Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 03:40 PM BST

PDB ID	:	6S3U
Title	:	Adhesin P140 from Mycoplasma Genitalium
Authors	:	Fita, I.; Aparicio, D.
Deposited on	:	2019-06-26
Resolution	:	3.24 Å(reported)

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

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

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

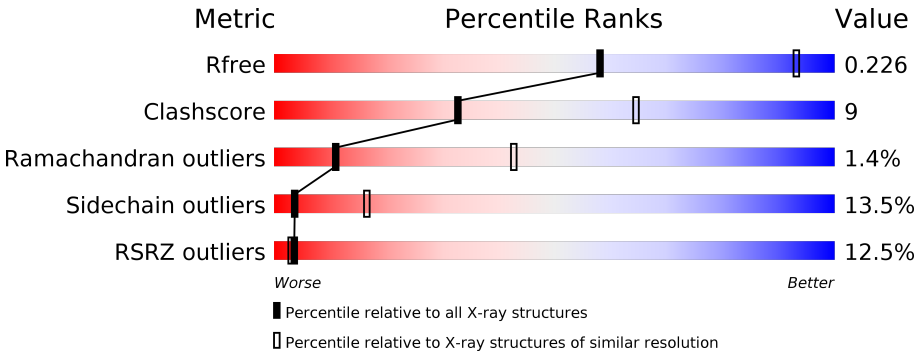
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 3.24 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	1619 (3.28-3.20)
Clashscore	141614	1755 (3.28-3.20)
Ramachandran outliers	138981	1728 (3.28-3.20)
Sidechain outliers	138945	1727 (3.28-3.20)
RSRZ outliers	127900	1567 (3.28-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1304	68% 26%
1	B	1304	68% 26%
1	C	1304	70% 25%
1	D	1304	69% 24%
1	E	1304	34% 69% 24%
1	F	1304	33% 69% 24%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 59767 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 Adhesin P1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1278	Total	C	N	O	S	0	0	0
			10016	6351	1692	1960	13			
1	B	1275	Total	C	N	O	S	0	0	0
			9999	6340	1689	1957	13			
1	C	1274	Total	C	N	O	S	0	0	0
			9993	6339	1688	1953	13			
1	D	1271	Total	C	N	O	S	0	0	0
			9976	6328	1685	1950	13			
1	E	1262	Total	C	N	O	S	0	0	0
			9886	6272	1666	1935	13			
1	F	1262	Total	C	N	O	S	0	0	0
			9897	6281	1668	1935	13			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1352	HIS	-	expression tag	UNP P20796
A	1353	HIS	-	expression tag	UNP P20796
A	1354	HIS	-	expression tag	UNP P20796
A	1355	HIS	-	expression tag	UNP P20796
A	1356	HIS	-	expression tag	UNP P20796
A	1357	HIS	-	expression tag	UNP P20796
B	1352	HIS	-	expression tag	UNP P20796
B	1353	HIS	-	expression tag	UNP P20796
B	1354	HIS	-	expression tag	UNP P20796
B	1355	HIS	-	expression tag	UNP P20796
B	1356	HIS	-	expression tag	UNP P20796
B	1357	HIS	-	expression tag	UNP P20796
C	1352	HIS	-	expression tag	UNP P20796
C	1353	HIS	-	expression tag	UNP P20796
C	1354	HIS	-	expression tag	UNP P20796
C	1355	HIS	-	expression tag	UNP P20796
C	1356	HIS	-	expression tag	UNP P20796

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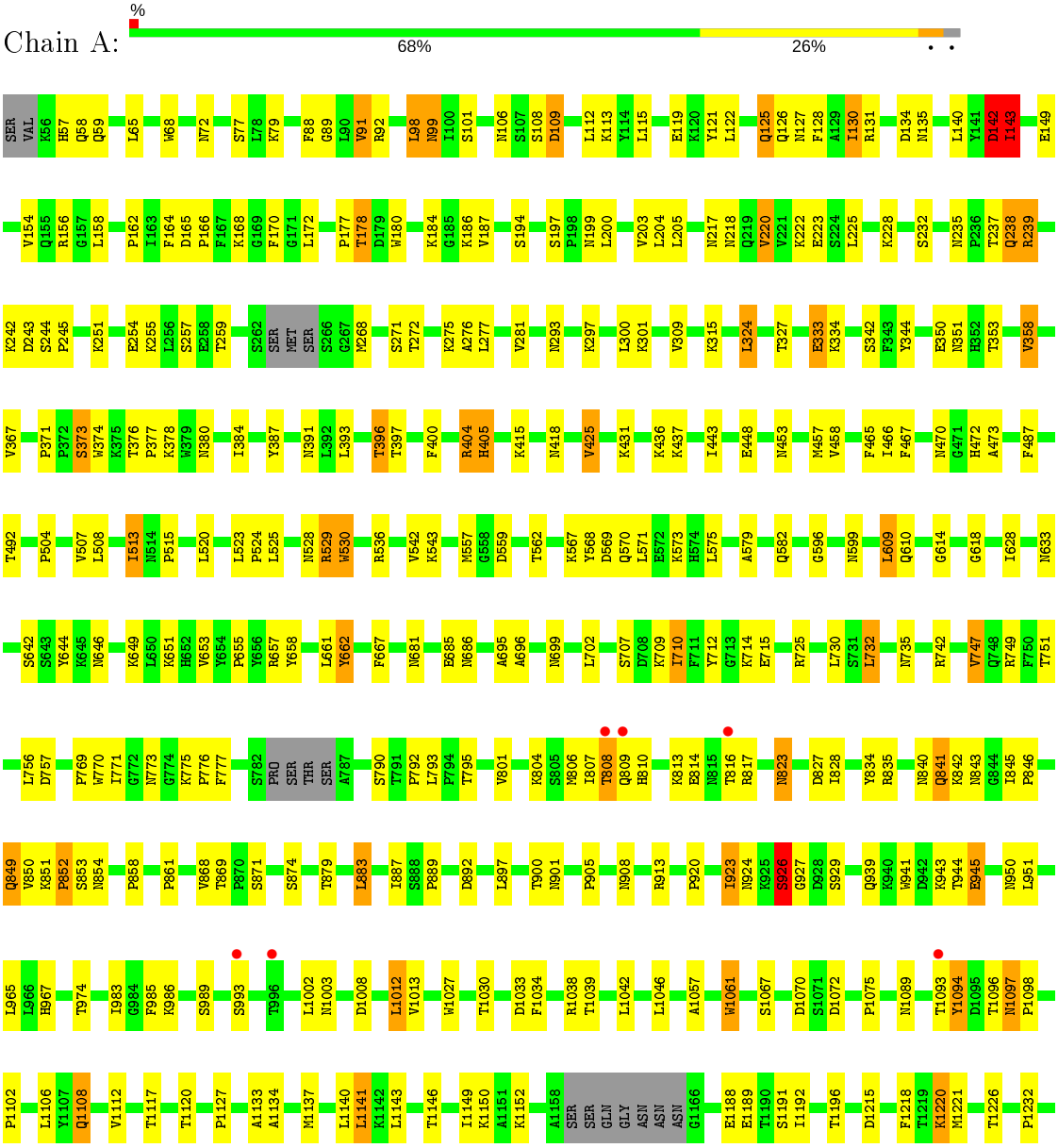
Chain	Residue	Modelled	Actual	Comment	Reference
C	1357	HIS	-	expression tag	UNP P20796
D	1352	HIS	-	expression tag	UNP P20796
D	1353	HIS	-	expression tag	UNP P20796
D	1354	HIS	-	expression tag	UNP P20796
D	1355	HIS	-	expression tag	UNP P20796
D	1356	HIS	-	expression tag	UNP P20796
D	1357	HIS	-	expression tag	UNP P20796
E	1352	HIS	-	expression tag	UNP P20796
E	1353	HIS	-	expression tag	UNP P20796
E	1354	HIS	-	expression tag	UNP P20796
E	1355	HIS	-	expression tag	UNP P20796
E	1356	HIS	-	expression tag	UNP P20796
E	1357	HIS	-	expression tag	UNP P20796
F	1352	HIS	-	expression tag	UNP P20796
F	1353	HIS	-	expression tag	UNP P20796
F	1354	HIS	-	expression tag	UNP P20796
F	1355	HIS	-	expression tag	UNP P20796
F	1356	HIS	-	expression tag	UNP P20796
F	1357	HIS	-	expression tag	UNP P20796

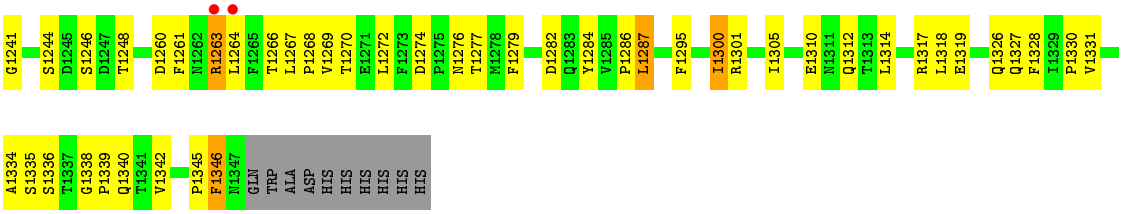
3 Residue-property plots (i)

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: Adhesin P1

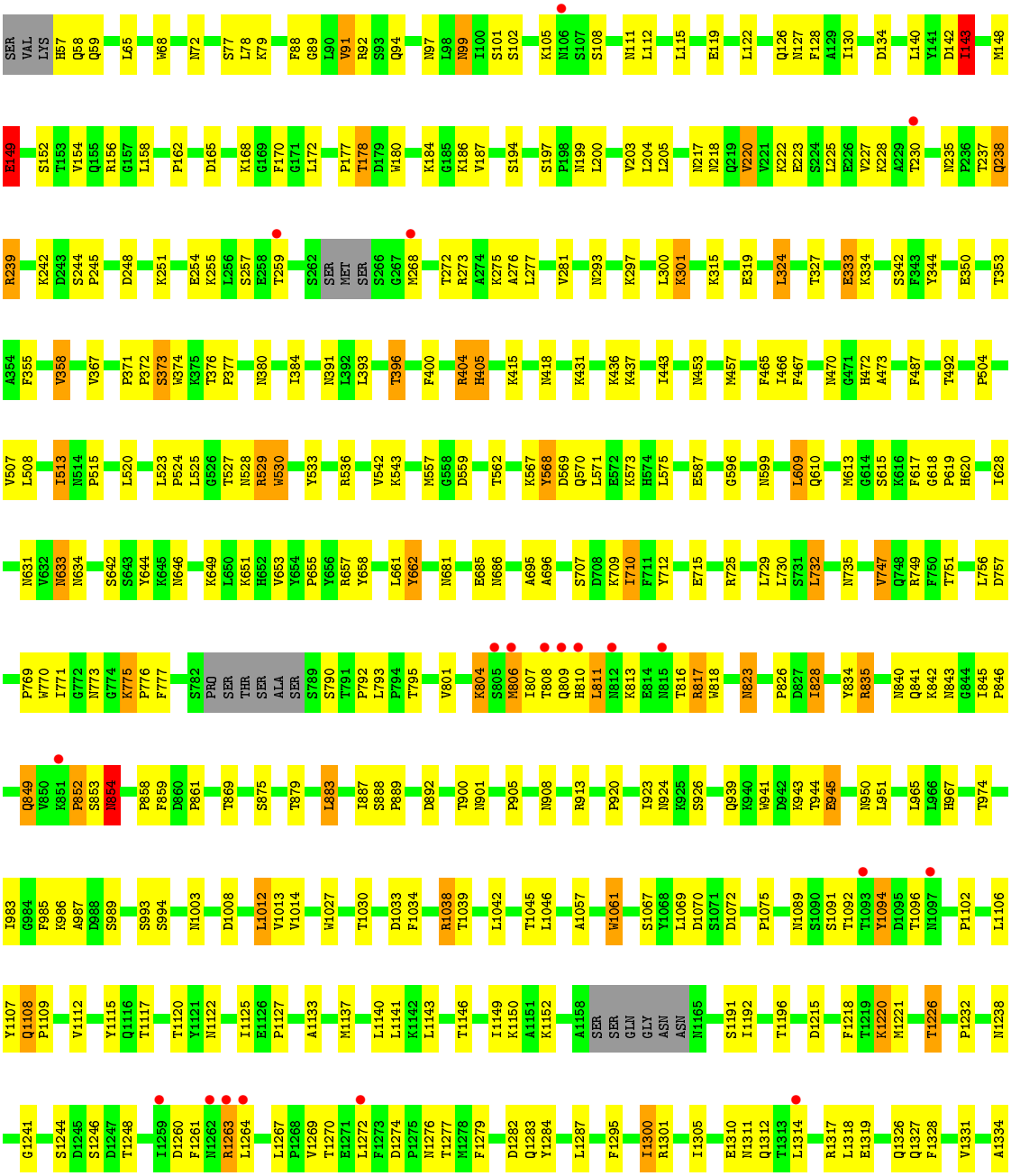
Chain A:

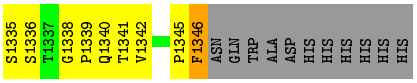




- Molecule 1: Adhesin P1

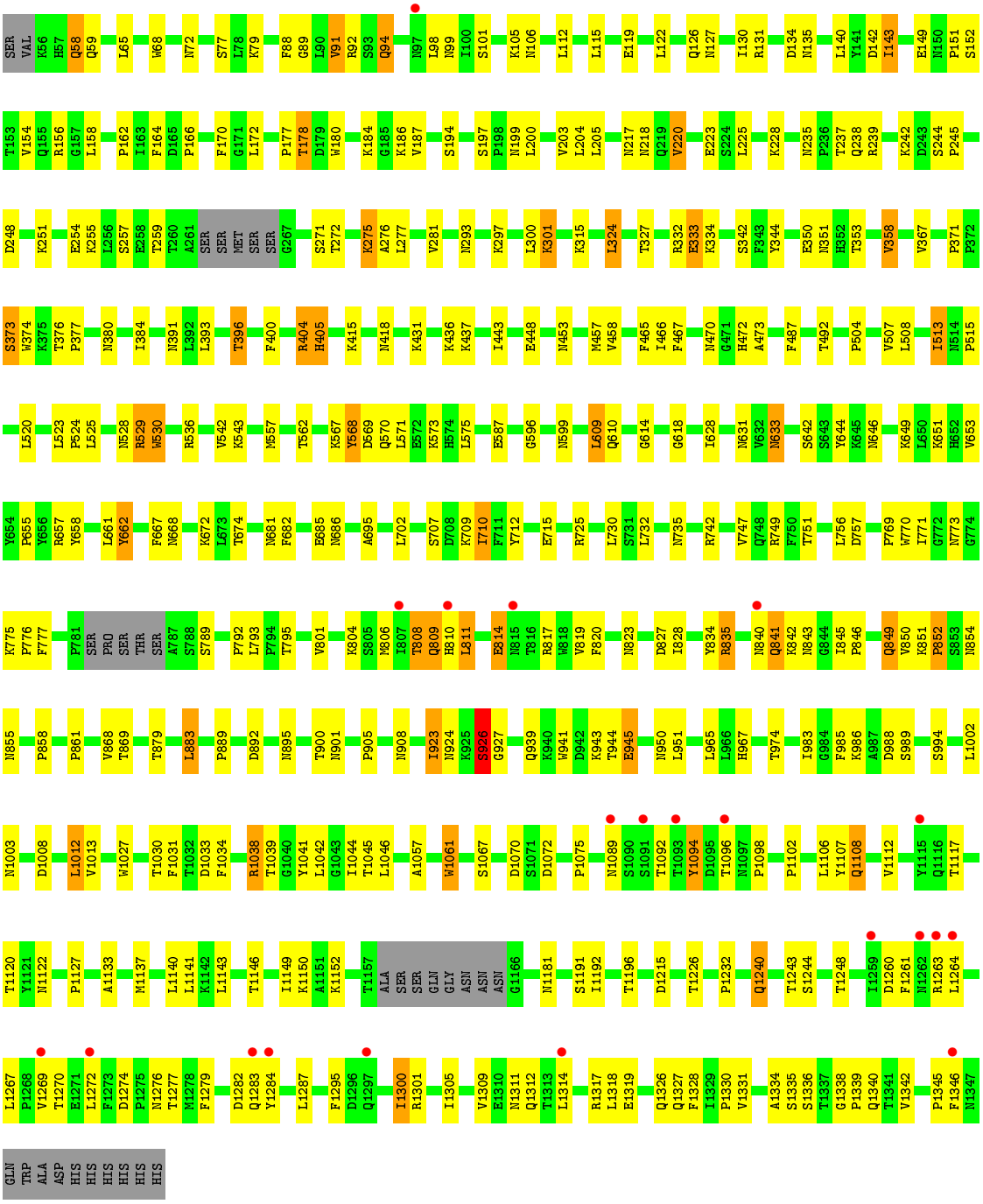
Chain B:





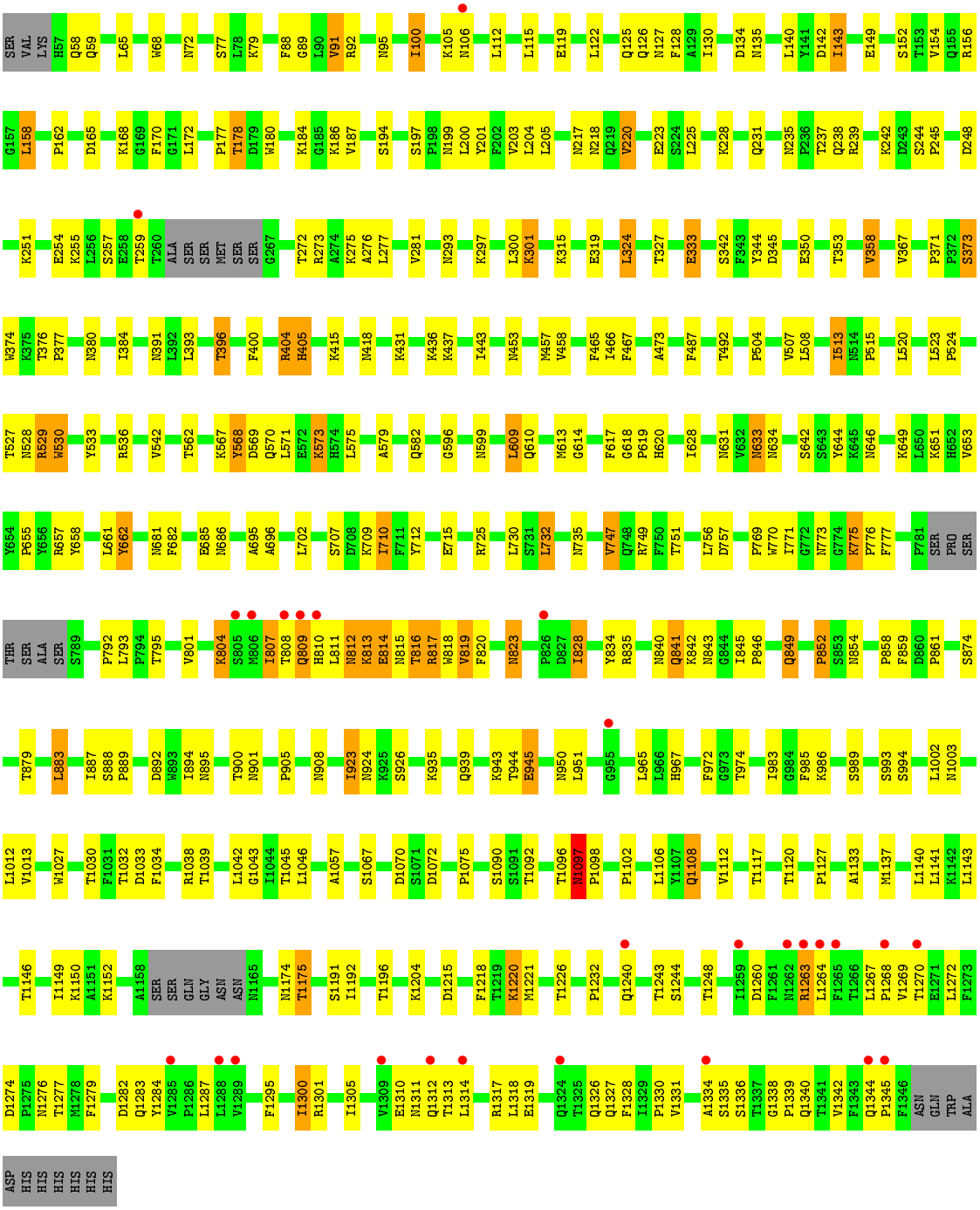
- Molecule 1: Adhesin P1

Chain C:



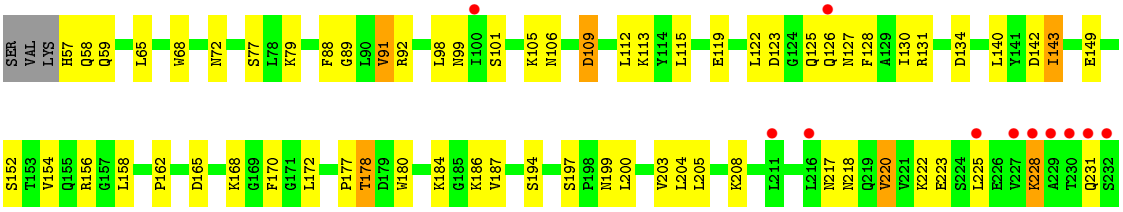
- Molecule 1: Adhesin P1

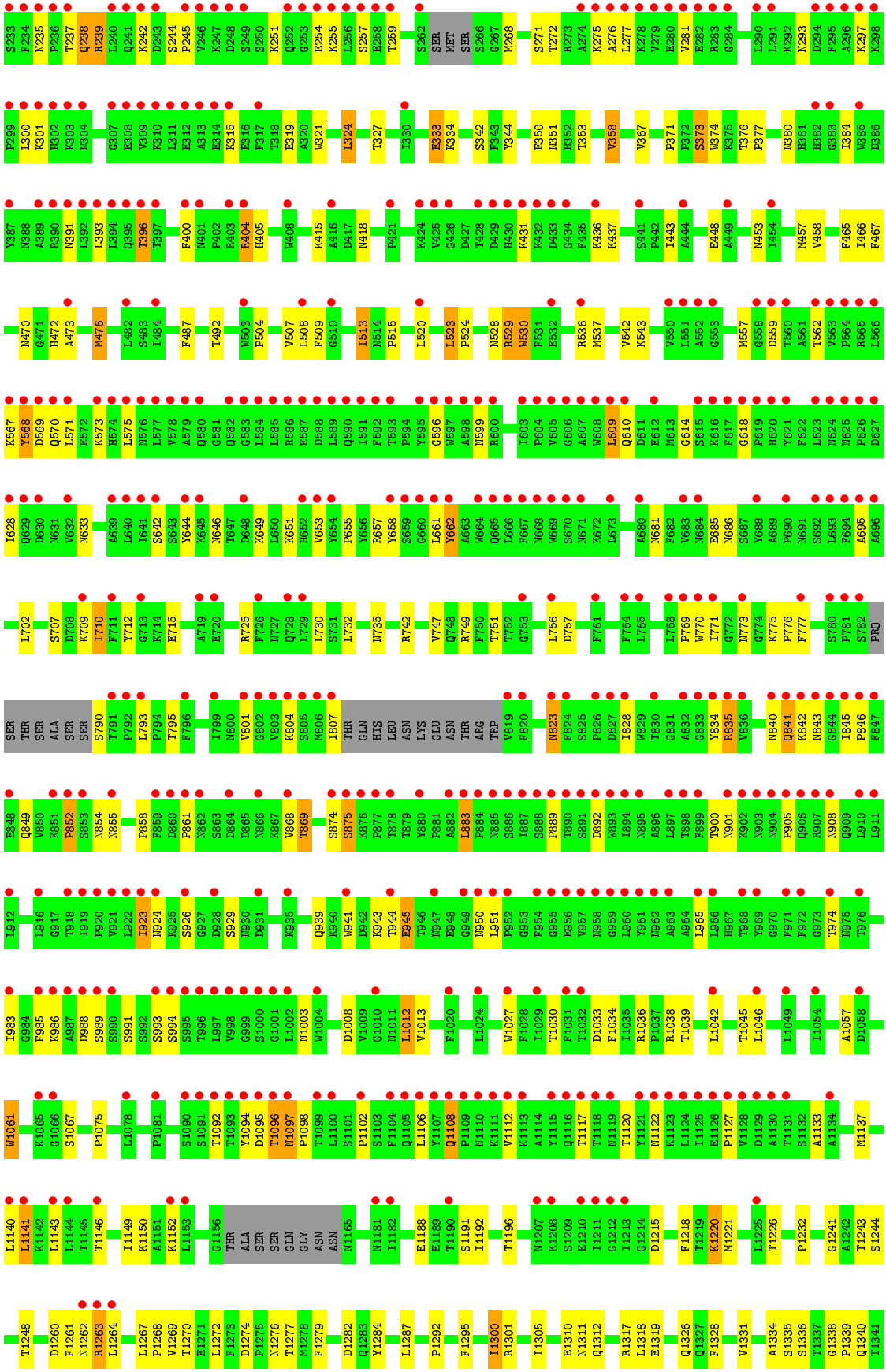
Chain D:



