Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:28 am BST

PDB ID	:	5TBZ
Title	:	E. Coli RNA Polymerase complexed with NusG
Authors	:	Liu, B.; Steitz, T.A.
Deposited on	:	2016-09-13
Resolution	:	7.00 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:

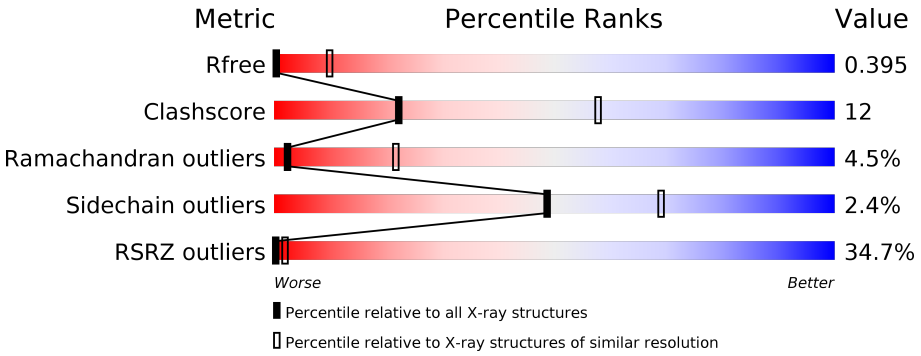
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 7.00 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	1004 (10.00-3.90)
Clashscore	141614	1069 (10.00-3.90)
Ramachandran outliers	138981	1002 (10.00-3.90)
Sidechain outliers	138945	1002 (10.00-3.86)
RSRZ outliers	127900	1004 (9.50-3.80)

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	242	26% 73% 18% • 7%
1	B	242	47% 69% 18% • 11%
1	F	242	23% 72% 20% • 7%
1	G	242	38% 71% 17% • 11%
2	C	1342	32% 77% 20% • •
2	H	1342	34% 75% 21% • •

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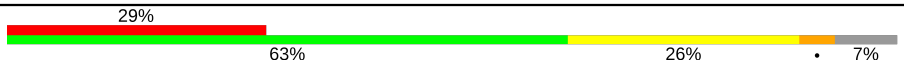
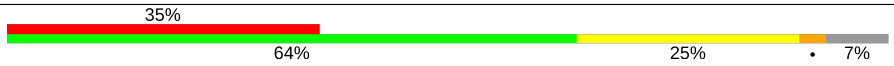
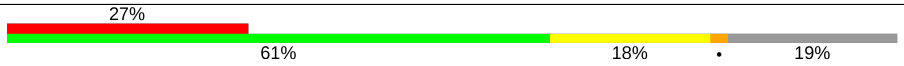
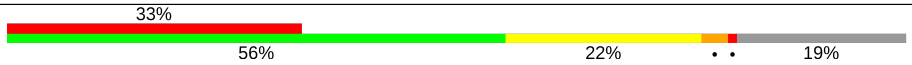
Mol	Chain	Length	Quality of chain
3	D	1407	
3	I	1407	
4	J	181	
4	K	181	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 50147 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1740	1082	309	343	6			
1	B	215	Total	C	N	O	S	0	0	0
			1657	1034	291	326	6			
1	F	225	Total	C	N	O	S	0	0	0
			1740	1082	309	343	6			
1	G	216	Total	C	N	O	S	0	0	0
			1667	1040	294	327	6			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ALA	-	expression tag	UNP P0A7Z6
A	-5	HIS	-	expression tag	UNP P0A7Z6
A	-4	HIS	-	expression tag	UNP P0A7Z6
A	-3	HIS	-	expression tag	UNP P0A7Z6
A	-2	HIS	-	expression tag	UNP P0A7Z6
A	-1	HIS	-	expression tag	UNP P0A7Z6
A	0	HIS	-	expression tag	UNP P0A7Z6
B	-6	ALA	-	expression tag	UNP P0A7Z6
B	-5	HIS	-	expression tag	UNP P0A7Z6
B	-4	HIS	-	expression tag	UNP P0A7Z6
B	-3	HIS	-	expression tag	UNP P0A7Z6
B	-2	HIS	-	expression tag	UNP P0A7Z6
B	-1	HIS	-	expression tag	UNP P0A7Z6
B	0	HIS	-	expression tag	UNP P0A7Z6
F	-6	ALA	-	expression tag	UNP P0A7Z6
F	-5	HIS	-	expression tag	UNP P0A7Z6
F	-4	HIS	-	expression tag	UNP P0A7Z6
F	-3	HIS	-	expression tag	UNP P0A7Z6
F	-2	HIS	-	expression tag	UNP P0A7Z6
F	-1	HIS	-	expression tag	UNP P0A7Z6
F	0	HIS	-	expression tag	UNP P0A7Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-6	ALA	-	expression tag	UNP P0A7Z6
G	-5	HIS	-	expression tag	UNP P0A7Z6
G	-4	HIS	-	expression tag	UNP P0A7Z6
G	-3	HIS	-	expression tag	UNP P0A7Z6
G	-2	HIS	-	expression tag	UNP P0A7Z6
G	-1	HIS	-	expression tag	UNP P0A7Z6
G	0	HIS	-	expression tag	UNP P0A7Z6

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1319	Total	C	N	O	S	0	1	0
			10401	6524	1814	2020	43			
2	H	1319	Total	C	N	O	S	0	1	0
			10401	6524	1814	2020	43			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1302	Total	C	N	O	S	0	0	0
			10085	6326	1800	1911	48			
3	I	1306	Total	C	N	O	S	0	0	0
			10126	6353	1809	1916	48			

- Molecule 4 is a protein called Transcription termination/antitermination protein NusG.

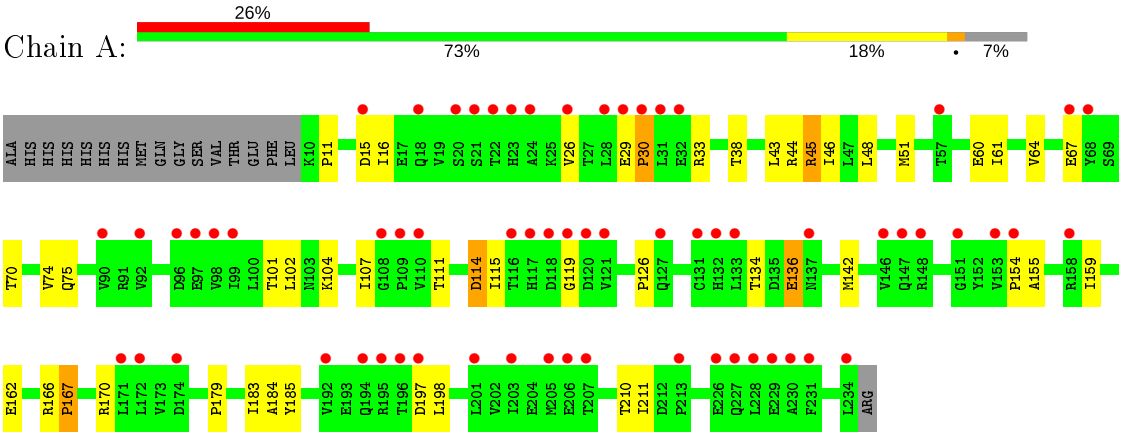
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	147	Total	C	N	O	S	0	0	0
			1165	740	201	217	7			
4	K	147	Total	C	N	O	S	0	0	0
			1165	740	201	217	7			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

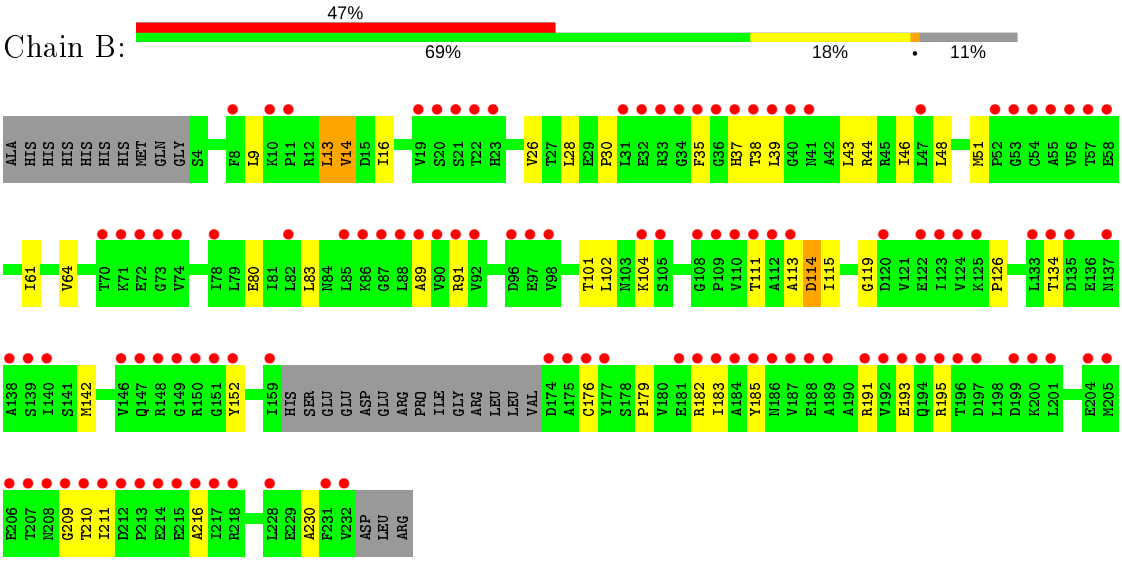
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



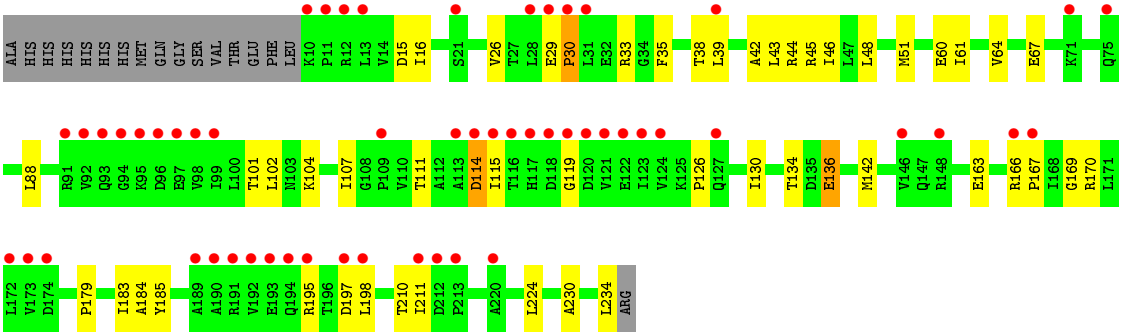
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B:



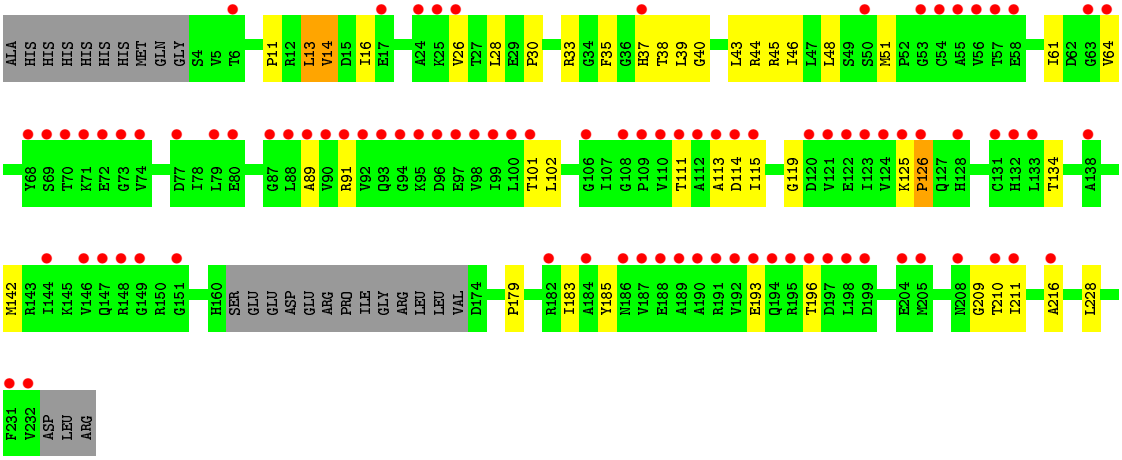
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain F:



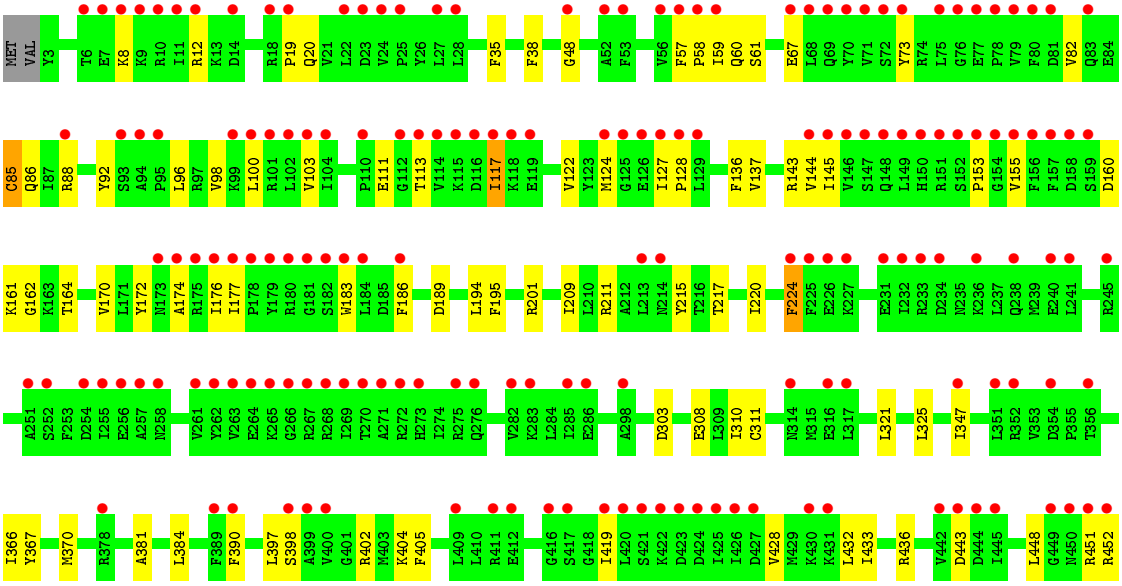
• Molecule 1: DNA-directed RNA polymerase subunit alpha

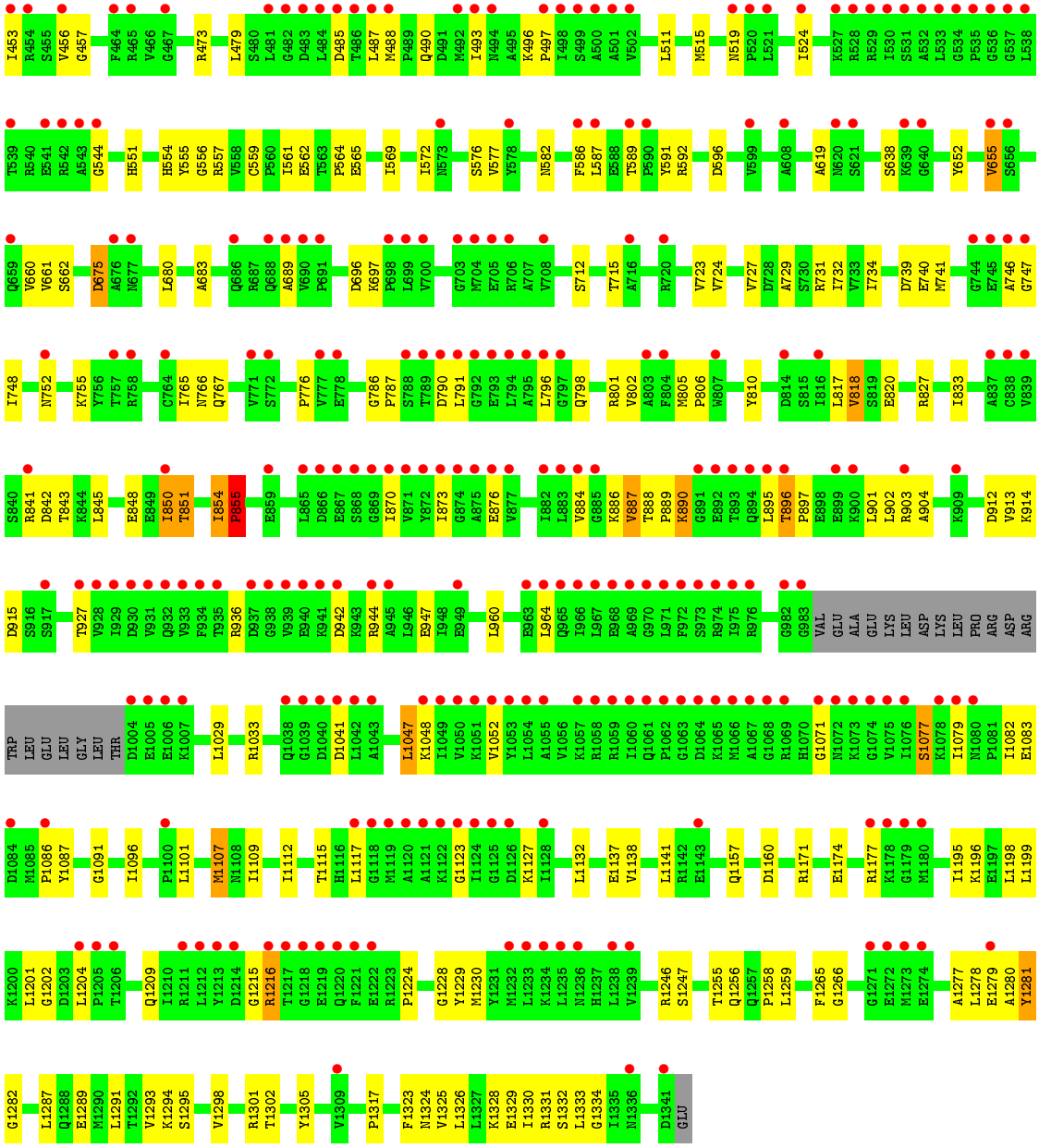
Chain G:



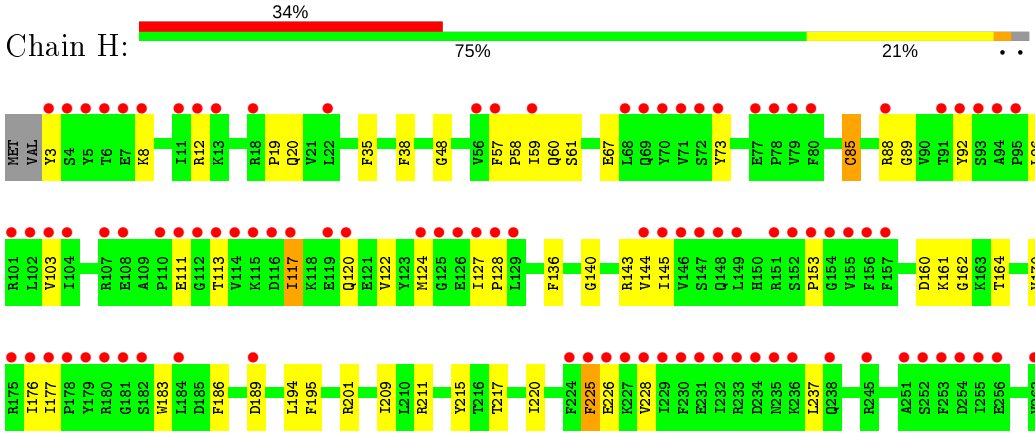
• Molecule 2: DNA-directed RNA polymerase subunit beta

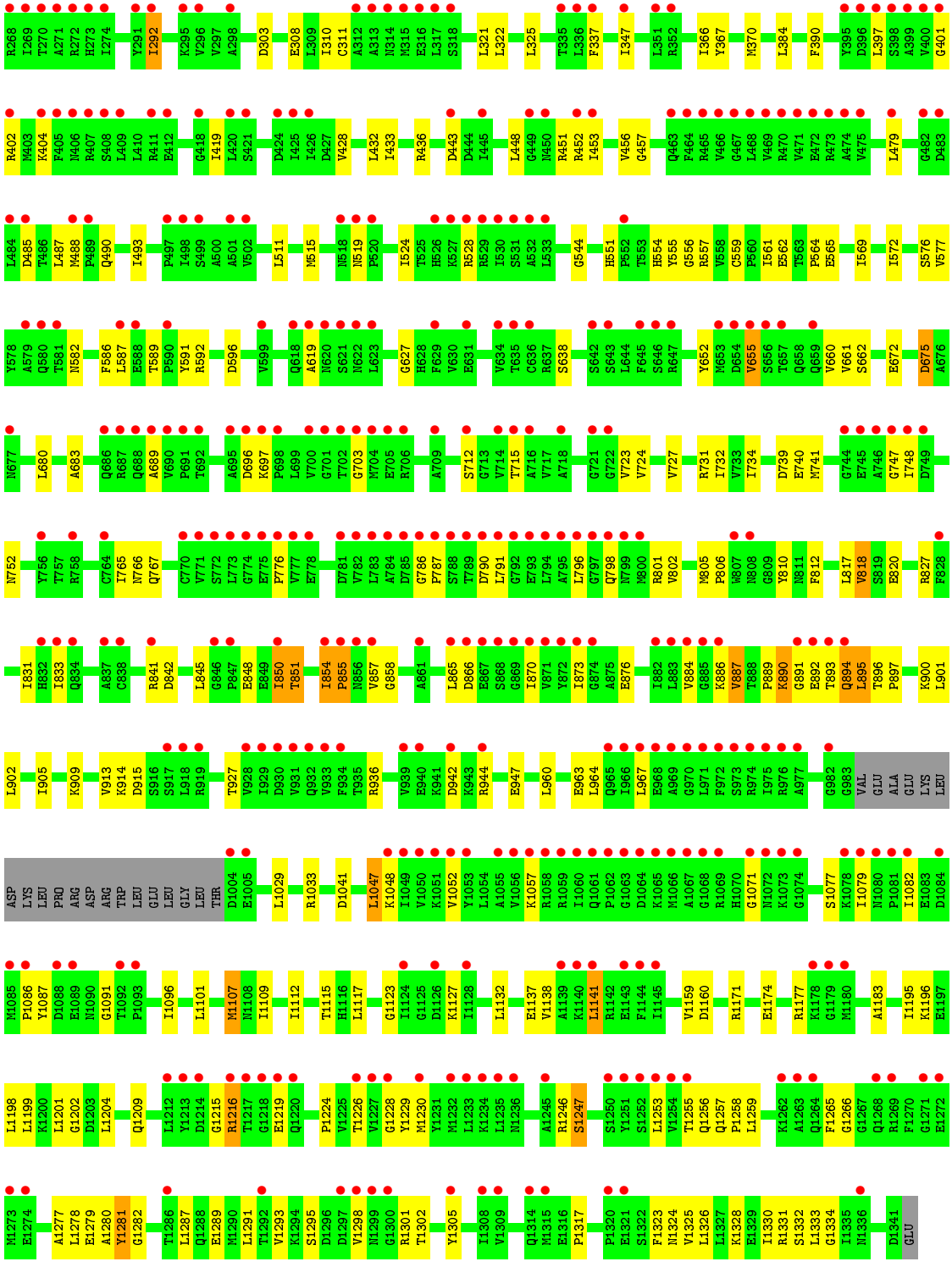
Chain C:



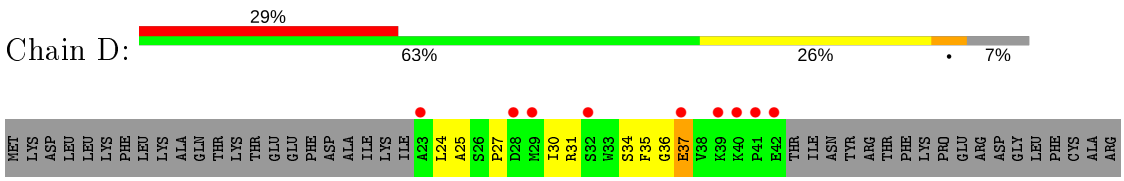


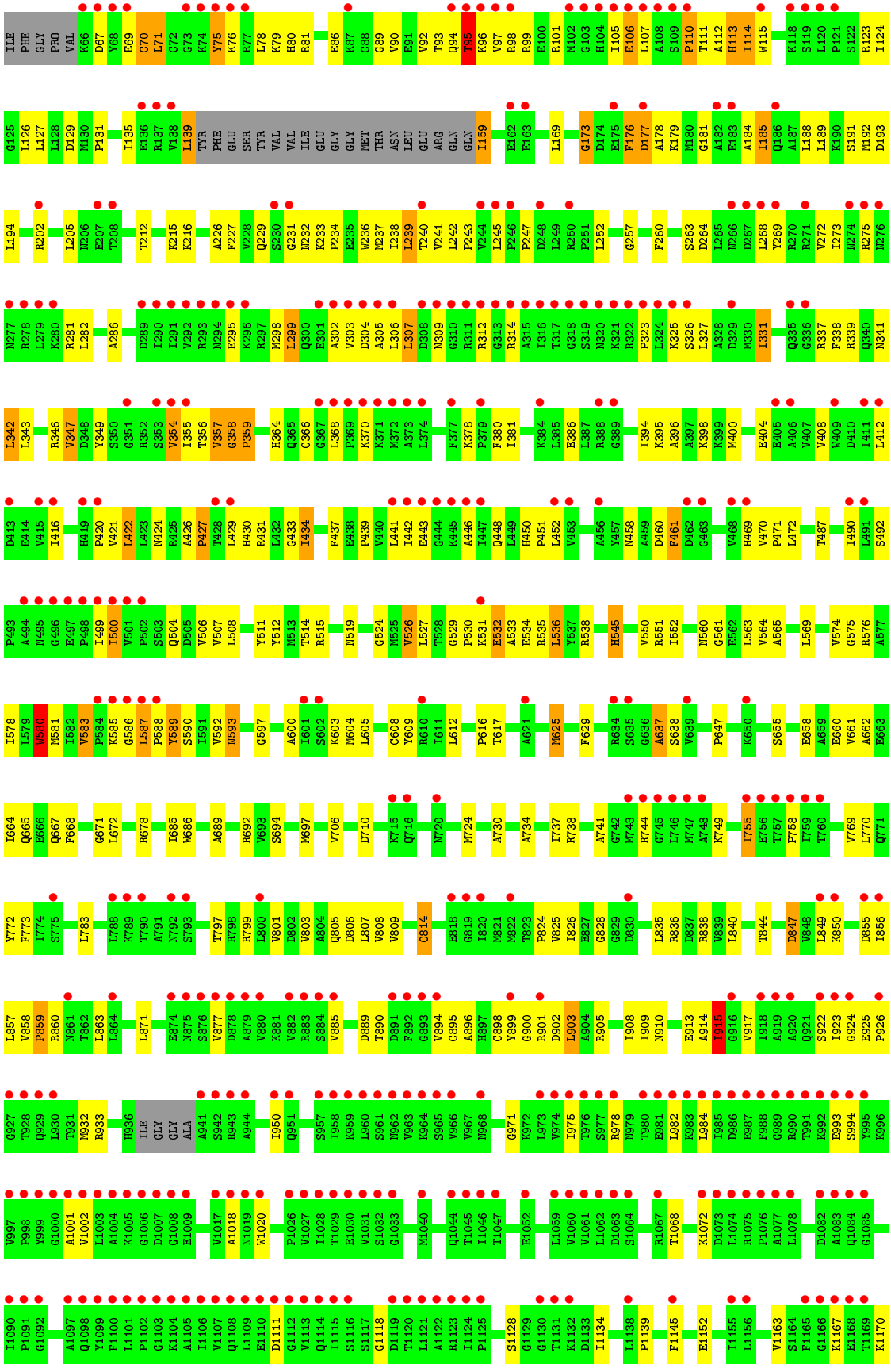
• Molecule 2: DNA-directed RNA polymerase subunit beta

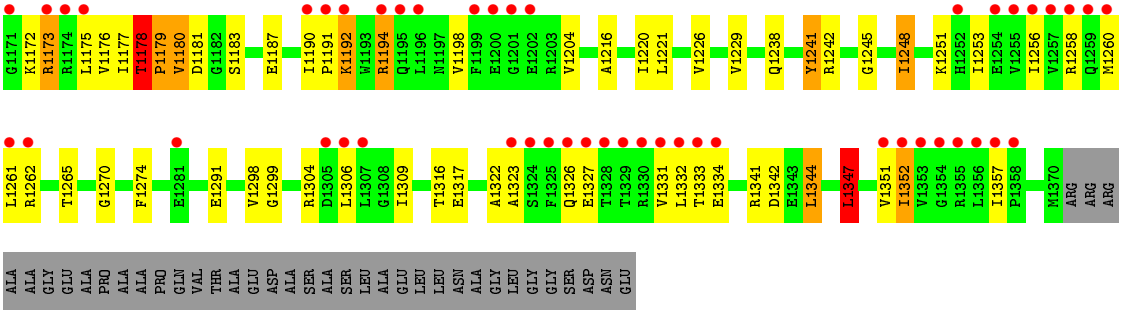




• Molecule 3: DNA-directed RNA polymerase subunit beta'

