Full wwPDB EM Validation Report (i)

Aug 5, 2026 – 08:28 AM EDT

PDB ID	:	7ML1 / pdb_00007ml1
EMDB ID	:	EMD-23905
Title	:	RNA polymerase II pre-initiation complex (PIC2)
Authors	:	Yang, C.; Fujiwara, R.; Kim, H.J.; Gorbea Colon, J.J.; Steimle, S.; Garcia, B.A.; Murakami, K.
Deposited on	:	2021-04-27
Resolution	:	4.00 Å(reported)
Based on initial model	:	5OQJ

This is a Full wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

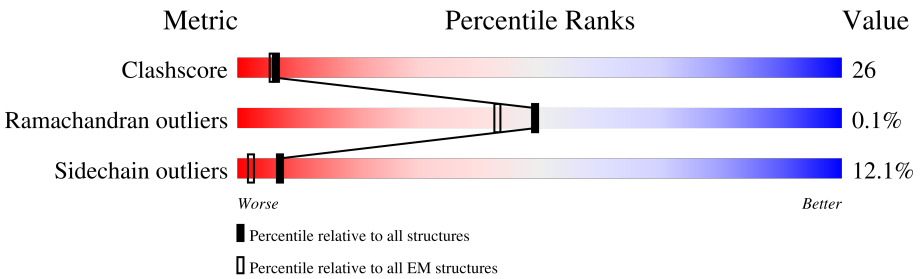
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

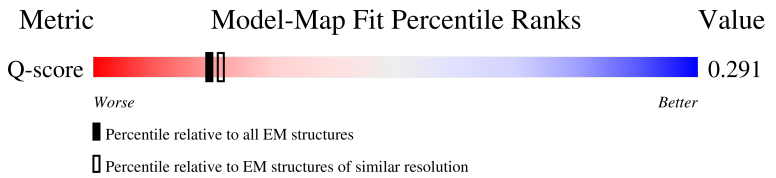
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	542	17% 37% 27% • 32%
2	4	338	9% 39% 39% 6% 16%
3	0	778	20% 32% 58% 8% •
4	6	461	7% 29% 40% 7% 24%

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Mol	Chain	Length	Quality of chain
5	2	513	9% 48% 35% 7% 10%
6	5	72	17% 25% 51% 15% 8%
7	7	843	15% 27% 39% 9% 25%
8	3	321	38% 28% 14% • 57%
9	O	240	42% 40% 34% • 25%
10	N	57	26% 30% 70%
11	T	57	23% 74% 26%
12	A	1733	• 45% 31% • 19%
13	B	1224	• 54% 36% • 6%
14	C	318	54% 25% • 18%
15	D	221	23% 30% 37% • 29%
16	E	215	45% 48% 6% •
17	F	155	34% 17% • 46%
18	G	171	12% 43% 51% 6%
19	H	146	• 46% 39% 8% • 7%
20	I	122	13% 49% 43% • 5%
21	J	70	• 46% 37% 10% 7%
22	K	120	10% 53% 38% • 7%
23	L	70	7% 27% 29% 9% 36%
24	M	345	42% 41% 36% • 19%
25	Q	735	• 12% 7% • 80%
26	R	400	15% 31% 15% • 52%
27	U	286	15% 6% 9% 85%
28	V	122	40% 23% 15% • 59%
29	W	482	20% 20% 19% • 60%

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Mol	Chain	Length	Quality of chain
30	X	328	25% 38% 9% • 52%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	SF4	0	801	-	-	X	-

2 Entry composition (i)

There are 33 unique types of molecules in this entry. The entry contains 64538 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Tfb1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	367	2411	1536	438	430	7	0	0

- Molecule 2 is a protein called General transcription and DNA repair factor IIH subunit TFB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	4	284	2041	1310	343	376	12	0	0

- Molecule 3 is a protein called General transcription and DNA repair factor IIH helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	0	754	6108	3891	1032	1147	38	0	0

- Molecule 4 is a protein called General transcription and DNA repair factor IIH subunit SSL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	6	351	2527	1590	454	456	27	0	0

- Molecule 5 is a protein called RNA polymerase II transcription factor B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	2	460	3011	1856	562	584	9	0	0

- Molecule 6 is a protein called General transcription and DNA repair factor IIH subunit TFB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	66	498	314	89	93	2	0	0

- Molecule 7 is a protein called General transcription and DNA repair factor IIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	7	634	4447	2722	827	874	24	0	0

- Molecule 8 is a protein called BJ4_G0050160.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	3	138	860	533	160	160	7	0	0

- Molecule 9 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	O	180	1416	921	242	247	6	0	0

- Molecule 10 is a DNA chain called non-template strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
10	N	57	1178	562	227	332	57	0	0

- Molecule 11 is a DNA chain called template strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
11	T	57	1159	559	191	352	57	0	0

- Molecule 12 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	A	1398	10997	6931	1927	2078	61	0	0

- Molecule 13 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	B	1147	9132	5775	1602	1700	55	0	0

- Molecule 14 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	C	262	2061	1299	343	406	13	0	0

- Molecule 15 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	D	157	1253	779	220	252	2	0	0

- Molecule 16 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	E	213	1744	1107	308	318	11	0	0

- Molecule 17 is a protein called DNA-directed RNA polymerases I,II,and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	F	83	670	428	114	125	3	0	0

- Molecule 18 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	G	171	1340	861	222	249	8	0	0

- Molecule 19 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	H	136	1089	686	184	215	4	0	0

- Molecule 20 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	I	116	944	581	172	181	10	0	0

- Molecule 21 is a protein called DNA-directed RNA polymerases II subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	J	65	532	339	93	94	6	0	0

- Molecule 22 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	K	112	904	580	154	168	2	0	0

- Molecule 23 is a protein called DNA-directed RNA polymerases II subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	L	45	358	221	71	62	4	0	0

- Molecule 24 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	M	279	2175	1382	373	403	17	0	0

- Molecule 25 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Q	148	1144	733	195	212	4	0	0

- Molecule 26 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	R	190	1303	812	238	246	7	0	0

- Molecule 27 is a protein called Transcription initiation factor IIA large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	U	44	366	233	64	66	3	0	0

- Molecule 28 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	V	50	389	245	65	76	3	0	0

- Molecule 29 is a protein called Transcription initiation factor IIE subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	W	191	1469	932	254	277	6	0	0

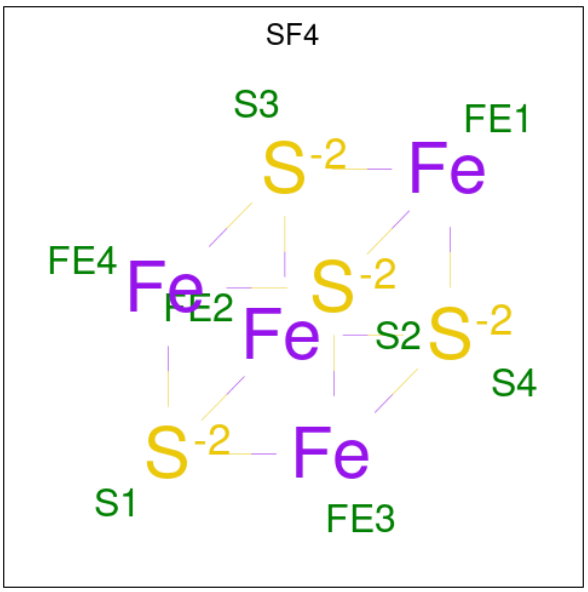
- Molecule 30 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	X	156	984	608	180	192	4	0	0

- Molecule 31 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
31	4	1	1	1	0
31	6	4	4	4	0
31	3	2	2	2	0
31	A	3	3	3	0
31	B	1	1	1	0
31	C	1	1	1	0
31	I	2	2	2	0
31	J	1	1	1	0
31	L	1	1	1	0
31	M	1	1	1	0
31	W	1	1	1	0
31	X	1	1	1	0

- Molecule 32 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
32	0	1	8	4	4	0

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

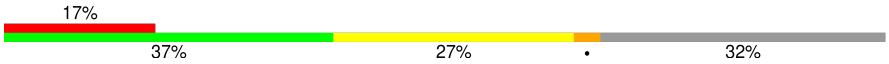
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
33	A	1	1	1	0

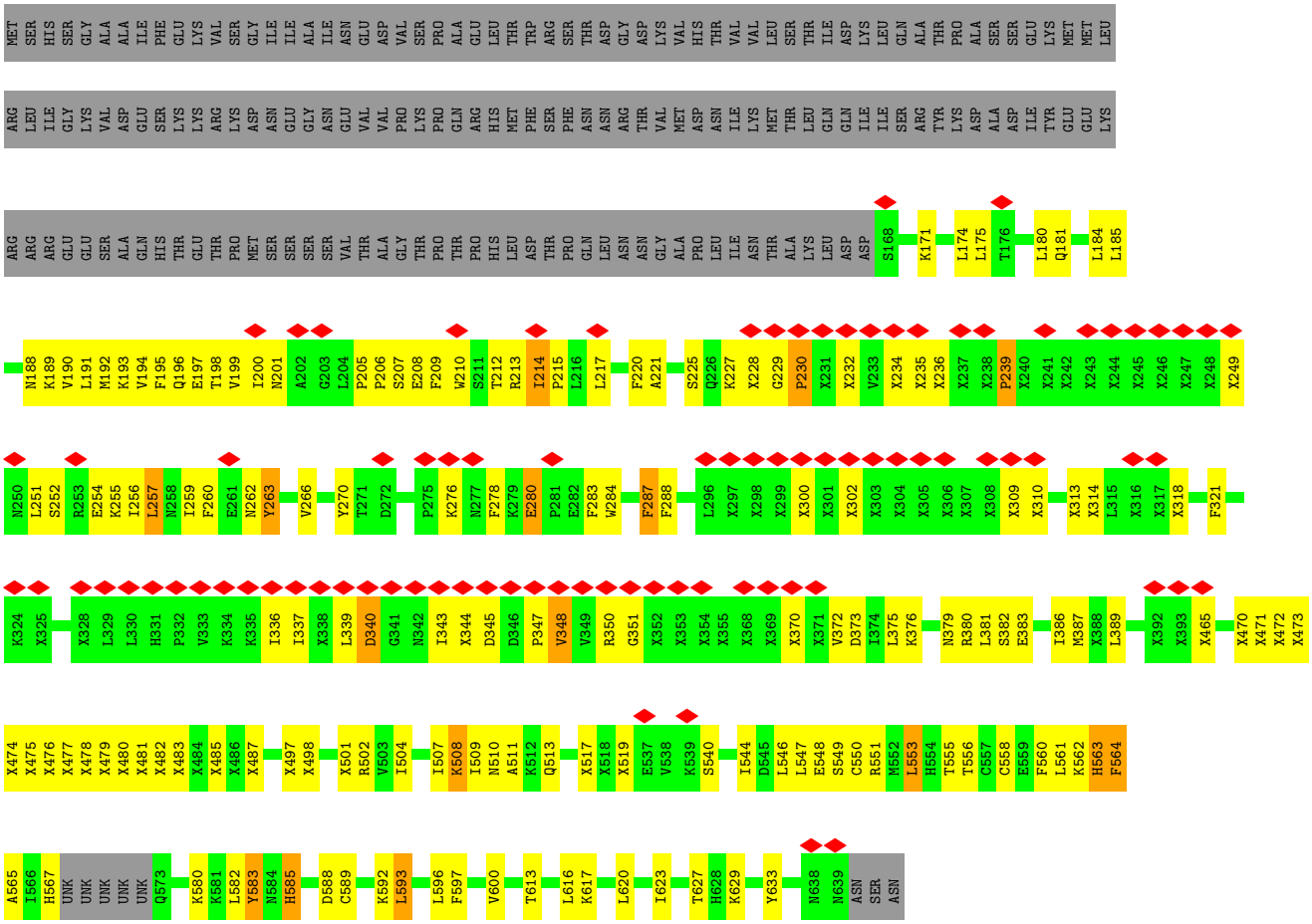
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Tfb1

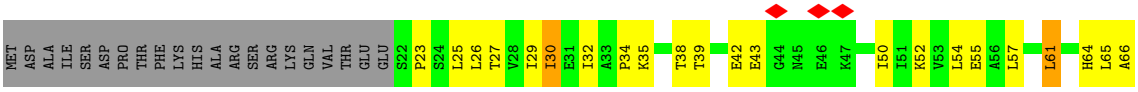
Chain 1:

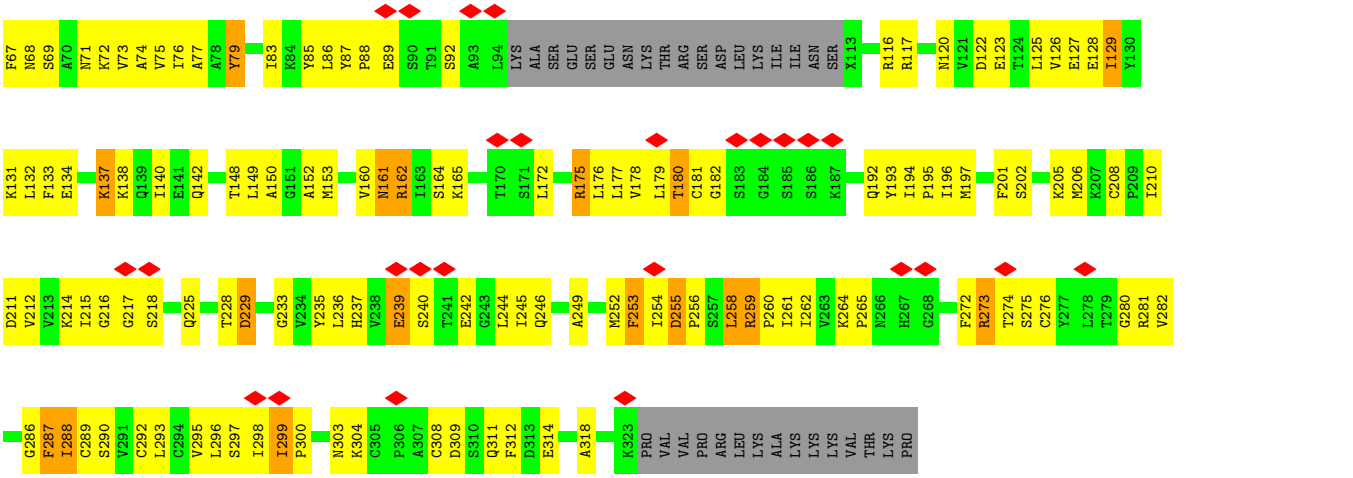




- Molecule 2: General transcription and DNA repair factor IIH subunit TFB4

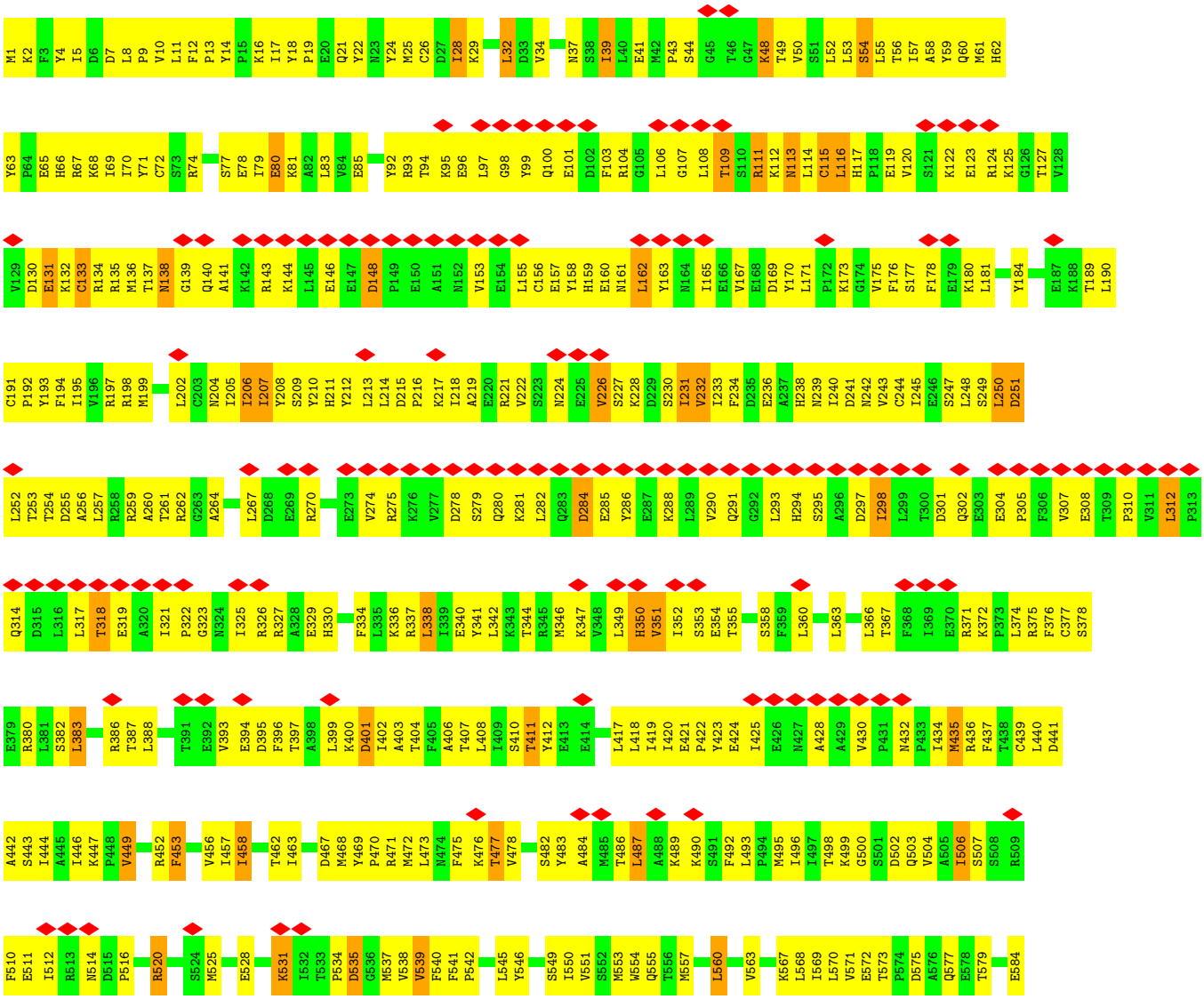
Chain 4:

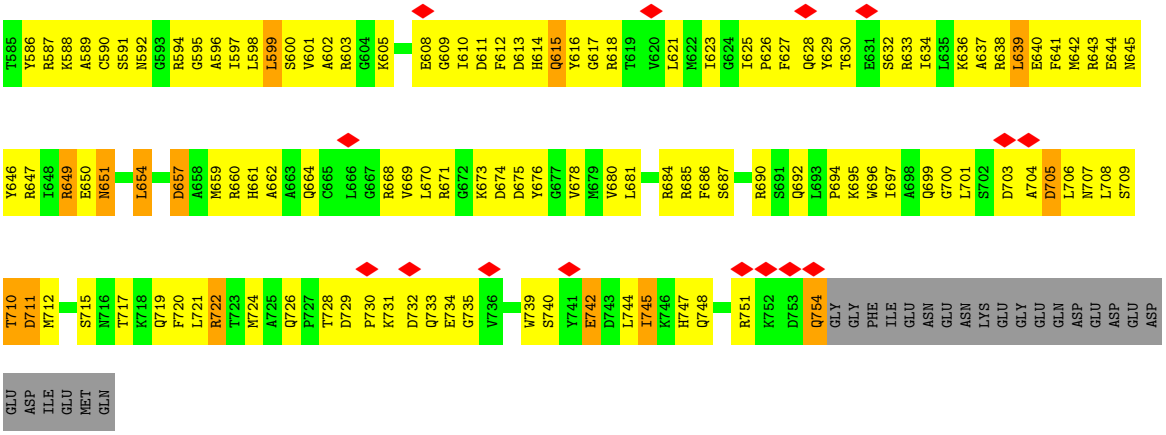




• Molecule 3: General transcription and DNA repair factor IIH helicase subunit XPD

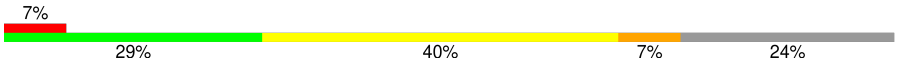
Chain 0:

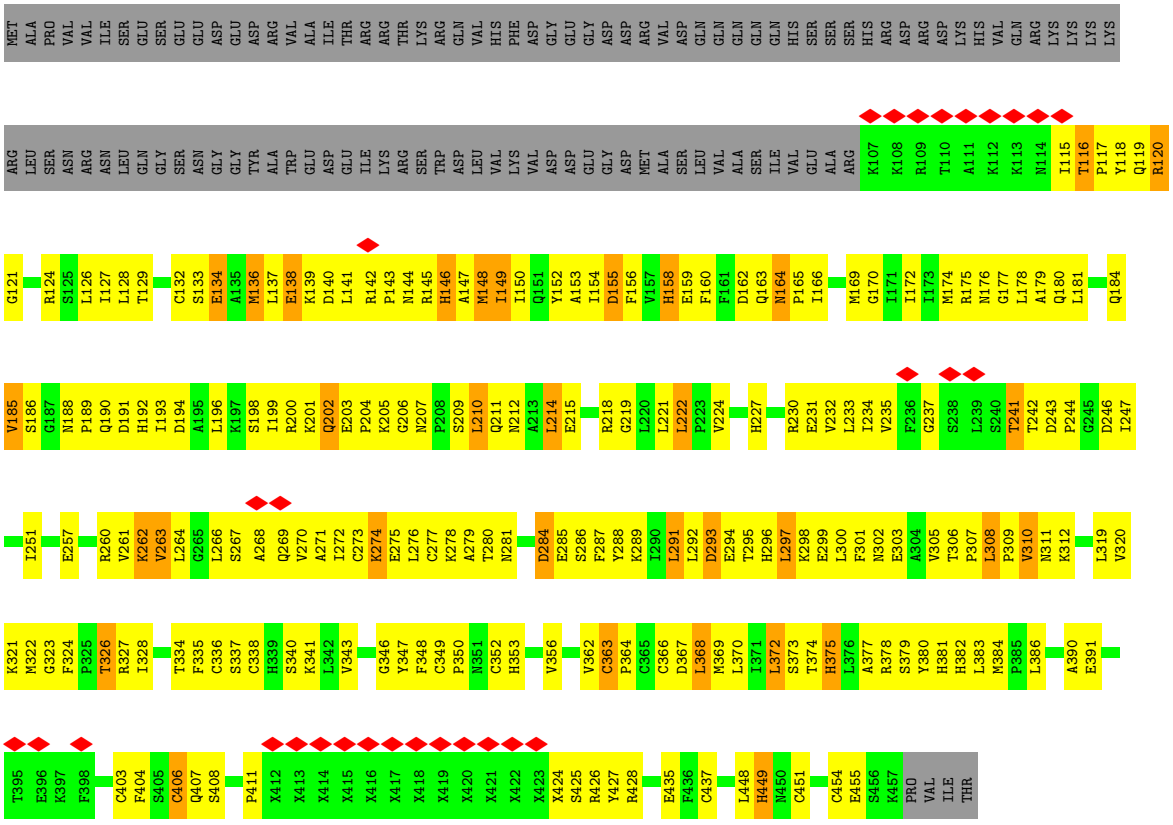




• Molecule 4: General transcription and DNA repair factor IIH subunit SSL1

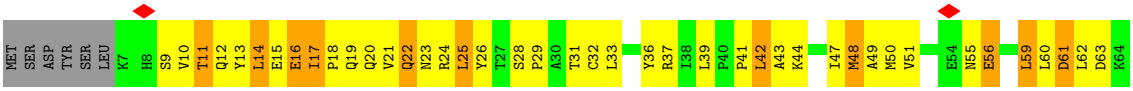
Chain 6:

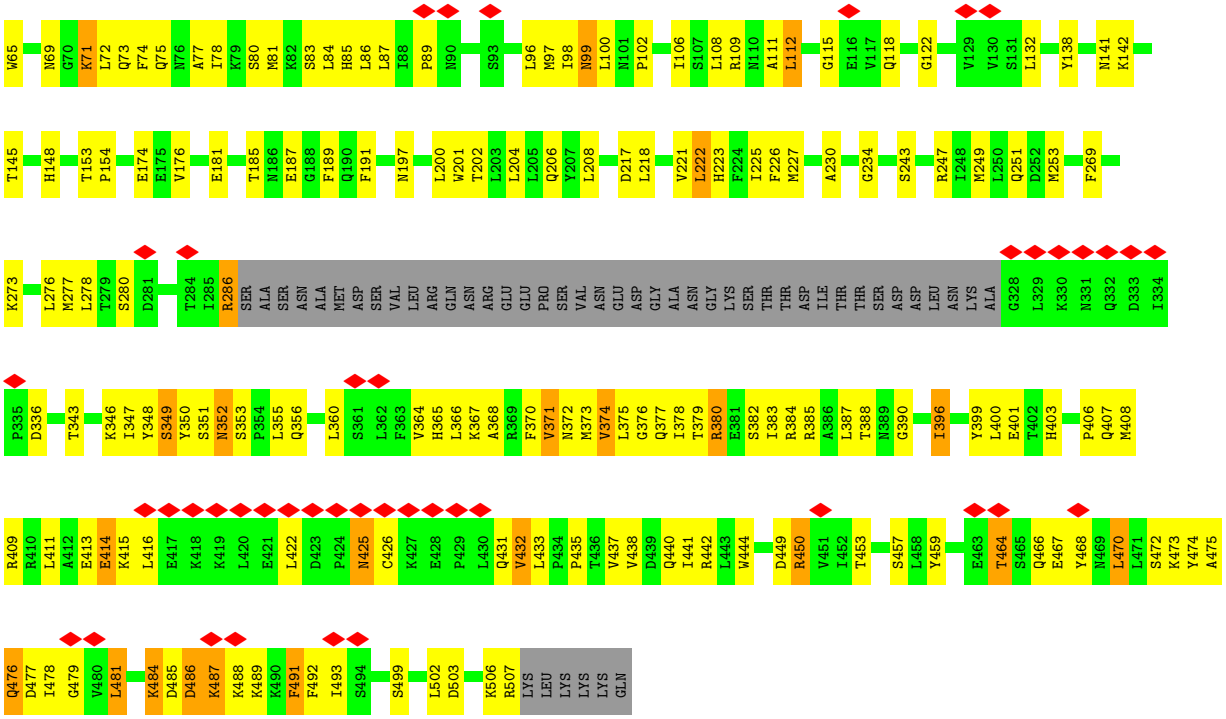




• Molecule 5: RNA polymerase II transcription factor B subunit 2

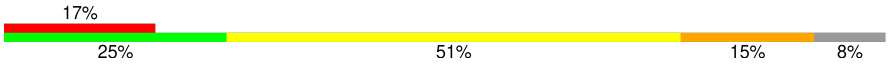
Chain 2:

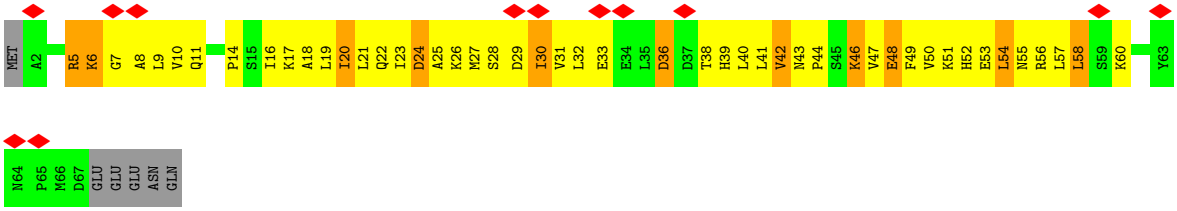




- Molecule 6: General transcription and DNA repair factor IIH subunit TFB5

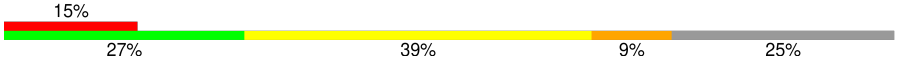
Chain 5:

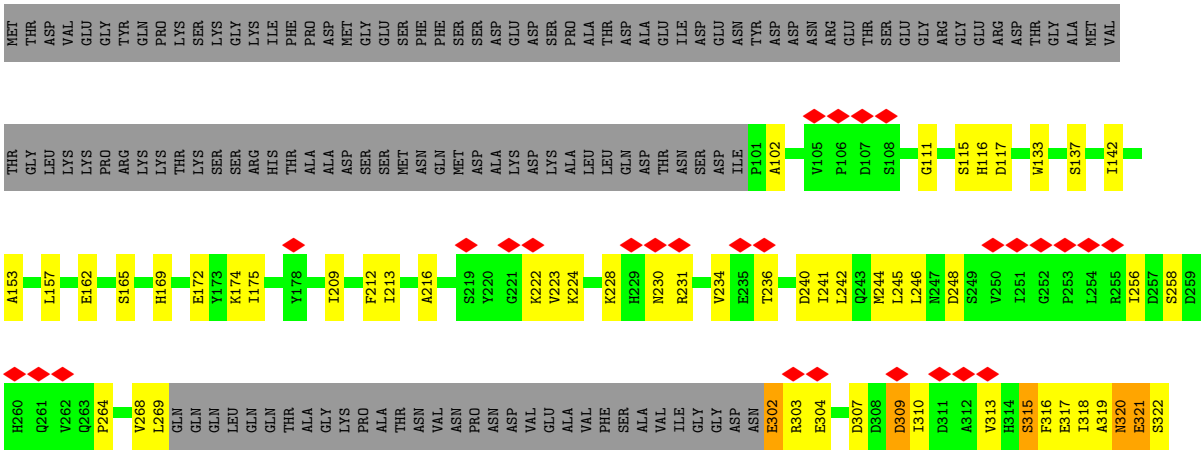


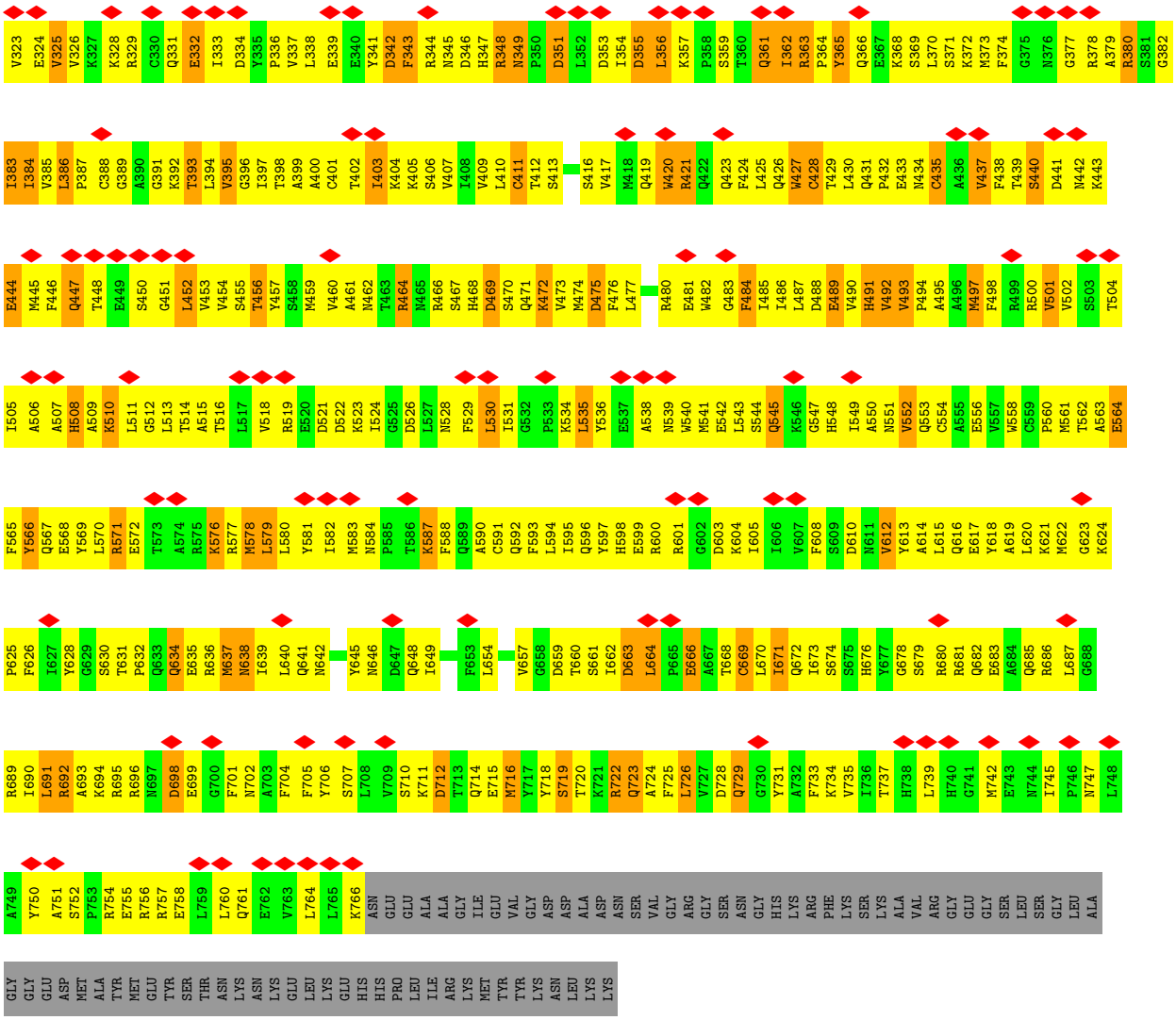


- Molecule 7: General transcription and DNA repair factor IIH helicase subunit XPB

