASP
1	A	122	ASN
1	A	136	PHE
1	A	144	LEU
1	A	180	SER
1	A	191	SER
1	A	194	PHE
1	A	196	ASP
1	A	197	ASN
1	A	201	GLU
1	A	221	LEU
1	A	230	THR
1	A	258	ASN
1	A	270	ASP

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Mol	Chain	Res	Type
1	A	273	THR
1	A	278	ASP
1	A	281	LYS
1	A	290	GLN
1	A	301	ASP
1	A	305	GLU
1	A	326	ASP
1	A	336	GLU
1	A	348	ARG
1	A	354	GLN
1	A	402	ARG
1	A	421	ILE
1	A	428	GLU
1	A	436	PHE
1	A	440	GLU
1	A	441	ASN
1	A	443	TYR
1	A	447	ASN
1	A	455	ASP
1	A	456	ASP
1	A	464	TYR
1	A	465	GLU
1	A	468	LEU
1	A	475	PHE
1	A	486	GLU
1	A	487	LYS
1	A	491	THR
1	A	506	THR
1	A	515	ASN
1	A	532	GLU
1	A	554	PHE
1	A	591	SER
1	A	598	ASP
1	A	608	LEU
1	A	625	LEU
1	A	634	LEU
1	A	658	ASP
1	A	674	ARG
1	A	690	MET
1	A	696	GLN
1	A	703	GLN
1	A	705	TYR

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Mol	Chain	Res	Type
1	A	716	LYS
1	A	725	SER
1	A	733	GLU
1	A	734	LEU
1	A	735	THR
1	A	738	TYR
1	A	755	MET
1	A	781	LYS
1	A	795	ASN
1	A	821	ASN
1	A	838	SER
1	A	839	TYR
1	A	842	LYS
1	A	869	ASP
1	A	886	ASN
1	A	893	ASP
1	A	897	GLU
1	A	903	ASN
1	A	904	ASP
1	A	905	TYR
1	A	907	ILE
1	A	918	SER
1	A	930	ILE
1	A	938	THR
1	A	1002	ASP
1	A	1016	SER
1	A	1020	LEU
1	A	1027	ASP
1	A	1037	SER
1	A	1040	ARG
1	A	1045	ARG
1	A	1052	LYS
1	A	1053	GLU
1	A	1083	ASP
1	A	1088	LEU
1	A	1099	ASP
1	A	1103	ASP
1	A	1104	SER
1	A	1105	THR
1	A	1134	ASN
1	A	1143	ARG
1	A	1169	THR

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Mol	Chain	Res	Type
1	A	1170	ASN
1	A	1197	CYS
1	A	1205	ASN
1	A	1217	ASP
1	A	1230	ARG
1	A	1250	GLN
1	C	16	ARG
1	C	17	THR
1	C	19	LEU
1	C	50	THR
1	C	53	GLN
1	C	65	ASP
1	C	93	ARG
1	C	108	SER
1	C	121	ASP
1	C	122	ASN
1	C	136	PHE
1	C	144	LEU
1	C	180	SER
1	C	191	SER
1	C	194	PHE
1	C	196	ASP
1	C	197	ASN
1	C	201	GLU
1	C	221	LEU
1	C	230	THR
1	C	258	ASN
1	C	270	ASP
1	C	273	THR
1	C	278	ASP
1	C	281	LYS
1	C	290	GLN
1	C	301	ASP
1	C	305	GLU
1	C	326	ASP
1	C	336	GLU
1	C	348	ARG
1	C	354	GLN
1	C	402	ARG
1	C	421	ILE
1	C	422	ARG
1	C	428	GLU

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Mol	Chain	Res	Type
1	C	436	PHE
1	C	440	GLU
1	C	441	ASN
1	C	443	TYR
1	C	447	ASN
1	C	456	ASP
1	C	464	TYR
1	C	465	GLU
1	C	468	LEU
1	C	475	PHE
1	C	486	GLU
1	C	487	LYS
1	C	491	THR
1	C	506	THR
1	C	515	ASN
1	C	532	GLU
1	C	554	PHE
1	C	591	SER
1	C	598	ASP
1	C	608	LEU
1	C	625	LEU
1	C	634	LEU
1	C	658	ASP
1	C	690	MET
1	C	696	GLN
1	C	703	GLN
1	C	705	TYR
1	C	716	LYS
1	C	725	SER
1	C	733	GLU
1	C	734	LEU
1	C	735	THR
1	C	738	TYR
1	C	755	MET
1	C	781	LYS
1	C	795	ASN
1	C	821	ASN
1	C	831	THR
1	C	838	SER
1	C	839	TYR
1	C	842	LYS
1	C	869	ASP