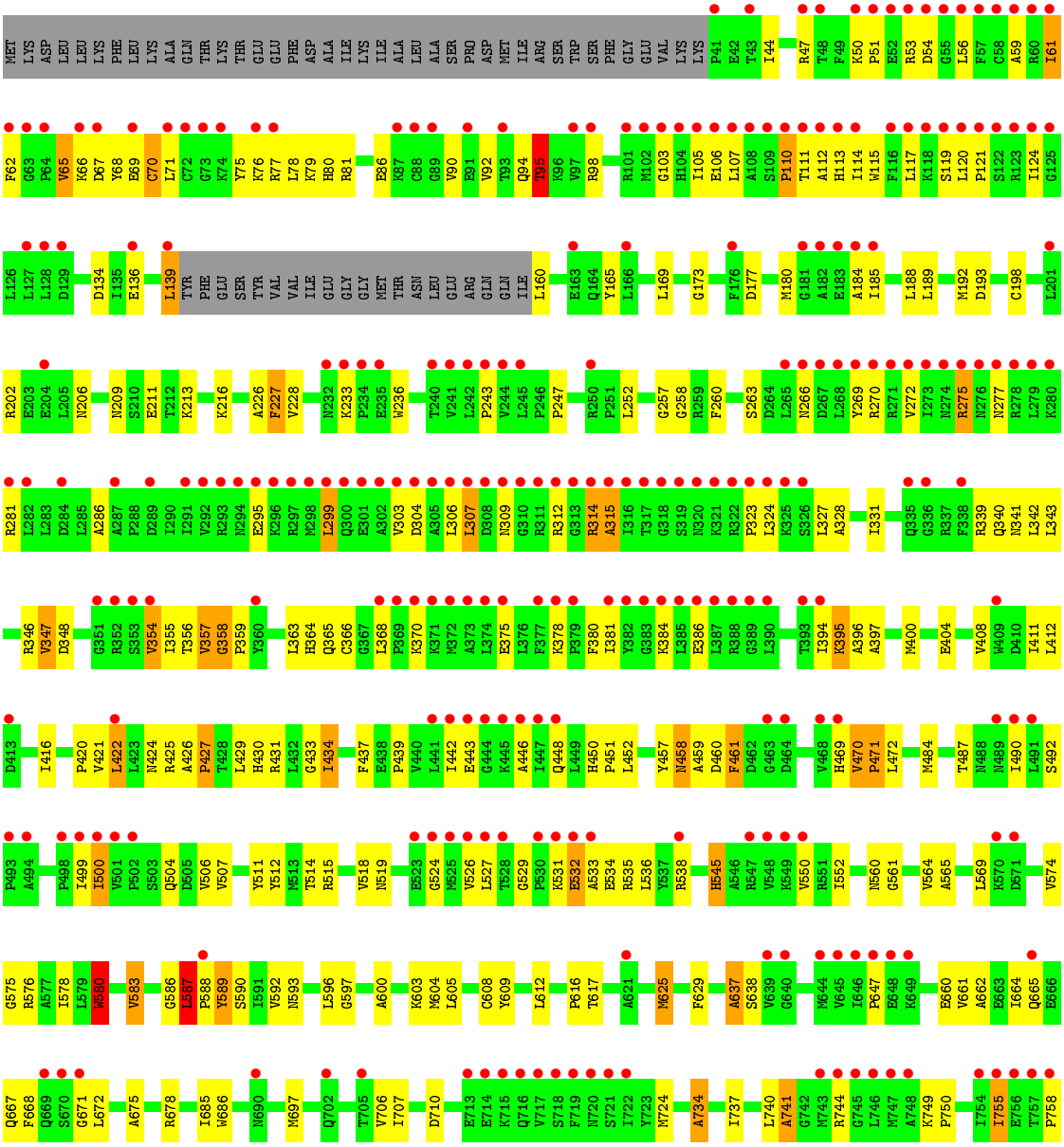


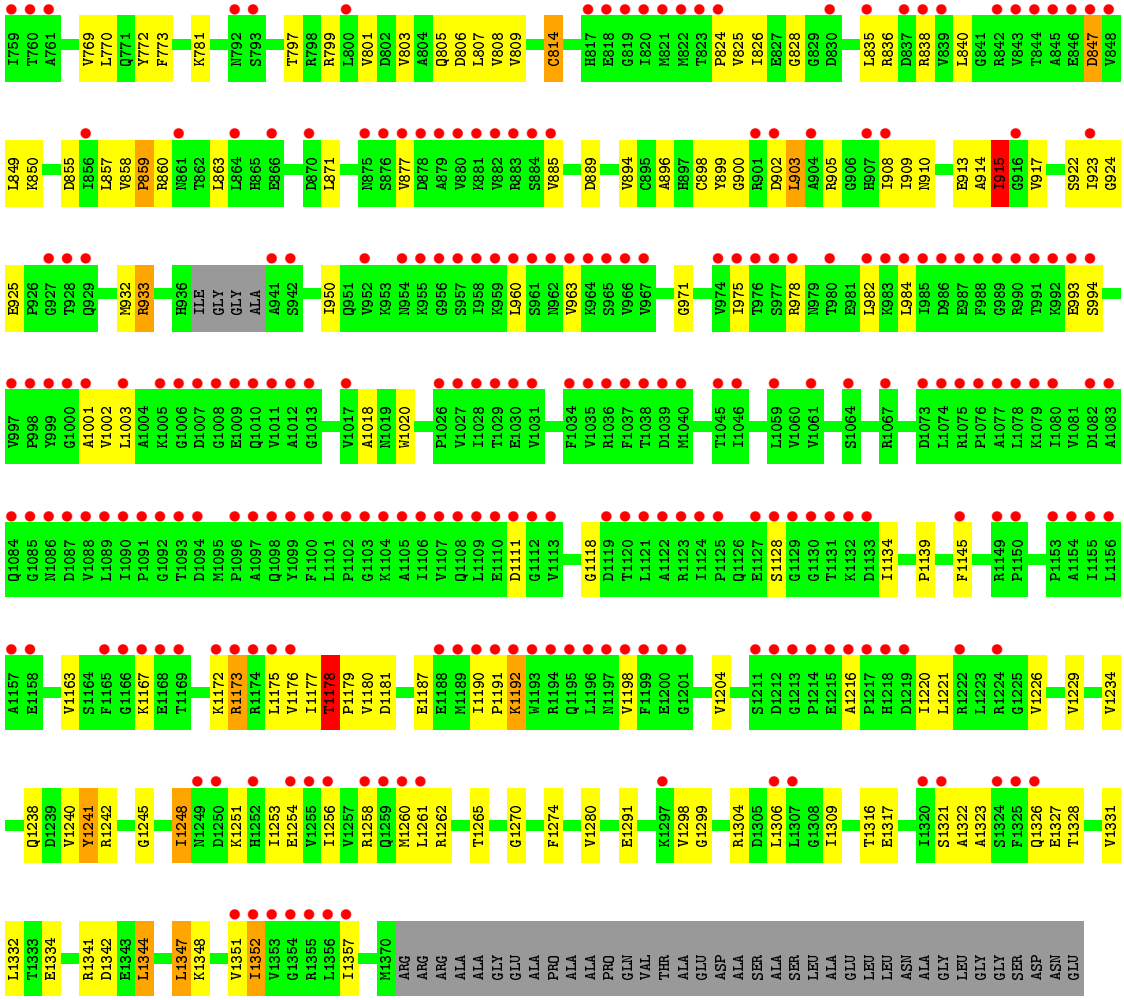

ILE PHE GLY PRO VAL K66 D67 Y68 E69 C70 L71 C72 G73 K74 Y75 K76 R77 L78 K79 H80 R81 E86 K87 C88 G89 V90 E91 V92 T93 Q94 T95 K96 V97 R98 R99 E100 R101 M102 G103 H104 I105 E106 L107 A108 S109 P110 T111 A112 H113 I114 W115 K118 S119 L120 P121 S122 R123 I124
G126 L126 L127 L128 D129 M130 P131 I135 E136 R137 V138 L139 TYR PHE GLU SER TYR VAL VAL ILE GLU GLY GLY MET THR ASN LEU GLU ARG GLN GLN I159 E162 E163 L169 G173 D174 E175 F176 D177 A178 K179 M180 G181 A182 E183 A184 I185 Q186 A187 L188 L189 K190 S191 M192 D193
L194 R202 L205 N206 E207 T208 T212 K215 K216 A226 F227 V228 Q229 S230 G231 N232 K233 P234 E235 W236 M237 I238 L239 T240 V241 L242 P243 V244 L245 P246 P247 D248 L249 R250 P251 L252 G257 F260 S263 D264 L265 N266 D267 L268 Y269 R270 R271 V272 I273 N274 R275 N276
N277 R278 L279 K280 R281 L282 A286 D289 I290 I291 V292 R293 N294 E295 K296 R297 M298 L299 Q300 E301 A302 V303 D304 A305 L306 L307 D308 N309 G310 R311 R312 G313 R314 A315 I316 T317 G318 S319 N320 K321 R322 P323 L324 K325 S326 L327 A328 D329 M330 I331 Q335 G336 R337 F338 R339 Q340 N341
L342 L343 R346 V347 D348 Y349 S350 G351 R352 S353 V354 I355 T356 V357 G358 P359 H364 Q365 C366 G367 L368 P369 K370 K371 M372 A373 L374 F377 K378 P379 F380 I381 K384 L385 E386 L387 R388 G389 I394 K395 A396 A397 K398 K399 M400 E404 E405 A406 V407 V408 W409 D410 I411 L412
D413 E414 V415 I416 H419 P420 V421 L422 L423 N424 R425 A426 P427 T428 L429 H430 R431 L432 G433 I434 F437 E438 P439 V440 L441 I442 E443 G444 K445 A446 I447 Q448 L449 H450 P451 L452 V453 A456 Y457 N458 A459 D460 P461 D462 G463 V468 H469 V470 P471 L472 T487 I490 L491 S492
P493 A494 N495 G496 E497 P498 T499 I500 V501 P502 S503 Q504 D505 V506 V507 L508 Y511 Y512 M513 T514 R515 N519 G524 M525 V526 L527 T528 G529 P530 K531 E532 A533 E534 R535 L536 Y537 R538 H545 V550 R551 I552 N560 G561 E562 L563 V564 A565 L569 V574 G575 R576 A577
I578 L579 M580 M581 I582 V583 P584 K585 G586 L587 P588 Y589 S590 I591 V592 N593 G597 A600 I601 S602 K603 M604 L605 C608 Y609 R610 I611 L612 P616 T617 A621 M625 F629 R634 S635 G636 A637 S638 V639 P647 K650 S655 E658 A659 E660 V661 A662 E663
I664 Q665 E666 Q667 F668 G671 L672 R678 I685 W686 A689 R692 V693 S694 M697 V706 D710 K715 Q716 M720 M724 A730 A734 I737 R738 A741 G742 M743 R744 G745 L746 M747 A748 K749 I755 E756 T757 P758 I759 T760 V769 L770 Q771
Y772 F773 I774 S775 L783 L788 K789 T790 A791 N792 S793 T797 R798 R799 L800 V801 D802 V803 A804 Q805 D806 L807 V808 V809 C814 E818 G819 I820 M821 M822 T823 P824 V825 I826 E827 G828 G829 D830 L835 R836 D837 R838 V839 L840 T844 D847 V848 L849 K850 D855 I856
L857 V858 P859 R860 N861 T862 L863 L864 L871 E874 N875 S876 V877 D878 A879 V880 K881 V882 R883 S884 V885 D889 T890 D891 F892 G893 V894 C895 A896 H897 C898 Y899 G900 R901 D902 L903 A904 R905 I908 I909 N910 E913 A914 I915 G916 V917 I918 A919 A920 Q921 S922 I923 G924 E925 P926
G927 T928 Q929 L930 T931 M932 R933 H936 ILE GLY GLY ALA A941 S942 R943 A944 I950 Q951 S957 I958 K959 L960 S961 N962 V963 K964 S965 V966 V967 N968 G971 K972 L973 V974 I975 T976 S977 R978 N979 T980 E981 L982 K983 L984 I985 D986 E987 F988 G989 R990 T991 K992 E993 S994 Y995 K996
V997 P998 Y999 G1000 A1001 V1002 L1003 A1004 K1005 G1006 D1007 G1008 E1009 V1017 A1018 N1019 W1020 P1026 V1027 I1028 T1029 E1030 V1031 S1032 G1033 M1040 Q1044 T1045 I1046 T1047 E1052 L1059 Y1060 V1061 L1062 D1063 S1064 R1067 T1068 K1072 D1073 L1074 R1075 P1076 A1077 L1078 D1082 A1083 Q1084 G1085
I1090 P1091 G1092 A1097 Q1098 Y1099 F1100 L1101 P1102 G1103 K1104 A1105 I1106 V1107 Q1108 L1109 E1110 D1111 G1112 V1113 Q1114 I1115 S1116 S1117 G1118 D1119 T1120 L1121 A1122 R1123 I1124 P1125 S1128 G1129 G1130 T1131 K1132 D1133 I1134 L1138 P1139 F1145 E1152 I1155 L1156 V1163 S1164 F1165 G1166 K1167 E1168 T1169 K1170



• Molecule 3: DNA-directed RNA polymerase subunit beta'

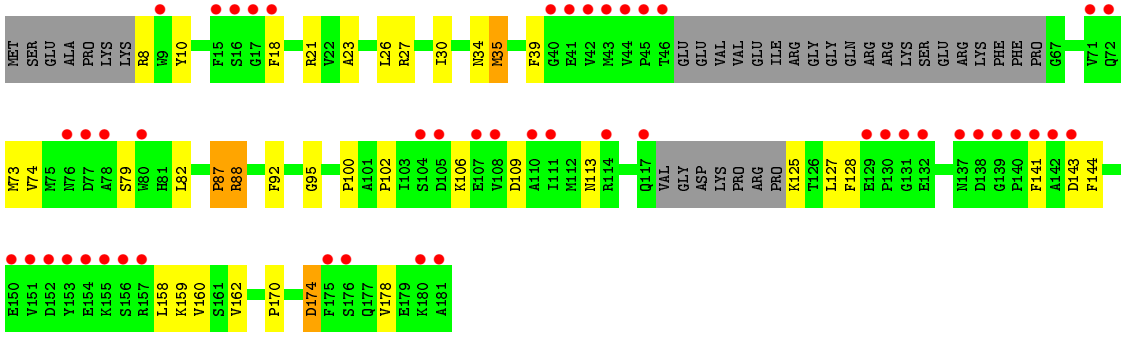
Chain I:





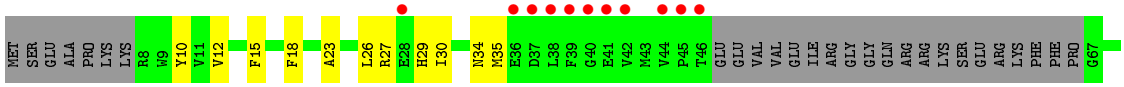
• Molecule 4: Transcription termination/antitermination protein NusG

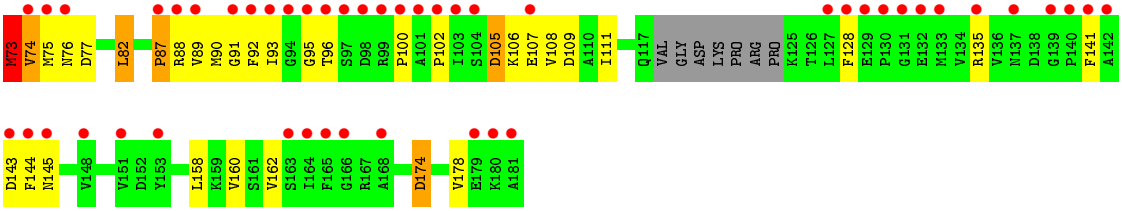
Chain J:



• Molecule 4: Transcription termination/antitermination protein NusG

Chain K:




M73
V74
M75
N76
D77
L82
P87
R88
V89
M90
G91
F92
I93
G94
G95
T96
S97
D98
R99
P100
A101
P102
T103
S104
D105
K106
E107
V108
D109
A110
I111
Q117
VAL
GLY
ASP
LYS
PRO
ARG
PRO
K125
T126
L127
F128
E129
P130
G131
E132
M133
V134
R135
V136
N137
D138
G139
P140
F141
A142
D143
F144
N145
V148
V151
D152
Y153
L158
K159
V160
S161
V162
S163
I164
F165
G166
R167
A168
D174
V178
E179
K180
A181

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	248.16Å 313.78Å 162.79Å 90.00° 130.23° 90.00°	Depositor
Resolution (Å)	162.19 – 7.00 49.91 – 7.00	Depositor EDS
% Data completeness (in resolution range)	96.0 (162.19-7.00) 93.3 (49.91-7.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.04 (at 6.68Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.330 , 0.395 0.330 , 0.395	Depositor DCC
R_{free} test set	707 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	314.0	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 500.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.35$, $< L^2 > = 0.18$	Xtriage
Estimated twinning fraction	0.185 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.78	EDS
Total number of atoms	50147	wwPDB-VP
Average B, all atoms (Å^2)	330.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% 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	0.45	0/1761	0.72	0/2387
1	B	0.46	0/1676	0.71	0/2271
1	F	0.45	0/1761	0.74	0/2387
1	G	0.47	0/1687	0.70	0/2286
2	C	0.43	0/10569	0.67	0/14258
2	H	0.43	0/10569	0.67	0/14258
3	D	0.44	0/10233	0.76	5/13816 (0.0%)
3	I	0.44	0/10277	0.74	1/13877 (0.0%)
4	J	0.50	0/1188	0.70	0/1603
4	K	0.50	0/1188	0.74	1/1603 (0.1%)
All	All	0.44	0/50909	0.71	7/68746 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	2
2	H	0	2
3	D	0	1
3	I	0	1
4	K	0	1
All	All	0	7

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1194	ARG	NE-CZ-NH2	-6.82	116.89	120.30
3	D	239	LEU	CA-CB-CG	5.33	127.56	115.30
3	D	173	GLY	N-CA-C	5.30	126.36	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	117	LEU	CA-CB-CG	5.29	127.46	115.30
4	K	73	MET	C-N-CA	5.27	134.87	121.70
3	D	71	LEU	CA-CB-CG	5.13	127.09	115.30
3	D	1347	LEU	CA-CB-CG	5.11	127.06	115.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	57	PHE	Peptide
2	C	855	PRO	Peptide
3	D	1178	THR	Peptide
2	H	57	PHE	Peptide
2	H	855	PRO	Peptide
3	I	1178	THR	Peptide
4	K	73	MET	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1740	0	1767	40	0
1	B	1657	0	1686	40	0
1	F	1740	0	1767	38	0
1	G	1667	0	1693	35	0
2	C	10401	0	10414	216	0
2	H	10401	0	10414	232	0
3	D	10085	0	10303	380	2
3	I	10126	0	10341	316	0
4	J	1165	0	1145	26	0
4	K	1165	0	1145	30	0
All	All	50147	0	50675	1182	2

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 12.