Chain 7:

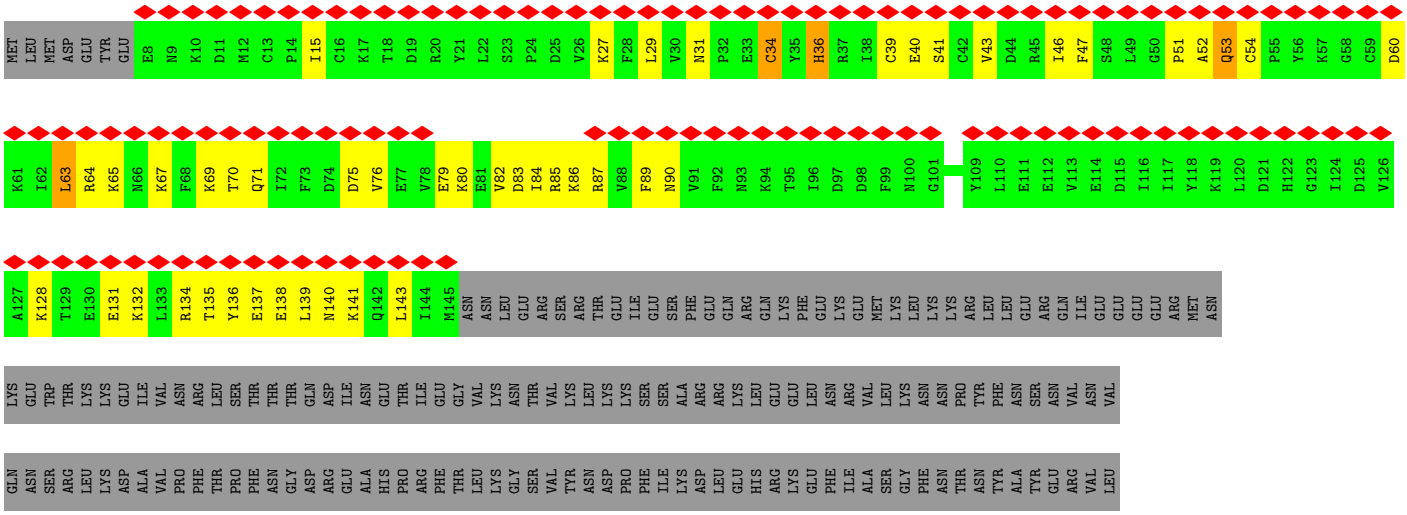


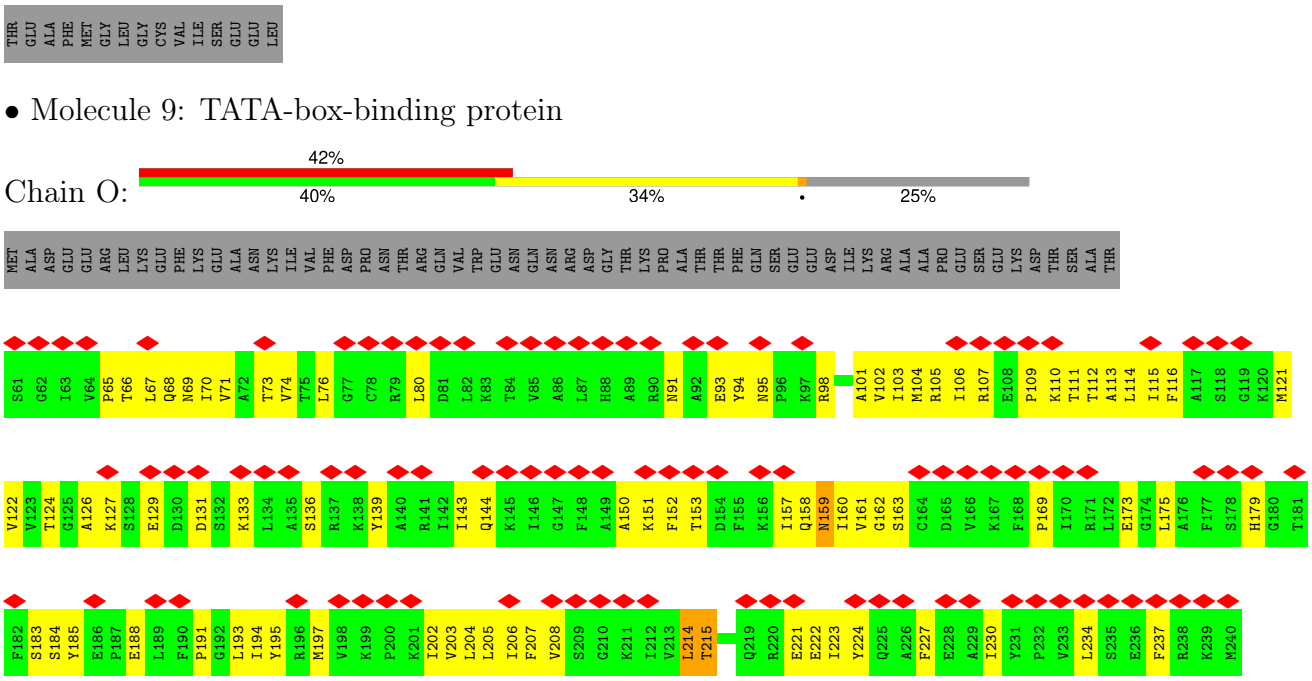


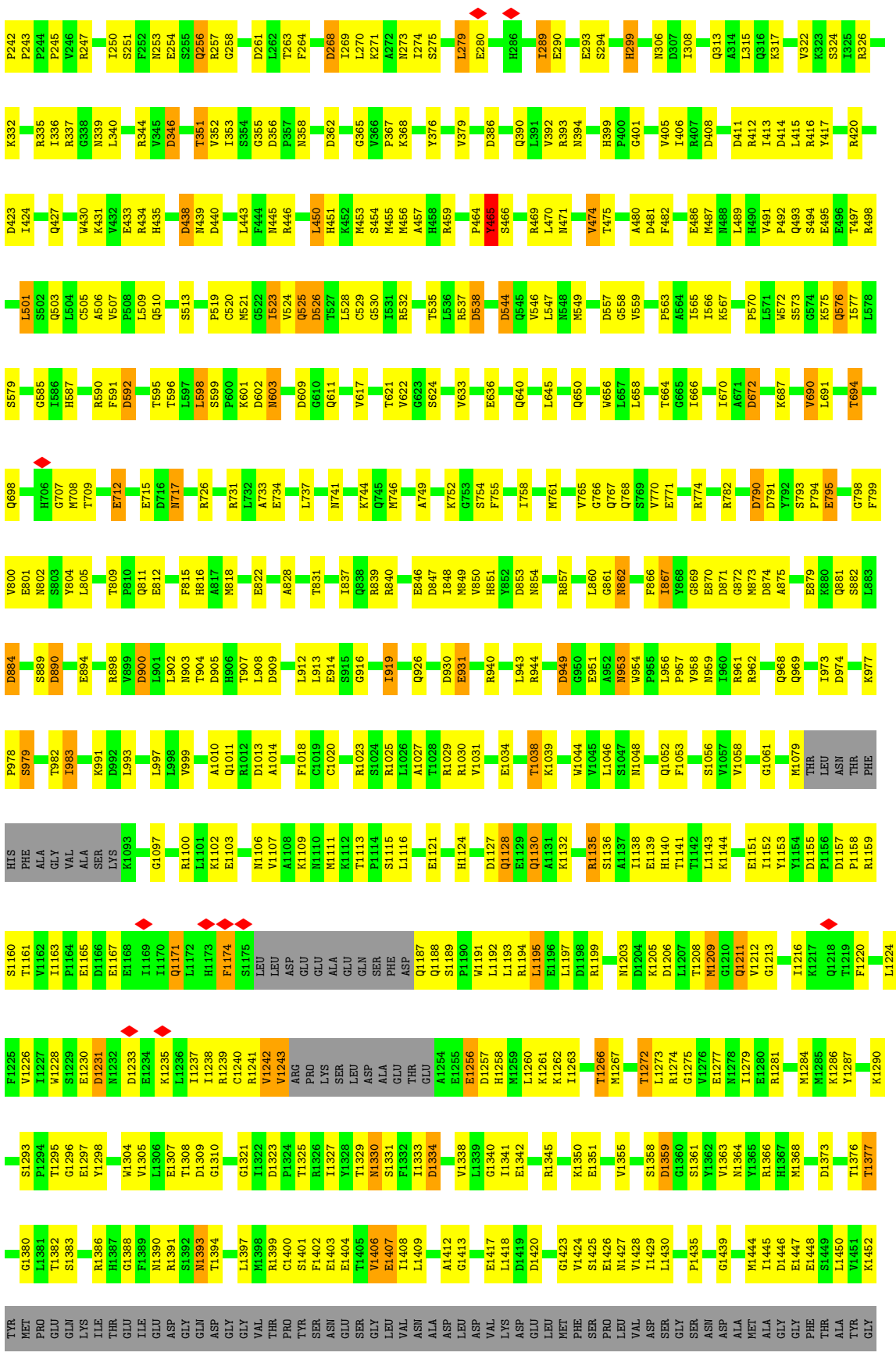


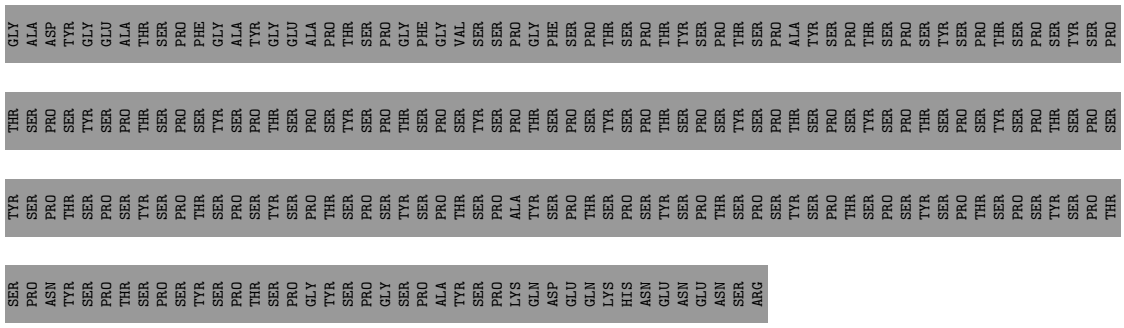
- Molecule 8: BJ4_G0050160.mRNA.1.CDS.1

Chain 3:



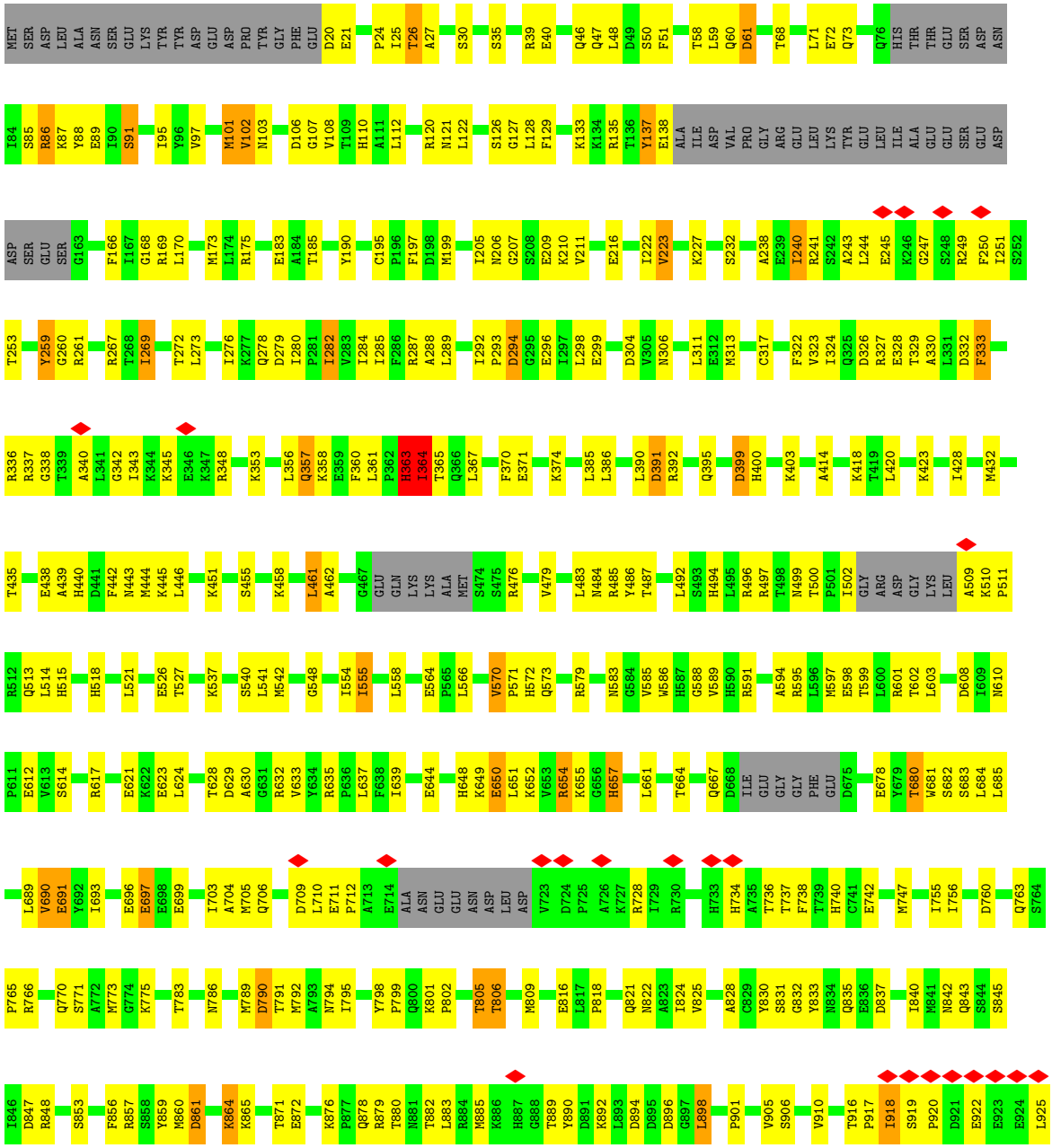

THR GLU ALA PHE MET GLY LEU GLY CYS VAL ILE SER GLU GLU LEU
• Molecule 9: TATA-box-binding protein
Chain O:
42%
40%
34%
25%
MET ALA ASP GLU GLU ARG LEU LYS GLU PHE LYS GLU ALA ASN LYS ILE VAL PHE ASP PRO ASN THR ARG GLN VAL TRP GLU ASN GLN ASN ARG ASP GLY THR LYS PRO ALA THR THR PHE GLN SER GLU GLU ASP ILE LYS ARG ALA ALA PRO GLU SER GLU LYS ASP THR SER ALA THR
S61 G62 I63 V64 P65 T66 L67 Q68 N69 I70 V71 A72 T73 V74 T75 L76 G77 C78 R79 L80 D81 L82 K83 T84 V85 A86 L87 H88 A89 R90 N91 A92 E93 Y94 N95 P96 K97 R98 A101 V102 I103 M104 R105 I106 R107 E108 P109 K110 T111 T112 A113 L114 I115 F116 A117 S118 G119 K120 M121
V122 V123 T124 G125 A126 K127 S128 E129 D130 D131 S132 K133 L134 A135 S136 R137 K138 Y139 A140 R141 I142 I143 Q144 K145 I146 G147 F148 A149 A150 K151 F152 T153 D154 F155 K156 I157 Q158 N159 I160 V161 G162 S163 C164 D165 V166 K167 F168 P169 I170 R171 L172 E173 G174 L175 A176 F177 S178 H179 G180 T181
F182 S183 S184 Y185 E186 P187 E188 L189 F190 P191 G192 L193 I194 Y195 R196 M197 V198 K199 P200 K201 I202 V203 L204 L205 I206 F207 V208 S209 G210 K211 I212 V213 L214 T215 Q219 R220 E221 E222 I223 Y224 Q225 A226 F227 E228 A229 I230 Y231 P232 V233 L234 S235 E236 F237 R238 K239 M240
• Molecule 10: non-template strand DNA
Chain N:
26%
30%
70%
A2 A3 A4 A5 A6 A7 A8 A9 A10 A11 G12 G13 C14 G15 C16 G17 T20 A21 T22 A23 A24 A25 A26 G27 T28 T29 T30 C31 A32 A33 T34 G35 T36 C37 G38 C39 G40 A41 A42 T43 T44 C45 G46 G47 G50 T51 T55 A56 C57 A58
• Molecule 11: template strand DNA
Chain T:
23%
74%
26%
T108 C120 T124 A130 C131 A132 T133 T134 G135 A136 A137 A138 A144 T145 G150 C151 G152 C153 C154 T155 T156 T157 T158 T159 T160 T161 T162 T163 T164
• Molecule 12: DNA-directed RNA polymerase subunit
Chain A:
45%
31%
19%
MET VAL G3 Q4 V14 K15 E16 S23 P24 E25 E26 V27 R28 A29 I30 I35 M41 D42 T46 R47 A48 K49 L53 N54 D55 L58 G59 S60 I61 D62 L65 K66 T69 C70 Q71 E72 G73 M74 N75 E76 C77 P78 G79 H80 F81 I84 K88 P89 V90
F91 F95 V106 C107 M108 H109 L114 E120 R123 Q124 I128 K129 D130 S131 K132 K133 R134 T140 L141 C142 K143 T144 K145 M146 V147 C148 E149 T150 D151 V152 P153 S154 GLU ASP ASP PRO THR GLN LEU VAL SER R164 G165 G166 C167 T170 Q171 P172 T173 I174 R175 K176
D177 L181 V182 G183 S184 W185 K186 K187 ASP ARG ALA THR GLY ASP ALA ASP GLU P197 E198 L199 R200 V201 L202 S203 T204 E205 E206 I207 L208 N209 I210 F211 K212 H213 V216 K217 D218 F219 T220 S221 L222 G223 F224 N225 E226 V227 F228 S229 R230 P231 E232 W233 M234 I235 L236 L239

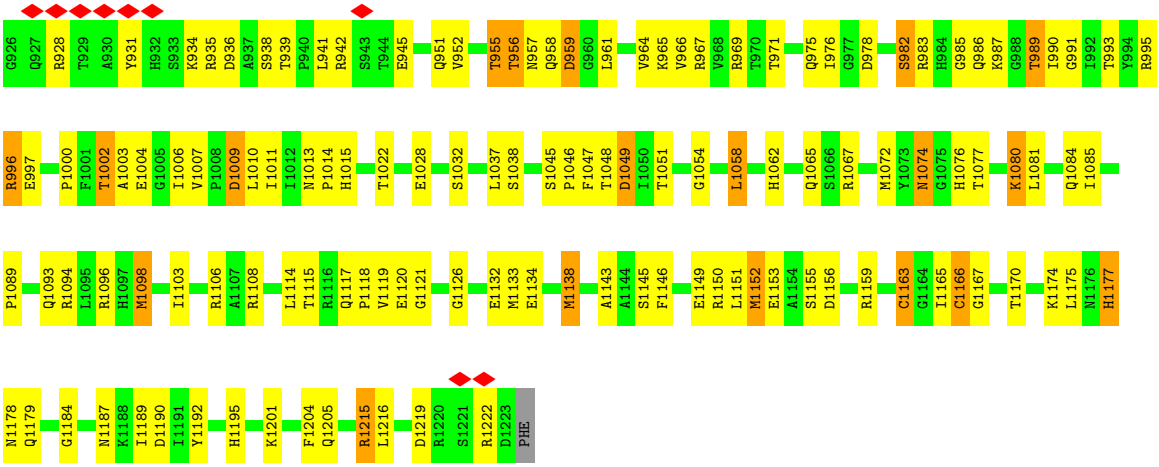

TYR MET PRO GLU GLN LYS ILE THR GLU ILE GLU ASP GLY GLN ASP GLY GLY VAL THR PRO TYR SER SER ASN GLU SER GLY GLU VAL ASN ALA ASP LEU ASP VAL LYS ASP GLU LEU MET PHE SER PRO LEU VAL ASP SER GLY SER ASN ASP ALA MET ALA GLY GLY PHE THR ALA TYR GLY
G1380 L1381 T1382 S1383 R1386 H1387 G1388 F1389 N1390 R1391 S1392 N1393 T1394 L1397 M1398 R1399 C1400 S1401 F1402 E1403 E1404 T1405 V1406 E1407 I1408 L1409 A1412 G1413 E1417 L1418 D1419 D1420 G1423 V1424 S1425 E1426 N1427 V1428 I1429 L1430 P1435 G1439 M1444 I1445 D1446 E1447 E1448 S1449 L1450 V1451 K1452
S1293 P1294 T1295 G1296 E1297 Y1298 W1304 V1305 L1306 E1307 T1308 D1309 G1310 G1321 I1322 D1323 P1324 T1325 R1326 I1327 Y1328 T1329 N1330 S1331 F1332 I1333 D1334 V1338 L1339 G1340 I1341 E1342 R1345 K1350 E1351 V1355 S1358 D1359 G1360 S1361 Y1362 V1363 N1364 Y1365 R1366 H1367 M1368 D1373 T1376 T1377
F1225 V1226 I1227 W1228 S1229 E1230 D1231 N1232 D1233 E1234 K1235 L1236 I1237 I1238 R1239 C1240 R1241 V1242 V1243 ARG PRO LYS SER LEU ASP ALA GLU THR GLU A1254 E1255 E1256 D1257 H1258 M1259 L1260 K1261 K1262 I1263 T1266 M1267 T1272 L1273 R1274 G1275 V1276 E1277 N1278 I1279 E1280 R1281 M1284 M1285 K1286 Y1287 K1290
S1160 T1161 V1162 I1163 P1164 E1165 D1166 E1167 E1168 I1169 I1170 Q1171 L1172 H1173 F1174 S1175 LEU LEU ASP GLU GLU GLN SER PHE ASP Q1187 Q1188 S1189 P1190 W1191 L1192 L1193 R1194 L1195 E1196 L1197 D1198 R1199 N1203 D1204 K1205 D1206 L1207 T1208 M1209 G1210 Q1211 V1212 G1213 I1216 K1217 Q1218 T1219 F1220 L1224
HIS PHE ALA GLY VAL ALA SER LYS K1093 G1097 R1100 L1101 K1102 E1103 N1106 V1107 A1108 K1109 N1110 M1111 K1112 T1113 P1114 S1115 L1116 E1121 H1124 D1127 Q1128 E1129 Q1130 A1131 K1132 R1135 S1136 A1137 I1138 E1139 H1140 T1141 T1142 L1143 K1144 E1151 I1152 Y1153 Y1154 D1155 P1156 D1157 P1158 R1159
P978 S979 T982 I983 K991 D992 L993 L997 L998 V999 A1010 Q1011 R1012 D1013 A1014 F1018 C1019 C1020 R1023 S1024 R1025 L1026 A1027 T1028 R1029 R1030 V1031 E1034 T1038 K1039 W1044 V1045 L1046 S1047 N1048 Q1052 F1053 S1056 V1057 V1058 G1061 M1079 THR LEU ASN THR PHE
D884 S889 D890 E894 R898 V899 D900 L901 L902 N903 T904 D905 H906 T907 L908 D909 L912 L913 E914 S915 G916 I919 Q926 D930 E931 R940 L943 R944 D949 G950 E951 A952 N953 W954 P955 L956 P957 V958 N959 I960 R961 R962 Q968 Q969 I973 D974 K977
V800 E801 N802 S803 Y804 L805 T809 P810 Q811 E812 F815 H816 A817 M818 E822 A828 T831 I837 Q838 R839 R840 E846 D847 I848 M849 V850 H851 Y852 D853 N854 R857 L860 G861 N862 F866 I867 Y868 G869 E870 D871 G872 M873 D874 A875 E879 K880 Q881 S882 L883
Q698 H706 G707 M708 T709 E712 E715 D716 N717 R726 R731 L732 A733 E734 L737 N741 K744 Q745 M746 A749 K752 G753 S754 F755 I758 M761 V765 G766 Q767 Q768 S769 V770 E771 R774 R782 D790 D791 Y792 S793 P794 E795 G798 F799
S579 G585 I586 H587 R590 F591 D592 T595 T596 L597 L598 S599 P600 K601 D602 N603 D609 G610 Q611 V617 T621 V622 G623 S624 V633 E636 Q640 L645 Q650 W656 L657 L658 T664 G665 I666 I670 A671 D672 K687 V690 L691 T694
L501 S502 Q503 L504 C505 A506 V507 P508 L509 Q510 S513 P519 C520 M521 G522 I523 V524 Q525 D526 T527 L528 C529 G530 I531 R532 T535 L536 R537 D538 D544 Q545 V546 L547 N548 M549 D557 G558 V559 P563 A564 I565 I566 K567 P570 L571 W572 S573 G574 K575 Q576 I577 L578
D423 I424 Q427 W430 K431 V432 E433 R434 H435 D438 N439 D440 L443 F444 N445 R446 L450 H451 K452 M453 S454 M455 M456 A457 H458 R459 P464 Y465 S466 R469 L470 N471 V474 T475 A480 D481 F482 E486 M487 N488 L489 H490 V491 P492 Q493 S494 E495 E496 T497 R498
K332 R335 I336 R337 G338 N339 L340 R344 V345 D346 T351 V352 I353 S354 G355 D356 P357 N358 D362 G365 V366 P367 K368 Y376 V379 D386 Q390 L391 V392 R393 N394 H399 P400 G401 V405 I406 R407 D408 D411 R412 I413 D414 L415 R416 Y417 R420
P242 P243 P244 P245 V246 R247 I250 S251 F252 N253 E254 S255 Q256 R257 G258 D261 L262 T263 F264 D268 I269 L270 K271 A272 N273 I274 S275 L279 E280 H286 I289 E290 E293 S294 H299 N306 D307 I308 Q313 A314 L315 Q316 K317 V322 K323 S324 I325 R326



• Molecule 13: DNA-directed RNA polymerase subunit beta

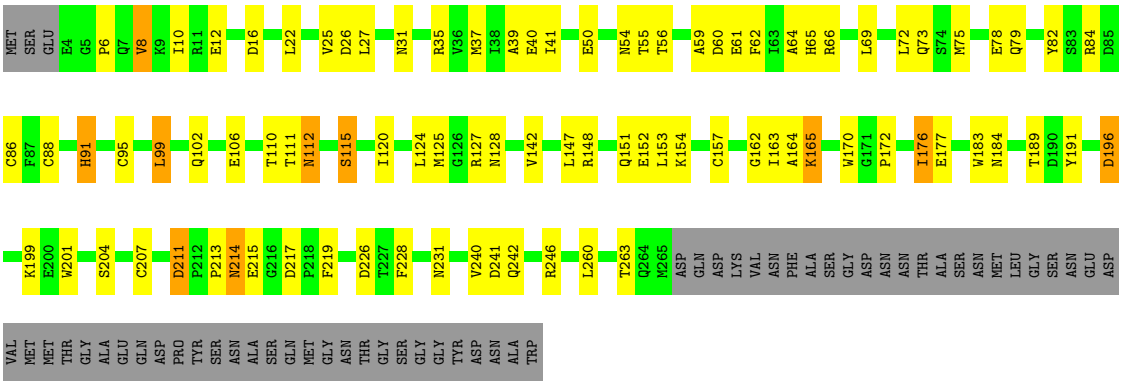
Chain B: 54% 36% • 6%





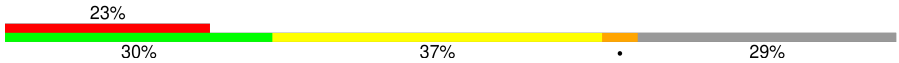
- Molecule 14: DNA-directed RNA polymerase II subunit RPB3

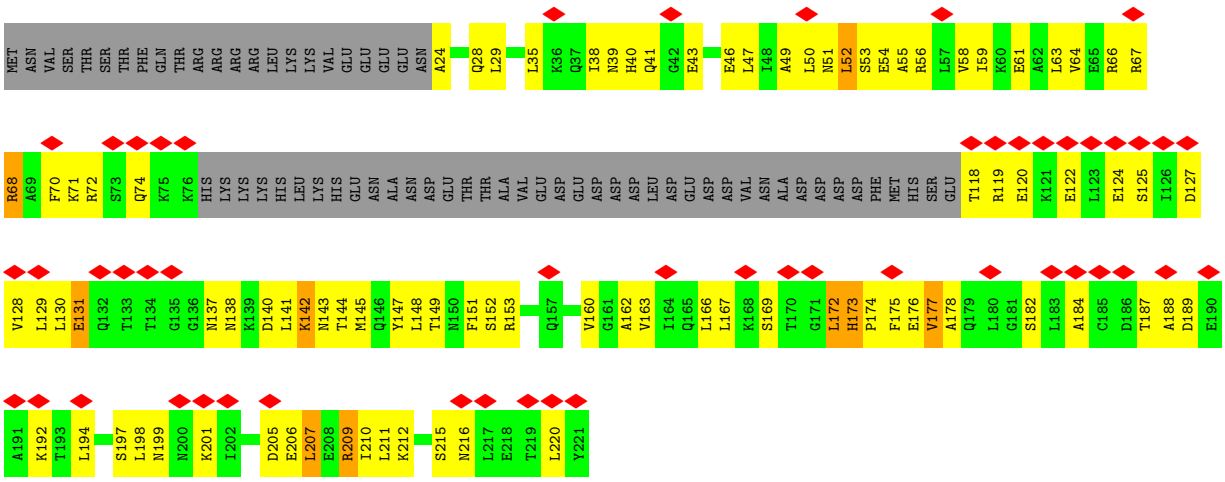
Chain C:



- Molecule 15: DNA-directed RNA polymerase II subunit RPB4

Chain D:





- Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 45% 48% 6% •

MET ASP Q3 E6 R7 N8 I9 S10 R11 L12 V19 K20 V23 K24 Y28 F29 I30 T31 Q32 E33 E34 V35 E36 L37 P38 L39 E40 D41 F42 K43 A44 K45 Y46 C47 D48 S49 M50 G51 R52 R55 K56 M57 M58 S59 F60 Q61 A62 N63 P64 T65 E66 E67 S68 I69 S70

K71 F72 P73 D74 M75 G76 S77 L78 W79 V80 E81 D84 T92 M93 I98 H99 I100 Q101 E102 F105 Q106 T107 G108 I109 Q113 N114 N115 I116 T117 P118 S119 A120 M121 K122 L123 V124 P125 S126 T131 I132 E133 T134 E137 L140 N143 I144 T145 H146 L156 S157

E160 E163 L164 L165 K166 R167 Y168 R169 L170 K171 E172 S173 R177 I178 Q179 R180 A181 D182 P183 V184 A185 L186 Y187 I188 G189 L190 K191 R192 G193 E194 V195 V196 K197 I198 I199 R200 K201 S202 E203 T204 S205 G206 R207 Y211 R212 I213 C214 M215

• Molecule 17: DNA-directed RNA polymerases I,II,and III subunit RPABC2

Chain F: 34% 17% • 46%

MET SER ASP TYR GLU GLU ALA PHE ASN ASP GLY ASN GLU ASN PHE GLU ASP PHE ASP VAL GLU HIS PHE SER ASP GLU GLU THR TYR GLU GLU LYS PRO GLN PHE LYS ASP GLY GLU THR THR ASP ALA ASN GLY LYS THR ILE VAL THR GLY GLY ASN GLY PRO GLU ASP PHE GLN GLN

HIS GLU GLN ILE ARG ARG LYS THR LEU LYS GLU K72 A73 I74 R79 A80 T81 T82 M85 T86 E89 R90 A91 R92 I93 T96 R97 A98 L99 Q100 I101 S102 D110 L111 E112 G113 E114 T115 D116 R119 I130 V133 I134 R135 R136 D140 G141 S142 W146 S147

V148 E149 E150 D154 LEU

• Molecule 18: DNA-directed RNA polymerase II subunit RPB7

Chain G: 12% 43% 51% 6%

M1 F2 F3 I4 K5 D6 L7 S8 L9 H14 P15 S16 F17 F18 R21 M22 Y25 L26 K29 E33 V34 E35 G36 S37 C38 T39 G40 K41 F42 G43 Y44 I45 L46 C47 V48 L49 D50 I56 Q57 R58 G59 R60 I61 T64 D65 G66 S67 A68 V72 K73 Y74 R75