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Mol	Chain	Res	Type
1	C	886	ASN
1	C	893	ASP
1	C	897	GLU
1	C	903	ASN
1	C	904	ASP
1	C	905	TYR
1	C	907	ILE
1	C	918	SER
1	C	930	ILE
1	C	938	THR
1	C	1002	ASP
1	C	1016	SER
1	C	1020	LEU
1	C	1027	ASP
1	C	1037	SER
1	C	1040	ARG
1	C	1045	ARG
1	C	1052	LYS
1	C	1053	GLU
1	C	1083	ASP
1	C	1088	LEU
1	C	1099	ASP
1	C	1103	ASP
1	C	1104	SER
1	C	1105	THR
1	C	1134	ASN
1	C	1143	ARG
1	C	1146	ASP
1	C	1169	THR
1	C	1170	ASN
1	C	1183	ARG
1	C	1197	CYS
1	C	1205	ASN
1	C	1217	ASP
1	C	1230	ARG
1	C	1250	GLN
1	E	16	ARG
1	E	17	THR
1	E	19	LEU
1	E	50	THR
1	E	53	GLN
1	E	65	ASP

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Mol	Chain	Res	Type
1	E	93	ARG
1	E	108	SER
1	E	121	ASP
1	E	122	ASN
1	E	136	PHE
1	E	144	LEU
1	E	180	SER
1	E	191	SER
1	E	194	PHE
1	E	196	ASP
1	E	197	ASN
1	E	201	GLU
1	E	221	LEU
1	E	230	THR
1	E	258	ASN
1	E	273	THR
1	E	278	ASP
1	E	281	LYS
1	E	290	GLN
1	E	305	GLU
1	E	326	ASP
1	E	336	GLU
1	E	348	ARG
1	E	354	GLN
1	E	367	SER
1	E	402	ARG
1	E	421	ILE
1	E	422	ARG
1	E	428	GLU
1	E	436	PHE
1	E	440	GLU
1	E	441	ASN
1	E	443	TYR
1	E	447	ASN
1	E	455	ASP
1	E	456	ASP
1	E	464	TYR
1	E	465	GLU
1	E	468	LEU
1	E	475	PHE
1	E	486	GLU
1	E	487	LYS

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Mol	Chain	Res	Type
1	E	491	THR
1	E	506	THR
1	E	532	GLU
1	E	554	PHE
1	E	591	SER
1	E	598	ASP
1	E	608	LEU
1	E	625	LEU
1	E	634	LEU
1	E	658	ASP
1	E	690	MET
1	E	696	GLN
1	E	703	GLN
1	E	705	TYR
1	E	716	LYS
1	E	725	SER
1	E	733	GLU
1	E	734	LEU
1	E	735	THR
1	E	738	TYR
1	E	755	MET
1	E	781	LYS
1	E	795	ASN
1	E	821	ASN
1	E	838	SER
1	E	839	TYR
1	E	842	LYS
1	E	869	ASP
1	E	886	ASN
1	E	893	ASP
1	E	897	GLU
1	E	903	ASN
1	E	904	ASP
1	E	905	TYR
1	E	907	ILE
1	E	918	SER
1	E	930	ILE
1	E	938	THR
1	E	1002	ASP
1	E	1016	SER
1	E	1020	LEU
1	E	1027	ASP

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Mol	Chain	Res	Type
1	E	1037	SER
1	E	1040	ARG
1	E	1045	ARG
1	E	1052	LYS
1	E	1053	GLU
1	E	1083	ASP
1	E	1088	LEU
1	E	1099	ASP
1	E	1103	ASP
1	E	1104	SER
1	E	1105	THR
1	E	1128	LYS
1	E	1134	ASN
1	E	1143	ARG
1	E	1169	THR
1	E	1170	ASN
1	E	1197	CYS
1	E	1205	ASN
1	E	1217	ASP
1	E	1230	ARG
1	E	1250	GLN
2	B	14	ASP
2	B	23	SER
2	B	41	ILE
2	B	63	ILE
2	B	68	PHE
2	B	70	SER
2	B	152	TYR
2	B	153	TYR
2	B	179	ASP
2	B	207	ASP
2	B	248	TYR
2	B	253	LYS
2	B	267	ASN
2	B	272	LYS
2	B	291	PHE
2	B	300	GLU
2	B	304	SER
2	B	319	ASN
2	B	335	TYR
2	B	351	THR
2	B	400	ASN