- Molecule 1: Adhesin P1

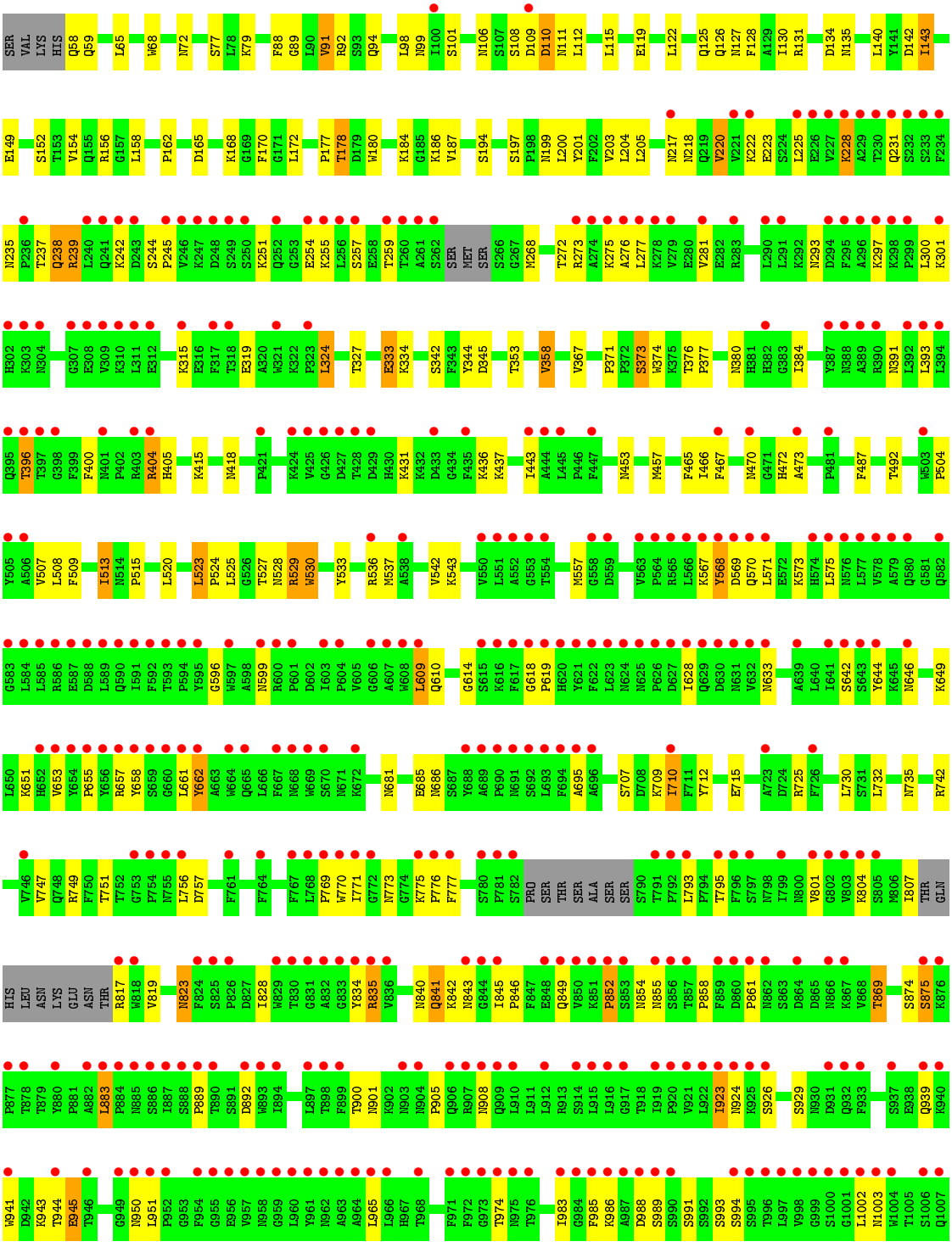
Chain E:

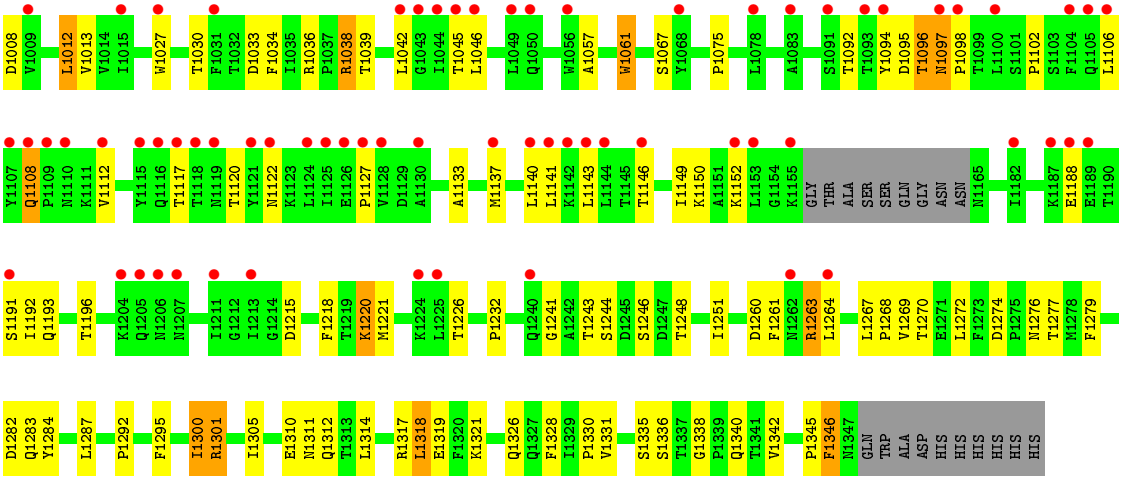



S233 F234 N235 P236 T237 Q238 R239 L240 Q241 K242 D243 S244 P245 V246 K247 D248 S249 S250 K251 Q252 G253 E254 K255 L256 S257 E258 T259 S262 SER MET SER S266 G267 M268 S271 T272 R273 A274 K275 A276 L277 K278 V279 E280 V281 E282 R283 G284 L290 L291 K292 N293 D294 F295 A296 K297 K298
P299 L300 K301 H302 K303 N304 G307 E308 V309 K310 L311 E312 A313 E314 K315 E316 F317 T318 E319 A320 W321 L324 T327 I330 E333 K334 S342 F343 Y344 E350 N351 H352 T353 V358 V367 P371 P372 S373 W374 K375 T376 P377 N380 H381 H382 G383 I384 W385 D386
Y387 N388 A389 R390 N391 L392 L393 L394 Q395 T396 T397 P400 N401 P402 R403 R404 H405 W408 K415 A416 D417 N418 P421 K424 V425 G426 D427 T428 D429 H430 K431 K432 D433 G434 F435 K436 K437 S441 P442 I443 A444 E448 A449 N453 I454 N457 V458 F465 I466 F467
N470 G471 H472 A473 M476 L482 S483 I484 F487 T492 W503 P504 V507 L508 F509 G510 I513 N514 P515 L520 L523 P524 N528 R529 W530 F531 E532 R536 M537 V542 K543 V550 L551 A552 G553 M557 G558 D559 T560 A561 T562 V563 P564 R565 L566
K567 Y568 D569 Q570 L571 E572 K573 H574 L575 N576 L577 V578 A579 Q580 G581 Q582 G583 L584 L585 R586 E587 D588 L589 Q590 I591 F592 T593 P594 Y595 G596 W597 A598 N599 R600 I603 P604 V605 G606 A607 W608 L609 Q610 D611 E612 H613 G614 S615 K616 F617 G618 P619 H620 Y621 F622 L623 N624 N625 P626 D627
I628 D629 M630 N631 V632 M633 A639 L640 I641 S642 S643 Y644 K645 W646 T647 D648 K649 L650 K651 H652 V653 Y654 P655 Y656 R657 Y658 S659 G660 L661 V662 A663 W664 Q665 L666 F667 N668 W669 S670 N671 K672 L673 A680 V681 F682 V683 N684 B685 N686 S687 Y688 A689 P690 H691 S692 L693 F694 A695 A696
L702 S707 D708 K709 I710 F711 Y712 G713 K714 E715 A719 E720 R725 F726 N727 Q728 L729 L730 S731 L732 N735 R742 V747 Q748 R749 F750 T751 T752 G753 L756 D757 F761 F764 L765 L768 P769 W770 T771 G772 N773 G774 K775 P776 F777 S780 P781 S782 PRO
SER THR SER ALA SER SER S790 T791 P792 L793 P794 T795 F796 I799 N800 V801 G802 V803 K804 S805 M806 I807 THR GLN HIS LEU ASN LYS GLU ASN THR ARG TRP V819 F820 N823 F824 S825 P826 D827 I828 W829 T830 G831 A832 G833 Y834 R835 V836 N840 Q841 K842 N843 G844 I845 P846 F847
E848 Q849 V850 K851 P852 S853 N854 N855 P858 F859 D860 P861 N862 S863 D864 D865 N866 K867 V868 T869 S874 S875 K876 P877 T878 T879 Y880 P881 A882 L883 P884 N885 S886 I887 S888 P889 T890 S891 D892 W893 I894 N895 A896 L897 T898 F899 T900 N901 K902 N903 N904 P905 Q906 R907 N908 Q909 L910 L911
L912 L916 G917 T918 I919 P920 V921 L922 I923 N924 K925 S926 G927 D928 S929 N930 D931 K935 Q939 K940 W941 D942 K943 T944 E945 T946 N947 E948 G949 N950 L951 P952 G953 F954 G955 E956 W957 N958 G959 L960 Y961 N962 A963 L965 L966 H967 T968 Y969 G970 F971 F972 G973 T974 N975 T976
I983 G984 F985 K986 A987 D988 S989 S990 S991 S992 S993 S994 S995 T996 L997 V998 G999 S1000 G1001 L1002 N1003 W1004 D1008 V1009 G1010 N1011 L1012 V1013 F1020 L1024 W1027 F1028 I1029 T1030 F1031 T1032 D1033 F1034 I1035 R1036 P1037 R1038 T1039 L1042 T1045 L1046 L1049 I1064 A1057 D1058
W1061 K1065 G1066 S1067 P1075 L1078 P1081 S1090 S1091 T1092 T1093 Y1094 D1095 T1096 N1097 P1098 T1099 L1100 S1101 P1102 S1103 F1104 Q1105 L1106 Y1107 Q1108 P1109 N1110 K1111 V1112 K1113 A1114 Y1115 Q1116 T1117 T1118 N1119 T1120 Y1121 N1122 K1123 L1124 I1125 E1126 P1127 V1128 D1129 A1130 T1131 S1132 A1133 A1134 M1137
L1140 L1141 K1142 L1143 L1144 T1145 T1146 I1149 K1150 A1151 K1152 L1153 G1156 THR ALA SER SER GLN GLY ASN ASN N1165 N1181 I1182 E1188 E1189 T1190 S1191 I1192 T1196 N1207 K1208 S1209 E1210 I1211 G1212 I1213 G1214 D1215 F1218 T1219 K1220 M1221 L1225 T1226 P1232 G1241 A1242 T1243 S1244
T1248 D1260 F1261 N1262 R1263 L1264 L1267 P1268 V1269 T1270 E1271 L1272 F1273 D1274 P1275 N1276 T1277 M1278 F1279 D1282 Q1283 Y1284 L1287 P1292 F1295 I1300 R1301 I1305 E1310 N1311 Q1312 R1317 L1318 E1319 Q1326 Q1327 F1328 V1331 A1334 S1335 S1336 T1337 G1338 P1339 Q1340 T1341

- Molecule 1: Adhesin P1

Chain F:




D1008 V1009 L1012 V1013 Y1014 I1015 W1027 T1030 F1031 T1032 D1033 F1034 I1035 R1036 P1037 R1038 T1039 L1042 G1043 I1044 T1045 L1046 L1049 Q1050 W1056 A1057 W1061 S1067 Y1068 P1075 L1078 A1083 S1091 T1092 T1093 Y1094 D1095 T1096 N1097 P1098 T1099 L1100 S1101 P1102 S1103 F1104 Q1105 L1106
Y1107 Q1108 P1109 N1110 K1111 V1112 Y1115 Q1116 T1117 T1118 N1119 T1120 Y1121 N1122 K1123 L1124 I1125 E1126 P1127 V1128 D1129 A1130 A1133 M1137 L1140 L1141 K1142 L1143 L1144 T1145 T1146 I1149 K1150 A1151 K1152 L1153 G1154 K1155 GLY THR ALA SER SER GLN GLY ASN ASN N1165 I1182 K1187 E1188 E1189 T1190
S1191 I1192 Q1193 T1196 K1204 Q1205 N1206 N1207 T1211 G1212 I1213 G1214 D1215 F1218 T1219 K1220 M1221 K1224 L1225 T1226 P1232 Q1240 G1241 A1242 T1243 S1244 D1245 S1246 D1247 T1248 I1251 D1260 F1261 N1262 R1263 L1264 L1267 P1268 V1269 T1270 E1271 L1272 F1273 D1274 P1275 N1276 T1277 M1278 F1279
D1282 Q1283 Y1284 L1287 P1292 F1295 I1300 R1301 I1305 E1310 N1311 Q1312 T1313 L1314 R1317 L1318 E1319 F1320 K1321 Q1326 Q1327 F1328 I1329 P1330 V1331 S1335 S1336 T1337 G1338 P1339 Q1340 T1341 V1342 P1345 F1346 N1347 GLN TRP ALA ASP HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	459.19Å 116.66Å 285.64Å 90.00° 124.20° 90.00°	Depositor
Resolution (Å)	37.36 – 3.24 236.25 – 3.24	Depositor EDS
% Data completeness (in resolution range)	61.7 (37.36-3.24) 61.8 (236.25-3.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 3.26Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.184 , 0.205 0.203 , 0.226	Depositor DCC
R_{free} test set	6155 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	59.0	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 96.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	59767	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.52	0/10269	0.78	6/13978 (0.0%)
1	B	0.49	0/10252	0.76	3/13956 (0.0%)
1	C	0.50	0/10246	0.76	1/13947 (0.0%)
1	D	0.50	0/10229	0.76	3/13925 (0.0%)
1	E	0.45	0/10135	0.73	2/13795 (0.0%)
1	F	0.45	0/10147	0.73	2/13812 (0.0%)
All	All	0.49	0/61278	0.75	17/83413 (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
1	A	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	476	MET	CB-CG-SD	7.17	133.92	112.40
1	E	861	PRO	N-CA-C	-6.71	94.65	112.10
1	F	861	PRO	N-CA-C	-6.65	94.81	112.10
1	A	109	ASP	C-N-CA	6.20	137.21	121.70
1	A	806	MET	C-N-CA	6.17	137.12	121.70
1	A	143	ILE	N-CA-C	-5.86	95.19	111.00
1	B	849	GLN	C-N-CA	5.72	136.00	121.70
1	D	849	GLN	C-N-CA	5.72	136.00	121.70
1	B	853	SER	C-N-CA	5.62	135.76	121.70
1	D	1174	ASN	C-N-CA	5.61	135.73	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	849	GLN	C-N-CA	5.58	135.65	121.70
1	A	849	GLN	C-N-CA	5.53	135.51	121.70
1	A	1093	THR	C-N-CA	5.40	135.21	121.70
1	B	149	GLU	N-CA-C	-5.34	96.58	111.00
1	F	110	ASP	C-N-CA	5.28	134.91	121.70
1	A	142	ASP	N-CA-C	-5.14	97.12	111.00
1	D	812	ASN	C-N-CA	5.13	134.53	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	926	SER	Mainchain
1	C	926	SER	Mainchain