A76 V77 V78 F79 K80 P81 F82 K83 V86 V87 D88 S93 C94 S95 Q96 F99 E100 V101 Q102 V103 G104 V108 F109 K112 M115 P116 Q117 D118 L119 A123 G124 S125 N126 P127 P128 S129 Y130 Q131 S132 S133 E134 D135 T138 I139 K140 S141 R144 V145 K146 I147 E148

G149 C150 I151 S152 S155 S156 I157 H158 A159 I160 G161 S162 I163 K164 E165 D166 Y167 L168 G169 A170 I171

• Molecule 19: DNA-directed RNA polymerases I, II, and III subunit RPABC3

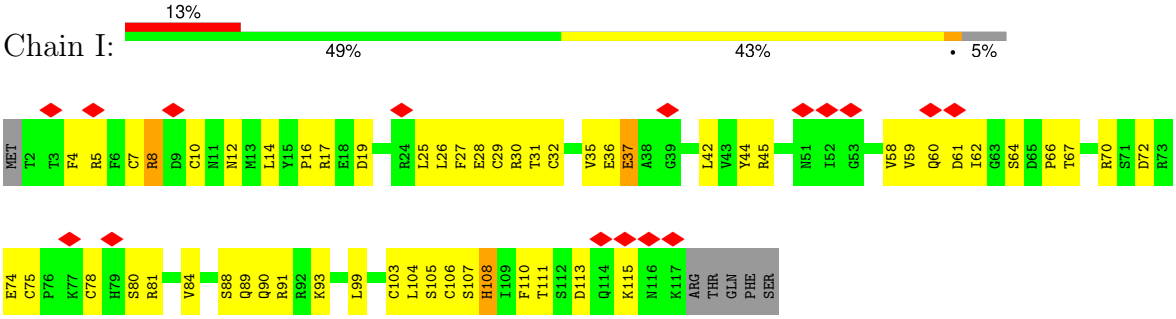
Chain H: • 46% 39% 8% • 7%

MET S2 N3 T4 L5 F6 D7 D8 I9 F10 Q11 V12 S13 E14 V15 D16 V23 C24 R25 I26 E27 A28 Q33 D34 Q35 L38 T39 L40 D41 I42 N43 V44 E45 L46 T56 V57 T58 S61 L65 GLU ASP THR PRO ALA ASN ASP SER SER A75 T76 R77 S78 W79 R80

P81 P82 Q83 A84 G85 D86 R87 S88 L89 A90 D91 D92 Y93 D94 Y95 V96 M97 A101 F104 K109 D110 L111 I112 Y116 S117 F118 L121 L122 M123 R124 L125 E126 G127 N128 Y129 R130 N131 L132 N133 N134 L135 K136 Q137 L142 L143 I144 R145 R146

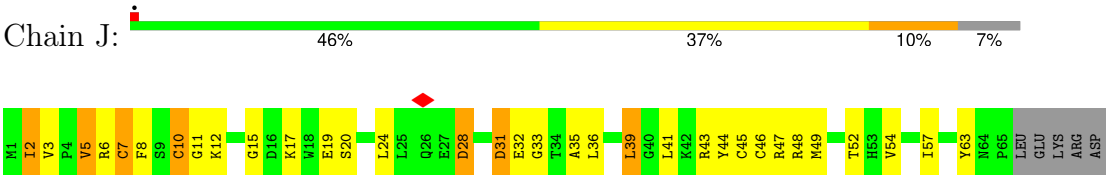
• Molecule 20: DNA-directed RNA polymerase II subunit RPB9

Chain I:



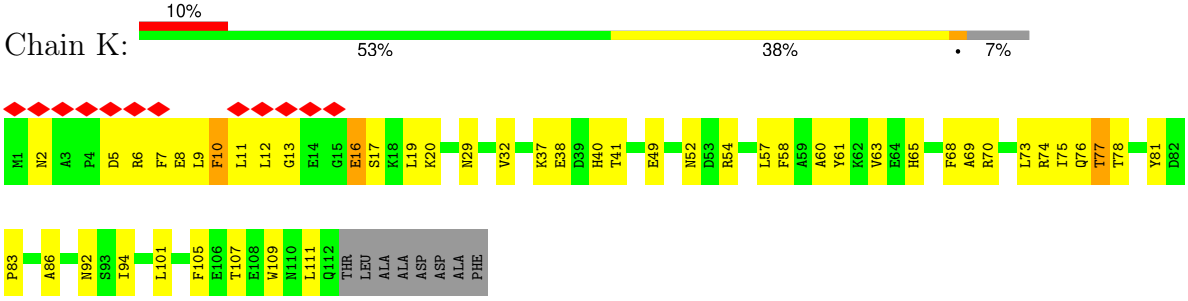
• Molecule 21: DNA-directed RNA polymerases II subunit RPABC5

Chain J:



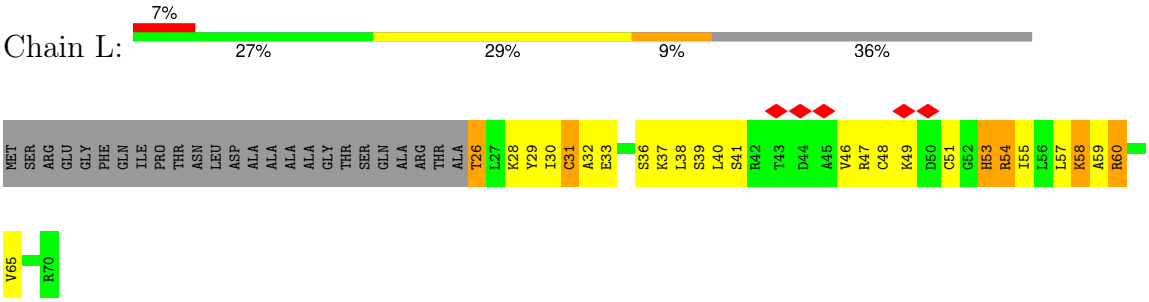
• Molecule 22: DNA-directed RNA polymerase II subunit RPB11

Chain K:



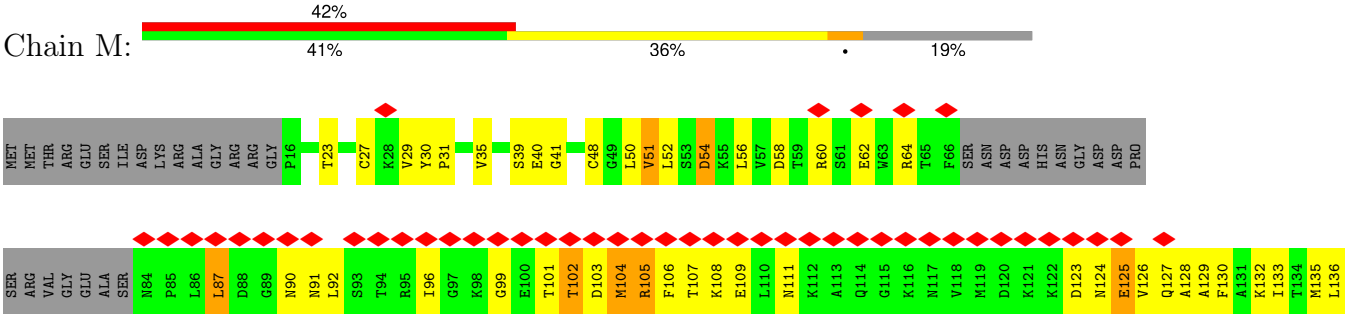
• Molecule 23: DNA-directed RNA polymerases II subunit RPABC4

Chain L:



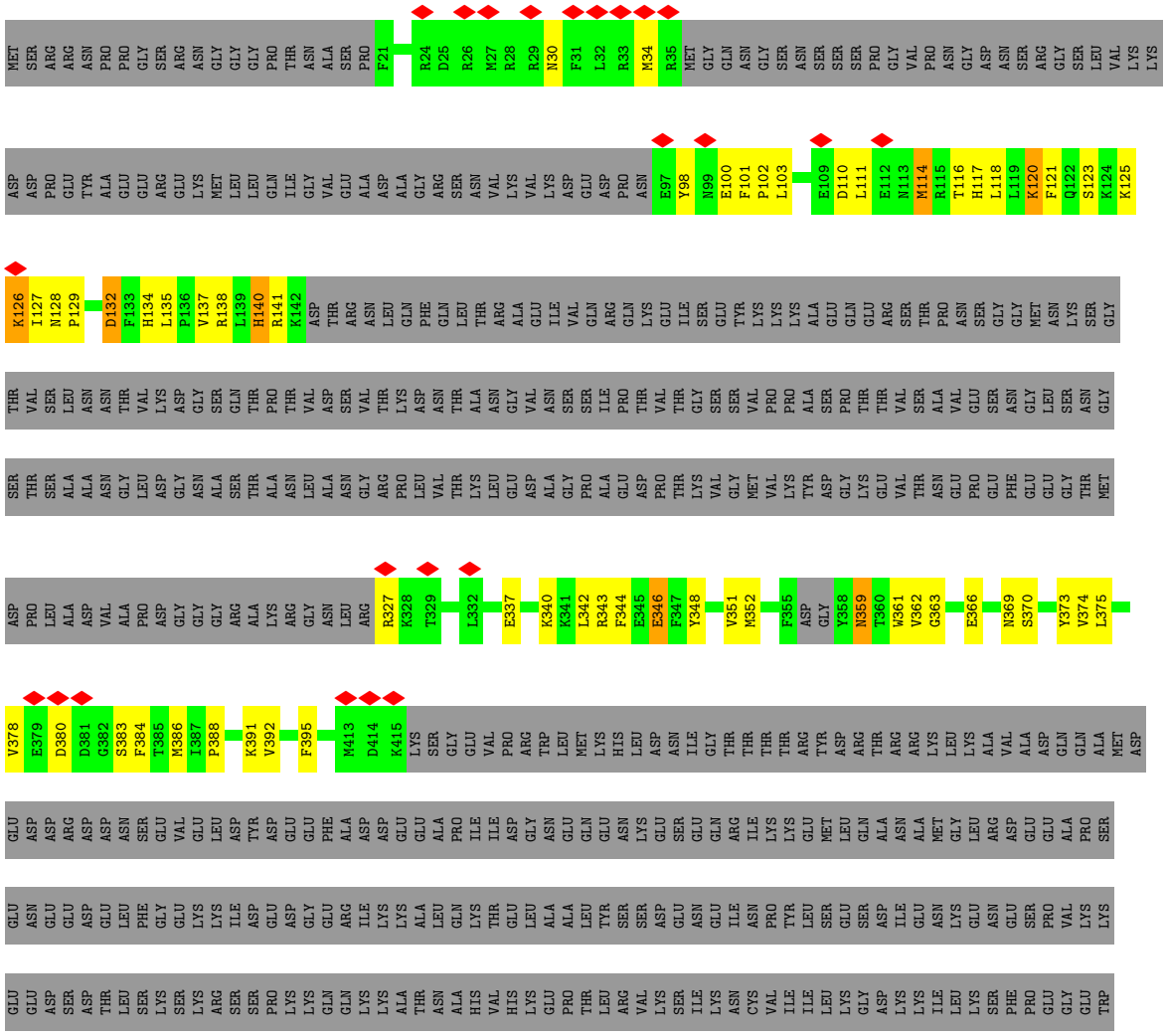
• Molecule 24: Transcription initiation factor IIB

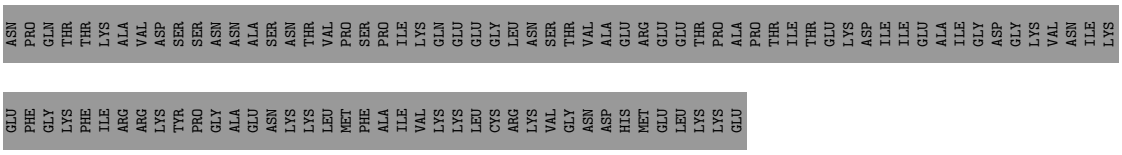
Chain M:



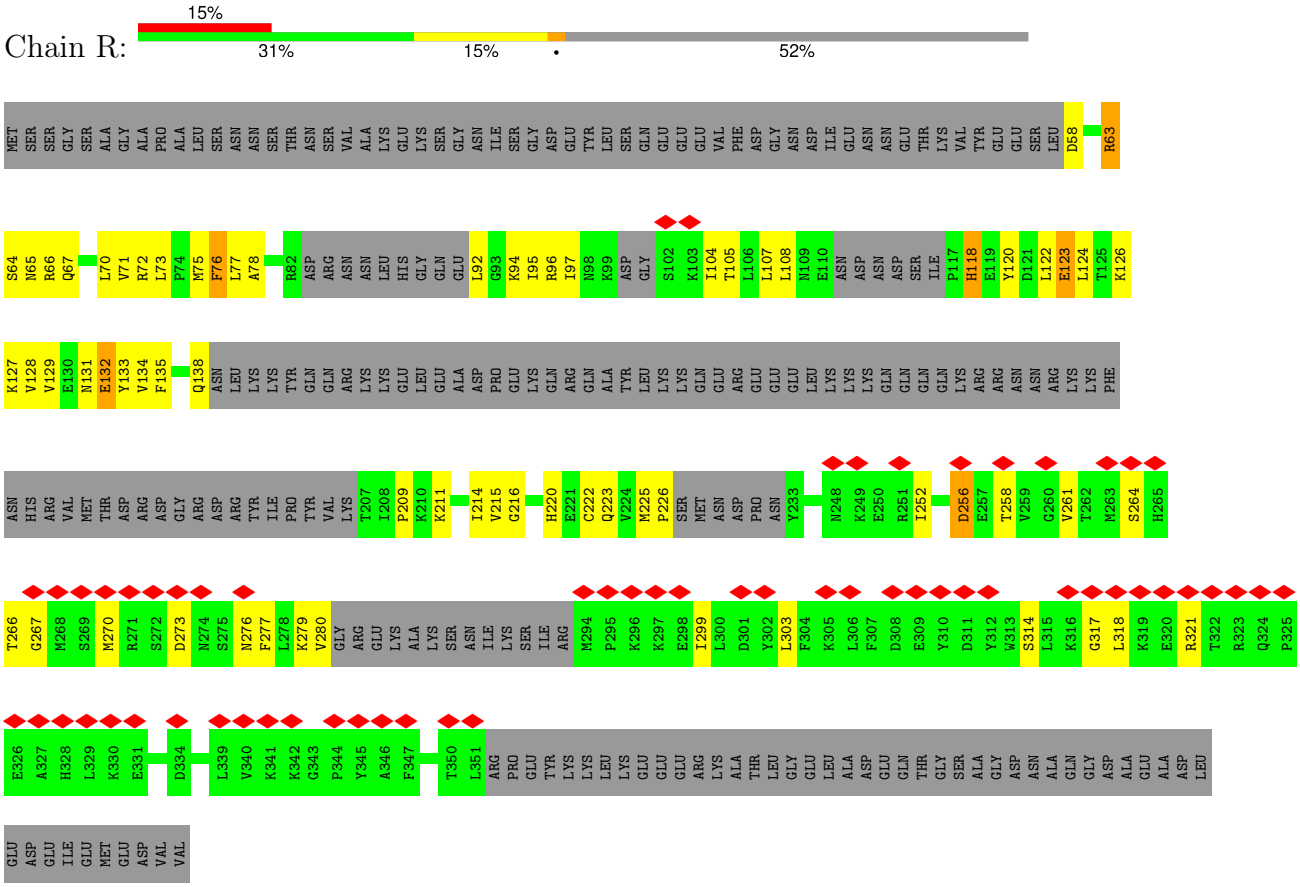
• Molecule 25: Transcription initiation factor IIF subunit alpha

Chain Q:

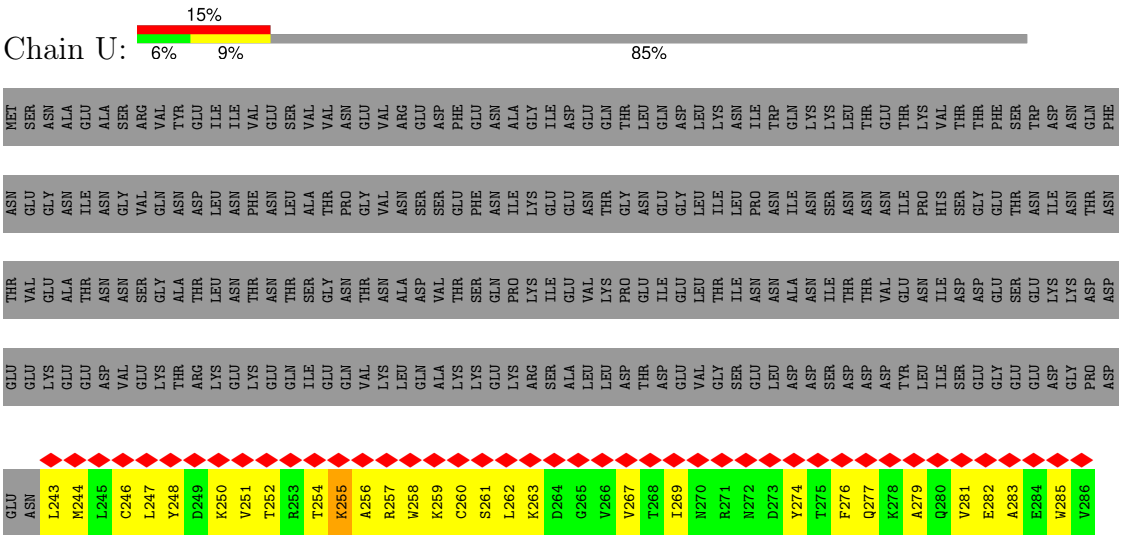




• Molecule 26: Transcription initiation factor IIF subunit beta



• Molecule 27: Transcription initiation factor IIA large subunit



• Molecule 28: Transcription initiation factor IIA subunit 2

Chain V: 40% 23% 15% • 59%

MET ALA VAL PRO GLY TYR TYR GLU LEU TYR ARG ARG SER THR ILE GLY ASN SER LEU VAL ASP ALA LEU ASP THR LEU ILE SER ASP GLY ARG ILE GLU ALA SER LEU ALA MET ARG VAL LEU GLU THR PHE ASP LYS VAL VAL ALA GLU THR LEU LYS ASP N55 T56 Q57 S58 K59 L60

T61 V62 K63 G64 N65 L66 D67 T68 Y69 G70 F71 C72 D73 D74 V75 W76 T77 F78 I79 V80 K81 N82 C83 Q84 V85 T86 V87 E88 ASP SER HIS ARG ASP ALA SER GLN ASN GLY SER GLY ASP SER GLN S104 V105 I106 S107 V108 D109 K110 L111 R112 I113 V114 A115 C116 N117 S118 K119 LYS

SER GLU

- Molecule 29: Transcription initiation factor IIE subunit alpha

Chain W: 20% 20% 19% • 60%

MET ASP ARG P4 I5 D6 D7 I8 V9 K10 N11 L12 L13 K14 F15 V16 V17 R18 G19 F20 Y21 G22 G23 S24 F25 V26 L27 V28 L29 D30 A31 I32 L33 F34 H35 S36 V37 L38 A39 E40 L43 K44 L47 S48 I49 N50 K51 T52 E53 L54 G55 P56 L57 I58 A59 R60 L61 R62

S63 D64 R65 L66 I67 S68 I69 H70 K71 Q72 R73 E74 Y75 P76 P77 N78 S79 K80 S81 V82 E83 R84 V85 Y86 Y87 Y88 V89 K90 Y91 P92 H93 A94 I95 D96 A97 I98 K99 W100 K101 V102 H103 Q104 V105 V106 Q107 R108 L109 K110 D111 N116 S117 E118 P119 N120 G121 Y122 M123 C124 P125

I126 C127 L128 T129 K130 Y131 T132 Q133 L134 E135 A136 L139 L140 N141 F142 D143 R144 T145 E146 F147 L148 C149 S150 L151 C152 D153 E154 P155 L156 V157 E158 D159 D160 K163 K164 N165 K166 E167 K168 Q169 D170 K171 L172 N173 R174 L175 M176 D177 Q178 I179 Q180 I183 D184 S185 L186 K187 K188

I189 D190 D191 S192 R193 I194 GLU GLU ASN THR PHE GLU ILE ALA LEU ALA ARG LEU ILE PRO PRO GLN ASN GLN SER HIS ALA ALA TYR THR TYR ASN PRO LYS LYS GLY SER THR MET PHE ARG PRO GLY ASP SER ALA PRO LEU PRO ASN LEU MET GLY THR ALA LEU GLY ASN ASP SER

SER ARG ARG ALA GLY ALA ASN SER GLN ALA THR LEU HIS ILE ASN ILE THR THR ALA SER ASP GLU VAL ALA GLN ARG GLU LEU GLN GLU ARG GLN ALA GLU GLU LYS ARG LYS GLN ASN ALA VAL PRO GLU TRP HIS LYS GLN SER THR ILE GLY LYS THR ALA LEU GLY ARG LEU ASP

ASN GLU GLU GLU PHE ASP PRO VAL VAL THR ALA SER ALA MET ASP SER ILE ASN PRO ASP ASN GLU PRO ALA GLN GLU THR SER TYR GLN ASN ASN ARG THR LEU THR GLU GLN GLU MET GLU GLU ARG GLU ASN GLU LYS THR LEU ASN ASP TYR TYR ALA ALA LEU ALA LYS GLN

ALA LYS LEU ASN LYS GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU MET GLU ASP VAL MET ASP ASP ASN ASP GLU THR ALA ARG GLU ASN ALA LEU GLU ASP GLU PHE GLU ASP VAL THR ASP THR ALA GLY THR ALA ALA LYS THR GLU SER ASN

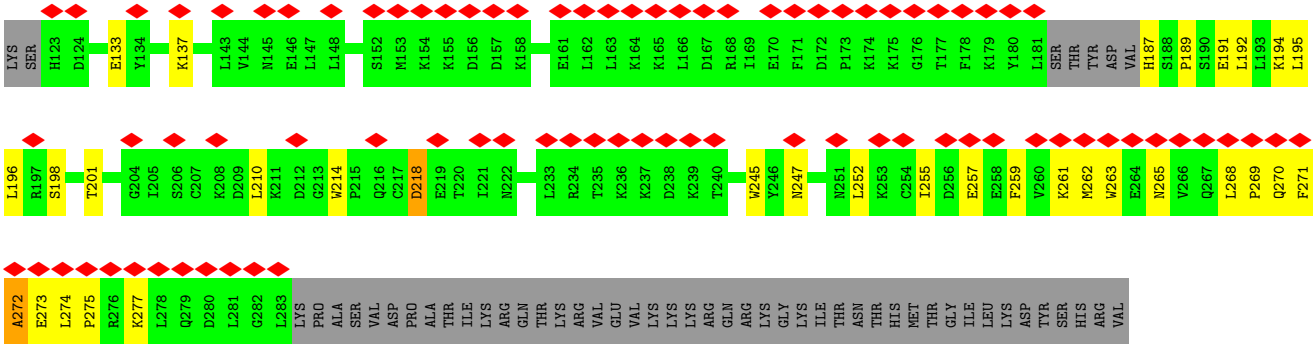
THR SER ASN ASP VAL LYS GLN GLU SER ILE ASN ASP LYS THR GLU ASP ALA VAL ASN ALA THR ALA THR ALA SER GLY PRO SER ALA ASN ALA LYS PRO ASN ASP GLY ASP ASP ASP ASP ASP ASP ASP ASP GLU MET ASP ILE GLU PHE GLU ASP VAL

- Molecule 30: Transcription initiation factor IIE subunit beta

Chain X: 25% 38% 9% • 52%

MET SER LYS ASN ARG ASP PRO LEU LEU ALA ASN LEU ASN ALA PHE LYS SER LYS VAL LYS SER ALA PRO VAL ILE ALA PRO ALA LYS VAL GLY GLN LYS LYS THR ASN ASP THR VAL ILE THR ILE ASP GLY ASN THR ARG LYS ARG THR ALA SER GLU ARG ALA ALA GLN GLU ASN THR LEU

ASN SER ALA LYS ASN PRO VAL LEU VAL ASP ILE LYS LYS GLU ALA GLY SER ASN SER SER ASN ALA ILE SER LEU ASP ASP ASP ASP ASP GLU ASP PHE GLY SER SER PRO SER LYS LYS VAL ARG PRO GLY SER ILE ALA ALA ALA ALA LEU GLN ALA ASN GLN THR ASP ILE SER


LYS SER H123 D124 E133 Y134 K137 L143 V144 N145 E146 L147 L148 S152 M153 K154 K155 D156 D157 K158 E161 L162 L163 K164 K165 L166 D167 R168 I169 E170 F171 D172 P173 K174 K175 G176 T177 F178 K179 Y180 L181 SER THR TYR ASP VAL H187 S188 P189 S190 E191 L192 L193 K194 L195
L196 R197 S198 T201 G204 I205 S206 C207 K208 D209 L210 K211 D212 G213 W214 P215 Q216 C217 D218 E219 T220 I221 N222 L233 R234 T235 K236 K237 D238 K239 T240 W245 Y246 N247 N251 L252 K253 C254 I255 D256 E257 E258 F259 V260 K261 M262 W263 E264 N265 V266 Q267 L268 P269 Q270 F271
A272 E273 L274 P275 R276 K277 L278 Q279 D280 L281 G282 L283 LYS PRO ALA SER VAL ASP PRO ALA THR ILE LYS ARG GLN THR LYS ARG VAL GLU VAL LYS LYS LYS ARG GLN ARG LYS GLY LYS ILE THR ASN THR HIS MET THR GLY ILE LEU LYS ASP TYR SER HIS ARG VAL

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33150	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.048	Depositor
Minimum map value	0.000	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0135	Depositor
Map size (Å)	453.67996, 405.97998, 419.75998	wwPDB
Map dimensions	428, 383, 396	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SF4, MG

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	1	0.14	0/1896	0.35	1/2543 (0.0%)
2	4	0.17	0/2062	0.46	3/2805 (0.1%)
3	0	0.14	0/6226	0.38	0/8407
4	6	0.16	0/2506	0.41	0/3402
5	2	0.16	0/3057	0.39	0/4071
6	5	0.18	0/502	0.46	0/677
7	7	0.19	0/4521	0.47	0/6036
8	3	0.13	0/870	0.36	0/1190
9	O	0.12	0/1443	0.31	0/1942
10	N	0.24	0/1326	0.48	0/2045
11	T	0.21	0/1294	0.42	0/1994
12	A	0.27	0/11192	0.39	0/15128
13	B	0.29	0/9311	0.38	0/12558
14	C	0.31	0/2099	0.39	0/2845
15	D	0.15	0/1262	0.37	0/1693
16	E	0.26	0/1780	0.37	0/2395
17	F	0.30	0/682	0.41	0/922
18	G	0.18	0/1368	0.36	0/1844
19	H	0.26	0/1107	0.42	0/1499
20	I	0.20	0/962	0.41	0/1295
21	J	0.34	0/541	0.51	0/727
22	K	0.28	0/922	0.40	0/1244
23	L	0.25	0/360	0.55	0/478
24	M	0.16	0/2204	0.42	0/2963
25	Q	0.20	0/1168	0.37	0/1579
26	R	0.17	0/1312	0.37	0/1777
27	U	0.12	0/372	0.33	0/500
28	V	0.11	0/392	0.27	0/529
29	W	0.11	0/1490	0.28	0/2014
30	X	0.10	0/993	0.31	0/1357
All	All	0.22	0/65220	0.40	4/88459 (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	4	0	1
4	6	0	1
7	7	0	1
12	A	0	2
13	B	0	2
24	M	0	1
All	All	0	8

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	4	298	ILE	CA-C-N	8.43	125.55	120.24
2	4	298	ILE	C-N-CA	8.43	125.55	120.24
1	1	336	ILE	N-CA-C	-5.28	107.45	111.62
2	4	299	ILE	CB-CA-C	-5.14	108.90	114.35