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Mol	Chain	Res	Type
2	B	435	GLU
2	B	438	TYR
2	B	453	ILE
2	B	481	ASN
2	B	483	SER
2	B	484	SER
2	B	491	SER
2	B	499	SER
2	B	504	THR
2	B	518	ASP
2	B	566	THR
2	B	570	PHE
2	B	580	ILE
2	B	588	ASN
2	B	593	LYS
2	B	601	SER
2	B	620	CYS
2	B	643	SER
2	B	656	VAL
2	B	678	SER
2	B	697	ARG
2	B	754	ASN
2	B	756	ASN
2	B	787	ASN
2	B	791	GLU
2	B	793	LEU
2	B	830	LYS
2	B	845	LEU
2	B	856	ASN
2	B	863	LEU
2	B	865	ASN
2	B	876	LEU
2	B	899	PHE
2	B	910	ASP
2	B	928	TRP
2	B	954	GLU
2	B	958	GLU
2	B	969	SER
2	B	974	ASN
2	B	986	ASN
2	B	987	LYS
2	B	1002	LEU

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Mol	Chain	Res	Type
2	B	1013	GLU
2	B	1024	PHE
2	B	1030	GLU
2	B	1075	ASP
2	B	1095	ASN
2	B	1097	ARG
2	B	1140	TYR
2	B	1142	TRP
2	B	1145	CYS
2	B	1147	LEU
2	B	1148	ASN
2	B	1158	TRP
2	D	14	ASP
2	D	23	SER
2	D	41	ILE
2	D	63	ILE
2	D	68	PHE
2	D	70	SER
2	D	152	TYR
2	D	153	TYR
2	D	207	ASP
2	D	248	TYR
2	D	253	LYS
2	D	258	THR
2	D	267	ASN
2	D	272	LYS
2	D	291	PHE
2	D	300	GLU
2	D	304	SER
2	D	319	ASN
2	D	335	TYR
2	D	351	THR
2	D	400	ASN
2	D	438	TYR
2	D	445	ASP
2	D	453	ILE
2	D	481	ASN
2	D	483	SER
2	D	484	SER
2	D	491	SER
2	D	499	SER
2	D	504	THR

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Mol	Chain	Res	Type
2	D	518	ASP
2	D	566	THR
2	D	570	PHE
2	D	580	ILE
2	D	588	ASN
2	D	593	LYS
2	D	601	SER
2	D	620	CYS
2	D	643	SER
2	D	656	VAL
2	D	678	SER
2	D	697	ARG
2	D	703	SER
2	D	754	ASN
2	D	756	ASN
2	D	787	ASN
2	D	791	GLU
2	D	793	LEU
2	D	830	LYS
2	D	845	LEU
2	D	863	LEU
2	D	865	ASN
2	D	876	LEU
2	D	899	PHE
2	D	910	ASP
2	D	928	TRP
2	D	954	GLU
2	D	958	GLU
2	D	969	SER
2	D	974	ASN
2	D	986	ASN
2	D	987	LYS
2	D	1002	LEU
2	D	1013	GLU
2	D	1024	PHE
2	D	1030	GLU
2	D	1075	ASP
2	D	1095	ASN
2	D	1097	ARG
2	D	1140	TYR
2	D	1142	TRP
2	D	1145	CYS

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Mol	Chain	Res	Type
2	D	1147	LEU
2	D	1148	ASN
2	D	1158	TRP
2	F	14	ASP
2	F	23	SER
2	F	41	ILE
2	F	56	ASP
2	F	63	ILE
2	F	68	PHE
2	F	70	SER
2	F	74	GLU
2	F	152	TYR
2	F	153	TYR
2	F	207	ASP
2	F	248	TYR
2	F	253	LYS
2	F	267	ASN
2	F	272	LYS
2	F	291	PHE
2	F	300	GLU
2	F	304	SER
2	F	319	ASN
2	F	335	TYR
2	F	351	THR
2	F	400	ASN
2	F	438	TYR
2	F	445	ASP
2	F	453	ILE
2	F	481	ASN
2	F	483	SER
2	F	484	SER
2	F	491	SER
2	F	499	SER
2	F	504	THR
2	F	518	ASP
2	F	566	THR
2	F	570	PHE
2	F	580	ILE
2	F	588	ASN
2	F	593	LYS
2	F	601	SER
2	F	620	CYS

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Mol	Chain	Res	Type
2	F	643	SER
2	F	656	VAL
2	F	678	SER
2	F	697	ARG
2	F	754	ASN
2	F	756	ASN
2	F	791	GLU
2	F	793	LEU
2	F	830	LYS
2	F	845	LEU
2	F	855	THR
2	F	856	ASN
2	F	863	LEU
2	F	865	ASN
2	F	876	LEU
2	F	899	PHE
2	F	910	ASP
2	F	928	TRP
2	F	954	GLU
2	F	958	GLU
2	F	969	SER
2	F	974	ASN
2	F	986	ASN
2	F	987	LYS
2	F	1002	LEU
2	F	1013	GLU
2	F	1024	PHE
2	F	1030	GLU
2	F	1075	ASP
2	F	1095	ASN
2	F	1097	ARG
2	F	1140	TYR
2	F	1142	TRP
2	F	1145	CYS
2	F	1147	LEU
2	F	1148	ASN
2	F	1158	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (110) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	ASN