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	10016	0	9726	182	0
1	B	9999	0	9707	183	0
1	C	9993	0	9706	182	0
1	D	9976	0	9687	205	0
1	E	9886	0	9597	156	0
1	F	9897	0	9610	163	0
All	All	59767	0	58033	1029	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (1029) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:ILE:CD1	1:D:100:ILE:CG1	1.76	1.57
1:D:812:ASN:ND2	1:D:815:ASN:HD22	1.28	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1279:PHE:CE2	1:F:1301:ARG:HD2	1.78	1.18
1:A:1266:THR:HG21	1:C:1264:LEU:HD11	1.19	1.15
1:A:1264:LEU:HG	1:C:1283:GLN:HB2	1.30	1.09
1:F:1279:PHE:HE2	1:F:1301:ARG:HD2	1.09	1.05
1:C:1279:PHE:CE2	1:C:1301:ARG:HD2	1.93	1.02
1:F:1279:PHE:CE2	1:F:1301:ARG:CD	2.42	1.01
1:D:812:ASN:ND2	1:D:815:ASN:ND2	2.09	1.00
1:D:1279:PHE:CE1	1:D:1301:ARG:HD2	2.00	0.96
1:E:1279:PHE:CE1	1:E:1301:ARG:HD2	2.00	0.96
1:A:1287:LEU:HD22	1:D:158:LEU:HD21	1.46	0.96
1:B:1279:PHE:CE1	1:B:1301:ARG:HD2	2.01	0.96
1:A:1279:PHE:CE1	1:A:1301:ARG:HD2	2.01	0.93
1:F:1301:ARG:HG2	1:F:1328:PHE:CE2	2.03	0.92
1:A:528:ASN:HD22	1:A:530:TRP:HE3	1.15	0.92
1:F:1301:ARG:HG2	1:F:1328:PHE:CD2	2.04	0.92
1:E:528:ASN:HD22	1:E:530:TRP:HE3	1.17	0.90
1:F:528:ASN:HD22	1:F:530:TRP:HE3	1.17	0.90
1:C:667:PHE:HE2	1:D:815:ASN:O	1.53	0.90
1:C:808:THR:HB	1:D:634:ASN:OD1	1.72	0.90
1:C:528:ASN:HD22	1:C:530:TRP:HE3	1.18	0.89
1:D:528:ASN:HD22	1:D:530:TRP:HE3	1.18	0.89
1:D:277:LEU:HD13	1:D:620:HIS:NE2	1.87	0.89
1:B:528:ASN:HD22	1:B:530:TRP:HE3	1.17	0.89
1:B:277:LEU:HD13	1:B:620:HIS:NE2	1.89	0.88
1:A:387:TYR:CE2	1:A:425:VAL:HG21	2.09	0.87
1:D:812:ASN:HD21	1:D:815:ASN:HD22	1.21	0.87
1:D:813:LYS:H	1:D:817:ARG:HH12	1.23	0.86
1:A:1134:ALA:HA	1:A:1137:MET:CE	2.07	0.85
1:C:667:PHE:CE2	1:D:815:ASN:O	2.29	0.85
1:A:1274:ASP:HB3	1:A:1277:THR:HG22	1.59	0.84
1:F:1274:ASP:HB3	1:F:1277:THR:HG22	1.58	0.84
1:A:1264:LEU:HD13	1:A:1284:TYR:HE1	1.42	0.83
1:D:1274:ASP:HB3	1:D:1277:THR:HG22	1.60	0.83
1:E:1274:ASP:HB3	1:E:1277:THR:HG22	1.60	0.83
1:B:1226:THR:H	1:B:1238:ASN:HD21	1.25	0.83
1:B:1274:ASP:HB3	1:B:1277:THR:HG22	1.59	0.83
1:A:1266:THR:CG2	1:C:1264:LEU:HD11	2.07	0.82
1:C:1274:ASP:HB3	1:C:1277:THR:HG22	1.63	0.80
1:E:1264:LEU:HD13	1:E:1284:TYR:HE2	1.47	0.80
1:C:674:THR:HG21	1:D:814:GLU:OE2	1.81	0.80
1:A:1134:ALA:HA	1:A:1137:MET:HE2	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ASP:HB2	1:A:113:LYS:HD2	1.64	0.79
1:C:820:PHE:HE2	1:D:682:PHE:HE2	1.30	0.79
1:B:237:THR:HG22	1:B:1108:GLN:HG3	1.66	0.78
1:C:1264:LEU:HD13	1:C:1284:TYR:HE1	1.47	0.77
1:F:1264:LEU:HD13	1:F:1284:TYR:HE1	1.49	0.77
1:A:1264:LEU:HG	1:C:1283:GLN:CB	2.13	0.76
1:E:237:THR:HG22	1:E:1108:GLN:HG3	1.68	0.76
1:F:237:THR:HG22	1:F:1108:GLN:HG3	1.68	0.76
1:C:237:THR:HG22	1:C:1108:GLN:HG3	1.68	0.75
1:D:237:THR:HG22	1:D:1108:GLN:HG3	1.69	0.75
1:D:810:HIS:CG	1:D:818:TRP:CZ3	2.76	0.74
1:A:1097:ASN:HB3	1:A:1098:PRO:CD	2.17	0.74
1:B:1264:LEU:HD13	1:B:1284:TYR:HE1	1.52	0.74
1:D:811:LEU:CD1	1:D:894:ILE:HG13	2.17	0.74
1:D:1264:LEU:HD13	1:D:1284:TYR:HE1	1.52	0.73
1:D:813:LYS:H	1:D:817:ARG:NH1	1.86	0.73
1:D:813:LYS:N	1:D:817:ARG:HH12	1.87	0.73
1:E:869:THR:HG23	1:E:875:SER:H	1.54	0.72
1:A:237:THR:HG22	1:A:1108:GLN:HG3	1.69	0.72
1:D:1097:ASN:HB2	1:D:1098:PRO:HD3	1.70	0.72
1:A:528:ASN:ND2	1:A:530:TRP:HE3	1.86	0.72
1:C:1279:PHE:HE2	1:C:1301:ARG:HD2	1.48	0.72
1:E:528:ASN:ND2	1:E:530:TRP:HE3	1.88	0.71
1:F:869:THR:HG23	1:F:875:SER:H	1.53	0.71
1:B:923:ILE:HG22	1:B:1140:LEU:HD23	1.72	0.71
1:C:528:ASN:ND2	1:C:530:TRP:HE3	1.88	0.71
1:D:1305:ILE:HD11	1:D:1317:ARG:HB3	1.73	0.71
1:A:923:ILE:HG22	1:A:1140:LEU:HD23	1.72	0.71
1:B:617:PHE:CD2	1:B:859:PHE:HD2	2.09	0.71
1:C:820:PHE:HE2	1:D:682:PHE:CE2	2.09	0.71
1:D:923:ILE:HG22	1:D:1140:LEU:HD23	1.72	0.71
1:B:987:ALA:HB1	1:B:1115:TYR:CD2	2.25	0.71
1:D:528:ASN:ND2	1:D:530:TRP:HE3	1.89	0.71
1:A:1264:LEU:HD13	1:A:1284:TYR:CE1	2.25	0.70
1:B:528:ASN:ND2	1:B:530:TRP:HE3	1.89	0.70
1:D:810:HIS:CD2	1:D:818:TRP:CZ3	2.79	0.70
1:C:769:PRO:HA	1:C:776:PRO:HA	1.74	0.69
1:A:387:TYR:HE2	1:A:425:VAL:HG21	1.58	0.69
1:D:194:SER:HB2	1:D:200:LEU:HD23	1.74	0.69
1:A:109:ASP:CB	1:A:113:LYS:HD2	2.22	0.69
1:A:98:LEU:HD12	1:A:125:GLN:HG2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:923:ILE:HG22	1:F:1140:LEU:HD23	1.75	0.69
1:A:1305:ILE:HD11	1:A:1317:ARG:HB3	1.75	0.68
1:B:769:PRO:HA	1:B:776:PRO:HA	1.76	0.68
1:B:1305:ILE:HD11	1:B:1317:ARG:HB3	1.74	0.68
1:B:277:LEU:HD13	1:B:620:HIS:CD2	2.29	0.68
1:C:923:ILE:HG22	1:C:1140:LEU:HD23	1.74	0.68
1:F:1305:ILE:HD11	1:F:1317:ARG:HB3	1.75	0.68
1:F:769:PRO:HA	1:F:776:PRO:HA	1.76	0.68
1:E:194:SER:HB2	1:E:200:LEU:HD23	1.76	0.68
1:A:1287:LEU:HD22	1:D:158:LEU:CD2	2.21	0.67
1:F:528:ASN:ND2	1:F:530:TRP:HE3	1.89	0.67
1:F:988:ASP:OD2	1:F:991:SER:O	2.12	0.67
1:F:194:SER:HB2	1:F:200:LEU:HD23	1.75	0.67
1:A:1266:THR:HG21	1:C:1264:LEU:CD1	2.13	0.67
1:C:1264:LEU:HD13	1:C:1284:TYR:CE1	2.28	0.67
1:E:923:ILE:HG22	1:E:1140:LEU:HD23	1.76	0.67
1:A:769:PRO:HA	1:A:776:PRO:HA	1.76	0.67
1:F:1263:ARG:HG3	1:F:1264:LEU:HD12	1.76	0.67
1:E:1264:LEU:HD13	1:E:1284:TYR:CE2	2.30	0.67
1:E:1305:ILE:HD11	1:E:1317:ARG:HB3	1.76	0.67
1:B:1263:ARG:HG3	1:B:1264:LEU:HD12	1.77	0.67
1:B:194:SER:HB2	1:B:200:LEU:HD23	1.77	0.66
1:A:1263:ARG:HG3	1:A:1264:LEU:HD12	1.78	0.66
1:D:1263:ARG:HG3	1:D:1264:LEU:HD12	1.77	0.66
1:A:809:GLN:HG2	1:B:634:ASN:HB2	1.76	0.66
1:C:1305:ILE:HD11	1:C:1317:ARG:HB3	1.77	0.66
1:C:570:GLN:HG2	1:C:596:GLY:HA2	1.77	0.66
1:E:1263:ARG:HG3	1:E:1264:LEU:HD12	1.77	0.66
1:D:769:PRO:HA	1:D:776:PRO:HA	1.76	0.66
1:D:617:PHE:CD2	1:D:859:PHE:HD2	2.14	0.65
1:E:988:ASP:OD2	1:E:991:SER:O	2.13	0.65
1:E:646:ASN:HB2	1:F:823:ASN:HA	1.77	0.65
1:A:570:GLN:HG2	1:A:596:GLY:HA2	1.78	0.65
1:E:769:PRO:HA	1:E:776:PRO:HA	1.77	0.65
1:D:95:ASN:HD21	1:D:125:GLN:HG3	1.62	0.65
1:F:1264:LEU:HD13	1:F:1284:TYR:CE1	2.31	0.65
1:A:194:SER:HB2	1:A:200:LEU:HD23	1.79	0.65
1:C:194:SER:HB2	1:C:200:LEU:HD23	1.78	0.65
1:B:777:PHE:O	1:B:795:THR:HG22	1.98	0.64
1:A:1097:ASN:HB3	1:A:1098:PRO:HD3	1.80	0.64
1:D:277:LEU:HD13	1:D:620:HIS:CD2	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:777:PHE:O	1:A:795:THR:HG22	1.98	0.63
1:D:217:ASN:HB3	1:D:220:VAL:HG23	1.80	0.63
1:D:244:SER:HB2	1:D:568:TYR:O	1.99	0.63
1:B:570:GLN:HG2	1:B:596:GLY:HA2	1.80	0.63
1:D:1264:LEU:HD13	1:D:1284:TYR:CE1	2.33	0.63
1:F:570:GLN:HG2	1:F:596:GLY:HA2	1.80	0.63
1:B:217:ASN:HB3	1:B:220:VAL:HG23	1.81	0.63
1:C:820:PHE:CE2	1:D:682:PHE:HE2	2.13	0.63
1:B:681:ASN:HB2	1:B:730:LEU:HD22	1.80	0.63
1:D:570:GLN:HG2	1:D:596:GLY:HA2	1.79	0.63
1:B:58:GLN:NE2	1:B:149:GLU:O	2.32	0.63
1:C:1263:ARG:HG3	1:C:1264:LEU:HD12	1.80	0.63
1:C:777:PHE:O	1:C:795:THR:HG22	1.99	0.63
1:A:244:SER:HB3	1:A:571:LEU:HB2	1.80	0.62
1:D:777:PHE:O	1:D:795:THR:HG22	1.99	0.62
1:B:244:SER:HB3	1:B:571:LEU:HB2	1.82	0.62
1:B:1264:LEU:HD13	1:B:1284:TYR:CE1	2.33	0.62
1:D:812:ASN:HD21	1:D:815:ASN:ND2	1.86	0.62
1:A:808:THR:HB	1:B:634:ASN:OD1	1.99	0.62
1:C:809:GLN:HE22	1:C:811:LEU:HD23	1.64	0.62
1:E:777:PHE:O	1:E:795:THR:HG22	2.00	0.62
1:F:1279:PHE:CE2	1:F:1301:ARG:HD3	2.33	0.62
1:B:834:TYR:OH	1:B:945:GLU:HG2	2.00	0.62
1:C:681:ASN:HB2	1:C:730:LEU:HD22	1.80	0.62
1:F:79:LYS:HD3	1:F:1232:PRO:HA	1.82	0.62
1:C:244:SER:HB3	1:C:571:LEU:HB2	1.82	0.62
1:E:1003:ASN:HB3	1:E:1102:PRO:HG2	1.82	0.62
1:B:244:SER:HB2	1:B:568:TYR:O	2.00	0.61
1:A:1003:ASN:HB3	1:A:1102:PRO:HG2	1.82	0.61
1:B:1248:THR:HB	1:B:1331:VAL:HG13	1.82	0.61
1:E:1279:PHE:HE1	1:E:1301:ARG:HD2	1.64	0.61
1:E:570:GLN:HG2	1:E:596:GLY:HA2	1.81	0.61
1:B:1033:ASP:OD1	1:B:1038:ARG:HG3	1.99	0.61
1:C:1248:THR:HB	1:C:1331:VAL:HG13	1.83	0.61
1:D:1248:THR:HB	1:D:1331:VAL:HG13	1.82	0.61
1:C:217:ASN:HB3	1:C:220:VAL:HG23	1.82	0.61
1:E:244:SER:HB3	1:E:571:LEU:HB2	1.82	0.61
1:E:79:LYS:HD3	1:E:1232:PRO:HA	1.83	0.61
1:C:244:SER:HB2	1:C:568:TYR:O	2.01	0.61
1:A:1248:THR:HB	1:A:1331:VAL:HG13	1.83	0.61
1:C:1033:ASP:OD1	1:C:1038:ARG:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1248:THR:HB	1:F:1331:VAL:HG13	1.83	0.61
1:A:217:ASN:HB3	1:A:220:VAL:HG23	1.82	0.61
1:C:811:LEU:HD11	1:C:895:ASN:O	2.01	0.61
1:F:1301:ARG:HG2	1:F:1328:PHE:HD2	1.63	0.61
1:F:244:SER:HB2	1:F:568:TYR:O	2.01	0.61
1:F:244:SER:HB3	1:F:571:LEU:HB2	1.82	0.61
1:F:777:PHE:O	1:F:795:THR:HG22	2.00	0.60
1:B:277:LEU:HD13	1:B:620:HIS:HE2	1.66	0.60
1:C:1003:ASN:HB3	1:C:1102:PRO:HG2	1.83	0.60
1:D:244:SER:HB3	1:D:571:LEU:HB2	1.83	0.60
1:D:935:LYS:HB3	1:D:972:PHE:HD2	1.66	0.60
1:D:1003:ASN:HB3	1:D:1102:PRO:HG2	1.84	0.60
1:E:742:ARG:HH12	1:F:1036:ARG:HH21	1.50	0.60
1:A:244:SER:HB2	1:A:568:TYR:O	2.01	0.60
1:D:79:LYS:HD3	1:D:1232:PRO:HA	1.84	0.60
1:E:852:PRO:HA	1:E:858:PRO:HA	1.84	0.60
1:F:1003:ASN:HB3	1:F:1102:PRO:HG2	1.83	0.60
1:C:457:MET:HA	1:C:465:PHE:O	2.02	0.59
1:C:817:ARG:HG2	1:C:817:ARG:HH21	1.67	0.59
1:C:94:GLN:HA	1:C:94:GLN:HE21	1.67	0.59
1:E:457:MET:HA	1:E:465:PHE:O	2.02	0.59
1:F:217:ASN:HB3	1:F:220:VAL:HG23	1.84	0.59
1:A:79:LYS:HD3	1:A:1232:PRO:HA	1.85	0.59
1:C:105:LYS:HZ2	1:C:105:LYS:HB2	1.66	0.59
1:D:614:GLY:HA3	1:D:854:ASN:HD21	1.67	0.59
1:F:457:MET:HA	1:F:465:PHE:O	2.01	0.59
1:E:244:SER:HB2	1:E:568:TYR:O	2.02	0.59
1:A:1134:ALA:HA	1:A:1137:MET:HE1	1.83	0.59
1:C:810:HIS:NE2	1:C:814:GLU:HA	2.18	0.59
1:F:1301:ARG:HG2	1:F:1328:PHE:HE2	1.64	0.59
1:B:457:MET:HA	1:B:465:PHE:O	2.02	0.59
1:D:834:TYR:OH	1:D:945:GLU:HG2	2.03	0.59
1:F:1033:ASP:OD1	1:F:1038:ARG:HG3	2.02	0.59
1:A:817:ARG:HG2	1:A:817:ARG:HH21	1.68	0.59
1:B:1003:ASN:HB3	1:B:1102:PRO:HG2	1.85	0.58
1:E:217:ASN:HB3	1:E:220:VAL:HG23	1.84	0.58
1:C:122:LEU:HB3	1:C:126:GLN:HE21	1.68	0.58
1:E:742:ARG:HH12	1:F:1036:ARG:NH2	2.01	0.58
1:A:681:ASN:HB2	1:A:730:LEU:HD22	1.85	0.58
1:A:852:PRO:HA	1:A:858:PRO:HA	1.85	0.58
1:C:852:PRO:HA	1:C:858:PRO:HA	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:PHE:CE2	1:B:816:THR:HG23	2.38	0.58
1:A:59:GLN:HB2	1:A:142:ASP:O	2.03	0.58
1:D:457:MET:HA	1:D:465:PHE:O	2.03	0.58
1:D:811:LEU:HA	1:D:817:ARG:HH11	1.67	0.58
1:F:852:PRO:HA	1:F:858:PRO:HA	1.84	0.58
1:B:79:LYS:HD3	1:B:1232:PRO:HA	1.85	0.58
1:F:681:ASN:HB2	1:F:730:LEU:HD22	1.86	0.58
1:E:681:ASN:HB2	1:E:730:LEU:HD22	1.85	0.58
1:A:457:MET:HA	1:A:465:PHE:O	2.04	0.58
1:C:513:ILE:HD12	1:C:515:PRO:HD2	1.86	0.58
1:D:813:LYS:HA	1:D:817:ARG:HH12	1.69	0.58
1:F:1261:PHE:HE1	1:F:1345:PRO:HA	1.69	0.57
1:B:852:PRO:HA	1:B:858:PRO:HA	1.85	0.57
1:D:646:ASN:HD22	1:D:651:LYS:HA	1.70	0.57
1:D:809:GLN:CG	1:D:894:ILE:HG21	2.34	0.57
1:C:105:LYS:NZ	1:C:105:LYS:HB2	2.19	0.57
1:D:852:PRO:HA	1:D:858:PRO:HA	1.87	0.57
1:B:804:LYS:HD3	1:B:804:LYS:H	1.70	0.57
1:C:834:TYR:OH	1:C:945:GLU:HG2	2.05	0.57
1:D:95:ASN:ND2	1:D:125:GLN:HG3	2.18	0.57
1:D:277:LEU:HD13	1:D:620:HIS:HE2	1.64	0.57
1:E:834:TYR:OH	1:E:945:GLU:HG2	2.05	0.57
1:C:939:GLN:HE21	1:C:950:ASN:HD22	1.53	0.57
1:B:1295:PHE:HE2	1:B:1300:ILE:HG12	1.69	0.57
1:C:79:LYS:HD3	1:C:1232:PRO:HA	1.86	0.57
1:C:819:VAL:HG23	1:C:820:PHE:HD1	1.70	0.57
1:D:614:GLY:HA3	1:D:854:ASN:ND2	2.20	0.57
1:F:58:GLN:OE1	1:F:149:GLU:HB3	2.04	0.56
1:F:834:TYR:OH	1:F:945:GLU:HG2	2.04	0.56
1:D:804:LYS:H	1:D:804:LYS:HD3	1.68	0.56
1:C:674:THR:CG2	1:D:814:GLU:OE2	2.52	0.56
1:C:199:ASN:O	1:C:344:TYR:HA	2.05	0.56
1:A:646:ASN:HD22	1:A:651:LYS:HA	1.71	0.56
1:D:1295:PHE:HE2	1:D:1300:ILE:HG12	1.69	0.56
1:D:681:ASN:HB2	1:D:730:LEU:HD22	1.86	0.56
1:C:1096:THR:HG22	1:C:1098:PRO:HD2	1.87	0.56
1:A:834:TYR:OH	1:A:945:GLU:HG2	2.05	0.56
1:A:939:GLN:HE21	1:A:950:ASN:HD22	1.53	0.56
1:C:820:PHE:CE2	1:D:682:PHE:CE2	2.93	0.56
1:E:1295:PHE:HE2	1:E:1300:ILE:HG12	1.71	0.56
1:F:646:ASN:HD22	1:F:651:LYS:HA	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:646:ASN:HD22	1:B:651:LYS:HA	1.71	0.56
1:A:1264:LEU:CG	1:C:1283:GLN:HB2	2.20	0.56
1:C:646:ASN:HD22	1:C:651:LYS:HA	1.71	0.56
1:D:513:ILE:HD12	1:D:515:PRO:HD2	1.86	0.56
1:F:1335:SER:HB3	1:F:1338:GLY:O	2.06	0.56
1:D:1030:THR:HB	1:D:1045:THR:OG1	2.06	0.56
1:D:122:LEU:HB3	1:D:126:GLN:HE21	1.71	0.56
1:E:1248:THR:HB	1:E:1331:VAL:HG13	1.86	0.56
1:B:1261:PHE:HE1	1:B:1345:PRO:HA	1.71	0.55
1:E:646:ASN:HD22	1:E:651:LYS:HA	1.71	0.55
1:F:1218:PHE:HE2	1:F:1220:LYS:HG2	1.71	0.55
1:B:770:TRP:HE3	1:B:773:ASN:HB2	1.71	0.55
1:E:58:GLN:OE1	1:E:149:GLU:HB3	2.05	0.55
1:E:255:LYS:HD2	1:E:609:LEU:HB2	1.89	0.55
1:A:255:LYS:HD2	1:A:609:LEU:HB2	1.89	0.55
1:A:813:LYS:HA	1:B:817:ARG:HG2	1.88	0.55
1:E:695:ALA:HB3	1:E:751:THR:HG22	1.89	0.55
1:F:134:ASP:HB3	1:F:140:LEU:HD21	1.89	0.55
1:F:695:ALA:HB3	1:F:751:THR:HG22	1.89	0.55
1:F:939:GLN:HE21	1:F:950:ASN:HD22	1.55	0.55
1:D:813:LYS:CA	1:D:817:ARG:HH12	2.18	0.55
1:B:1115:TYR:HE1	1:B:1125:ILE:HG21	1.72	0.55
1:A:122:LEU:HB3	1:A:126:GLN:HE21	1.71	0.55
1:C:255:LYS:HD2	1:C:609:LEU:HB2	1.88	0.55
1:F:770:TRP:HE3	1:F:773:ASN:HB2	1.72	0.55
1:A:77:SER:HA	1:A:89:GLY:HA2	1.89	0.54
1:B:199:ASN:O	1:B:344:TYR:HA	2.07	0.54
1:C:1030:THR:HB	1:C:1045:THR:OG1	2.07	0.54
1:A:770:TRP:HE3	1:A:773:ASN:HB2	1.72	0.54
1:B:1335:SER:HB3	1:B:1338:GLY:O	2.07	0.54
1:E:1335:SER:HB3	1:E:1338:GLY:O	2.07	0.54
1:F:255:LYS:HD2	1:F:609:LEU:HB2	1.88	0.54
1:A:1295:PHE:HE2	1:A:1300:ILE:HG12	1.71	0.54
1:E:68:TRP:CD1	1:E:92:ARG:HB2	2.43	0.54
1:A:58:GLN:OE1	1:A:149:GLU:HB3	2.06	0.54
1:B:924:ASN:HB2	1:B:985:PHE:HA	1.90	0.54
1:D:770:TRP:HE3	1:D:773:ASN:HB2	1.72	0.54
1:E:134:ASP:HB3	1:E:140:LEU:HD21	1.89	0.54
1:C:614:GLY:HA3	1:C:854:ASN:HD21	1.73	0.54
1:A:1335:SER:HB3	1:A:1338:GLY:O	2.08	0.54
1:A:199:ASN:O	1:A:344:TYR:HA	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1335:SER:HB3	1:C:1338:GLY:O	2.08	0.54
1:F:122:LEU:HB3	1:F:126:GLN:HE21	1.73	0.54
1:C:924:ASN:HB2	1:C:985:PHE:HA	1.89	0.54
1:E:770:TRP:HE3	1:E:773:ASN:HB2	1.72	0.54
1:E:939:GLN:HE21	1:E:950:ASN:HD22	1.55	0.54
1:B:65:LEU:HB3	1:B:91:VAL:HG13	1.90	0.54
1:E:823:ASN:HA	1:F:646:ASN:HB2	1.90	0.54
1:B:122:LEU:HB3	1:B:126:GLN:HE21	1.72	0.53
1:E:199:ASN:O	1:E:344:TYR:HA	2.08	0.53
1:F:1295:PHE:HE2	1:F:1300:ILE:HG12	1.72	0.53
1:B:1143:LEU:HD23	1:B:1149:ILE:HG12	1.89	0.53
1:B:1030:THR:HB	1:B:1045:THR:OG1	2.08	0.53
1:A:1218:PHE:HE2	1:A:1220:LYS:HG2	1.73	0.53
1:A:529:ARG:HB2	1:A:715:GLU:O	2.08	0.53
1:D:134:ASP:HB3	1:D:140:LEU:HD21	1.91	0.53
1:E:321:TRP:HE1	1:E:476:MET:CE	2.21	0.53
1:A:134:ASP:HB3	1:A:140:LEU:HD21	1.91	0.53
1:B:939:GLN:HE21	1:B:950:ASN:HD22	1.55	0.53
1:E:524:PRO:HD2	1:E:557:MET:HE2	1.90	0.53
1:B:1218:PHE:HE2	1:B:1220:LYS:HG2	1.73	0.53
1:C:770:TRP:HE3	1:C:773:ASN:HB2	1.73	0.53
1:C:614:GLY:HA3	1:C:854:ASN:ND2	2.24	0.53
1:C:77:SER:HA	1:C:89:GLY:HA2	1.91	0.53
1:D:924:ASN:HB2	1:D:985:PHE:HA	1.89	0.53
1:E:1218:PHE:HE2	1:E:1220:LYS:HG2	1.73	0.53
1:D:255:LYS:HD2	1:D:609:LEU:HB2	1.90	0.53
1:B:134:ASP:HB3	1:B:140:LEU:HD21	1.90	0.53
1:B:695:ALA:HB3	1:B:751:THR:HG22	1.91	0.53
1:D:812:ASN:H	1:D:817:ARG:HH11	1.56	0.53
1:C:668:ASN:ND2	1:D:816:THR:OG1	2.36	0.53
1:D:846:PRO:HG2	1:D:849:GLN:HE22	1.73	0.53
1:C:1143:LEU:HD23	1:C:1149:ILE:HG12	1.91	0.53
1:D:939:GLN:HE21	1:D:950:ASN:HD22	1.56	0.53
1:F:65:LEU:HB3	1:F:91:VAL:HG13	1.91	0.53
1:F:924:ASN:HB2	1:F:985:PHE:HA	1.91	0.53
1:A:924:ASN:HB2	1:A:985:PHE:HA	1.91	0.52
1:C:134:ASP:HB3	1:C:140:LEU:HD21	1.91	0.52
1:D:396:THR:HG21	1:D:404:ARG:HE	1.75	0.52
1:E:1030:THR:HB	1:E:1045:THR:OG1	2.09	0.52
1:F:817:ARG:HH21	1:F:817:ARG:HG2	1.73	0.52
1:A:513:ILE:HD12	1:A:515:PRO:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:695:ALA:HB3	1:D:751:THR:HG22	1.92	0.52
1:D:1335:SER:HB3	1:D:1338:GLY:O	2.09	0.52
1:C:808:THR:CB	1:D:634:ASN:OD1	2.53	0.52
1:E:77:SER:HA	1:E:89:GLY:HA2	1.91	0.52
1:E:924:ASN:HB2	1:E:985:PHE:HA	1.91	0.52
1:F:1030:THR:HB	1:F:1045:THR:OG1	2.09	0.52
1:F:513:ILE:HD12	1:F:515:PRO:HD2	1.91	0.52
1:B:255:LYS:HD2	1:B:609:LEU:HB2	1.90	0.52
1:C:248:ASP:HB2	1:C:301:LYS:HB2	1.92	0.52
1:D:199:ASN:O	1:D:344:TYR:HA	2.08	0.52
1:E:1003:ASN:HD21	1:E:1146:THR:HG21	1.74	0.52
1:F:199:ASN:O	1:F:344:TYR:HA	2.09	0.52
1:D:1218:PHE:HE2	1:D:1220:LYS:HG2	1.73	0.52
1:D:816:THR:HB	1:D:819:VAL:HG22	1.92	0.52
1:C:846:PRO:HG2	1:C:849:GLN:HE22	1.73	0.52
1:C:892:ASP:HA	1:C:900:THR:HG23	1.92	0.52
1:D:248:ASP:HB2	1:D:301:LYS:HB2	1.92	0.52
1:B:228:LYS:HE2	1:B:230:THR:HB	1.91	0.52
1:B:248:ASP:HB2	1:B:301:LYS:HB2	1.92	0.52
1:D:1313:THR:HG22	1:D:1344:GLN:HG3	1.91	0.52
1:A:695:ALA:HB3	1:A:751:THR:HG22	1.92	0.51
1:C:1295:PHE:HE2	1:C:1300:ILE:HG12	1.73	0.51
1:F:846:PRO:HG2	1:F:849:GLN:HE22	1.74	0.51
1:F:68:TRP:CD1	1:F:92:ARG:HB2	2.45	0.51
1:A:68:TRP:CD1	1:A:92:ARG:HB2	2.45	0.51
1:B:529:ARG:HB2	1:B:715:GLU:O	2.10	0.51
1:D:529:ARG:HB2	1:D:715:GLU:O	2.10	0.51
1:D:809:GLN:HG3	1:D:894:ILE:HG21	1.92	0.51
1:D:77:SER:HA	1:D:89:GLY:HA2	1.92	0.51
1:E:846:PRO:HG2	1:E:849:GLN:HE22	1.74	0.51
1:A:65:LEU:HB3	1:A:91:VAL:HG13	1.92	0.51
1:B:846:PRO:HG2	1:B:849:GLN:HE22	1.74	0.51
1:C:695:ALA:HB3	1:C:751:THR:HG22	1.91	0.51
1:F:529:ARG:HB2	1:F:715:GLU:O	2.09	0.51
1:B:59:GLN:HB2	1:B:143:ILE:H	1.76	0.51
1:F:1003:ASN:HD21	1:F:1146:THR:HG21	1.76	0.51
1:A:1261:PHE:HE1	1:A:1345:PRO:HA	1.76	0.51
1:B:68:TRP:CD1	1:B:92:ARG:HB2	2.46	0.51
1:E:513:ILE:HD12	1:E:515:PRO:HD2	1.93	0.51
1:A:897:LEU:CD2	1:B:816:THR:HG21	2.41	0.51
1:B:834:TYR:CZ	1:B:945:GLU:HG2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1003:ASN:HD21	1:C:1146:THR:HG21	1.76	0.51
1:E:122:LEU:HB3	1:E:126:GLN:HE21	1.74	0.51
1:B:1014:VAL:O	1:B:1069:LEU:HD22	2.11	0.51
1:C:529:ARG:HB2	1:C:715:GLU:O	2.11	0.51
1:B:817:ARG:HB3	1:B:818:TRP:CD1	2.46	0.51
1:D:58:GLN:OE1	1:D:149:GLU:HB3	2.11	0.51
1:D:65:LEU:HB3	1:D:91:VAL:HG13	1.93	0.50
1:D:834:TYR:CZ	1:D:945:GLU:HG2	2.47	0.50
1:F:77:SER:HA	1:F:89:GLY:HA2	1.93	0.50
1:B:112:LEU:HD11	1:B:333:GLU:HG2	1.92	0.50
1:D:68:TRP:CD1	1:D:92:ARG:HB2	2.46	0.50
1:F:1027:TRP:CE3	1:F:1046:LEU:HB3	2.47	0.50
1:A:1003:ASN:HD21	1:A:1146:THR:HG21	1.75	0.50
1:C:65:LEU:HB3	1:C:91:VAL:HG13	1.92	0.50
1:D:809:GLN:HG3	1:D:894:ILE:CG2	2.41	0.50
1:E:529:ARG:HB2	1:E:715:GLU:O	2.10	0.50
1:E:834:TYR:CZ	1:E:945:GLU:HG2	2.47	0.50
1:B:892:ASP:HA	1:B:900:THR:HG23	1.93	0.50
1:C:98:LEU:O	1:C:98:LEU:HD12	2.11	0.50
1:D:186:LYS:HB3	1:D:205:LEU:HB3	1.94	0.50
1:A:154:VAL:HG23	1:A:170:PHE:HB3	1.94	0.50
1:A:504:PRO:HG2	1:A:507:VAL:HG23	1.94	0.50
1:E:1027:TRP:CE3	1:E:1046:LEU:HB3	2.46	0.50
1:E:1261:PHE:HE1	1:E:1345:PRO:HA	1.77	0.50
1:F:523:LEU:HG	1:F:557:MET:CE	2.42	0.50
1:A:1027:TRP:CE3	1:A:1046:LEU:HB3	2.46	0.50
1:A:377:PRO:HG3	1:A:443:ILE:HG13	1.94	0.50
1:A:396:THR:HG21	1:A:404:ARG:HE	1.76	0.50
1:A:892:ASP:HA	1:A:900:THR:HG23	1.93	0.50
1:B:513:ILE:HD12	1:B:515:PRO:HD2	1.93	0.50
1:B:869:THR:HG22	1:B:875:SER:OG	2.11	0.50
1:C:1261:PHE:HE1	1:C:1345:PRO:HA	1.76	0.50
1:D:276:ALA:HB2	1:D:655:PRO:HD3	1.93	0.50
1:D:810:HIS:CD2	1:D:818:TRP:HZ3	2.26	0.50
1:E:614:GLY:HA3	1:E:854:ASN:HD21	1.77	0.50
1:E:742:ARG:NH1	1:F:1036:ARG:HH21	2.09	0.50
1:C:1027:TRP:CE3	1:C:1046:LEU:HB3	2.46	0.50
1:A:186:LYS:HB3	1:A:205:LEU:HB3	1.94	0.50
1:A:254:GLU:O	1:A:297:LYS:HB3	2.12	0.50
1:C:396:THR:HG21	1:C:404:ARG:HE	1.77	0.50
1:C:674:THR:CB	1:D:814:GLU:OE2	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:892:ASP:HA	1:E:900:THR:HG23	1.93	0.50
1:F:892:ASP:HA	1:F:900:THR:HG23	1.93	0.50
1:F:254:GLU:O	1:F:297:LYS:HB3	2.12	0.49
1:E:371:PRO:HD2	1:E:374:TRP:CD2	2.47	0.49
1:B:396:THR:HG21	1:B:404:ARG:HE	1.77	0.49
1:B:77:SER:HA	1:B:89:GLY:HA2	1.94	0.49
1:E:321:TRP:HE1	1:E:476:MET:HE3	1.78	0.49
1:E:65:LEU:HB3	1:E:91:VAL:HG13	1.92	0.49
1:A:926:SER:O	1:A:983:ILE:HG12	2.12	0.49
1:B:813:LYS:HA	1:B:817:ARG:HH22	1.78	0.49
1:C:254:GLU:O	1:C:297:LYS:HB3	2.12	0.49
1:F:614:GLY:HA3	1:F:854:ASN:HD21	1.77	0.49
1:A:112:LEU:HD11	1:A:333:GLU:HG2	1.93	0.49
1:A:327:THR:HG21	1:A:367:VAL:HG21	1.95	0.49
1:A:834:TYR:CZ	1:A:945:GLU:HG2	2.48	0.49
1:B:1226:THR:H	1:B:1238:ASN:ND2	2.03	0.49
1:C:58:GLN:OE1	1:C:149:GLU:HB3	2.13	0.49
1:C:834:TYR:CZ	1:C:945:GLU:HG2	2.47	0.49
1:D:1143:LEU:HD23	1:D:1149:ILE:HG12	1.95	0.49
1:D:327:THR:HG21	1:D:367:VAL:HG21	1.94	0.49
1:D:812:ASN:H	1:D:817:ARG:NH1	2.10	0.49
1:E:59:GLN:HB2	1:E:143:ILE:H	1.78	0.49
1:A:1143:LEU:HD23	1:A:1149:ILE:HG12	1.94	0.49
1:D:112:LEU:HD11	1:D:333:GLU:HG2	1.93	0.49
1:A:846:PRO:HG2	1:A:849:GLN:HE22	1.77	0.49
1:C:68:TRP:CD1	1:C:92:ARG:HB2	2.47	0.49
1:B:1003:ASN:HD21	1:B:1146:THR:HG21	1.77	0.49
1:C:391:ASN:HD22	1:C:418:ASN:HD22	1.61	0.49
1:D:1027:TRP:CE3	1:D:1046:LEU:HB3	2.47	0.49
1:D:811:LEU:CD1	1:D:894:ILE:CG1	2.88	0.49
1:F:777:PHE:HB3	1:F:795:THR:CG2	2.43	0.49
1:A:98:LEU:O	1:A:99:ASN:C	2.49	0.49
1:B:466:ILE:HB	1:B:487:PHE:HB2	1.94	0.49
1:C:371:PRO:HD2	1:C:374:TRP:CD2	2.48	0.49
1:C:994:SER:HB2	1:C:1137:MET:CE	2.42	0.49
1:D:275:LYS:HG2	1:D:644:TYR:HE1	1.78	0.49
1:D:254:GLU:O	1:D:297:LYS:HB3	2.12	0.49
1:B:186:LYS:HB3	1:B:205:LEU:HB3	1.95	0.49
1:B:987:ALA:HA	1:B:1115:TYR:CE2	2.48	0.49
1:E:466:ILE:HB	1:E:487:PHE:HB2	1.95	0.49
1:E:994:SER:HB2	1:E:1137:MET:CE	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:396:THR:HG21	1:F:404:ARG:HE	1.78	0.49
1:D:777:PHE:HB3	1:D:795:THR:CG2	2.43	0.48
1:B:994:SER:HB2	1:B:1137:MET:HE3	1.95	0.48
1:C:777:PHE:HB3	1:C:795:THR:CG2	2.43	0.48
1:E:1143:LEU:HD23	1:E:1149:ILE:HG12	1.95	0.48
1:F:59:GLN:HB2	1:F:143:ILE:H	1.78	0.48
1:F:834:TYR:CZ	1:F:945:GLU:HG2	2.47	0.48
1:D:391:ASN:HD22	1:D:418:ASN:HD22	1.62	0.48
1:A:651:LYS:CE	1:B:823:ASN:HD21	2.26	0.48
1:B:987:ALA:CB	1:B:1115:TYR:CD2	2.96	0.48
1:E:112:LEU:HD11	1:E:333:GLU:HG2	1.95	0.48
1:B:809:GLN:HB3	1:B:826:PRO:HB2	1.95	0.48
1:C:277:LEU:HB2	1:C:653:VAL:HB	1.96	0.48
1:D:1003:ASN:HD21	1:D:1146:THR:HG21	1.79	0.48
1:E:154:VAL:HG23	1:E:170:PHE:HB3	1.96	0.48
1:E:777:PHE:HB3	1:E:795:THR:CG2	2.44	0.48
1:A:98:LEU:O	1:A:121:TYR:OH	2.31	0.48
1:B:1312:GLN:O	1:B:1345:PRO:HD2	2.13	0.48
1:B:617:PHE:CE2	1:B:859:PHE:HB2	2.48	0.48
1:C:1143:LEU:O	1:C:1149:ILE:HD11	2.14	0.48
1:C:466:ILE:HB	1:C:487:PHE:HB2	1.95	0.48
1:F:276:ALA:HB2	1:F:655:PRO:HD3	1.96	0.48
1:A:1097:ASN:CB	1:A:1098:PRO:CD	2.90	0.48
1:D:994:SER:HB2	1:D:1137:MET:CE	2.43	0.48
1:F:523:LEU:HG	1:F:557:MET:HE2	1.96	0.48
1:A:277:LEU:HB2	1:A:653:VAL:HB	1.96	0.48
1:B:58:GLN:OE1	1:B:149:GLU:HB3	2.13	0.48
1:B:520:LEU:HD23	1:B:757:ASP:HA	1.95	0.48
1:C:186:LYS:HB3	1:C:205:LEU:HB3	1.96	0.48
1:D:154:VAL:HG23	1:D:170:PHE:HB3	1.95	0.48
1:D:892:ASP:HA	1:D:900:THR:HG23	1.95	0.48
1:F:112:LEU:HD11	1:F:333:GLU:HG2	1.96	0.48
1:E:254:GLU:O	1:E:297:LYS:HB3	2.13	0.48
1:F:1312:GLN:O	1:F:1345:PRO:HD2	2.14	0.48
1:B:1027:TRP:CE3	1:B:1046:LEU:HB3	2.48	0.48
1:B:806:MET:HB2	1:B:843:ASN:OD1	2.13	0.48
1:B:994:SER:HB2	1:B:1137:MET:CE	2.44	0.48
1:C:889:PRO:HD2	1:C:951:LEU:HD21	1.95	0.48
1:E:523:LEU:HB3	1:E:557:MET:HE1	1.96	0.48
1:F:377:PRO:HB2	1:F:400:PHE:O	2.14	0.48
1:C:154:VAL:HG23	1:C:170:PHE:HB3	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:ALA:HB2	1:C:655:PRO:HD3	1.96	0.47
1:C:377:PRO:HG3	1:C:443:ILE:HG13	1.95	0.47
1:E:396:THR:HG21	1:E:404:ARG:HE	1.79	0.47
1:A:245:PRO:HG2	1:A:568:TYR:HB2	1.96	0.47
1:C:327:THR:HG21	1:C:367:VAL:HG21	1.96	0.47
1:D:371:PRO:HD2	1:D:374:TRP:CD2	2.49	0.47
1:F:186:LYS:HB3	1:F:205:LEU:HB3	1.96	0.47
1:A:391:ASN:HD22	1:A:418:ASN:HD22	1.62	0.47
1:B:276:ALA:HB2	1:B:655:PRO:HD3	1.96	0.47
1:B:377:PRO:HB2	1:B:400:PHE:O	2.14	0.47
1:C:112:LEU:HD11	1:C:333:GLU:HG2	1.96	0.47
1:E:231:GLN:HG3	1:E:1096:THR:HA	1.97	0.47
1:F:994:SER:HB2	1:F:1137:MET:CE	2.43	0.47
1:F:371:PRO:HD2	1:F:374:TRP:CD2	2.48	0.47
1:C:520:LEU:HD23	1:C:757:ASP:HA	1.97	0.47
1:C:245:PRO:HG2	1:C:568:TYR:HB2	1.97	0.47
1:C:845:ILE:HG22	1:C:883:LEU:O	2.15	0.47
1:E:276:ALA:HB2	1:E:655:PRO:HD3	1.96	0.47
1:F:277:LEU:HB2	1:F:653:VAL:HB	1.96	0.47
1:A:614:GLY:HA3	1:A:854:ASN:HD21	1.80	0.47
1:B:254:GLU:O	1:B:297:LYS:HB3	2.14	0.47
1:D:59:GLN:HB2	1:D:143:ILE:H	1.79	0.47