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	4	255	ASP	Peptide
4	6	116	THR	Peptide
7	7	321	GLU	Peptide
12	A	465	TYR	Peptide
12	A	71	GLN	Peptide
13	B	137	TYR	Peptide
13	B	363	HIS	Peptide
24	M	272	LYS	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	1	2411	0	1880	132	0
2	4	2041	0	1954	120	0
3	0	6108	0	6168	433	0
4	6	2527	0	2322	187	0
5	2	3011	0	2600	184	0
6	5	498	0	506	49	0
7	7	4447	0	3905	440	0
8	3	860	0	622	34	0
9	O	1416	0	1493	79	0
10	N	1178	0	642	52	0
11	T	1159	0	652	17	0
12	A	10997	0	11081	434	0
13	B	9132	0	9146	346	0
14	C	2061	0	2029	63	0
15	D	1253	0	1275	67	0
16	E	1744	0	1772	83	0
17	F	670	0	690	21	0
18	G	1340	0	1357	79	0
19	H	1089	0	1062	58	0
20	I	944	0	899	45	0
21	J	532	0	542	34	0
22	K	904	0	911	34	0
23	L	358	0	381	29	0
24	M	2175	0	2283	98	0
25	Q	1144	0	1034	65	0
26	R	1303	0	1110	60	0
27	U	366	0	372	41	0
28	V	389	0	394	31	0
29	W	1469	0	1432	78	0
30	X	984	0	722	27	0
31	3	2	0	0	0	0
31	4	1	0	0	0	0
31	6	4	0	0	0	0
31	A	3	0	0	0	0
31	B	1	0	0	0	0
31	C	1	0	0	0	0
31	I	2	0	0	0	0
31	J	1	0	0	0	0
31	L	1	0	0	0	0
31	M	1	0	0	0	0
31	W	1	0	0	0	0
31	X	1	0	0	0	0
32	0	8	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	A	1	0	0	0	0
All	All	64538	0	61236	3180	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (3180) 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)
3:0:133:CYS:HB2	32:0:801:SF4:S4	1.97	1.03
7:7:303:ARG:H	7:7:323:VAL:HG13	1.29	0.97
7:7:477:LEU:HA	7:7:482:TRP:HE1	1.36	0.91
7:7:592:GLN:HE22	7:7:747:ASN:HB3	1.38	0.89
7:7:234:VAL:H	7:7:316:PHE:H	1.20	0.88
12:A:70:CYS:SG	12:A:80:HIS:CE1	2.64	0.86
12:A:1239:ARG:HH12	12:A:1241:ARG:HH21	1.23	0.86
13:B:794:ASN:HD22	13:B:1096:ARG:HE	1.25	0.84
20:I:75:CYS:SG	20:I:103:CYS:HB2	2.18	0.83
10:N:11:DA:H5'	10:N:11:DA:C8	2.15	0.82
10:N:10:DA:H1'	10:N:11:DA:N7	1.95	0.82
7:7:428:CYS:SG	7:7:429:THR:N	2.53	0.81
26:R:277:PHE:H	26:R:279:LYS:HE2	1.45	0.81
29:W:17:VAL:HG22	29:W:25:PHE:HB3	1.61	0.81
29:W:132:THR:HG22	29:W:135:GLU:HG2	1.62	0.81
3:0:63:TYR:O	3:0:67:ARG:NH2	2.14	0.81
7:7:403:ILE:HG13	7:7:405:LYS:H	1.44	0.81
3:0:719:GLN:HA	3:0:722:ARG:HD3	1.61	0.80
9:O:158:GLN:HB3	10:N:23:DA:H4'	1.62	0.80
12:A:60:SER:HB2	12:A:65:LEU:HB2	1.64	0.80
13:B:959:ASP:N	13:B:959:ASP:OD1	2.15	0.80
25:Q:378:VAL:O	26:R:66:ARG:NH1	2.14	0.80
1:1:251:LEU:HB3	1:1:254:GLU:HB2	1.64	0.79
7:7:411:CYS:SG	7:7:412:THR:N	2.53	0.79
9:O:114:LEU:HB2	9:O:122:VAL:HB	1.64	0.79
16:E:100:ILE:HG23	16:E:105:PHE:HB2	1.64	0.79
27:U:248:TYR:HB3	28:V:115:ALA:HB1	1.64	0.79
7:7:487:LEU:HB2	7:7:512:GLY:HA2	1.63	0.79
7:7:343:PHE:HD2	7:7:380:ARG:HB2	1.47	0.78
7:7:604:LYS:HG2	7:7:666:GLU:HB2	1.63	0.78
7:7:389:GLY:HA2	7:7:692:ARG:HG2	1.66	0.78
7:7:682:GLN:NE2	7:7:685:GLN:OE1	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:370:PHE:HB2	5:2:373:MET:H	1.49	0.77
7:7:302:GLU:O	7:7:321:GLU:N	2.17	0.77
7:7:604:LYS:HD3	7:7:694:LYS:HZ1	1.50	0.77
12:A:326:ARG:HG2	12:A:1406:VAL:HG11	1.67	0.76
12:A:1128:GLN:NE2	12:A:1284:MET:SD	2.56	0.76
7:7:554:CYS:HA	7:7:705:PHE:HB3	1.67	0.76
12:A:268:ASP:OD2	12:A:299:HIS:NE2	2.18	0.76
5:2:75:GLN:NE2	5:2:503:ASP:OD2	2.18	0.76
7:7:303:ARG:HB3	7:7:323:VAL:HG22	1.68	0.76
7:7:613:TYR:O	7:7:617:GLU:N	2.15	0.76
23:L:47:ARG:NH2	23:L:48:CYS:O	2.19	0.76
7:7:365:TYR:H	7:7:548:HIS:HB2	1.50	0.76
7:7:425:LEU:HB3	7:7:430:LEU:HB3	1.67	0.76
2:4:116:ARG:O	2:4:120:ASN:ND2	2.18	0.76
25:Q:127:ILE:O	26:R:133:TYR:OH	2.04	0.75
12:A:1209:MET:N	12:A:1209:MET:SD	2.59	0.75
7:7:302:GLU:HB2	7:7:321:GLU:H	1.51	0.75
28:V:78:PHE:HB2	28:V:113:ILE:HB	1.69	0.75
7:7:668:THR:OG1	7:7:694:LYS:NZ	2.18	0.75
13:B:894:ASP:OD2	23:L:58:LYS:NZ	2.19	0.75
5:2:343:THR:OG1	5:2:415:LYS:NZ	2.18	0.75
24:M:281:SER:O	24:M:285:ASN:ND2	2.19	0.75
3:0:297:ASP:O	3:0:386:ARG:NH1	2.18	0.74
5:2:373:MET:HE3	5:2:375:LEU:HA	1.68	0.74
7:7:698:ASP:OD1	7:7:698:ASP:N	2.18	0.74
3:0:259:ARG:HG2	3:0:262:ARG:HH21	1.51	0.74
4:6:286:SER:O	4:6:289:LYS:NZ	2.21	0.74
16:E:197:LYS:HG3	16:E:211:TYR:HE1	1.53	0.74
12:A:55:ASP:N	12:A:55:ASP:OD1	2.20	0.74
4:6:211:GLN:HB3	4:6:244:PRO:HD2	1.70	0.74
7:7:407:VAL:HG13	7:7:484:PHE:HB3	1.69	0.74
15:D:144:THR:O	15:D:148:LEU:N	2.20	0.74
2:4:289:CYS:SG	2:4:290:SER:N	2.61	0.73
7:7:579:LEU:HD13	7:7:766:LYS:HB3	1.69	0.73
3:0:535:ASP:HB3	3:0:595:GLY:HA2	1.70	0.73
7:7:343:PHE:HB2	7:7:344:ARG:HH21	1.53	0.73
12:A:269:ILE:HG12	12:A:299:HIS:HB3	1.70	0.73
4:6:156:PHE:HB2	4:6:301:PHE:HD2	1.52	0.73
2:4:275:SER:HA	2:4:282:VAL:HA	1.70	0.73
3:0:167:VAL:HG22	3:0:198:ARG:HD2	1.71	0.73
12:A:451:HIS:HB2	12:A:454:SER:H	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:368:LYS:HE3	7:7:543:LEU:HD23	1.70	0.73
12:A:882:SER:O	12:A:1025:ARG:NH2	2.22	0.73
20:I:88:SER:O	20:I:91:ARG:NH2	2.17	0.73
3:0:535:ASP:HB2	3:0:590:CYS:HA	1.70	0.73
5:2:69:ASN:HA	5:2:71:LYS:HE3	1.69	0.73
26:R:138:GLN:HB2	26:R:211:LYS:HB2	1.69	0.73
4:6:141:LEU:HD23	4:6:145:ARG:HA	1.71	0.73
7:7:536:TYR:OH	7:7:540:TRP:NE1	2.21	0.73
13:B:706:GLN:HB2	13:B:709:ASP:HB3	1.70	0.72
12:A:862:ASN:OD1	12:A:862:ASN:N	2.23	0.72
29:W:65:ARG:NH2	30:X:270:GLN:O	2.22	0.72
7:7:372:LYS:O	7:7:380:ARG:NH2	2.23	0.72
10:N:43:DT:N3	11:T:124:DT:O2	2.23	0.72
14:C:211:ASP:OD1	14:C:211:ASP:N	2.16	0.72
4:6:127:ILE:HG13	4:6:170:GLY:H	1.53	0.72
3:0:111:ARG:NE	3:0:133:CYS:SG	2.62	0.72
5:2:102:PRO:O	5:2:106:ILE:N	2.23	0.72
14:C:142:VAL:HG13	21:J:15:GLY:HA3	1.71	0.72
2:4:228:THR:O	2:4:233:GLY:N	2.20	0.72
5:2:59:LEU:HD13	5:2:96:LEU:HD12	1.72	0.72
7:7:739:LEU:HB2	7:7:742:MET:HB3	1.71	0.72
7:7:370:LEU:HD21	7:7:395:VAL:HG13	1.71	0.72
16:E:180:ARG:HH21	16:E:191:LYS:HA	1.54	0.72
9:O:70:ILE:HG13	9:O:160:ILE:HG12	1.71	0.72
1:1:210:TRP:HB3	1:1:217:LEU:HD11	1.72	0.71
13:B:367:LEU:HB2	13:B:370:PHE:HE1	1.54	0.71
3:0:687:SER:HA	3:0:706:LEU:HD12	1.72	0.71
28:V:81:LYS:HE2	28:V:110:LYS:HG3	1.70	0.71
4:6:224:VAL:O	4:6:230:ARG:NH2	2.24	0.71
12:A:456:MET:HE2	12:A:507:VAL:HG22	1.72	0.71
7:7:572:GLU:O	7:7:577:ARG:NH2	2.23	0.71
13:B:24:PRO:O	13:B:655:LYS:NZ	2.22	0.71
13:B:919:SER:HB3	13:B:922:GLU:HB2	1.73	0.71
7:7:302:GLU:HB3	7:7:319:ALA:HB3	1.71	0.71
13:B:399:ASP:OD1	13:B:399:ASP:N	2.24	0.71
14:C:56:THR:HG22	14:C:147:LEU:HD21	1.71	0.71
19:H:56:THR:OG1	19:H:146:ARG:NH1	2.23	0.71
5:2:109:ARG:HA	5:2:112:LEU:HD22	1.73	0.71
3:0:108:LEU:HB3	3:0:208:TYR:HB3	1.72	0.71
1:1:379:ASN:HD21	3:0:571:VAL:H	1.37	0.71
7:7:363:ARG:HB2	7:7:548:HIS:CG	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:624:LYS:NZ	7:7:648:GLN:O	2.24	0.71
25:Q:375:LEU:HG	26:R:70:LEU:HD13	1.72	0.71
3:0:295:SER:HA	3:0:298:ILE:HG22	1.73	0.70
13:B:103:ASN:O	13:B:958:GLN:NE2	2.23	0.70
5:2:384:ARG:NH1	5:2:444:TRP:O	2.24	0.70
12:A:636:GLU:OE2	12:A:962:ARG:NH1	2.23	0.70
7:7:309:ASP:OD1	7:7:309:ASP:N	2.24	0.70
3:0:252:LEU:HD12	3:0:435:MET:HB3	1.73	0.70
8:3:46:ILE:HG23	8:3:52:ALA:HB3	1.72	0.70
29:W:5:ILE:HD11	29:W:189:ILE:HA	1.71	0.70
7:7:434:ASN:HB3	7:7:451:GLY:HA3	1.73	0.70
12:A:53:LEU:O	12:A:247:ARG:NH2	2.23	0.70
12:A:406:ILE:HB	12:A:431:LYS:HB2	1.74	0.70
2:4:64:HIS:O	2:4:71:ASN:ND2	2.23	0.70
12:A:346:ASP:OD1	12:A:346:ASP:N	2.24	0.70
13:B:199:MET:N	13:B:199:MET:SD	2.64	0.70
12:A:451:HIS:HB3	12:A:453:MET:HE2	1.74	0.70
12:A:881:GLN:NE2	12:A:957:PRO:O	2.24	0.70
1:1:174:LEU:O	1:1:181:GLN:NE2	2.24	0.70
7:7:407:VAL:HB	7:7:452:LEU:HD13	1.73	0.70
3:0:1:MET:HE3	3:0:742:GLU:H	1.57	0.69
3:0:587:ARG:NH2	3:0:611:ASP:O	2.25	0.69
5:2:486:ASP:OD1	5:2:486:ASP:N	2.24	0.69
12:A:592:ASP:OD1	12:A:592:ASP:N	2.26	0.69
13:B:20:ASP:OD1	13:B:21:GLU:N	2.25	0.69
29:W:121:GLY:HA2	29:W:132:THR:HA	1.74	0.69
7:7:256:ILE:N	7:7:317:GLU:O	2.25	0.69
9:O:203:VAL:HG11	10:N:21:DA:H4'	1.74	0.69
29:W:172:LEU:HB3	29:W:176:MET:HE3	1.73	0.69
24:M:195:LEU:HD23	24:M:196:ILE:HG13	1.73	0.69
25:Q:141:ARG:HH22	25:Q:343:ARG:HH12	1.40	0.69
7:7:477:LEU:HB3	7:7:505:ILE:HG13	1.73	0.69
13:B:232:SER:O	13:B:261:ARG:NH1	2.24	0.69
1:1:597:PHE:HA	1:1:600:VAL:HB	1.74	0.69
29:W:44:LYS:NZ	29:W:49:ILE:O	2.24	0.69
2:4:23:PRO:HG2	2:4:172:LEU:HG	1.73	0.69
3:0:484:ALA:HA	3:0:696:TRP:HB3	1.72	0.69
7:7:642:ASN:HA	7:7:646:ASN:HB3	1.74	0.69
19:H:12:VAL:HG11	19:H:15:VAL:HG23	1.73	0.69
27:U:260:CYS:HB3	27:U:281:VAL:HB	1.74	0.69
7:7:556:GLU:HG3	7:7:707:SER:HB3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:879:GLU:OE2	12:A:962:ARG:NH2	2.26	0.69
13:B:842:ASN:OD1	13:B:845:SER:N	2.19	0.69
15:D:172:LEU:HB3	15:D:177:VAL:HG12	1.75	0.69
27:U:246:CYS:SG	27:U:247:LEU:N	2.63	0.69
25:Q:386:MET:N	25:Q:386:MET:SD	2.65	0.69
18:G:57:GLN:OE1	18:G:57:GLN:N	2.23	0.69
2:4:162:ARG:NH2	4:6:407:GLN:O	2.26	0.68
5:2:22:GLN:O	5:2:26:TYR:N	2.26	0.68
12:A:1386:ARG:O	12:A:1391:ARG:NH1	2.26	0.68
24:M:264:LYS:HE3	24:M:265:GLU:HG3	1.74	0.68
4:6:132:CYS:HB2	4:6:175:ARG:HG2	1.75	0.68
7:7:674:SER:O	7:7:686:ARG:NH1	2.26	0.68
13:B:801:LYS:O	21:J:52:THR:OG1	2.10	0.68
16:E:48:ASP:OD1	16:E:52:ARG:N	2.26	0.68
3:0:496:ILE:HD12	3:0:686:PHE:HB3	1.73	0.68
7:7:264:PRO:O	7:7:268:VAL:N	2.26	0.68
7:7:344:ARG:NH2	7:7:379:ALA:O	2.26	0.68
7:7:554:CYS:HB2	7:7:733:PHE:HA	1.73	0.68
13:B:363:HIS:O	13:B:365:THR:N	2.26	0.68
13:B:443:ASN:HD22	13:B:446:LEU:HG	1.57	0.68
14:C:86:CYS:HB2	14:C:88:CYS:SG	2.33	0.68
15:D:52:LEU:HG	15:D:182:SER:HB2	1.74	0.68
16:E:182:ASP:OD1	16:E:185:ALA:N	2.20	0.68
12:A:544:ASP:OD1	12:A:544:ASP:N	2.24	0.68
12:A:603:ASN:N	12:A:603:ASN:OD1	2.25	0.68
15:D:153:ARG:NH2	15:D:182:SER:O	2.26	0.68
18:G:94:CYS:SG	18:G:130:TYR:OH	2.51	0.68
2:4:292:CYS:HB2	2:4:308:CYS:SG	2.33	0.68
3:0:221:ARG:HD3	3:0:221:ARG:H	1.58	0.68
12:A:1423:GLY:O	12:A:1427:ASN:ND2	2.26	0.68
13:B:364:ILE:HG22	13:B:585:VAL:HG13	1.75	0.68
7:7:473:VAL:O	7:7:477:LEU:N	2.22	0.68
3:0:476:LYS:NZ	3:0:477:THR:O	2.24	0.68
12:A:898:ARG:O	12:A:1029:ARG:NH2	2.27	0.68
7:7:209:ILE:O	7:7:213:ILE:N	2.25	0.68
7:7:370:LEU:O	7:7:374:PHE:N	2.18	0.68
9:O:74:VAL:HB	9:O:121:MET:HB3	1.76	0.68
24:M:54:ASP:OD1	24:M:54:ASP:N	2.25	0.68
7:7:696:ARG:HB3	7:7:702:ASN:HB3	1.75	0.68
10:N:9:DA:H1'	10:N:10:DA:H5'	1.76	0.68
4:6:262:LYS:HE2	4:6:289:LYS:HE2	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:61:ASP:N	5:2:61:ASP:OD1	2.26	0.67
23:L:36:SER:OG	23:L:48:CYS:SG	2.50	0.67
3:0:215:ASP:HB3	3:0:218:ILE:HG12	1.75	0.67
3:0:722:ARG:HH21	4:6:292:LEU:HB2	1.59	0.67
9:O:67:LEU:HA	9:O:162:GLY:HA2	1.76	0.67
16:E:67:GLU:OE1	16:E:68:SER:N	2.28	0.67
18:G:34:VAL:HG12	18:G:45:ILE:HG21	1.75	0.67
5:2:364:VAL:HA	5:2:382:SER:HB3	1.76	0.67
3:0:77:SER:OG	3:0:81:LYS:NZ	2.28	0.67
7:7:615:LEU:O	7:7:619:ALA:N	2.24	0.67
13:B:71:LEU:HD22	13:B:432:MET:HE3	1.76	0.67
13:B:1074:ASN:OD1	13:B:1077:THR:N	2.25	0.67
3:0:259:ARG:HH22	3:0:395:ASP:HA	1.60	0.67
4:6:134:GLU:HA	4:6:137:LEU:HD12	1.76	0.67
4:6:175:ARG:HH21	4:6:205:LYS:HB2	1.58	0.67
5:2:352:ASN:ND2	5:2:370:PHE:O	2.27	0.67
12:A:443:LEU:HD21	12:A:455:MET:HE3	1.75	0.67
12:A:746:MET:HE1	13:B:1015:HIS:HA	1.75	0.67
24:M:270:ALA:HB1	24:M:277:ILE:HG21	1.77	0.67
1:1:510:ASN:OD1	1:1:513:GLN:NE2	2.28	0.67
3:0:563:VAL:HG22	3:0:569:ILE:HD11	1.77	0.67
4:6:272:ILE:O	4:6:276:LEU:N	2.25	0.67
29:W:69:ILE:HA	29:W:87:TYR:HA	1.77	0.67
3:0:232:VAL:O	3:0:457:ILE:N	2.25	0.66
5:2:48:MET:HE3	5:2:49:ALA:HA	1.78	0.66
3:0:157:GLU:O	3:0:161:ASN:ND2	2.27	0.66
26:R:71:VAL:HG13	26:R:223:GLN:HA	1.75	0.66
4:6:237:GLY:HA2	4:6:266:LEU:HG	1.77	0.66
1:1:351:GLY:O	3:0:436:ARG:NH1	2.28	0.66
5:2:218:LEU:O	5:2:222:LEU:N	2.27	0.66
12:A:974:ASP:HB2	12:A:977:LYS:HD3	1.77	0.66
14:C:61:GLU:OE1	14:C:61:GLU:N	2.26	0.66
24:M:316:LEU:HD13	24:M:319:HIS:HD2	1.60	0.66
29:W:28:VAL:HG21	29:W:57:LEU:HB3	1.78	0.66
1:1:560:PHE:O	1:1:563:HIS:ND1	2.28	0.66
7:7:577:ARG:HA	7:7:580:LEU:HB2	1.78	0.66
7:7:663:ASP:OD1	7:7:663:ASP:N	2.21	0.66
19:H:101:ALA:HA	19:H:116:TYR:HA	1.78	0.66
1:1:232:UNK:O	1:1:236:UNK:N	2.28	0.66
2:4:153:MET:HE1	2:4:196:ILE:HG12	1.76	0.66
4:6:188:ASN:HD21	4:6:190:GLN:HB3	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:416:ARG:NH2	24:M:40:GLU:OE2	2.28	0.66
14:C:41:ILE:HB	14:C:172:PRO:HG3	1.75	0.66
19:H:110:ASP:OD2	19:H:130:ARG:NH2	2.28	0.66
3:0:499:LYS:HB3	3:0:503:GLN:HA	1.77	0.66
4:6:262:LYS:HB2	4:6:287:PHE:HD2	1.61	0.66
13:B:496:ARG:NH2	13:B:540:SER:O	2.28	0.66
13:B:728:ARG:NH1	13:B:1048:THR:O	2.29	0.66
15:D:127:ASP:HB3	15:D:142:LYS:HE2	1.76	0.66
19:H:90:ALA:HA	19:H:93:TYR:HB2	1.77	0.66
25:Q:141:ARG:NH2	25:Q:346:GLU:O	2.29	0.66
4:6:124:ARG:NH2	4:6:306:THR:O	2.25	0.66
4:6:128:LEU:HG	4:6:233:LEU:HB3	1.76	0.66
12:A:804:TYR:OH	12:A:816:HIS:NE2	2.28	0.66
16:E:40:GLU:HA	16:E:43:LYS:HE2	1.77	0.66
16:E:67:GLU:O	16:E:70:SER:OG	2.11	0.66
20:I:19:ASP:HB2	20:I:26:LEU:HG	1.77	0.66
21:J:33:GLY:O	21:J:47:ARG:NH2	2.28	0.66
23:L:26:THR:OG1	23:L:39:SER:O	2.14	0.66
11:T:136:DA:H2'	11:T:137:DA:C8	2.31	0.66
12:A:818:MET:HG2	13:B:514:LEU:HB3	1.78	0.66
12:A:908:LEU:HD11	12:A:912:LEU:HD12	1.78	0.66
13:B:705:MET:HG3	13:B:706:GLN:HG3	1.78	0.66
2:4:150:ALA:HB2	2:4:192:GLN:HB2	1.78	0.66
5:2:346:LYS:NZ	5:2:347:ILE:O	2.29	0.66
7:7:303:ARG:N	7:7:323:VAL:HG13	2.06	0.66
13:B:996:ARG:HD2	13:B:1007:VAL:HG21	1.78	0.66
4:6:174:MET:HA	4:6:179:ALA:HA	1.78	0.65
7:7:344:ARG:HD2	7:7:378:ARG:HD2	1.77	0.65
7:7:409:VAL:HB	7:7:454:VAL:HA	1.78	0.65
7:7:464:ARG:HH21	7:7:466:ARG:HH12	1.44	0.65
12:A:997:LEU:O	12:A:1011:GLN:NE2	2.29	0.65
18:G:47:CYS:H	18:G:77:VAL:HG22	1.61	0.65
29:W:141:ASN:OD1	29:W:141:ASN:N	2.28	0.65
3:0:211:HIS:O	3:0:215:ASP:N	2.29	0.65
4:6:169:MET:O	4:6:192:HIS:NE2	2.30	0.65
4:6:347:TYR:N	4:6:356:VAL:O	2.29	0.65
7:7:594:LEU:O	7:7:598:HIS:ND1	2.28	0.65
21:J:10:CYS:SG	21:J:12:LYS:N	2.68	0.65
2:4:258:LEU:HB2	2:4:260:PRO:HD3	1.79	0.65
3:0:117:HIS:N	32:0:801:SF4:S3	2.69	0.65
12:A:446:ARG:HB2	12:A:487:MET:HG2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:445:LYS:NZ	26:R:267:GLY:O	2.28	0.65
6:5:32:LEU:N	6:5:41:LEU:O	2.29	0.65
15:D:119:ARG:NH1	15:D:149:THR:O	2.28	0.65
24:M:91:ASN:ND2	24:M:123:ASP:OD2	2.29	0.65
3:0:711:ASP:OD1	3:0:711:ASP:N	2.24	0.65
7:7:541:MET:SD	7:7:545:GLN:NE2	2.61	0.65
8:3:39:CYS:SG	8:3:41:SER:OG	2.54	0.65
3:0:37:ASN:ND2	3:0:476:LYS:O	2.30	0.65
3:0:643:ARG:HH11	3:0:650:GLU:HG3	1.61	0.65
6:5:16:ILE:HG23	6:5:19:LEU:HD12	1.77	0.65
7:7:111:GLY:N	7:7:175:ILE:O	2.30	0.65
10:N:5:DA:H2"	10:N:6:DA:H8	1.60	0.65
13:B:241:ARG:HH21	13:B:251:ILE:HA	1.62	0.65
13:B:802:PRO:HG3	13:B:809:MET:HE1	1.79	0.65
18:G:96:GLN:OE1	29:W:145:THR:OG1	2.14	0.65
27:U:267:VAL:HB	27:U:274:TYR:HB2	1.77	0.65
29:W:14:LYS:NZ	29:W:30:ASP:OD1	2.28	0.65
1:1:593:LEU:HD21	1:1:620:LEU:HD12	1.78	0.65
2:4:150:ALA:HA	2:4:153:MET:HE2	1.78	0.65
2:4:217:GLY:O	2:4:237:HIS:NE2	2.30	0.65
3:0:215:ASP:O	3:0:219:ALA:N	2.29	0.65
25:Q:127:ILE:HG23	25:Q:129:PRO:HD3	1.79	0.65
3:0:363:LEU:O	3:0:367:THR:N	2.30	0.65
30:X:187:HIS:HA	30:X:214:TRP:HB2	1.79	0.65
3:0:74:ARG:HH21	3:0:236:GLU:HB3	1.60	0.65
4:6:116:THR:O	4:6:118:TYR:N	2.30	0.65
5:2:353:SER:HB2	5:2:356:GLN:HB3	1.77	0.65
7:7:583:MET:O	7:7:618:TYR:OH	2.15	0.65
12:A:537:ARG:NE	12:A:602:ASP:OD2	2.30	0.65
13:B:392:ARG:HG2	20:I:90:GLN:HE22	1.62	0.65
7:7:363:ARG:HG2	7:7:695:ARG:HB2	1.79	0.65
7:7:386:LEU:O	7:7:392:LYS:NZ	2.29	0.65
14:C:115:SER:OG	14:C:142:VAL:N	2.29	0.65
1:1:227:LYS:O	4:6:212:ASN:ND2	2.25	0.64
3:0:191:CYS:SG	3:0:194:PHE:HB2	2.37	0.64
3:0:371:ARG:O	3:0:410:SER:OG	2.15	0.64
5:2:132:LEU:O	5:2:286:ARG:NH2	2.30	0.64
7:7:578:MET:SD	7:7:581:TYR:OH	2.55	0.64
8:3:128:LYS:O	8:3:132:LYS:N	2.26	0.64
13:B:763:GLN:HG2	13:B:765:PRO:HD2	1.79	0.64
14:C:177:GLU:HB2	14:C:231:ASN:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Q:114:MET:HB2	26:R:138:GLN:HG2	1.79	0.64
2:4:52:LYS:NZ	2:4:240:SER:O	2.30	0.64
5:2:370:PHE:N	5:2:373:MET:O	2.30	0.64
12:A:90:VAL:O	12:A:236:LEU:N	2.30	0.64
13:B:287:ARG:NE	13:B:292:ILE:O	2.29	0.64
20:I:29:CYS:SG	20:I:31:THR:OG1	2.55	0.64
7:7:614:ALA:HA	7:7:617:GLU:HB3	1.79	0.64
12:A:526:ASP:OD1	12:A:526:ASP:N	2.17	0.64
27:U:281:VAL:HG13	28:V:62:VAL:HB	1.79	0.64
1:1:343:ILE:O	1:1:345:ASP:N	2.26	0.64
1:1:507:ILE:HG23	2:4:264:LYS:HG2	1.80	0.64
3:0:322:PRO:HB2	3:0:325:ILE:HB	1.78	0.64
13:B:121:ASN:HA	13:B:207:GLY:HA3	1.78	0.64
24:M:175:SER:O	24:M:179:GLY:N	2.30	0.64
2:4:29:ILE:HB	2:4:178:VAL:HG22	1.78	0.64
4:6:293:ASP:O	4:6:297:LEU:N	2.30	0.64
12:A:767:GLN:NE2	12:A:768:GLN:O	2.25	0.64
13:B:101:MET:HE1	13:B:127:GLY:H	1.62	0.64
3:0:353:SER:HA	3:0:419:ILE:HA	1.77	0.64
3:0:375:ARG:HA	3:0:407:THR:HA	1.79	0.64
4:6:451:CYS:O	4:6:455:GLU:N	2.30	0.64
5:2:396:ILE:HA	5:2:399:TYR:HB3	1.78	0.64
9:O:76:LEU:HD12	9:O:80:LEU:HD11	1.80	0.64
19:H:13:SER:N	19:H:27:GLU:O	2.30	0.64
3:0:148:ASP:N	3:0:148:ASP:OD1	2.30	0.64
12:A:198:GLU:OE1	12:A:200:ARG:NH1	2.31	0.64
12:A:1386:ARG:HB3	12:A:1403:GLU:HG3	1.80	0.64
17:F:110:ASP:OD1	17:F:110:ASP:N	2.30	0.64
5:2:349:SER:OG	5:2:373:MET:SD	2.51	0.64
7:7:347:HIS:O	7:7:405:LYS:NZ	2.23	0.64
7:7:489:GLU:OE1	7:7:685:GLN:NE2	2.29	0.64
12:A:351:THR:OG1	12:A:352:VAL:N	2.28	0.64
13:B:287:ARG:HD3	13:B:292:ILE:HA	1.80	0.64
21:J:10:CYS:SG	21:J:11:GLY:N	2.71	0.64
25:Q:359:ASN:N	25:Q:359:ASN:OD1	2.31	0.64
3:0:217:LYS:HB2	3:0:308:GLU:HG3	1.80	0.64
3:0:360:LEU:HD11	3:0:371:ARG:HB2	1.80	0.64
6:5:8:ALA:HB3	6:5:42:VAL:H	1.63	0.64
12:A:362:ASP:OD2	12:A:459:ARG:NE	2.29	0.64
12:A:931:GLU:OE2	12:A:991:LYS:NZ	2.30	0.64
20:I:108:HIS:CE1	20:I:110:PHE:HB3	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:343:ILE:HG21	3:0:605:LYS:HD3	1.80	0.64
3:0:112:LYS:NZ	3:0:123:GLU:O	2.31	0.64
7:7:469:ASP:N	7:7:469:ASP:OD1	2.28	0.64
12:A:1013:ASP:OD1	16:E:207:ARG:NH1	2.31	0.64
12:A:1334:ASP:N	12:A:1334:ASP:OD1	2.27	0.64
15:D:148:LEU:O	15:D:152:SER:N	2.31	0.64
9:O:184:SER:HB3	9:O:194:ILE:HB	1.79	0.63
10:N:15:DG:OP1	27:U:257:ARG:NH2	2.31	0.63
13:B:205:ILE:HD11	13:B:461:LEU:HD23	1.80	0.63
18:G:108:VAL:HG22	18:G:159:ALA:HB3	1.80	0.63
7:7:222:LYS:N	7:7:336:PRO:O	2.30	0.63
7:7:302:GLU:HA	7:7:318:ILE:HG22	1.79	0.63
7:7:495:ALA:HA	7:7:498:PHE:HB3	1.79	0.63
16:E:76:GLY:N	16:E:106:GLN:OE1	2.29	0.63
18:G:88:ASP:HA	18:G:144:ARG:HA	1.79	0.63
1:1:582:LEU:O	1:1:585:HIS:ND1	2.31	0.63
2:4:255:ASP:O	2:4:259:ARG:NH1	2.31	0.63
3:0:224:ASN:OD1	3:0:452:ARG:NH2	2.31	0.63
9:O:66:THR:N	9:O:163:SER:O	2.22	0.63
10:N:24:DA:H2'	10:N:25:DA:C8	2.33	0.63
14:C:40:GLU:OE2	14:C:165:LYS:NZ	2.31	0.63
26:R:65:ASN:O	26:R:67:GLN:NE2	2.31	0.63