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Mol	Chain	Res	Type
1	A	122	ASN
1	A	125	HIS
1	A	195	ASN
1	A	197	ASN
1	A	204	GLN
1	A	235	GLN
1	A	261	ASN
1	A	379	ASN
1	A	441	ASN
1	A	661	ASN
1	A	669	ASN
1	A	711	GLN
1	A	957	ASN
1	A	1060	GLN
1	A	1170	ASN
1	A	1228	HIS
1	C	111	ASN
1	C	122	ASN
1	C	125	HIS
1	C	195	ASN
1	C	197	ASN
1	C	235	GLN
1	C	261	ASN
1	C	379	ASN
1	C	441	ASN
1	C	661	ASN
1	C	669	ASN
1	C	841	ASN
1	C	932	ASN
1	C	956	HIS
1	C	957	ASN
1	C	1060	GLN
1	C	1170	ASN
1	E	111	ASN
1	E	122	ASN
1	E	125	HIS
1	E	142	HIS
1	E	195	ASN
1	E	197	ASN
1	E	204	GLN
1	E	235	GLN
1	E	261	ASN

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Mol	Chain	Res	Type
1	E	379	ASN
1	E	441	ASN
1	E	661	ASN
1	E	669	ASN
1	E	711	GLN
1	E	932	ASN
1	E	956	HIS
1	E	957	ASN
1	E	1060	GLN
1	E	1170	ASN
1	E	1228	HIS
2	B	67	ASN
2	B	171	GLN
2	B	208	ASN
2	B	289	GLN
2	B	324	HIS
2	B	377	ASN
2	B	452	ASN
2	B	636	GLN
2	B	644	GLN
2	B	677	ASN
2	B	684	ASN
2	B	704	GLN
2	B	762	HIS
2	B	849	ASN
2	B	865	ASN
2	B	1003	ASN
2	B	1034	ASN
2	B	1130	ASN
2	B	1137	ASN
2	D	67	ASN
2	D	171	GLN
2	D	208	ASN
2	D	289	GLN
2	D	324	HIS
2	D	452	ASN
2	D	636	GLN
2	D	644	GLN
2	D	677	ASN
2	D	684	ASN
2	D	704	GLN
2	D	762	HIS

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Mol	Chain	Res	Type
2	D	849	ASN
2	D	865	ASN
2	D	925	ASN
2	D	1003	ASN
2	D	1034	ASN
2	D	1130	ASN
2	D	1137	ASN
2	F	67	ASN
2	F	92	ASN
2	F	171	GLN
2	F	208	ASN
2	F	289	GLN
2	F	324	HIS
2	F	452	ASN
2	F	636	GLN
2	F	644	GLN
2	F	677	ASN
2	F	684	ASN
2	F	704	GLN
2	F	762	HIS
2	F	865	ASN
2	F	1003	ASN
2	F	1034	ASN
2	F	1130	ASN
2	F	1137	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	1235/1252 (98%)	-0.69	1 (0%)	95	91	53, 120, 189, 296	0
1	C	1235/1252 (98%)	-0.66	3 (0%)	95	89	46, 129, 207, 364	0
1	E	1235/1252 (98%)	-0.67	5 (0%)	92	82	62, 143, 214, 391	0
2	B	1114/1163 (95%)	-0.69	1 (0%)	95	91	37, 109, 179, 274	0
2	D	1114/1163 (95%)	-0.68	4 (0%)	92	82	48, 129, 194, 278	0
2	F	1114/1163 (95%)	-0.61	10 (0%)	84	66	51, 143, 220, 328	0
All	All	7047/7245 (97%)	-0.67	24 (0%)	94	85	37, 129, 203, 391	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	657	SER	9.4
1	E	655	GLY	7.5
1	E	657	SER	7.4
2	B	275	ASN	6.8
1	E	656	SER	4.7
2	F	852	ILE	4.4
1	E	658	ASP	4.2
1	C	656	SER	3.9
2	F	434	ASP	3.7
2	F	1158	TRP	3.4
1	C	803	ILE	3.4
1	E	420	GLY	3.2
2	F	843	ILE	3.2
1	A	498	ILE	2.9
2	D	275	ASN	2.8
2	F	275	ASN	2.3
2	F	279	ILE	2.2
2	F	278	TYR	2.2
2	F	380	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	843	ILE	2.1
2	D	1158	TRP	2.1
2	F	873	LEU	2.1
2	F	979	ILE	2.0
2	D	863	LEU	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	C	1301	1/1	0.98	0.17	83,83,83,83	0
3	ZN	E	1301	1/1	0.98	0.14	99,99,99,99	0
3	ZN	A	1301	1/1	0.99	0.18	86,86,86,86	0

6.5 Other polymers (i)

There are no such residues in this entry.