1:F:377:PRO:HG3	1:F:443:ILE:HG13	1.97	0.47
1:A:277:LEU:HD21	1:A:610:GLN:HG3	1.97	0.47
1:B:777:PHE:HB3	1:B:795:THR:CG2	2.45	0.47
1:D:811:LEU:HD13	1:D:894:ILE:HG13	1.95	0.47
1:B:277:LEU:HD21	1:B:610:GLN:CG	2.45	0.47
1:E:186:LYS:HB3	1:E:205:LEU:HB3	1.97	0.47
1:E:277:LEU:HB2	1:E:653:VAL:HB	1.96	0.47
1:E:377:PRO:HB2	1:E:400:PHE:O	2.15	0.47
1:E:520:LEU:HD23	1:E:757:ASP:HA	1.96	0.47
1:E:614:GLY:HA3	1:E:854:ASN:ND2	2.30	0.47
1:A:777:PHE:HB3	1:A:795:THR:CG2	2.45	0.47
1:C:793:LEU:HD22	1:C:801:VAL:HG13	1.96	0.47
1:D:889:PRO:HD2	1:D:951:LEU:HD21	1.96	0.47
1:F:1261:PHE:CE1	1:F:1345:PRO:HA	2.50	0.47
1:A:570:GLN:HG2	1:A:596:GLY:CA	2.45	0.47
1:B:178:THR:O	1:B:358:VAL:HG11	2.15	0.47
1:B:391:ASN:HD22	1:B:418:ASN:HD22	1.62	0.47
1:E:889:PRO:HD2	1:E:951:LEU:HD21	1.97	0.47
1:E:1036:ARG:HH21	1:F:742:ARG:HH12	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1143:LEU:O	1:A:1149:ILE:HD11	2.16	0.46
1:C:377:PRO:HB2	1:C:400:PHE:O	2.15	0.46
1:A:1013:VAL:HG11	1:A:1075:PRO:HB3	1.98	0.46
1:A:178:THR:O	1:A:358:VAL:HG11	2.15	0.46
1:A:371:PRO:HD2	1:A:374:TRP:CD2	2.50	0.46
1:A:466:ILE:HB	1:A:487:PHE:HB2	1.96	0.46
1:B:154:VAL:HG23	1:B:170:PHE:HB3	1.96	0.46
1:B:275:LYS:HG3	1:B:644:TYR:HE1	1.81	0.46
1:D:520:LEU:HD23	1:D:757:ASP:HA	1.97	0.46
1:E:448:GLU:HG2	1:E:448:GLU:H	1.48	0.46
1:F:1143:LEU:HD23	1:F:1149:ILE:HG12	1.95	0.46
1:A:559:ASP:OD2	1:A:562:THR:HB	2.16	0.46
1:E:1143:LEU:O	1:E:1149:ILE:HD11	2.15	0.46
1:F:889:PRO:HD2	1:F:951:LEU:HD21	1.97	0.46
1:B:1345:PRO:O	1:B:1346:PHE:HB2	2.15	0.46
1:D:845:ILE:HG22	1:D:883:LEU:O	2.16	0.46
1:A:770:TRP:CE3	1:A:773:ASN:HB2	2.51	0.46
1:A:793:LEU:HD22	1:A:801:VAL:HG13	1.97	0.46
1:B:327:THR:HG21	1:B:367:VAL:HG21	1.97	0.46
1:B:373:SER:HB2	1:B:374:TRP:HD1	1.79	0.46
1:B:277:LEU:HB2	1:B:653:VAL:HB	1.98	0.46
1:C:1191:SER:HB2	1:C:1196:THR:HG23	1.98	0.46
1:C:570:GLN:HG2	1:C:596:GLY:CA	2.46	0.46
1:C:710:ILE:HD11	1:C:712:TYR:CZ	2.49	0.46
1:E:228:LYS:NZ	1:E:1096:THR:HG21	2.30	0.46
1:E:327:THR:HG21	1:E:367:VAL:HG21	1.97	0.46
1:E:1036:ARG:NH2	1:F:742:ARG:HH12	2.13	0.46
1:A:92:ARG:HG3	1:A:128:PHE:CE1	2.51	0.46
1:C:945:GLU:H	1:C:945:GLU:HG3	1.24	0.46
1:D:277:LEU:HD21	1:D:610:GLN:CG	2.45	0.46
1:F:162:PRO:HG3	1:F:344:TYR:CE2	2.51	0.46
1:A:276:ALA:HB2	1:A:655:PRO:HD3	1.97	0.46
1:A:275:LYS:HG3	1:A:644:TYR:HE1	1.81	0.46
1:F:614:GLY:HA3	1:F:854:ASN:ND2	2.31	0.46
1:A:983:ILE:HD11	1:A:1152:LYS:HD2	1.98	0.46
1:C:281:VAL:HG22	1:C:293:ASN:HA	1.98	0.46
1:D:281:VAL:HG22	1:D:293:ASN:HA	1.98	0.46
1:D:373:SER:HB2	1:D:374:TRP:HD1	1.81	0.46
1:E:177:PRO:HG2	1:E:180:TRP:CE3	2.51	0.46
1:F:1143:LEU:O	1:F:1149:ILE:HD11	2.15	0.46
1:A:1286:PRO:HG2	1:D:158:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:PRO:HB2	1:A:400:PHE:O	2.16	0.46
1:D:817:ARG:HD2	1:D:817:ARG:N	2.30	0.46
1:E:275:LYS:HG3	1:E:644:TYR:HE1	1.81	0.46
1:E:504:PRO:HG2	1:E:507:VAL:HG23	1.97	0.46
1:F:245:PRO:HG2	1:F:568:TYR:HB2	1.98	0.46
1:F:504:PRO:HG2	1:F:507:VAL:HG23	1.98	0.46
1:B:377:PRO:HG3	1:B:443:ILE:HG13	1.98	0.46
1:D:524:PRO:HD3	1:D:905:PRO:HG3	1.98	0.46
1:E:391:ASN:HD22	1:E:418:ASN:HD22	1.64	0.46
1:A:277:LEU:HD21	1:A:610:GLN:CG	2.47	0.45
1:B:277:LEU:HD21	1:B:610:GLN:HG3	1.98	0.45
1:B:770:TRP:CE3	1:B:773:ASN:HB2	2.50	0.45
1:B:889:PRO:HD2	1:B:951:LEU:HD21	1.98	0.45
1:D:377:PRO:HB2	1:D:400:PHE:O	2.16	0.45
1:D:861:PRO:HB3	1:D:879:THR:HG21	1.98	0.45
1:E:1274:ASP:CB	1:E:1277:THR:HG22	2.41	0.45
1:F:154:VAL:HG23	1:F:170:PHE:HB3	1.97	0.45
1:F:520:LEU:HD23	1:F:757:ASP:HA	1.96	0.45
1:A:614:GLY:HA3	1:A:854:ASN:ND2	2.30	0.45
1:A:845:ILE:HG22	1:A:883:LEU:O	2.17	0.45
1:A:889:PRO:HD2	1:A:951:LEU:HD21	1.98	0.45
1:B:371:PRO:HD2	1:B:374:TRP:CD2	2.51	0.45
1:C:749:ARG:NH1	1:C:1034:PHE:O	2.49	0.45
1:D:396:THR:CG2	1:D:404:ARG:HE	2.29	0.45
1:D:570:GLN:HG2	1:D:596:GLY:CA	2.44	0.45
1:E:178:THR:O	1:E:358:VAL:HG11	2.16	0.45
1:F:277:LEU:HD21	1:F:610:GLN:HG3	1.98	0.45
1:F:841:GLN:HE22	1:F:843:ASN:HB2	1.81	0.45
1:A:115:LEU:HD11	1:A:324:LEU:HD13	1.99	0.45
1:C:524:PRO:HD3	1:C:905:PRO:HG3	1.98	0.45
1:E:1008:ASP:HB3	1:E:1061:TRP:CD1	2.52	0.45
1:F:1112:VAL:HA	1:F:1127:PRO:HA	1.99	0.45
1:B:115:LEU:HD11	1:B:324:LEU:HD13	1.98	0.45
1:B:277:LEU:HD22	1:B:620:HIS:CD2	2.51	0.45
1:D:1013:VAL:HG11	1:D:1075:PRO:HB3	1.99	0.45
1:D:770:TRP:CE3	1:D:773:ASN:HB2	2.51	0.45
1:D:377:PRO:HG3	1:D:443:ILE:HG13	1.98	0.45
1:D:466:ILE:HB	1:D:487:PHE:HB2	1.97	0.45
1:F:1269:VAL:HA	1:F:1272:LEU:HD12	1.99	0.45
1:A:448:GLU:H	1:A:448:GLU:HG2	1.46	0.45
1:B:1112:VAL:HA	1:B:1127:PRO:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1191:SER:HB2	1:B:1196:THR:HG23	1.98	0.45
1:B:245:PRO:HG2	1:B:568:TYR:HB2	1.99	0.45
1:B:281:VAL:HG22	1:B:293:ASN:HA	1.99	0.45
1:D:1312:GLN:O	1:D:1345:PRO:HD2	2.17	0.45
1:E:377:PRO:HG3	1:E:443:ILE:HG13	1.97	0.45
1:E:770:TRP:CE3	1:E:773:ASN:HB2	2.50	0.45
1:F:391:ASN:HD22	1:F:418:ASN:HD22	1.64	0.45
1:A:281:VAL:HG22	1:A:293:ASN:HA	1.99	0.45
1:B:504:PRO:HG2	1:B:507:VAL:HG23	1.99	0.45
1:C:1269:VAL:HA	1:C:1272:LEU:HD12	1.98	0.45
1:C:275:LYS:HG3	1:C:644:TYR:HE1	1.80	0.45
1:D:277:LEU:HD22	1:D:620:HIS:CD2	2.52	0.45
1:E:162:PRO:HG3	1:E:344:TYR:CE2	2.52	0.45
1:E:524:PRO:HD3	1:E:905:PRO:HG3	1.97	0.45
1:E:841:GLN:HE22	1:E:843:ASN:HB2	1.82	0.45
1:F:1321:LYS:HB2	1:F:1328:PHE:CE1	2.52	0.45
1:C:115:LEU:HD11	1:C:324:LEU:HD13	1.98	0.45
1:C:841:GLN:HE22	1:C:843:ASN:HB2	1.81	0.45
1:D:793:LEU:HD22	1:D:801:VAL:HG13	1.98	0.45
1:E:245:PRO:HG2	1:E:568:TYR:HB2	1.98	0.45
1:F:793:LEU:HD22	1:F:801:VAL:HG13	1.99	0.45
1:A:520:LEU:HD23	1:A:757:ASP:HA	1.99	0.45
1:D:1143:LEU:O	1:D:1149:ILE:HD11	2.17	0.45
1:C:651:LYS:HE3	1:D:823:ASN:HD21	1.82	0.45
1:E:277:LEU:HD21	1:E:610:GLN:HG3	1.98	0.45
1:F:570:GLN:HG2	1:F:596:GLY:CA	2.46	0.45
1:C:770:TRP:CE3	1:C:773:ASN:HB2	2.51	0.45
1:F:277:LEU:HD21	1:F:610:GLN:CG	2.46	0.45
1:F:178:THR:O	1:F:358:VAL:HG11	2.16	0.45
1:A:732:LEU:HD13	1:A:732:LEU:HA	1.87	0.44
1:B:467:PHE:CG	1:B:542:VAL:HG21	2.52	0.44
1:D:811:LEU:HD23	1:D:817:ARG:CZ	2.48	0.44
1:E:1269:VAL:HA	1:E:1272:LEU:HD12	1.99	0.44
1:E:277:LEU:HD21	1:E:610:GLN:CG	2.46	0.44
1:F:845:ILE:HG22	1:F:883:LEU:O	2.17	0.44
1:A:1003:ASN:ND2	1:A:1146:THR:HG21	2.32	0.44
1:A:749:ARG:NH1	1:A:1034:PHE:O	2.51	0.44
1:A:525:LEU:HD21	1:A:557:MET:HG2	1.98	0.44
1:B:628:ILE:HD12	1:B:657:ARG:HD3	1.99	0.44
1:D:162:PRO:HG3	1:D:344:TYR:CE2	2.52	0.44
1:F:1013:VAL:HG11	1:F:1075:PRO:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:373:SER:HB2	1:F:374:TRP:HD1	1.82	0.44
1:F:466:ILE:HB	1:F:487:PHE:HB2	1.97	0.44
1:A:1112:VAL:HA	1:A:1127:PRO:HA	1.98	0.44
1:A:710:ILE:HD11	1:A:712:TYR:CZ	2.52	0.44
1:A:524:PRO:HD3	1:A:905:PRO:HG3	2.00	0.44
1:A:792:PRO:HG3	1:A:967:HIS:CE1	2.53	0.44
1:B:162:PRO:HG3	1:B:344:TYR:CE2	2.53	0.44
1:C:672:LYS:NZ	1:D:814:GLU:O	2.42	0.44
1:F:1191:SER:HB2	1:F:1196:THR:HG23	1.99	0.44
1:F:165:ASP:HB3	1:F:168:LYS:HB2	1.98	0.44
1:F:238:GLN:HE21	1:F:239:ARG:HG2	1.81	0.44
1:A:177:PRO:HG2	1:A:180:TRP:CE3	2.53	0.44
1:B:1269:VAL:HA	1:B:1272:LEU:HD12	1.98	0.44
1:B:177:PRO:HG2	1:B:180:TRP:CE3	2.53	0.44
1:B:710:ILE:HD11	1:B:712:TYR:CZ	2.52	0.44
1:C:1013:VAL:HG11	1:C:1075:PRO:HB3	1.99	0.44
1:C:58:GLN:OE1	1:C:149:GLU:CB	2.65	0.44
1:D:277:LEU:HB2	1:D:653:VAL:HB	1.98	0.44
1:F:275:LYS:HG3	1:F:644:TYR:HE1	1.82	0.44
1:A:1269:VAL:HA	1:A:1272:LEU:HD12	1.99	0.44
1:A:92:ARG:HG3	1:A:128:PHE:CD1	2.53	0.44
1:A:1334:ALA:HB3	1:A:1339:PRO:HA	2.00	0.44
1:B:1109:PRO:HB3	1:B:1137:MET:SD	2.57	0.44
1:B:570:GLN:HG2	1:B:596:GLY:CA	2.46	0.44
1:C:926:SER:O	1:C:983:ILE:HG12	2.18	0.44
1:A:378:LYS:O	1:A:397:THR:HG23	2.17	0.44
1:B:749:ARG:NH1	1:B:1034:PHE:O	2.51	0.44
1:E:1003:ASN:ND2	1:E:1146:THR:HG21	2.32	0.44
1:E:91:VAL:HG21	1:E:131:ARG:CZ	2.47	0.44
1:E:524:PRO:HD2	1:E:557:MET:CE	2.48	0.44
1:F:749:ARG:NH1	1:F:1034:PHE:O	2.50	0.44
1:F:228:LYS:NZ	1:F:1096:THR:HG21	2.31	0.44
1:F:525:LEU:HD21	1:F:557:MET:HG2	2.00	0.44
1:B:1334:ALA:HB3	1:B:1339:PRO:HA	2.00	0.44
1:A:651:LYS:HE3	1:B:823:ASN:HD21	1.83	0.44
1:C:1008:ASP:HB3	1:C:1061:TRP:CD1	2.51	0.44
1:C:178:THR:O	1:C:358:VAL:HG11	2.18	0.44
1:C:793:LEU:HD12	1:C:941:TRP:HE3	1.82	0.44
1:D:749:ARG:NH1	1:D:1034:PHE:O	2.51	0.44
1:A:1008:ASP:HB3	1:A:1061:TRP:CD1	2.52	0.44
1:A:396:THR:CG2	1:A:404:ARG:HE	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ASN:HB2	1:A:473:ALA:HB2	1.99	0.44
1:B:1143:LEU:O	1:B:1149:ILE:HD11	2.18	0.44
1:B:470:ASN:OD1	1:B:472:HIS:HB2	2.18	0.44
1:B:861:PRO:HB3	1:B:879:THR:HG21	2.00	0.44
1:C:1112:VAL:HA	1:C:1127:PRO:HA	1.99	0.44
1:E:152:SER:OG	1:E:172:LEU:HB3	2.18	0.44
1:F:1292:PRO:HG2	1:F:1295:PHE:HB2	2.00	0.44
1:D:100:ILE:H	1:D:100:ILE:HD12	1.83	0.44
1:D:245:PRO:HG2	1:D:568:TYR:HB2	2.00	0.44
1:E:1191:SER:HB2	1:E:1196:THR:HG23	2.00	0.44
1:E:845:ILE:HG22	1:E:883:LEU:O	2.17	0.44
1:B:536:ARG:NH1	1:B:686:ASN:HB3	2.33	0.43
1:C:135:ASN:HD22	1:C:1330:PRO:HD2	1.83	0.43
1:D:200:LEU:HD12	1:D:344:TYR:CE2	2.53	0.43
1:D:115:LEU:HD11	1:D:324:LEU:HD13	2.00	0.43
1:D:277:LEU:HD21	1:D:610:GLN:HG3	2.00	0.43
1:D:628:ILE:HD12	1:D:657:ARG:HD3	2.00	0.43
1:F:1008:ASP:HB3	1:F:1061:TRP:CD1	2.52	0.43
1:F:628:ILE:HD12	1:F:657:ARG:HD3	2.00	0.43
1:F:524:PRO:HD3	1:F:905:PRO:HG3	2.00	0.43
1:A:238:GLN:HE21	1:A:239:ARG:HG2	1.84	0.43
1:B:559:ASP:OD2	1:B:562:THR:HB	2.18	0.43
1:D:1112:VAL:HA	1:D:1127:PRO:HA	2.00	0.43
1:D:1269:VAL:HA	1:D:1272:LEU:HD12	1.99	0.43
1:D:177:PRO:HG2	1:D:180:TRP:CE3	2.53	0.43
1:E:793:LEU:HD22	1:E:801:VAL:HG13	1.99	0.43
1:F:470:ASN:OD1	1:F:472:HIS:HB2	2.18	0.43
1:A:373:SER:HB2	1:A:374:TRP:HD1	1.83	0.43
1:A:405:HIS:HE1	1:A:686:ASN:O	2.01	0.43
1:B:237:THR:HG21	1:B:575:LEU:HD13	2.01	0.43
1:C:237:THR:HG21	1:C:575:LEU:HD13	2.00	0.43
1:C:628:ILE:HD12	1:C:657:ARG:HD3	2.00	0.43
1:D:504:PRO:HG2	1:D:507:VAL:HG23	1.99	0.43
1:D:732:LEU:HD13	1:D:732:LEU:HA	1.87	0.43
1:A:200:LEU:HD12	1:A:344:TYR:CE2	2.52	0.43
1:D:152:SER:OG	1:D:172:LEU:HB3	2.18	0.43
1:E:1112:VAL:HA	1:E:1127:PRO:HA	1.99	0.43
1:E:1261:PHE:CE1	1:E:1345:PRO:HA	2.54	0.43
1:E:238:GLN:HE21	1:E:239:ARG:HG2	1.83	0.43
1:E:628:ILE:HD12	1:E:657:ARG:HD3	2.01	0.43
1:F:1193:GLN:HB3	1:F:1193:GLN:HE21	1.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:177:PRO:HG2	1:F:180:TRP:CE3	2.52	0.43
1:F:115:LEU:HD11	1:F:324:LEU:HD13	2.00	0.43
1:B:987:ALA:CA	1:B:1115:TYR:CD2	3.02	0.43
1:B:599:ASN:HB2	1:B:658:TYR:O	2.18	0.43
1:B:524:PRO:HD3	1:B:905:PRO:HG3	2.00	0.43
1:C:1003:ASN:ND2	1:C:1146:THR:HG21	2.32	0.43
1:C:72:ASN:HB2	1:C:473:ALA:HB2	2.01	0.43
1:E:467:PHE:CG	1:E:542:VAL:HG21	2.54	0.43
1:F:327:THR:HG21	1:F:367:VAL:HG21	1.99	0.43
1:F:770:TRP:CE3	1:F:773:ASN:HB2	2.51	0.43
1:A:793:LEU:HD12	1:A:941:TRP:HE3	1.83	0.43
1:B:92:ARG:HG3	1:B:128:PHE:CE1	2.54	0.43
1:C:373:SER:HB2	1:C:374:TRP:HD1	1.82	0.43
1:C:271:SER:HB2	1:C:868:VAL:HG22	2.01	0.43
1:D:237:THR:HG21	1:D:575:LEU:HD13	2.01	0.43
1:D:72:ASN:HB2	1:D:473:ALA:HB2	2.00	0.43
1:F:945:GLU:HG3	1:F:945:GLU:H	1.24	0.43
1:A:699:ASN:ND2	1:A:702:LEU:HB2	2.34	0.43
1:B:793:LEU:HD12	1:B:941:TRP:HE3	1.83	0.43
1:C:1334:ALA:HB3	1:C:1339:PRO:HA	2.01	0.43
1:E:1301:ARG:HG2	1:E:1328:PHE:CD2	2.54	0.43
1:F:1321:LYS:HA	1:F:1328:PHE:CD1	2.53	0.43
1:F:374:TRP:N	1:F:374:TRP:CD1	2.87	0.43
1:F:91:VAL:HG21	1:F:131:ARG:CZ	2.48	0.43
1:C:1041:TYR:CE1	1:C:1181:ASN:HB2	2.54	0.43
1:A:470:ASN:OD1	1:A:472:HIS:HB2	2.19	0.43
1:A:467:PHE:CG	1:A:542:VAL:HG21	2.54	0.43
1:C:396:THR:CG2	1:C:404:ARG:HE	2.31	0.43
1:C:599:ASN:HB2	1:C:658:TYR:O	2.19	0.43
1:D:1097:ASN:HB2	1:D:1098:PRO:CD	2.43	0.43
1:D:165:ASP:HB3	1:D:168:LYS:HB2	2.01	0.43
1:D:273:ARG:HD3	1:D:619:PRO:HB3	2.01	0.43
1:A:1191:SER:HB2	1:A:1196:THR:HG23	2.00	0.43
1:B:1003:ASN:ND2	1:B:1146:THR:HG21	2.33	0.43
1:B:277:LEU:HD22	1:B:620:HIS:HD2	1.84	0.43
1:C:277:LEU:HD21	1:C:610:GLN:CG	2.49	0.43
1:C:277:LEU:HD21	1:C:610:GLN:HG3	2.00	0.43
1:E:165:ASP:HB3	1:E:168:LYS:HB2	2.01	0.43
1:E:200:LEU:HD12	1:E:344:TYR:CE2	2.53	0.43
1:E:396:THR:CG2	1:E:404:ARG:HE	2.32	0.43
1:E:570:GLN:HG2	1:E:596:GLY:CA	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:PRO:HG3	1:A:344:TYR:CE2	2.54	0.42
1:B:1008:ASP:HB3	1:B:1061:TRP:CD1	2.54	0.42
1:B:396:THR:CG2	1:B:404:ARG:HE	2.31	0.42
1:B:273:ARG:HD3	1:B:619:PRO:HB3	2.01	0.42
1:B:793:LEU:HD22	1:B:801:VAL:HG13	2.01	0.42
1:B:913:ARG:NH2	1:B:920:PRO:HD3	2.34	0.42
1:C:1070:ASP:HB3	1:C:1072:ASP:OD1	2.19	0.42
1:C:172:LEU:HD11	1:C:351:ASN:HB3	2.01	0.42
1:C:504:PRO:HG2	1:C:507:VAL:HG23	2.01	0.42
1:C:811:LEU:HD21	1:C:895:ASN:O	2.19	0.42
1:D:811:LEU:HD23	1:D:817:ARG:NE	2.34	0.42
1:E:281:VAL:HG22	1:E:293:ASN:HA	2.00	0.42
1:E:72:ASN:HB2	1:E:473:ALA:HB2	2.01	0.42
1:A:861:PRO:HB3	1:A:879:THR:HG21	2.01	0.42
1:A:913:ARG:NH2	1:A:920:PRO:HD3	2.34	0.42
1:B:148:MET:HE1	1:B:355:PHE:HZ	1.84	0.42
1:C:228:LYS:NZ	1:C:239:ARG:HH12	2.17	0.42
1:C:983:ILE:HD11	1:C:1152:LYS:HD2	2.00	0.42
1:D:1191:SER:HB2	1:D:1196:THR:HG23	2.00	0.42
1:D:92:ARG:HG3	1:D:128:PHE:CD1	2.54	0.42
1:D:194:SER:CB	1:D:200:LEU:HD23	2.48	0.42
1:F:152:SER:OG	1:F:172:LEU:HB3	2.18	0.42
1:F:467:PHE:CG	1:F:542:VAL:HG21	2.54	0.42
1:A:1319:GLU:HB3	1:A:1328:PHE:HB3	2.00	0.42
1:B:525:LEU:HD21	1:B:557:MET:HG2	2.00	0.42
1:C:59:GLN:HB2	1:C:143:ILE:H	1.84	0.42
1:D:1319:GLU:HB3	1:D:1328:PHE:HB3	2.01	0.42
1:D:178:THR:O	1:D:358:VAL:HG11	2.19	0.42
1:E:1292:PRO:HG2	1:E:1295:PHE:HB2	2.00	0.42
1:E:373:SER:HB2	1:E:374:TRP:HD1	1.84	0.42
1:F:281:VAL:HG22	1:F:293:ASN:HA	2.00	0.42
1:F:396:THR:CG2	1:F:404:ARG:HE	2.31	0.42
1:F:994:SER:HB2	1:F:1137:MET:HE2	2.01	0.42
1:A:1070:ASP:HB3	1:A:1072:ASP:OD1	2.20	0.42
1:B:792:PRO:HG3	1:B:967:HIS:CE1	2.54	0.42
1:C:448:GLU:H	1:C:448:GLU:HG2	1.48	0.42
1:C:651:LYS:CE	1:D:823:ASN:HD21	2.32	0.42
1:D:405:HIS:HE1	1:D:686:ASN:O	2.02	0.42
1:D:841:GLN:HE22	1:D:843:ASN:HB2	1.85	0.42
1:D:811:LEU:HD11	1:D:895:ASN:OD1	2.20	0.42
1:E:470:ASN:OD1	1:E:472:HIS:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:749:ARG:NH1	1:E:1034:PHE:O	2.52	0.42
1:A:244:SER:HA	1:A:571:LEU:HD22	2.01	0.42
1:A:628:ILE:HD12	1:A:657:ARG:HD3	2.00	0.42
1:B:165:ASP:HB3	1:B:168:LYS:HB2	2.02	0.42
1:B:72:ASN:HB2	1:B:473:ALA:HB2	2.00	0.42
1:D:1334:ALA:HB3	1:D:1339:PRO:HA	2.01	0.42
1:D:467:PHE:CG	1:D:542:VAL:HG21	2.54	0.42
1:D:92:ARG:HG3	1:D:128:PHE:CE1	2.55	0.42
1:F:1274:ASP:CB	1:F:1277:THR:HG22	2.40	0.42
1:F:201:TYR:CE1	1:F:345:ASP:HB3	2.55	0.42
1:A:165:ASP:HB3	1:A:168:LYS:HB2	2.02	0.42
1:B:1261:PHE:CE1	1:B:1345:PRO:HA	2.52	0.42
1:C:177:PRO:HG2	1:C:180:TRP:CE3	2.54	0.42
1:C:817:ARG:HA	1:C:817:ARG:NE	2.34	0.42
1:D:1070:ASP:HB3	1:D:1072:ASP:OD1	2.19	0.42
1:D:994:SER:HB2	1:D:1137:MET:HE3	2.02	0.42
1:E:1013:VAL:HG11	1:E:1075:PRO:HB3	2.02	0.42
1:F:1301:ARG:CG	1:F:1328:PHE:HE2	2.32	0.42
1:A:749:ARG:HG3	1:A:749:ARG:HH21	1.84	0.42
1:A:817:ARG:HA	1:A:817:ARG:NE	2.35	0.42
1:A:841:GLN:HE22	1:A:843:ASN:HB2	1.84	0.42
1:B:405:HIS:HE1	1:B:686:ASN:O	2.03	0.42
1:D:710:ILE:HD11	1:D:712:TYR:CZ	2.54	0.42
1:E:994:SER:HB2	1:E:1137:MET:HE3	2.02	0.42
1:F:1003:ASN:ND2	1:F:1146:THR:HG21	2.33	0.42
1:F:536:ARG:NH1	1:F:686:ASN:HB3	2.35	0.42
1:F:72:ASN:HB2	1:F:473:ALA:HB2	2.02	0.42
1:B:987:ALA:HA	1:B:1115:TYR:CD2	2.55	0.42
1:B:152:SER:OG	1:B:172:LEU:HB3	2.20	0.42
1:A:1189:GLU:OE2	1:B:729:LEU:HD11	2.20	0.42
1:B:732:LEU:HA	1:B:732:LEU:HD13	1.90	0.42
1:C:244:SER:HA	1:C:571:LEU:HD22	2.02	0.42
1:C:536:ARG:NH1	1:C:686:ASN:HB3	2.34	0.42
1:D:122:LEU:HB3	1:D:126:GLN:NE2	2.35	0.42
1:D:617:PHE:CE2	1:D:859:PHE:HB2	2.54	0.42
1:D:773:ASN:HB3	1:D:775:LYS:HB2	2.01	0.42
1:E:543:LYS:HD2	1:E:1012:LEU:HB3	2.02	0.42
1:E:1097:ASN:HB3	1:E:1098:PRO:HD3	2.02	0.42
1:E:557:MET:HB3	1:E:557:MET:HE2	1.85	0.42
1:F:543:LYS:HD2	1:F:1012:LEU:HB3	2.02	0.42
1:F:599:ASN:HB2	1:F:658:TYR:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1312:GLN:O	1:A:1345:PRO:HD2	2.20	0.42
1:B:1070:ASP:HB3	1:B:1072:ASP:OD1	2.19	0.42
1:B:587:GLU:HG3	1:B:1107:TYR:HE1	1.85	0.42
1:C:152:SER:OG	1:C:172:LEU:HB3	2.20	0.42
1:D:1003:ASN:ND2	1:D:1146:THR:HG21	2.34	0.42
1:E:115:LEU:HD11	1:E:324:LEU:HD13	2.01	0.42
1:A:1141:LEU:HA	1:A:1141:LEU:HD12	1.93	0.42
1:B:1319:GLU:HB3	1:B:1328:PHE:HB3	2.01	0.42
1:B:374:TRP:CD1	1:B:374:TRP:N	2.87	0.42
1:B:92:ARG:HG3	1:B:128:PHE:CD1	2.54	0.42
1:C:470:ASN:OD1	1:C:472:HIS:HB2	2.18	0.42
1:C:467:PHE:CG	1:C:542:VAL:HG21	2.55	0.42
1:C:994:SER:HB2	1:C:1137:MET:HE3	2.01	0.42
1:E:509:PHE:HZ	1:E:537:MET:HE1	1.84	0.42
1:E:92:ARG:HG3	1:E:128:PHE:CE2	2.54	0.42
1:F:237:THR:HG21	1:F:575:LEU:HD13	2.02	0.42
1:F:793:LEU:HD12	1:F:941:TRP:HE3	1.85	0.42
1:F:983:ILE:HD11	1:F:1152:LYS:HD2	2.02	0.42
1:A:1097:ASN:HB3	1:A:1098:PRO:HD2	1.99	0.41
1:B:238:GLN:HE21	1:B:239:ARG:HG2	1.85	0.41
1:C:661:LEU:HD13	1:C:901:ASN:HD21	1.85	0.41
1:D:536:ARG:NH1	1:D:686:ASN:HB3	2.35	0.41
1:D:923:ILE:HA	1:D:923:ILE:HD13	1.85	0.41
1:E:109:ASP:HB3	1:E:113:LYS:HD3	2.02	0.41
1:F:543:LYS:HB2	1:F:1012:LEU:HD13	2.02	0.41
1:C:391:ASN:ND2	1:C:418:ASN:HD22	2.18	0.41
1:C:850:VAL:CG2	1:C:851:LYS:N	2.83	0.41
1:D:631:ASN:OD1	1:D:633:ASN:HB2	2.20	0.41
1:D:599:ASN:HB2	1:D:658:TYR:O	2.20	0.41
1:A:1279:PHE:HE1	1:A:1301:ARG:HD2	1.72	0.41
1:B:1013:VAL:HG11	1:B:1075:PRO:HB3	2.02	0.41
1:B:244:SER:HA	1:B:571:LEU:HD22	2.03	0.41
1:B:888:SER:HB2	1:B:889:PRO:HD2	2.02	0.41
1:C:164:PHE:CZ	1:C:166:PRO:HA	2.55	0.41
1:C:162:PRO:HG3	1:C:344:TYR:CE2	2.54	0.41
1:C:810:HIS:CE1	1:C:814:GLU:HG2	2.54	0.41
1:E:172:LEU:HD11	1:E:351:ASN:HB3	2.03	0.41
1:E:374:TRP:CD1	1:E:374:TRP:N	2.87	0.41
1:F:509:PHE:HZ	1:F:537:MET:HE1	1.85	0.41
1:B:696:ALA:HB1	1:B:747:VAL:HG12	2.01	0.41
1:C:200:LEU:HD12	1:C:344:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:939:GLN:HE21	1:C:950:ASN:HB2	1.84	0.41
1:D:100:ILE:CD1	1:D:100:ILE:H	2.33	0.41
1:D:945:GLU:H	1:D:945:GLU:HG3	1.25	0.41
1:D:924:ASN:CB	1:D:985:PHE:HA	2.51	0.41
1:E:983:ILE:HD11	1:E:1152:LYS:HD2	2.03	0.41
1:A:1137:MET:HB2	1:A:1137:MET:HE2	1.57	0.41
1:A:237:THR:HG21	1:A:575:LEU:HD13	2.01	0.41
1:B:194:SER:CB	1:B:200:LEU:HD23	2.49	0.41
1:B:923:ILE:HA	1:B:923:ILE:HD13	1.87	0.41
1:C:122:LEU:HB3	1:C:126:GLN:NE2	2.33	0.41
1:E:237:THR:HG21	1:E:575:LEU:HD13	2.02	0.41
1:E:710:ILE:HD11	1:E:712:TYR:CZ	2.55	0.41
1:F:835:ARG:HB3	1:F:1122:ASN:HA	2.02	0.41
1:A:135:ASN:HD22	1:A:1330:PRO:HD2	1.86	0.41
1:A:599:ASN:HB2	1:A:658:TYR:O	2.20	0.41
1:B:810:HIS:ND1	1:B:817:ARG:HD3	2.35	0.41
1:C:1312:GLN:O	1:C:1345:PRO:HD2	2.21	0.41
1:C:1319:GLU:HB3	1:C:1328:PHE:HB3	2.01	0.41
1:C:631:ASN:OD1	1:C:633:ASN:HB2	2.20	0.41
1:C:846:PRO:HG2	1:C:849:GLN:NE2	2.36	0.41
1:D:846:PRO:HG2	1:D:849:GLN:NE2	2.35	0.41
1:F:1097:ASN:HB3	1:F:1098:PRO:HD3	2.03	0.41
1:F:135:ASN:HD22	1:F:1330:PRO:HD2	1.84	0.41
1:A:164:PHE:CZ	1:A:166:PRO:HA	2.55	0.41
1:B:1301:ARG:HG2	1:B:1328:PHE:CD2	2.56	0.41
1:B:845:ILE:HG22	1:B:883:LEU:O	2.21	0.41
1:C:525:LEU:HD21	1:C:557:MET:HG2	2.03	0.41
1:C:861:PRO:HB3	1:C:879:THR:HG21	2.03	0.41
1:C:91:VAL:HG21	1:C:131:ARG:CZ	2.51	0.41
1:D:135:ASN:HD22	1:D:1330:PRO:HD2	1.85	0.41
1:E:1036:ARG:HH21	1:F:742:ARG:NH1	2.19	0.41
1:E:1312:GLN:O	1:E:1345:PRO:HD2	2.19	0.41
1:E:271:SER:HB2	1:E:868:VAL:HG22	2.02	0.41
1:A:850:VAL:CG2	1:A:851:LYS:N	2.84	0.41
1:B:99:ASN:ND2	1:B:102:SER:HB3	2.35	0.41
1:B:122:LEU:HB3	1:B:126:GLN:NE2	2.35	0.41
1:B:467:PHE:CD1	1:B:542:VAL:HG21	2.56	0.41
1:C:374:TRP:CD1	1:C:374:TRP:N	2.88	0.41
1:C:702:LEU:HD12	1:C:702:LEU:HA	1.87	0.41
1:D:696:ALA:HB1	1:D:747:VAL:HG12	2.02	0.41
1:F:527:THR:HB	1:F:533:TYR:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:SER:HB2	1:A:868:VAL:HG22	2.03	0.41
1:B:809:GLN:HB2	1:B:828:ILE:CD1	2.50	0.41
1:B:615:SER:N	1:B:854:ASN:HD21	2.18	0.41
1:B:939:GLN:HE21	1:B:950:ASN:HB2	1.85	0.41
1:C:835:ARG:HB3	1:C:1122:ASN:HA	2.02	0.41
1:E:92:ARG:HG3	1:E:128:PHE:CD2	2.56	0.41
1:F:1248:THR:HA	1:F:1251:ILE:HD12	2.03	0.41
1:F:92:ARG:HG3	1:F:128:PHE:CE2	2.55	0.41
1:F:1319:GLU:HB3	1:F:1328:PHE:HB3	2.02	0.41
1:F:1321:LYS:HA	1:F:1328:PHE:HD1	1.86	0.41
1:A:122:LEU:HB3	1:A:126:GLN:NE2	2.34	0.41
1:A:243:ASP:HB2	1:A:309:VAL:HG11	2.03	0.41
1:B:543:LYS:HD2	1:B:1012:LEU:HB3	2.03	0.41
1:B:749:ARG:HG3	1:B:749:ARG:HH21	1.85	0.41
1:C:587:GLU:HG3	1:C:1107:TYR:HE1	1.86	0.41
1:C:1261:PHE:CE1	1:C:1345:PRO:HA	2.56	0.41
1:C:405:HIS:HE1	1:C:686:ASN:O	2.03	0.41
1:C:926:SER:O	1:C:983:ILE:HG23	2.20	0.41
1:D:1032:THR:OG1	1:D:1043:GLY:HA2	2.20	0.41
1:E:1334:ALA:HB3	1:E:1339:PRO:HA	2.02	0.41
1:E:661:LEU:HD13	1:E:901:ASN:HD21	1.85	0.41
1:F:122:LEU:HB3	1:F:126:GLN:NE2	2.36	0.41
1:A:172:LEU:HD11	1:A:351:ASN:HB3	2.03	0.41
1:A:696:ALA:HB1	1:A:747:VAL:HG12	2.03	0.41
1:B:987:ALA:CA	1:B:1115:TYR:HD2	2.34	0.41
1:C:543:LYS:HB2	1:C:1012:LEU:HD13	2.03	0.41
1:D:201:TYR:CE1	1:D:345:ASP:HB3	2.56	0.41
1:D:244:SER:HA	1:D:571:LEU:HD22	2.03	0.41
1:E:1319:GLU:HB3	1:E:1328:PHE:HB3	2.02	0.41
1:E:702:LEU:HA	1:E:702:LEU:HD12	1.92	0.41
1:E:793:LEU:HD12	1:E:941:TRP:HE3	1.86	0.41
1:E:945:GLU:HG3	1:E:945:GLU:H	1.24	0.41
1:F:244:SER:HA	1:F:571:LEU:HD22	2.03	0.41
1:A:130:ILE:HG13	1:A:143:ILE:HG23	2.03	0.40
1:A:543:LYS:HD2	1:A:1012:LEU:HB3	2.03	0.40
1:A:661:LEU:HD13	1:A:901:ASN:HD21	1.86	0.40
1:B:983:ILE:HD11	1:B:1152:LYS:HD2	2.01	0.40
1:B:773:ASN:HB3	1:B:775:LYS:HB2	2.03	0.40
1:C:792:PRO:HG3	1:C:967:HIS:CE1	2.56	0.40
1:D:115:LEU:HA	1:D:115:LEU:HD23	1.88	0.40
1:D:391:ASN:ND2	1:D:418:ASN:HD22	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:273:ARG:HD3	1:F:619:PRO:HB3	2.03	0.40
1:A:91:VAL:HG21	1:A:131:ARG:CZ	2.52	0.40
1:A:397:THR:HG22	1:A:418:ASN:OD1	2.21	0.40
1:A:579:ALA:HA	1:A:582:GLN:HB2	2.04	0.40
1:A:923:ILE:HA	1:A:923:ILE:HD13	1.87	0.40
1:B:527:THR:HB	1:B:533:TYR:HB3	2.02	0.40
1:C:1031:PHE:CE1	1:C:1044:ILE:HD11	2.56	0.40
1:C:682:PHE:HE2	1:D:820:PHE:CE1	2.40	0.40
1:D:809:GLN:NE2	1:D:828:ILE:HD12	2.36	0.40
1:D:888:SER:HB2	1:D:889:PRO:HD2	2.04	0.40
1:E:1141:LEU:HA	1:E:1141:LEU:HD12	1.95	0.40
1:A:109:ASP:HB3	1:A:113:LYS:HD2	2.00	0.40
1:A:467:PHE:CD1	1:A:542:VAL:HG21	2.55	0.40
1:A:823:ASN:HD21	1:B:651:LYS:HE3	1.86	0.40
1:B:631:ASN:OD1	1:B:633:ASN:HB2	2.22	0.40
1:C:151:PRO:HG3	1:C:180:TRP:CE2	2.57	0.40
1:D:983:ILE:HD11	1:D:1152:LYS:HD2	2.03	0.40
1:D:1301:ARG:HG2	1:D:1328:PHE:CD2	2.56	0.40
1:D:527:THR:HB	1:D:533:TYR:HB3	2.03	0.40
1:D:570:GLN:HG3	1:D:573:LYS:HE2	2.03	0.40
1:D:792:PRO:HG3	1:D:967:HIS:CE1	2.56	0.40
1:D:811:LEU:HD13	1:D:894:ILE:CG1	2.51	0.40
1:E:123:ASP:OD1	1:E:208:LYS:HE2	2.20	0.40
1:E:599:ASN:HB2	1:E:658:TYR:O	2.20	0.40
1:E:536:ARG:NH1	1:E:686:ASN:HB3	2.36	0.40
1:E:835:ARG:HB3	1:E:1122:ASN:HA	2.02	0.40
1:F:1318:LEU:HB3	1:F:1331:VAL:HB	2.03	0.40
1:F:231:GLN:HG3	1:F:1096:THR:HA	2.02	0.40
1:A:374:TRP:N	1:A:374:TRP:CD1	2.86	0.40
1:A:536:ARG:NH1	1:A:686:ASN:HB3	2.36	0.40
1:B:835:ARG:HB3	1:B:1122:ASN:HA	2.03	0.40
1:D:702:LEU:HD12	1:D:702:LEU:HA	1.87	0.40
1:D:749:ARG:HH21	1:D:749:ARG:HG3	1.86	0.40
1:D:661:LEU:HD13	1:D:901:ASN:HD21	1.85	0.40
1:E:939:GLN:HE21	1:E:950:ASN:HB2	1.87	0.40
1:F:200:LEU:HD12	1:F:344:TYR:CE2	2.55	0.40
1:F:661:LEU:HD13	1:F:901:ASN:HD21	1.85	0.40
1:A:817:ARG:NH2	1:A:817:ARG:HG2	2.35	0.40
1:B:661:LEU:HD13	1:B:901:ASN:HD21	1.87	0.40
1:D:467:PHE:CD1	1:D:542:VAL:HG21	2.56	0.40
1:D:579:ALA:HA	1:D:582:GLN:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:559:ASP:OD2	1:E:562:THR:HB	2.22	0.40
1:F:710:ILE:HD11	1:F:712:TYR:CZ	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1270/1304 (97%)	1128 (89%)	122 (10%)	20 (2%)	9 40
1	B	1267/1304 (97%)	1136 (90%)	114 (9%)	17 (1%)	12 44
1	C	1266/1304 (97%)	1128 (89%)	123 (10%)	15 (1%)	13 46
1	D	1263/1304 (97%)	1127 (89%)	117 (9%)	19 (2%)	10 41
1	E	1252/1304 (96%)	1118 (89%)	117 (9%)	17 (1%)	11 43
1	F	1252/1304 (96%)	1114 (89%)	119 (10%)	19 (2%)	10 41
All	All	7570/7824 (97%)	6751 (89%)	712 (9%)	107 (1%)	11 43