All (1182) 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)
3:I:1001:ALA:HA	3:I:1020:TRP:HE1	1.12	1.13
4:K:29:HIS:HB3	4:K:82:LEU:HG	1.35	1.06
3:D:226:ALA:HB1	3:D:227:PHE:HA	1.31	1.06
3:D:1001:ALA:HA	3:D:1020:TRP:HE1	1.12	1.06
3:D:247:PRO:HB3	3:I:53:ARG:HH12	1.18	1.06
3:D:247:PRO:HB3	3:I:53:ARG:NH1	1.74	1.03
3:D:885:VAL:HB	3:D:1258:ARG:HD3	1.40	1.02
2:C:12[A]:ARG:HG3	2:C:12[A]:ARG:HH11	1.20	1.02
3:I:885:VAL:HB	3:I:1258:ARG:HD3	1.40	1.02
3:D:1001:ALA:HA	3:D:1020:TRP:NE1	1.75	1.02
3:D:272:VAL:HG22	3:D:306:LEU:CD1	1.90	1.02
4:K:107:GLU:HG2	4:K:135:ARG:HG3	1.37	1.02
3:I:1001:ALA:HA	3:I:1020:TRP:NE1	1.75	1.01
3:D:272:VAL:HG22	3:D:306:LEU:HD11	1.42	1.00
3:I:65:VAL:HG23	3:I:71:LEU:HD22	1.44	1.00
2:C:697:LYS:HE2	2:C:790:ASP:HB3	1.44	0.99
2:H:697:LYS:HE2	2:H:790:ASP:HB3	1.45	0.98
3:D:535:ARG:HG2	3:D:538:ARG:NH1	1.80	0.96
3:I:535:ARG:HG2	3:I:538:ARG:NH1	1.80	0.96
3:D:34:SER:HB2	3:D:105:ILE:HG12	1.48	0.95
2:H:1334:GLY:HA3	3:I:113:HIS:HE1	1.32	0.94
2:H:619:ALA:HB3	3:I:769:VAL:HG21	1.47	0.93
3:D:113:HIS:NE2	3:D:239:LEU:HG	1.84	0.92
1:G:179:PRO:HA	1:G:209:GLY:HA3	1.52	0.91
3:D:275:ARG:NH1	3:D:298:MET:O	2.04	0.91
2:H:226:GLU:HB2	2:H:337:PHE:CE2	2.07	0.90
3:I:420:PRO:HA	3:I:439:PRO:HD3	1.54	0.90
1:B:179:PRO:HA	1:B:209:GLY:HA3	1.53	0.88
3:D:420:PRO:HA	3:D:439:PRO:HD3	1.54	0.88
3:D:395:LYS:HZ3	2:H:905:ILE:HB	1.37	0.88
3:D:508:LEU:HD21	3:D:730:ALA:HB2	1.56	0.87
3:I:252:LEU:HD23	3:I:263:SER:HB3	1.57	0.85
3:D:808:VAL:HG13	3:D:914:ALA:HA	1.58	0.84
3:I:808:VAL:HG13	3:I:914:ALA:HA	1.58	0.84
2:H:1334:GLY:HA3	3:I:113:HIS:CE1	2.12	0.84
3:D:226:ALA:CB	3:D:227:PHE:HA	2.07	0.83
2:H:887:VAL:HG13	2:H:909:LYS:HE2	1.60	0.83
3:D:275:ARG:NH1	3:D:302:ALA:H	1.77	0.82
4:K:87:PRO:HB2	4:K:88:ARG:HA	1.62	0.82
4:J:87:PRO:HB2	4:J:88:ARG:HA	1.61	0.81
3:D:395:LYS:HE3	2:H:901:LEU:O	1.80	0.80
3:D:113:HIS:CD2	3:D:238:ILE:HA	2.17	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:252:LEU:HD13	3:D:260:PHE:HB3	1.63	0.79
3:D:252:LEU:HD23	3:D:263:SER:HB3	1.63	0.79
3:D:86:GLU:HB3	2:H:1253:LEU:CD2	2.13	0.79
1:A:45:ARG:HD3	1:B:38:THR:HG22	1.65	0.79
2:C:12[A]:ARG:HG3	2:C:12[A]:ARG:NH1	1.96	0.79
2:C:619:ALA:HB3	3:D:769:VAL:HG21	1.62	0.79
3:D:331:ILE:HG21	3:D:1332:LEU:CD1	2.13	0.78
3:D:169:LEU:HB3	3:D:176:PHE:CZ	2.18	0.77
3:D:139:LEU:HD13	3:D:185:ILE:HD11	1.65	0.77
2:C:1332:SER:HA	3:D:243:PRO:HB2	1.66	0.77
1:A:45:ARG:HB2	1:B:38:THR:CG2	2.15	0.77
3:D:34:SER:CB	3:D:105:ILE:HG12	2.15	0.76
3:D:506:VAL:HG22	3:D:629:PHE:CZ	2.20	0.76
3:I:849:LEU:HD22	3:I:877:VAL:HG11	1.66	0.75
3:D:327:LEU:O	3:D:331:ILE:HG13	1.86	0.75
2:H:855:PRO:HB3	2:H:914:LYS:HD3	1.69	0.75
3:I:506:VAL:HG22	3:I:629:PHE:CZ	2.20	0.75
3:D:86:GLU:HB3	2:H:1253:LEU:HD22	1.66	0.74
2:H:805:MET:HE3	2:H:806:PRO:HD2	1.69	0.74
3:I:1226:VAL:HG22	3:I:1304:ARG:HH22	1.52	0.74
2:H:1330:ILE:HA	2:H:1333:LEU:HD12	1.68	0.74
2:C:1330:ILE:HA	2:C:1333:LEU:HD12	1.67	0.74
3:D:1152:GLU:C	3:D:1194:ARG:HH22	1.91	0.74
3:D:124:ILE:HG22	3:D:135:ILE:HD13	1.70	0.73
3:D:272:VAL:HG22	3:D:306:LEU:HD13	1.69	0.73
2:C:497:PRO:HB3	4:J:8:ARG:HD3	1.71	0.73
3:D:275:ARG:CZ	3:D:298:MET:O	2.36	0.73
2:C:810:TYR:HA	3:D:357:VAL:HG11	1.71	0.73
3:D:664:ILE:HD11	3:D:685:ILE:HD12	1.71	0.72
4:K:107:GLU:CG	4:K:135:ARG:HG3	2.16	0.72
2:C:35:PHE:CZ	2:C:456:VAL:HB	2.25	0.72
3:D:275:ARG:HH12	3:D:302:ALA:H	1.37	0.72
3:D:81:ARG:HD3	2:H:890:LYS:HE3	1.70	0.72
2:H:35:PHE:CZ	2:H:456:VAL:HB	2.25	0.72
3:D:849:LEU:HD22	3:D:877:VAL:HG11	1.71	0.72
3:D:123:ARG:HH12	3:D:1333:THR:HB	1.55	0.71
3:D:647:PRO:HD3	3:D:697:MET:SD	2.31	0.71
2:C:801:ARG:HG3	2:C:1229:TYR:CE1	2.25	0.71
3:D:113:HIS:HD2	3:D:238:ILE:HA	1.56	0.71
3:I:664:ILE:HD11	3:I:685:ILE:HD12	1.70	0.71
3:I:425:ARG:NH2	3:I:457:TYR:HB2	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:331:ILE:HB	3:I:1328:THR:OG1	1.91	0.71
2:H:801:ARG:HG3	2:H:1229:TYR:CE1	2.25	0.70
2:C:1295:SER:HA	2:C:1301:ARG:HH21	1.56	0.70
3:D:71:LEU:O	3:I:66:LYS:HA	1.91	0.70
1:F:45:ARG:NH2	1:G:37:HIS:HB3	2.05	0.70
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.72	0.70
2:C:1326:LEU:HG	3:D:341:ASN:ND2	2.05	0.70
2:C:1209:GLN:HB3	2:C:1224:PRO:HB2	1.72	0.70
2:C:559:CYS:SG	2:C:576:SER:HA	2.32	0.70
2:H:1209:GLN:HB3	2:H:1224:PRO:HB2	1.72	0.70
2:C:896:THR:HB	2:C:897:PRO:HD2	1.72	0.70
2:H:19:PRO:HB2	2:H:20:GLN:HG3	1.73	0.69
3:D:431:ARG:HH22	3:D:914:ALA:HB3	1.57	0.69
2:H:896:THR:HB	2:H:897:PRO:HD2	1.74	0.69
3:I:430:HIS:CE1	3:I:922:SER:HA	2.28	0.69
3:I:647:PRO:HD3	3:I:697:MET:SD	2.33	0.69
2:H:226:GLU:CB	2:H:337:PHE:CE2	2.75	0.69
3:I:114:ILE:HG12	3:I:304:ASP:HA	1.75	0.69
1:A:51:MET:HB3	1:A:179:PRO:HD2	1.74	0.69
2:H:559:CYS:SG	2:H:576:SER:HA	2.32	0.69
1:A:45:ARG:HD3	1:B:38:THR:CG2	2.23	0.69
3:I:431:ARG:HH22	3:I:914:ALA:HB3	1.58	0.69
3:D:71:LEU:HD21	3:I:51:PRO:HD3	1.75	0.68
2:H:1295:SER:HA	2:H:1301:ARG:HH21	1.56	0.68
3:D:536:LEU:HD13	3:D:574:VAL:HG13	1.76	0.68
1:B:182:ARG:HH22	3:D:581:MET:HG3	1.58	0.68
3:D:430:HIS:CE1	3:D:922:SER:HA	2.27	0.68
3:I:424:ASN:OD1	3:I:434:ILE:HA	1.93	0.68
3:D:424:ASN:OD1	3:D:434:ILE:HA	1.93	0.68
3:I:169:LEU:O	3:I:173:GLY:HA3	1.94	0.68
1:F:51:MET:HB3	1:F:179:PRO:HD2	1.76	0.68
2:H:226:GLU:HB2	2:H:337:PHE:HE2	1.58	0.68
4:K:87:PRO:HB2	4:K:88:ARG:CA	2.23	0.68
4:K:143:ASP:O	4:K:144:PHE:HD1	1.77	0.68
4:J:87:PRO:HB2	4:J:88:ARG:CA	2.24	0.67
3:I:202:ARG:NH1	3:I:216:LYS:HB2	2.08	0.67
2:H:122:VAL:HG21	2:H:493:ILE:HB	1.77	0.67
3:D:1261:LEU:HA	3:D:1306:LEU:HD22	1.76	0.67
3:D:305:ALA:HB2	3:D:314:ARG:HD3	1.77	0.67
2:C:122:VAL:HG21	2:C:493:ILE:HB	1.76	0.67
3:I:1261:LEU:HA	3:I:1306:LEU:HD22	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:46:ILE:HG12	1:G:35:PHE:CE1	2.30	0.67
3:I:425:ARG:CZ	3:I:459:ALA:HB2	2.24	0.67
3:D:113:HIS:CE1	3:D:239:LEU:HG	2.30	0.67
3:D:93:THR:HG22	2:H:890:LYS:HZ1	1.59	0.67
3:D:114:ILE:HG12	3:D:304:ASP:HA	1.77	0.67
3:D:127:LEU:HD13	3:D:234:PRO:HB3	1.78	0.66
2:C:12[A]:ARG:CG	2:C:12[A]:ARG:HH11	2.03	0.66
2:C:211:ARG:HA	2:C:215:TYR:O	1.96	0.66
2:H:211:ARG:HA	2:H:215:TYR:O	1.96	0.66
3:I:202:ARG:HH12	3:I:216:LYS:HB2	1.61	0.66
3:I:303:VAL:HA	3:I:306:LEU:HD12	1.77	0.66
3:I:365:GLN:O	3:I:450:HIS:CE1	2.48	0.66
3:I:315:ALA:HB3	3:I:324:LEU:HD23	1.78	0.66
2:C:889:PRO:C	3:I:78:LEU:HD12	2.16	0.66
3:I:536:LEU:HD13	3:I:574:VAL:HG13	1.78	0.66
3:D:421:VAL:HG23	3:D:439:PRO:HG3	1.78	0.66
2:C:1333:LEU:HD23	3:D:307:LEU:HB3	1.78	0.66
2:C:1329:GLU:HG2	3:D:245:LEU:HD21	1.78	0.66
1:A:70:THR:HG21	2:C:755:LYS:HD3	1.77	0.66
3:I:978:ARG:HH12	3:I:1198:VAL:HA	1.61	0.66
2:H:226:GLU:CB	2:H:337:PHE:HE2	2.07	0.66
3:I:189:LEU:HA	3:I:192:MET:HB2	1.78	0.66
3:I:327:LEU:O	3:I:331:ILE:HG12	1.95	0.65
1:G:51:MET:HB3	1:G:179:PRO:HD2	1.78	0.65
3:D:978:ARG:HH12	3:D:1198:VAL:HA	1.59	0.65
1:F:48:LEU:HD11	2:H:1087:TYR:OH	1.96	0.65
3:I:228:VAL:HG23	3:I:1341:ARG:CZ	2.26	0.65
4:K:107:GLU:HB2	4:K:145:ASN:HB3	1.77	0.65
1:A:179:PRO:HG3	1:A:211:ILE:HD12	1.79	0.65
3:D:398:LYS:HG2	2:H:901:LEU:HD22	1.79	0.65
2:H:592:ARG:HG3	2:H:655:VAL:HG22	1.79	0.65
3:D:105:ILE:HD13	4:K:18:PHE:CE2	2.32	0.65
3:D:24:LEU:HB2	3:D:236:TRP:HB3	1.77	0.65
2:C:1295:SER:HB3	3:D:347:VAL:HG22	1.77	0.64
2:H:675:ASP:OD1	2:H:1107:MET:HB2	1.98	0.64
2:H:189:ASP:HB2	2:H:195:PHE:CE2	2.33	0.64
3:I:421:VAL:HG23	3:I:439:PRO:HG3	1.78	0.64
3:I:587:LEU:HB2	3:I:589:TYR:CE1	2.32	0.64
3:D:809:VAL:HB	3:D:913:GLU:H	1.61	0.64
2:C:189:ASP:HB2	2:C:195:PHE:CE2	2.33	0.64
2:C:903:ARG:HB2	3:I:395:LYS:HZ2	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:909:ILE:HG22	3:D:910:ASN:H	1.62	0.64
2:H:1331:ARG:O	3:I:243:PRO:HG2	1.97	0.64
3:I:809:VAL:HB	3:I:913:GLU:H	1.61	0.64
2:C:82:VAL:HA	2:C:92:TYR:HE1	1.62	0.64
3:D:303:VAL:HA	3:D:306:LEU:HD12	1.77	0.64
3:D:587:LEU:HB2	3:D:589:TYR:CE1	2.32	0.64
2:H:820:GLU:HB2	2:H:1082:ILE:HG13	1.80	0.64
3:D:24:LEU:HB2	3:D:236:TRP:CB	2.28	0.63
4:K:73:MET:HG2	4:K:74:VAL:O	1.98	0.63
1:B:51:MET:HB3	1:B:179:PRO:HD2	1.78	0.63
2:C:913:VAL:O	2:C:914:LYS:HG3	1.98	0.63
2:H:1291:LEU:HD22	3:I:343:LEU:O	1.98	0.63
3:I:909:ILE:HG22	3:I:910:ASN:H	1.63	0.63
4:K:75:MET:CE	4:K:100:PRO:HG2	2.28	0.63
2:C:592:ARG:HG3	2:C:655:VAL:HG22	1.79	0.63
3:D:124:ILE:HG13	3:D:237:MET:HE3	1.79	0.63
2:H:1302:THR:HA	2:H:1305:TYR:CD2	2.34	0.63
4:K:108:VAL:O	4:K:111:ILE:HG22	1.98	0.63
1:A:45:ARG:HB2	1:B:38:THR:HG21	1.80	0.63
2:C:820:GLU:HB2	2:C:1082:ILE:HG13	1.81	0.63
2:C:675:ASP:OD1	2:C:1107:MET:HB2	1.98	0.63
3:D:252:LEU:HG	3:I:86:GLU:HB2	1.78	0.63
1:F:179:PRO:HG3	1:F:211:ILE:HD12	1.80	0.63
2:H:557:ARG:HB3	2:H:587:LEU:HD22	1.81	0.63
2:H:85:CYS:HA	2:H:88:ARG:HB2	1.81	0.63
3:I:50:LYS:HB3	3:I:51:PRO:HD2	1.81	0.63
3:D:269:TYR:HA	3:D:272:VAL:HG23	1.80	0.62
2:C:805:MET:HE3	2:C:806:PRO:HD2	1.79	0.62
2:C:1302:THR:HA	2:C:1305:TYR:CD2	2.33	0.62
1:F:35:PHE:CE1	1:G:46:ILE:HG12	2.35	0.62
2:H:1333:LEU:HD13	3:I:115:TRP:HE1	1.64	0.62
2:H:884:VAL:HG23	2:H:1052:VAL:HG23	1.82	0.62
3:D:189:LEU:HA	3:D:192:MET:HB2	1.82	0.62
3:I:885:VAL:HB	3:I:1258:ARG:CD	2.25	0.62
2:C:85:CYS:HA	2:C:88:ARG:HB2	1.81	0.62
3:I:1221:LEU:HG	3:I:1229:VAL:HG21	1.82	0.62
1:A:74:VAL:O	2:C:729:ALA:HB2	2.00	0.61
2:C:557:ARG:HB3	2:C:587:LEU:HD22	1.82	0.61
3:I:365:GLN:O	3:I:450:HIS:HE1	1.83	0.61
2:H:96:LEU:HD11	2:H:127:ILE:HD12	1.83	0.61
2:C:876:GLU:HG2	2:C:927:THR:HG22	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1238:GLN:O	3:D:1242:ARG:HB2	2.01	0.61
3:D:97:VAL:HG21	3:I:47:ARG:HD3	1.82	0.61
3:D:395:LYS:NZ	2:H:905:ILE:HB	2.14	0.61
3:I:269:TYR:HA	3:I:272:VAL:HG23	1.80	0.61
2:C:884:VAL:HG23	2:C:1052:VAL:HG23	1.81	0.61
3:I:1238:GLN:O	3:I:1242:ARG:HB2	2.01	0.61
3:I:807:LEU:HD22	3:I:1262:ARG:HH12	1.66	0.61
3:I:408:VAL:O	3:I:412:LEU:HG	2.01	0.61
3:D:807:LEU:HD22	3:D:1262:ARG:HH12	1.65	0.61
2:C:848:GLU:HG2	2:C:889:PRO:HD3	1.81	0.61
3:D:408:VAL:O	3:D:412:LEU:HG	2.01	0.61
4:K:160:VAL:HG21	4:K:178:VAL:HG11	1.82	0.61
3:D:1173:ARG:HB3	3:D:1190:ILE:O	2.00	0.61
3:D:1221:LEU:HG	3:D:1229:VAL:HG21	1.82	0.61
3:D:395:LYS:O	3:D:398:LYS:HG3	2.01	0.61
1:F:46:ILE:HG12	1:G:35:PHE:HE1	1.64	0.61
3:D:81:ARG:NH1	2:H:890:LYS:H	1.98	0.61
2:H:1332:SER:HA	3:I:243:PRO:HB2	1.83	0.61
2:C:802:VAL:HG21	2:C:1230:MET:HB2	1.83	0.61
3:D:982:LEU:O	3:D:994:SER:HB2	2.00	0.61
3:I:1173:ARG:HB3	3:I:1190:ILE:O	2.01	0.61
3:I:425:ARG:CZ	3:I:457:TYR:HB3	2.31	0.61
3:D:205:LEU:HD13	3:D:212:THR:HG21	1.83	0.60
1:G:61:ILE:HG12	1:G:142:MET:HE1	1.82	0.60
2:H:855:PRO:HD2	2:H:886:LYS:HD2	1.82	0.60
2:H:1295:SER:HB3	3:I:347:VAL:HG22	1.82	0.60
2:C:1330:ILE:HD11	3:D:1332:LEU:HD22	1.82	0.60
2:C:96:LEU:HD11	2:C:127:ILE:HD12	1.81	0.60
3:I:78:LEU:HD13	3:I:81:ARG:NH2	2.16	0.60
2:H:453:ILE:HD11	2:H:587:LEU:HG	1.83	0.60
3:I:982:LEU:O	3:I:994:SER:HB2	2.01	0.60
3:D:605:LEU:O	3:D:609:TYR:HD2	1.85	0.60
2:C:1137:GLU:HA	2:C:1141:LEU:HD12	1.83	0.60
2:H:802:VAL:HG21	2:H:1230:MET:HB2	1.83	0.60
3:I:309:ASN:HB2	3:I:324:LEU:HD13	1.83	0.60
2:H:1333:LEU:HD22	3:I:115:TRP:NE1	2.16	0.60
3:I:1241:TYR:HB2	3:I:1248:ILE:HD11	1.82	0.60
3:I:605:LEU:O	3:I:609:TYR:HD2	1.85	0.60
3:D:81:ARG:HA	3:D:92:VAL:HB	1.84	0.60
3:I:119:SER:C	3:I:121:PRO:HD3	2.22	0.60
3:I:1238:GLN:HG3	3:I:1253:ILE:CD1	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1331:VAL:HA	3:I:1334:GLU:HB2	1.83	0.60
3:D:1256:ILE:O	3:D:1260:MET:HG2	2.02	0.59
1:F:107:ILE:HD11	1:F:136:GLU:HG2	1.84	0.59
3:I:425:ARG:HH12	3:I:458:ASN:C	2.05	0.59
3:D:1238:GLN:HG3	3:D:1253:ILE:CD1	2.32	0.59
2:H:35:PHE:HZ	2:H:456:VAL:HB	1.66	0.59
3:I:984:LEU:HD12	3:I:993:GLU:HB2	1.84	0.59
2:C:194:LEU:HD11	2:C:433:ILE:HD11	1.83	0.59
2:C:805:MET:HE1	3:D:637:ALA:H	1.66	0.59
3:I:1256:ILE:O	3:I:1260:MET:HG2	2.02	0.59
3:I:597:GLY:HA2	3:I:600:ALA:HB3	1.84	0.59
4:J:160:VAL:HG21	4:J:178:VAL:HG11	1.83	0.59
2:C:453:ILE:HD11	2:C:587:LEU:HG	1.84	0.59
3:D:885:VAL:CB	3:D:1258:ARG:HD3	2.26	0.59
3:D:78:LEU:HD13	3:D:81:ARG:HH21	1.67	0.59
3:I:226:ALA:HB1	3:I:1341:ARG:CZ	2.33	0.59
3:D:90:VAL:HA	3:I:260:PHE:HE1	1.68	0.59
3:D:597:GLY:HA2	3:D:600:ALA:HB3	1.85	0.59
3:D:797:THR:O	3:D:801:VAL:HG23	2.03	0.59
4:J:95:GLY:HA3	4:J:102:PRO:HG2	1.84	0.59
1:A:48:LEU:HB2	2:C:1083:GLU:HG2	1.84	0.59
1:F:234:LEU:HD13	1:G:13:LEU:H	1.68	0.59
2:H:1295:SER:HA	2:H:1301:ARG:NH2	2.18	0.59
2:C:1295:SER:HA	2:C:1301:ARG:NH2	2.18	0.58
2:C:82:VAL:O	2:C:92:TYR:OH	2.21	0.58
3:D:239:LEU:HD22	3:D:241:VAL:O	2.03	0.58
3:D:275:ARG:HB3	3:D:299:LEU:HD22	1.85	0.58
1:A:101:THR:O	1:A:115:ILE:HG23	2.04	0.58
3:D:1241:TYR:HB2	3:D:1248:ILE:HD11	1.84	0.58
2:H:226:GLU:HB2	2:H:337:PHE:CD2	2.37	0.58
3:I:550:VAL:HB	3:I:552:ILE:HG13	1.85	0.58
2:C:855:PRO:HG3	2:C:914:LYS:HD3	1.85	0.58
1:F:234:LEU:HB3	1:G:13:LEU:HD12	1.83	0.58
3:D:1001:ALA:CA	3:D:1020:TRP:HE1	2.02	0.58
3:D:86:GLU:HB3	2:H:1253:LEU:HD21	1.85	0.58
2:H:1137:GLU:HA	2:H:1141:LEU:HD12	1.84	0.58
2:H:1326:LEU:HG	3:I:341:ASN:ND2	2.18	0.58
3:I:797:THR:O	3:I:801:VAL:HG23	2.04	0.58
3:D:189:LEU:HD22	3:D:234:PRO:HB2	1.85	0.58
2:H:562:GLU:HG2	2:H:683:ALA:HB1	1.85	0.58
2:C:731:ARG:HG2	2:C:752:ASN:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:169:LEU:HB3	3:D:176:PHE:HZ	1.63	0.58
2:C:35:PHE:HZ	2:C:456:VAL:HB	1.66	0.57
3:D:550:VAL:HB	3:D:552:ILE:HG13	1.85	0.57
2:H:194:LEU:HD11	2:H:433:ILE:HD11	1.84	0.57
2:H:524:ILE:HD11	2:H:712:SER:HB3	1.87	0.57
2:H:845:LEU:HB2	2:H:890:LYS:HG2	1.86	0.57
3:D:247:PRO:CB	3:I:53:ARG:HH12	2.03	0.57
3:I:932:MET:HA	3:I:1139:PRO:HD3	1.86	0.57
3:D:1331:VAL:HA	3:D:1334:GLU:HB2	1.84	0.57
3:I:384:LYS:HD3	3:I:411:ILE:HG22	1.85	0.57
1:A:159:ILE:O	1:A:162:GLU:HG3	2.05	0.57
3:D:885:VAL:HB	3:D:1258:ARG:CD	2.25	0.57
2:H:145:ILE:HG23	2:H:511:LEU:HB3	1.86	0.57
2:C:176:ILE:HD11	2:C:428:VAL:HG11	1.86	0.57
2:C:524:ILE:HD11	2:C:712:SER:HB3	1.87	0.57
3:D:984:LEU:HD12	3:D:993:GLU:HB2	1.86	0.57
2:C:562:GLU:HG2	2:C:683:ALA:HB1	1.86	0.57
3:D:194:LEU:HD13	3:D:231:GLY:O	2.04	0.57
3:D:81:ARG:HH12	2:H:890:LYS:N	2.02	0.57
1:F:104:LYS:HE2	1:F:114:ASP:HB2	1.86	0.57
3:D:1220:ILE:HG22	3:D:1229:VAL:HG22	1.86	0.57
3:D:113:HIS:CD2	3:D:239:LEU:HG	2.40	0.57
4:K:107:GLU:HG2	4:K:135:ARG:CG	2.24	0.57
2:C:904:ALA:HB3	3:I:395:LYS:HD2	1.85	0.56
3:D:70:CYS:HB2	3:D:75:TYR:HB2	1.85	0.56
1:G:13:LEU:HD23	1:G:28:LEU:HG	1.87	0.56
2:H:225:PHE:HE2	2:H:347:ILE:HB	1.69	0.56
2:C:765:ILE:HG23	2:C:787:PRO:HG3	1.86	0.56
2:C:1330:ILE:CD1	3:D:1332:LEU:HD22	2.35	0.56
2:H:765:ILE:HG23	2:H:787:PRO:HG3	1.86	0.56
3:I:105:ILE:HG21	4:J:18:PHE:HE2	1.70	0.56
2:H:1123:GLY:HA3	2:H:1204:LEU:HD11	1.87	0.56
2:H:893:THR:O	2:H:894:GLN:HB2	2.06	0.56
2:C:1115:THR:HB	2:C:1228:GLY:HA3	1.88	0.56
3:D:514:THR:HB	3:D:576:ARG:HE	1.70	0.56
2:H:715:THR:HG22	2:H:786:GLY:H	1.70	0.56
2:H:731:ARG:HG2	2:H:752:ASN:HA	1.87	0.56
2:C:1289:GLU:HA	2:C:1293:VAL:HB	1.87	0.56
2:C:404:LYS:HD2	2:C:452:ARG:HH21	1.71	0.56
2:H:848:GLU:HA	2:H:889:PRO:HD3	1.87	0.56
3:D:81:ARG:NH1	2:H:890:LYS:N	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:514:THR:HB	3:I:576:ARG:HE	1.71	0.56
2:H:176:ILE:HD11	2:H:428:VAL:HG11	1.88	0.56
3:I:198:CYS:SG	3:I:216:LYS:HD3	2.45	0.56
2:H:805:MET:HE1	3:I:637:ALA:H	1.70	0.56
2:C:224:PHE:CE1	2:C:347:ILE:HD13	2.40	0.56
4:J:39:PHE:HZ	4:J:79:SER:HG	1.53	0.56
4:K:23:ALA:HA	4:K:26:LEU:HD12	1.87	0.56
3:I:1220:ILE:HG22	3:I:1229:VAL:HG22	1.88	0.56
3:I:1316:THR:OG1	3:I:1322:ALA:HB2	2.06	0.56
3:I:580:TRP:HE1	3:I:590:SER:HA	1.71	0.56
3:I:661:VAL:HG23	3:I:685:ILE:HG22	1.88	0.56
1:B:91:ARG:HG3	1:B:210:THR:HB	1.87	0.55
2:C:145:ILE:HG23	2:C:511:LEU:HB3	1.88	0.55
2:C:390:PHE:HA	2:C:419:ILE:HG23	1.88	0.55
3:D:885:VAL:HG22	3:D:899:TYR:CD1	2.41	0.55
2:H:390:PHE:HA	2:H:419:ILE:HG23	1.87	0.55
3:D:932:MET:HA	3:D:1139:PRO:HD3	1.88	0.55
3:D:1316:THR:OG1	3:D:1322:ALA:HB2	2.05	0.55
3:D:252:LEU:HD12	3:I:75:TYR:OH	2.07	0.55
4:K:95:GLY:HA3	4:K:102:PRO:HG2	1.88	0.55
3:D:668:PHE:CZ	3:D:678:ARG:HB3	2.41	0.55
3:D:749:LYS:HE3	3:D:755:ILE:HG12	1.88	0.55
2:H:1107:MET:HE3	3:I:740:LEU:HG	1.88	0.55
2:H:1115:THR:HB	2:H:1228:GLY:HA3	1.88	0.55
3:D:1216:ALA:O	3:D:1220:ILE:HG13	2.07	0.55
3:D:535:ARG:HG2	3:D:538:ARG:HH12	1.67	0.55
3:I:227:PHE:C	3:I:1341:ARG:HH12	2.10	0.55
2:C:1333:LEU:HD13	3:D:115:TRP:HE1	1.71	0.55
2:C:1333:LEU:HD22	3:D:115:TRP:NE1	2.22	0.55
3:I:114:ILE:HD12	3:I:307:LEU:HB2	1.88	0.55
4:J:106:LYS:HB2	4:J:143:ASP:HA	1.88	0.55
4:K:87:PRO:CB	4:K:88:ARG:HA	2.34	0.55
1:B:179:PRO:HA	1:B:209:GLY:CA	2.33	0.55
2:C:1333:LEU:HD22	3:D:115:TRP:HE1	1.71	0.55
3:D:661:VAL:HG23	3:D:685:ILE:HG22	1.89	0.55
4:J:23:ALA:HA	4:J:26:LEU:HD12	1.86	0.55
1:A:104:LYS:HE2	1:A:114:ASP:HB2	1.89	0.55
3:I:668:PHE:CZ	3:I:678:ARG:HB3	2.41	0.55
2:C:697:LYS:HZ1	2:C:791:LEU:HB2	1.72	0.55
3:I:78:LEU:HB3	3:I:81:ARG:HH21	1.72	0.55
3:I:885:VAL:HG22	3:I:899:TYR:CD1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:715:THR:HG22	2:C:786:GLY:H	1.71	0.55
3:D:194:LEU:HD21	3:D:232:ASN:O	2.07	0.55
1:G:91:ARG:HG3	1:G:210:THR:HB	1.88	0.55
2:H:805:MET:CE	2:H:806:PRO:HD2	2.37	0.55
3:I:206:ASN:HA	3:I:209:ASN:O	2.07	0.55
3:I:81:ARG:HA	3:I:92:VAL:HB	1.88	0.55
2:C:1109:ILE:HA	2:C:1112:ILE:HD12	1.90	0.54
2:C:1256:GLN:HB3	2:C:1298:VAL:HG23	1.90	0.54
2:C:1323:PHE:CE1	3:D:1352:ILE:HG23	2.42	0.54
2:C:496:LYS:HG2	4:J:102:PRO:HB3	1.89	0.54
3:D:309:ASN:ND2	3:D:326:SER:HB3	2.22	0.54
3:D:380:PHE:HE2	3:D:472:LEU:HD22	1.72	0.54
3:D:81:ARG:NH2	2:H:913:VAL:HG11	2.22	0.54
3:D:331:ILE:HG12	3:D:337:ARG:NH2	2.22	0.54
1:G:89:ALA:HB1	1:G:210:THR:HG23	1.89	0.54
2:H:404:LYS:HD2	2:H:452:ARG:HH21	1.70	0.54
2:C:818:VAL:HB	2:C:1079:ILE:HG12	1.89	0.54
2:C:144:VAL:HB	2:C:515:MET:SD	2.47	0.54
3:D:189:LEU:HD13	3:D:234:PRO:O	2.07	0.54
3:D:123:ARG:HB2	3:D:237:MET:HE1	1.90	0.54
2:C:1123:GLY:HA3	2:C:1204:LEU:HD11	1.89	0.54
2:H:561:ILE:HA	2:H:680:LEU:HD23	1.90	0.54
1:B:179:PRO:HG3	1:B:211:ILE:HD12	1.88	0.54
1:B:43:LEU:HA	1:B:46:ILE:HD12	1.89	0.54
2:C:805:MET:CE	2:C:806:PRO:HD2	2.37	0.54
3:I:79:LYS:HB3	3:I:80:HIS:CD2	2.43	0.54
1:A:43:LEU:HA	1:A:46:ILE:HD12	1.90	0.54
1:B:89:ALA:HB1	1:B:210:THR:HG23	1.88	0.54
1:A:75:GLN:HE21	2:C:727:VAL:HG11	1.72	0.54
1:G:43:LEU:HA	1:G:46:ILE:HD12	1.88	0.54
3:D:395:LYS:HE2	2:H:905:ILE:HD12	1.90	0.54
3:I:1323:ALA:HB1	3:I:1332:LEU:HD23	1.90	0.54
2:C:92:TYR:O	2:C:128:PRO:HA	2.08	0.54
3:D:576:ARG:HD3	3:D:593:ASN:HB3	1.90	0.54
2:H:1256:GLN:HB3	2:H:1298:VAL:HG23	1.90	0.54
4:J:92:PHE:CD1	4:J:100:PRO:HG3	2.43	0.54
4:K:27:ARG:HA	4:K:30:ILE:HD12	1.90	0.54
2:C:890:LYS:HD3	3:I:77:ARG:HA	1.89	0.54
3:D:1238:GLN:HG3	3:D:1253:ILE:HD13	1.90	0.54
3:D:587:LEU:HB3	3:D:588:PRO:HD2	1.89	0.54
2:H:1289:GLU:HA	2:H:1293:VAL:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1330:ILE:CD1	3:I:1332:LEU:HD22	2.37	0.54
1:B:13:LEU:HD23	1:B:28:LEU:HG	1.89	0.54
2:C:1101:LEU:HD13	3:D:504:GLN:HB3	1.89	0.54
3:D:806:ASP:HA	3:D:1347:LEU:HG	1.90	0.54
2:H:160:ASP:HB3	2:H:164:THR:HG21	1.90	0.54
3:I:1317:GLU:HB2	3:I:1344:LEU:HD11	1.90	0.54
2:C:1255:THR:HG22	2:C:1325:VAL:HG21	1.89	0.53
3:D:1072:LYS:NZ	3:D:1170:LYS:HE3	2.23	0.53
3:D:580:TRP:HE1	3:D:590:SER:HA	1.71	0.53
1:F:43:LEU:HA	1:F:46:ILE:HD12	1.90	0.53
2:H:144:VAL:HB	2:H:515:MET:SD	2.47	0.53
3:I:1001:ALA:CA	3:I:1020:TRP:HE1	2.03	0.53
3:I:1178:THR:HG22	3:I:1187:GLU:HG2	1.90	0.53
2:H:897:PRO:O	2:H:901:LEU:HG	2.08	0.53
3:I:1216:ALA:O	3:I:1220:ILE:HG13	2.07	0.53
3:D:264:ASP:HB3	3:D:325:LYS:HD2	1.90	0.53
3:D:807:LEU:CD2	3:D:1262:ARG:HH12	2.22	0.53
2:C:473:ARG:HD3	4:J:74:VAL:HG21	1.90	0.53
2:C:12[A]:ARG:CG	2:C:12[A]:ARG:NH1	2.66	0.53
2:C:561:ILE:HA	2:C:680:LEU:HD23	1.91	0.53
2:C:887:VAL:HG22	2:C:914:LYS:HG2	1.91	0.53
3:D:233:LYS:HB2	3:D:236:TRP:CD1	2.44	0.53
1:B:48:LEU:HD21	3:D:534:GLU:OE2	2.08	0.53
2:H:1109:ILE:HA	2:H:1112:ILE:HD12	1.89	0.53
2:C:496:LYS:HD3	4:J:102:PRO:HD3	1.91	0.53
2:C:1333:LEU:O	3:D:307:LEU:HD13	2.09	0.53
3:D:1317:GLU:HB2	3:D:1344:LEU:HD11	1.90	0.53
3:D:69:GLU:HG2	3:D:76:LYS:HA	1.90	0.53
2:C:1246:ARG:HD2	2:C:1266:GLY:H	1.74	0.53
2:C:20:GLN:HG3	2:C:1157:GLN:HE21	1.73	0.53
3:D:395:LYS:HE3	2:H:902:LEU:HA	1.91	0.53
2:H:1333:LEU:HD22	3:I:115:TRP:HE1	1.72	0.53
2:H:1333:LEU:HD21	3:I:327:LEU:HB2	1.90	0.53
3:I:807:LEU:CD2	3:I:1262:ARG:HH12	2.21	0.53
2:C:473:ARG:CD	4:J:74:VAL:HG21	2.38	0.53
3:D:1323:ALA:HB1	3:D:1332:LEU:HD23	1.90	0.53
2:H:818:VAL:HB	2:H:1079:ILE:HG12	1.90	0.53
3:I:233:LYS:HB2	3:I:236:TRP:CD1	2.44	0.53
3:I:69:GLU:HG2	3:I:76:LYS:HA	1.90	0.53
1:B:182:ARG:NH2	3:D:581:MET:HG3	2.24	0.53
2:C:1333:LEU:HD11	3:D:331:ILE:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:179:PRO:HA	1:G:209:GLY:CA	2.32	0.53
4:J:87:PRO:CB	4:J:88:ARG:HA	2.36	0.53
2:C:160:ASP:HB3	2:C:164:THR:HG21	1.91	0.53
2:C:1328:LYS:NZ	3:D:99:ARG:HB3	2.24	0.53
2:H:1246:ARG:HD2	2:H:1266:GLY:H	1.74	0.53
3:I:576:ARG:HD3	3:I:593:ASN:HB3	1.90	0.52
3:D:194:LEU:HD11	3:D:233:LYS:N	2.24	0.52
2:C:680:LEU:HD13	3:D:783:LEU:HD11	1.90	0.52
3:I:59:ALA:O	3:I:90:VAL:HG22	2.08	0.52
2:H:92:TYR:O	2:H:128:PRO:HA	2.09	0.52
3:I:160:LEU:N	3:I:165:TYR:HH	2.07	0.52
3:I:309:ASN:HD22	3:I:324:LEU:HB2	1.73	0.52
4:K:105:ASP:O	4:K:107:GLU:N	2.43	0.52
2:C:367:TYR:OH	2:C:384:LEU:C	2.48	0.52
3:D:357:VAL:HG12	3:D:358:GLY:N	2.25	0.52
2:H:172:TYR:CD2	2:H:436:ARG:HD2	2.45	0.52
3:I:535:ARG:HG2	3:I:538:ARG:HH12	1.68	0.52
2:C:1258:PRO:HB3	2:C:1265:PHE:CD2	2.44	0.52
2:C:172:TYR:CD2	2:C:436:ARG:HD2	2.45	0.52
3:D:890:THR:HG1	3:D:895:CYS:HG	1.58	0.52
3:I:70:CYS:HB2	3:I:75:TYR:HB2	1.91	0.52
1:F:48:LEU:CD1	2:H:1087:TYR:OH	2.57	0.52
2:H:186:PHE:HE1	2:H:209:ILE:HD12	1.74	0.52
3:I:53:ARG:HA	3:I:59:ALA:HB3	1.91	0.52
4:K:90:MET:HB3	4:K:91:GLY:HA3	1.91	0.52
2:C:82:VAL:HA	2:C:92:TYR:CE1	2.42	0.52
2:H:96:LEU:HB2	2:H:124:MET:HB2	1.92	0.52
2:H:367:TYR:OH	2:H:384:LEU:C	2.48	0.52
3:I:806:ASP:HA	3:I:1347:LEU:HG	1.90	0.52
3:I:533:ALA:HA	3:I:578:ILE:HG12	1.91	0.52
3:I:277:ASN:HB3	3:I:281:ARG:HD2	1.92	0.52
3:I:536:LEU:HD13	3:I:574:VAL:CG1	2.40	0.52
1:B:102:LEU:HD23	1:B:115:ILE:HG12	1.91	0.52
3:D:422:LEU:HB2	3:D:469:HIS:HB2	1.92	0.52
1:G:48:LEU:HG	1:G:183:ILE:HD12	1.91	0.52
3:I:885:VAL:CB	3:I:1258:ARG:HD3	2.25	0.51
3:I:1241:TYR:HB2	3:I:1248:ILE:CD1	2.40	0.51
1:A:107:ILE:HD11	1:A:136:GLU:HG2	1.91	0.51
2:C:1086:PRO:HA	2:C:1215:GLY:H	1.75	0.51
2:C:577:VAL:HG23	2:C:661:VAL:O	2.10	0.51
3:D:536:LEU:HD13	3:D:574:VAL:CG1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:45:ARG:HH21	2:H:1219:GLU:HG3	1.75	0.51
2:H:577:VAL:HG23	2:H:661:VAL:O	2.10	0.51
3:I:314:ARG:HD3	3:I:315:ALA:H	1.74	0.51
3:D:114:ILE:HD12	3:D:307:LEU:HB2	1.93	0.51
2:H:1086:PRO:HA	2:H:1215:GLY:H	1.75	0.51
2:H:60:GLN:HG2	2:H:67:GLU:HG2	1.93	0.51
3:I:105:ILE:HG21	4:J:18:PHE:CE2	2.45	0.51
3:I:1238:GLN:HG3	3:I:1253:ILE:HD13	1.90	0.51
3:D:1178:THR:HG22	3:D:1187:GLU:HG2	1.92	0.51
3:D:123:ARG:HH12	3:D:1333:THR:CB	2.23	0.51
2:H:841:ARG:HH11	2:H:1047:LEU:HD22	1.75	0.51
4:K:29:HIS:CB	4:K:82:LEU:HG	2.25	0.51
1:F:234:LEU:CB	1:G:13:LEU:HD12	2.40	0.51
2:C:310:ILE:HG23	2:C:325:LEU:HD22	1.93	0.51
3:D:78:LEU:HD13	3:D:81:ARG:NH2	2.25	0.51
2:H:1258:PRO:HB3	2:H:1265:PHE:CD2	2.46	0.51
3:I:386:GLU:HG2	3:I:394:ILE:HA	1.93	0.51
2:C:189:ASP:HB2	2:C:195:PHE:HE2	1.76	0.51
3:D:1241:TYR:HB2	3:D:1248:ILE:CD1	2.41	0.51
3:D:381:ILE:HG23	3:D:412:LEU:HD21	1.93	0.51
2:H:876:GLU:HG2	2:H:927:THR:HG22	1.93	0.51
1:A:166:ARG:H	1:A:167:PRO:HD3	1.76	0.51
2:C:96:LEU:HB2	2:C:124:MET:HB2	1.92	0.51
2:C:889:PRO:O	3:I:78:LEU:CD1	2.59	0.51
3:D:202:ARG:HD3	3:D:216:LYS:HG3	1.93	0.51
3:D:27:PRO:HB3	3:D:240:THR:OG1	2.11	0.51
3:D:734:ALA:HA	3:D:737:ILE:HD12	1.93	0.51
3:D:93:THR:HG22	2:H:890:LYS:NZ	2.24	0.51
3:I:228:VAL:HG23	3:I:1341:ARG:NH1	2.26	0.51
1:B:48:LEU:HG	1:B:183:ILE:HD12	1.92	0.50
3:D:113:HIS:CD2	3:D:237:MET:O	2.63	0.50
2:H:1328:LYS:HA	2:H:1331:ARG:HD2	1.93	0.50
3:I:357:VAL:HG12	3:I:358:GLY:N	2.25	0.50
3:I:425:ARG:NH2	3:I:457:TYR:CB	2.73	0.50
3:I:59:ALA:CB	3:I:71:LEU:HD11	2.41	0.50
2:C:1077:SER:HB2	3:D:357:VAL:HB	1.92	0.50
2:C:1224:PRO:O	3:D:638:SER:HB3	2.11	0.50
3:D:79:LYS:HB3	3:D:80:HIS:CD2	2.46	0.50
2:C:186:PHE:HE1	2:C:209:ILE:HD12	1.76	0.50
3:D:531:LYS:HD3	3:D:535:ARG:HH21	1.76	0.50
3:I:136:GLU:O	3:I:312:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:452:LEU:HG	3:D:625:MET:SD	2.51	0.50
1:G:102:LEU:HD23	1:G:115:ILE:HG12	1.93	0.50
2:H:310:ILE:HG23	2:H:325:LEU:HD22	1.92	0.50
3:I:667:GLN:HG2	3:I:672:LEU:HD12	1.93	0.50
3:D:226:ALA:CB	3:D:227:PHE:CA	2.87	0.50
2:C:1291:LEU:HD22	3:D:343:LEU:O	2.11	0.50
2:H:697:LYS:HZ1	2:H:791:LEU:HB2	1.75	0.50
1:B:16:ILE:HG12	1:B:26:VAL:HG13	1.94	0.50
3:D:1326:GLN:HB2	3:D:1331:VAL:HG21	1.94	0.50
2:C:1328:LYS:HA	2:C:1331:ARG:HD2	1.93	0.50
3:D:331:ILE:HG21	3:D:1332:LEU:HD11	1.92	0.50
3:D:667:GLN:HG2	3:D:672:LEU:HD12	1.94	0.50
3:I:169:LEU:O	3:I:173:GLY:CA	2.60	0.50
1:A:16:ILE:HG12	1:A:26:VAL:HG13	1.94	0.50
3:D:799:ARG:O	3:D:803:VAL:HG23	2.12	0.50
2:C:92:TYR:CD2	2:C:137:VAL:HB	2.47	0.50
2:H:189:ASP:HB2	2:H:195:PHE:HE2	1.76	0.50
2:C:519:ASN:HD21	2:C:689:ALA:HB3	1.76	0.49
3:I:139:LEU:HD13	3:I:185:ILE:HD11	1.94	0.49
3:I:364:HIS:HB3	3:I:487:THR:HG22	1.93	0.49
3:I:600:ALA:HA	3:I:603:LYS:HB2	1.94	0.49
1:A:74:VAL:O	2:C:729:ALA:N	2.46	0.49
3:D:272:VAL:CG2	3:D:306:LEU:HD13	2.42	0.49
3:D:378:LYS:HA	3:D:381:ILE:HD12	1.93	0.49
3:D:364:HIS:HB3	3:D:487:THR:HG22	1.93	0.49
1:B:182:ARG:HH22	3:D:581:MET:CG	2.22	0.49
2:C:724:VAL:HG22	2:C:734:ILE:HG12	1.94	0.49
1:G:179:PRO:HG3	1:G:211:ILE:HD12	1.95	0.49
4:J:27:ARG:HA	4:J:30:ILE:HD12	1.94	0.49
3:D:978:ARG:NH1	3:D:1198:VAL:HA	2.27	0.49
2:H:870:ILE:HD12	2:H:944:ARG:HD2	1.95	0.49
3:D:242:LEU:HD22	3:D:303:VAL:HG11	1.92	0.49
3:D:281:ARG:HG2	3:I:107:LEU:CD1	2.42	0.49
3:D:600:ALA:HA	3:D:603:LYS:HB2	1.94	0.49
2:H:895:LEU:HD22	2:H:900:LYS:HG3	1.95	0.49
3:I:750:PRO:HA	3:I:781:LYS:HE2	1.94	0.49
1:A:101:THR:HA	1:A:142:MET:O	2.13	0.49
2:C:224:PHE:CZ	2:C:347:ILE:HG21	2.48	0.49
3:D:337:ARG:HB3	3:D:341:ASN:ND2	2.27	0.49
3:D:366:CYS:HB2	3:D:437:PHE:HB2	1.94	0.49
1:F:16:ILE:HG12	1:F:26:VAL:HG13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:122:VAL:HG22	2:H:490:GLN:HA	1.94	0.49
2:H:1255:THR:HG22	2:H:1325:VAL:HG21	1.93	0.49
2:H:321:LEU:O	2:H:325:LEU:HG	2.12	0.49
2:H:724:VAL:HG22	2:H:734:ILE:HG12	1.94	0.49
3:I:422:LEU:HB2	3:I:469:HIS:HB2	1.94	0.49
3:I:580:TRP:HE1	3:I:593:ASN:HB2	1.77	0.49
1:A:48:LEU:HG	1:A:183:ILE:HD12	1.95	0.49
2:C:321:LEU:O	2:C:325:LEU:HG	2.13	0.49
2:C:367:TYR:HA	2:C:370:MET:HB2	1.95	0.49
2:C:122:VAL:HG22	2:C:490:GLN:HA	1.94	0.49
3:D:113:HIS:CD2	3:D:239:LEU:N	2.81	0.49
1:G:101:THR:HA	1:G:142:MET:O	2.13	0.49
2:H:851:THR:HG23	2:H:886:LYS:H	1.78	0.49
3:I:425:ARG:CZ	3:I:457:TYR:CB	2.91	0.49
2:H:1281:TYR:HD1	3:I:484:MET:HG3	1.76	0.49