3:0:420:ILE:HG12	3:0:435:MET:HG3	1.80	0.63
3:0:424:GLU:OE1	3:0:432:ASN:ND2	2.30	0.63
4:6:158:HIS:O	4:6:162:ASP:N	2.31	0.63
6:5:24:ASP:HA	6:5:27:MET:HG3	1.80	0.63
24:M:271:GLY:HA3	24:M:274:PRO:HA	1.80	0.63
2:4:75:VAL:HG12	2:4:86:LEU:HD23	1.80	0.63
3:0:111:ARG:HD2	3:0:130:ASP:HA	1.79	0.63
9:O:162:GLY:N	9:O:214:LEU:O	2.27	0.63
12:A:968:GLN:HA	12:A:973:ILE:HG12	1.79	0.63
13:B:336:ARG:HD2	13:B:348:ARG:HD3	1.80	0.63
1:1:214:ILE:HG23	1:1:215:PRO:HD3	1.81	0.63
3:0:83:LEU:HB3	3:0:177:SER:HA	1.81	0.63
3:0:507:SER:HB2	3:0:684:ARG:HG2	1.79	0.63
7:7:223:VAL:N	7:7:336:PRO:O	2.31	0.63
7:7:519:ARG:NH2	7:7:521:ASP:OD2	2.32	0.63
12:A:107:CYS:SG	12:A:171:GLN:NE2	2.71	0.63
3:0:307:VAL:HB	3:0:382:SER:HB3	1.81	0.63
3:0:534:PRO:O	3:0:567:LYS:NZ	2.30	0.63
4:6:149:ILE:O	4:6:153:ALA:N	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:516:THR:OG1	7:7:681:ARG:O	2.16	0.63
13:B:885:MET:HG2	13:B:936:ASP:HB2	1.81	0.63
15:D:66:ARG:NH2	18:G:35:GLU:OE2	2.29	0.63
19:H:130:ARG:O	19:H:133:ASN:ND2	2.26	0.63
3:0:109:THR:OG1	3:0:113:ASN:ND2	2.30	0.63
7:7:365:TYR:HB3	7:7:548:HIS:HB3	1.81	0.63
9:O:91:ASN:OD1	9:O:107:ARG:NH2	2.32	0.63
1:1:209:PHE:O	1:1:213:ARG:NH1	2.32	0.62
3:0:326:ARG:O	3:0:380:ARG:NH2	2.32	0.62
3:0:327:ARG:HD2	3:0:329:GLU:HG2	1.81	0.62
3:0:377:CYS:HG	3:0:407:THR:HG1	1.39	0.62
3:0:407:THR:O	3:0:411:THR:OG1	2.14	0.62
10:N:23:DA:H2'	10:N:24:DA:C8	2.33	0.62
12:A:218:ASP:O	12:A:221:SER:OG	2.16	0.62
29:W:122:TYR:O	29:W:131:TYR:N	2.28	0.62
1:1:259:ILE:HG22	1:1:266:VAL:HG11	1.81	0.62
7:7:162:GLU:O	7:7:174:LYS:N	2.32	0.62
12:A:355:GLY:O	12:A:469:ARG:NH1	2.31	0.62
13:B:361:LEU:HD22	13:B:363:HIS:HE1	1.64	0.62
19:H:109:LYS:O	19:H:111:LEU:N	2.31	0.62
19:H:112:ILE:HG23	19:H:132:LEU:HD12	1.80	0.62
2:4:304:LYS:HG3	2:4:309:ASP:HA	1.81	0.62
12:A:225:ASN:OD1	12:A:228:PHE:N	2.33	0.62
12:A:399:HIS:O	12:A:435:HIS:ND1	2.33	0.62
12:A:1345:ARG:NE	12:A:1373:ASP:OD1	2.31	0.62
7:7:685:GLN:HG3	7:7:689:ARG:HD2	1.80	0.62
13:B:860:MET:HB2	13:B:965:LYS:HG2	1.81	0.62
16:E:98:ILE:O	16:E:102:GLU:N	2.25	0.62
29:W:19:GLY:HA2	30:X:252:LEU:HD12	1.80	0.62
8:3:136:TYR:O	8:3:140:ASN:N	2.27	0.62
12:A:526:ASP:OD2	13:B:1013:ASN:ND2	2.31	0.62
12:A:1188:GLN:HA	12:A:1243:VAL:HA	1.82	0.62
18:G:9:LEU:N	18:G:72:VAL:O	2.30	0.62
8:3:79:GLU:O	8:3:83:ASP:N	2.25	0.62
12:A:76:GLU:OE2	13:B:1159:ARG:NH2	2.32	0.62
13:B:365:THR:HG21	13:B:370:PHE:HB2	1.79	0.62
15:D:211:LEU:O	15:D:215:SER:N	2.30	0.62
3:0:304:GLU:HB3	3:0:386:ARG:HD3	1.80	0.62
3:0:443:SER:HB3	3:0:473:LEU:HA	1.80	0.62
5:2:379:THR:H	5:2:382:SER:HB2	1.63	0.62
7:7:456:THR:HG23	7:7:459:MET:HE3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:5:DA:H2"	10:N:6:DA:C8	2.34	0.62
10:N:8:DA:C2	10:N:9:DA:C6	2.88	0.62
3:0:286:TYR:HE1	3:0:380:ARG:HH22	1.48	0.62
7:7:423:GLN:NE2	7:7:663:ASP:O	2.31	0.62
7:7:568:GLU:HG3	7:7:577:ARG:HD3	1.82	0.62
7:7:707:SER:OG	7:7:722:ARG:NH1	2.33	0.62
7:7:752:SER:HG	7:7:754:ARG:HG3	1.64	0.62
9:O:227:PHE:HA	9:O:230:ILE:HG22	1.82	0.62
12:A:88:LYS:HG2	12:A:293:GLU:HG3	1.80	0.62
12:A:368:LYS:HD2	22:K:2:ASN:HB3	1.81	0.62
12:A:457:ALA:HB2	12:A:501:LEU:HD12	1.82	0.62
13:B:486:TYR:HA	13:B:1096:ARG:HH22	1.63	0.62
3:0:120:VAL:HG22	3:0:132:LYS:HD2	1.82	0.62
5:2:99:ASN:N	5:2:99:ASN:OD1	2.32	0.62
7:7:359:SER:OG	7:7:427:TRP:O	2.15	0.62
13:B:771:SER:O	13:B:775:LYS:NZ	2.32	0.62
4:6:262:LYS:HD2	4:6:287:PHE:HA	1.81	0.62
5:2:73:GLN:O	5:2:77:ALA:N	2.31	0.62
7:7:348:ARG:HA	7:7:348:ARG:HE	1.63	0.62
13:B:195:CYS:SG	13:B:783:THR:OG1	2.57	0.62
3:0:742:GLU:HA	3:0:745:ILE:HD11	1.82	0.61
4:6:221:LEU:HD23	4:6:230:ARG:HB3	1.82	0.61
4:6:262:LYS:HA	4:6:287:PHE:HB3	1.82	0.61
7:7:407:VAL:H	7:7:452:LEU:HD22	1.65	0.61
29:W:127:CYS:SG	29:W:129:THR:OG1	2.52	0.61
2:4:286:GLY:N	4:6:322:MET:O	2.33	0.61
13:B:1163:CYS:SG	13:B:1166:CYS:N	2.67	0.61
20:I:74:GLU:HA	20:I:81:ARG:HA	1.82	0.61
2:4:57:LEU:O	2:4:61:LEU:N	2.31	0.61
3:0:5:ILE:O	3:0:29:LYS:NZ	2.34	0.61
3:0:567:LYS:HE3	3:0:597:ILE:HD11	1.82	0.61
4:6:277:CYS:O	4:6:281:ASN:ND2	2.26	0.61
5:2:62:LEU:HA	5:2:65:TRP:HD1	1.66	0.61
7:7:568:GLU:HG2	7:7:580:LEU:HD22	1.80	0.61
7:7:628:TYR:O	7:7:631:THR:OG1	2.14	0.61
7:7:634:GLN:HA	7:7:637:MET:HB2	1.81	0.61
7:7:720:THR:HA	7:7:723:GLN:HB3	1.81	0.61
9:O:191:PRO:HG3	24:M:272:LYS:HA	1.82	0.61
12:A:1342:GLU:OE2	16:E:212:ARG:NE	2.32	0.61
13:B:211:VAL:HG21	13:B:483:LEU:HD13	1.82	0.61
13:B:901:PRO:HG3	23:L:58:LYS:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:H:85:GLY:O	19:H:87:ARG:NH2	2.33	0.61
7:7:617:GLU:OE2	7:7:621:LYS:NZ	2.32	0.61
14:C:99:LEU:O	14:C:157:CYS:N	2.33	0.61
15:D:184:ALA:H	18:G:144:ARG:HH22	1.48	0.61
5:2:475:ALA:HA	5:2:478:ILE:HG12	1.81	0.61
7:7:630:SER:H	7:7:657:VAL:HG21	1.66	0.61
7:7:726:LEU:HD12	7:7:733:PHE:HD1	1.65	0.61
12:A:871:ASP:OD2	12:A:1366:ARG:NH2	2.34	0.61
1:1:283:PHE:HD1	1:1:284:TRP:HD1	1.48	0.61
4:6:137:LEU:HA	4:6:144:ASN:HD22	1.66	0.61
13:B:818:PRO:HG3	21:J:54:VAL:HG21	1.82	0.61
14:C:75:MET:SD	14:C:246:ARG:NH2	2.74	0.61
1:1:510:ASN:O	1:1:513:GLN:NE2	2.32	0.61
3:0:17:ILE:HG13	3:0:18:TYR:H	1.65	0.61
7:7:577:ARG:HG2	7:7:580:LEU:HB2	1.83	0.61
15:D:67:ARG:HG2	15:D:71:LYS:HE3	1.83	0.61
1:1:251:LEU:HD22	1:1:255:LYS:HE3	1.83	0.61
5:2:222:LEU:HA	5:2:225:ILE:HB	1.82	0.61
13:B:650:GLU:HB3	13:B:654:ARG:HH22	1.64	0.61
2:4:288:ILE:HG13	2:4:293:LEU:HA	1.83	0.61
4:6:177:GLY:N	4:6:207:ASN:O	2.29	0.61
4:6:196:LEU:O	4:6:200:ARG:N	2.25	0.61
4:6:406:CYS:SG	4:6:407:GLN:N	2.74	0.61
7:7:595:ILE:O	7:7:599:GLU:N	2.31	0.61
12:A:337:ARG:NE	13:B:1132:GLU:OE2	2.27	0.61
12:A:926:GLN:NE2	12:A:930:ASP:OD1	2.34	0.61
2:4:182:GLY:N	2:4:215:ILE:O	2.29	0.60
3:0:111:ARG:NH1	3:0:130:ASP:OD1	2.33	0.60
6:5:53:GLU:HA	6:5:56:ARG:HB2	1.83	0.60
7:7:384:ILE:HG23	7:7:536:TYR:HD2	1.65	0.60
7:7:541:MET:HE1	7:7:552:VAL:HG11	1.83	0.60
12:A:427:GLN:HB2	12:A:430:TRP:CE2	2.36	0.60
12:A:791:ASP:OD1	12:A:793:SER:OG	2.19	0.60
12:A:1152:ILE:HB	20:I:44:TYR:HB3	1.83	0.60
13:B:901:PRO:HD3	23:L:58:LYS:HG3	1.82	0.60
21:J:7:CYS:HB2	21:J:49:MET:HG3	1.82	0.60
3:0:19:PRO:HB2	3:0:486:THR:HG21	1.83	0.60
7:7:115:SER:N	7:7:137:SER:O	2.31	0.60
7:7:551:ASN:ND2	7:7:702:ASN:OD1	2.32	0.60
8:3:27:LYS:HB3	8:3:29:LEU:HG	1.82	0.60
9:O:68:GLN:O	9:O:127:LYS:NZ	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:T:130:DA:H2"	11:T:131:DC:H5"	1.83	0.60
13:B:120:ARG:NH2	13:B:956:THR:OG1	2.35	0.60
1:1:284:TRP:HA	1:1:287:PHE:HB3	1.83	0.60
4:6:328:ILE:N	4:6:346:GLY:O	2.29	0.60
4:6:175:ARG:NH2	4:6:203:GLU:O	2.35	0.60
4:6:336:CYS:N	4:6:341:LYS:O	2.34	0.60
7:7:722:ARG:O	7:7:726:LEU:N	2.33	0.60
12:A:860:LEU:HD11	12:A:1394:THR:HA	1.83	0.60
13:B:260:GLY:O	13:B:267:ARG:NH2	2.30	0.60
15:D:71:LYS:HA	15:D:74:GLN:HB3	1.82	0.60
16:E:8:ASN:OD1	16:E:8:ASN:N	2.34	0.60
5:2:80:SER:O	5:2:83:SER:OG	2.14	0.60
7:7:351:ASP:HA	7:7:405:LYS:HG2	1.83	0.60
1:1:478:UNK:O	1:1:482:UNK:N	2.34	0.60
5:2:399:TYR:O	5:2:403:HIS:N	2.24	0.60
7:7:497:MET:HA	7:7:500:ARG:HE	1.65	0.60
11:T:131:DC:OP1	25:Q:327:ARG:N	2.35	0.60
12:A:951:GLU:OE2	12:A:953:ASN:ND2	2.34	0.60
13:B:1134:GLU:OE1	13:B:1134:GLU:N	2.30	0.60
14:C:8:VAL:HG11	22:K:105:PHE:HD1	1.66	0.60
15:D:39:ASN:ND2	15:D:43:GLU:OE1	2.35	0.60
7:7:421:ARG:HG3	7:7:454:VAL:HG11	1.83	0.60
7:7:556:GLU:HB2	7:7:733:PHE:CE1	2.36	0.60
12:A:306:ASN:HB2	12:A:324:SER:HB3	1.82	0.60
12:A:506:ALA:HB3	12:A:509:LEU:HG	1.81	0.60
14:C:69:LEU:O	21:J:6:ARG:NH2	2.34	0.60
3:0:97:LEU:O	3:0:100:GLN:NE2	2.33	0.60
3:0:439:CYS:SG	3:0:440:LEU:N	2.75	0.60
5:2:221:VAL:O	5:2:225:ILE:N	2.30	0.60
7:7:353:ASP:OD1	7:7:404:LYS:NZ	2.35	0.60
7:7:674:SER:O	7:7:722:ARG:NH2	2.34	0.60
12:A:475:THR:OG1	12:A:480:ALA:O	2.18	0.60
20:I:14:LEU:HB3	20:I:27:PHE:HB3	1.84	0.60
20:I:59:VAL:HG23	20:I:61:ASP:H	1.66	0.60
1:1:194:VAL:O	1:1:198:THR:OG1	2.17	0.60
1:1:382:SER:O	1:1:386:ILE:N	2.32	0.60
3:0:21:GLN:O	3:0:25:MET:N	2.30	0.60
7:7:391:GLY:HA2	7:7:394:LEU:HD13	1.84	0.60
7:7:515:ALA:HB1	7:7:685:GLN:HB2	1.84	0.60
12:A:250:ILE:O	12:A:258:GLY:N	2.35	0.60
13:B:652:LYS:HB3	13:B:689:LEU:HD22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:D:198:LEU:HD23	15:D:201:LYS:HG3	1.83	0.60
16:E:28:TYR:HA	16:E:64:PRO:HA	1.82	0.60
18:G:45:ILE:HG13	18:G:78:VAL:HG12	1.82	0.60
24:M:298:VAL:HG13	24:M:302:LEU:HD13	1.84	0.60
6:5:42:VAL:HB	6:5:47:VAL:HG22	1.82	0.60
7:7:371:SER:HA	7:7:374:PHE:HB2	1.84	0.60
7:7:597:TYR:HA	7:7:600:ARG:HH21	1.67	0.60
12:A:335:ARG:HH21	13:B:1114:LEU:HD21	1.66	0.60
20:I:103:CYS:SG	20:I:105:SER:N	2.75	0.60
1:1:498:UNK:O	1:1:502:ARG:N	2.34	0.59
3:0:644:GLU:O	3:0:647:ARG:NH1	2.35	0.59
21:J:32:GLU:OE1	21:J:32:GLU:N	2.30	0.59
27:U:269:ILE:HG12	28:V:111:LEU:HD21	1.82	0.59
3:0:44:SER:HA	3:0:48:LYS:HZ3	1.67	0.59
3:0:675:ASP:OD1	3:0:676:TYR:N	2.36	0.59
3:0:751:ARG:O	3:0:754:GLN:NE2	2.35	0.59
7:7:598:HIS:CD2	7:7:603:ASP:HB2	2.37	0.59
11:T:135:DG:H2'	11:T:136:DA:C8	2.37	0.59
12:A:250:ILE:HG23	24:M:62:GLU:HB2	1.84	0.59
18:G:100:GLU:HA	18:G:109:PHE:HA	1.84	0.59
24:M:39:SER:OG	24:M:40:GLU:OE1	2.19	0.59
29:W:143:ASP:OD1	29:W:143:ASP:N	2.29	0.59
2:4:52:LYS:NZ	2:4:242:GLU:O	2.31	0.59
7:7:242:LEU:O	7:7:246:LEU:N	2.27	0.59
7:7:345:ASN:O	7:7:508:HIS:NE2	2.35	0.59
12:A:999:VAL:H	12:A:1011:GLN:HE22	1.50	0.59
13:B:975:GLN:N	13:B:978:ASP:OD2	2.30	0.59
15:D:197:SER:O	15:D:201:LYS:NZ	2.28	0.59
16:E:192:ARG:NH1	16:E:215:MET:O	2.35	0.59
3:0:68:LYS:HG3	3:0:226:VAL:HA	1.84	0.59
3:0:210:TYR:O	3:0:214:LEU:N	2.32	0.59
3:0:274:VAL:O	3:0:278:ASP:N	2.32	0.59
3:0:573:THR:OG1	3:0:575:ASP:O	2.19	0.59
5:2:484:LYS:NZ	5:2:486:ASP:OD1	2.35	0.59
12:A:175:ARG:HH22	12:A:184:SER:HB2	1.67	0.59
3:0:692:GLN:OE1	3:0:692:GLN:N	2.35	0.59
7:7:461:ALA:HB1	7:7:500:ARG:HB3	1.83	0.59
7:7:669:CYS:HA	7:7:704:PHE:HB2	1.84	0.59
13:B:68:THR:HG22	13:B:91:SER:HB3	1.85	0.59
16:E:61:GLN:HG3	16:E:105:PHE:HE1	1.68	0.59
6:5:14:PRO:HA	6:5:17:LYS:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:699:GLU:O	7:7:702:ASN:ND2	2.36	0.59
3:0:489:LYS:NZ	3:0:728:THR:OG1	2.33	0.59
7:7:303:ARG:HG2	7:7:304:GLU:H	1.68	0.59
7:7:366:GLN:O	7:7:370:LEU:N	2.29	0.59
7:7:593:PHE:HA	7:7:596:GLN:HG2	1.83	0.59
12:A:491:VAL:O	13:B:1150:ARG:NH2	2.34	0.59
12:A:1444:MET:HB2	17:F:133:VAL:HG13	1.84	0.59
14:C:75:MET:O	14:C:246:ARG:NH2	2.31	0.59
18:G:33:GLU:HG3	18:G:34:VAL:HG23	1.84	0.59
4:6:162:ASP:O	4:6:378:ARG:NH2	2.35	0.59
4:6:176:ASN:HA	4:6:206:GLY:HA3	1.85	0.59
5:2:50:MET:HB3	5:2:100:LEU:HG	1.83	0.59
7:7:386:LEU:HD12	7:7:513:LEU:HD22	1.85	0.59
7:7:409:VAL:O	7:7:455:SER:N	2.35	0.59
7:7:474:MET:HA	7:7:477:LEU:HB2	1.85	0.59
7:7:477:LEU:HA	7:7:482:TRP:NE1	2.12	0.59
7:7:603:ASP:OD1	7:7:696:ARG:NH1	2.36	0.59
7:7:635:GLU:O	7:7:638:ASN:ND2	2.36	0.59
13:B:46:GLN:OE1	13:B:46:GLN:N	2.36	0.59
13:B:324:ILE:HG21	13:B:330:ALA:HB2	1.83	0.59
3:0:227:SER:OG	3:0:452:ARG:NH2	2.30	0.59
3:0:250:LEU:N	3:0:437:PHE:O	2.35	0.59
4:6:260:ARG:HG2	4:6:281:ASN:HA	1.85	0.59
5:2:352:ASN:N	5:2:352:ASN:OD1	2.35	0.59
7:7:331:GLN:HE22	7:7:523:LYS:HB2	1.68	0.59
7:7:387:PRO:HG2	7:7:540:TRP:HZ2	1.68	0.59
7:7:439:THR:O	7:7:440:SER:OG	2.18	0.59
12:A:525:GLN:HG3	13:B:835:GLN:HB3	1.83	0.59
19:H:110:ASP:OD1	19:H:110:ASP:N	2.31	0.59
3:0:50:VAL:O	3:0:54:SER:OG	2.17	0.59
5:2:32:CYS:HB3	5:2:108:LEU:HB2	1.85	0.59
12:A:438:ASP:OD1	12:A:438:ASP:N	2.33	0.59
12:A:767:GLN:NE2	12:A:798:GLY:O	2.36	0.59
13:B:843:GLN:NE2	13:B:847:ASP:OD1	2.34	0.59
19:H:8:ASP:OD1	19:H:9:ILE:N	2.36	0.59
25:Q:102:PRO:O	25:Q:383:SER:OG	2.19	0.59
28:V:62:VAL:HA	28:V:85:VAL:HA	1.84	0.59
3:0:625:ILE:HD12	3:0:626:PRO:HD2	1.84	0.58
5:2:378:ILE:HD11	5:2:383:ILE:HG22	1.84	0.58
7:7:413:SER:O	7:7:417:VAL:HG23	2.03	0.58
12:A:326:ARG:NH2	12:A:1407:GLU:OE2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:413:ILE:HG12	24:M:50:LEU:HD12	1.85	0.58
12:A:417:TYR:HE2	24:M:35:VAL:HG21	1.68	0.58
12:A:782:ARG:NH2	13:B:699:GLU:O	2.36	0.58
12:A:1209:MET:HB2	12:A:1228:TRP:CD1	2.38	0.58
13:B:451:LYS:O	13:B:455:SER:OG	2.16	0.58
15:D:151:PHE:O	15:D:153:ARG:NH1	2.36	0.58
16:E:191:LYS:N	16:E:194:GLU:OE1	2.36	0.58
7:7:443:LYS:NZ	7:7:444:GLU:O	2.36	0.58
7:7:757:ARG:O	7:7:761:GLN:NE2	2.35	0.58
18:G:152:SER:HA	18:G:157:ILE:HG12	1.85	0.58
23:L:30:ILE:HB	23:L:57:LEU:HB2	1.85	0.58
24:M:251:GLN:OE1	24:M:251:GLN:N	2.33	0.58
25:Q:141:ARG:NE	25:Q:348:TYR:O	2.35	0.58
29:W:110:LYS:HZ2	29:W:172:LEU:HD13	1.68	0.58
1:1:249:UNK:O	1:1:252:SER:OG	2.20	0.58
3:0:169:ASP:O	3:0:198:ARG:NH1	2.26	0.58
5:2:453:THR:HG23	6:5:10:VAL:HA	1.85	0.58
12:A:42:ASP:HB3	12:A:46:THR:H	1.68	0.58
13:B:629:ASP:O	13:B:632:ARG:NH2	2.35	0.58
25:Q:343:ARG:O	25:Q:343:ARG:NH2	2.35	0.58
3:0:92:TYR:OH	3:0:96:GLU:OE2	2.20	0.58
4:6:200:ARG:NH1	5:2:425:ASN:O	2.36	0.58
5:2:450:ARG:HH11	6:5:16:ILE:HG13	1.69	0.58
9:O:93:GLU:O	9:O:103:ILE:N	2.30	0.58
12:A:261:ASP:HB3	12:A:322:VAL:HG13	1.84	0.58
12:A:433:GLU:OE2	13:B:1108:ARG:NH2	2.36	0.58
12:A:1010:ALA:O	12:A:1014:ALA:N	2.36	0.58
14:C:120:ILE:HD13	14:C:124:LEU:HD21	1.85	0.58
18:G:125:SER:OG	18:G:129:SER:N	2.36	0.58
20:I:7:CYS:HB3	20:I:12:ASN:H	1.68	0.58
4:6:277:CYS:HB3	4:6:287:PHE:HB2	1.85	0.58
6:5:55:ASN:HA	6:5:58:LEU:HD23	1.84	0.58
13:B:21:GLU:HA	13:B:655:LYS:HB2	1.85	0.58
25:Q:366:GLU:OE1	25:Q:366:GLU:N	2.36	0.58
2:4:161:ASN:O	2:4:165:LYS:N	2.35	0.58
3:0:238:HIS:O	3:0:660:ARG:NH1	2.37	0.58
4:6:136:MET:O	4:6:144:ASN:ND2	2.37	0.58
4:6:218:ARG:NH1	4:6:257:GLU:OE2	2.36	0.58
9:O:144:GLN:NE2	9:O:150:ALA:O	2.36	0.58
18:G:86:VAL:HA	18:G:146:LYS:HA	1.85	0.58
21:J:17:LYS:HG2	21:J:41:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:L:28:LYS:HA	23:L:39:SER:HA	1.86	0.58
27:U:281:VAL:HG21	28:V:113:ILE:HG12	1.86	0.58
2:4:193:TYR:HA	2:4:196:ILE:HD12	1.84	0.58
5:2:485:ASP:HB2	5:2:487:LYS:HG2	1.84	0.58
7:7:584:ASN:HB3	7:7:587:LYS:HB3	1.85	0.58
9:O:68:GLN:N	9:O:161:VAL:O	2.29	0.58
12:A:47:ARG:H	12:A:47:ARG:HD3	1.68	0.58
12:A:731:ARG:NH1	12:A:734:GLU:OE1	2.37	0.58
15:D:66:ARG:O	15:D:70:PHE:N	2.34	0.58
28:V:78:PHE:O	28:V:113:ILE:N	2.33	0.58
30:X:196:LEU:HD22	30:X:245:TRP:H	1.69	0.58
1:1:548:GLU:HA	1:1:551:ARG:HB3	1.86	0.58
3:0:722:ARG:HG2	4:6:267:SER:HB2	1.85	0.58
7:7:224:LYS:H	7:7:337:VAL:HG12	1.68	0.58
7:7:412:THR:HA	7:7:457:TYR:CD2	2.37	0.58
8:3:83:ASP:O	8:3:87:ARG:N	2.26	0.58
9:O:102:VAL:HB	9:O:115:ILE:HB	1.86	0.58
15:D:39:ASN:ND2	15:D:41:GLN:OE1	2.36	0.58
19:H:93:TYR:HA	19:H:145:ARG:HB3	1.85	0.58
30:X:218:ASP:OD1	30:X:218:ASP:N	2.36	0.58
3:0:353:SER:HB2	3:0:417:LEU:HD11	1.86	0.58
4:6:159:GLU:O	4:6:163:GLN:NE2	2.37	0.58
4:6:210:LEU:HB3	4:6:241:THR:HB	1.86	0.58
4:6:293:ASP:OD2	4:6:295:THR:OG1	2.16	0.58
5:2:384:ARG:O	5:2:388:THR:N	2.36	0.58
6:5:43:ASN:HB3	6:5:46:LYS:HG3	1.84	0.58
9:O:195:TYR:HB3	9:O:204:LEU:HB2	1.86	0.58
12:A:526:ASP:O	12:A:530:GLY:N	2.27	0.58
12:A:771:GLU:N	12:A:822:GLU:OE2	2.32	0.58
12:A:1111:MET:SD	12:A:1330:ASN:ND2	2.77	0.58
12:A:1293:SER:N	12:A:1297:GLU:O	2.37	0.58
24:M:133:ILE:HA	24:M:136:LEU:HB2	1.85	0.58
1:1:207:SER:OG	1:1:208:GLU:OE1	2.19	0.58
1:1:483:UNK:O	1:1:485:UNK:N	2.37	0.58
10:N:37:DC:H2'	10:N:38:DG:C8	2.38	0.58
12:A:672:ASP:OD1	12:A:672:ASP:N	2.37	0.58
12:A:1079:MET:HE3	12:A:1359:ASP:HB3	1.86	0.58
12:A:1141:THR:OG1	12:A:1274:ARG:N	2.36	0.58
3:0:99:TYR:OH	3:0:173:LYS:NZ	2.34	0.57
3:0:286:TYR:O	3:0:326:ARG:NH1	2.28	0.57
3:0:690:ARG:NH2	3:0:701:LEU:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:378:ARG:O	4:6:382:HIS:ND1	2.37	0.57
7:7:582:ILE:HG12	7:7:673:ILE:HG22	1.86	0.57
7:7:654:LEU:HD22	7:7:662:ILE:HD11	1.86	0.57
13:B:298:LEU:HD23	13:B:311:LEU:HD22	1.84	0.57
18:G:138:THR:O	18:G:141:SER:OG	2.21	0.57
29:W:32:ILE:HD11	29:W:58:ILE:HD12	1.86	0.57
2:4:66:ALA:O	5:2:37:ARG:NE	2.37	0.57
3:0:354:GLU:N	3:0:418:LEU:O	2.37	0.57
4:6:188:ASN:ND2	4:6:191:ASP:OD1	2.37	0.57
5:2:11:THR:HA	5:2:14:LEU:HD22	1.86	0.57
7:7:682:GLN:O	7:7:686:ARG:N	2.37	0.57
14:C:102:GLN:HG3	14:C:154:LYS:HG2	1.85	0.57
1:1:475:UNK:O	1:1:479:UNK:N	2.38	0.57
3:0:288:LYS:O	3:0:291:GLN:NE2	2.37	0.57
5:2:42:LEU:H	5:2:42:LEU:HD22	1.69	0.57
6:5:27:MET:HE2	6:5:49:PHE:HD2	1.67	0.57
7:7:234:VAL:N	7:7:316:PHE:H	1.95	0.57
7:7:244:MET:O	7:7:248:ASP:N	2.38	0.57
12:A:658:LEU:HD12	13:B:831:SER:HA	1.84	0.57
13:B:1049:ASP:OD1	13:B:1049:ASP:N	2.35	0.57
20:I:10:CYS:SG	20:I:31:THR:OG1	2.62	0.57
2:4:288:ILE:HD12	2:4:293:LEU:HD13	1.85	0.57
5:2:350:TYR:H	5:2:407:GLN:CD	2.11	0.57
7:7:712:ASP:N	7:7:716:MET:SD	2.72	0.57
12:A:1044:TRP:O	12:A:1048:ASN:ND2	2.33	0.57
12:A:1141:THR:HG22	12:A:1205:LYS:HD2	1.84	0.57
13:B:323:VAL:HG23	13:B:324:ILE:HG13	1.86	0.57
1:1:547:LEU:O	1:1:551:ARG:N	2.30	0.57
1:1:558:CYS:O	1:1:562:LYS:N	2.33	0.57
3:0:647:ARG:O	3:0:649:ARG:NH2	2.28	0.57
7:7:576:LYS:HG2	7:7:579:LEU:HD12	1.86	0.57
7:7:724:ALA:O	7:7:728:ASP:N	2.38	0.57
12:A:41:MET:O	24:M:90:ASN:ND2	2.37	0.57
13:B:861:ASP:OD2	13:B:939:THR:OG1	2.16	0.57
13:B:1219:ASP:N	13:B:1219:ASP:OD1	2.38	0.57
16:E:118:PRO:O	16:E:122:LYS:N	2.34	0.57
3:0:645:ASN:O	3:0:647:ARG:NH2	2.37	0.57
5:2:384:ARG:HA	5:2:387:LEU:HB2	1.86	0.57
13:B:356:LEU:O	13:B:374:LYS:NZ	2.32	0.57
22:K:58:PHE:HE2	22:K:74:ARG:HD3	1.69	0.57
24:M:189:PHE:O	24:M:193:GLN:N	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:83:ILE:HG21	2:4:152:ALA:HB2	1.86	0.57
6:5:14:PRO:O	6:5:18:ALA:N	2.30	0.57
7:7:343:PHE:CD2	7:7:380:ARG:HB2	2.34	0.57
7:7:366:GLN:HE22	7:7:394:LEU:HB2	1.69	0.57
7:7:608:PHE:HB2	7:7:690:ILE:HG21	1.87	0.57
15:D:66:ARG:NH2	18:G:48:VAL:O	2.36	0.57
23:L:53:HIS:O	23:L:54:ARG:NH1	2.37	0.57
29:W:109:LEU:HD21	29:W:171:LYS:HB3	1.87	0.57
8:3:86:LYS:O	8:3:90:ASN:N	2.36	0.57
14:C:55:THR:HG1	14:C:152:GLU:H	1.53	0.57
18:G:87:VAL:N	18:G:145:VAL:O	2.26	0.57
24:M:315:ILE:O	24:M:319:HIS:NE2	2.38	0.57
1:1:544:ILE:O	1:1:548:GLU:N	2.30	0.57
3:0:1:MET:HB2	3:0:12:PHE:HB3	1.87	0.57
3:0:78:GLU:HA	3:0:81:LYS:HD2	1.87	0.57
3:0:117:HIS:CE1	3:0:119:GLU:HB3	2.39	0.57
6:5:24:ASP:HB3	6:5:29:ASP:CG	2.29	0.57
7:7:434:ASN:OD1	7:7:450:SER:OG	2.23	0.57
7:7:461:ALA:HB3	7:7:501:VAL:HG12	1.87	0.57
12:A:1287:TYR:OH	12:A:1307:GLU:OE2	2.22	0.57
13:B:364:ILE:HG13	13:B:365:THR:HG22	1.85	0.57
14:C:184:ASN:ND2	14:C:189:THR:O	2.34	0.57
25:Q:100:GLU:HG3	26:R:94:LYS:HG2	1.87	0.57
3:0:104:ARG:O	3:0:204:ASN:N	2.37	0.57
3:0:212:TYR:HA	3:0:218:ILE:HG13	1.87	0.57
5:2:59:LEU:HD11	5:2:507:ARG:HH12	1.70	0.57
7:7:361:GLN:HG2	7:7:424:PHE:HE1	1.69	0.57