All (107) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	SER
1	A	1094	TYR
1	A	1097	ASN
1	A	1241	GLY
1	B	811	LEU
1	B	926	SER
1	B	1241	GLY
1	C	926	SER
1	C	1240	GLN
1	D	874	SER

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Mol	Chain	Res	Type
1	D	926	SER
1	D	1096	THR
1	D	1097	ASN
1	D	1175	THR
1	D	1240	GLN
1	E	926	SER
1	E	1241	GLY
1	F	111	ASN
1	F	926	SER
1	F	1241	GLY
1	A	99	ASN
1	A	618	GLY
1	A	827	ASP
1	A	926	SER
1	A	1057	ALA
1	A	1096	THR
1	A	1346	PHE
1	B	618	GLY
1	B	854	ASN
1	B	1057	ALA
1	C	143	ILE
1	C	618	GLY
1	C	827	ASP
1	C	1057	ALA
1	D	618	GLY
1	D	807	ILE
1	D	1057	ALA
1	E	618	GLY
1	E	874	SER
1	E	875	SER
1	E	1057	ALA
1	E	1096	THR
1	E	1346	PHE
1	F	108	SER
1	F	618	GLY
1	F	874	SER
1	F	875	SER
1	F	1057	ALA
1	F	1096	THR
1	F	1346	PHE
1	A	662	TYR
1	A	927	GLY