3:I:749:LYS:HE3	3:I:755:ILE:HG12	1.95	0.49
3:I:430:HIS:CE1	3:I:925:GLU:HB2	2.48	0.49
3:D:185:ILE:HA	3:D:188:LEU:HG	1.95	0.49
1:F:48:LEU:HG	1:F:183:ILE:HD12	1.94	0.49
2:H:367:TYR:HA	2:H:370:MET:HB2	1.95	0.49
4:J:174:ASP:O	4:J:178:VAL:HG22	2.13	0.49
2:C:802:VAL:HA	2:C:1096:ILE:O	2.12	0.49
3:I:363:LEU:HD23	3:I:450:HIS:HB3	1.94	0.49
3:I:506:VAL:HG22	3:I:629:PHE:CE1	2.48	0.49
3:I:62:PHE:CD1	3:I:247:PRO:HD3	2.48	0.49
4:J:159:LYS:HE3	4:J:170:PRO:HB2	1.94	0.49
2:C:841:ARG:HH11	2:C:1047:LEU:HD22	1.76	0.49
1:F:101:THR:HA	1:F:142:MET:O	2.13	0.49
2:H:519:ASN:HD21	2:H:689:ALA:HB3	1.77	0.49
2:H:870:ILE:HG23	2:H:884:VAL:HG22	1.95	0.49
2:C:60:GLN:HG2	2:C:67:GLU:HG2	1.94	0.48
2:C:870:ILE:HG23	2:C:884:VAL:HG22	1.94	0.48
3:D:1002:VAL:HG23	3:D:1020:TRP:CZ2	2.48	0.48
3:D:106:GLU:OE2	3:D:273:ILE:HG12	2.13	0.48
3:D:90:VAL:HA	3:I:260:PHE:CE1	2.48	0.48
3:D:81:ARG:CZ	2:H:890:LYS:HB2	2.42	0.48
3:I:531:LYS:HD3	3:I:535:ARG:HH21	1.78	0.48
2:H:810:TYR:HB3	2:H:817:LEU:CD2	2.43	0.48
2:H:854:ILE:HD13	2:H:865:LEU:HD13	1.94	0.48
3:I:452:LEU:HG	3:I:625:MET:SD	2.53	0.48
3:I:660:GLU:HB3	3:I:685:ILE:CG2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:75:MET:HE2	4:K:100:PRO:HG2	1.95	0.48
4:K:174:ASP:O	4:K:178:VAL:HG22	2.13	0.48
2:C:117:ILE:HD11	2:C:485:ASP:HB3	1.94	0.48
2:C:1279:GLU:HA	2:C:1287:LEU:HD11	1.95	0.48
3:I:661:VAL:HG21	3:I:686:TRP:CD1	2.49	0.48
3:I:70:CYS:SG	3:I:90:VAL:HB	2.53	0.48
3:I:59:ALA:HB2	3:I:71:LEU:HD11	1.94	0.48
3:D:386:GLU:HG2	3:D:394:ILE:HA	1.95	0.48
1:F:210:THR:O	1:F:211:ILE:HG13	2.14	0.48
3:I:56:LEU:HD11	3:I:270:ARG:HG3	1.94	0.48
3:D:512:TYR:HA	3:D:515:ARG:CZ	2.44	0.48
3:D:430:HIS:CE1	3:D:925:GLU:HB2	2.48	0.48
3:I:799:ARG:O	3:I:803:VAL:HG23	2.13	0.48
3:D:30:ILE:HG21	3:D:243:PRO:HG3	1.94	0.48
3:D:366:CYS:HB3	3:D:439:PRO:HA	1.95	0.48
3:D:661:VAL:HG21	3:D:686:TRP:CD1	2.49	0.48
1:G:16:ILE:HG12	1:G:26:VAL:HG13	1.95	0.48
1:F:42:ALA:HA	1:G:38:THR:HG22	1.94	0.48
3:I:416:ILE:HG23	3:I:439:PRO:HB2	1.95	0.48
1:A:60:GLU:HG3	1:A:170:ARG:HG3	1.96	0.48
3:D:368:LEU:HD21	3:D:421:VAL:HG21	1.96	0.48
1:B:101:THR:HA	1:B:142:MET:O	2.13	0.48
2:C:851:THR:HG23	2:C:886:LYS:H	1.79	0.48
3:D:580:TRP:HE1	3:D:593:ASN:HB2	1.78	0.48
2:H:802:VAL:HA	2:H:1096:ILE:O	2.12	0.48
3:D:394:ILE:HG22	2:H:901:LEU:HD23	1.96	0.48
2:C:38:PHE:HD1	2:C:48:GLY:HA2	1.79	0.48
3:D:275:ARG:CZ	3:D:302:ALA:HB3	2.44	0.48
2:H:366:ILE:O	2:H:370:MET:HG2	2.14	0.48
2:H:831:ILE:HG12	2:H:1057:LYS:HG2	1.95	0.48
3:I:1002:VAL:HG23	3:I:1020:TRP:CZ2	2.48	0.48
3:I:512:TYR:HA	3:I:515:ARG:CZ	2.44	0.48
3:I:612:LEU:HB3	3:I:616:PRO:HG2	1.95	0.48
2:C:843:THR:HB	3:I:81:ARG:CZ	2.44	0.48
3:D:416:ILE:HG23	3:D:439:PRO:HB2	1.96	0.48
3:D:612:LEU:HB3	3:D:616:PRO:HG2	1.96	0.48
3:I:1326:GLN:HB2	3:I:1331:VAL:HG21	1.96	0.48
2:C:1277:ALA:HB1	2:C:1281:TYR:HE2	1.79	0.47
2:C:741:MET:HG2	2:C:747:GLY:HA2	1.96	0.47
3:D:212:THR:HG22	3:D:215:LYS:HD2	1.96	0.47
2:H:38:PHE:HD1	2:H:48:GLY:HA2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:141:PHE:HB3	4:K:162:VAL:HG21	1.96	0.47
1:A:210:THR:O	1:A:211:ILE:HG13	2.14	0.47
3:D:202:ARG:HG2	3:D:212:THR:HB	1.95	0.47
3:D:272:VAL:CG2	3:D:306:LEU:CD1	2.79	0.47
2:H:1277:ALA:HB1	2:H:1281:TYR:HE2	1.79	0.47
3:I:978:ARG:NH1	3:I:1198:VAL:HA	2.27	0.47
2:H:1330:ILE:HD11	3:I:1332:LEU:HD22	1.95	0.47
3:I:425:ARG:CZ	3:I:459:ALA:CB	2.92	0.47
2:C:559:CYS:SG	2:C:662:SER:N	2.87	0.47
2:H:12[B]:ARG:HD2	2:H:1183:ALA:HB2	1.95	0.47
3:I:114:ILE:CG1	3:I:304:ASP:HA	2.42	0.47
3:I:381:ILE:HG12	3:I:412:LEU:HD22	1.96	0.47
3:I:660:GLU:HB3	3:I:685:ILE:HG21	1.96	0.47
3:I:68:TYR:CG	3:I:78:LEU:CD2	2.98	0.47
3:I:896:ALA:HA	3:I:899:TYR:CE2	2.49	0.47
1:A:74:VAL:O	2:C:729:ALA:CB	2.62	0.47
2:C:810:TYR:HB3	2:C:817:LEU:CD2	2.44	0.47
3:D:107:LEU:HD23	3:D:241:VAL:HG22	1.96	0.47
3:D:424:ASN:HD21	3:D:434:ILE:HG12	1.79	0.47
3:D:660:GLU:HB3	3:D:685:ILE:CG2	2.44	0.47
2:H:812:PHE:HB2	3:I:357:VAL:HG22	1.95	0.47
2:H:944:ARG:HA	2:H:947:GLU:HB2	1.96	0.47
2:C:366:ILE:O	2:C:370:MET:HG2	2.14	0.47
3:D:896:ALA:HA	3:D:899:TYR:CE2	2.49	0.47
3:D:71:LEU:CD2	3:I:51:PRO:HD3	2.44	0.47
2:C:174:ALA:HB2	2:C:432:LEU:CD2	2.45	0.47
3:D:78:LEU:HB3	3:D:81:ARG:HH21	1.78	0.47
1:G:33:ARG:NH2	1:G:196:THR:OG1	2.47	0.47
2:H:524:ILE:HG21	2:H:528:ARG:HH21	1.79	0.47
2:H:857:VAL:H	2:H:858:GLY:HA3	1.80	0.47
3:D:35:PHE:CZ	3:D:101:ARG:HG2	2.50	0.47
3:D:506:VAL:HG22	3:D:629:PHE:CE1	2.47	0.47
4:K:111:ILE:HD12	4:K:135:ARG:HH12	1.80	0.47
3:D:660:GLU:HB3	3:D:685:ILE:HG21	1.97	0.47
2:H:559:CYS:SG	2:H:662:SER:N	2.87	0.47
3:I:366:CYS:HB3	3:I:439:PRO:HA	1.95	0.47
3:I:902:ASP:C	3:I:903:LEU:HG	2.35	0.47
2:C:1196:LYS:HA	2:C:1199:LEU:HD12	1.96	0.47
3:D:902:ASP:C	3:D:903:LEU:HG	2.35	0.47
3:D:809:VAL:HG23	3:D:915:ILE:HD11	1.96	0.47
2:H:591:TYR:HB3	2:H:652:TYR:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:TYR:CZ	3:D:538:ARG:CZ	2.98	0.47
2:C:565:GLU:HA	2:C:569:ILE:HG12	1.97	0.47
2:C:895:LEU:HB2	2:H:1302:THR:HG21	1.96	0.47
1:F:107:ILE:HG13	1:F:136:GLU:HA	1.97	0.47
2:H:12[B]:ARG:CZ	2:H:703:GLY:HA2	2.45	0.47
3:I:424:ASN:HD21	3:I:434:ILE:HG12	1.79	0.47
2:C:1246:ARG:HD2	2:C:1266:GLY:N	2.30	0.47
3:D:1221:LEU:HG	3:D:1229:VAL:HG11	1.97	0.47
3:I:1172:LYS:HG3	3:I:1173:ARG:H	1.79	0.47
3:I:357:VAL:HG12	3:I:358:GLY:H	1.80	0.47
3:I:381:ILE:HG23	3:I:412:LEU:HD21	1.96	0.47
3:I:575:GLY:HA2	3:I:578:ILE:HD12	1.96	0.47
3:D:564:VAL:HG12	3:D:565:ALA:H	1.80	0.46
3:I:366:CYS:HB2	3:I:437:PHE:HB2	1.95	0.46
2:C:591:TYR:HB3	2:C:652:TYR:HB3	1.97	0.46
3:D:268:LEU:O	3:D:306:LEU:HD21	2.14	0.46
2:H:1226:THR:HG23	3:I:638:SER:HB2	1.97	0.46
2:H:1280:ALA:C	2:H:1282:GLY:H	2.18	0.46
2:H:741:MET:HG2	2:H:747:GLY:HA2	1.96	0.46
3:I:185:ILE:HA	3:I:188:LEU:HG	1.96	0.46
3:I:564:VAL:HG12	3:I:565:ALA:H	1.80	0.46
1:A:61:ILE:HG12	1:A:142:MET:HE1	1.97	0.46
2:C:841:ARG:HD3	2:C:1047:LEU:HD13	1.97	0.46
2:C:1132:LEU:HD13	2:C:1177:ARG:NE	2.30	0.46
3:D:903:LEU:HD13	3:D:909:ILE:HG13	1.97	0.46
2:H:225:PHE:CE2	2:H:347:ILE:HB	2.49	0.46
2:H:3:TYR:CE2	2:H:1159:VAL:HG11	2.50	0.46
3:I:903:LEU:HD13	3:I:909:ILE:HG13	1.98	0.46
3:I:809:VAL:HG23	3:I:915:ILE:HD11	1.96	0.46
3:D:662:ALA:HA	3:D:665:GLN:HB2	1.98	0.46
3:D:94:GLN:HB3	3:D:95:THR:H	1.57	0.46
2:H:556:GLY:HA2	2:H:660:VAL:HA	1.98	0.46
3:I:396:ALA:O	3:I:400:MET:HG2	2.15	0.46
3:I:534:GLU:O	3:I:538:ARG:N	2.46	0.46
2:C:1280:ALA:C	2:C:1282:GLY:H	2.19	0.46
2:C:1294:LYS:HZ2	3:D:349:TYR:HE2	1.63	0.46
2:C:944:ARG:HA	2:C:947:GLU:HB2	1.98	0.46
3:D:37:GLU:H	3:D:105:ILE:CD1	2.29	0.46
2:H:1279:GLU:HA	2:H:1287:LEU:HD11	1.96	0.46
2:H:1324:ASN:HB3	2:H:1328:LYS:HE3	1.98	0.46
3:I:587:LEU:HB3	3:I:588:PRO:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ARG:N	1:A:167:PRO:HD3	2.30	0.46
3:D:123:ARG:HB3	3:D:237:MET:HE2	1.98	0.46
3:D:533:ALA:HA	3:D:578:ILE:HG12	1.96	0.46
2:H:1196:LYS:HA	2:H:1199:LEU:HD12	1.96	0.46
2:H:1246:ARG:HD2	2:H:1266:GLY:N	2.30	0.46
2:H:565:GLU:HA	2:H:569:ILE:HG12	1.97	0.46
3:I:368:LEU:HD21	3:I:421:VAL:HG21	1.97	0.46
3:I:378:LYS:HA	3:I:381:ILE:HD12	1.97	0.46
3:I:395:LYS:C	3:I:397:ALA:H	2.18	0.46
3:D:900:GLY:HA3	3:D:1251:LYS:HE2	1.96	0.46
3:D:242:LEU:HD22	3:D:303:VAL:CG1	2.44	0.46
3:D:338:PHE:HA	3:D:342:LEU:HB2	1.97	0.46
3:I:797:THR:HG22	3:I:924:GLY:CA	2.46	0.46
2:C:767:GLN:HA	2:C:786:GLY:HA2	1.97	0.46
3:D:593:ASN:HA	3:D:593:ASN:HD22	1.53	0.46
3:D:252:LEU:CG	3:I:86:GLU:HB2	2.44	0.46
2:C:473:ARG:HH11	4:J:74:VAL:HG21	1.80	0.46
2:C:174:ALA:HB2	2:C:432:LEU:HD22	1.97	0.46
3:D:123:ARG:HB3	3:D:237:MET:CE	2.46	0.46
3:D:331:ILE:HG12	3:D:337:ARG:CZ	2.46	0.46
3:I:307:LEU:O	3:I:328:ALA:HB2	2.16	0.46
2:H:672:GLU:HA	3:I:772:TYR:OH	2.16	0.46
1:A:48:LEU:HD11	2:C:1087:TYR:OH	2.16	0.46
1:B:113:ALA:O	1:B:115:ILE:N	2.45	0.46
2:C:851:THR:HA	2:C:887:VAL:HG21	1.98	0.46
3:D:575:GLY:HA2	3:D:578:ILE:HD12	1.98	0.46
3:D:814:CYS:SG	3:D:898:CYS:N	2.89	0.46
3:D:885:VAL:HG13	3:D:894:VAL:HG11	1.98	0.46
3:D:896:ALA:HA	3:D:899:TYR:HE2	1.81	0.46
1:F:61:ILE:HG12	1:F:142:MET:HE1	1.98	0.46
2:H:936:ARG:HB2	2:H:1047:LEU:HD23	1.98	0.46
3:I:923:ILE:HD13	3:I:1256:ILE:HD11	1.99	0.46
2:H:1107:MET:CE	3:I:740:LEU:HG	2.45	0.46
4:J:141:PHE:HB3	4:J:162:VAL:HG21	1.98	0.46
3:D:357:VAL:HG12	3:D:358:GLY:H	1.81	0.45
2:H:766:ASN:H	2:H:787:PRO:HB3	1.80	0.45
2:H:851:THR:HA	2:H:887:VAL:HG21	1.98	0.45
3:I:885:VAL:HG13	3:I:894:VAL:HG11	1.97	0.45
2:C:556:GLY:HA2	2:C:660:VAL:HA	1.98	0.45
2:C:766:ASN:H	2:C:787:PRO:HB3	1.80	0.45
3:D:131:PRO:HB3	3:D:159:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:GLU:O	3:D:551:ARG:NH2	2.48	0.45
3:I:429:LEU:HD22	3:I:797:THR:HG21	1.98	0.45
3:I:814:CYS:SG	3:I:898:CYS:N	2.89	0.45
3:D:609:TYR:HA	3:D:617:THR:HG21	1.99	0.45
2:H:117:ILE:HD11	2:H:485:ASP:HB3	1.99	0.45
3:I:1270:GLY:HA3	3:I:1298:VAL:HG13	1.97	0.45
3:D:797:THR:HG22	3:D:924:GLY:CA	2.47	0.45
2:H:841:ARG:HD3	2:H:1047:LEU:HD13	1.97	0.45
2:H:1132:LEU:HD13	2:H:1177:ARG:NE	2.31	0.45
2:H:767:GLN:HA	2:H:786:GLY:HA2	1.97	0.45
3:I:180:MET:CE	3:I:184:ALA:HB2	2.47	0.45
3:I:206:ASN:HD21	3:I:213:LYS:HD2	1.81	0.45
2:H:810:TYR:HA	3:I:357:VAL:HG11	1.97	0.45
3:I:580:TRP:CE3	3:I:580:TRP:HA	2.51	0.45
3:D:1270:GLY:HA3	3:D:1298:VAL:HG13	1.99	0.45
1:F:184:ALA:HB2	2:H:1091:GLY:HA3	1.96	0.45
2:H:103:VAL:HG13	2:H:113:THR:HG22	1.98	0.45
3:D:96:LYS:HE3	2:H:892:GLU:HB3	1.97	0.45
4:K:15:PHE:HB2	4:K:89:VAL:HB	1.97	0.45
1:B:176:CYS:SG	3:D:535:ARG:NH2	2.89	0.45
3:D:97:VAL:HG12	3:D:101:ARG:HG3	1.99	0.45
3:D:139:LEU:HA	3:D:181:GLY:HA2	1.98	0.45
1:F:30:PRO:HA	1:F:198:LEU:HD13	1.99	0.45
3:I:363:LEU:HA	3:I:450:HIS:ND1	2.31	0.45
1:B:191:ARG:NE	3:D:441:LEU:HB3	2.32	0.45
2:C:103:VAL:HG13	2:C:113:THR:HG22	1.98	0.45
2:C:1334:GLY:HA2	3:D:239:LEU:HD21	1.98	0.45
3:D:396:ALA:O	3:D:400:MET:HG2	2.16	0.45
3:I:975:ILE:HB	3:I:1001:ALA:HB3	1.99	0.45
3:I:803:VAL:HG21	3:I:1309:ILE:HG12	1.98	0.45
3:I:44:ILE:HG21	3:I:260:PHE:CE2	2.52	0.45
3:I:896:ALA:HA	3:I:899:TYR:HE2	1.81	0.45
3:I:933:ARG:HH21	3:I:1240:VAL:HG13	1.82	0.45
1:F:88:LEU:HD21	1:F:130:ILE:HG12	1.99	0.45
2:H:1101:LEU:HD13	3:I:504:GLN:HB3	1.98	0.45
3:I:121:PRO:HG2	3:I:124:ILE:HD12	1.99	0.45
3:I:180:MET:HE2	3:I:184:ALA:HB2	1.98	0.45
3:I:609:TYR:HA	3:I:617:THR:HG21	1.98	0.45
2:C:889:PRO:O	3:I:78:LEU:HD11	2.17	0.45
2:C:557:ARG:HG3	2:C:589:THR:HG23	1.99	0.45
2:C:805:MET:HE1	3:D:637:ALA:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1002:VAL:H	3:D:1020:TRP:HE1	1.65	0.45
3:D:123:ARG:NH2	3:D:1333:THR:OG1	2.49	0.45
2:H:390:PHE:HA	2:H:419:ILE:CG2	2.47	0.45
3:D:395:LYS:HD3	2:H:905:ILE:N	2.31	0.45
3:D:260:PHE:CD2	3:I:75:TYR:CD1	3.05	0.45
3:D:1072:LYS:HZ2	3:D:1170:LYS:HE3	1.82	0.45
3:D:1172:LYS:HG2	3:D:1173:ARG:H	1.81	0.45
3:D:123:ARG:CB	3:D:237:MET:HE1	2.46	0.45
3:D:770:LEU:HA	3:D:773:PHE:CD2	2.52	0.45
2:H:174:ALA:HB2	2:H:432:LEU:CD2	2.46	0.45
2:H:174:ALA:HB2	2:H:432:LEU:HD22	1.98	0.45
1:A:11:PRO:HG2	1:B:230:ALA:HB3	1.98	0.44
2:C:854:ILE:HG23	2:C:886:LYS:HD2	1.98	0.44
2:C:888:THR:OG1	2:C:915:ASP:OD2	2.36	0.44
3:D:239:LEU:HD13	3:D:242:LEU:HA	1.99	0.44
3:D:25:ALA:HB1	3:D:30:ILE:CG1	2.47	0.44
3:D:515:ARG:NH2	3:D:724:MET:HB3	2.32	0.44
2:C:1333:LEU:HA	3:D:307:LEU:HD22	1.99	0.44
3:D:923:ILE:HD13	3:D:1256:ILE:HD11	1.99	0.44
3:D:550:VAL:O	3:D:569:LEU:HA	2.17	0.44
3:D:580:TRP:HA	3:D:580:TRP:CE3	2.52	0.44
2:H:855:PRO:HB3	2:H:914:LYS:CD	2.44	0.44
3:I:1221:LEU:HG	3:I:1229:VAL:HG11	1.97	0.44
3:I:515:ARG:NH2	3:I:724:MET:HB3	2.32	0.44
3:D:398:LYS:HD3	2:H:901:LEU:HB3	1.98	0.44
3:I:1002:VAL:H	3:I:1020:TRP:HE1	1.65	0.44
3:I:900:GLY:HA3	3:I:1251:LYS:HE2	1.99	0.44
3:D:1323:ALA:HB1	3:D:1332:LEU:CD2	2.48	0.44
3:D:512:TYR:HA	3:D:515:ARG:NH1	2.33	0.44
3:D:545:HIS:CD2	3:D:574:VAL:HG11	2.53	0.44
3:D:70:CYS:SG	3:D:90:VAL:HB	2.58	0.44
1:F:230:ALA:HB3	1:G:11:PRO:HG2	2.00	0.44
2:H:61:SER:HB3	2:H:479:LEU:HB3	2.00	0.44
2:H:848:GLU:HG2	2:H:889:PRO:HD3	2.00	0.44
3:I:550:VAL:O	3:I:569:LEU:HA	2.18	0.44
2:C:936:ARG:HB2	2:C:1047:LEU:HD23	1.99	0.44
2:C:896:THR:HB	2:C:897:PRO:CD	2.43	0.44
3:D:114:ILE:CG1	3:D:304:ASP:HA	2.44	0.44
3:D:71:LEU:HD13	3:I:98:ARG:HH22	1.83	0.44
2:H:292:ILE:O	2:H:322:LEU:HD11	2.17	0.44
2:H:557:ARG:HG3	2:H:589:THR:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:545:HIS:CD2	3:I:574:VAL:HG11	2.53	0.44
2:C:61:SER:HB3	2:C:479:LEU:HB3	2.00	0.44
3:D:113:HIS:CD2	3:D:238:ILE:CA	2.94	0.44
3:D:600:ALA:O	3:D:604:MET:N	2.50	0.44
3:I:662:ALA:HA	3:I:665:GLN:HB2	1.99	0.44
2:C:1029:LEU:HD22	2:C:1033:ARG:HH21	1.82	0.44
2:H:136:PHE:HB2	2:H:143:ARG:O	2.18	0.44
2:H:564:PRO:HD2	2:H:572:ILE:O	2.18	0.44
2:C:397:LEU:HB2	2:C:402:ARG:HE	1.83	0.44
3:D:975:ILE:HB	3:D:1001:ALA:HB3	1.99	0.44
3:D:1226:VAL:HG22	3:D:1304:ARG:HH22	1.83	0.44
2:C:1323:PHE:CD1	3:D:341:ASN:HB3	2.52	0.44
2:H:1117:LEU:HG	2:H:1195:ILE:HG23	2.00	0.44
2:H:582:ASN:HB2	2:H:586:PHE:H	1.83	0.44
4:K:87:PRO:HG2	4:K:88:ARG:HG2	2.00	0.44
1:A:107:ILE:HG13	1:A:136:GLU:HA	1.99	0.43
2:C:136:PHE:HB2	2:C:143:ARG:O	2.18	0.43
2:C:161:LYS:HG2	2:C:170:VAL:HG13	2.00	0.43
3:D:1179:PRO:HB2	3:D:1180:VAL:H	1.58	0.43
3:D:229:GLN:NE2	3:D:1341:ARG:HB2	2.33	0.43
3:D:507:VAL:HG13	3:D:511:TYR:HE2	1.83	0.43
3:I:770:LEU:HA	3:I:773:PHE:CD2	2.52	0.43
3:D:1177:ILE:O	3:D:1187:GLU:HA	2.18	0.43
3:D:1261:LEU:HD22	3:D:1306:LEU:HD13	2.00	0.43
3:D:429:LEU:HD22	3:D:797:THR:HG21	1.99	0.43
3:D:836:ARG:HG2	3:D:871:LEU:HD22	2.00	0.43
1:F:101:THR:O	1:F:115:ILE:HG23	2.18	0.43
2:H:854:ILE:HG23	2:H:886:LYS:HD2	1.98	0.43
3:I:309:ASN:ND2	3:I:324:LEU:HB2	2.33	0.43
3:I:470:VAL:HA	3:I:471:PRO:HD3	1.88	0.43
3:I:68:TYR:CB	3:I:78:LEU:HD23	2.48	0.43
2:C:38:PHE:CD2	2:C:457:GLY:HA3	2.54	0.43
2:C:73:TYR:HD1	2:C:98:VAL:HG22	1.83	0.43
3:D:803:VAL:HG21	3:D:1309:ILE:HG12	1.99	0.43
3:D:370:LYS:HE2	3:D:443:GLU:HB3	2.00	0.43
3:D:79:LYS:HA	2:H:915:ASP:CG	2.38	0.43
2:H:1029:LEU:HD22	2:H:1033:ARG:HH21	1.82	0.43
3:I:857:LEU:HD13	3:I:860:ARG:HD2	2.00	0.43
3:I:836:ARG:HG2	3:I:871:LEU:HD22	1.99	0.43
1:A:46:ILE:HG12	1:B:35:PHE:HE1	1.83	0.43
2:C:675:ASP:CG	2:C:1107:MET:HB2	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:110:PRO:HB2	3:D:111:THR:H	1.68	0.43
3:I:1261:LEU:HD22	3:I:1306:LEU:HD13	1.99	0.43
3:I:492:SER:HB3	3:I:499:ILE:HG13	2.00	0.43
4:K:128:PHE:CD2	4:K:158:LEU:HD11	2.53	0.43
1:A:45:ARG:NH2	1:B:37:HIS:HB3	2.34	0.43
2:C:1256:GLN:HG3	3:D:99:ARG:NH1	2.33	0.43
2:C:211:ARG:HG3	2:C:220:ILE:HD11	2.01	0.43
3:D:534:GLU:O	3:D:538:ARG:N	2.47	0.43
3:D:75:TYR:N	3:D:75:TYR:CD2	2.87	0.43
2:H:397:LEU:HB2	2:H:402:ARG:HE	1.84	0.43
3:D:93:THR:HA	2:H:890:LYS:HZ3	1.83	0.43
3:I:1234:VAL:HG21	3:I:1254:GLU:HG2	2.01	0.43
3:I:380:PHE:HE2	3:I:472:LEU:HD22	1.82	0.43
3:I:424:ASN:ND2	3:I:434:ILE:HG12	2.34	0.43
3:I:600:ALA:O	3:I:604:MET:N	2.50	0.43
4:J:10:TYR:CD2	4:J:73:MET:HB3	2.53	0.43
2:C:1278:LEU:HG	3:D:434:ILE:HD13	2.00	0.43
2:H:38:PHE:CD2	2:H:457:GLY:HA3	2.53	0.43
2:H:73:TYR:HD1	2:H:98:VAL:HG22	1.84	0.43
3:I:357:VAL:CG1	3:I:358:GLY:N	2.81	0.43
3:I:355:ILE:HG21	3:I:461:PHE:HB3	2.00	0.43
2:C:153:PRO:O	2:C:452:ARG:NH2	2.52	0.43
2:H:1127:LYS:HD2	2:H:1202:GLY:HA2	2.00	0.43
2:H:798:GLN:OE1	2:H:827:ARG:HB3	2.18	0.43
3:D:394:ILE:HG21	2:H:900:LYS:O	2.19	0.43
3:I:512:TYR:HA	3:I:515:ARG:NH1	2.33	0.43
1:A:44:ARG:HH21	1:A:185:TYR:HB2	1.84	0.43
3:D:127:LEU:HD13	3:D:234:PRO:CB	2.47	0.43
3:D:202:ARG:HB2	3:D:216:LYS:HE3	2.01	0.43
3:D:355:ILE:HG21	3:D:461:PHE:HB3	2.00	0.43
3:D:356:THR:HG23	3:D:446:ALA:CB	2.49	0.43
3:D:527:LEU:HD12	3:D:532:GLU:HG2	2.00	0.43
3:D:563:LEU:HD22	3:D:585:LYS:HB3	2.01	0.43
3:D:769:VAL:HG12	3:D:770:LEU:HD23	2.01	0.43
1:F:46:ILE:HD13	1:F:224:LEU:HG	2.01	0.43
2:H:226:GLU:HB3	2:H:337:PHE:HE2	1.80	0.43
2:C:551:HIS:H	2:C:554:HIS:HD2	1.67	0.43
2:C:582:ASN:HB2	2:C:586:PHE:H	1.83	0.43
3:D:123:ARG:CB	3:D:237:MET:CE	2.97	0.43
3:D:580:TRP:HA	3:D:580:TRP:HE3	1.84	0.43
3:I:1167:LYS:HD2	3:I:1176:VAL:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1351:VAL:HG22	3:I:1357:ILE:HD11	2.00	0.43
3:I:275:ARG:HB3	3:I:299:LEU:HD22	2.01	0.43
2:C:390:PHE:HA	2:C:419:ILE:CG2	2.47	0.43
2:C:727:VAL:HG13	2:C:732:ILE:HG12	2.01	0.43
3:D:452:LEU:HD22	3:D:500:ILE:HG23	2.01	0.43
1:F:60:GLU:CG	1:F:170:ARG:HG3	2.49	0.43
1:F:39:LEU:HD22	1:G:228:LEU:HD21	2.01	0.43
2:H:1101:LEU:HD22	3:I:504:GLN:HB3	2.00	0.43
2:H:1247:SER:HB3	3:I:375:GLU:O	2.19	0.43
2:H:696:ASP:O	2:H:697:LYS:HB2	2.19	0.43
2:H:1281:TYR:CD1	3:I:484:MET:HG3	2.53	0.43
3:I:511:TYR:HD1	3:I:596:LEU:HD22	1.84	0.43
3:I:580:TRP:HA	3:I:580:TRP:HE3	1.84	0.43
4:J:144:PHE:HB3	4:J:162:VAL:HG13	2.00	0.43
2:C:1077:SER:CB	3:D:357:VAL:HB	2.48	0.42
2:C:798:GLN:OE1	2:C:827:ARG:HB3	2.18	0.42
2:C:850:ILE:HG12	2:C:1048:LYS:HE2	2.00	0.42
2:C:86:GLN:N	2:C:92:TYR:OH	2.51	0.42
1:F:234:LEU:CD1	1:G:13:LEU:H	2.31	0.42
3:I:1177:ILE:O	3:I:1187:GLU:HA	2.18	0.42
3:I:1248:ILE:H	3:I:1248:ILE:HG13	1.74	0.42
3:I:1323:ALA:HB1	3:I:1332:LEU:CD2	2.48	0.42
3:I:356:THR:OG1	3:I:448:GLN:HA	2.19	0.42
2:C:889:PRO:O	3:I:78:LEU:HD12	2.18	0.42
3:D:1167:LYS:HD2	3:D:1176:VAL:HB	2.01	0.42
3:D:357:VAL:CG1	3:D:358:GLY:N	2.82	0.42
3:D:426:ALA:HB3	3:D:427:PRO:HD3	2.00	0.42
2:C:1328:LYS:HZ2	3:D:99:ARG:HB3	1.82	0.42
1:G:38:THR:O	1:G:40:GLY:N	2.46	0.42
2:H:675:ASP:CG	2:H:1107:MET:HB2	2.38	0.42
2:H:1278:LEU:HG	3:I:434:ILE:HD13	2.00	0.42
2:H:1323:PHE:CE1	3:I:1352:ILE:HG23	2.54	0.42
2:H:697:LYS:HE2	2:H:790:ASP:CB	2.32	0.42
3:I:858:VAL:HB	3:I:859:PRO:HD3	2.00	0.42
2:C:564:PRO:HD2	2:C:572:ILE:O	2.18	0.42
2:C:723:VAL:HA	2:C:776:PRO:HA	2.01	0.42
3:D:295:GLU:O	3:D:299:LEU:N	2.52	0.42
3:D:381:ILE:HG12	3:D:412:LEU:HD22	2.01	0.42
3:D:424:ASN:ND2	3:D:434:ILE:HG12	2.34	0.42
1:F:33:ARG:HE	1:F:197:ASP:HB2	1.84	0.42
2:H:161:LYS:HG2	2:H:170:VAL:HG13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:139:LEU:CD1	3:I:185:ILE:HD11	2.48	0.42
3:I:356:THR:HG23	3:I:446:ALA:CB	2.49	0.42
3:I:825:VAL:HG22	3:I:838:ARG:NH2	2.34	0.42
1:B:102:LEU:HB2	1:B:142:MET:HB2	2.02	0.42
2:C:1117:LEU:HG	2:C:1195:ILE:HG23	2.00	0.42
2:C:1174:GLU:HA	2:C:1177:ARG:CZ	2.49	0.42
3:D:1221:LEU:HD22	3:D:1306:LEU:CD1	2.49	0.42
3:D:272:VAL:CG2	3:D:306:LEU:HD11	2.31	0.42
3:D:583:VAL:HG22	3:D:589:TYR:CE1	2.54	0.42
1:F:30:PRO:HB3	1:F:195:ARG:NH1	2.34	0.42
2:H:524:ILE:CG2	2:H:528:ARG:HH21	2.32	0.42
2:H:851:THR:CG2	2:H:886:LYS:H	2.32	0.42
3:I:950:ILE:HD12	3:I:1018:ALA:HB3	2.01	0.42
2:C:1323:PHE:CD1	3:D:1352:ILE:HG23	2.55	0.42
2:C:1324:ASN:HB3	2:C:1328:LYS:HE3	2.00	0.42
2:C:845:LEU:HB2	3:I:81:ARG:HH12	1.84	0.42
3:D:339:ARG:HA	3:D:343:LEU:HD12	2.00	0.42
1:G:211:ILE:HG21	1:G:216:ALA:HB2	2.01	0.42
2:H:1330:ILE:HD13	3:I:1332:LEU:HD22	2.00	0.42
3:I:744:ARG:NH2	3:I:772:TYR:OH	2.53	0.42
4:J:128:PHE:CD2	4:J:158:LEU:HD11	2.54	0.42
3:D:744:ARG:NH2	3:D:772:TYR:OH	2.52	0.42
3:D:899:TYR:CE1	3:D:915:ILE:HD13	2.55	0.42
1:G:102:LEU:HB2	1:G:142:MET:HB2	2.02	0.42
1:G:91:ARG:HE	1:G:210:THR:HB	1.85	0.42
2:H:153:PRO:O	2:H:452:ARG:NH2	2.52	0.42
2:H:850:ILE:HG12	2:H:1048:LYS:HE2	2.00	0.42
3:I:1234:VAL:HG21	3:I:1254:GLU:CG	2.49	0.42
3:I:429:LEU:HB2	3:I:925:GLU:HG3	2.01	0.42
3:I:356:THR:HG23	3:I:446:ALA:HB1	2.02	0.42
3:I:507:VAL:HG13	3:I:511:TYR:HE2	1.85	0.42
3:I:583:VAL:HG22	3:I:589:TYR:CE1	2.53	0.42
3:D:950:ILE:HD12	3:D:1018:ALA:HB3	2.01	0.42
1:F:44:ARG:HH21	1:F:185:TYR:HB2	1.84	0.42
1:G:44:ARG:HH21	1:G:185:TYR:HB2	1.85	0.42
2:H:98:VAL:HG12	2:H:100:LEU:HG	2.00	0.42
2:H:551:HIS:H	2:H:554:HIS:HD2	1.68	0.42
3:I:295:GLU:O	3:I:299:LEU:N	2.52	0.42
3:I:426:ALA:HB3	3:I:427:PRO:HD3	2.00	0.42
2:C:855:PRO:HG3	2:C:914:LYS:CD	2.48	0.42
2:C:902:LEU:HB3	2:C:912:ASP:CG	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:857:LEU:HD13	3:D:860:ARG:HD2	2.02	0.42
1:F:107:ILE:CG1	1:F:136:GLU:HA	2.49	0.42
2:H:1298:VAL:O	2:H:1302:THR:HG23	2.20	0.42
2:H:727:VAL:HG13	2:H:732:ILE:HG12	2.01	0.42
3:I:339:ARG:HA	3:I:343:LEU:HD12	2.01	0.42
3:I:734:ALA:HA	3:I:737:ILE:HD12	2.02	0.42
1:B:91:ARG:HE	1:B:210:THR:HB	1.85	0.42
2:C:696:ASP:O	2:C:697:LYS:HB2	2.20	0.42
3:D:1191:PRO:O	3:D:1192:LYS:HB2	2.19	0.42
3:D:395:LYS:HZ3	2:H:905:ILE:CB	2.21	0.42
1:B:83:LEU:HD21	3:D:526:VAL:O	2.20	0.42
2:H:1198:LEU:HD23	2:H:1201:LEU:HD12	2.02	0.42
2:H:896:THR:HB	2:H:897:PRO:CD	2.46	0.42
2:H:960:LEU:O	2:H:964:LEU:HG	2.20	0.42
3:I:1321:SER:CB	3:I:1348:LYS:HB3	2.50	0.42
1:A:60:GLU:CG	1:A:170:ARG:HG3	2.50	0.42
1:B:9:LEU:HD12	1:B:195:ARG:HH22	1.84	0.42
2:C:38:PHE:HA	2:C:48:GLY:HA3	2.02	0.42
2:C:960:LEU:O	2:C:964:LEU:HG	2.20	0.42
3:D:808:VAL:HG21	3:D:1347:LEU:HD21	2.01	0.42
3:D:268:LEU:C	3:D:306:LEU:HD21	2.40	0.42
3:D:356:THR:OG1	3:D:448:GLN:HA	2.19	0.42
2:H:448:LEU:HD23	2:H:451:ARG:HD2	2.01	0.42
3:I:1163:VAL:CG2	3:I:1204:VAL:HB	2.50	0.42
4:K:10:TYR:CD2	4:K:73:MET:HB3	2.55	0.42
1:A:107:ILE:CG1	1:A:136:GLU:HA	2.50	0.41
1:A:61:ILE:HB	1:A:64:VAL:O	2.20	0.41
3:D:694:SER:HB2	3:D:738:ARG:HD3	2.02	0.41
3:D:825:VAL:HG22	3:D:838:ARG:NH2	2.35	0.41
3:I:1172:LYS:HG3	3:I:1173:ARG:N	2.35	0.41
3:I:56:LEU:HD13	3:I:266:ASN:ND2	2.35	0.41
2:C:843:THR:HG22	3:I:78:LEU:O	2.20	0.41
1:B:211:ILE:HG21	1:B:216:ALA:HB2	2.02	0.41
2:C:98:VAL:HG12	2:C:100:LEU:HG	2.01	0.41
2:C:448:LEU:HD23	2:C:451:ARG:HD2	2.01	0.41
3:D:492:SER:HB3	3:D:499:ILE:HG13	2.02	0.41
3:D:587:LEU:HD11	3:D:608:CYS:SG	2.60	0.41
3:D:903:LEU:HD22	3:D:909:ILE:HG13	2.02	0.41
2:H:1174:GLU:HA	2:H:1177:ARG:CZ	2.50	0.41
3:I:425:ARG:NH2	3:I:459:ALA:CB	2.84	0.41
3:I:490:ILE:HA	3:I:500:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:527:LEU:HD12	3:I:532:GLU:HG2	2.02	0.41
3:I:518:VAL:HG11	3:I:707:ILE:HD13	2.02	0.41
1:A:166:ARG:N	1:A:167:PRO:CD	2.83	0.41
3:D:1145:PHE:HB3	3:D:1309:ILE:HD12	2.02	0.41
3:D:233:LYS:HD2	3:D:236:TRP:HE1	1.86	0.41
3:D:31:ARG:HA	3:D:34:SER:OG	2.20	0.41
3:D:858:VAL:HB	3:D:859:PRO:HD3	2.01	0.41
1:F:61:ILE:HB	1:F:64:VAL:O	2.20	0.41
2:H:723:VAL:HA	2:H:776:PRO:HA	2.02	0.41
3:I:65:VAL:CG2	3:I:71:LEU:HD22	2.33	0.41
2:C:810:TYR:CE2	3:D:359:PRO:HG2	2.55	0.41
3:D:37:GLU:H	3:D:105:ILE:HG13	1.85	0.41
3:D:534:GLU:HB3	3:D:538:ARG:NE	2.35	0.41
3:D:655:SER:HA	3:D:658:GLU:HB2	2.02	0.41
1:G:125:LYS:HA	1:G:126:PRO:HD3	1.91	0.41
3:D:89:GLY:O	3:I:252:LEU:HD12	2.19	0.41
3:I:899:TYR:CE1	3:I:915:ILE:HD13	2.56	0.41
1:A:30:PRO:HA	1:A:198:LEU:HD13	2.01	0.41
1:B:44:ARG:HH21	1:B:185:TYR:HB2	1.84	0.41
2:C:1127:LYS:HD2	2:C:1202:GLY:HA2	2.02	0.41
3:D:1351:VAL:HG22	3:D:1357:ILE:HD11	2.02	0.41
2:H:237:LEU:HD13	2:H:292:ILE:HD12	2.03	0.41
2:H:551:HIS:H	2:H:554:HIS:CD2	2.38	0.41
1:B:104:LYS:HE2	1:B:114:ASP:HB2	2.01	0.41
2:C:1198:LEU:HD23	2:C:1201:LEU:HD12	2.03	0.41
3:D:429:LEU:HB2	3:D:925:GLU:HG3	2.02	0.41
2:C:1280:ALA:HB1	3:D:431:ARG:NE	2.35	0.41
3:D:356:THR:HG23	3:D:446:ALA:HB1	2.02	0.41
2:H:177:ILE:HG12	2:H:183:TRP:HZ3	1.84	0.41
2:H:19:PRO:HB2	2:H:20:GLN:CG	2.47	0.41
2:H:211:ARG:HG3	2:H:220:ILE:HD11	2.01	0.41
3:D:1068:THR:O	3:D:1072:LYS:HE3	2.21	0.41
3:D:1248:ILE:HG13	3:D:1248:ILE:H	1.73	0.41
2:H:89:GLY:HA2	2:H:140:GLY:HA3	2.03	0.41
2:H:909:LYS:HE3	2:H:914:LYS:HG2	2.01	0.41
3:I:94:GLN:O	3:I:95:THR:OG1	2.39	0.41
4:K:12:VAL:HG22	4:K:92:PHE:CD1	2.54	0.41
1:A:33:ARG:HE	1:A:197:ASP:HB2	1.85	0.41
2:C:551:HIS:H	2:C:554:HIS:CD2	2.38	0.41
2:C:1334:GLY:CA	3:D:239:LEU:HD21	2.51	0.41
1:G:113:ALA:O	1:G:115:ILE:N	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:210:THR:O	1:G:211:ILE:HG13	2.20	0.41
2:H:303:ASP:HB2	2:H:308:GLU:H	1.86	0.41
2:H:38:PHE:HA	2:H:48:GLY:HA3	2.02	0.41
2:H:401:GLY:HA2	2:H:452:ARG:HH22	1.85	0.41
3:D:395:LYS:HZ3	2:H:905:ILE:H	1.69	0.41
3:I:1003:LEU:HD23	3:I:1018:ALA:HB2	2.02	0.41
1:B:61:ILE:HG12	1:B:142:MET:CE	2.51	0.41
2:C:1323:PHE:CE1	3:D:341:ASN:HB3	2.56	0.41
2:C:303:ASP:HB2	2:C:308:GLU:H	1.86	0.41
2:C:850:ILE:H	2:C:850:ILE:HG13	1.73	0.41
3:D:105:ILE:HD13	4:K:18:PHE:HE2	1.83	0.41
3:D:1163:VAL:CG2	3:D:1204:VAL:HB	2.51	0.41
1:B:182:ARG:NH2	3:D:530:PRO:HA	2.36	0.41
3:D:689:ALA:HA	3:D:692:ARG:HB2	2.03	0.41
2:H:855:PRO:CB	2:H:914:LYS:HD3	2.45	0.41
3:I:808:VAL:HG21	3:I:1347:LEU:HD21	2.02	0.41
3:I:347:VAL:HG12	3:I:348:ASP:O	2.21	0.41
4:J:125:LYS:HD3	4:J:127:LEU:HD12	2.02	0.41
2:C:155:VAL:HG23	2:C:405:PHE:CD1	2.56	0.41
3:D:123:ARG:HA	3:D:126:LEU:HD12	2.03	0.41
3:D:809:VAL:N	3:D:915:ILE:HD11	2.36	0.41
1:F:29:GLU:HB2	1:F:30:PRO:HD3	2.03	0.41
1:F:60:GLU:HA	1:F:169:GLY:O	2.21	0.41
3:I:233:LYS:HD2	3:I:236:TRP:HE1	1.85	0.41
3:I:755:ILE:HG13	3:I:755:ILE:H	1.63	0.41
3:D:452:LEU:HD13	3:D:500:ILE:HG23	2.02	0.41
3:D:515:ARG:NH1	3:D:724:MET:HG3	2.36	0.41
2:H:561:ILE:CD1	2:H:661:VAL:HG22	2.51	0.41
3:I:592:VAL:HG21	3:I:604:MET:SD	2.61	0.41
3:I:75:TYR:N	3:I:75:TYR:CD2	2.89	0.41
2:C:177:ILE:HG12	2:C:183:TRP:HZ3	1.86	0.40
3:D:490:ILE:HA	3:D:500:ILE:HD12	2.03	0.40
2:C:680:LEU:CD1	3:D:783:LEU:HD11	2.51	0.40
2:H:1257:GLN:NE2	3:I:340:GLN:O	2.54	0.40
2:H:963:GLU:O	2:H:967:LEU:HG	2.22	0.40
3:I:1002:VAL:N	3:I:1020:TRP:HE1	2.19	0.40
3:I:61:ILE:HG23	3:I:103:GLY:HA3	2.04	0.40
3:I:370:LYS:HE2	3:I:443:GLU:HB3	2.03	0.40
3:I:506:VAL:HG13	3:I:625:MET:HA	2.03	0.40
3:I:534:GLU:HB3	3:I:538:ARG:NE	2.36	0.40
1:A:102:LEU:HB2	1:A:142:MET:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:GLU:HB2	1:A:30:PRO:HD3	2.03	0.40
1:B:61:ILE:HB	1:B:64:VAL:O	2.21	0.40
2:C:1298:VAL:O	2:C:1302:THR:HG23	2.21	0.40
3:D:312:ARG:HD2	3:D:314:ARG:NH2	2.36	0.40
3:D:824:PRO:HG3	3:D:835:LEU:HG	2.04	0.40
3:D:901:ARG:H	3:D:1251:LYS:HZ1	1.70	0.40
3:D:429:LEU:HD12	3:D:925:GLU:HG2	2.03	0.40
3:I:110:PRO:HB2	3:I:111:THR:H	1.72	0.40
3:I:1163:VAL:HG21	3:I:1204:VAL:HB	2.02	0.40
3:I:50:LYS:HB3	3:I:51:PRO:CD	2.49	0.40
3:I:809:VAL:N	3:I:915:ILE:HD11	2.36	0.40
3:I:824:PRO:HG3	3:I:835:LEU:HG	2.03	0.40
1:B:61:ILE:HG12	1:B:142:MET:HE1	2.02	0.40
3:D:923:ILE:HA	3:D:926:PRO:HG2	2.04	0.40
1:F:102:LEU:HB2	1:F:142:MET:HB2	2.03	0.40
3:I:587:LEU:HD11	3:I:608:CYS:SG	2.62	0.40
3:I:960:LEU:HD13	3:I:963:VAL:HG21	2.03	0.40
2:C:1171:ARG:HA	2:C:1174:GLU:HB2	2.04	0.40
2:C:19:PRO:HA	2:C:1157:GLN:HG3	2.03	0.40
3:D:844:THR:HG21	3:D:856:ILE:HG21	2.04	0.40
1:G:61:ILE:HB	1:G:64:VAL:O	2.21	0.40
2:H:1171:ARG:HA	2:H:1174:GLU:HB2	2.04	0.40
3:I:1191:PRO:O	3:I:1192:LYS:HB2	2.20	0.40
1:B:51:MET:HE2	1:B:179:PRO:HG2	2.04	0.40
2:C:1196:LYS:HA	2:C:1199:LEU:HB2	2.03	0.40
2:C:367:TYR:CE2	2:C:381:ALA:HA	2.56	0.40
2:H:120:GLN:HB3	2:H:490:GLN:HG3	2.04	0.40
2:H:225:PHE:HB3	2:H:226:GLU:H	1.65	0.40
3:I:1145:PHE:HB3	3:I:1309:ILE:HD12	2.02	0.40
3:I:452:LEU:HD22	3:I:500:ILE:HG23	2.04	0.40
3:I:675:ALA:HA	3:I:678:ARG:HD2	2.04	0.40
3:I:697:MET:HE1	3:I:741:ALA:HB1	2.04	0.40
3:D:282:LEU:HG	4:J:21:ARG:HH21	1.86	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:184:ALA:O	3:D:191:SER:OG[2_957]	2.03	0.17
3:D:1183:SER:OG	3:D:1183:SER:OG[2_957]	2.12	0.08