7:7:396:GLY:O	7:7:400:ALA:N	2.24	0.57
13:B:756:ILE:HG12	13:B:770:GLN:HG2	1.87	0.57
20:I:78:CYS:SG	20:I:105:SER:OG	2.62	0.57
5:2:200:LEU:O	5:2:204:LEU:N	2.31	0.56
5:2:351:SER:N	5:2:407:GLN:OE1	2.29	0.56
5:2:437:VAL:O	5:2:441:ILE:N	2.33	0.56
7:7:212:PHE:O	7:7:216:ALA:N	2.32	0.56
7:7:625:PRO:HB2	7:7:639:ILE:HG12	1.86	0.56
12:A:54:ASN:OD1	12:A:54:ASN:N	2.37	0.56
12:A:1193:LEU:HD23	12:A:1240:CYS:HB3	1.87	0.56
13:B:101:MET:N	13:B:101:MET:SD	2.77	0.56
19:H:40:LEU:HD13	19:H:123:MET:HB2	1.86	0.56
3:0:8:LEU:HD23	3:0:62:HIS:HB3	1.86	0.56
3:0:80:GLU:HB3	3:0:178:PHE:HD2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:489:GLU:HB2	7:7:491:HIS:CE1	2.40	0.56
7:7:725:PHE:O	7:7:729:GLN:NE2	2.37	0.56
14:C:6:PRO:HG2	22:K:101:LEU:HD13	1.87	0.56
15:D:39:ASN:HD21	15:D:41:GLN:HB2	1.70	0.56
25:Q:337:GLU:CD	25:Q:340:LYS:H	2.12	0.56
26:R:75:MET:SD	26:R:76:PHE:N	2.78	0.56
2:4:32:ILE:HD11	2:4:79:TYR:HD1	1.70	0.56
3:0:116:LEU:N	32:0:801:SF4:S3	2.78	0.56
3:0:208:TYR:CD2	3:0:212:TYR:HB2	2.40	0.56
3:0:587:ARG:HH21	3:0:612:PHE:HA	1.69	0.56
12:A:340:LEU:HD13	12:A:1429:ILE:HG23	1.87	0.56
12:A:690:VAL:O	12:A:694:THR:OG1	2.23	0.56
12:A:890:ASP:O	12:A:894:GLU:N	2.32	0.56
22:K:29:ASN:ND2	22:K:77:THR:OG1	2.38	0.56
24:M:181:ARG:NH1	24:M:234:GLN:OE1	2.38	0.56
1:1:561:LEU:HA	1:1:564:PHE:HB2	1.85	0.56
2:4:122:ASP:O	2:4:126:VAL:N	2.38	0.56
4:6:379:SER:O	4:6:383:LEU:N	2.35	0.56
4:6:403:CYS:HB2	4:6:437:CYS:HB3	1.86	0.56
6:5:20:ILE:HA	6:5:23:ILE:HB	1.88	0.56
7:7:258:SER:O	7:7:317:GLU:N	2.28	0.56
10:N:6:DA:C2	10:N:7:DA:C5	2.94	0.56
12:A:114:LEU:HD13	12:A:145:LYS:HB3	1.87	0.56
13:B:216:GLU:OE1	13:B:537:LYS:NZ	2.39	0.56
16:E:55:ARG:NH1	16:E:113:GLN:OE1	2.39	0.56
16:E:173:SER:O	16:E:177:ARG:NH1	2.36	0.56
2:4:274:THR:HG23	2:4:295:VAL:HG11	1.87	0.56
2:4:303:ASN:HA	2:4:312:PHE:H	1.71	0.56
4:6:310:VAL:HG13	4:6:311:ASN:H	1.70	0.56
4:6:390:ALA:N	4:6:428:ARG:O	2.38	0.56
6:5:27:MET:O	6:5:28:SER:OG	2.21	0.56
7:7:372:LYS:HB3	7:7:535:LEU:HD12	1.88	0.56
7:7:670:LEU:N	7:7:704:PHE:O	2.35	0.56
7:7:752:SER:HG	7:7:755:GLU:H	1.51	0.56
16:E:19:VAL:HG22	16:E:140:LEU:HD13	1.88	0.56
5:2:197:ASN:O	5:2:201:TRP:N	2.35	0.56
7:7:315:SER:OG	7:7:316:PHE:N	2.33	0.56
7:7:348:ARG:H	7:7:508:HIS:CE1	2.23	0.56
7:7:383:ILE:HG13	7:7:528:ASN:HA	1.85	0.56
7:7:457:TYR:HH	7:7:488:ASP:H	1.53	0.56
19:H:5:LEU:HD11	19:H:61:SER:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Q:370:SER:HB3	25:Q:392:VAL:HG12	1.88	0.56
2:4:117:ARG:HA	2:4:120:ASN:HD21	1.70	0.56
3:0:32:LEU:HB3	3:0:59:TYR:CZ	2.40	0.56
3:0:394:GLU:O	3:0:397:THR:OG1	2.22	0.56
5:2:50:MET:HE2	5:2:100:LEU:H	1.70	0.56
7:7:491:HIS:CG	7:7:681:ARG:HH11	2.23	0.56
7:7:554:CYS:O	7:7:734:LYS:N	2.39	0.56
7:7:566:TYR:O	7:7:570:LEU:N	2.34	0.56
12:A:146:MET:HA	12:A:171:GLN:HB2	1.88	0.56
12:A:809:THR:OG1	12:A:812:GLU:OE2	2.23	0.56
13:B:969:ARG:NH2	14:C:60:ASP:OD2	2.39	0.56
13:B:1187:ASN:ND2	13:B:1190:ASP:O	2.39	0.56
18:G:101:VAL:N	18:G:108:VAL:O	2.25	0.56
2:4:162:ARG:HD2	4:6:406:CYS:HB2	1.87	0.56
3:0:291:GLN:HE22	3:0:294:HIS:HA	1.70	0.56
3:0:690:ARG:HG3	3:0:701:LEU:HD23	1.87	0.56
3:0:740:SER:H	3:0:744:LEU:HD22	1.69	0.56
7:7:485:ILE:HB	7:7:510:LYS:HA	1.87	0.56
12:A:405:VAL:HG23	12:A:415:LEU:HD21	1.86	0.56
12:A:1143:LEU:HB2	12:A:1273:LEU:HD21	1.88	0.56
13:B:71:LEU:O	13:B:88:TYR:N	2.27	0.56
13:B:693:ILE:HG23	13:B:697:GLU:HB3	1.87	0.56
13:B:983:ARG:NH2	13:B:1028:GLU:OE2	2.35	0.56
3:0:744:LEU:O	3:0:748:GLN:N	2.32	0.56
4:6:200:ARG:HH21	4:6:201:LYS:HE3	1.70	0.56
6:5:49:PHE:HA	6:5:52:HIS:CD2	2.41	0.56
7:7:363:ARG:HA	7:7:695:ARG:CZ	2.35	0.56
7:7:476:PHE:O	7:7:480:ARG:N	2.33	0.56
13:B:294:ASP:OD1	13:B:294:ASP:N	2.38	0.56
13:B:603:LEU:HB3	13:B:608:ASP:HB2	1.88	0.56
18:G:49:LEU:HD21	18:G:75:ARG:HG2	1.87	0.56
19:H:80:ARG:HG2	22:K:57:LEU:HD22	1.88	0.56
24:M:253:THR:O	24:M:257:GLU:N	2.34	0.56
25:Q:374:VAL:HG22	25:Q:388:PRO:HB3	1.88	0.56
26:R:258:THR:HG22	26:R:261:VAL:HG22	1.88	0.56
1:1:350:ARG:NH1	3:0:401:ASP:OD1	2.38	0.56
2:4:258:LEU:H	2:4:258:LEU:HD12	1.69	0.56
5:2:473:LYS:O	5:2:477:ASP:N	2.39	0.56
7:7:468:HIS:ND1	7:7:471:GLN:OE1	2.39	0.56
7:7:591:CYS:HA	7:7:594:LEU:HD12	1.87	0.56
12:A:225:ASN:N	12:A:229:SER:OG	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:849:MET:HE2	12:A:1061:GLY:HA2	1.87	0.56
13:B:982:SER:OG	13:B:983:ARG:N	2.37	0.56
25:Q:340:LYS:O	25:Q:344:PHE:N	2.36	0.56
1:1:348:VAL:HG12	3:0:127:THR:HG22	1.87	0.55
3:0:314:GLN:HA	3:0:317:LEU:HD13	1.88	0.55
5:2:56:GLU:HB2	5:2:99:ASN:HB3	1.88	0.55
7:7:637:MET:N	7:7:637:MET:SD	2.79	0.55
8:3:31:ASN:HB3	8:3:34:CYS:HB2	1.87	0.55
12:A:599:SER:O	12:A:599:SER:OG	2.17	0.55
13:B:805:THR:OG1	13:B:806:THR:N	2.40	0.55
18:G:35:GLU:OE2	18:G:48:VAL:N	2.32	0.55
19:H:81:PRO:O	19:H:83:GLN:NE2	2.38	0.55
3:0:256:ALA:O	3:0:260:ALA:N	2.36	0.55
3:0:378:SER:OG	3:0:403:ALA:O	2.23	0.55
3:0:625:ILE:HG22	3:0:685:ARG:HH21	1.72	0.55
4:6:156:PHE:HB2	4:6:301:PHE:CD2	2.40	0.55
5:2:62:LEU:HA	5:2:65:TRP:CD1	2.41	0.55
5:2:202:THR:O	5:2:206:GLN:N	2.33	0.55
5:2:222:LEU:HD22	5:2:225:ILE:HD12	1.87	0.55
12:A:217:LYS:O	12:A:217:LYS:NZ	2.38	0.55
12:A:230:ARG:HB2	12:A:233:TRP:CD2	2.41	0.55
13:B:573:GLN:OE1	13:B:573:GLN:N	2.39	0.55
15:D:140:ASP:O	15:D:144:THR:N	2.26	0.55
19:H:87:ARG:NH1	19:H:91:ASP:OD2	2.39	0.55
25:Q:123:SER:HB3	25:Q:361:TRP:HH2	1.71	0.55
25:Q:351:VAL:HG22	25:Q:362:VAL:HG22	1.87	0.55
1:1:510:ASN:HB3	2:4:264:LYS:HG3	1.88	0.55
6:5:22:GLN:H	6:5:22:GLN:CD	2.13	0.55
7:7:580:LEU:HD11	7:7:764:LEU:HA	1.87	0.55
7:7:596:GLN:HA	7:7:599:GLU:HB2	1.88	0.55
12:A:900:ASP:N	12:A:900:ASP:OD1	2.39	0.55
16:E:157:SER:N	16:E:160:GLU:OE1	2.39	0.55
25:Q:374:VAL:HA	25:Q:388:PRO:HA	1.87	0.55
5:2:234:GLY:O	5:2:269:PHE:N	2.40	0.55
7:7:365:TYR:HB2	7:7:543:LEU:O	2.06	0.55
7:7:694:LYS:HG3	7:7:696:ARG:HB2	1.88	0.55
12:A:367:PRO:HB3	12:A:466:SER:HA	1.87	0.55
12:A:840:ARG:NH1	12:A:1106:ASN:OD1	2.36	0.55
13:B:766:ARG:NH1	13:B:985:GLY:O	2.39	0.55
24:M:41:GLY:HA2	24:M:56:LEU:HD23	1.87	0.55
29:W:65:ARG:HB3	29:W:93:HIS:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:185:LEU:HD12	1:1:191:LEU:HB3	1.89	0.55
12:A:78:PRO:O	13:B:1201:LYS:NZ	2.29	0.55
16:E:24:LYS:NZ	16:E:32:GLN:OE1	2.38	0.55
25:Q:361:TRP:HB3	25:Q:395:PHE:HD2	1.72	0.55
1:1:195:PHE:O	1:1:199:VAL:N	2.39	0.55
3:0:131:GLU:OE2	3:0:135:ARG:NH2	2.40	0.55
3:0:573:THR:OG1	3:0:579:THR:OG1	2.22	0.55
7:7:366:GLN:HG3	7:7:548:HIS:HE1	1.72	0.55
7:7:495:ALA:N	7:7:521:ASP:OD1	2.39	0.55
9:O:129:GLU:HB2	9:O:157:ILE:HD11	1.88	0.55
10:N:5:DA:C2	10:N:6:DA:C5	2.95	0.55
22:K:83:PRO:HA	22:K:86:ALA:HB3	1.89	0.55
24:M:132:LYS:HA	24:M:135:MET:HE2	1.88	0.55
25:Q:369:ASN:OD1	26:R:72:ARG:NH2	2.39	0.55
2:4:202:SER:O	2:4:206:MET:N	2.34	0.55
7:7:372:LYS:HE2	7:7:543:LEU:HD21	1.87	0.55
7:7:446:PHE:HB3	7:7:473:VAL:HG22	1.89	0.55
7:7:757:ARG:HH11	7:7:758:GLU:HA	1.72	0.55
9:O:158:GLN:HE21	10:N:23:DA:H4'	1.70	0.55
12:A:585:GLY:N	12:A:609:ASP:OD1	2.34	0.55
13:B:1074:ASN:ND2	13:B:1076:HIS:H	2.04	0.55
14:C:196:ASP:OD2	14:C:199:LYS:N	2.36	0.55
19:H:35:GLN:OE1	19:H:35:GLN:N	2.39	0.55
19:H:38:LEU:HB2	19:H:125:LEU:HD13	1.89	0.55
22:K:58:PHE:HB3	22:K:76:GLN:HB3	1.88	0.55
22:K:68:PHE:HB2	22:K:70:ARG:HG2	1.88	0.55
1:1:550:CYS:HA	1:1:553:LEU:HB3	1.88	0.55
3:0:116:LEU:HB3	3:0:158:TYR:CE2	2.42	0.55
9:O:66:THR:O	9:O:163:SER:N	2.39	0.55
13:B:120:ARG:NH2	13:B:957:ASN:O	2.39	0.55
15:D:63:LEU:HB3	15:D:130:LEU:HD22	1.89	0.55
15:D:212:LYS:O	15:D:216:ASN:N	2.38	0.55
2:4:182:GLY:HA3	2:4:216:GLY:HA3	1.88	0.55
5:2:176:VAL:O	5:2:181:GLU:N	2.37	0.55
5:2:187:GLU:O	5:2:191:PHE:N	2.40	0.55
6:5:51:LYS:HA	6:5:54:LEU:HB3	1.89	0.55
12:A:469:ARG:NH2	13:B:991:GLY:O	2.39	0.55
13:B:122:LEU:O	13:B:207:GLY:N	2.40	0.55
19:H:96:VAL:HA	19:H:142:LEU:O	2.06	0.55
3:0:137:THR:HG23	3:0:156:CYS:H	1.72	0.55
5:2:226:PHE:O	5:2:230:ALA:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:538:ASP:OD1	12:A:538:ASP:N	2.39	0.55
13:B:238:ALA:HB2	13:B:385:LEU:HD13	1.89	0.55
16:E:55:ARG:HG2	16:E:58:MET:HE2	1.89	0.55
16:E:84:ASP:O	16:E:113:GLN:NE2	2.39	0.55
18:G:39:THR:OG1	18:G:42:PHE:N	2.40	0.55
30:X:187:HIS:N	30:X:191:GLU:OE1	2.40	0.55
4:6:172:ILE:HA	4:6:181:LEU:HA	1.88	0.54
7:7:329:ARG:O	7:7:333:ILE:N	2.26	0.54
7:7:403:ILE:O	7:7:405:LYS:HG3	2.07	0.54
12:A:1323:ASP:OD1	12:A:1325:THR:OG1	2.20	0.54
13:B:127:GLY:HA2	13:B:169:ARG:HA	1.90	0.54
13:B:952:VAL:O	23:L:58:LYS:HB2	2.08	0.54
15:D:64:VAL:HG22	15:D:67:ARG:HH12	1.72	0.54
15:D:212:LYS:HA	15:D:215:SER:HB3	1.88	0.54
19:H:132:LEU:HA	19:H:135:LEU:HD21	1.89	0.54
24:M:40:GLU:OE1	24:M:40:GLU:N	2.40	0.54
29:W:101:LYS:NZ	30:X:263:TRP:O	2.30	0.54
4:6:189:PRO:O	4:6:193:ILE:N	2.34	0.54
6:5:24:ASP:O	6:5:29:ASP:N	2.40	0.54
7:7:384:ILE:HG23	7:7:536:TYR:CD2	2.41	0.54
7:7:544:SER:HB2	7:7:549:ILE:HB	1.90	0.54
13:B:806:THR:HG23	13:B:1045:SER:HA	1.88	0.54
14:C:54:ASN:ND2	14:C:60:ASP:OD1	2.34	0.54
19:H:28:ALA:HB3	19:H:38:LEU:HB3	1.89	0.54
1:1:254:GLU:OE1	1:1:254:GLU:N	2.34	0.54
1:1:375:LEU:HB3	3:0:571:VAL:HG11	1.89	0.54
2:4:137:LYS:H	2:4:140:ILE:HB	1.70	0.54
3:0:601:VAL:HG12	3:0:603:ARG:H	1.71	0.54
3:0:729:ASP:O	3:0:731:LYS:NZ	2.41	0.54
5:2:352:ASN:HB3	5:2:374:VAL:HG22	1.88	0.54
8:3:53:GLN:HG3	8:3:60:ASP:HA	1.89	0.54
13:B:129:PHE:HE2	26:R:266:THR:HG21	1.72	0.54
15:D:178:ALA:O	15:D:182:SER:N	2.31	0.54
24:M:58:ASP:OD1	24:M:60:ARG:N	2.33	0.54
27:U:282:GLU:N	28:V:62:VAL:O	2.40	0.54
2:4:180:THR:HG23	2:4:214:LYS:HA	1.89	0.54
3:0:419:ILE:HG23	3:0:436:ARG:HB3	1.89	0.54
6:5:36:ASP:HB2	6:5:39:HIS:CE1	2.42	0.54
9:O:161:VAL:HA	9:O:215:THR:HA	1.88	0.54
12:A:1364:ASN:HD21	12:A:1366:ARG:HH11	1.55	0.54
14:C:79:GLN:HB3	14:C:127:ARG:HE	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:D:118:THR:OG1	15:D:120:GLU:OE1	2.25	0.54
25:Q:140:HIS:HB3	26:R:209:PRO:HB3	1.89	0.54
3:0:139:GLY:HA3	3:0:302:GLN:HE21	1.73	0.54
3:0:337:ARG:HB3	3:0:367:THR:HG21	1.89	0.54
4:6:209:SER:HA	4:6:242:THR:HB	1.89	0.54
4:6:390:ALA:O	4:6:428:ARG:N	2.26	0.54
7:7:719:SER:O	7:7:723:GLN:N	2.40	0.54
9:O:76:LEU:O	9:O:151:LYS:N	2.36	0.54
24:M:283:TYR:HA	24:M:286:ILE:HG22	1.89	0.54
1:1:228:UNK:C	4:6:244:PRO:HG3	2.38	0.54
4:6:262:LYS:HZ3	4:6:287:PHE:C	2.14	0.54
5:2:370:PHE:CD2	5:2:373:MET:HB3	2.42	0.54
11:T:150:DG:H5”	24:M:276:THR:HG21	1.89	0.54
12:A:866:PHE:HE2	16:E:211:TYR:H	1.56	0.54
18:G:149:GLY:O	18:G:160:ILE:N	2.33	0.54
27:U:247:LEU:HB3	28:V:118:SER:HB3	1.90	0.54
2:4:27:THR:HG21	2:4:160:VAL:HG22	1.90	0.54
4:6:176:ASN:HA	4:6:207:ASN:H	1.72	0.54
5:2:21:VAL:HA	5:2:24:ARG:HB2	1.89	0.54
5:2:349:SER:HA	5:2:407:GLN:HE22	1.72	0.54
8:3:82:VAL:O	8:3:86:LYS:N	2.30	0.54
12:A:1239:ARG:NH1	12:A:1241:ARG:HH21	1.99	0.54
13:B:1174:LYS:O	13:B:1178:ASN:N	2.41	0.54
21:J:31:ASP:OD1	21:J:31:ASP:N	2.41	0.54
3:0:137:THR:HG21	3:0:159:HIS:HB3	1.89	0.54
4:6:121:GLY:H	4:6:308:LEU:H	1.55	0.54
7:7:553:GLN:HB2	7:7:701:PHE:HB3	1.89	0.54
8:3:75:ASP:O	8:3:79:GLU:N	2.29	0.54
13:B:955:THR:HG21	23:L:55:ILE:HG12	1.88	0.54
3:0:103:PHE:O	3:0:104:ARG:NH1	2.41	0.54
3:0:171:LEU:HD22	3:0:184:TYR:HE2	1.72	0.54
7:7:354:ILE:HG22	7:7:355:ASP:H	1.73	0.54
7:7:725:PHE:HA	7:7:728:ASP:HB2	1.90	0.54
12:A:439:ASN:OD1	12:A:459:ARG:NH1	2.36	0.54
12:A:587:HIS:CD2	12:A:969:GLN:HG3	2.43	0.54
13:B:667:GLN:NE2	13:B:667:GLN:O	2.41	0.54
13:B:853:SER:OG	13:B:1094:ARG:NH1	2.41	0.54
2:4:129:ILE:O	2:4:133:PHE:N	2.41	0.54
3:0:1:MET:N	3:0:92:TYR:OH	2.41	0.54
3:0:487:LEU:HD12	3:0:489:LYS:H	1.72	0.54
5:2:111:ALA:HA	5:2:115:GLY:HA3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:406:SER:HB2	7:7:482:TRP:CE3	2.43	0.54
7:7:540:TRP:O	7:7:544:SER:N	2.41	0.54
7:7:582:ILE:HG23	7:7:673:ILE:HG21	1.89	0.54
12:A:1393:ASN:OD1	12:A:1393:ASN:N	2.37	0.54
13:B:816:GLU:OE1	13:B:816:GLU:N	2.41	0.54
20:I:7:CYS:SG	20:I:8:ARG:N	2.81	0.54
29:W:95:ILE:HB	29:W:99:LYS:HE2	1.90	0.54
3:0:215:ASP:OD1	3:0:217:LYS:NZ	2.29	0.53
4:6:428:ARG:HA	4:6:435:GLU:HA	1.88	0.53
20:I:103:CYS:SG	20:I:107:SER:N	2.81	0.53
1:1:623:ILE:O	1:1:627:THR:N	2.32	0.53
6:5:7:GLY:HA3	6:5:41:LEU:HD23	1.90	0.53
6:5:20:ILE:O	6:5:24:ASP:N	2.28	0.53
7:7:556:GLU:HB2	7:7:733:PHE:HE1	1.73	0.53
7:7:584:ASN:ND2	7:7:710:SER:OG	2.28	0.53
9:O:71:VAL:HB	9:O:159:ASN:HB3	1.91	0.53
9:O:94:TYR:HB2	9:O:102:VAL:HG22	1.90	0.53
12:A:401:GLY:O	12:A:435:HIS:ND1	2.41	0.53
12:A:1420:ASP:N	12:A:1420:ASP:OD1	2.34	0.53
13:B:273:LEU:HB2	13:B:276:ILE:HG13	1.90	0.53
14:C:125:MET:SD	14:C:125:MET:N	2.82	0.53
19:H:131:ASN:OD1	19:H:131:ASN:N	2.33	0.53
26:R:273:ASP:HA	26:R:279:LYS:HE3	1.90	0.53
28:V:76:TRP:HB2	28:V:115:ALA:HB3	1.91	0.53
3:0:115:CYS:SG	3:0:120:VAL:HB	2.48	0.53
5:2:467:GLU:HA	5:2:470:LEU:HB2	1.90	0.53
9:O:183:SER:HB3	9:O:193:LEU:HD11	1.88	0.53
12:A:344:ARG:NH2	13:B:1120:GLU:OE1	2.41	0.53
13:B:279:ASP:OD1	13:B:279:ASP:N	2.35	0.53
13:B:326:ASP:O	13:B:329:THR:OG1	2.27	0.53
13:B:661:LEU:HD11	13:B:684:LEU:HD11	1.90	0.53
18:G:8:SER:HA	18:G:73:LYS:HA	1.89	0.53
22:K:8:GLU:O	22:K:37:LYS:HD2	2.09	0.53
3:0:37:ASN:HD22	3:0:475:PHE:HD2	1.56	0.53
3:0:553:MET:SD	3:0:554:TRP:N	2.82	0.53
7:7:341:TYR:CE2	7:7:343:PHE:HA	2.44	0.53
7:7:351:ASP:OD1	7:7:351:ASP:N	2.42	0.53
12:A:494:SER:O	12:A:497:THR:OG1	2.23	0.53
12:A:590:ARG:NH2	12:A:621:THR:OG1	2.31	0.53
12:A:1100:ARG:NH2	12:A:1351:GLU:OE2	2.33	0.53
13:B:299:GLU:HG2	13:B:571:PRO:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:586:TRP:CD1	13:B:588:GLY:H	2.26	0.53
20:I:103:CYS:SG	20:I:106:CYS:N	2.81	0.53
24:M:246:LEU:HB2	24:M:248:LEU:HD11	1.91	0.53
25:Q:346:GLU:OE1	25:Q:391:LYS:NZ	2.40	0.53
29:W:136:ALA:O	29:W:140:LEU:N	2.42	0.53
3:0:176:PHE:HA	3:0:180:LYS:HD3	1.91	0.53
3:0:539:VAL:HB	3:0:623:ILE:HD11	1.89	0.53
7:7:556:GLU:HB3	7:7:735:VAL:HG22	1.90	0.53
12:A:25:GLU:OE1	12:A:25:GLU:N	2.36	0.53
13:B:289:LEU:HD22	13:B:371:GLU:HB3	1.90	0.53
14:C:39:ALA:HA	14:C:164:ALA:HB3	1.89	0.53
15:D:173:HIS:HB3	15:D:176:GLU:HG3	1.90	0.53
26:R:96:ARG:O	26:R:105:THR:OG1	2.26	0.53
26:R:134:VAL:HB	26:R:215:VAL:HB	1.90	0.53
3:0:71:TYR:HB3	3:0:207:ILE:HG23	1.91	0.53
3:0:275:ARG:HA	3:0:279:SER:HB2	1.89	0.53
3:0:468:MET:O	3:0:472:MET:N	2.35	0.53
3:0:500:GLY:O	3:0:503:GLN:NE2	2.41	0.53
4:6:251:ILE:HG12	4:6:276:LEU:HD13	1.90	0.53
7:7:588:PHE:CZ	7:7:621:LYS:HB3	2.44	0.53
12:A:423:ASP:OD1	12:A:424:ILE:N	2.42	0.53
12:A:503:GLN:OE1	17:F:90:ARG:NH1	2.39	0.53
12:A:884:ASP:OD1	12:A:884:ASP:N	2.41	0.53
13:B:1189:ILE:HG21	18:G:41:LYS:HB2	1.91	0.53
17:F:86:THR:OG1	17:F:89:GLU:OE1	2.16	0.53
18:G:138:THR:HG22	18:G:139:ILE:H	1.74	0.53
1:1:551:ARG:HD3	4:6:340:SER:HA	1.91	0.53
3:0:651:ASN:HA	3:0:654:LEU:HB2	1.90	0.53
5:2:12:GLN:OE1	5:2:12:GLN:N	2.42	0.53
5:2:365:HIS:NE2	5:2:377:GLN:O	2.41	0.53
7:7:302:GLU:HG3	7:7:322:SER:H	1.74	0.53
7:7:343:PHE:HB3	7:7:380:ARG:HA	1.90	0.53
7:7:365:TYR:HB3	7:7:548:HIS:CB	2.39	0.53
10:N:26:DA:H2'	10:N:27:DG:C8	2.44	0.53
12:A:120:GLU:HG2	12:A:123:ARG:HD2	1.91	0.53
16:E:197:LYS:HG3	16:E:211:TYR:CE1	2.40	0.53
21:J:10:CYS:SG	21:J:43:ARG:NH2	2.75	0.53
21:J:46:CYS:O	21:J:49:MET:N	2.41	0.53
23:L:47:ARG:HA	23:L:53:HIS:O	2.09	0.53
29:W:171:LYS:HG2	29:W:174:ARG:HH11	1.73	0.53
3:0:11:LEU:HD21	3:0:97:LEU:HG	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:498:THR:HB	3:0:707:ASN:HA	1.90	0.53
7:7:325:VAL:HA	7:7:328:LYS:HB2	1.90	0.53
7:7:625:PRO:HG2	7:7:649:ILE:HG12	1.90	0.53
12:A:793:SER:OG	12:A:795:GLU:OE1	2.22	0.53
1:1:310:UNK:O	1:1:314:UNK:N	2.42	0.53
1:1:370:UNK:O	1:1:372:VAL:N	2.38	0.53
1:1:379:ASN:O	1:1:383:GLU:N	2.37	0.53
2:4:273:ARG:NH2	4:6:372:LEU:HB2	2.23	0.53
4:6:291:LEU:HA	4:6:296:HIS:CE1	2.44	0.53
5:2:20:GLN:O	5:2:24:ARG:N	2.38	0.53
7:7:576:LYS:HZ3	7:7:579:LEU:HB2	1.72	0.53
12:A:41:MET:N	24:M:90:ASN:HD21	2.07	0.53
12:A:565:ILE:HG12	19:H:97:MET:HG2	1.90	0.53
12:A:853:ASP:N	12:A:853:ASP:OD1	2.38	0.53
12:A:1257:ASP:N	12:A:1257:ASP:OD1	2.41	0.53
13:B:86:ARG:NE	13:B:138:GLU:OE2	2.38	0.53
13:B:843:GLN:HB3	13:B:995:ARG:HA	1.91	0.53
16:E:3:GLN:N	16:E:6:GLU:OE1	2.41	0.53
18:G:86:VAL:HG12	18:G:146:LYS:HB2	1.90	0.53
19:H:4:THR:HG21	19:H:7:ASP:HB2	1.91	0.53
1:1:185:LEU:HD13	1:1:210:TRP:HH2	1.74	0.53
3:0:490:LYS:NZ	3:0:700:GLY:O	2.31	0.53
3:0:528:GLU:OE2	3:0:710:THR:OG1	2.26	0.53
3:0:611:ASP:OD1	3:0:612:PHE:N	2.42	0.53
3:0:633:ARG:O	3:0:637:ALA:N	2.31	0.53
5:2:9:SER:O	5:2:12:GLN:N	2.37	0.53
7:7:462:ASN:HA	7:7:500:ARG:NH2	2.24	0.53
12:A:1158:PRO:HB2	12:A:1159:ARG:HH11	1.74	0.53
12:A:1191:TRP:NE1	12:A:1256:GLU:OE1	2.34	0.53
13:B:106:ASP:OD1	13:B:107:GLY:N	2.42	0.53
13:B:241:ARG:NH2	13:B:250:PHE:O	2.41	0.53
14:C:162:GLY:HA3	14:C:170:TRP:CE2	2.44	0.53
24:M:160:GLU:HB2	24:M:163:LEU:HG	1.90	0.53
1:1:380:ARG:HA	1:1:383:GLU:HB2	1.91	0.52
2:4:286:GLY:H	4:6:323:GLY:HA2	1.74	0.52
4:6:175:ARG:N	4:6:178:LEU:O	2.38	0.52
7:7:303:ARG:HH12	7:7:505:ILE:HB	1.73	0.52
7:7:622:MET:HE1	7:7:624:LYS:HB2	1.91	0.52
12:A:392:VAL:HG13	12:A:415:LEU:HD11	1.91	0.52
13:B:654:ARG:H	13:B:657:HIS:CE1	2.26	0.52
18:G:50:ASP:OD2	18:G:75:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:W:190:ASP:OD1	29:W:193:ARG:NH1	2.41	0.52
2:4:38:THR:O	2:4:42:GLU:N	2.40	0.52
2:4:75:VAL:HB	2:4:87:TYR:H	1.74	0.52
7:7:412:THR:OG1	7:7:413:SER:N	2.42	0.52
12:A:219:PHE:HA	12:A:222:LEU:HD12	1.91	0.52
12:A:850:VAL:O	12:A:1061:GLY:N	2.29	0.52
13:B:597:MET:HG3	13:B:601:ARG:HE	1.74	0.52
16:E:59:SER:HB3	16:E:80:VAL:O	2.09	0.52
17:F:140:ASP:OD1	17:F:142:SER:N	2.40	0.52
21:J:5:VAL:HG12	21:J:6:ARG:H	1.74	0.52
25:Q:380:ASP:OD1	25:Q:380:ASP:N	2.43	0.52
7:7:362:ILE:O	7:7:695:ARG:NH2	2.33	0.52
7:7:365:TYR:HD2	7:7:548:HIS:CG	2.27	0.52
7:7:490:VAL:HB	7:7:519:ARG:HH22	1.74	0.52
12:A:209:ASN:OD1	12:A:213:HIS:NE2	2.42	0.52
12:A:353:ILE:HG13	12:A:482:PHE:HD1	1.74	0.52
13:B:345:LYS:HD3	13:B:348:ARG:HH11	1.75	0.52
13:B:737:THR:OG1	20:I:66:PRO:O	2.23	0.52
15:D:194:LEU:HB3	18:G:86:VAL:HG21	1.91	0.52
16:E:185:ALA:O	16:E:189:GLY:N	2.42	0.52
27:U:282:GLU:HB2	28:V:63:LYS:HG2	1.91	0.52
30:X:189:PRO:HA	30:X:192:LEU:HB3	1.90	0.52
4:6:120:ARG:HH11	4:6:307:PRO:HB2	1.74	0.52
4:6:326:THR:O	4:6:348:PHE:N	2.43	0.52
4:6:424:UNK:O	4:6:426:ARG:N	2.43	0.52
7:7:608:PHE:HB3	7:7:672:GLN:HA	1.91	0.52
12:A:365:GLY:N	12:A:469:ARG:O	2.28	0.52
13:B:798:TYR:O	13:B:821:GLN:NE2	2.43	0.52
23:L:26:THR:HB	23:L:41:SER:HB3	1.91	0.52
23:L:31:CYS:HB2	23:L:48:CYS:SG	2.50	0.52