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Mol	Chain	Res	Type
1	A	1133	ALA
1	B	662	TYR
1	C	662	TYR
1	C	927	GLY
1	C	1094	TYR
1	C	1346	PHE
1	D	662	TYR
1	D	808	THR
1	D	1090	SER
1	E	662	TYR
1	F	662	TYR
1	A	823	ASN
1	B	143	ILE
1	B	808	THR
1	B	823	ASN
1	B	1133	ALA
1	C	1133	ALA
1	D	143	ILE
1	D	823	ASN
1	E	143	ILE
1	E	1097	ASN
1	E	1133	ALA
1	F	143	ILE
1	F	1092	THR
1	F	1097	ASN
1	F	1133	ALA
1	A	232	SER
1	B	568	TYR
1	B	1089	ASN
1	C	568	TYR
1	C	809	GLN
1	C	823	ASN
1	D	568	TYR
1	D	813	LYS
1	D	1133	ALA
1	E	568	TYR
1	E	823	ASN
1	E	1092	THR
1	F	568	TYR
1	F	823	ASN
1	A	816	THR
1	A	852	PRO

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Mol	Chain	Res	Type
1	B	227	VAL
1	B	790	SER
1	B	1094	TYR
1	C	852	PRO
1	A	1268	PRO
1	B	852	PRO
1	D	852	PRO
1	E	852	PRO
1	E	1268	PRO
1	F	852	PRO
1	F	1268	PRO
1	A	143	ILE
1	D	1268	PRO

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	1121/1146 (98%)	964 (86%)	157 (14%)	3 15
1	B	1120/1146 (98%)	965 (86%)	155 (14%)	3 15
1	C	1118/1146 (98%)	973 (87%)	145 (13%)	4 18
1	D	1117/1146 (98%)	969 (87%)	148 (13%)	4 17
1	E	1107/1146 (97%)	958 (86%)	149 (14%)	4 16
1	F	1108/1146 (97%)	958 (86%)	150 (14%)	4 16
All	All	6691/6876 (97%)	5787 (86%)	904 (14%)	4 16

All (904) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	88	PHE
1	A	91	VAL
1	A	98	LEU
1	A	101	SER

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Mol	Chain	Res	Type
1	A	106	ASN
1	A	119	GLU
1	A	125	GLN
1	A	127	ASN
1	A	130	ILE
1	A	142	ASP
1	A	143	ILE
1	A	156	ARG
1	A	158	LEU
1	A	178	THR
1	A	184	LYS
1	A	187	VAL
1	A	197	SER
1	A	203	VAL
1	A	204	LEU
1	A	218	ASN
1	A	220	VAL
1	A	222	LYS
1	A	223	GLU
1	A	225	LEU
1	A	228	LYS
1	A	235	ASN
1	A	238	GLN
1	A	239	ARG
1	A	242	LYS
1	A	251	LYS
1	A	257	SER
1	A	259	THR
1	A	268	MET
1	A	272	THR
1	A	300	LEU
1	A	301	LYS
1	A	315	LYS
1	A	324	LEU
1	A	333	GLU
1	A	334	LYS
1	A	342	SER
1	A	350	GLU
1	A	353	THR
1	A	358	VAL
1	A	373	SER
1	A	376	THR

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Mol	Chain	Res	Type
1	A	380	ASN
1	A	384	ILE
1	A	393	LEU
1	A	396	THR
1	A	404	ARG
1	A	405	HIS
1	A	415	LYS
1	A	425	VAL
1	A	431	LYS
1	A	436	LYS
1	A	437	LYS
1	A	453	ASN
1	A	458	VAL
1	A	492	THR
1	A	508	LEU
1	A	513	ILE
1	A	523	LEU
1	A	529	ARG
1	A	530	TRP
1	A	567	LYS
1	A	569	ASP
1	A	573	LYS
1	A	609	LEU
1	A	633	ASN
1	A	642	SER
1	A	649	LYS
1	A	662	TYR
1	A	685	GLU
1	A	707	SER
1	A	709	LYS
1	A	710	ILE
1	A	714	LYS
1	A	725	ARG
1	A	732	LEU
1	A	735	ASN
1	A	742	ARG
1	A	747	VAL
1	A	756	LEU
1	A	771	ILE
1	A	775	LYS
1	A	790	SER
1	A	804	LYS

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Mol	Chain	Res	Type
1	A	807	ILE
1	A	808	THR
1	A	810	HIS
1	A	814	GLU
1	A	828	ILE
1	A	835	ARG
1	A	840	ASN
1	A	841	GLN
1	A	842	LYS
1	A	853	SER
1	A	869	THR
1	A	871	SER
1	A	874	SER
1	A	883	LEU
1	A	887	ILE
1	A	908	ASN
1	A	923	ILE
1	A	929	SER
1	A	943	LYS
1	A	944	THR
1	A	945	GLU
1	A	965	LEU
1	A	974	THR
1	A	986	LYS
1	A	989	SER
1	A	993	SER
1	A	1002	LEU
1	A	1012	LEU
1	A	1030	THR
1	A	1033	ASP
1	A	1038	ARG
1	A	1039	THR
1	A	1042	LEU
1	A	1061	TRP
1	A	1067	SER
1	A	1089	ASN
1	A	1094	TYR
1	A	1106	LEU
1	A	1108	GLN
1	A	1117	THR
1	A	1120	THR
1	A	1141	LEU

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Mol	Chain	Res	Type
1	A	1150	LYS
1	A	1188	GLU
1	A	1192	ILE
1	A	1215	ASP
1	A	1220	LYS
1	A	1221	MET
1	A	1226	THR
1	A	1244	SER
1	A	1246	SER
1	A	1260	ASP
1	A	1263	ARG
1	A	1267	LEU
1	A	1270	THR
1	A	1276	ASN
1	A	1282	ASP
1	A	1287	LEU
1	A	1300	ILE
1	A	1310	GLU
1	A	1314	LEU
1	A	1318	LEU
1	A	1326	GLN
1	A	1327	GLN
1	A	1336	SER
1	A	1340	GLN
1	A	1342	VAL
1	A	1346	PHE
1	B	57	HIS
1	B	78	LEU
1	B	88	PHE
1	B	91	VAL
1	B	94	GLN
1	B	97	ASN
1	B	99	ASN
1	B	101	SER
1	B	105	LYS
1	B	108	SER
1	B	111	ASN
1	B	119	GLU
1	B	127	ASN
1	B	130	ILE
1	B	142	ASP
1	B	143	ILE

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Mol	Chain	Res	Type
1	B	149	GLU
1	B	156	ARG
1	B	158	LEU
1	B	178	THR
1	B	184	LYS
1	B	187	VAL
1	B	197	SER
1	B	203	VAL
1	B	204	LEU
1	B	218	ASN
1	B	220	VAL
1	B	222	LYS
1	B	223	GLU
1	B	225	LEU
1	B	235	ASN
1	B	238	GLN
1	B	239	ARG
1	B	242	LYS
1	B	251	LYS
1	B	257	SER
1	B	259	THR
1	B	268	MET
1	B	272	THR
1	B	300	LEU
1	B	301	LYS
1	B	315	LYS
1	B	319	GLU
1	B	324	LEU
1	B	333	GLU
1	B	334	LYS
1	B	342	SER
1	B	350	GLU
1	B	353	THR
1	B	358	VAL
1	B	372	PRO
1	B	373	SER
1	B	376	THR
1	B	380	ASN
1	B	384	ILE
1	B	393	LEU
1	B	396	THR
1	B	404	ARG

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Mol	Chain	Res	Type
1	B	405	HIS
1	B	415	LYS
1	B	431	LYS
1	B	436	LYS
1	B	437	LYS
1	B	453	ASN
1	B	492	THR
1	B	508	LEU
1	B	513	ILE
1	B	523	LEU
1	B	529	ARG
1	B	530	TRP
1	B	567	LYS
1	B	569	ASP
1	B	573	LYS
1	B	609	LEU
1	B	613	MET
1	B	633	ASN
1	B	642	SER
1	B	649	LYS
1	B	662	TYR
1	B	685	GLU
1	B	707	SER
1	B	709	LYS
1	B	710	ILE
1	B	725	ARG
1	B	732	LEU
1	B	735	ASN
1	B	747	VAL
1	B	756	LEU
1	B	771	ILE
1	B	775	LYS
1	B	804	LYS
1	B	806	MET
1	B	807	ILE
1	B	811	LEU
1	B	817	ARG
1	B	828	ILE
1	B	835	ARG
1	B	840	ASN
1	B	841	GLN
1	B	842	LYS

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Mol	Chain	Res	Type
1	B	854	ASN
1	B	883	LEU
1	B	887	ILE
1	B	908	ASN
1	B	943	LYS
1	B	944	THR
1	B	945	GLU
1	B	965	LEU
1	B	974	THR
1	B	986	LYS
1	B	989	SER
1	B	993	SER
1	B	1012	LEU
1	B	1038	ARG
1	B	1039	THR
1	B	1042	LEU
1	B	1061	TRP
1	B	1067	SER
1	B	1091	SER
1	B	1092	THR
1	B	1094	TYR
1	B	1096	THR
1	B	1106	LEU
1	B	1108	GLN
1	B	1117	THR
1	B	1120	THR
1	B	1141	LEU
1	B	1150	LYS
1	B	1192	ILE
1	B	1215	ASP
1	B	1220	LYS
1	B	1221	MET
1	B	1226	THR
1	B	1244	SER
1	B	1246	SER
1	B	1260	ASP
1	B	1263	ARG
1	B	1267	LEU
1	B	1270	THR
1	B	1276	ASN
1	B	1282	ASP
1	B	1283	GLN

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Mol	Chain	Res	Type
1	B	1287	LEU
1	B	1300	ILE
1	B	1310	GLU
1	B	1311	ASN
1	B	1314	LEU
1	B	1318	LEU
1	B	1326	GLN
1	B	1327	GLN
1	B	1336	SER
1	B	1340	GLN
1	B	1341	THR
1	B	1342	VAL
1	B	1346	PHE
1	C	58	GLN
1	C	88	PHE
1	C	91	VAL
1	C	94	GLN
1	C	99	ASN
1	C	101	SER
1	C	106	ASN
1	C	119	GLU
1	C	127	ASN
1	C	130	ILE
1	C	142	ASP
1	C	156	ARG
1	C	158	LEU
1	C	178	THR
1	C	184	LYS
1	C	187	VAL
1	C	197	SER
1	C	203	VAL
1	C	204	LEU
1	C	218	ASN
1	C	220	VAL
1	C	223	GLU
1	C	225	LEU
1	C	235	ASN
1	C	238	GLN
1	C	242	LYS
1	C	251	LYS
1	C	257	SER
1	C	259	THR

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Mol	Chain	Res	Type
1	C	272	THR
1	C	275	LYS
1	C	300	LEU
1	C	301	LYS
1	C	315	LYS
1	C	324	LEU
1	C	332	ARG
1	C	333	GLU
1	C	334	LYS
1	C	342	SER
1	C	350	GLU
1	C	353	THR
1	C	358	VAL
1	C	373	SER
1	C	376	THR
1	C	380	ASN
1	C	384	ILE
1	C	393	LEU
1	C	396	THR
1	C	404	ARG
1	C	405	HIS
1	C	415	LYS
1	C	431	LYS
1	C	436	LYS
1	C	437	LYS
1	C	453	ASN
1	C	458	VAL
1	C	492	THR
1	C	508	LEU
1	C	513	ILE
1	C	523	LEU
1	C	529	ARG
1	C	530	TRP
1	C	562	THR
1	C	567	LYS
1	C	569	ASP
1	C	573	LYS
1	C	609	LEU
1	C	633	ASN
1	C	642	SER
1	C	649	LYS
1	C	662	TYR

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Mol	Chain	Res	Type
1	C	685	GLU
1	C	707	SER
1	C	709	LYS
1	C	710	ILE
1	C	725	ARG
1	C	732	LEU
1	C	735	ASN
1	C	742	ARG
1	C	747	VAL
1	C	756	LEU
1	C	771	ILE
1	C	775	LYS
1	C	789	SER
1	C	804	LYS
1	C	806	MET
1	C	808	THR
1	C	811	LEU
1	C	814	GLU
1	C	828	ILE
1	C	835	ARG
1	C	840	ASN
1	C	841	GLN
1	C	842	LYS
1	C	855	ASN
1	C	869	THR
1	C	883	LEU
1	C	908	ASN
1	C	923	ILE
1	C	943	LYS
1	C	944	THR
1	C	945	GLU
1	C	965	LEU
1	C	974	THR
1	C	986	LYS
1	C	988	ASP
1	C	989	SER
1	C	1002	LEU
1	C	1012	LEU
1	C	1038	ARG
1	C	1039	THR
1	C	1042	LEU
1	C	1061	TRP

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Mol	Chain	Res	Type
1	C	1067	SER
1	C	1089	ASN
1	C	1092	THR
1	C	1094	TYR
1	C	1106	LEU
1	C	1108	GLN
1	C	1117	THR
1	C	1120	THR
1	C	1141	LEU
1	C	1150	LYS
1	C	1192	ILE
1	C	1215	ASP
1	C	1226	THR
1	C	1240	GLN
1	C	1243	THR
1	C	1244	SER
1	C	1260	ASP
1	C	1267	LEU
1	C	1270	THR
1	C	1276	ASN
1	C	1282	ASP
1	C	1287	LEU
1	C	1300	ILE
1	C	1309	VAL
1	C	1311	ASN
1	C	1314	LEU
1	C	1318	LEU
1	C	1326	GLN
1	C	1327	GLN
1	C	1336	SER
1	C	1340	GLN
1	C	1342	VAL
1	D	88	PHE
1	D	91	VAL
1	D	100	ILE
1	D	105	LYS
1	D	106	ASN
1	D	119	GLU
1	D	127	ASN
1	D	130	ILE
1	D	142	ASP
1	D	156	ARG