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	223/242 (92%)	182 (82%)	29 (13%)	12 (5%)	2 19
1	B	211/242 (87%)	175 (83%)	27 (13%)	9 (4%)	2 22
1	F	223/242 (92%)	183 (82%)	28 (13%)	12 (5%)	2 19
1	G	212/242 (88%)	177 (84%)	26 (12%)	9 (4%)	3 22
2	C	1316/1342 (98%)	1108 (84%)	172 (13%)	36 (3%)	5 31
2	H	1316/1342 (98%)	1110 (84%)	168 (13%)	38 (3%)	4 29
3	D	1294/1407 (92%)	1023 (79%)	190 (15%)	81 (6%)	1 17
3	I	1300/1407 (92%)	1024 (79%)	197 (15%)	79 (6%)	1 17
4	J	141/181 (78%)	123 (87%)	15 (11%)	3 (2%)	7 36
4	K	141/181 (78%)	117 (83%)	18 (13%)	6 (4%)	2 22
All	All	6377/6828 (93%)	5222 (82%)	870 (14%)	285 (4%)	2 22

All (285) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	67	GLU
1	A	114	ASP
1	A	155	ALA
1	B	114	ASP
1	B	193	GLU
2	C	58	PRO
2	C	842	ASP
2	C	851	THR
2	C	890	LYS
2	C	1216	ARG
2	C	1317	PRO
3	D	37	GLU
3	D	98	ARG