25:Q:137:VAL:O	26:R:58:ASP:N	2.42	0.52
3:0:28:ILE:HD13	3:0:55:LEU:HB3	1.91	0.52
3:0:512:ILE:HG13	3:0:630:THR:HG23	1.91	0.52
4:6:327:ARG:HA	4:6:347:TYR:HA	1.91	0.52
5:2:108:LEU:HD12	5:2:111:ALA:HB3	1.91	0.52
7:7:153:ALA:O	7:7:157:LEU:N	2.28	0.52
7:7:642:ASN:HB3	7:7:649:ILE:HB	1.91	0.52
12:A:790:ASP:N	12:A:790:ASP:OD1	2.42	0.52
17:F:130:ILE:HB	17:F:148:VAL:HG21	1.91	0.52
26:R:256:ASP:N	26:R:256:ASP:OD1	2.42	0.52
29:W:149:CYS:O	29:W:153:ASP:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:342:LEU:O	3:0:346:MET:N	2.42	0.52
3:0:747:HIS:O	3:0:751:ARG:HG2	2.09	0.52
12:A:1053:PHE:O	12:A:1056:SER:OG	2.24	0.52
14:C:214:ASN:O	14:C:214:ASN:ND2	2.38	0.52
30:X:257:GLU:O	30:X:261:LYS:N	2.31	0.52
7:7:395:VAL:O	7:7:398:THR:OG1	2.27	0.52
7:7:545:GLN:HA	7:7:550:ALA:HA	1.91	0.52
9:O:74:VAL:N	9:O:121:MET:O	2.41	0.52
10:N:21:DA:H61	11:T:145:DT:H3	1.57	0.52
12:A:715:GLU:OE1	12:A:774:ARG:NH1	2.33	0.52
18:G:1:MET:N	18:G:80:LYS:O	2.43	0.52
27:U:251:VAL:HG22	27:U:260:CYS:HA	1.91	0.52
2:4:68:ASN:O	5:2:37:ARG:NH2	2.43	0.52
3:0:103:PHE:H	3:0:173:LYS:HE3	1.75	0.52
4:6:334:THR:HA	4:6:343:VAL:O	2.09	0.52
5:2:41:PRO:HA	5:2:44:LYS:HB2	1.92	0.52
6:5:57:LEU:HA	6:5:60:LYS:HD3	1.92	0.52
7:7:417:VAL:HG21	7:7:456:THR:HA	1.92	0.52
13:B:443:ASN:HD21	13:B:445:LYS:HD2	1.75	0.52
14:C:226:ASP:N	14:C:226:ASP:OD1	2.42	0.52
16:E:62:ALA:HB3	16:E:78:LEU:HB3	1.90	0.52
16:E:68:SER:O	16:E:72:PHE:N	2.32	0.52
23:L:38:LEU:HD12	23:L:40:LEU:HD23	1.91	0.52
3:0:507:SER:OG	3:0:685:ARG:NH2	2.34	0.52
12:A:1205:LYS:HB3	12:A:1274:ARG:HH21	1.74	0.52
12:A:1290:LYS:HB3	12:A:1298:TYR:HB3	1.92	0.52
13:B:680:THR:O	13:B:683:SER:OG	2.27	0.52
3:0:11:LEU:HD22	3:0:93:ARG:HG3	1.92	0.52
7:7:491:HIS:CD2	7:7:681:ARG:HH11	2.28	0.52
12:A:408:ASP:H	12:A:430:TRP:CD1	2.28	0.52
15:D:138:ASN:O	15:D:141:LEU:HB3	2.09	0.52
16:E:6:GLU:HA	16:E:9:ILE:HB	1.92	0.52
22:K:29:ASN:ND2	22:K:78:THR:O	2.43	0.52
30:X:262:MET:HA	30:X:265:ASN:HB2	1.92	0.52
4:6:347:TYR:HB2	4:6:356:VAL:HG13	1.91	0.51
5:2:486:ASP:HA	5:2:489:LYS:HD3	1.91	0.51
7:7:349:ASN:OD1	7:7:349:ASN:N	2.24	0.51
9:O:133:LYS:HG3	9:O:152:PHE:HZ	1.76	0.51
12:A:902:LEU:HD22	12:A:926:GLN:HG2	1.90	0.51
15:D:205:ASP:OD1	15:D:206:GLU:N	2.42	0.51
22:K:17:SER:O	22:K:20:LYS:NZ	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:181:GLN:O	1:1:185:LEU:N	2.34	0.51
3:0:120:VAL:HG13	3:0:132:LYS:HB3	1.92	0.51
5:2:368:ALA:H	5:2:375:LEU:HB3	1.73	0.51
21:J:3:VAL:HG12	21:J:15:GLY:HA2	1.92	0.51
3:0:157:GLU:HA	3:0:160:GLU:HG2	1.92	0.51
4:6:156:PHE:CE2	4:6:160:PHE:HB2	2.45	0.51
5:2:488:LYS:NZ	6:5:36:ASP:OD2	2.43	0.51
7:7:348:ARG:HB3	7:7:405:LYS:HD3	1.92	0.51
12:A:1187:GLN:HG3	12:A:1188:GLN:HG3	1.92	0.51
12:A:1231:ASP:OD1	12:A:1231:ASP:N	2.43	0.51
13:B:438:GLU:OE1	13:B:440:HIS:NE2	2.43	0.51
14:C:66:ARG:NH1	21:J:2:ILE:O	2.44	0.51
2:4:74:ALA:HA	2:4:87:TYR:HD2	1.75	0.51
5:2:223:HIS:O	5:2:227:MET:N	2.42	0.51
5:2:472:SER:O	5:2:476:GLN:NE2	2.39	0.51
7:7:388:CYS:N	7:7:689:ARG:HG2	2.26	0.51
11:T:144:DA:OP2	27:U:255:LYS:NZ	2.35	0.51
12:A:559:VAL:HG13	19:H:78:SER:HB2	1.92	0.51
12:A:563:PRO:HD2	19:H:79:TRP:CD1	2.46	0.51
25:Q:98:TYR:HB2	26:R:95:ILE:O	2.11	0.51
25:Q:110:ASP:OD1	25:Q:111:LEU:N	2.43	0.51
29:W:13:LEU:HB3	29:W:29:LEU:HD11	1.93	0.51
29:W:144:ARG:HH22	29:W:146:GLU:HB2	1.75	0.51
1:1:309:UNK:O	1:1:313:UNK:N	2.44	0.51
2:4:69:SER:HA	5:2:37:ARG:HH12	1.76	0.51
3:0:39:ILE:HG22	3:0:477:THR:HG21	1.91	0.51
3:0:636:LYS:O	3:0:640:GLU:N	2.24	0.51
4:6:219:GLY:HA2	4:6:222:LEU:HD23	1.91	0.51
5:2:72:LEU:HD23	5:2:72:LEU:H	1.75	0.51
9:O:133:LYS:HG3	9:O:152:PHE:CZ	2.46	0.51
12:A:134:ARG:NH1	12:A:221:SER:O	2.43	0.51
12:A:874:ASP:OD1	12:A:875:ALA:N	2.43	0.51
13:B:97:VAL:HG12	26:R:252:ILE:HG21	1.91	0.51
13:B:510:LYS:HD2	13:B:511:PRO:HD2	1.93	0.51
16:E:65:THR:OG1	16:E:68:SER:OG	2.24	0.51
18:G:6:ASP:OD1	18:G:75:ARG:HB2	2.10	0.51
25:Q:343:ARG:NH2	25:Q:346:GLU:O	2.41	0.51
3:0:499:LYS:O	3:0:709:SER:HA	2.11	0.51
7:7:425:LEU:HG	7:7:430:LEU:HD23	1.92	0.51
7:7:590:ALA:O	7:7:594:LEU:HG	2.10	0.51
7:7:622:MET:SD	7:7:623:GLY:N	2.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:172:PRO:HB3	12:A:185:TRP:CD2	2.46	0.51
12:A:376:TYR:OH	12:A:495:GLU:OE2	2.28	0.51
12:A:390:GLN:OE1	12:A:393:ARG:NH1	2.35	0.51
12:A:513:SER:HB3	12:A:520:CYS:HB3	1.91	0.51
13:B:340:ALA:O	13:B:348:ARG:NH2	2.43	0.51
20:I:103:CYS:SG	20:I:104:LEU:N	2.83	0.51
24:M:41:GLY:C	24:M:56:LEU:HB3	2.36	0.51
29:W:122:TYR:CZ	29:W:158:GLU:HG2	2.46	0.51
4:6:293:ASP:OD2	4:6:296:HIS:N	2.33	0.51
7:7:475:ASP:OD1	7:7:475:ASP:N	2.44	0.51
12:A:386:ASP:N	12:A:386:ASP:OD1	2.43	0.51
12:A:591:PHE:HA	12:A:595:THR:HG21	1.91	0.51
12:A:698:GLN:CD	20:I:99:LEU:HD11	2.36	0.51
12:A:846:GLU:OE2	12:A:1425:SER:OG	2.29	0.51
2:4:25:LEU:HD23	2:4:160:VAL:HG13	1.93	0.51
3:0:80:GLU:HA	3:0:83:LEU:HB2	1.93	0.51
7:7:610:ASP:N	7:7:610:ASP:OD1	2.43	0.51
9:O:103:ILE:HG23	9:O:112:THR:HG23	1.93	0.51
12:A:95:PHE:HB3	12:A:234:MET:SD	2.51	0.51
12:A:547:LEU:HB3	22:K:60:ALA:HB2	1.93	0.51
13:B:790:ASP:N	13:B:790:ASP:OD1	2.42	0.51
23:L:54:ARG:N	23:L:54:ARG:HD2	2.26	0.51
1:1:208:GLU:OE1	1:1:208:GLU:N	2.37	0.51
1:1:230:PRO:HD3	4:6:244:PRO:HA	1.93	0.51
3:0:493:LEU:H	3:0:678:VAL:HA	1.76	0.51
3:0:528:GLU:HA	3:0:531:LYS:HE3	1.91	0.51
7:7:560:PRO:HA	7:7:711:LYS:HE2	1.93	0.51
12:A:280:GLU:HG2	12:A:289:ILE:HD12	1.92	0.51
13:B:760:ASP:N	13:B:760:ASP:OD1	2.43	0.51
13:B:1187:ASN:HD21	13:B:1190:ASP:C	2.18	0.51
19:H:7:ASP:OD1	19:H:8:ASP:N	2.44	0.51
29:W:109:LEU:HG	29:W:172:LEU:HG	1.92	0.51
6:5:31:VAL:HG11	6:5:40:LEU:HD22	1.92	0.51
7:7:409:VAL:HA	7:7:486:ILE:HB	1.93	0.51
10:N:36:DT:H2"	10:N:37:DC:C5	2.46	0.51
10:N:46:DG:H1'	10:N:47:DG:N7	2.25	0.51
14:C:26:ASP:OD1	14:C:26:ASP:N	2.42	0.51
14:C:111:THR:N	14:C:147:LEU:O	2.39	0.51
16:E:30:ILE:HG23	16:E:34:GLU:CD	2.36	0.51
20:I:80:SER:OG	20:I:105:SER:OG	2.27	0.51
23:L:32:ALA:HB3	23:L:53:HIS:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:75:VAL:H	2:4:88:PRO:HD3	1.76	0.50
3:0:628:GLN:N	3:0:628:GLN:OE1	2.44	0.50
3:0:695:LYS:O	3:0:699:GLN:N	2.33	0.50
4:6:349:CYS:HB3	4:6:353:HIS:H	1.76	0.50
7:7:388:CYS:HB2	7:7:392:LYS:HD2	1.91	0.50
7:7:489:GLU:O	7:7:491:HIS:ND1	2.39	0.50
7:7:548:HIS:CD2	7:7:693:ALA:HB1	2.45	0.50
12:A:264:PHE:O	12:A:268:ASP:N	2.34	0.50
13:B:241:ARG:CZ	13:B:243:ALA:HB2	2.41	0.50
13:B:356:LEU:HA	13:B:360:PHE:HB3	1.93	0.50
13:B:789:MET:SD	13:B:951:GLN:NE2	2.69	0.50
13:B:892:LYS:HD3	13:B:905:VAL:HG12	1.92	0.50
25:Q:378:VAL:HG22	25:Q:384:PHE:CE1	2.47	0.50
29:W:183:ILE:O	29:W:187:LYS:HG2	2.11	0.50
3:0:43:PRO:HD3	3:0:483:TYR:HB2	1.92	0.50
3:0:60:GLN:HE22	3:0:204:ASN:HB3	1.75	0.50
3:0:587:ARG:HA	3:0:590:CYS:HB2	1.94	0.50
3:0:639:LEU:HA	3:0:642:MET:HB3	1.93	0.50
4:6:188:ASN:O	4:6:192:HIS:ND1	2.44	0.50
7:7:393:THR:HB	7:7:424:PHE:CE2	2.46	0.50
7:7:670:LEU:O	7:7:706:TYR:N	2.44	0.50
9:O:93:GLU:OE2	9:O:105:ARG:NH1	2.45	0.50
10:N:6:DA:C2	10:N:7:DA:C6	2.99	0.50
12:A:109:HIS:CE1	12:A:185:TRP:HE1	2.29	0.50
12:A:733:ALA:O	12:A:737:LEU:HG	2.11	0.50
12:A:1158:PRO:HB3	12:A:1188:GLN:HB2	1.92	0.50
24:M:188:THR:N	24:M:191:GLU:OE1	2.43	0.50
29:W:62:ARG:HD3	29:W:69:ILE:H	1.75	0.50
1:1:256:ILE:O	1:1:260:PHE:N	2.39	0.50
3:0:39:ILE:HD11	3:0:463:ILE:HG21	1.93	0.50
4:6:144:ASN:HD21	4:6:146:HIS:HB3	1.77	0.50
7:7:680:ARG:HA	7:7:683:GLU:HB2	1.93	0.50
8:3:40:GLU:HA	8:3:43:VAL:HG12	1.92	0.50
10:N:3:DA:H2"	10:N:4:DA:C8	2.46	0.50
12:A:1309:ASP:OD1	12:A:1310:GLY:N	2.44	0.50
13:B:223:VAL:HA	13:B:240:ILE:HB	1.93	0.50
13:B:594:ALA:HA	13:B:617:ARG:HH12	1.76	0.50
13:B:1080:LYS:HG2	14:C:189:THR:OG1	2.11	0.50
24:M:129:ALA:HA	24:M:132:LYS:HE3	1.93	0.50
29:W:97:ALA:HA	30:X:274:LEU:HD21	1.94	0.50
29:W:123:MET:HG3	29:W:130:LYS:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:34:PRO:O	2:4:38:THR:N	2.34	0.50
7:7:236:THR:H	7:7:313:VAL:HG21	1.77	0.50
7:7:548:HIS:HD2	7:7:693:ALA:HB1	1.75	0.50
12:A:182:VAL:HA	12:A:201:VAL:HA	1.93	0.50
12:A:1341:ILE:HD11	12:A:1376:THR:HB	1.93	0.50
13:B:400:HIS:NE2	13:B:699:GLU:OE2	2.45	0.50
3:0:103:PHE:HE1	3:0:205:ILE:HG22	1.77	0.50
3:0:350:HIS:HA	3:0:422:PRO:HG3	1.92	0.50
3:0:463:ILE:HG23	3:0:469:TYR:CE1	2.46	0.50
7:7:373:MET:HA	7:7:535:LEU:HG	1.94	0.50
7:7:424:PHE:HD2	7:7:425:LEU:HD22	1.76	0.50
9:O:214:LEU:HD21	9:O:227:PHE:HB2	1.94	0.50
12:A:798:GLY:HA2	12:A:815:PHE:CD2	2.47	0.50
13:B:278:GLN:CD	13:B:337:ARG:HH11	2.20	0.50
13:B:1002:THR:OG1	13:B:1003:ALA:N	2.44	0.50
15:D:145:MET:HA	15:D:148:LEU:HB2	1.93	0.50
18:G:7:LEU:O	18:G:74:TYR:N	2.34	0.50
1:1:284:TRP:O	1:1:288:PHE:N	2.34	0.50
2:4:175:ARG:HA	2:4:208:CYS:SG	2.52	0.50
3:0:103:PHE:N	3:0:173:LYS:HE3	2.27	0.50
4:6:155:ASP:O	4:6:159:GLU:HG2	2.11	0.50
7:7:567:GLN:O	7:7:571:ARG:N	2.45	0.50
7:7:578:MET:HA	7:7:581:TYR:CZ	2.47	0.50
8:3:76:VAL:O	8:3:80:LYS:N	2.34	0.50
10:N:4:DA:C4	10:N:5:DA:C8	3.00	0.50
12:A:754:SER:OG	12:A:755:PHE:N	2.45	0.50
14:C:241:ASP:OD1	14:C:242:GLN:N	2.45	0.50
15:D:40:HIS:CG	18:G:73:LYS:HB3	2.47	0.50
25:Q:337:GLU:HG3	25:Q:340:LYS:HB3	1.94	0.50
2:4:85:TYR:HD2	2:4:88:PRO:HG2	1.76	0.50
3:0:58:ALA:O	3:0:62:HIS:N	2.44	0.50
3:0:256:ALA:HA	3:0:259:ARG:HB2	1.94	0.50
4:6:152:TYR:HB3	4:6:301:PHE:CZ	2.47	0.50
5:2:17:ILE:HG23	5:2:21:VAL:HG23	1.93	0.50
5:2:19:GLN:HG3	5:2:85:HIS:CG	2.47	0.50
7:7:464:ARG:HA	7:7:466:ARG:HG3	1.94	0.50
10:N:9:DA:C6	10:N:10:DA:C6	3.00	0.50
12:A:1187:GLN:HE21	12:A:1188:GLN:HE21	1.60	0.50
13:B:521:LEU:HD22	13:B:633:VAL:HG12	1.92	0.50
24:M:268:GLU:OE2	24:M:319:HIS:NE2	2.44	0.50
29:W:131:TYR:OH	29:W:149:CYS:SG	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:W:149:CYS:N	29:W:154:GLU:O	2.45	0.50
1:1:551:ARG:O	1:1:555:THR:OG1	2.27	0.50
3:0:354:GLU:OE1	3:0:358:SER:OG	2.28	0.50
3:0:493:LEU:HB2	3:0:678:VAL:HG13	1.92	0.50
3:0:603:ARG:HH21	3:0:626:PRO:HB2	1.77	0.50
5:2:350:TYR:HA	5:2:372:ASN:HD22	1.77	0.50
7:7:365:TYR:CD1	7:7:543:LEU:HB3	2.46	0.50
7:7:636:ARG:HA	7:7:639:ILE:HB	1.93	0.50
13:B:435:THR:HG21	13:B:442:PHE:CD1	2.47	0.50
13:B:651:LEU:O	13:B:654:ARG:NH2	2.45	0.50
16:E:163:GLU:OE2	16:E:167:ARG:NE	2.44	0.50
25:Q:117:HIS:HB2	26:R:135:PHE:CE1	2.46	0.50
1:1:278:PHE:O	1:1:283:PHE:HB2	2.12	0.50
3:0:274:VAL:HG23	3:0:282:LEU:HD11	1.94	0.50
3:0:730:PRO:HG2	3:0:734:GLU:HG3	1.94	0.50
4:6:211:GLN:HA	4:6:214:LEU:HB2	1.94	0.50
7:7:755:GLU:HA	7:7:758:GLU:HG2	1.93	0.50
12:A:326:ARG:NE	12:A:1406:VAL:HG21	2.27	0.50
12:A:1135:ARG:HB3	12:A:1135:ARG:HH11	1.77	0.50
13:B:206:ASN:OD1	13:B:458:LYS:NZ	2.35	0.50
13:B:917:PRO:HG3	13:B:934:LYS:HE3	1.93	0.50
13:B:952:VAL:HG22	13:B:966:VAL:HG22	1.92	0.50
13:B:1074:ASN:HD21	13:B:1076:HIS:HB2	1.77	0.50
21:J:36:LEU:HA	21:J:39:LEU:HB2	1.94	0.50
25:Q:132:ASP:N	25:Q:132:ASP:OD1	2.44	0.50
28:V:85:VAL:HG13	28:V:106:ILE:HB	1.93	0.50
3:0:234:PHE:N	3:0:457:ILE:O	2.45	0.49
3:0:321:ILE:HG13	3:0:323:GLY:H	1.76	0.49
3:0:498:THR:HG23	3:0:684:ARG:HA	1.94	0.49
4:6:124:ARG:NH1	4:6:164:ASN:OD1	2.45	0.49
5:2:336:ASP:O	5:2:351:SER:HB3	2.11	0.49
6:5:24:ASP:HB3	6:5:29:ASP:HA	1.93	0.49
7:7:671:ILE:HG13	7:7:706:TYR:HB2	1.94	0.49
12:A:481:ASP:OD1	12:A:481:ASP:N	2.45	0.49
13:B:435:THR:HG21	13:B:442:PHE:HD1	1.75	0.49
16:E:6:GLU:O	16:E:10:SER:N	2.32	0.49
16:E:62:ALA:N	16:E:78:LEU:O	2.29	0.49
17:F:81:THR:OG1	17:F:136:ARG:NH1	2.45	0.49
18:G:14:HIS:HB3	18:G:17:PHE:CE1	2.47	0.49
24:M:211:LYS:HA	24:M:214:LEU:HD12	1.94	0.49
1:1:540:SER:O	1:1:544:ILE:N	2.34	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:628:GLN:NE2	3:0:657:ASP:OD1	2.45	0.49
4:6:363:CYS:SG	4:6:366:CYS:N	2.85	0.49
7:7:370:LEU:HD11	7:7:395:VAL:HA	1.93	0.49
7:7:751:ALA:O	7:7:756:ARG:NE	2.34	0.49
12:A:1153:TYR:CD1	20:I:42:LEU:HA	2.46	0.49
13:B:1004:GLU:HA	14:C:177:GLU:HG2	1.94	0.49
22:K:12:LEU:HD12	22:K:13:GLY:N	2.27	0.49
1:1:188:ASN:HB3	1:1:191:LEU:HB2	1.93	0.49
1:1:337:ILE:HG13	3:0:584:GLU:HB3	1.93	0.49
2:4:50:ILE:O	2:4:54:LEU:N	2.32	0.49
2:4:201:PHE:CZ	4:6:377:ALA:HB3	2.48	0.49
3:0:349:LEU:HD23	3:0:349:LEU:H	1.76	0.49
5:2:87:LEU:HG	5:2:89:PRO:HD3	1.94	0.49
6:5:11:GLN:HE22	6:5:38:THR:HB	1.76	0.49
7:7:228:LYS:N	7:7:231:ARG:O	2.45	0.49
9:O:69:ASN:H	9:O:161:VAL:HB	1.77	0.49
12:A:1030:ARG:NE	12:A:1034:GLU:OE1	2.42	0.49
12:A:1109:LYS:HD3	12:A:1333:ILE:HD13	1.94	0.49
15:D:176:GLU:HB3	15:D:198:LEU:HD11	1.94	0.49
28:V:62:VAL:HG22	28:V:85:VAL:HB	1.94	0.49
30:X:195:LEU:HD23	30:X:210:LEU:HD21	1.95	0.49
3:0:79:ILE:O	3:0:83:LEU:N	2.39	0.49
3:0:244:CYS:O	3:0:247:SER:OG	2.24	0.49
7:7:347:HIS:CE1	7:7:349:ASN:HA	2.48	0.49
7:7:366:GLN:HG3	7:7:548:HIS:CE1	2.48	0.49
7:7:430:LEU:HD11	7:7:435:CYS:HB2	1.94	0.49
9:O:202:ILE:HD11	9:O:222:GLU:HB3	1.94	0.49
12:A:837:ILE:HD11	12:A:1102:LYS:HG2	1.94	0.49
12:A:873:MET:HB2	12:A:1366:ARG:HH21	1.77	0.49
13:B:1084:GLN:HG2	14:C:201:TRP:CH2	2.48	0.49
13:B:1121:GLY:O	13:B:1126:GLY:N	2.45	0.49
25:Q:125:LYS:HB3	25:Q:128:ASN:HB2	1.94	0.49
3:0:234:PHE:HB2	3:0:458:ILE:HA	1.95	0.49
3:0:302:GLN:CD	3:0:302:GLN:H	2.20	0.49
3:0:720:PHE:HD2	3:0:721:LEU:HD12	1.77	0.49
4:6:363:CYS:SG	4:6:367:ASP:N	2.86	0.49
7:7:594:LEU:HD13	7:7:706:TYR:CD2	2.47	0.49
9:O:214:LEU:HB2	9:O:223:ILE:HG23	1.94	0.49
10:N:20:DT:O4	10:N:21:DA:N6	2.46	0.49
12:A:30:ILE:HD13	13:B:1170:THR:HG21	1.94	0.49
12:A:903:ASN:OD1	12:A:904:THR:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:D:189:ASP:HA	15:D:192:LYS:HG3	1.94	0.49
23:L:32:ALA:HB2	23:L:55:ILE:HB	1.94	0.49
25:Q:363:GLY:HA2	25:Q:395:PHE:HA	1.93	0.49
26:R:108:LEU:HB2	26:R:118:HIS:O	2.12	0.49
27:U:258:TRP:O	27:U:283:ALA:N	2.45	0.49
3:0:615:GLN:OE1	3:0:616:TYR:N	2.46	0.49
3:0:638:ARG:O	3:0:642:MET:N	2.38	0.49
4:6:294:GLU:O	4:6:298:LYS:N	2.45	0.49
5:2:449:ASP:O	5:2:450:ARG:HG3	2.11	0.49
7:7:696:ARG:HH11	7:7:699:GLU:HB2	1.77	0.49
12:A:75:ASN:N	12:A:75:ASN:OD1	2.46	0.49
12:A:365:GLY:HA3	12:A:469:ARG:HB2	1.95	0.49
12:A:557:ASP:OD1	12:A:558:GLY:N	2.46	0.49
12:A:944:ARG:NH2	12:A:1296:GLY:O	2.45	0.49
12:A:1355:VAL:O	12:A:1358:SER:OG	2.16	0.49
14:C:204:SER:N	14:C:207:CYS:SG	2.85	0.49
20:I:16:PRO:HB2	20:I:25:LEU:HD11	1.93	0.49
24:M:108:LYS:HD3	24:M:111:ASN:HB2	1.94	0.49
1:1:190:VAL:HA	1:1:193:LYS:HB2	1.95	0.49
3:0:176:PHE:HB3	3:0:181:LEU:HB2	1.95	0.49
5:2:18:PRO:HB2	5:2:20:GLN:HE22	1.78	0.49
5:2:350:TYR:HA	5:2:372:ASN:ND2	2.28	0.49
5:2:422:LEU:O	5:2:426:CYS:N	2.39	0.49
7:7:421:ARG:HH21	7:7:426:GLN:CD	2.20	0.49
12:A:35:ILE:HG21	12:A:53:LEU:HD12	1.94	0.49
12:A:61:ILE:HA	12:A:74:MET:HG3	1.93	0.49
12:A:993:LEU:HD13	12:A:1046:LEU:HD22	1.94	0.49
12:A:1187:GLN:HE21	12:A:1188:GLN:NE2	2.11	0.49
13:B:120:ARG:NE	13:B:956:THR:O	2.42	0.49
13:B:635:ARG:NH2	13:B:742:GLU:OE2	2.37	0.49
17:F:89:GLU:OE1	17:F:89:GLU:N	2.42	0.49
25:Q:141:ARG:HH22	25:Q:343:ARG:NH1	2.06	0.49
27:U:269:ILE:HD11	28:V:111:LEU:HD11	1.93	0.49
3:0:104:ARG:N	3:0:204:ASN:OD1	2.39	0.49
3:0:233:ILE:HA	3:0:457:ILE:HB	1.95	0.49
4:6:184:GLN:O	4:6:192:HIS:NE2	2.46	0.49
4:6:232:VAL:H	4:6:261:VAL:HG22	1.78	0.49
5:2:75:GLN:NE2	5:2:499:SER:O	2.46	0.49
12:A:1159:ARG:HD2	12:A:1174:PHE:CE2	2.48	0.49
12:A:1258:HIS:O	12:A:1262:LYS:HG2	2.12	0.49
13:B:342:GLY:O	13:B:348:ARG:NH1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:824:ILE:N	13:B:1009:ASP:OD2	2.31	0.49
13:B:1032:SER:HB3	13:B:1089:PRO:HG2	1.94	0.49
15:D:35:LEU:HG	15:D:46:GLU:HG3	1.94	0.49
24:M:60:ARG:HB3	24:M:64:ARG:HH21	1.77	0.49
30:X:269:PRO:HG2	30:X:274:LEU:HD22	1.95	0.49
1:1:340:ASP:OD1	3:0:577:GLN:N	2.45	0.49
3:0:138:ASN:HB3	3:0:141:ALA:H	1.77	0.49
3:0:538:VAL:HG22	3:0:598:LEU:HB3	1.94	0.49
3:0:570:LEU:HD13	3:0:586:TYR:HD1	1.77	0.49
4:6:381:HIS:HB2	4:6:449:HIS:CD2	2.48	0.49
7:7:423:GLN:NE2	7:7:662:ILE:HB	2.27	0.49
7:7:423:GLN:HG2	7:7:663:ASP:CG	2.37	0.49
7:7:569:TYR:HA	7:7:577:ARG:CZ	2.43	0.49
7:7:576:LYS:NZ	7:7:579:LEU:HB2	2.28	0.49
7:7:576:LYS:HZ1	7:7:580:LEU:HG	1.78	0.49
9:O:175:LEU:O	9:O:179:HIS:ND1	2.43	0.49
11:T:151:DC:H2'	11:T:152:DG:C8	2.48	0.49
12:A:130:ASP:OD1	12:A:132:LYS:N	2.46	0.49
12:A:358:ASN:OD1	13:B:833:TYR:OH	2.25	0.49
12:A:881:GLN:CD	12:A:959:ASN:HA	2.37	0.49
13:B:322:PHE:CZ	20:I:30:ARG:HB3	2.48	0.49
13:B:806:THR:HB	13:B:809:MET:HG3	1.94	0.49
15:D:56:ARG:HB2	15:D:148:LEU:HD13	1.95	0.49
4:6:215:GLU:OE1	4:6:218:ARG:NE	2.40	0.49
5:2:185:THR:O	5:2:189:PHE:N	2.26	0.49
7:7:754:ARG:O	7:7:758:GLU:N	2.46	0.49
12:A:839:ARG:NH2	12:A:1402:PHE:O	2.46	0.49
12:A:1446:ASP:OD1	12:A:1447:GLU:N	2.44	0.49
14:C:217:ASP:N	14:C:217:ASP:OD1	2.45	0.49
27:U:252:THR:O	27:U:257:ARG:NH1	2.45	0.49
2:4:76:ILE:HG12	2:4:85:TYR:HA	1.95	0.48
7:7:309:ASP:HB3	7:7:337:VAL:HB	1.95	0.48
7:7:334:ASP:O	7:7:336:PRO:HD3	2.13	0.48
8:3:132:LYS:O	8:3:136:TYR:N	2.31	0.48
12:A:737:LEU:HB2	12:A:744:LYS:HD2	1.95	0.48
12:A:1256:GLU:O	12:A:1260:LEU:N	2.32	0.48
13:B:333:PHE:O	13:B:337:ARG:HG2	2.13	0.48
13:B:391:ASP:N	13:B:391:ASP:OD1	2.46	0.48
13:B:486:TYR:HB3	13:B:1096:ARG:HH12	1.78	0.48
15:D:174:PRO:HA	15:D:177:VAL:HG13	1.95	0.48
30:X:271:PHE:O	30:X:273:GLU:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:175:ARG:NH1	2:4:252:MET:O	2.45	0.48
3:0:211:HIS:HA	3:0:214:LEU:HB2	1.95	0.48
4:6:335:PHE:N	4:6:343:VAL:H	2.11	0.48
5:2:84:LEU:HD11	5:2:86:LEU:HD23	1.94	0.48
9:O:103:ILE:HA	9:O:113:ALA:O	2.13	0.48
12:A:206:GLU:O	12:A:210:ILE:HG12	2.13	0.48
12:A:1038:THR:OG1	12:A:1039:LYS:N	2.45	0.48
13:B:27:ALA:O	13:B:30:SER:OG	2.29	0.48
15:D:51:ASN:OD1	15:D:53:SER:OG	2.19	0.48
15:D:188:ALA:HA	15:D:207:LEU:HD22	1.94	0.48
1:1:229:GLY:HA3	4:6:242:THR:HG22	1.93	0.48
1:1:257:LEU:HA	1:1:260:PHE:HB2	1.94	0.48
2:4:29:ILE:HD13	2:4:153:MET:HA	1.94	0.48
4:6:271:ALA:O	4:6:275:GLU:N	2.39	0.48
7:7:491:HIS:CD2	7:7:681:ARG:HG2	2.49	0.48
12:A:362:ASP:OD1	12:A:459:ARG:NH2	2.45	0.48
12:A:523:ILE:O	12:A:528:LEU:HB2	2.13	0.48
12:A:871:ASP:OD2	16:E:204:THR:OG1	2.30	0.48
27:U:248:TYR:OH	28:V:74:ASP:OD2	2.30	0.48
1:1:549:SER:O	1:1:553:LEU:N	2.38	0.48
3:0:41:GLU:HB3	3:0:482:SER:HA	1.95	0.48
3:0:254:THR:HA	3:0:257:LEU:HB2	1.94	0.48
3:0:473:LEU:HB2	3:0:475:PHE:CE1	2.49	0.48
5:2:464:THR:OG1	5:2:466:GLN:OE1	2.20	0.48
7:7:365:TYR:HD1	7:7:543:LEU:HD22	1.77	0.48
7:7:719:SER:HA	7:7:722:ARG:HD2	1.96	0.48
12:A:451:HIS:HB2	12:A:454:SER:N	2.27	0.48
12:A:737:LEU:HB3	12:A:741:ASN:HD22	1.78	0.48
13:B:494:HIS:HA	13:B:497:ARG:NH1	2.29	0.48
15:D:50:LEU:HB2	15:D:55:ALA:HB2	1.96	0.48
18:G:81:PRO:HG2	18:G:157:ILE:HG21	1.95	0.48