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Mol	Chain	Res	Type
1	D	158	LEU
1	D	178	THR
1	D	184	LYS
1	D	187	VAL
1	D	197	SER
1	D	203	VAL
1	D	204	LEU
1	D	218	ASN
1	D	220	VAL
1	D	223	GLU
1	D	225	LEU
1	D	228	LYS
1	D	231	GLN
1	D	235	ASN
1	D	238	GLN
1	D	239	ARG
1	D	242	LYS
1	D	251	LYS
1	D	257	SER
1	D	259	THR
1	D	272	THR
1	D	300	LEU
1	D	301	LYS
1	D	315	LYS
1	D	319	GLU
1	D	324	LEU
1	D	333	GLU
1	D	342	SER
1	D	350	GLU
1	D	353	THR
1	D	358	VAL
1	D	373	SER
1	D	376	THR
1	D	380	ASN
1	D	384	ILE
1	D	393	LEU
1	D	396	THR
1	D	404	ARG
1	D	405	HIS
1	D	415	LYS
1	D	431	LYS
1	D	436	LYS

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Mol	Chain	Res	Type
1	D	437	LYS
1	D	453	ASN
1	D	458	VAL
1	D	492	THR
1	D	508	LEU
1	D	513	ILE
1	D	523	LEU
1	D	529	ARG
1	D	530	TRP
1	D	562	THR
1	D	567	LYS
1	D	569	ASP
1	D	573	LYS
1	D	609	LEU
1	D	613	MET
1	D	633	ASN
1	D	642	SER
1	D	649	LYS
1	D	662	TYR
1	D	685	GLU
1	D	707	SER
1	D	709	LYS
1	D	710	ILE
1	D	725	ARG
1	D	732	LEU
1	D	735	ASN
1	D	747	VAL
1	D	756	LEU
1	D	771	ILE
1	D	775	LYS
1	D	804	LYS
1	D	807	ILE
1	D	809	GLN
1	D	814	GLU
1	D	816	THR
1	D	817	ARG
1	D	819	VAL
1	D	828	ILE
1	D	835	ARG
1	D	840	ASN
1	D	841	GLN
1	D	842	LYS

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Mol	Chain	Res	Type
1	D	883	LEU
1	D	887	ILE
1	D	908	ASN
1	D	923	ILE
1	D	943	LYS
1	D	944	THR
1	D	945	GLU
1	D	965	LEU
1	D	974	THR
1	D	986	LYS
1	D	989	SER
1	D	993	SER
1	D	1002	LEU
1	D	1012	LEU
1	D	1033	ASP
1	D	1038	ARG
1	D	1039	THR
1	D	1042	LEU
1	D	1067	SER
1	D	1092	THR
1	D	1097	ASN
1	D	1106	LEU
1	D	1108	GLN
1	D	1117	THR
1	D	1120	THR
1	D	1141	LEU
1	D	1150	LYS
1	D	1175	THR
1	D	1192	ILE
1	D	1204	LYS
1	D	1215	ASP
1	D	1220	LYS
1	D	1221	MET
1	D	1226	THR
1	D	1243	THR
1	D	1244	SER
1	D	1260	ASP
1	D	1263	ARG
1	D	1267	LEU
1	D	1270	THR
1	D	1276	ASN
1	D	1282	ASP

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Mol	Chain	Res	Type
1	D	1283	GLN
1	D	1287	LEU
1	D	1300	ILE
1	D	1310	GLU
1	D	1311	ASN
1	D	1314	LEU
1	D	1318	LEU
1	D	1326	GLN
1	D	1327	GLN
1	D	1336	SER
1	D	1340	GLN
1	D	1342	VAL
1	E	57	HIS
1	E	88	PHE
1	E	91	VAL
1	E	98	LEU
1	E	99	ASN
1	E	101	SER
1	E	105	LYS
1	E	106	ASN
1	E	109	ASP
1	E	119	GLU
1	E	125	GLN
1	E	127	ASN
1	E	130	ILE
1	E	142	ASP
1	E	156	ARG
1	E	158	LEU
1	E	178	THR
1	E	184	LYS
1	E	187	VAL
1	E	197	SER
1	E	203	VAL
1	E	204	LEU
1	E	218	ASN
1	E	220	VAL
1	E	222	LYS
1	E	223	GLU
1	E	225	LEU
1	E	228	LYS
1	E	235	ASN
1	E	238	GLN

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Mol	Chain	Res	Type
1	E	239	ARG
1	E	242	LYS
1	E	251	LYS
1	E	257	SER
1	E	259	THR
1	E	268	MET
1	E	272	THR
1	E	300	LEU
1	E	301	LYS
1	E	315	LYS
1	E	319	GLU
1	E	324	LEU
1	E	333	GLU
1	E	334	LYS
1	E	342	SER
1	E	350	GLU
1	E	353	THR
1	E	358	VAL
1	E	373	SER
1	E	376	THR
1	E	380	ASN
1	E	384	ILE
1	E	393	LEU
1	E	396	THR
1	E	404	ARG
1	E	405	HIS
1	E	415	LYS
1	E	431	LYS
1	E	436	LYS
1	E	437	LYS
1	E	453	ASN
1	E	458	VAL
1	E	492	THR
1	E	508	LEU
1	E	513	ILE
1	E	523	LEU
1	E	529	ARG
1	E	530	TRP
1	E	567	LYS
1	E	569	ASP
1	E	573	LYS
1	E	609	LEU

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Mol	Chain	Res	Type
1	E	633	ASN
1	E	642	SER
1	E	649	LYS
1	E	662	TYR
1	E	685	GLU
1	E	707	SER
1	E	709	LYS
1	E	710	ILE
1	E	725	ARG
1	E	732	LEU
1	E	735	ASN
1	E	747	VAL
1	E	756	LEU
1	E	771	ILE
1	E	775	LYS
1	E	790	SER
1	E	804	LYS
1	E	807	ILE
1	E	828	ILE
1	E	835	ARG
1	E	840	ASN
1	E	841	GLN
1	E	842	LYS
1	E	855	ASN
1	E	869	THR
1	E	883	LEU
1	E	908	ASN
1	E	923	ILE
1	E	929	SER
1	E	943	LYS
1	E	944	THR
1	E	945	GLU
1	E	965	LEU
1	E	974	THR
1	E	986	LYS
1	E	989	SER
1	E	993	SER
1	E	1012	LEU
1	E	1033	ASP
1	E	1038	ARG
1	E	1039	THR
1	E	1042	LEU

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Mol	Chain	Res	Type
1	E	1061	TRP
1	E	1067	SER
1	E	1094	TYR
1	E	1095	ASP
1	E	1106	LEU
1	E	1108	GLN
1	E	1117	THR
1	E	1120	THR
1	E	1141	LEU
1	E	1150	LYS
1	E	1188	GLU
1	E	1192	ILE
1	E	1215	ASP
1	E	1220	LYS
1	E	1221	MET
1	E	1226	THR
1	E	1243	THR
1	E	1244	SER
1	E	1260	ASP
1	E	1262	ASN
1	E	1263	ARG
1	E	1267	LEU
1	E	1270	THR
1	E	1276	ASN
1	E	1282	ASP
1	E	1287	LEU
1	E	1300	ILE
1	E	1310	GLU
1	E	1311	ASN
1	E	1318	LEU
1	E	1326	GLN
1	E	1336	SER
1	E	1340	GLN
1	E	1342	VAL
1	E	1346	PHE
1	F	88	PHE
1	F	91	VAL
1	F	94	GLN
1	F	98	LEU
1	F	99	ASN
1	F	101	SER
1	F	106	ASN

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Mol	Chain	Res	Type
1	F	109	ASP
1	F	110	ASP
1	F	119	GLU
1	F	125	GLN
1	F	127	ASN
1	F	130	ILE
1	F	142	ASP
1	F	156	ARG
1	F	158	LEU
1	F	178	THR
1	F	184	LYS
1	F	187	VAL
1	F	197	SER
1	F	203	VAL
1	F	204	LEU
1	F	218	ASN
1	F	220	VAL
1	F	222	LYS
1	F	223	GLU
1	F	225	LEU
1	F	228	LYS
1	F	235	ASN
1	F	238	GLN
1	F	239	ARG
1	F	242	LYS
1	F	251	LYS
1	F	257	SER
1	F	259	THR
1	F	268	MET
1	F	272	THR
1	F	300	LEU
1	F	301	LYS
1	F	315	LYS
1	F	319	GLU
1	F	324	LEU
1	F	333	GLU
1	F	334	LYS
1	F	342	SER
1	F	353	THR
1	F	358	VAL
1	F	373	SER
1	F	376	THR

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Mol	Chain	Res	Type
1	F	380	ASN
1	F	384	ILE
1	F	393	LEU
1	F	396	THR
1	F	404	ARG
1	F	405	HIS
1	F	415	LYS
1	F	431	LYS
1	F	436	LYS
1	F	437	LYS
1	F	453	ASN
1	F	492	THR
1	F	508	LEU
1	F	513	ILE
1	F	523	LEU
1	F	529	ARG
1	F	530	TRP
1	F	567	LYS
1	F	569	ASP
1	F	573	LYS
1	F	609	LEU
1	F	633	ASN
1	F	642	SER
1	F	649	LYS
1	F	662	TYR
1	F	685	GLU
1	F	707	SER
1	F	709	LYS
1	F	710	ILE
1	F	725	ARG
1	F	732	LEU
1	F	735	ASN
1	F	747	VAL
1	F	756	LEU
1	F	771	ILE
1	F	775	LYS
1	F	804	LYS
1	F	807	ILE
1	F	819	VAL
1	F	828	ILE
1	F	835	ARG
1	F	840	ASN

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Mol	Chain	Res	Type
1	F	841	GLN
1	F	842	LYS
1	F	855	ASN
1	F	869	THR
1	F	883	LEU
1	F	908	ASN
1	F	923	ILE
1	F	929	SER
1	F	943	LYS
1	F	944	THR
1	F	945	GLU
1	F	965	LEU
1	F	974	THR
1	F	986	LYS
1	F	989	SER
1	F	993	SER
1	F	1002	LEU
1	F	1012	LEU
1	F	1038	ARG
1	F	1039	THR
1	F	1042	LEU
1	F	1061	TRP
1	F	1067	SER
1	F	1094	TYR
1	F	1095	ASP
1	F	1106	LEU
1	F	1108	GLN
1	F	1117	THR
1	F	1120	THR
1	F	1141	LEU
1	F	1150	LYS
1	F	1188	GLU
1	F	1192	ILE
1	F	1215	ASP
1	F	1220	LYS
1	F	1221	MET
1	F	1226	THR
1	F	1243	THR
1	F	1244	SER
1	F	1246	SER
1	F	1260	ASP
1	F	1263	ARG

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Mol	Chain	Res	Type
1	F	1267	LEU
1	F	1270	THR
1	F	1276	ASN
1	F	1282	ASP
1	F	1283	GLN
1	F	1287	LEU
1	F	1300	ILE
1	F	1301	ARG
1	F	1310	GLU
1	F	1311	ASN
1	F	1314	LEU
1	F	1318	LEU
1	F	1326	GLN
1	F	1336	SER
1	F	1340	GLN
1	F	1342	VAL
1	F	1346	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (174) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	94	GLN
1	A	111	ASN
1	A	125	GLN
1	A	126	GLN
1	A	175	ASN
1	A	217	ASN
1	A	235	ASN
1	A	238	GLN
1	A	380	ASN
1	A	391	ASN
1	A	395	GLN
1	A	610	GLN
1	A	629	GLN
1	A	646	ASN
1	A	668	ASN
1	A	681	ASN
1	A	728	GLN
1	A	735	ASN
1	A	737	ASN
1	A	841	GLN

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Mol	Chain	Res	Type
1	A	849	GLN
1	A	854	ASN
1	A	885	ASN
1	A	908	ASN
1	A	909	GLN
1	A	924	ASN
1	A	939	GLN
1	A	947	ASN
1	A	1003	ASN
1	A	1122	ASN
1	A	1327	GLN
1	B	71	ASN
1	B	94	GLN
1	B	97	ASN
1	B	125	GLN
1	B	126	GLN
1	B	175	ASN
1	B	217	ASN
1	B	235	ASN
1	B	238	GLN
1	B	380	ASN
1	B	391	ASN
1	B	610	GLN
1	B	629	GLN
1	B	646	ASN
1	B	681	ASN
1	B	728	GLN
1	B	735	ASN
1	B	737	ASN
1	B	823	ASN
1	B	841	GLN
1	B	849	GLN
1	B	854	ASN
1	B	885	ASN
1	B	908	ASN
1	B	909	GLN
1	B	932	GLN
1	B	939	GLN
1	B	947	ASN
1	B	1122	ASN
1	B	1238	ASN
1	B	1327	GLN

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Mol	Chain	Res	Type
1	C	71	ASN
1	C	94	GLN
1	C	111	ASN
1	C	126	GLN
1	C	235	ASN
1	C	238	GLN
1	C	380	ASN
1	C	391	ASN
1	C	395	GLN
1	C	610	GLN
1	C	646	ASN
1	C	728	GLN
1	C	735	ASN
1	C	737	ASN
1	C	809	GLN
1	C	815	ASN
1	C	841	GLN
1	C	849	GLN
1	C	854	ASN
1	C	908	ASN
1	C	909	GLN
1	C	924	ASN
1	C	939	GLN
1	C	947	ASN
1	C	1327	GLN
1	D	71	ASN
1	D	95	ASN
1	D	111	ASN
1	D	125	GLN
1	D	126	GLN
1	D	175	ASN
1	D	235	ASN
1	D	238	GLN
1	D	380	ASN
1	D	391	ASN
1	D	480	ASN
1	D	610	GLN
1	D	646	ASN
1	D	681	ASN
1	D	728	GLN
1	D	735	ASN
1	D	737	ASN

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Mol	Chain	Res	Type
1	D	810	HIS
1	D	812	ASN
1	D	841	GLN
1	D	849	GLN
1	D	854	ASN
1	D	885	ASN
1	D	908	ASN
1	D	909	GLN
1	D	924	ASN
1	D	939	GLN
1	D	947	ASN
1	D	1097	ASN
1	D	1122	ASN
1	D	1193	GLN
1	D	1327	GLN
1	E	71	ASN
1	E	125	GLN
1	E	126	GLN
1	E	175	ASN
1	E	217	ASN
1	E	235	ASN
1	E	238	GLN
1	E	380	ASN
1	E	391	ASN
1	E	395	GLN
1	E	610	GLN
1	E	646	ASN
1	E	681	ASN
1	E	728	GLN
1	E	733	ASN
1	E	735	ASN
1	E	737	ASN
1	E	841	GLN
1	E	849	GLN
1	E	854	ASN
1	E	885	ASN
1	E	908	ASN
1	E	909	GLN
1	E	939	GLN
1	E	947	ASN
1	E	1122	ASN
1	F	71	ASN

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Mol	Chain	Res	Type
1	F	125	GLN
1	F	126	GLN
1	F	175	ASN
1	F	217	ASN
1	F	235	ASN
1	F	238	GLN
1	F	380	ASN
1	F	391	ASN
1	F	395	GLN
1	F	610	GLN
1	F	646	ASN
1	F	681	ASN
1	F	728	GLN
1	F	733	ASN
1	F	735	ASN
1	F	737	ASN
1	F	841	GLN
1	F	849	GLN
1	F	854	ASN
1	F	885	ASN
1	F	908	ASN
1	F	909	GLN
1	F	939	GLN
1	F	947	ASN
1	F	1122	ASN
1	F	1193	GLN
1	F	1326	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	1278/1304 (98%)	0.15	8 (0%) 89 85	13, 49, 106, 165	0
1	B	1275/1304 (97%)	0.28	20 (1%) 72 63	24, 60, 127, 238	0
1	C	1274/1304 (97%)	0.24	21 (1%) 72 63	11, 50, 128, 234	0
1	D	1271/1304 (97%)	0.32	27 (2%) 63 53	18, 58, 132, 228	0
1	E	1262/1304 (96%)	1.91	445 (35%) 0 0	25, 156, 238, 252	0
1	F	1262/1304 (96%)	1.75	431 (34%) 0 0	21, 149, 229, 244	0
All	All	7622/7824 (97%)	0.77	952 (12%) 3 3	11, 68, 224, 252	0

All (952) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	920	PRO	20.2
1	F	836	VAL	14.6
1	F	920	PRO	14.3
1	E	1125	ILE	14.1
1	F	961	TYR	13.9
1	E	626	PRO	13.8
1	F	1125	ILE	13.5
1	E	903	ASN	12.6
1	E	609	LEU	12.5
1	F	659	SER	12.5
1	E	782	SER	12.4
1	F	632	VAL	12.1
1	E	1109	PRO	11.7
1	E	1107	TYR	11.3
1	F	955	GLY	10.9
1	E	957	VAL	10.7
1	E	1119	ASN	10.6
1	E	807	ILE	10.6
1	F	887	ILE	10.5

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Mol	Chain	Res	Type	RSRZ
1	F	921	VAL	10.4
1	E	921	VAL	10.3
1	E	591	ILE	10.2
1	F	922	LEU	10.2
1	E	658	TYR	10.1
1	E	887	ILE	10.1
1	E	1124	LEU	9.9
1	E	257	SER	9.8
1	E	299	PRO	9.7
1	F	884	PRO	9.4
1	F	1106	LEU	9.3
1	E	595	TYR	9.3
1	F	883	LEU	9.3
1	E	1115	TYR	9.2
1	E	625	ASN	9.2
1	F	972	PHE	9.1
1	F	589	LEU	9.1
1	E	256	LEU	8.9
1	E	922	LEU	8.9
1	E	961	TYR	8.8
1	E	599	ASN	8.7
1	E	242	LYS	8.6
1	E	604	PRO	8.6
1	F	956	GLU	8.5
1	E	923	ILE	8.5
1	F	885	ASN	8.5
1	F	1126	GLU	8.5
1	E	1106	LEU	8.3
1	F	886	SER	8.3
1	E	836	VAL	8.2
1	E	799	ILE	8.2
1	E	884	PRO	8.1
1	F	256	LEU	8.1
1	F	877	PRO	8.0
1	F	658	TYR	8.0
1	E	919	ILE	7.9
1	E	1143	LEU	7.9
1	D	1264	LEU	7.9
1	F	803	VAL	7.9
1	E	309	VAL	7.9
1	E	619	PRO	7.8
1	E	1110	ASN	7.8

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Mol	Chain	Res	Type	RSRZ
1	E	968	THR	7.8
1	C	1264	LEU	7.8
1	E	247	LYS	7.8
1	E	392	LEU	7.7
1	F	392	LEU	7.7
1	E	582	GLN	7.7
1	F	899	PHE	7.7
1	E	311	LEU	7.6
1	E	659	SER	7.6
1	A	1264	LEU	7.6
1	F	851	LYS	7.5
1	E	998	VAL	7.5
1	E	566	LEU	7.5
1	E	425	VAL	7.4
1	E	254	GLU	7.4
1	F	853	SER	7.4
1	E	877	PRO	7.3
1	F	310	LYS	7.3
1	F	1127	PRO	7.3
1	F	1000	SER	7.3
1	E	886	SER	7.2
1	E	851	LYS	7.2
1	E	570	GLN	7.2
1	B	1264	LEU	7.1
1	F	878	THR	7.1
1	E	574	HIS	7.1
1	F	626	PRO	7.1
1	F	595	TYR	7.1
1	F	311	LEU	7.0
1	E	1127	PRO	7.0
1	F	575	LEU	6.9
1	E	433	ASP	6.9
1	F	424	LYS	6.9
1	F	1143	LEU	6.8
1	F	603	ILE	6.8
1	D	808	THR	6.8
1	B	809	GLN	6.8
1	E	580	GLN	6.7
1	F	889	PRO	6.7
1	E	668	ASN	6.7
1	F	892	ASP	6.6
1	E	1212	GLY	6.6

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Mol	Chain	Res	Type	RSRZ
1	F	304	ASN	6.6
1	F	590	GLN	6.6
1	E	1112	VAL	6.6
1	F	957	VAL	6.6
1	F	963	ALA	6.5
1	F	818	TRP	6.5
1	F	1124	LEU	6.5
1	F	580	GLN	6.5
1	F	582	GLN	6.5
1	E	806	MET	6.5
1	F	782	SER	6.5
1	E	295	PHE	6.5
1	F	1093	THR	6.4
1	E	1152	LYS	6.4
1	F	1119	ASN	6.4
1	E	859	PHE	6.4
1	F	844	GLY	6.3
1	F	996	THR	6.3
1	F	960	LEU	6.3
1	E	1117	THR	6.3
1	E	571	LEU	6.3
1	E	805	SER	6.2
1	F	625	ASN	6.2
1	F	591	ILE	6.2
1	E	669	TRP	6.2
1	E	893	TRP	6.2
1	F	866	ASN	6.2
1	F	1107	TYR	6.2
1	E	298	LYS	6.2
1	E	883	LEU	6.2
1	F	243	ASP	6.1
1	F	309	VAL	6.1
1	E	424	LYS	6.1
1	F	893	TRP	6.1
1	E	252	GLN	6.1
1	E	303	LYS	6.1
1	F	923	ILE	6.1
1	E	1097	ASN	6.1
1	E	889	PRO	6.1
1	E	253	GLY	6.0
1	E	802	GLY	6.0
1	E	1264	LEU	6.0

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Mol	Chain	Res	Type	RSRZ
1	E	803	VAL	6.0
1	F	247	LYS	6.0
1	E	997	LEU	6.0
1	E	593	THR	5.9
1	D	809	GLN	5.9
1	E	1094	TYR	5.9
1	E	885	ASN	5.9
1	E	588	ASP	5.9
1	F	919	ILE	5.9
1	F	824	PHE	5.8
1	F	669	TRP	5.8
1	E	612	GLU	5.8
1	F	558	GLY	5.8
1	E	820	PHE	5.8
1	F	242	LYS	5.8
1	F	624	ASN	5.8
1	F	259	THR	5.7
1	E	300	LEU	5.7
1	F	826	PRO	5.7
1	E	291	LEU	5.7
1	E	1000	SER	5.7
1	F	629	GLN	5.7
1	F	1118	THR	5.7
1	E	1129	ASP	5.7
1	F	974	THR	5.7
1	E	632	VAL	5.7
1	E	761	PHE	5.7
1	E	592	PHE	5.6
1	E	996	THR	5.6
1	F	804	LYS	5.6
1	E	951	LEU	5.6
1	E	434	GLY	5.6
1	F	565	ARG	5.5
1	E	832	ALA	5.5
1	E	589	LEU	5.5
1	E	567	LYS	5.5
1	F	254	GLU	5.5
1	F	398	GLY	5.5
1	E	1108	GLN	5.5
1	E	988	ASP	5.4
1	E	1146	THR	5.4
1	E	987	ALA	5.4

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Mol	Chain	Res	Type	RSRZ
1	E	249	SER	5.4
1	E	833	GLY	5.4
1	E	899	PHE	5.3
1	F	593	THR	5.3
1	E	624	ASN	5.3
1	F	278	LYS	5.3
1	E	875	SER	5.3
1	F	832	ALA	5.3
1	F	695	ALA	5.3
1	E	1004	TRP	5.3
1	F	769	PRO	5.3
1	F	387	TYR	5.3
1	F	859	PHE	5.2
1	F	1122	ASN	5.2
1	E	1131	THR	5.2
1	F	792	PRO	5.2
1	A	1093	THR	5.2
1	E	426	GLY	5.2
1	E	1122	ASN	5.2
1	E	1140	LEU	5.2
1	E	853	SER	5.2
1	D	810	HIS	5.2
1	E	393	LEU	5.1
1	B	1259	ILE	5.1
1	E	1116	GLN	5.1
1	E	600	ARG	5.1
1	E	660	GLY	5.1
1	E	575	LEU	5.1
1	F	888	SER	5.1
1	E	243	ASP	5.1
1	F	574	HIS	5.1
1	F	563	VAL	5.1
1	F	587	GLU	5.1
1	F	606	GLY	5.1
1	E	296	ALA	5.1
1	F	230	THR	5.1
1	E	950	ASN	5.1
1	E	615	SER	5.0
1	F	566	LEU	5.0
1	E	830	THR	5.0
1	F	425	VAL	5.0
1	E	906	GLN	5.0