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Mol	Chain	Res	Type
3	D	110	PRO
3	D	112	ALA
3	D	173	GLY
3	D	178	ALA
3	D	323	PRO
3	D	587	LEU
3	D	1179	PRO
3	D	1180	VAL
1	F	15	ASP
1	F	67	GLU
1	F	114	ASP
1	G	114	ASP
1	G	193	GLU
2	H	58	PRO
2	H	228	VAL
2	H	311	CYS
2	H	842	ASP
2	H	851	THR
2	H	890	LYS
2	H	894	GLN
2	H	1216	ARG
3	I	65	VAL
3	I	110	PRO
3	I	323	PRO
3	I	461	PHE
3	I	587	LEU
3	I	741	ALA
3	I	1179	PRO
3	I	1180	VAL
4	J	34	ASN
4	J	87	PRO
4	K	74	VAL
4	K	87	PRO
4	K	93	ILE
4	K	106	LYS
1	A	111	THR
1	A	119	GLY
1	B	39	LEU
1	B	111	THR
1	B	119	GLY
2	C	117	ILE
2	C	311	CYS

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Mol	Chain	Res	Type
2	C	796	LEU
2	C	818	VAL
2	C	855	PRO
2	C	1077	SER
3	D	129	ASP
3	D	257	GLY
3	D	347	VAL
3	D	354	VAL
3	D	357	VAL
3	D	434	ILE
3	D	458	ASN
3	D	461	PHE
3	D	519	ASN
3	D	545	HIS
3	D	589	TYR
3	D	741	ALA
3	D	828	GLY
3	D	855	ASP
3	D	915	ILE
3	D	1192	LYS
3	D	1274	PHE
3	D	1299	GLY
1	F	111	THR
1	F	119	GLY
1	F	136	GLU
1	F	163	GLU
1	G	39	LEU
1	G	111	THR
1	G	119	GLY
2	H	117	ILE
2	H	796	LEU
2	H	818	VAL
2	H	895	LEU
2	H	1077	SER
2	H	1317	PRO
3	I	112	ALA
3	I	120	LEU
3	I	347	VAL
3	I	354	VAL
3	I	357	VAL
3	I	434	ILE
3	I	458	ASN

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Mol	Chain	Res	Type
3	I	519	ASN
3	I	586	GLY
3	I	589	TYR
3	I	734	ALA
3	I	828	GLY
3	I	855	ASP
3	I	915	ILE
3	I	1192	LYS
3	I	1274	PHE
3	I	1299	GLY
1	A	38	THR
1	A	136	GLU
1	A	154	PRO
2	C	8	LYS
2	C	487	LEU
2	C	555	TYR
2	C	596	ASP
3	D	36	GLY
3	D	67	ASP
3	D	95	THR
3	D	177	ASP
3	D	286	ALA
3	D	359	PRO
3	D	404	GLU
3	D	471	PRO
3	D	560	ASN
3	D	586	GLY
3	D	625	MET
3	D	637	ALA
3	D	758	PRO
3	D	840	LEU
3	D	859	PRO
3	D	905	ARG
3	D	933	ARG
3	D	1128	SER
3	D	1134	ILE
3	D	1173	ARG
3	D	1342	ASP
1	F	38	THR
2	H	8	LYS
2	H	225	PHE
2	H	487	LEU

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Mol	Chain	Res	Type
2	H	555	TYR
2	H	596	ASP
3	I	67	ASP
3	I	359	PRO
3	I	471	PRO
3	I	545	HIS
3	I	560	ASN
3	I	625	MET
3	I	637	ALA
3	I	840	LEU
3	I	859	PRO
3	I	863	LEU
3	I	905	ARG
3	I	933	ARG
3	I	1128	SER
3	I	1245	GLY
4	K	34	ASN
2	C	488	MET
2	C	854	ILE
3	D	176	PHE
3	D	346	ARG
3	D	532	GLU
3	D	561	GLY
3	D	580	TRP
3	D	583	VAL
3	D	710	ASP
3	D	847	ASP
3	D	850	LYS
3	D	863	LEU
3	D	1245	GLY
3	D	1291	GLU
3	D	1327	GLU
2	H	111	GLU
2	H	201	ARG
2	H	488	MET
2	H	854	ILE
2	H	887	VAL
3	I	95	THR
3	I	258	GLY
3	I	286	ALA
3	I	315	ALA
3	I	404	GLU

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Mol	Chain	Res	Type
3	I	532	GLU
3	I	561	GLY
3	I	583	VAL
3	I	710	ASP
3	I	758	PRO
3	I	847	ASP
3	I	850	LYS
3	I	1134	ILE
3	I	1173	ARG
3	I	1291	GLU
3	I	1327	GLU
3	I	1342	ASP
4	K	105	ASP
1	A	30	PRO
1	B	13	LEU
1	B	30	PRO
2	C	111	GLU
2	C	201	ARG
2	C	224	PHE
2	C	398	SER
2	C	638	SER
2	C	740	GLU
2	C	748	ILE
2	C	887	VAL
2	C	1138	VAL
2	C	1247	SER
2	C	1281	TYR
3	D	106	GLU
3	D	113	HIS
3	D	179	LYS
3	D	805	GLN
3	D	908	ILE
3	D	971	GLY
3	D	1175	LEU
3	D	1352	ILE
1	F	30	PRO
1	F	166	ARG
1	G	13	LEU
1	G	30	PRO
2	H	638	SER
2	H	740	GLU
2	H	748	ILE

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Mol	Chain	Res	Type
2	H	1138	VAL
2	H	1247	SER
2	H	1281	TYR
3	I	227	PHE
3	I	346	ARG
3	I	580	TRP
3	I	805	GLN
3	I	908	ILE
3	I	1175	LEU
4	J	35	MET
1	A	167	PRO
2	C	746	ALA
3	D	427	PRO
3	D	706	VAL
3	D	1178	THR
3	I	106	GLU
3	I	177	ASP
3	I	211	GLU
3	I	427	PRO
3	I	500	ILE
3	I	706	VAL
3	I	971	GLY
3	I	1178	THR
3	I	1352	ILE
2	C	162	GLY
2	C	873	ILE
3	D	500	ILE
3	D	529	GLY
3	D	1118	GLY
3	I	529	GLY
2	C	544	GLY
2	C	655	VAL
2	C	1071	GLY
3	D	451	PRO
3	D	524	GLY
2	H	162	GLY
2	H	544	GLY
2	H	655	VAL
2	H	1071	GLY
3	I	1118	GLY
3	D	358	GLY
3	D	433	GLY

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Mol	Chain	Res	Type
3	D	671	GLY
2	H	627	GLY
3	I	358	GLY
3	I	433	GLY
3	I	451	PRO
3	I	524	GLY
3	I	671	GLY
1	A	126	PRO
1	F	126	PRO
1	F	167	PRO
1	G	14	VAL
2	H	292	ILE
2	H	873	ILE
2	H	891	GLY
3	I	257	GLY
1	B	14	VAL
1	B	126	PRO
2	C	896	THR
1	G	126	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	193/208 (93%)	191 (99%)	2 (1%)	76	86
1	B	184/208 (88%)	182 (99%)	2 (1%)	73	84
1	F	193/208 (93%)	192 (100%)	1 (0%)	88	93
1	G	185/208 (89%)	183 (99%)	2 (1%)	73	84
2	C	1137/1157 (98%)	1121 (99%)	16 (1%)	67	80
2	H	1137/1157 (98%)	1120 (98%)	17 (2%)	65	80
3	D	1087/1168 (93%)	1048 (96%)	39 (4%)	35	59
3	I	1091/1168 (93%)	1054 (97%)	37 (3%)	37	60
4	J	128/158 (81%)	122 (95%)	6 (5%)	26	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	K	128/158 (81%)	121 (94%)	7 (6%)	21 47
All	All	5463/5798 (94%)	5334 (98%)	129 (2%)	49 69

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ARG
1	A	134	THR
1	B	14	VAL
1	B	134	THR
2	C	59	ILE
2	C	85	CYS
2	C	217	THR
2	C	443	ASP
2	C	675	ASP
2	C	739	ASP
2	C	833	ILE
2	C	850	ILE
2	C	901	LEU
2	C	942	ASP
2	C	1041	ASP
2	C	1047	LEU
2	C	1107	MET
2	C	1160	ASP
2	C	1216	ARG
2	C	1259	LEU
3	D	70	CYS
3	D	75	TYR
3	D	95	THR
3	D	114	ILE
3	D	139	LEU
3	D	159	ILE
3	D	177	ASP
3	D	185	ILE
3	D	193	ASP
3	D	299	LEU
3	D	307	LEU
3	D	331	ILE
3	D	342	LEU
3	D	354	VAL
3	D	422	LEU
3	D	442	ILE

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Mol	Chain	Res	Type
3	D	450	HIS
3	D	460	ASP
3	D	470	VAL
3	D	526	VAL
3	D	536	LEU
3	D	580	TRP
3	D	592	VAL
3	D	593	ASN
3	D	755	ILE
3	D	814	CYS
3	D	826	ILE
3	D	847	ASP
3	D	889	ASP
3	D	903	LEU
3	D	915	ILE
3	D	917	VAL
3	D	1111	ASP
3	D	1181	ASP
3	D	1241	TYR
3	D	1248	ILE
3	D	1265	THR
3	D	1344	LEU
3	D	1347	LEU
1	F	134	THR
1	G	14	VAL
1	G	134	THR
2	H	59	ILE
2	H	85	CYS
2	H	217	THR
2	H	443	ASP
2	H	675	ASP
2	H	739	ASP
2	H	833	ILE
2	H	850	ILE
2	H	866	ASP
2	H	942	ASP
2	H	1041	ASP
2	H	1047	LEU
2	H	1107	MET
2	H	1141	LEU
2	H	1160	ASP
2	H	1216	ARG

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Mol	Chain	Res	Type
2	H	1259	LEU
3	I	54	ASP
3	I	61	ILE
3	I	70	CYS
3	I	95	THR
3	I	134	ASP
3	I	139	LEU
3	I	193	ASP
3	I	275	ARG
3	I	299	LEU
3	I	307	LEU
3	I	314	ARG
3	I	342	LEU
3	I	354	VAL
3	I	395	LYS
3	I	422	LEU
3	I	442	ILE
3	I	460	ASP
3	I	470	VAL
3	I	526	VAL
3	I	580	TRP
3	I	587	LEU
3	I	755	ILE
3	I	814	CYS
3	I	826	ILE
3	I	847	ASP
3	I	889	ASP
3	I	903	LEU
3	I	915	ILE
3	I	917	VAL
3	I	1111	ASP
3	I	1181	ASP
3	I	1241	TYR
3	I	1248	ILE
3	I	1265	THR
3	I	1280	VAL
3	I	1344	LEU
3	I	1347	LEU
4	J	35	MET
4	J	82	LEU
4	J	88	ARG
4	J	109	ASP

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Mol	Chain	Res	Type
4	J	113	ASN
4	J	174	ASP
4	K	35	MET
4	K	76	ASN
4	K	77	ASP
4	K	82	LEU
4	K	96	THR
4	K	109	ASP
4	K	174	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	75	GLN
1	A	160	HIS
1	B	41	ASN
2	C	46	GLN
2	C	120	GLN
2	C	148	GLN
2	C	273	HIS
2	C	462	ASN
2	C	519	ASN
2	C	554	HIS
2	C	725	GLN
2	C	1099	ASN
2	C	1111	GLN
2	C	1157	GLN
2	C	1236	ASN
2	C	1257	GLN
3	D	80	HIS
3	D	113	HIS
3	D	186	GLN
3	D	229	GLN
3	D	274	ASN
3	D	276	ASN
3	D	341	ASN
3	D	495	ASN
3	D	519	ASN
3	D	593	ASN
3	D	777	HIS
3	D	1249	ASN

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Mol	Chain	Res	Type
3	D	1268	ASN
3	D	1366	HIS
1	F	41	ASN
1	F	75	GLN
1	F	160	HIS
1	G	41	ASN
2	H	120	GLN
2	H	148	GLN
2	H	273	HIS
2	H	462	ASN
2	H	519	ASN
2	H	554	HIS
2	H	725	GLN
2	H	1099	ASN
2	H	1111	GLN
2	H	1236	ASN
2	H	1256	GLN
2	H	1257	GLN
2	H	1268	GLN
3	I	94	GLN
3	I	113	HIS
3	I	186	GLN
3	I	206	ASN
3	I	274	ASN
3	I	300	GLN
3	I	309	ASN
3	I	341	ASN
3	I	495	ASN
3	I	519	ASN
3	I	1249	ASN
3	I	1268	ASN
3	I	1366	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	225/242 (92%)	1.34	64 (28%) 0 2	267, 330, 380, 416	0
1	B	215/242 (88%)	2.69	114 (53%) 0 1	266, 335, 388, 430	0
1	F	225/242 (92%)	1.26	55 (24%) 0 2	248, 320, 383, 403	0
1	G	216/242 (89%)	2.11	91 (42%) 0 1	279, 337, 380, 412	0
2	C	1319/1342 (98%)	1.62	431 (32%) 0 2	232, 313, 384, 510	0
2	H	1319/1342 (98%)	1.75	450 (34%) 0 2	231, 315, 383, 482	0
3	D	1302/1407 (92%)	1.65	415 (31%) 0 2	230, 326, 424, 473	0
3	I	1306/1407 (92%)	2.06	498 (38%) 0 1	231, 332, 431, 492	0
4	J	147/181 (81%)	1.64	49 (33%) 0 2	300, 384, 446, 483	0
4	K	147/181 (81%)	2.13	59 (40%) 0 1	324, 413, 469, 491	0
All	All	6421/6828 (94%)	1.78	2226 (34%) 0 2	230, 324, 419, 510	0

All (2226) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	314	ARG	18.1
3	I	989	GLY	17.0
2	H	788	SER	16.3
3	I	315	ALA	15.7
3	D	315	ALA	15.4
3	D	1001	ALA	14.6
1	B	55	ALA	14.4
3	I	1076	PRO	14.2
3	D	318	GLY	13.7
3	I	106	GLU	13.6
3	I	304	ASP	13.3
3	I	991	THR	13.3
3	D	324	LEU	13.3

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Mol	Chain	Res	Type	RSRZ
3	I	819	GLY	13.1
3	I	986	ASP	13.0
2	H	792	GLY	12.7
3	D	316	ILE	12.6
3	I	1099	TYR	12.5
2	C	869	GLY	12.5
3	D	1000	GLY	12.3
3	I	295	GLU	12.3
2	C	116	ASP	12.2
3	D	974	VAL	12.2
3	I	302	ALA	12.2
2	H	621	SER	12.1
3	I	305	ALA	11.9
1	B	147	GLN	11.8
3	I	1112	GLY	11.8
2	H	772	SER	11.8
2	H	93	SER	11.7
3	I	443	GLU	11.6
3	I	444	GLY	11.6
3	I	990	ARG	11.4
4	K	129	GLU	11.4
1	B	89	ALA	11.3
3	I	63	GLY	11.1
3	I	847	ASP	10.9
2	H	314	ASN	10.9
2	H	794	LEU	10.9
2	H	793	GLU	10.8
3	I	105	ILE	10.8
2	H	869	GLY	10.7
3	I	369	PRO	10.6
3	D	1002	VAL	10.6
2	H	619	ALA	10.4
3	D	305	ALA	10.2
2	H	72	SER	10.1
4	K	94	GLY	10.1
3	I	745	GLY	10.0
2	H	868	SER	10.0
2	H	795	ALA	10.0
3	D	1004	ALA	10.0
3	I	310	GLY	9.9
3	I	993	GLU	9.9
2	H	620	ASN	9.9

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Mol	Chain	Res	Type	RSRZ
3	I	312	ARG	9.9
1	G	54	CYS	9.9
2	H	689	ALA	9.8
1	G	89	ALA	9.8
4	K	131	GLY	9.8
3	I	1107	VAL	9.7
3	I	1098	GLN	9.7
2	C	117	ILE	9.7
3	I	987	GLU	9.7
2	H	789	THR	9.6
1	B	57	THR	9.6
2	H	705	GLU	9.6
3	I	956	GLY	9.5
2	H	316	GLU	9.5
1	B	37	HIS	9.4
2	C	102	LEU	9.4
2	C	1064	ASP	9.4
2	C	175	ARG	9.4
3	I	976	THR	9.3
1	B	56	VAL	9.3
3	I	1077	ALA	9.3
2	C	871	VAL	9.3
3	I	977	SER	9.3
3	I	442	ILE	9.2
1	B	176	CYS	9.2
3	I	985	ILE	9.2
3	I	1168	GLU	9.2
2	H	746	ALA	9.2
3	D	991	THR	9.1
3	I	1122	ALA	9.1
3	D	317	THR	9.1
2	H	690	VAL	9.1
3	I	878	ASP	9.1
3	I	882	VAL	9.1
2	H	885	GLY	9.0
3	I	1111	ASP	9.0
2	H	128	PRO	9.0
1	B	54	CYS	9.0
2	C	868	SER	9.0
3	I	1110	GLU	9.0
4	K	95	GLY	8.9
3	I	1108	GLN	8.9

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Mol	Chain	Res	Type	RSRZ
3	I	267	ASP	8.8
3	D	975	ILE	8.8
1	B	36	GLY	8.8
3	D	1102	PRO	8.8
1	F	119	GLY	8.8
1	G	91	ARG	8.8
3	I	292	VAL	8.8
2	C	1066	MET	8.7
3	I	314	ARG	8.7
3	I	1166	GLY	8.7
3	I	294	ASN	8.7
2	H	884	VAL	8.6
2	H	745	GLU	8.6
3	D	984	LEU	8.6
2	C	1072	ASN	8.6
1	G	191	ARG	8.5
3	I	324	LEU	8.5
3	I	1097	ALA	8.5
3	I	1101	LEU	8.5
3	D	1110	GLU	8.5
2	H	71	VAL	8.5
2	H	790	ASP	8.5
2	H	796	LEU	8.5
3	D	745	GLY	8.4
3	I	957	SER	8.4
3	I	303	VAL	8.4
3	I	278	ARG	8.4
2	C	884	VAL	8.4
3	D	977	SER	8.4
2	H	1062	PRO	8.3
3	D	758	PRO	8.3
3	D	1169	THR	8.3
2	C	531	SER	8.3
2	H	147	SER	8.2
3	I	111	THR	8.2
3	I	1006	GLY	8.2
4	J	155	LYS	8.2
3	I	266	ASN	8.2
3	D	1101	LEU	8.2
2	H	1234	LYS	8.2
2	C	932	GLN	8.2
2	C	1234	LYS	8.1

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Mol	Chain	Res	Type	RSRZ
3	I	992	LYS	8.1
2	H	866	ASP	8.1
3	D	354	VAL	8.1
3	D	109	SER	8.0
1	B	97	GLU	8.0
2	H	656	SER	8.0
2	H	102	LEU	8.0
3	D	976	THR	7.9
2	H	92	TYR	7.9
3	I	881	LYS	7.9
3	D	1076	PRO	7.9
3	I	1100	PHE	7.9
4	J	154	GLU	7.9
3	I	955	LYS	7.9
3	D	983	LYS	7.9
2	H	771	VAL	7.9
3	D	1028	ILE	7.8
2	C	874	GLY	7.8
2	C	933	VAL	7.8
2	H	871	VAL	7.8
3	I	1109	LEU	7.8
3	D	310	GLY	7.8
3	I	306	LEU	7.7
1	B	38	THR	7.7
1	F	29	GLU	7.7
3	D	747	MET	7.7
3	I	61	ILE	7.7
1	B	149	GLY	7.7
3	D	993	GLU	7.7
2	C	483	ASP	7.7
4	J	44	VAL	7.7
3	D	1073	ASP	7.7
2	H	891	GLY	7.6
1	F	30	PRO	7.6
2	C	931	VAL	7.6
3	I	1102	PRO	7.6
2	H	467	GLY	7.6
2	C	176	ILE	7.6
3	I	370	LYS	7.6
3	D	1105	ALA	7.5
4	K	96	THR	7.5
3	I	1106	ILE	7.5

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Mol	Chain	Res	Type	RSRZ
2	C	70	TYR	7.5
2	C	178	PRO	7.5
3	I	107	LEU	7.5
3	D	309	ASN	7.5
3	I	524	GLY	7.5
3	I	747	MET	7.5
4	K	46	THR	7.5
1	B	191	ARG	7.4
2	H	797	GLY	7.4
2	C	174	ALA	7.4
3	D	992	LYS	7.4
1	G	122	GLU	7.4
3	I	118	LYS	7.4
2	C	147	SER	7.4
2	C	182	SER	7.4
2	H	870	ILE	7.4
3	I	984	LEU	7.4
3	I	1007	ASP	7.4
3	D	1103	GLY	7.4
3	I	1083	ALA	7.3
2	C	485	ASP	7.2
3	I	316	ILE	7.2
1	B	91	ARG	7.2
3	I	758	PRO	7.2
3	D	1168	GLU	7.2
3	D	1045	THR	7.2
1	F	190	ALA	7.2
2	C	421	SER	7.2
3	I	317	THR	7.2
3	D	942	SER	7.2
3	D	369	PRO	7.1
3	D	965	SER	7.1
1	G	55	ALA	7.1
2	H	100	LEU	7.1
3	D	1100	PHE	7.1
3	I	757	THR	7.0
4	K	97	SER	7.0
2	H	655	VAL	7.0
1	B	193	GLU	7.0
1	G	111	THR	7.0
2	H	1064	ASP	7.0
2	H	155	VAL	7.0

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Mol	Chain	Res	Type	RSRZ
2	H	1063	GLY	7.0
1	F	120	ASP	7.0
2	H	1066	MET	6.9
1	F	121	VAL	6.9
1	B	88	LEU	6.9
2	H	94	ALA	6.9
1	G	112	ALA	6.9
2	C	177	ILE	6.9
1	B	208	ASN	6.9
3	I	58	CYS	6.9
3	D	1109	LEU	6.9
3	I	1078	LEU	6.9
4	K	140	PRO	6.9
2	C	796	LEU	6.9
3	D	973	LEU	6.8
2	H	73	TYR	6.8
3	I	244	VAL	6.8
3	I	59	ALA	6.8
1	A	120	ASP	6.8
3	D	1006	GLY	6.8
3	I	1090	ILE	6.8
3	I	1127	GLU	6.8
3	I	62	PHE	6.7
1	F	118	ASP	6.7
3	I	469	HIS	6.7
3	D	757	THR	6.7
2	H	398	SER	6.7
2	C	870	ILE	6.7
3	D	1074	LEU	6.7
3	I	820	ILE	6.7
3	D	1003	LEU	6.7
2	C	488	MET	6.7
3	D	1122	ALA	6.7
3	I	301	GLU	6.6
4	K	132	GLU	6.6
1	F	192	VAL	6.6
3	D	319	SER	6.6
3	I	275	ARG	6.6
3	D	1099	TYR	6.6
3	I	1091	PRO	6.6
1	B	96	ASP	6.6
1	B	146	VAL	6.6

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Mol	Chain	Res	Type	RSRZ
2	C	1051	LYS	6.6
2	H	233	ARG	6.6
3	I	394	ILE	6.6
3	I	445	LYS	6.6
3	D	312	ARG	6.5
3	D	878	ASP	6.5
3	D	1018	ALA	6.5
3	I	1084	GLN	6.5
2	C	930	ASP	6.5
2	C	1062	PRO	6.5
2	H	931	VAL	6.5
2	H	691	PRO	6.5
3	I	822	MET	6.5
3	I	879	ALA	6.5
3	I	371	LYS	6.5
2	H	1084	ASP	6.5
2	C	173	ASN	6.5
3	D	999	TYR	6.4
3	I	966	VAL	6.4
2	H	1061	GLN	6.4
3	D	294	ASN	6.4
2	H	883	LEU	6.4
2	H	116	ASP	6.4
4	J	152	ASP	6.4
4	K	180	LYS	6.4
3	I	121	PRO	6.4
3	I	1167	LYS	6.4
3	D	313	GLY	6.4
1	B	187	VAL	6.4
3	I	962	ASN	6.4
3	I	388	ARG	6.4
3	I	242	LEU	6.4
3	I	856	ILE	6.4
3	I	570	LYS	6.4
1	G	90	VAL	6.4
4	K	104	SER	6.4
3	D	292	VAL	6.3
3	D	1258	ARG	6.3
2	C	158	ASP	6.3
4	K	100	PRO	6.3
2	C	968	GLU	6.3
2	C	125	GLY	6.3

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Mol	Chain	Res	Type	RSRZ
2	H	483	ASP	6.3
3	D	268	LEU	6.3
2	C	885	GLY	6.3
2	C	1120	ALA	6.3
3	I	313	GLY	6.3
2	H	622	ASN	6.3
2	H	688	GLN	6.3
2	H	70	TYR	6.2
2	C	894	GLN	6.2
2	C	705	GLU	6.2
4	J	42	VAL	6.2
3	D	118	LYS	6.2
2	C	1220	GLN	6.2
2	H	867	GLU	6.2
2	H	1081	PRO	6.2
2	H	932	GLN	6.2
1	B	87	GLY	6.2
3	I	323	PRO	6.2
3	D	958	ILE	6.2
2	C	1061	GLN	6.1
3	I	296	LYS	6.1
2	H	468	LEU	6.1
2	H	892	GLU	6.1
1	B	34	GLY	6.1
3	I	756	GLU	6.1
2	C	1074	GLY	6.1
2	H	263	VAL	6.1
3	I	877	VAL	6.1
4	K	130	PRO	6.1
1	G	92	VAL	6.1
2	H	777	VAL	6.1
1	G	98	VAL	6.1
2	H	99	LYS	6.1
2	H	933	VAL	6.1
2	C	126	GLU	6.1
3	D	293	ARG	6.0
1	A	119	GLY	6.0
2	H	791	LEU	6.0
1	G	56	VAL	6.0
3	I	965	SER	6.0
4	K	98	ASP	6.0
1	A	118	ASP	6.0

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Mol	Chain	Res	Type	RSRZ
2	H	774	GLY	6.0
2	H	930	ASP	6.0
3	D	311	ARG	6.0
3	D	1324	SER	6.0
3	I	1074	LEU	6.0
3	I	975	ILE	6.0
3	D	370	LYS	6.0
3	I	1075	ARG	6.0
1	B	174	ASP	6.0
2	C	690	VAL	6.0
3	I	268	LEU	5.9
2	H	1059	ARG	5.9
3	D	274	ASN	5.9
3	I	299	LEU	5.9
3	I	490	ILE	5.9
2	C	745	GLU	5.9
2	C	867	GLU	5.9
2	H	781	ASP	5.9
4	J	43	MET	5.9
3	D	325	LYS	5.9
3	I	1165	PHE	5.9
1	A	98	VAL	5.9
3	I	958	ILE	5.9
2	H	396	ASP	5.9
3	I	1195	GLN	5.9
2	H	127	ILE	5.9
2	H	976	ARG	5.9
3	D	1005	LYS	5.9
3	I	325	LYS	5.9
1	B	138	ALA	5.9
2	C	1063	GLY	5.9
3	I	880	VAL	5.9
2	C	873	ILE	5.9
4	K	44	VAL	5.9
2	C	94	ALA	5.9
2	H	1069	ARG	5.9
3	D	323	PRO	5.9
1	B	39	LEU	5.9
3	D	96	LYS	5.9
3	D	1083	ALA	5.9
3	D	944	ALA	5.8
3	I	104	HIS	5.8

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Mol	Chain	Res	Type	RSRZ
4	K	76	ASN	5.8
3	I	1088	VAL	5.8
4	K	93	ILE	5.8
2	C	533	LEU	5.8
4	K	88	ARG	5.8
1	G	71	LYS	5.8
1	B	175	ALA	5.8
3	D	295	GLU	5.8
2	C	1233	LEU	5.8
3	D	1075	ARG	5.8
1	B	32	GLU	5.8
2	C	127	ILE	5.8
3	I	311	ARG	5.8
2	H	313	ALA	5.8
2	C	146	VAL	5.7
3	I	119	SER	5.7
3	I	1092	GLY	5.7
2	H	485	ASP	5.7
2	C	1041	ASP	5.7
3	I	108	ALA	5.7
1	G	210	THR	5.7
3	I	276	ASN	5.7
3	D	107	LEU	5.7
2	C	1053	TYR	5.7
2	C	838	CYS	5.7
3	D	1046	ILE	5.7
3	D	304	ASP	5.7
2	C	1179	GLY	5.7
2	H	775	GLU	5.7
2	C	128	PRO	5.7
2	H	847	PRO	5.7
2	H	1058	ARG	5.6
3	D	1026	PRO	5.6
2	C	76	GLY	5.6
2	C	72	SER	5.6
3	I	525	MET	5.6
3	I	1132	LYS	5.6
2	H	706	ARG	5.6
3	I	1011	VAL	5.6
3	I	1194	ARG	5.6
2	C	940	GLU	5.6
3	I	571	ASP	5.6

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Mol	Chain	Res	Type	RSRZ
3	I	300	GLN	5.6
4	J	45	PRO	5.6
2	C	1050	VAL	5.6
1	G	125	LYS	5.6
4	J	17	GLY	5.6
1	A	97	GLU	5.6
3	I	54	ASP	5.6
3	I	279	LEU	5.6
3	I	441	LEU	5.6
3	I	876	SER	5.6
1	B	98	VAL	5.5
3	D	960	LEU	5.5
3	D	1007	ASP	5.5
2	H	1272	GLU	5.5
3	D	1084	GLN	5.5
2	C	794	LEU	5.5
1	B	216	ALA	5.5
2	H	893	THR	5.5
2	C	1121	ALA	5.5
3	D	746	LEU	5.5
1	B	148	ARG	5.5
2	C	262	TYR	5.5
3	I	1005	LYS	5.5
3	D	1027	VAL	5.5
2	C	532	ALA	5.5
3	D	498	PRO	5.5
3	I	1121	LEU	5.5
1	B	125	LYS	5.5
3	I	60	ARG	5.5
4	K	37	ASP	5.4
2	H	1072	ASN	5.4
3	I	954	ASN	5.4
4	K	102	PRO	5.4
2	H	1080	ASN	5.4
4	K	41	GLU	5.4
1	A	147	GLN	5.4
2	C	893	THR	5.4
2	C	487	LEU	5.4
4	K	75	MET	5.4
2	H	103	VAL	5.4
3	D	966	VAL	5.4
2	C	263	VAL	5.4