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Mol	Chain	Res	Type	RSRZ
1	E	628	ILE	5.0
1	E	771	ILE	5.0
1	E	228	LYS	5.0
1	E	616	LYS	5.0
1	E	1118	THR	5.0
1	F	791	THR	5.0
1	E	947	ASN	5.0
1	E	768	LEU	5.0
1	F	631	ASN	4.9
1	F	652	HIS	4.9
1	E	610	GLN	4.9
1	E	662	TYR	4.9
1	E	652	HIS	4.9
1	E	792	PRO	4.9
1	E	1130	ALA	4.9
1	E	894	ILE	4.9
1	E	1054	ILE	4.9
1	F	295	PHE	4.9
1	F	971	PHE	4.9
1	F	299	PRO	4.9
1	F	229	ALA	4.9
1	E	972	PHE	4.9
1	E	1128	VAL	4.9
1	E	231	GLN	4.9
1	E	1126	GLU	4.8
1	F	607	ALA	4.8
1	E	563	VAL	4.8
1	E	590	GLN	4.8
1	E	801	VAL	4.8
1	E	1093	THR	4.8
1	E	618	GLY	4.8
1	F	246	VAL	4.8
1	F	255	LYS	4.8
1	E	661	LEU	4.8
1	E	726	PHE	4.8
1	F	599	ASN	4.8
1	E	916	LEU	4.8
1	E	584	LEU	4.8
1	F	577	LEU	4.8
1	F	843	ASN	4.8
1	F	302	HIS	4.8
1	F	799	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
1	E	394	LEU	4.8
1	E	902	LYS	4.7
1	F	564	PRO	4.7
1	E	888	SER	4.7
1	E	840	ASN	4.7
1	F	835	ARG	4.7
1	F	1002	LEU	4.7
1	E	560	THR	4.7
1	F	998	VAL	4.7
1	C	1283	GLN	4.7
1	E	233	SER	4.7
1	F	248	ASP	4.7
1	F	260	THR	4.7
1	F	692	SER	4.7
1	E	835	ARG	4.7
1	F	628	ILE	4.6
1	E	290	LEU	4.6
1	E	892	ASP	4.6
1	E	963	ALA	4.6
1	E	586	ARG	4.6
1	E	769	PRO	4.6
1	E	428	THR	4.6
1	E	971	PHE	4.6
1	E	804	LYS	4.6
1	F	756	LEU	4.6
1	E	603	ILE	4.6
1	E	234	PHE	4.5
1	E	259	THR	4.5
1	E	955	GLY	4.5
1	F	984	GLY	4.5
1	E	245	PRO	4.5
1	E	956	GLU	4.5
1	E	315	LYS	4.5
1	F	600	ARG	4.5
1	E	688	TYR	4.5
1	F	660	GLY	4.5
1	F	657	ARG	4.5
1	E	862	ASN	4.5
1	E	796	PHE	4.5
1	E	255	LYS	4.4
1	E	908	ASN	4.4
1	E	1121	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
1	F	584	LEU	4.4
1	F	965	LEU	4.4
1	E	597	TRP	4.4
1	F	1109	PRO	4.4
1	F	664	TRP	4.4
1	F	404	ARG	4.4
1	E	954	PHE	4.4
1	F	1027	TRP	4.4
1	F	594	PRO	4.3
1	F	231	GLN	4.3
1	E	695	ALA	4.3
1	F	966	LEU	4.3
1	E	965	LEU	4.3
1	F	1144	LEU	4.3
1	F	608	TRP	4.3
1	E	665	GLN	4.3
1	E	904	ASN	4.3
1	A	808	THR	4.3
1	E	640	LEU	4.3
1	E	664	TRP	4.3
1	F	825	SER	4.3
1	E	645	LYS	4.2
1	E	935	LYS	4.2
1	F	388	ASN	4.2
1	F	630	ASP	4.2
1	E	989	SER	4.2
1	E	317	PHE	4.2
1	F	834	TYR	4.2
1	F	1049	LEU	4.2
1	E	232	SER	4.2
1	B	1314	LEU	4.2
1	E	629	GLN	4.2
1	E	828	ILE	4.2
1	F	1204	LYS	4.2
1	E	421	PRO	4.2
1	F	802	GLY	4.2
1	F	962	ASN	4.2
1	F	444	ALA	4.2
1	F	609	LEU	4.2
1	E	959	GLY	4.2
1	F	951	LEU	4.2
1	E	1104	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	397	THR	4.2
1	F	890	THR	4.1
1	E	834	TYR	4.1
1	F	862	ASN	4.1
1	F	924	ASN	4.1
1	F	396	THR	4.1
1	F	298	LYS	4.1
1	F	585	LEU	4.1
1	F	586	ARG	4.1
1	F	903	ASN	4.1
1	F	620	HIS	4.1
1	E	793	LEU	4.1
1	F	559	ASP	4.1
1	F	552	ALA	4.0
1	F	726	PHE	4.0
1	E	898	THR	4.0
1	E	389	ALA	4.0
1	F	908	ASN	4.0
1	E	297	LYS	4.0
1	F	897	LEU	4.0
1	F	553	GLY	4.0
1	E	229	ALA	4.0
1	F	1182	ILE	4.0
1	E	878	THR	4.0
1	E	585	LEU	4.0
1	E	895	ASN	4.0
1	F	1108	GLN	4.0
1	E	897	LEU	4.0
1	E	667	PHE	4.0
1	E	1182	ILE	4.0
1	F	245	PRO	3.9
1	F	303	LYS	3.9
1	E	641	ILE	3.9
1	F	588	ASP	3.9
1	F	654	TYR	3.9
1	E	608	TRP	3.9
1	F	988	ASP	3.9
1	E	429	ASP	3.9
1	E	842	LYS	3.9
1	F	619	PRO	3.9
1	E	583	GLY	3.9
1	F	994	SER	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	1309	VAL	3.9
1	E	577	LEU	3.9
1	E	302	HIS	3.9
1	F	1205	GLN	3.9
1	D	1345	PRO	3.8
1	F	592	PHE	3.8
1	E	246	VAL	3.8
1	E	294	ASP	3.8
1	E	901	ASN	3.8
1	F	393	LEU	3.8
1	E	1207	ASN	3.8
1	F	1110	ASN	3.8
1	F	597	TRP	3.8
1	F	394	LEU	3.8
1	E	764	PHE	3.8
1	F	941	TRP	3.8
1	F	926	SER	3.8
1	F	768	LEU	3.8
1	E	781	PRO	3.8
1	F	225	LEU	3.8
1	E	868	VAL	3.8
1	F	667	PHE	3.8
1	E	282	GLU	3.8
1	F	1042	LEU	3.8
1	E	876	LYS	3.7
1	E	994	SER	3.7
1	F	906	GLN	3.7
1	F	554	THR	3.7
1	F	987	ALA	3.7
1	E	670	SER	3.7
1	F	1141	LEU	3.7
1	E	278	LYS	3.7
1	F	1115	TYR	3.7
1	F	857	THR	3.7
1	F	421	PRO	3.7
1	E	313	ALA	3.7
1	F	845	ILE	3.7
1	F	801	VAL	3.7
1	F	848	GLU	3.7
1	E	237	THR	3.6
1	F	989	SER	3.6
1	F	427	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	225	LEU	3.6
1	F	604	PRO	3.6
1	E	536	ARG	3.6
1	F	691	ASN	3.6
1	F	776	PRO	3.6
1	F	1056	TRP	3.6
1	E	1123	LYS	3.6
1	B	810	HIS	3.6
1	F	656	TYR	3.6
1	E	551	LEU	3.6
1	E	1141	LEU	3.6
1	F	997	LEU	3.6
1	F	855	ASN	3.6
1	E	843	ASN	3.6
1	F	551	LEU	3.6
1	B	808	THR	3.6
1	E	753	GLY	3.6
1	F	1121	TYR	3.6
1	E	960	LEU	3.5
1	E	436	LYS	3.5
1	F	764	PHE	3.5
1	F	964	ALA	3.5
1	F	1097	ASN	3.5
1	E	553	GLY	3.5
1	E	275	LYS	3.5
1	E	605	VAL	3.5
1	F	1207	ASN	3.5
1	F	317	PHE	3.5
1	E	683	VAL	3.5
1	F	262	SER	3.5
1	D	1240	GLN	3.5
1	E	565	ARG	3.5
1	D	1259	ILE	3.5
1	E	692	SER	3.5
1	F	771	ILE	3.5
1	F	898	THR	3.5
1	F	882	ALA	3.5
1	E	279	VAL	3.5
1	F	234	PHE	3.5
1	E	1002	LEU	3.5
1	F	222	LYS	3.5
1	F	1105	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	383	GLY	3.5
1	E	958	ASN	3.5
1	E	1153	LEU	3.5
1	F	641	ILE	3.5
1	F	672	LYS	3.5
1	E	431	LYS	3.4
1	E	1213	ILE	3.4
1	E	844	GLY	3.4
1	F	279	VAL	3.4
1	E	587	GLU	3.4
1	E	653	VAL	3.4
1	E	666	LEU	3.4
1	E	880	TYR	3.4
1	E	770	TRP	3.4
1	F	1188	GLU	3.4
1	D	1314	LEU	3.4
1	F	571	LEU	3.4
1	E	236	PRO	3.4
1	E	1027	TRP	3.4
1	E	819	VAL	3.4
1	F	949	GLY	3.4
1	F	403	ARG	3.4
1	F	567	LYS	3.4
1	F	227	VAL	3.4
1	F	538	ALA	3.4
1	F	390	ARG	3.4
1	F	876	LYS	3.4
1	F	1153	LEU	3.4
1	E	240	LEU	3.4
1	F	655	PRO	3.4
1	F	273	ARG	3.4
1	F	226	GLU	3.3
1	E	693	LEU	3.3
1	E	552	ALA	3.3
1	E	396	THR	3.3
1	F	696	ALA	3.3
1	E	1134	ALA	3.3
1	F	894	ILE	3.3
1	E	1263	ARG	3.3
1	F	775	LYS	3.3
1	E	573	LYS	3.3
1	F	308	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	1015	ILE	3.3
1	F	952	PRO	3.3
1	F	1046	LEU	3.3
1	E	630	ASP	3.3
1	F	627	ASP	3.3
1	D	826	PRO	3.3
1	F	723	ALA	3.3
1	F	688	TYR	3.3
1	F	976	THR	3.3
1	F	767	PHE	3.3
1	F	1140	LEU	3.3
1	F	937	SER	3.3
1	E	241	GLN	3.3
1	F	1240	GLN	3.3
1	F	986	LYS	3.3
1	E	627	ASP	3.3
1	E	281	VAL	3.3
1	E	861	PRO	3.3
1	F	622	PHE	3.3
1	F	232	SER	3.3
1	F	830	THR	3.3
1	B	815	ASN	3.2
1	F	481	PRO	3.2
1	E	969	TYR	3.2
1	E	728	GLN	3.2
1	E	852	PRO	3.2
1	F	618	GLY	3.2
1	E	1099	THR	3.2
1	E	274	ALA	3.2
1	F	746	VAL	3.2
1	F	1191	SER	3.2
1	D	1289	VAL	3.2
1	F	995	SER	3.2
1	F	274	ALA	3.2
1	F	1104	PHE	3.2
1	F	221	VAL	3.2
1	F	1004	TRP	3.2
1	E	100	ILE	3.2
1	E	277	LEU	3.2
1	F	925	LYS	3.2
1	F	954	PHE	3.2
1	F	990	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	1288	LEU	3.2
1	F	1043	GLY	3.2
1	F	1142	LYS	3.2
1	E	952	PRO	3.1
1	E	983	ILE	3.1
1	F	915	LEU	3.1
1	F	401	ASN	3.1
1	F	916	LEU	3.1
1	E	432	LYS	3.1
1	F	261	ALA	3.1
1	F	301	LYS	3.1
1	F	661	LEU	3.1
1	E	648	ASP	3.1
1	E	382	HIS	3.1
1	E	826	PRO	3.1
1	F	1137	MET	3.1
1	E	777	PHE	3.1
1	E	550	VAL	3.1
1	E	1144	LEU	3.1
1	E	578	VAL	3.1
1	E	284	GLY	3.1
1	C	1263	ARG	3.1
1	F	690	PRO	3.1
1	E	391	ASN	3.1
1	F	670	SER	3.1
1	E	1029	ILE	3.1
1	F	975	ASN	3.1
1	F	428	THR	3.1
1	E	621	TYR	3.0
1	F	447	PHE	3.0
1	F	940	LYS	3.0
1	E	694	PHE	3.0
1	E	330	ILE	3.0
1	F	852	PRO	3.0
1	E	280	GLU	3.0
1	E	397	THR	3.0
1	E	126	GLN	3.0
1	E	642	SER	3.0
1	E	974	THR	3.0
1	F	983	ILE	3.0
1	F	503	TRP	3.0
1	F	1031	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	949	GLY	3.0
1	F	275	LYS	3.0
1	E	564	PRO	3.0
1	E	620	HIS	3.0
1	F	781	PRO	3.0
1	F	433	ASP	3.0
1	F	753	GLY	3.0
1	E	1111	LYS	3.0
1	E	235	ASN	3.0
1	E	918	THR	3.0
1	B	268	MET	3.0
1	F	754	PRO	3.0
1	E	598	ALA	3.0
1	F	653	VAL	3.0
1	F	323	PRO	3.0
1	E	510	GLY	3.0
1	C	807	ILE	3.0
1	E	227	VAL	3.0
1	E	864	ASP	3.0
1	F	644	TYR	3.0
1	F	569	ASP	2.9
1	E	390	ARG	2.9
1	E	907	ARG	2.9
1	E	508	LEU	2.9
1	F	761	PHE	2.9
1	E	307	GLY	2.9
1	E	1046	LEU	2.9
1	E	995	SER	2.9
1	E	845	ILE	2.9
1	F	1117	THR	2.9
1	F	568	TYR	2.9
1	F	1083	ALA	2.9
1	F	1146	THR	2.9
1	E	596	GLY	2.9
1	C	1259	ILE	2.9
1	E	855	ASN	2.9
1	E	1262	ASN	2.9
1	E	1100	LEU	2.9
1	E	579	ALA	2.9
1	E	719	ALA	2.9
1	F	252	GLN	2.9
1	D	1262	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	985	PHE	2.9
1	E	310	LYS	2.9
1	F	693	LEU	2.9
1	F	109	ASP	2.9
1	C	810	HIS	2.9
1	F	1044	ILE	2.8
1	F	395	GLN	2.8
1	D	1344	GLN	2.8
1	E	910	LEU	2.8
1	D	1263	ARG	2.8
1	E	484	ILE	2.8
1	E	482	LEU	2.8
1	E	569	ASP	2.8
1	F	985	PHE	2.8
1	F	958	ASN	2.8
1	F	281	VAL	2.8
1	F	850	VAL	2.8
1	E	780	SER	2.8
1	E	1210	GLU	2.8
1	D	1285	VAL	2.8
1	F	249	SER	2.8
1	E	558	GLY	2.8
1	E	860	ASP	2.8
1	F	1009	VAL	2.8
1	E	941	TRP	2.7
1	F	321	TRP	2.7
1	B	805	SER	2.7
1	F	861	PRO	2.7
1	F	294	ASP	2.7
1	E	993	SER	2.7
1	E	401	ASN	2.7
1	E	890	THR	2.7
1	F	228	LYS	2.7
1	F	315	LYS	2.7
1	E	400	PHE	2.7
1	B	106	ASN	2.7
1	F	429	ASP	2.7
1	E	696	ALA	2.7
1	E	403	ARG	2.7
1	A	809	GLN	2.7
1	F	1094	TYR	2.7
1	E	430	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	426	GLY	2.7
1	F	793	LEU	2.7
1	E	387	TYR	2.7
1	E	848	GLU	2.7
1	F	910	LEU	2.7
1	E	999	GLY	2.7
1	D	106	ASN	2.7
1	E	301	LYS	2.7
1	E	623	LEU	2.7
1	F	290	LEU	2.6
1	F	780	SER	2.6
1	E	617	PHE	2.6
1	E	449	ALA	2.6
1	F	233	SER	2.6
1	F	860	ASP	2.6
1	E	924	ASN	2.6
1	A	816	THR	2.6
1	B	259	THR	2.6
1	F	1187	LYS	2.6
1	B	230	THR	2.6
1	E	408	TRP	2.6
1	E	823	ASN	2.6
1	F	100	ILE	2.6
1	F	443	ILE	2.6
1	D	1265	PHE	2.6
1	E	1066	GLY	2.6
1	E	1024	LEU	2.6
1	E	1211	ILE	2.6
1	F	1152	LYS	2.6
1	E	690	PRO	2.6
1	E	395	GLN	2.6
1	F	909	GLN	2.6
1	E	230	THR	2.6
1	F	1003	ASN	2.6
1	F	283	ARG	2.6
1	E	639	ALA	2.6
1	F	933	PHE	2.6
1	B	806	MET	2.6
1	F	615	SER	2.6
1	F	880	TYR	2.5
1	F	856	SER	2.5
1	F	1189	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	986	LYS	2.5
1	E	905	PRO	2.5
1	E	568	TYR	2.5
1	E	607	ALA	2.5
1	F	576	ASN	2.5
1	F	318	THR	2.5
1	E	283	ARG	2.5
1	F	1213	ILE	2.5
1	C	1262	ASN	2.5
1	E	416	ALA	2.5
1	E	276	ALA	2.5
1	F	639	ALA	2.5
1	F	1155	LYS	2.5
1	B	1262	ASN	2.5
1	F	668	ASN	2.5
1	E	944	THR	2.5
1	F	579	ALA	2.5
1	F	689	ALA	2.5
1	E	729	LEU	2.5
1	F	968	THR	2.5
1	E	654	TYR	2.5
1	F	550	VAL	2.5
1	F	1112	VAL	2.5
1	F	796	PHE	2.5
1	E	962	ASN	2.5
1	E	644	TYR	2.5
1	E	756	LEU	2.5
1	D	1270	THR	2.5
1	F	633	ASN	2.5
1	F	907	ARG	2.5
1	C	1272	LEU	2.5
1	E	520	LEU	2.5
1	F	1116	GLN	2.5
1	E	1078	LEU	2.5
1	F	833	GLY	2.5
1	F	473	ALA	2.5
1	F	1264	LEU	2.5
1	D	1268	PRO	2.5
1	F	257	SER	2.5
1	F	875	SER	2.5
1	E	1065	LYS	2.4
1	C	97	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	882	ALA	2.4
1	E	562	THR	2.4
1	E	931	ASP	2.4
1	E	912	LEU	2.4
1	F	797	SER	2.4
1	F	912	LEU	2.4
1	F	276	ALA	2.4
1	F	694	PHE	2.4
1	E	308	GLU	2.4
1	E	1190	THR	2.4
1	E	1092	THR	2.4
1	F	939	GLN	2.4
1	E	673	LEU	2.4
1	E	1001	GLY	2.4
1	E	262	SER	2.4
1	E	866	ASN	2.4
1	F	904	ASN	2.4
1	F	1050	GLN	2.4
1	E	911	LEU	2.4
1	F	917	GLY	2.4
1	A	993	SER	2.4
1	F	250	SER	2.4
1	F	570	GLN	2.4
1	D	805	SER	2.4
1	F	642	SER	2.4
1	F	382	HIS	2.4
1	F	241	GLN	2.4
1	F	849	GLN	2.4
1	F	646	ASN	2.4
1	C	1297	GLN	2.4
1	E	576	ASN	2.4
1	F	1098	PRO	2.4
1	E	1113	LYS	2.4
1	F	616	LYS	2.4
1	E	791	THR	2.4
1	E	1049	LEU	2.4
1	F	291	LEU	2.4
1	F	795	THR	2.4
1	E	1010	GLY	2.3
1	E	990	SER	2.3
1	F	805	SER	2.3
1	C	1284	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	473	ALA	2.3
1	F	662	TYR	2.3
1	E	765	LEU	2.3
1	F	944	THR	2.3
1	E	1031	PHE	2.3
1	E	1102	PRO	2.3
1	C	1269	VAL	2.3
1	E	606	GLY	2.3
1	F	864	ASP	2.3
1	F	623	LEU	2.3
1	F	959	GLY	2.3
1	F	1128	VAL	2.3
1	F	617	PHE	2.3
1	C	1096	THR	2.3
1	E	385	TRP	2.3
1	E	404	ARG	2.3
1	F	307	GLY	2.3
1	E	709	LYS	2.3
1	F	772	GLY	2.3
1	E	258	GLU	2.3
1	F	999	GLY	2.3
1	E	312	GLU	2.3
1	F	770	TRP	2.3
1	F	1206	ASN	2.3
1	E	503	TRP	2.3
1	E	1225	LEU	2.3
1	F	914	SER	2.3
1	F	829	TRP	2.3
1	F	643	SER	2.3
1	E	314	GLU	2.2
1	B	851	LYS	2.2
1	D	259	THR	2.2
1	E	824	PHE	2.2
1	E	1081	PRO	2.2
1	F	601	PRO	2.2
1	D	955	GLY	2.2
1	C	1314	LEU	2.2
1	C	1093	THR	2.2
1	E	928	ASP	2.2
1	F	1262	ASN	2.2
1	F	932	GLN	2.2
1	F	867	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	966	LEU	2.2
1	F	445	LEU	2.2
1	E	559	ASP	2.2
1	F	536	ARG	2.2
1	F	297	LYS	2.2
1	F	583	GLY	2.2
1	F	1001	GLY	2.2
1	D	806	MET	2.2
1	F	1091	SER	2.2
1	F	435	PHE	2.2
1	F	312	GLU	2.2
1	E	444	ALA	2.2
1	F	506	ALA	2.2
1	E	216	LEU	2.2
1	F	277	LEU	2.2
1	E	713	GLY	2.2
1	F	236	PRO	2.2
1	F	1006	SER	2.2
1	C	1115	TYR	2.2
1	E	846	PRO	2.2
1	F	665	GLN	2.2
1	F	296	ALA	2.2
1	E	1058	ASP	2.2
1	E	976	THR	2.2
1	E	1020	PHE	2.2
1	F	973	GLY	2.2
1	D	1334	ALA	2.2
1	E	841	GLN	2.2
1	B	1097	ASN	2.2
1	F	470	ASN	2.2
1	B	1263	ARG	2.2
1	F	817	ARG	2.2
1	F	389	ALA	2.2
1	C	1091	SER	2.1
1	D	1324	GLN	2.1
1	E	874	SER	2.1
1	A	996	THR	2.1
1	F	1045	THR	2.1
1	E	847	PHE	2.1
1	E	441	SER	2.1
1	C	1346	PHE	2.1
1	E	532	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	211	LEU	2.1
1	F	1224	LYS	2.1
1	E	926	SER	2.1
1	A	1263	ARG	2.1
1	F	1130	ALA	2.1
1	E	1096	THR	2.1
1	E	1181	ASN	2.1
1	F	710	ILE	2.1
1	E	1042	LEU	2.1
1	E	1208	LYS	2.1
1	E	680	ALA	2.1
1	C	840	ASN	2.1
1	E	454	ILE	2.1
1	E	1032	THR	2.1
1	F	217	ASN	2.1
1	F	831	GLY	2.1
1	F	621	TYR	2.1
1	E	248	ASP	2.1
1	F	578	VAL	2.1
1	B	812	ASN	2.1
1	C	815	ASN	2.1
1	F	755	ASN	2.1
1	E	827	ASP	2.1
1	E	1095	ASP	2.1
1	D	1312	GLN	2.1
1	F	1211	ILE	2.1
1	F	1100	LEU	2.1
1	E	720	GLU	2.1
1	E	773	ASN	2.0
1	E	711	PHE	2.0
1	B	1093	THR	2.0
1	E	684	ASN	2.0
1	F	946	THR	2.0
1	F	1078	LEU	2.0
1	F	1225	LEU	2.0
1	E	891	SER	2.0
1	F	931	ASP	2.0
1	F	240	LEU	2.0
1	E	671	ASN	2.0
1	F	777	PHE	2.0
1	E	1105	GLN	2.0
1	E	1090	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	467	PHE	2.0
1	E	304	ASN	2.0
1	F	950	ASN	2.0
1	B	1272	LEU	2.0
1	E	1091	SER	2.0
1	F	505	TYR	2.0
1	F	1068	TYR	2.0
1	C	1089	ASN	2.0
1	F	1007	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.