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Mol	Chain	Res	Type	RSRZ
2	H	471	VAL	5.4
3	I	53	ARG	5.4
2	H	715	THR	5.4
3	I	1324	SER	5.4
3	D	943	ARG	5.4
1	B	90	VAL	5.3
3	I	1082	ASP	5.3
1	G	149	GLY	5.3
2	C	69	GLN	5.3
4	J	77	ASP	5.3
3	D	1111	ASP	5.3
3	I	988	PHE	5.3
3	D	500	ILE	5.3
3	I	309	ASN	5.3
2	C	967	LEU	5.3
2	H	126	GLU	5.3
2	H	714	VAL	5.3
3	I	963	VAL	5.3
3	D	963	VAL	5.3
2	C	180	ARG	5.3
2	C	939	VAL	5.3
2	C	1004	ASP	5.3
4	K	40	GLY	5.3
2	C	942	ASP	5.3
1	A	121	VAL	5.3
3	I	110	PRO	5.3
1	A	172	LEU	5.3
3	D	302	ALA	5.2
2	C	73	TYR	5.2
2	H	101	ARG	5.2
2	C	115	LYS	5.2
2	C	1042	LEU	5.2
3	D	877	VAL	5.2
2	C	793	GLU	5.2
2	H	972	PHE	5.2
3	D	1260	MET	5.2
2	C	1124	ILE	5.2
2	C	530	ILE	5.2
2	C	929	ILE	5.2
2	H	782	VAL	5.2
3	D	445	LYS	5.2
3	D	959	LYS	5.2

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Mol	Chain	Res	Type	RSRZ
4	K	163	SER	5.2
3	I	277	ASN	5.2
2	H	776	PRO	5.2
3	D	1061	VAL	5.2
2	H	872	TYR	5.2
1	F	117	HIS	5.1
2	H	146	VAL	5.1
4	K	45	PRO	5.1
1	G	133	LEU	5.1
1	B	199	ASP	5.1
3	I	755	ILE	5.1
3	I	759	ILE	5.1
2	C	676	ALA	5.1
2	C	746	ALA	5.1
1	B	213	PRO	5.1
2	C	148	GLN	5.1
1	B	210	THR	5.1
2	H	1271	GLY	5.1
1	G	193	GLU	5.1
3	I	117	LEU	5.1
3	I	746	LEU	5.1
2	H	917	SER	5.1
2	H	465	ARG	5.1
1	G	96	ASP	5.1
3	I	1113	VAL	5.1
4	K	142	ALA	5.1
2	C	866	ASP	5.1
3	D	1261	LEU	5.1
3	I	1250	ASP	5.1
3	D	443	GLU	5.1
4	K	139	GLY	5.1
2	C	68	LEU	5.1
3	I	446	ALA	5.1
2	C	872	TYR	5.1
3	D	110	PRO	5.1
2	C	267	ARG	5.0
3	D	326	SER	5.0
3	I	240	THR	5.0
1	G	70	THR	5.0
1	G	110	VAL	5.0
2	C	934	PHE	5.0
2	C	227	LYS	5.0

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Mol	Chain	Res	Type	RSRZ
2	H	529	ARG	5.0
1	B	86	LYS	5.0
2	H	472	GLU	5.0
3	D	230	SER	5.0
3	D	1121	LEU	5.0
3	I	1103	GLY	5.0
2	H	531	SER	5.0
3	D	108	ALA	5.0
3	D	1029	THR	5.0
2	C	1065	LYS	5.0
3	D	76	LYS	5.0
1	B	71	LYS	5.0
2	C	444	ASP	5.0
3	I	838	ARG	5.0
4	K	128	PHE	5.0
2	C	1217	THR	5.0
3	D	874	GLU	5.0
3	D	267	ASP	4.9
3	D	962	ASN	4.9
2	C	77	GLU	4.9
4	K	42	VAL	4.9
2	C	941	LYS	4.9
2	H	151	ARG	4.9
2	H	1060	ILE	4.9
3	I	274	ASN	4.9
4	K	166	GLY	4.9
1	G	57	THR	4.9
3	I	293	ARG	4.9
2	C	498	ILE	4.9
2	H	273	HIS	4.9
2	C	972	PHE	4.9
2	H	6	THR	4.9
2	C	1067	ALA	4.9
2	C	1071	GLY	4.9
3	D	66	LYS	4.9
2	H	57	PHE	4.9
2	C	1069	ARG	4.9
4	K	151	VAL	4.9
2	C	422	LYS	4.9
3	D	74	LYS	4.9
2	C	744	GLY	4.9
2	H	1315	MET	4.9

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Mol	Chain	Res	Type	RSRZ
3	D	29	MET	4.9
1	G	88	LEU	4.9
3	D	69	GLU	4.9
1	G	113	ALA	4.9
3	D	1325	PHE	4.8
2	C	314	ASN	4.8
2	C	621	SER	4.8
2	C	1005	GLU	4.8
3	I	1212	ASP	4.8
1	B	92	VAL	4.8
3	I	64	PRO	4.8
2	C	266	GLY	4.8
2	H	156	PHE	4.8
1	B	73	GLY	4.8
1	G	73	GLY	4.8
3	D	1329	THR	4.8
2	C	1123	GLY	4.8
3	I	109	SER	4.8
4	J	140	PRO	4.8
3	D	760	THR	4.8
3	I	719	PHE	4.8
2	H	778	GLU	4.8
3	D	989	GLY	4.8
2	C	689	ALA	4.8
1	A	109	PRO	4.8
1	G	190	ALA	4.8
2	H	967	LEU	4.8
3	D	490	ILE	4.8
4	J	78	ALA	4.8
2	C	1073	LYS	4.8
2	H	654	ASP	4.8
3	D	957	SER	4.8
3	I	548	VAL	4.8
2	H	1264	GLN	4.8
3	I	1105	ALA	4.8
3	D	277	ASN	4.7
3	I	760	THR	4.7
2	H	470	ARG	4.7
4	J	41	GLU	4.7
3	I	999	TYR	4.7
2	H	1065	LYS	4.7
2	H	498	ILE	4.7

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Mol	Chain	Res	Type	RSRZ
2	C	271	ALA	4.7
3	D	879	ALA	4.7
3	I	298	MET	4.7
3	I	1120	THR	4.7
2	H	397	LEU	4.7
3	I	1027	VAL	4.7
3	D	275	ARG	4.7
3	I	978	ARG	4.7
1	A	22	THR	4.7
3	I	372	MET	4.7
2	H	695	ALA	4.7
4	J	156	SER	4.7
2	C	256	GLU	4.7
2	C	499	SER	4.7
2	C	1206	THR	4.7
2	H	255	ILE	4.7
2	H	1217	THR	4.7
1	B	35	PHE	4.7
3	D	990	ARG	4.7
3	I	55	GLY	4.7
3	D	39	LYS	4.7
2	H	1050	VAL	4.7
2	C	772	SER	4.6
1	F	98	VAL	4.6
3	I	974	VAL	4.6
2	C	1219	GLU	4.6
3	I	1325	PHE	4.6
1	F	195	ARG	4.6
3	D	37	GLU	4.6
1	G	108	GLY	4.6
2	C	484	LEU	4.6
3	I	1037	PHE	4.6
3	I	1089	LEU	4.6
2	H	148	GLN	4.6
3	D	444	GLY	4.6
1	B	215	GLU	4.6
4	J	46	THR	4.6
3	I	280	LYS	4.6
2	H	180	ARG	4.6
3	D	1256	ILE	4.6
3	I	269	TYR	4.6
3	I	1197	ASN	4.6

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Mol	Chain	Res	Type	RSRZ
4	K	87	PRO	4.6
2	C	1239	VAL	4.6
2	C	486	THR	4.6
2	H	519	ASN	4.6
3	I	718	SER	4.6
1	G	189	ALA	4.6
2	H	580	GLN	4.6
1	F	122	GLU	4.6
3	I	883	ARG	4.6
3	I	308	ASP	4.6
3	I	271	ARG	4.6
2	H	965	GLN	4.6
3	D	1123	ARG	4.6
2	H	4	SER	4.6
2	H	929	ILE	4.6
3	D	1257	VAL	4.6
2	C	157	PHE	4.6
2	C	1272	GLU	4.6
2	H	254	ASP	4.5
2	H	256	GLU	4.5
1	A	108	GLY	4.5
2	C	706	ARG	4.5
2	H	267	ARG	4.5
2	C	103	VAL	4.5
2	H	968	GLU	4.5
4	K	143	ASP	4.5
3	I	122	SER	4.5
2	C	1084	ASP	4.5
2	C	252	SER	4.5
2	C	57	PHE	4.5
1	B	124	VAL	4.5
3	D	67	ASP	4.5
2	C	450	ASN	4.5
2	H	315	MET	4.5
3	D	964	LYS	4.5
3	I	393	THR	4.5
2	C	983	GLY	4.5
3	D	920	ALA	4.5
3	I	1174	ARG	4.5
3	D	1306	LEU	4.5
3	I	1191	PRO	4.5
3	I	1008	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
2	H	69	GLN	4.5
2	C	152	SER	4.5
2	H	1336	ASN	4.4
3	D	499	ILE	4.5
2	H	291	TYR	4.4
2	C	501	ALA	4.4
3	I	1149	ARG	4.4
3	I	112	ALA	4.4
3	D	276	ASN	4.4
3	D	1174	ARG	4.4
3	D	759	ILE	4.4
2	H	918	LEU	4.4
4	J	139	GLY	4.4
2	C	529	ARG	4.4
3	D	335	GLN	4.4
1	B	31	LEU	4.4
1	B	104	LYS	4.4
3	I	1175	LEU	4.4
3	I	48	THR	4.4
3	I	818	GLU	4.4
3	I	1176	VAL	4.4
3	D	497	GLU	4.4
3	D	1017	VAL	4.4
3	I	1040	MET	4.4
2	C	269	ILE	4.4
2	C	976	ARG	4.4
3	D	1281	GLU	4.4
1	F	172	LEU	4.4
2	C	420	LEU	4.4
2	C	795	ALA	4.4
2	C	156	PHE	4.4
3	I	670	SER	4.4
2	H	966	ILE	4.4
3	I	848	VAL	4.4
2	C	969	ALA	4.4
3	I	373	ALA	4.3
2	C	528	ARG	4.3
1	G	87	GLY	4.3
3	D	355	ILE	4.3
3	I	1169	THR	4.3
3	I	319	SER	4.3
2	H	974	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
2	H	1235	LEU	4.3
2	H	882	ILE	4.3
2	H	113	THR	4.3
3	D	1064	SER	4.3
3	I	1045	THR	4.3
2	C	788	SER	4.3
3	I	297	ARG	4.3
3	I	128	LEU	4.3
3	I	902	ASP	4.3
3	I	1028	ILE	4.3
4	J	151	VAL	4.3
2	C	184	LEU	4.3
3	D	280	LYS	4.3
1	G	188	GLU	4.3
2	H	970	GLY	4.3
3	D	1114	GLN	4.3
3	I	270	ARG	4.3
2	C	400	VAL	4.3
2	H	115	LYS	4.3
2	H	234	ASP	4.3
2	H	112	GLY	4.3
2	C	183	TRP	4.3
3	D	1330	ARG	4.3
2	H	129	LEU	4.3
3	D	162	GLU	4.3
3	I	1158	GLU	4.3
1	F	91	ARG	4.3
3	I	1073	ASP	4.3
3	I	318	GLY	4.3
3	I	1154	ALA	4.3
3	I	265	LEU	4.3
2	C	935	THR	4.3
2	C	251	ALA	4.3
2	H	484	LEU	4.3
1	G	132	HIS	4.3
2	H	785	ASP	4.3
3	D	998	PRO	4.3
4	K	137	ASN	4.3
3	D	75	TYR	4.2
2	H	463	GLN	4.2
2	H	642	SER	4.2
2	H	154	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
2	C	101	ARG	4.2
1	A	24	ALA	4.2
2	C	155	VAL	4.2
3	D	1115	ILE	4.2
2	H	940	GLU	4.2
3	I	241	VAL	4.2
2	C	883	LEU	4.2
3	I	124	ILE	4.2
3	D	1165	PHE	4.2
3	I	491	LEU	4.2
1	B	214	GLU	4.2
2	H	18	ARG	4.2
2	H	145	ILE	4.2
1	G	146	VAL	4.2
2	H	264	GLU	4.2
2	H	1216	ARG	4.2
3	D	501	VAL	4.2
2	C	270	THR	4.2
3	I	321	LYS	4.2
2	C	67	GLU	4.2
3	D	978	ARG	4.2
2	C	181	GLY	4.2
2	C	1060	ILE	4.2
2	C	151	ARG	4.2
2	H	125	GLY	4.2
1	G	231	PHE	4.2
3	D	1259	GLN	4.2
2	C	427	ASP	4.2
4	J	107	GLU	4.2
2	C	771	VAL	4.2
1	G	187	VAL	4.2
3	D	1262	ARG	4.2
3	I	720	ASN	4.2
2	H	855	PRO	4.2
3	D	1326	GLN	4.2
3	I	1326	GLN	4.2
2	C	1122	LYS	4.2
3	I	1354	GLY	4.1
3	D	1107	VAL	4.1
2	H	408	SER	4.1
3	I	72	CYS	4.1
1	G	93	GLN	4.1

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Mol	Chain	Res	Type	RSRZ
1	F	96	ASP	4.1
2	H	1088	ASP	4.1
2	C	226	GLU	4.1
2	C	691	PRO	4.1
3	D	994	SER	4.1
3	I	500	ILE	4.1
2	H	944	ARG	4.1
3	I	322	ARG	4.1
2	H	1308	ILE	4.1
3	I	527	LEU	4.1
1	F	116	THR	4.1
2	C	1052	VAL	4.1
2	C	316	GLU	4.1
2	H	1262	LYS	4.1
1	B	192	VAL	4.1
1	F	191	ARG	4.1
3	D	291	ILE	4.1
3	I	1123	ARG	4.1
2	C	656	SER	4.1
2	C	1235	LEU	4.1
2	H	865	LEU	4.1
2	C	95	PRO	4.1
3	D	950	ILE	4.1
3	I	1039	ASP	4.1
3	D	997	VAL	4.1
3	I	98	ARG	4.1
3	I	1190	ILE	4.1
2	H	838	CYS	4.1
3	I	493	PRO	4.1
4	K	181	ALA	4.1
3	D	306	LEU	4.1
3	I	1199	PHE	4.1
3	D	923	ILE	4.1
1	B	135	ASP	4.1
1	B	151	GLY	4.0
2	H	635	THR	4.0
2	C	677	ASN	4.0
1	A	21	SER	4.0
4	K	164	ILE	4.0
2	C	233	ARG	4.0
3	I	875	ASN	4.0
2	C	80	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
3	I	844	THR	4.0
2	C	578	TYR	4.0
2	C	88	ARG	4.0
2	H	152	SER	4.0
1	B	53	GLY	4.0
2	C	792	GLY	4.0
3	D	1120	THR	4.0
3	D	1009	GLU	4.0
2	C	797	GLY	4.0
2	H	464	PHE	4.0
3	I	1252	HIS	4.0
3	D	104	HIS	4.0
3	D	980	THR	4.0
2	H	79	VAL	4.0
2	H	445	ILE	4.0
3	D	927	GLY	4.0
3	I	245	LEU	4.0
1	B	20	SER	4.0
1	F	97	GLU	4.0
2	H	466	VAL	4.0
3	I	88	CYS	4.0
2	C	966	ILE	4.0
3	I	494	ALA	4.0
3	I	1093	THR	4.0
1	B	123	ILE	4.0
3	I	1129	GLY	4.0
2	C	145	ILE	4.0
2	C	1078	LYS	4.0
2	H	696	ASP	4.0
2	H	973	SER	4.0
3	D	119	SER	4.0
2	C	971	LEU	4.0
2	C	273	HIS	3.9
2	C	777	VAL	3.9
3	D	1166	GLY	3.9
2	H	399	ALA	3.9
2	H	886	LYS	3.9
2	C	317	LEU	3.9
1	A	23	HIS	3.9
2	H	225	PHE	3.9
3	I	368	LEU	3.9
3	D	1119	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
3	I	821	MET	3.9
3	I	964	LYS	3.9
2	H	969	ALA	3.9
3	D	1357	ILE	3.9
2	C	1216	ARG	3.9
3	D	278	ARG	3.9
1	F	31	LEU	3.9
2	H	975	ILE	3.9
1	B	21	SER	3.9
3	I	354	VAL	3.9
3	I	1306	LEU	3.9
3	D	1167	LYS	3.9
1	B	201	LEU	3.9
2	H	402	ARG	3.9
4	K	179	GLU	3.9
3	I	1035	VAL	3.9
3	D	995	TYR	3.9
2	H	418	GLY	3.9
3	I	927	GLY	3.9
3	D	502	PRO	3.9
3	I	717	VAL	3.9
1	B	139	SER	3.9
2	H	1051	LYS	3.9
3	D	1030	GLU	3.9
2	H	499	SER	3.9
2	H	939	VAL	3.9
3	I	463	GLY	3.9
2	C	426	ILE	3.9
3	I	291	ILE	3.9
2	C	114	VAL	3.9
2	C	272	ARG	3.9
2	H	1180	MET	3.9
1	B	185	TYR	3.9
3	I	163	GLU	3.9
1	G	109	PRO	3.9
2	H	317	LEU	3.9
3	D	368	LEU	3.9
3	I	379	PRO	3.9
3	I	1215	GLU	3.9
2	H	703	GLY	3.8
3	I	1085	GLY	3.8
3	I	1172	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
2	C	1040	ASP	3.8
3	I	489	ASN	3.8
3	D	1255	VAL	3.8
3	I	1009	GLU	3.8
2	C	10	ARG	3.8
2	H	489	PRO	3.8
3	D	371	LYS	3.8
1	F	28	LEU	3.8
2	C	1128	ILE	3.8
2	H	453	ILE	3.8
2	H	971	LEU	3.8
3	D	891	ASP	3.8
2	C	449	GLY	3.8
1	B	85	LEU	3.8
3	D	985	ILE	3.8
3	I	41	PRO	3.8
2	H	266	GLY	3.8
3	I	526	VAL	3.8
1	B	212	ASP	3.8
3	I	336	GLY	3.8
2	H	231	GLU	3.8
2	H	5	TYR	3.8
3	I	716	GLN	3.8
3	I	326	SER	3.8
3	D	389	GLY	3.8
1	B	177	TYR	3.8
3	I	1355	ARG	3.8
2	H	1067	ALA	3.8
2	H	1299	ASN	3.8
2	H	634	VAL	3.8
2	C	424	ASP	3.8
2	C	945	ALA	3.8
3	I	468	VAL	3.8
1	A	146	VAL	3.8
1	B	205	MET	3.8
2	H	783	LEU	3.8
2	H	226	GLU	3.8
2	C	452	ARG	3.8
3	D	409	TRP	3.8
3	D	1328	THR	3.8
1	F	21	SER	3.8
1	G	199	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
2	H	618	GLN	3.8
3	I	243	PRO	3.8
3	I	47	ARG	3.8
3	D	1191	PRO	3.8
2	H	119	GLU	3.7
2	C	527	LYS	3.7
2	H	1092	THR	3.7
2	H	798	GLN	3.7
3	D	177	ASP	3.7
3	I	184	ALA	3.7
1	F	123	ILE	3.7
2	C	423	ASP	3.7
1	A	195	ARG	3.7
4	J	104	SER	3.7
2	C	25	PRO	3.7
2	C	875	ALA	3.7
2	C	1336	ASN	3.7
2	C	586	PHE	3.7
3	I	43	THR	3.7
2	H	1218	GLY	3.7
3	D	41	PRO	3.7
2	C	113	THR	3.7
2	C	720	ARG	3.7
3	D	245	LEU	3.7
3	D	28	ASP	3.7
1	G	138	ALA	3.7
2	H	189	ASP	3.7
2	H	942	ASP	3.7
2	C	93	SER	3.7
2	C	179	TYR	3.7
3	I	69	GLU	3.7
3	I	1133	ASP	3.7
1	G	123	ILE	3.7
4	J	16	SER	3.7
3	D	602	SER	3.7
3	D	40	LYS	3.7
2	H	1179	GLY	3.7
2	C	804	PHE	3.7
2	C	1211	ARG	3.7
2	C	497	PRO	3.6
1	A	154	PRO	3.6
2	C	541	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
2	C	520	PRO	3.6
3	D	1008	GLY	3.6
1	B	211	ILE	3.6
2	H	520	PRO	3.6
3	I	928	THR	3.6
3	D	321	LYS	3.6
1	B	209	GLY	3.6
2	H	253	PHE	3.6
3	I	56	LEU	3.6
2	H	502	VAL	3.6
2	H	716	ALA	3.6
3	D	1200	GLU	3.6
3	I	1000	GLY	3.6
3	I	980	THR	3.6
2	C	1076	ILE	3.6
2	H	412	GLU	3.6
3	D	982	LEU	3.6
3	D	756	GLU	3.6
2	C	398	SER	3.6
3	D	290	ILE	3.6
3	D	353	SER	3.6
4	J	153	TYR	3.6
3	I	1001	ALA	3.6
2	H	78	PRO	3.6
3	I	1356	LEU	3.6
3	D	986	ASP	3.6
3	I	959	LYS	3.6
4	J	142	ALA	3.6
4	J	143	ASP	3.6
2	H	98	VAL	3.6
3	D	893	GLY	3.6
3	D	875	ASN	3.6
2	H	56	VAL	3.6
3	D	496	GLY	3.6
2	C	892	GLU	3.6
3	I	960	LEU	3.6
2	C	1038	GLN	3.6
2	H	1004	ASP	3.6
2	C	255	ILE	3.6
3	D	930	LEU	3.6
3	D	861	ASN	3.6
3	I	1128	SER	3.6

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Mol	Chain	Res	Type	RSRZ
3	I	102	MET	3.6
4	J	105	ASP	3.6
1	G	53	GLY	3.6
2	C	453	ILE	3.6
2	H	3	TYR	3.6
3	I	374	LEU	3.6
1	G	148	ARG	3.5
2	H	1227	VAL	3.5
3	I	1012	ALA	3.5
2	C	1049	ILE	3.5
2	H	452	ARG	3.5
2	H	657	THR	3.5
3	D	819	GLY	3.5
1	A	227	GLN	3.5
1	B	195	ARG	3.5
4	J	72	GLN	3.5
2	H	265	LYS	3.5
2	H	1124	ILE	3.5
3	I	523	GLU	3.5
1	F	198	LEU	3.5
3	I	413	ASP	3.5
2	C	837	ALA	3.5
3	I	923	ILE	3.5
1	G	147	GLN	3.5
4	J	130	PRO	3.5
2	H	1219	GLU	3.5
3	D	1354	GLY	3.5
3	I	386	GLU	3.5
2	H	1053	TYR	3.5
1	G	74	VAL	3.5
2	H	232	ILE	3.5
3	I	1087	ASP	3.5
1	G	211	ILE	3.5
3	D	1171	GLY	3.5
3	I	73	GLY	3.5
3	I	1256	ILE	3.5
2	H	1297	ASP	3.5
1	A	231	PHE	3.5
3	I	1030	GLU	3.5
3	D	372	MET	3.5
2	H	469	VAL	3.5
3	I	390	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
3	I	744	ARG	3.5
4	K	92	PHE	3.5
1	G	114	ASP	3.5
3	I	284	ASP	3.5
3	D	453	VAL	3.5
3	D	1124	ILE	3.5
1	G	95	LYS	3.5
2	H	1314	GLN	3.5
1	B	112	ALA	3.5
3	I	835	LEU	3.5
2	C	1075	VAL	3.5
2	C	686	GLN	3.5
2	C	1212	LEU	3.5
2	C	11	ILE	3.5
1	B	152	TYR	3.5
1	G	24	ALA	3.5
2	C	124	MET	3.5
3	I	389	GLY	3.5
3	I	793	SER	3.5
3	D	1116	SER	3.5
2	C	965	GLN	3.5
1	B	231	PHE	3.4
2	H	497	PRO	3.4
3	I	282	LEU	3.4
3	I	1029	THR	3.4
2	H	697	LYS	3.4
2	H	1128	ILE	3.4
3	I	1155	ILE	3.4
2	C	416	GLY	3.4
2	C	778	GLU	3.4
2	H	111	GLU	3.4
3	I	690	ASN	3.4
3	D	271	ARG	3.4
1	F	114	ASP	3.4
1	G	204	GLU	3.4
2	H	179	TYR	3.4
2	H	8	LYS	3.4
2	C	789	THR	3.4
2	H	91	THR	3.4
2	H	854	ILE	3.4
3	D	246	PRO	3.4
2	C	1214	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
2	H	807	TRP	3.4
2	C	704	MET	3.4
2	C	891	GLY	3.4
3	D	1252	HIS	3.4
1	A	68	TYR	3.4
2	C	431	LYS	3.4
2	C	859	GLU	3.4
2	C	502	VAL	3.4
3	I	87	LYS	3.4
4	K	135	ARG	3.4
3	D	1113	VAL	3.4
2	C	698	PRO	3.4
3	I	201	LEU	3.4
3	I	1214	PRO	3.4
2	H	747	GLY	3.4
1	B	10	LYS	3.4
3	D	849	LEU	3.4
3	D	941	ALA	3.4
3	D	1059	LEU	3.4
2	H	744	GLY	3.4
1	G	77	ASP	3.4
3	D	1108	GLN	3.4
2	C	258	ASN	3.4
1	F	12	ARG	3.4
1	A	230	ALA	3.4
3	I	823	THR	3.4
2	C	1271	GLY	3.4
3	D	1104	LYS	3.4
3	I	1096	PRO	3.4
4	J	150	GLU	3.4
1	B	33	ARG	3.4
2	H	1233	LEU	3.4
2	H	653	MET	3.3
2	H	828	PHE	3.3
2	C	1180	MET	3.3
2	C	443	ASP	3.3
3	I	360	TYR	3.3
4	K	103	ILE	3.3
3	I	952	VAL	3.3
1	G	25	LYS	3.3
2	C	1232	MET	3.3
3	D	289	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
3	D	1355	ARG	3.3
3	I	743	MET	3.3
2	C	1068	GLY	3.3
3	I	846	GLU	3.3
1	F	197	ASP	3.3
2	C	982	GLY	3.3
2	H	295	LYS	3.3
3	I	1153	PRO	3.3
2	H	1048	LYS	3.3
3	I	114	ILE	3.3
3	I	1173	ARG	3.3
1	B	105	SER	3.3
3	D	1072	LYS	3.3
3	I	1260	MET	3.3
2	C	1059	ARG	3.3
2	H	786	GLY	3.3
2	H	874	GLY	3.3
2	H	701	GLY	3.3
3	D	336	GLY	3.3
1	A	133	LEU	3.3
2	C	1079	ILE	3.3
3	D	1307	LEU	3.3
2	H	475	VAL	3.3
3	D	23	ALA	3.3
3	D	447	ILE	3.3
3	I	1131	THR	3.3
2	C	1213	TYR	3.3
3	D	452	LEU	3.3
3	I	89	GLY	3.3
3	I	549	LYS	3.3
3	I	1211	SER	3.3
3	I	1200	GLU	3.3
2	C	538	LEU	3.3
1	G	192	VAL	3.3
3	I	1061	VAL	3.3
3	D	715	LYS	3.3
1	B	72	GLU	3.3
3	D	1145	PHE	3.3
4	K	153	TYR	3.3
1	G	121	VAL	3.3
2	C	1039	GLY	3.3
2	H	274	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
3	I	1086	ASN	3.3
2	H	1274	GLU	3.3
3	I	1196	LEU	3.3
3	D	1063	ASP	3.2
4	J	138	ASP	3.2
1	G	99	ILE	3.2
1	F	11	PRO	3.2
2	H	95	PRO	3.2
2	C	492	MET	3.2
2	H	1251	TYR	3.2
3	D	855	ASP	3.2
4	K	148	VAL	3.2
1	B	111	THR	3.2
1	F	113	ALA	3.2
1	G	6	THR	3.2
3	D	463	GLY	3.2
4	J	111	ILE	3.2
2	C	110	PRO	3.2
2	C	465	ARG	3.2
3	I	941	ALA	3.2
3	D	244	VAL	3.2
2	C	264	GLU	3.2
2	C	347	ILE	3.2
3	I	645	VAL	3.2
3	I	1357	ILE	3.2
2	C	257	ALA	3.2
3	I	66	LYS	3.2
3	D	1098	GLN	3.2
3	I	182	ALA	3.2
3	I	320	ASN	3.2
2	C	758	ARG	3.2
2	H	700	VAL	3.2
3	I	994	SER	3.2
2	C	1274	GLU	3.2
2	C	590	PRO	3.2
2	H	1071	GLY	3.2
3	D	601	ILE	3.2
2	H	841	ARG	3.2
2	H	1254	VAL	3.2
3	I	929	GLN	3.2
2	H	443	ASP	3.2
3	I	830	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
2	H	758	ARG	3.2
1	G	144	ILE	3.2
2	C	445	ILE	3.2
3	I	447	ILE	3.2
3	I	1094	ASP	3.2
3	I	74	LYS	3.2
2	C	537	GLY	3.2
1	B	217	ILE	3.2
2	C	659	GLN	3.2
2	H	107	ARG	3.2
2	H	702	THR	3.2
3	I	377	PHE	3.2
1	G	196	THR	3.2
3	D	1082	ASP	3.2
3	D	1331	VAL	3.2
2	H	1232	MET	3.2
2	C	150	HIS	3.2
2	C	928	VAL	3.2
3	I	983	LYS	3.2
2	H	420	LEU	3.2
4	J	131	GLY	3.2
3	I	715	LYS	3.2
1	B	194	GLN	3.2
3	I	1079	LYS	3.2
3	I	103	GLY	3.1
3	I	1156	LEU	3.1
2	H	799	ASN	3.1
3	I	127	LEU	3.1
3	I	1150	PRO	3.1
1	A	92	VAL	3.1
3	D	207	GLU	3.1
3	D	981	GLU	3.1
2	C	944	ARG	3.1
2	C	71	VAL	3.1
2	H	599	VAL	3.1
2	C	27	LEU	3.1
3	D	95	THR	3.1
3	I	125	GLY	3.1
1	A	207	THR	3.1
2	H	636	CYS	3.1
3	I	997	VAL	3.1
2	H	873	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
2	C	19	PRO	3.1
3	D	42	GLU	3.1
3	D	87	LYS	3.1
3	I	378	LYS	3.1
3	D	924	GLY	3.1
2	H	406	ASN	3.1
3	D	462	ASP	3.1
2	C	791	LEU	3.1
2	H	298	ALA	3.1
2	H	501	ALA	3.1
1	A	234	LEU	3.1
2	C	655	VAL	3.1
3	D	367	GLY	3.1
3	D	1067	ARG	3.1
3	D	420	PRO	3.1
2	H	312	ALA	3.1
3	I	1189	MET	3.1
2	H	271	ALA	3.1
1	A	174	ASP	3.1
3	I	422	LEU	3.1
2	C	708	VAL	3.1
1	F	93	GLN	3.1
3	D	961	SER	3.1
1	B	206	GLU	3.1
2	C	964	LEU	3.1
2	H	533	LEU	3.1
3	I	532	GLU	3.1
3	D	1019	ASN	3.1
2	C	99	LYS	3.1
3	I	273	ILE	3.1
2	C	535	PRO	3.1
2	H	646	SER	3.1
3	I	531	LYS	3.1
2	C	1218	GLY	3.1
3	D	1332	LEU	3.1
3	I	1258	ARG	3.1
3	I	714	GLU	3.1
2	C	225	PHE	3.1
2	C	1204	LEU	3.1
2	H	623	LEU	3.1
2	H	1236	ASN	3.1
3	D	491	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
2	H	528	ARG	3.1
2	C	104	ILE	3.1
2	H	1082	ILE	3.1
1	G	100	LEU	3.0
1	G	115	ILE	3.0
2	C	841	ARG	3.1
3	D	1091	PRO	3.0
3	I	904	ALA	3.0
3	D	428	THR	3.0
3	D	1090	ILE	3.0
2	H	11	ILE	3.0
2	C	1221	PHE	3.0
2	H	252	SER	3.0
3	D	1199	PHE	3.0
2	H	482	GLY	3.0
3	I	181	GLY	3.0
1	B	140	ILE	3.0
2	C	118	LYS	3.0
2	H	426	ILE	3.0
4	K	99	ARG	3.0
2	C	22	LEU	3.0
1	B	23	HIS	3.0
2	H	687	ARG	3.0
3	D	916	GLY	3.0
2	C	100	LEU	3.0
1	A	99	ILE	3.0
2	H	177	ILE	3.0
3	D	1155	ILE	3.0
3	I	1067	ARG	3.0
3	D	987	GLU	3.0
3	I	1216	ALA	3.0
2	H	692	THR	3.0
3	I	1218	HIS	3.0
1	F	95	LYS	3.0
2	H	631	GLU	3.0
2	C	425	ILE	3.0
2	C	542	ARG	3.0
2	H	808	ASN	3.0
2	H	124	MET	3.0
3	D	163	GLU	3.0
2	C	688	GLN	3.0
2	H	230	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
3	D	1131	THR	3.0
2	H	1057	LYS	3.0
2	C	53	PHE	3.0
2	H	405	PHE	3.0
2	H	407	ARG	3.0
1	F	148	ARG	3.0
1	A	110	VAL	3.0
1	B	58	GLU	3.0
2	C	1118	GLY	3.0
3	D	1020	TRP	3.0
3	I	1064	SER	3.0
2	C	129	LEU	3.0
1	A	57	THR	3.0
4	K	38	LEU	3.0
2	H	837	ALA	3.0
3	D	1047	THR	3.0
1	A	29	GLU	3.0
1	F	75	GLN	3.0
2	H	1269	ARG	3.0
4	K	144	PHE	3.0
3	D	748	ALA	3.0
3	I	646	ILE	2.9
1	B	22	THR	2.9
2	H	104	ILE	2.9
1	B	40	GLY	2.9
3	D	1062	LEU	2.9
3	I	1219	ASP	2.9
2	C	144	VAL	2.9
2	C	9	LYS	2.9
2	H	488	MET	2.9
3	D	308	ASP	2.9
1	B	196	THR	2.9
3	D	1175	LEU	2.9
1	F	92	VAL	2.9
3	I	338	PHE	2.9
2	H	77	GLU	2.9
2	H	704	MET	2.9
2	C	1238	LEU	2.9
3	I	91	GLU	2.9
1	B	8	PHE	2.9
2	H	698	PRO	2.9
1	A	205	MET	2.9

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Mol	Chain	Res	Type	RSRZ
3	D	266	ASN	2.9
2	H	532	ALA	2.9
3	D	248	ASP	2.9
4	J	175	PHE	2.9
2	H	1068	GLY	2.9
2	H	1078	LYS	2.9
1	F	212	ASP	2.9
1	B	207	THR	2.9
2	H	1228	GLY	2.9
3	I	375	GLU	2.9
3	I	116	PHE	2.9
3	I	335	GLN	2.9
1	A	153	VAL	2.9
4	J	180	LYS	2.9
2	C	573	ASN	2.9
3	D	137	ARG	2.9
3	D	296	LYS	2.9
2	C	12[A]	ARG	2.9
4	K	101	ALA	2.9
1	F	174	ASP	2.9
1	B	184	ALA	2.9
2	H	773	LEU	2.9
1	F	166	ARG	2.9
2	C	1006	GLU	2.9
2	C	265	LYS	2.9
3	I	409	TRP	2.9
2	H	117	ILE	2.9
4	K	165	PHE	2.9
3	D	322	ARG	2.9
2	H	157	PHE	2.9
2	H	686	GLN	2.9
3	D	790	THR	2.9
3	D	1033	GLY	2.9
3	I	671	GLY	2.9
2	C	56	VAL	2.9
3	D	922	SER	2.9
3	D	1356	LEU	2.9
3	I	502	PRO	2.9
3	I	644	MET	2.8
1	B	181	GLU	2.8
3	I	538	ARG	2.8
1	B	109	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
2	C	1007	LYS	2.8
3	I	702	GLN	2.8
4	K	145	ASN	2.8
2	C	816	ILE	2.8
3	D	876	SER	2.8
1	G	184	ALA	2.8
3	D	919	ALA	2.8
3	I	1104	LYS	2.8
2	C	224	PHE	2.8
2	C	903	ARG	2.8
2	C	764	CYS	2.8
3	D	379	PRO	2.8
2	H	677	ASN	2.8
3	D	388	ARG	2.8
1	B	133	LEU	2.8
3	I	381	ILE	2.8
3	I	1353	VAL	2.8
1	G	72	GLU	2.8
3	D	892	PHE	2.8
3	I	1125	PRO	2.8
2	C	18	ARG	2.8
2	C	454	ARG	2.8
1	F	213	PRO	2.8
3	D	926	PRO	2.8
4	J	76	ASN	2.8
2	C	409	LEU	2.8
2	H	1052	VAL	2.8
3	D	894	VAL	2.8
1	B	232	VAL	2.8
2	H	718	ALA	2.8
3	I	387	LEU	2.8
1	F	115	ILE	2.8
3	D	818	GLU	2.8
1	B	41	ASN	2.8
2	C	524	ILE	2.8
1	A	116	THR	2.8
2	C	640	GLY	2.8
2	C	814	ASP	2.8
3	D	1085	GLY	2.8
2	H	181	GLY	2.8
3	I	1351	VAL	2.8
3	D	1201	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	124	VAL	2.8
2	H	108	GLU	2.8
3	D	441	LEU	2.8
3	D	951	GLN	2.8
3	I	845	ALA	2.8
2	H	272	ARG	2.8
3	D	320	ASN	2.8
2	C	149	LEU	2.8
3	I	1192	LYS	2.8
2	C	1058	ARG	2.8
3	D	585	LYS	2.8
3	D	882	VAL	2.8
2	C	442	VAL	2.8
2	C	970	GLY	2.8
3	D	231	GLY	2.8
3	D	429	LEU	2.8
3	I	843	VAL	2.8
1	F	167	PRO	2.8
3	D	32	SER	2.8
3	D	588	PRO	2.8
3	D	792	ASN	2.7
1	A	228	LEU	2.7
4	J	9	TRP	2.7
2	H	1178	LYS	2.7
1	A	132	HIS	2.7
1	G	50	SER	2.7
3	I	1254	GLU	2.7
3	I	1321	SER	2.7
2	C	703	GLY	2.7
2	H	1049	ILE	2.7
3	I	842	ARG	2.7
2	C	28	LEU	2.7
3	I	824	PRO	2.7
3	D	1190	ILE	2.7
2	C	1178	LYS	2.7
2	H	1086	PRO	2.7
3	D	880	VAL	2.7
3	I	204	GLU	2.7
3	I	817	HIS	2.7
3	I	1352	ILE	2.7
2	C	23	ASP	2.7
2	C	1043	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
2	H	629	PHE	2.7
2	H	787	PRO	2.7
2	C	81	ASP	2.7
3	D	279	LEU	2.7
3	I	384	LYS	2.7
3	I	385	LEU	2.7
2	H	1005	GLU	2.7
2	H	1212	LEU	2.7
3	I	176	PHE	2.7
2	H	80	PHE	2.7
2	H	336	LEU	2.7
2	H	832	HIS	2.7
1	A	148	ARG	2.7
3	D	621	ALA	2.7
1	G	208	ASN	2.7
3	D	1031	VAL	2.7
3	I	982	LEU	2.7
4	J	176	SER	2.7
2	H	227	LYS	2.7
3	I	665	GLN	2.7
3	D	586	GLY	2.7
1	G	128	HIS	2.7
2	C	500	ALA	2.7
3	D	94	GLN	2.7
3	I	97	VAL	2.7
3	I	748	ALA	2.7
3	I	1259	GLN	2.7
2	H	352	ARG	2.7
3	D	789	LYS	2.7
2	H	178	PRO	2.7
1	A	226	GLU	2.7
1	F	194	GLN	2.7
2	H	1300	GLY	2.7
3	D	351	GLY	2.7
3	I	1130	GLY	2.7
3	D	716	GLN	2.7
3	I	1036	ARG	2.7
2	C	975	ILE	2.7
2	H	176	ILE	2.7
2	H	68	LEU	2.7
4	K	141	PHE	2.7
3	I	352	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
3	I	1124	ILE	2.7
2	H	149	LEU	2.7
1	G	101	THR	2.7
3	D	929	GLN	2.7
3	I	307	LEU	2.7
3	I	1255	VAL	2.7
1	B	197	ASP	2.7
2	C	1119	MET	2.7
3	D	775	SER	2.7
3	I	235	GLU	2.7
3	D	1323	ALA	2.7
1	B	188	GLU	2.7
2	H	404	LYS	2.7
1	B	113	ALA	2.6
1	B	186	ASN	2.6
2	H	579	ALA	2.6
4	K	133	MET	2.6
2	H	411	ARG	2.6
3	D	1078	LEU	2.6
4	J	117	GLN	2.6
1	F	189	ALA	2.6
2	C	112	GLY	2.6
3	I	528	THR	2.6
2	C	8	LYS	2.6
3	I	272	VAL	2.6
2	H	1074	GLY	2.6
2	H	1321	GLU	2.6
3	I	77	ARG	2.6
3	I	51	PRO	2.6
3	I	382	TYR	2.6
2	H	401	GLY	2.6
3	D	1156	LEU	2.6
4	J	129	GLU	2.6
2	H	251	ALA	2.6
2	C	807	TRP	2.6
1	A	137	ASN	2.6
2	C	543	ALA	2.6
2	C	1126	ASP	2.6
2	H	1141	LEU	2.6
3	D	373	ALA	2.6
3	D	456	ALA	2.6
3	I	351	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
3	I	1320	ILE	2.6
2	H	1305	TYR	2.6
1	G	182	ARG	2.6
2	H	934	PHE	2.6
3	I	901	ARG	2.6
3	I	1188	GLU	2.6
1	B	183	ILE	2.6
3	D	115	TRP	2.6
3	I	648	GLU	2.6
3	I	884	SER	2.6
2	C	430	LYS	2.6
2	H	527	LYS	2.6
1	G	232	VAL	2.6
2	H	1085	MET	2.6
3	D	587	LEU	2.6
3	D	1040	MET	2.6
2	C	79	VAL	2.6
2	H	659	GLN	2.6
2	H	722	GLY	2.6
3	D	73	GLY	2.6
3	D	1112	GLY	2.6
2	H	1143	GLU	2.6
3	D	1254	GLU	2.6
3	I	123	ARG	2.6
2	H	645	PHE	2.6
2	C	232	ILE	2.6
2	H	421	SER	2.6
3	I	52	GLU	2.6
3	I	1034	PHE	2.6
1	F	127	GLN	2.6
2	C	882	ILE	2.6
2	H	12[A]	ARG	2.6
2	C	417	SER	2.6
2	C	747	GLY	2.6
2	H	590	PRO	2.6
3	D	303	VAL	2.6
2	H	850	ILE	2.6
3	D	1352	ILE	2.6
3	I	281	ARG	2.6
2	H	400	VAL	2.6
2	C	536	GLY	2.6
2	C	909	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
3	D	121	PRO	2.6
2	H	1252	SER	2.6
2	H	245	ARG	2.6
3	I	837	ASP	2.6
2	C	276	GLN	2.6
4	K	107	GLU	2.6
2	H	1292	THR	2.6
3	I	129	ASP	2.6
2	H	268	ARG	2.5
1	B	78	ILE	2.5
3	D	68	TYR	2.5
3	D	744	ARG	2.5
1	G	97	GLU	2.5
2	H	224	PHE	2.5
1	G	120	ASP	2.5
3	I	1157	ALA	2.5
3	D	103	GLY	2.5
3	I	233	LYS	2.5
3	I	649	LYS	2.5
3	I	861	ASN	2.5
3	D	120	LEU	2.5
3	D	442	ILE	2.5
1	G	63	GLY	2.5
2	C	467	GLY	2.5
2	C	963	GLU	2.5
3	D	419	HIS	2.5
3	I	588	PRO	2.5
2	C	716	ALA	2.5
3	D	494	ALA	2.5
3	I	1038	THR	2.5
2	C	240	GLU	2.5
3	D	639	VAL	2.5
3	D	1092	GLY	2.5
3	D	1202	GLU	2.5
3	I	185	ILE	2.5
2	C	938	GLY	2.5
2	C	1048	LYS	2.5
3	D	1192	LYS	2.5
2	C	1222	GLU	2.5
2	H	182	SER	2.5
2	C	451	ARG	2.5
1	F	10	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
3	D	885	VAL	2.5
2	C	7	GLU	2.5
3	D	1327	GLU	2.5
4	K	39	PHE	2.5
4	K	127	LEU	2.5
2	C	1080	ASN	2.5
2	H	581	THR	2.5
3	I	93	THR	2.5
2	C	482	GLY	2.5
2	C	534	GLY	2.5
2	H	833	ILE	2.5
3	D	1032	SER	2.5
3	I	1307	LEU	2.5
1	A	96	ASP	2.5
2	H	153	PRO	2.5
2	H	834	GLN	2.5
2	H	1139	ALA	2.5
2	C	456	VAL	2.5
2	H	229	ILE	2.5
3	D	988	PHE	2.5
3	I	383	GLY	2.5
2	C	354	ASP	2.5
2	C	378	ARG	2.5
2	C	587	LEU	2.5
2	H	409	LEU	2.5
2	H	1126	ASP	2.5
3	I	1201	GLY	2.5
1	F	13	LEU	2.5
3	D	136	GLU	2.5
3	I	1017	VAL	2.5
1	A	196	THR	2.5
1	B	70	THR	2.5
2	H	175	ARG	2.5
3	D	377	PHE	2.5
3	D	531	LYS	2.5
3	I	101	ARG	2.5
1	A	117	HIS	2.5
2	C	286	GLU	2.5
2	H	530	ILE	2.5
3	D	175	GLU	2.5
3	D	800	LEU	2.5
2	C	351	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	H	1079	ILE	2.5
3	D	468	VAL	2.5
2	C	1177	ARG	2.5
3	D	822	MET	2.5
3	I	547	ARG	2.5
2	H	335	THR	2.5
1	F	220	ALA	2.5
2	H	474	ALA	2.5
2	H	1230	MET	2.5
3	I	839	VAL	2.5
3	I	1059	LEU	2.5
2	C	544	GLY	2.5
3	I	1297	LYS	2.5
2	H	1320	PRO	2.5
2	C	352	ARG	2.5
3	D	901	ARG	2.5
3	D	240	THR	2.5
4	J	141	PHE	2.5
2	C	877	VAL	2.5
2	C	900	LYS	2.5
1	G	198	LEU	2.5
2	C	699	LEU	2.5
3	D	788	LEU	2.5
2	C	419	ILE	2.4
2	H	1089	GLU	2.4
3	D	610	ARG	2.4
3	D	1052	GLU	2.4
2	C	752	ASN	2.4
3	D	793	SER	2.4
4	J	114	ARG	2.4
2	C	494	ASN	2.4
1	F	173	VAL	2.4
1	A	171	LEU	2.4
2	C	927	THR	2.4
3	D	755	ILE	2.4
2	H	7	GLU	2.4
1	G	69	SER	2.4
3	D	411	ILE	2.4
3	D	928	THR	2.4
3	D	1106	ILE	2.4
3	I	120	LEU	2.4
3	I	464	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
4	J	40	GLY	2.4
1	A	203	ILE	2.4
3	D	1060	VAL	2.4
4	K	89	VAL	2.4
3	D	469	HIS	2.4
3	D	1358	PRO	2.4
2	C	850	ILE	2.4
3	I	967	VAL	2.4
2	C	153	PRO	2.4
3	I	250	ARG	2.4
1	A	127	GLN	2.4
1	B	19	VAL	2.4
2	H	1268	GLN	2.4
3	I	353	SER	2.4
3	I	448	GLN	2.4
3	I	864	LEU	2.4
1	G	151	GLY	2.4
3	I	1222	ARG	2.4
2	C	599	VAL	2.4
3	I	1003	LEU	2.4
2	H	1140	LYS	2.4
3	I	792	ASN	2.4
2	H	424	ASP	2.4
2	H	1214	ASP	2.4
3	D	186	GLN	2.4
1	A	28	LEU	2.4
2	C	411	ARG	2.4
2	H	1298	VAL	2.4
3	I	550	VAL	2.4
2	H	1263	ALA	2.4
3	D	1077	ALA	2.4
2	C	876	GLU	2.4
1	A	20	SER	2.4
2	C	1125	GLY	2.4
2	H	1273	MET	2.4
2	C	119	GLU	2.4
2	H	643	SER	2.4
2	H	709	ALA	2.4
1	A	151	GLY	2.4
2	C	481	LEU	2.4
2	C	298	ALA	2.4
1	B	228	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	254	ASP	2.4
3	I	67	ASP	2.4
1	A	229	GLU	2.4
3	I	1080	ILE	2.4
1	B	137	ASN	2.4
2	C	234	ASP	2.4
1	G	126	PRO	2.4
2	H	110	PRO	2.4
3	I	1261	LEU	2.4
2	H	13	LYS	2.4
3	D	884	SER	2.4
3	I	501	VAL	2.4
1	F	99	ILE	2.4
2	C	589	THR	2.4
2	H	764	CYS	2.4
3	D	1173	ARG	2.4
3	D	138	VAL	2.4
3	D	1351	VAL	2.4
4	J	80	TRP	2.4
3	D	384	LYS	2.4
2	C	974	ARG	2.4
3	I	1026	PRO	2.4
1	A	201	LEU	2.4
3	D	850	LYS	2.4
2	C	757	THR	2.4
2	H	235	ASN	2.4
4	J	181	ALA	2.4
2	C	390	PHE	2.3
3	D	918	ILE	2.3
2	C	1309	VAL	2.3
3	I	705	THR	2.3
1	A	90	VAL	2.3
1	B	52	PRO	2.3
2	H	1250	SER	2.3
1	B	150	ARG	2.3
3	D	634	ARG	2.3
3	I	907	HIS	2.3
2	C	790	ASP	2.3
3	I	639	VAL	2.3
2	H	1093	PRO	2.3
2	H	59	ILE	2.3
3	D	208	THR	2.3

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Mol	Chain	Res	Type	RSRZ
3	I	1031	VAL	2.3
2	C	620	ASN	2.3
2	C	1236	ASN	2.3
2	H	518	ASN	2.3
3	D	864	LEU	2.3
3	D	1138	LEU	2.3
3	I	289	ASP	2.3
4	J	18	PHE	2.3
2	C	285	ILE	2.3
2	H	88	ARG	2.3
2	H	856	ASN	2.3
2	H	1245	ALA	2.3
2	H	292	ILE	2.3
1	A	31	LEU	2.3
1	F	146	VAL	2.3
2	C	78	PRO	2.3
2	H	120	GLN	2.3
2	C	493	ILE	2.3
4	J	132	GLU	2.3
1	G	94	GLY	2.3
1	G	197	ASP	2.3
2	C	214	ASN	2.3
2	C	268	ARG	2.3
3	I	1145	PHE	2.3
2	C	52	ALA	2.3
2	C	283	LYS	2.3
2	C	464	PHE	2.3
2	H	977	ALA	2.3
2	H	1220	GLN	2.3
2	H	114	VAL	2.3
1	F	211	ILE	2.3
2	C	865	LEU	2.3
2	C	1273	MET	2.3
1	G	124	VAL	2.3
2	H	318	SER	2.3
2	H	748	ILE	2.3
3	D	406	ALA	2.3
1	A	206	GLU	2.3
2	H	184	LEU	2.3
2	H	552	PRO	2.3
2	C	1143	GLU	2.3
2	C	521	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	347	ILE	2.3
3	I	183	GLU	2.3
3	I	722	ILE	2.3
2	C	159	SER	2.3
2	H	800	MET	2.3
3	I	287	ALA	2.3
4	J	157	ARG	2.3
4	K	168	ALA	2.3
3	D	635	SER	2.3
3	I	57	PHE	2.3
2	H	270	THR	2.3
3	D	269	TYR	2.3
2	C	1117	LEU	2.3
3	I	640	GLY	2.3
2	C	973	SER	2.3
3	I	961	SER	2.3
1	B	82	LEU	2.3
1	B	134	THR	2.3
3	I	1249	ASN	2.3
3	D	97	VAL	2.3
2	H	296	VAL	2.2
1	B	11	PRO	2.2
1	B	74	VAL	2.2
1	G	68	TYR	2.2
3	I	71	LEU	2.2
3	D	412	LEU	2.2
3	D	1195	GLN	2.2
2	C	245	ARG	2.2
2	C	639	LYS	2.2
2	C	238	GLN	2.2
1	B	182	ARG	2.2
2	H	647	ARG	2.2
3	D	77	ARG	2.2
3	I	530	PRO	2.2
1	G	131	CYS	2.2
2	C	24	VAL	2.2
4	K	74	VAL	2.2
1	A	194	GLN	2.2
2	C	937	ASP	2.2
2	C	1086	PRO	2.2
3	D	1194	ARG	2.2
3	I	1193	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	192	VAL	2.2
2	C	700	VAL	2.2
3	I	721	SER	2.2
4	J	71	VAL	2.2
4	J	137	ASN	2.2
2	H	22	LEU	2.2
3	I	870	ASP	2.2
3	I	232	ASN	2.2
2	C	1057	LYS	2.2
2	C	1205	PRO	2.2
2	H	784	ALA	2.2
3	I	754	ILE	2.2
3	I	800	LEU	2.2
3	I	1213	GLY	2.2
1	B	47	LEU	2.2
1	G	194	GLN	2.2
2	C	275	ARG	2.2
3	D	856	ILE	2.2
1	G	195	ARG	2.2
2	C	236	LYS	2.2
4	K	91	GLY	2.2
2	C	213	LEU	2.2
2	C	399	ALA	2.2
2	C	899	GLU	2.2
3	D	743	MET	2.2
3	D	830	ASP	2.2
4	J	15	PHE	2.2
2	C	895	LEU	2.2
2	H	479	LEU	2.2
2	H	450	ASN	2.2
2	H	928	VAL	2.2
3	D	1334	GLU	2.2
3	I	50	LYS	2.2
3	D	899	TYR	2.2
1	A	213	PRO	2.2
2	H	449	GLY	2.2
3	D	968	ASN	2.2
1	A	26	VAL	2.2
2	H	144	VAL	2.2
1	B	122	GLU	2.2
1	B	218	ARG	2.2
1	F	94	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	186	ASN	2.2
3	D	650	LYS	2.2
2	H	395	TYR	2.2
3	I	166	LEU	2.2
1	A	131	CYS	2.2
1	A	15	ASP	2.2
1	B	204	GLU	2.2
2	H	1255	THR	2.2
3	D	301	GLU	2.2
3	D	495	ASN	2.2
1	G	216	ALA	2.2
2	H	337	PHE	2.2
3	I	113	HIS	2.2
3	I	139	LEU	2.2
2	H	919	ARG	2.2
3	D	1333	THR	2.2
2	H	588	GLU	2.2
3	I	998	PRO	2.2
3	I	1013	GLY	2.2
1	A	18	GLN	2.2
2	C	83	GLN	2.2
1	A	158	ARG	2.2
1	F	193	GLU	2.2
1	G	106	GLY	2.2
3	D	405	GLU	2.2
3	I	498	PRO	2.2
3	I	1217	PRO	2.2
1	B	189	ALA	2.2
4	J	110	ALA	2.2
3	D	1130	GLY	2.1
3	I	1046	ILE	2.2
1	B	120	ASP	2.1
2	C	231	GLU	2.1
2	C	608	ALA	2.1
3	I	76	LYS	2.1
2	C	839	VAL	2.1
2	H	473	ARG	2.1
3	D	105	ILE	2.1
3	D	1132	LYS	2.1
3	I	761	ALA	2.1
1	F	39	LEU	2.1
2	C	75	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	186	PHE	2.1
2	H	587	LEU	2.1
2	H	857	VAL	2.1
2	C	1341	ASP	2.1
3	D	416	ILE	2.1
3	D	1305	ASP	2.1
3	I	621	ALA	2.1
1	A	67	GLU	2.1
2	C	58	PRO	2.1
2	C	356	THR	2.1
3	I	499	ILE	2.1
2	H	526	HIS	2.1
3	D	446	ALA	2.1
2	H	236	LYS	2.1
2	C	48	GLY	2.1
2	H	770	CYS	2.1
3	I	1224	ARG	2.1
2	H	1253	LEU	2.1
3	D	1097	ALA	2.1
2	H	1226	THR	2.1
2	H	1286	THR	2.1
3	D	1044	GLN	2.1
2	H	712	SER	2.1
1	G	79	LEU	2.1
1	G	80	GLU	2.1
4	K	28	GLU	2.1
2	C	154	GLY	2.1
2	C	1055	ALA	2.1
2	H	1309	VAL	2.1
3	D	820	ILE	2.1
1	G	64	VAL	2.1
2	H	1056	VAL	2.1
1	G	37	HIS	2.1
2	C	241	LEU	2.1
2	C	1054	LEU	2.1
3	I	533	ALA	2.1
1	B	108	GLY	2.1
2	C	14	ASP	2.1
3	I	1119	ASP	2.1
2	C	6	THR	2.1
2	C	261	VAL	2.1
2	C	389	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	228	VAL	2.1
2	H	238	GLN	2.1
2	H	861	ALA	2.1
3	D	415	VAL	2.1
3	D	883	ARG	2.1
1	F	71	LYS	2.1
2	H	1055	ALA	2.1
3	D	98	ARG	2.1
2	C	1100	PRO	2.1
2	H	1213	TYR	2.1
1	A	32	GLU	2.1
1	A	197	ASP	2.1
2	C	519	ASN	2.1
2	H	269	ILE	2.1
3	I	1198	VAL	2.1
2	C	539	THR	2.1
2	H	1144	PHE	2.1
2	C	917	SER	2.1
3	I	942	SER	2.1
3	D	106	GLU	2.1
3	D	250	ARG	2.1
1	F	109	PRO	2.1
3	I	234	PRO	2.1
2	H	1145	ILE	2.1
4	K	36	GLU	2.1
1	G	205	MET	2.1
2	H	756	TYR	2.1
3	D	102	MET	2.1
1	B	200	LYS	2.1
1	G	26	VAL	2.1
3	D	1353	VAL	2.1
2	C	803	ALA	2.1
3	I	136	GLU	2.1
2	H	846	GLY	2.0
3	I	669	GLN	2.0
2	H	425	ILE	2.0
3	D	584	PRO	2.0
2	C	1279	GLU	2.0
2	H	721	GLY	2.0
3	D	329	ASP	2.0
1	G	17	GLU	2.0
3	D	1196	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
3	I	866	GLU	2.0
2	H	1073	LYS	2.0
2	H	894	GLN	2.0
3	D	374	LEU	2.0
1	A	30	PRO	2.0
2	H	351	LEU	2.0
1	B	110	VAL	2.0
3	I	885	VAL	2.0
1	G	58	GLU	2.0
2	C	59	ILE	2.0
2	C	412	GLU	2.0
2	H	982	GLY	2.0
3	D	182	ALA	2.0
3	D	1125	PRO	2.0
3	D	202	ARG	2.0
3	I	916	GLY	2.0
3	D	720	ASN	2.0
4	J	108	VAL	2.0
2	H	749	ASP	2.0
3	D	413	ASP	2.0
2	C	949	GLU	2.0
3	D	183	GLU	2.0
2	C	282	VAL	2.0
1	B	159	ILE	2.0
2	C	896	THR	2.0
3	I	647	PRO	2.0
3	I	908	ILE	2.0
3	I	1010	GLN	2.0
3	I	713	GLU	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 carbohydrates 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.