24:M:143:PRO:HG2	24:M:146:VAL:HG23	1.94	0.48
26:R:72:ARG:O	26:R:223:GLN:HG2	2.13	0.48
3:0:650:GLU:O	3:0:654:LEU:N	2.33	0.48
7:7:368:LYS:HZ1	7:7:543:LEU:HA	1.79	0.48
7:7:541:MET:O	7:7:545:GLN:HB2	2.14	0.48
7:7:604:LYS:HD3	7:7:694:LYS:NZ	2.26	0.48
7:7:604:LYS:O	7:7:669:CYS:N	2.44	0.48
7:7:631:THR:HB	7:7:636:ARG:HH21	1.78	0.48
8:3:139:LEU:O	8:3:143:LEU:N	2.42	0.48
9:O:65:PRO:HG2	9:O:224:TYR:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:46:DG:C2	11:T:120:DC:O2	2.66	0.48
12:A:802:ASN:ND2	12:A:812:GLU:OE2	2.46	0.48
13:B:129:PHE:CE2	26:R:266:THR:HG21	2.49	0.48
13:B:586:TRP:NE1	13:B:588:GLY:O	2.43	0.48
16:E:78:LEU:HD11	16:E:109:ILE:HG13	1.94	0.48
24:M:306:GLU:HA	24:M:309:ILE:HB	1.94	0.48
26:R:123:GLU:HG2	26:R:223:GLN:HB3	1.95	0.48
3:0:138:ASN:HD22	3:0:139:GLY:N	2.10	0.48
3:0:144:LYS:HB2	3:0:153:VAL:HG21	1.95	0.48
3:0:194:PHE:HA	3:0:197:ARG:HB3	1.95	0.48
7:7:133:TRP:O	7:7:142:ILE:N	2.40	0.48
7:7:241:ILE:O	7:7:245:LEU:N	2.42	0.48
7:7:423:GLN:HE22	7:7:662:ILE:HB	1.76	0.48
12:A:247:ARG:NH1	12:A:263:THR:OG1	2.46	0.48
12:A:573:SER:N	12:A:576:GLN:OE1	2.24	0.48
13:B:89:GLU:HB3	13:B:135:ARG:HB2	1.95	0.48
13:B:906:SER:O	13:B:941:LEU:HD23	2.14	0.48
13:B:920:PRO:O	13:B:928:ARG:HD2	2.14	0.48
16:E:8:ASN:O	16:E:12:LEU:N	2.37	0.48
16:E:183:PRO:O	16:E:187:TYR:N	2.36	0.48
17:F:147:SER:O	17:F:150:GLU:HG2	2.13	0.48
24:M:187:ARG:HH11	24:M:241:ARG:HD3	1.78	0.48
29:W:30:ASP:HB3	29:W:34:PHE:CZ	2.48	0.48
3:0:123:GLU:HB2	3:0:132:LYS:HZ2	1.79	0.48
3:0:227:SER:HG	3:0:453:PHE:HE1	1.60	0.48
3:0:301:ASP:HB3	3:0:304:GLU:HB2	1.94	0.48
5:2:473:LYS:NZ	5:2:477:ASP:OD1	2.47	0.48
7:7:321:GLU:HG2	7:7:322:SER:HB2	1.95	0.48
7:7:411:CYS:HB3	7:7:417:VAL:HG13	1.94	0.48
12:A:216:VAL:HA	12:A:219:PHE:CZ	2.48	0.48
12:A:535:THR:O	12:A:575:LYS:NZ	2.29	0.48
12:A:847:ASP:OD1	12:A:847:ASP:N	2.47	0.48
12:A:1151:GLU:OE2	20:I:45:ARG:NE	2.31	0.48
15:D:68:ARG:HD2	15:D:72:ARG:HH22	1.78	0.48
27:U:250:LYS:H	27:U:261:SER:HB3	1.77	0.48
29:W:116:ASN:HB3	29:W:164:LYS:HB2	1.95	0.48
7:7:368:LYS:O	7:7:372:LYS:HG3	2.14	0.48
9:O:221:GLU:OE1	9:O:221:GLU:N	2.40	0.48
12:A:243:PRO:HB2	12:A:245:PRO:HD2	1.95	0.48
12:A:251:SER:HA	12:A:257:ARG:HG3	1.96	0.48
13:B:72:GLU:HA	13:B:87:LYS:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:822:ASN:O	21:J:48:ARG:NH1	2.47	0.48
13:B:896:ASP:OD2	23:L:29:TYR:OH	2.32	0.48
16:E:168:TYR:HB3	16:E:170:LEU:HG	1.94	0.48
16:E:201:LYS:HA	16:E:206:GLY:O	2.14	0.48
18:G:26:LEU:HD13	18:G:56:ILE:HD11	1.96	0.48
24:M:173:ALA:HB2	24:M:196:ILE:HD12	1.96	0.48
1:1:504:ILE:O	1:1:508:LYS:N	2.38	0.48
2:4:175:ARG:NH2	2:4:211:ASP:OD2	2.46	0.48
3:0:477:THR:OG1	3:0:478:VAL:N	2.45	0.48
3:0:493:LEU:HB2	3:0:678:VAL:HG22	1.96	0.48
7:7:447:GLN:HG2	7:7:448:THR:HG23	1.95	0.48
12:A:958:VAL:HG21	12:A:1052:GLN:HB3	1.95	0.48
14:C:73:GLN:HG3	14:C:128:ASN:O	2.14	0.48
15:D:166:LEU:O	15:D:169:SER:OG	2.21	0.48
19:H:118:PHE:HB2	19:H:121:LEU:HB2	1.96	0.48
21:J:48:ARG:O	21:J:52:THR:HG22	2.14	0.48
1:1:340:ASP:OD2	3:0:124:ARG:NH2	2.47	0.48
2:4:249:ALA:O	2:4:253:PHE:HB2	2.14	0.48
3:0:642:MET:SD	3:0:646:TYR:HB2	2.53	0.48
7:7:616:GLN:HA	7:7:619:ALA:HB3	1.96	0.48
9:O:69:ASN:OD1	9:O:159:ASN:ND2	2.47	0.48
9:O:191:PRO:HG3	24:M:272:LYS:HD3	1.96	0.48
12:A:957:PRO:HG2	12:A:1018:PHE:CD1	2.49	0.48
13:B:403:LYS:NZ	13:B:696:GLU:OE2	2.46	0.48
13:B:860:MET:HE3	13:B:860:MET:HB3	1.83	0.48
23:L:47:ARG:HG2	23:L:48:CYS:N	2.29	0.48
23:L:48:CYS:HB3	23:L:51:CYS:O	2.14	0.48
1:1:197:GLU:HA	1:1:201:ASN:CG	2.38	0.47
2:4:67:PHE:O	5:2:44:LYS:NZ	2.41	0.47
2:4:239:GLU:OE1	2:4:240:SER:N	2.46	0.47
3:0:158:TYR:HA	3:0:161:ASN:HD21	1.79	0.47
3:0:259:ARG:HA	3:0:262:ARG:HB2	1.95	0.47
3:0:588:LYS:O	3:0:592:ASN:N	2.46	0.47
5:2:350:TYR:HA	5:2:372:ASN:HB2	1.95	0.47
5:2:360:LEU:HD21	5:2:403:HIS:HD1	1.79	0.47
5:2:468:TYR:O	5:2:472:SER:N	2.44	0.47
7:7:619:ALA:HA	7:7:622:MET:HG3	1.96	0.47
10:N:6:DA:H2"	10:N:7:DA:C8	2.49	0.47
12:A:242:PRO:HG2	12:A:247:ARG:HD3	1.95	0.47
12:A:670:ILE:HD13	12:A:805:LEU:HD21	1.96	0.47
13:B:1065:GLN:CD	13:B:1067:ARG:H	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:1096:ARG:O	13:B:1098:MET:N	2.47	0.47
16:E:61:GLN:HG3	16:E:105:PHE:CE1	2.49	0.47
23:L:33:GLU:H	23:L:53:HIS:HD2	1.62	0.47
29:W:108:ARG:HH22	29:W:109:LEU:HD13	1.79	0.47
1:1:561:LEU:O	1:1:565:ALA:N	2.35	0.47
3:0:37:ASN:HB2	3:0:477:THR:HA	1.96	0.47
4:6:142:ARG:HB2	4:6:143:PRO:HD3	1.95	0.47
4:6:391:GLU:HA	4:6:427:TYR:HA	1.95	0.47
5:2:84:LEU:HD21	5:2:86:LEU:HD23	1.96	0.47
7:7:456:THR:O	7:7:460:VAL:HG23	2.14	0.47
7:7:483:GLY:O	7:7:509:ALA:HB3	2.15	0.47
8:3:64:ARG:HG3	8:3:65:LYS:H	1.78	0.47
10:N:7:DA:C4	10:N:8:DA:C8	3.02	0.47
12:A:1226:VAL:HA	12:A:1239:ARG:O	2.13	0.47
17:F:74:ILE:HD11	17:F:142:SER:HB2	1.97	0.47
17:F:100:GLN:HB3	18:G:15:PRO:HB3	1.96	0.47
18:G:119:LEU:HD13	18:G:132:SER:HB3	1.95	0.47
22:K:40:HIS:NE2	22:K:63:VAL:HG21	2.29	0.47
26:R:317:GLY:O	26:R:321:ARG:N	2.42	0.47
27:U:244:MET:HE1	28:V:111:LEU:HB3	1.95	0.47
29:W:147:PHE:O	29:W:156:LEU:N	2.43	0.47
1:1:497:UNK:O	1:1:501:UNK:N	2.48	0.47
3:0:715:SER:O	3:0:719:GLN:NE2	2.40	0.47
5:2:100:LEU:O	5:2:102:PRO:HD3	2.15	0.47
5:2:506:LYS:HG3	5:2:507:ARG:H	1.78	0.47
6:5:48:GLU:HB2	6:5:52:HIS:CE1	2.49	0.47
7:7:303:ARG:HD2	7:7:502:VAL:O	2.13	0.47
9:O:112:THR:HB	9:O:124:THR:HG23	1.96	0.47
10:N:46:DG:N1	11:T:120:DC:C2	2.82	0.47
12:A:202:LEU:HB3	12:A:207:ILE:HD11	1.96	0.47
12:A:717:ASN:N	12:A:717:ASN:OD1	2.45	0.47
13:B:50:SER:OG	13:B:51:PHE:N	2.47	0.47
13:B:129:PHE:CE2	13:B:166:PHE:HB2	2.49	0.47
13:B:583:ASN:HD21	13:B:628:THR:H	1.62	0.47
18:G:15:PRO:HA	18:G:18:PHE:CE1	2.48	0.47
19:H:41:ASP:N	19:H:41:ASP:OD1	2.47	0.47
19:H:109:LYS:HG3	19:H:110:ASP:H	1.79	0.47
29:W:17:VAL:HG11	29:W:29:LEU:HD13	1.96	0.47
2:4:89:GLU:OE2	2:4:92:SER:OG	2.28	0.47
3:0:310:PRO:HG3	3:0:404:THR:HA	1.96	0.47
3:0:618:ARG:NH1	3:0:676:TYR:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:681:LEU:HB3	3:0:686:PHE:CE2	2.49	0.47
5:2:19:GLN:O	5:2:23:ASN:N	2.28	0.47
5:2:506:LYS:HG3	5:2:507:ARG:N	2.29	0.47
7:7:370:LEU:HB3	7:7:374:PHE:CE2	2.49	0.47
7:7:447:GLN:HA	7:7:476:PHE:CD1	2.50	0.47
7:7:635:GLU:O	7:7:639:ILE:N	2.44	0.47
8:3:15:ILE:HG23	29:W:176:MET:HG2	1.97	0.47
8:3:36:HIS:NE2	8:3:54:CYS:SG	2.88	0.47
9:O:74:VAL:HG21	9:O:136:SER:HB3	1.97	0.47
12:A:1100:ARG:NH1	12:A:1103:GLU:OE1	2.46	0.47
13:B:40:GLU:OE1	13:B:682:SER:N	2.41	0.47
15:D:140:ASP:O	15:D:144:THR:HG23	2.14	0.47
15:D:147:TYR:CE2	18:G:103:VAL:HA	2.50	0.47
19:H:26:ILE:O	19:H:39:THR:HA	2.14	0.47
20:I:26:LEU:HA	20:I:37:GLU:HA	1.95	0.47
23:L:30:ILE:HG13	23:L:59:ALA:HB2	1.95	0.47
24:M:103:ASP:OD1	24:M:104:MET:N	2.46	0.47
24:M:133:ILE:HG23	24:M:172:MET:HE3	1.97	0.47
27:U:246:CYS:SG	27:U:262:LEU:HB3	2.55	0.47
3:0:267:LEU:HD11	3:0:399:LEU:HD13	1.96	0.47
3:0:418:LEU:HD23	3:0:437:PHE:HB2	1.97	0.47
5:2:174:GLU:H	5:2:185:THR:H	1.61	0.47
5:2:382:SER:HA	5:2:385:ARG:HD3	1.95	0.47
5:2:459:TYR:HD2	5:2:491:PHE:HD1	1.61	0.47
7:7:269:LEU:HD13	7:7:304:GLU:HA	1.96	0.47
7:7:363:ARG:HB2	7:7:548:HIS:ND1	2.29	0.47
7:7:694:LYS:O	7:7:696:ARG:N	2.48	0.47
7:7:726:LEU:HD12	7:7:733:PHE:CD1	2.48	0.47
12:A:416:ARG:O	12:A:417:TYR:HB2	2.15	0.47
15:D:51:ASN:OD1	15:D:54:GLU:N	2.30	0.47
1:1:175:LEU:C	1:1:181:GLN:HE22	2.22	0.47
1:1:474:UNK:O	1:1:478:UNK:N	2.47	0.47
2:4:175:ARG:NH1	2:4:256:PRO:HD3	2.30	0.47
3:0:111:ARG:O	3:0:115:CYS:N	2.35	0.47
4:6:169:MET:C	4:6:185:VAL:HA	2.38	0.47
4:6:177:GLY:C	4:6:209:SER:HB2	2.39	0.47
7:7:304:GLU:HB3	7:7:507:ALA:O	2.14	0.47
7:7:363:ARG:HB2	7:7:548:HIS:CD2	2.50	0.47
12:A:940:ARG:HE	12:A:944:ARG:NH1	2.13	0.47
12:A:1141:THR:HG1	12:A:1274:ARG:H	1.59	0.47
13:B:175:ARG:HE	13:B:199:MET:HA	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:357:GLN:HE21	13:B:357:GLN:HB3	1.49	0.47
15:D:144:THR:HG22	18:G:104:GLY:C	2.39	0.47
20:I:70:ARG:HD3	20:I:84:VAL:HG13	1.96	0.47
1:1:192:MET:HA	1:1:195:PHE:HB3	1.97	0.47
1:1:196:GLN:HA	1:1:200:ILE:HG12	1.97	0.47
1:1:375:LEU:HB3	3:0:571:VAL:HG21	1.96	0.47
1:1:592:LYS:O	1:1:596:LEU:HG	2.14	0.47
1:1:613:THR:O	1:1:617:LYS:N	2.48	0.47
2:4:261:ILE:HG13	5:2:65:TRP:O	2.14	0.47
3:0:308:GLU:CD	3:0:308:GLU:H	2.23	0.47
3:0:568:LEU:N	3:0:595:GLY:O	2.40	0.47
4:6:377:ALA:HA	4:6:380:TYR:CD2	2.49	0.47
5:2:411:LEU:HA	5:2:414:GLU:HG2	1.97	0.47
7:7:320:ASN:OD1	7:7:320:ASN:N	2.48	0.47
7:7:363:ARG:NH1	7:7:693:ALA:HB3	2.29	0.47
7:7:603:ASP:HB3	7:7:668:THR:HB	1.95	0.47
7:7:608:PHE:HB3	7:7:672:GLN:HG2	1.97	0.47
8:3:29:LEU:HD22	8:3:70:THR:HA	1.96	0.47
9:O:70:ILE:HD13	9:O:127:LYS:HA	1.95	0.47
9:O:106:ILE:O	9:O:110:LYS:HA	2.15	0.47
10:N:45:DC:H2'	10:N:46:DG:C8	2.49	0.47
11:T:144:DA:H2"	11:T:145:DT:H5'	1.97	0.47
13:B:548:GLY:HA3	13:B:630:ALA:HB2	1.97	0.47
13:B:882:THR:OG1	13:B:885:MET:SD	2.69	0.47
14:C:204:SER:OG	14:C:207:CYS:SG	2.58	0.47
16:E:143:ASN:ND2	16:E:145:THR:OG1	2.47	0.47
17:F:97:ARG:HD2	17:F:100:GLN:OE1	2.13	0.47
18:G:35:GLU:HA	18:G:45:ILE:HG22	1.96	0.47
19:H:25:ARG:NH2	19:H:41:ASP:OD1	2.37	0.47
24:M:105:ARG:O	24:M:109:GLU:HB2	2.14	0.47
24:M:125:GLU:O	24:M:129:ALA:N	2.31	0.47
27:U:244:MET:HG2	27:U:267:VAL:HA	1.95	0.47
29:W:65:ARG:HH11	29:W:93:HIS:CE1	2.33	0.47
1:1:196:GLN:O	1:1:201:ASN:N	2.48	0.47
1:1:280:GLU:HB3	1:1:284:TRP:CE2	2.50	0.47
1:1:585:HIS:O	1:1:589:CYS:N	2.33	0.47
2:4:25:LEU:HA	2:4:72:LYS:O	2.14	0.47
2:4:126:VAL:O	2:4:129:ILE:HG23	2.15	0.47
3:0:613:ASP:O	3:0:617:GLY:N	2.24	0.47
4:6:126:LEU:HA	4:6:231:GLU:O	2.15	0.47
6:5:49:PHE:HA	6:5:52:HIS:CG	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:365:TYR:HA	7:7:368:LYS:HE2	1.95	0.47
7:7:467:SER:OG	7:7:468:HIS:N	2.47	0.47
7:7:592:GLN:HB3	7:7:745:ILE:HD13	1.96	0.47
7:7:676:HIS:N	7:7:715:GLU:OE2	2.45	0.47
9:O:91:ASN:ND2	9:O:105:ARG:O	2.48	0.47
9:O:159:ASN:HD21	9:O:161:VAL:HG23	1.79	0.47
12:A:306:ASN:ND2	12:A:313:GLN:OE1	2.48	0.47
13:B:1054:GLY:O	13:B:1058:LEU:HB2	2.15	0.47
15:D:199:ASN:OD1	15:D:199:ASN:N	2.48	0.47
18:G:163:ILE:HA	18:G:168:LEU:HD13	1.95	0.47
30:X:194:LYS:O	30:X:198:SER:N	2.48	0.47
2:4:304:LYS:HE2	2:4:304:LYS:HB2	1.81	0.47
3:0:224:ASN:CG	3:0:228:LYS:HB2	2.39	0.47
3:0:285:GLU:HA	3:0:288:LYS:HB2	1.95	0.47
3:0:504:VAL:HG22	7:7:377:GLY:HA2	1.97	0.47
5:2:401:GLU:HG3	5:2:433:LEU:HD13	1.97	0.47
7:7:409:VAL:HG22	7:7:486:ILE:HD12	1.96	0.47
13:B:1072:MET:HE2	13:B:1072:MET:HB3	1.83	0.47
18:G:112:LYS:HA	18:G:115:MET:HB2	1.97	0.47
4:6:133:SER:O	4:6:204:PRO:HB2	2.15	0.47
4:6:186:SER:HB2	4:6:192:HIS:CE1	2.50	0.47
6:5:5:ARG:HH12	6:5:33:GLU:CD	2.22	0.47
7:7:344:ARG:NE	7:7:378:ARG:HB3	2.29	0.47
7:7:687:LEU:HD13	7:7:726:LEU:HD22	1.97	0.47
12:A:313:GLN:H	24:M:99:GLY:HA3	1.80	0.47
12:A:1121:GLU:HB2	12:A:1321:GLY:O	2.16	0.47
12:A:1426:GLU:OE1	12:A:1426:GLU:N	2.42	0.47
13:B:554:ILE:O	13:B:558:LEU:N	2.41	0.47
17:F:116:ASP:OD2	17:F:119:ARG:N	2.38	0.47
24:M:176:ILE:O	24:M:180:CYS:N	2.26	0.47
3:0:132:LYS:O	3:0:136:MET:N	2.26	0.46
3:0:171:LEU:HD22	3:0:184:TYR:CE2	2.49	0.46
3:0:281:LYS:O	3:0:285:GLU:N	2.39	0.46
5:2:138:TYR:O	5:2:142:LYS:N	2.36	0.46
5:2:380:ARG:HH21	5:2:440:GLN:C	2.21	0.46
7:7:726:LEU:O	7:7:731:TYR:HB2	2.15	0.46
9:O:93:GLU:HG2	28:V:69:TYR:HE2	1.80	0.46
12:A:66:LYS:NZ	12:A:72:GLU:HB3	2.30	0.46
12:A:230:ARG:HB3	12:A:232:GLU:HG3	1.95	0.46
13:B:126:SER:O	13:B:170:LEU:N	2.48	0.46
13:B:599:THR:O	13:B:602:THR:OG1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:J:7:CYS:SG	21:J:10:CYS:N	2.83	0.46
27:U:243:LEU:HD23	28:V:112:ARG:HB2	1.97	0.46
27:U:262:LEU:HD11	28:V:113:ILE:HG23	1.96	0.46
29:W:67:ILE:HA	29:W:90:LYS:H	1.80	0.46
2:4:27:THR:HG22	2:4:74:ALA:HB3	1.98	0.46
2:4:86:LEU:HD12	2:4:128:GLU:HB3	1.97	0.46
3:0:109:THR:O	3:0:212:TYR:OH	2.23	0.46
4:6:128:LEU:HD11	4:6:233:LEU:HD22	1.97	0.46
7:7:363:ARG:HA	7:7:695:ARG:NE	2.31	0.46
7:7:439:THR:C	7:7:441:ASP:H	2.24	0.46
13:B:39:ARG:NH2	13:B:678:GLU:OE1	2.47	0.46
13:B:327:ARG:HH21	13:B:353:LYS:HE2	1.80	0.46
14:C:112:ASN:OD1	14:C:112:ASN:N	2.48	0.46
16:E:143:ASN:OD1	16:E:146:HIS:N	2.48	0.46
18:G:94:CYS:HA	18:G:99:PHE:HA	1.96	0.46
20:I:74:GLU:HB3	20:I:81:ARG:HG3	1.96	0.46
24:M:126:VAL:O	24:M:130:PHE:N	2.34	0.46
24:M:305:THR:HG22	24:M:307:GLY:H	1.80	0.46
29:W:68:SER:O	29:W:88:TYR:N	2.45	0.46
1:1:318:UNK:HA	1:1:321:PHE:HB3	1.97	0.46
1:1:351:GLY:O	3:0:251:ASP:HB2	2.14	0.46
3:0:214:LEU:HD11	3:0:240:ILE:HG23	1.98	0.46
3:0:241:ASP:OD1	3:0:241:ASP:N	2.46	0.46
3:0:270:ARG:NH2	3:0:388:LEU:O	2.31	0.46
3:0:322:PRO:HB3	3:0:376:PHE:HD2	1.80	0.46
3:0:495:MET:HB2	3:0:680:VAL:HA	1.97	0.46
3:0:514:ASN:HD21	3:0:549:SER:C	2.23	0.46
7:7:438:PHE:C	7:7:459:MET:HG3	2.41	0.46
7:7:694:LYS:NZ	7:7:696:ARG:HH21	2.13	0.46
12:A:270:LEU:O	12:A:274:ILE:N	2.47	0.46
12:A:356:ASP:OD2	22:K:65:HIS:NE2	2.42	0.46
12:A:1444:MET:HE3	17:F:135:ARG:CZ	2.45	0.46
13:B:40:GLU:OE1	13:B:680:THR:OG1	2.30	0.46
18:G:49:LEU:HD11	18:G:75:ARG:HE	1.81	0.46
24:M:103:ASP:O	24:M:107:THR:HG23	2.16	0.46
1:1:212:THR:HB	1:1:213:ARG:HH11	1.80	0.46
1:1:375:LEU:HD13	3:0:571:VAL:HG21	1.97	0.46
1:1:471:UNK:O	1:1:475:UNK:N	2.48	0.46
2:4:26:LEU:HB3	2:4:73:VAL:HG12	1.96	0.46
3:0:94:THR:O	3:0:98:GLY:N	2.39	0.46
3:0:393:VAL:O	3:0:397:THR:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:489:LYS:HE3	3:0:724:MET:HE1	1.97	0.46
5:2:475:ALA:O	5:2:479:GLY:N	2.42	0.46
6:5:24:ASP:HA	6:5:27:MET:SD	2.54	0.46
7:7:489:GLU:HB3	7:7:689:ARG:NH1	2.31	0.46
8:3:85:ARG:O	8:3:89:PHE:N	2.39	0.46
12:A:1140:HIS:NE2	12:A:1272:THR:HB	2.31	0.46
13:B:705:MET:H	13:B:710:LEU:HD12	1.80	0.46
16:E:98:ILE:HA	16:E:101:GLN:HB3	1.96	0.46
16:E:113:GLN:HA	16:E:137:GLU:CD	2.41	0.46
16:E:156:LEU:HB2	16:E:195:VAL:O	2.14	0.46
29:W:174:ARG:HD2	30:X:255:ILE:HD13	1.97	0.46
3:0:63:TYR:HB3	3:0:65:GLU:OE1	2.15	0.46
3:0:238:HIS:HB2	3:0:660:ARG:HD2	1.97	0.46
3:0:304:GLU:OE1	3:0:386:ARG:NH1	2.40	0.46
3:0:327:ARG:HB3	3:0:330:HIS:CD2	2.50	0.46
7:7:492:VAL:HG23	7:7:682:GLN:HE22	1.80	0.46
7:7:588:PHE:O	7:7:592:GLN:N	2.42	0.46
9:O:73:THR:OG1	9:O:158:GLN:OE1	2.22	0.46
12:A:376:TYR:CZ	12:A:498:ARG:HD2	2.51	0.46
12:A:1155:ASP:OD1	12:A:1161:THR:HA	2.16	0.46
12:A:1239:ARG:HH22	12:A:1241:ARG:NH2	2.14	0.46
20:I:27:PHE:N	20:I:36:GLU:O	2.43	0.46
25:Q:120:LYS:HB3	25:Q:120:LYS:HE2	1.73	0.46
27:U:267:VAL:HG23	27:U:276:PHE:CE1	2.50	0.46
1:1:551:ARG:HB2	1:1:616:LEU:HD11	1.97	0.46
3:0:24:TYR:O	3:0:28:ILE:HG22	2.16	0.46
3:0:32:LEU:HD23	3:0:59:TYR:CD1	2.51	0.46
3:0:603:ARG:NH2	3:0:626:PRO:O	2.48	0.46
3:0:709:SER:HB3	3:0:712:MET:HG2	1.98	0.46
4:6:120:ARG:CZ	4:6:309:PRO:HG3	2.46	0.46
5:2:13:TYR:HA	5:2:16:GLU:HB3	1.96	0.46
7:7:547:GLY:H	7:7:550:ALA:HB2	1.80	0.46
12:A:271:LYS:NZ	24:M:92:LEU:O	2.36	0.46
12:A:1341:ILE:HD13	12:A:1380:GLY:H	1.80	0.46
13:B:444:MET:SD	13:B:444:MET:N	2.88	0.46
18:G:5:LYS:HE3	18:G:6:ASP:H	1.79	0.46
1:1:372:VAL:O	1:1:376:LYS:HG3	2.16	0.46
3:0:195:ILE:O	3:0:199:MET:HB2	2.16	0.46
5:2:15:GLU:OE1	5:2:83:SER:HB2	2.16	0.46
6:5:24:ASP:HA	6:5:27:MET:CG	2.45	0.46
12:A:131:SER:OG	12:A:132:LYS:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:306:ASN:ND2	12:A:322:VAL:O	2.48	0.46
12:A:860:LEU:HB2	12:A:862:ASN:OD1	2.14	0.46
12:A:869:GLY:HA3	12:A:1366:ARG:HG2	1.97	0.46
12:A:1263:ILE:O	12:A:1267:MET:N	2.47	0.46
13:B:1152:MET:HE1	13:B:1195:HIS:HB3	1.97	0.46
14:C:16:ASP:OD1	14:C:16:ASP:N	2.47	0.46
24:M:204:GLY:HA2	24:M:207:LEU:HB3	1.98	0.46
1:1:221:ALA:O	1:1:225:SER:N	2.49	0.46
1:1:472:UNK:O	1:1:476:UNK:N	2.49	0.46
2:4:297:SER:O	2:4:300:PRO:HD3	2.15	0.46
3:0:131:GLU:HG3	3:0:393:VAL:HG21	1.97	0.46
3:0:211:HIS:HB3	3:0:215:ASP:HB2	1.98	0.46
7:7:356:LEU:H	7:7:404:LYS:HE2	1.80	0.46
7:7:424:PHE:O	7:7:428:CYS:HB3	2.16	0.46
7:7:659:ASP:HA	7:7:660:THR:HA	1.63	0.46
7:7:668:THR:HG1	7:7:694:LYS:NZ	2.11	0.46
7:7:739:LEU:H	7:7:742:MET:HE2	1.81	0.46
8:3:80:LYS:O	8:3:84:ILE:N	2.38	0.46
12:A:128:ILE:O	12:A:134:ARG:HD3	2.16	0.46
12:A:253:ASN:HB2	12:A:256:GLN:HG2	1.98	0.46
12:A:800:VAL:HG22	12:A:812:GLU:HB3	1.98	0.46
12:A:854:ASN:O	12:A:867:ILE:HA	2.15	0.46
13:B:87:LYS:N	13:B:137:TYR:O	2.38	0.46
23:L:58:LYS:HD2	23:L:58:LYS:HA	1.60	0.46
24:M:108:LYS:HD3	24:M:108:LYS:HA	1.74	0.46
24:M:148:ASP:HA	24:M:151:LYS:HB2	1.98	0.46
25:Q:337:GLU:OE2	25:Q:340:LYS:N	2.49	0.46
29:W:10:LYS:HE3	29:W:33:LEU:HD22	1.98	0.46
1:1:251:LEU:HB2	1:1:255:LYS:HG2	1.97	0.46
1:1:510:ASN:ND2	2:4:265:PRO:O	2.35	0.46
3:0:293:LEU:HD13	3:0:319:GLU:HA	1.98	0.46
3:0:629:TYR:CZ	3:0:636:LYS:HE2	2.50	0.46
7:7:321:GLU:HG3	7:7:504:THR:HA	1.96	0.46
7:7:341:TYR:OH	7:7:509:ALA:HB2	2.16	0.46
7:7:354:ILE:HD11	7:7:405:LYS:O	2.15	0.46
9:O:175:LEU:HD21	9:O:193:LEU:HD22	1.98	0.46
13:B:73:GLN:O	13:B:85:SER:OG	2.28	0.46
13:B:287:ARG:NH1	13:B:324:ILE:O	2.49	0.46
13:B:859:TYR:O	13:B:966:VAL:N	2.39	0.46
26:R:94:LYS:HE2	26:R:107:LEU:HG	1.96	0.46
27:U:257:ARG:HH11	27:U:259:LYS:HG3	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:605:LYS:HA	3:0:608:GLU:CD	2.40	0.46
3:0:632:SER:OG	3:0:633:ARG:N	2.49	0.46
3:0:681:LEU:HB3	3:0:686:PHE:CD2	2.51	0.46
7:7:383:ILE:HD11	7:7:531:ILE:HD13	1.98	0.46
7:7:562:THR:OG1	7:7:563:ALA:N	2.49	0.46
7:7:622:MET:HE2	7:7:622:MET:HB2	1.70	0.46
7:7:678:GLY:HA2	7:7:679:SER:HA	1.59	0.46
9:O:191:PRO:CG	24:M:272:LYS:HD3	2.46	0.46
10:N:7:DA:C2	10:N:8:DA:C5	3.04	0.46
12:A:42:ASP:HA	12:A:49:LYS:HB2	1.97	0.46
13:B:901:PRO:HD3	23:L:58:LYS:CG	2.46	0.46
25:Q:103:LEU:HB3	25:Q:386:MET:SD	2.55	0.46
28:V:69:TYR:HA	28:V:77:THR:O	2.16	0.46
1:1:300:UNK:O	1:1:302:UNK:N	2.48	0.45
2:4:312:PHE:HB3	4:6:319:LEU:HD11	1.96	0.45
3:0:70:ILE:HG13	3:0:206:ILE:HG13	1.98	0.45
3:0:123:GLU:OE1	3:0:125:LYS:N	2.49	0.45
3:0:294:HIS:CE1	3:0:297:ASP:HB3	2.52	0.45
3:0:327:ARG:HG3	3:0:330:HIS:H	1.80	0.45
3:0:440:LEU:HB3	3:0:641:PHE:CD2	2.51	0.45
5:2:432:VAL:HA	5:2:433:LEU:HA	1.69	0.45
6:5:53:GLU:CD	6:5:56:ARG:HB2	2.41	0.45
9:O:109:PRO:HG2	9:O:131:ASP:O	2.16	0.45
11:T:137:DA:H2"	11:T:138:DA:C8	2.51	0.45
13:B:1106:ARG:CZ	13:B:1118:PRO:HB3	2.45	0.45
15:D:127:ASP:HB3	15:D:142:LYS:HG3	1.97	0.45
15:D:128:VAL:HA	15:D:131:GLU:HB3	1.97	0.45
24:M:102:THR:HG23	24:M:106:PHE:HB2	1.97	0.45
25:Q:125:LYS:HB2	25:Q:125:LYS:HE3	1.70	0.45
29:W:97:ALA:HB1	30:X:268:LEU:HD13	1.96	0.45
1:1:476:UNK:O	1:1:480:UNK:N	2.49	0.45
2:4:30:ILE:HB	2:4:179:LEU:HD13	1.98	0.45
2:4:314:GLU:O	2:4:318:ALA:N	2.37	0.45
3:0:80:GLU:HB3	3:0:178:PHE:CD2	2.50	0.45
3:0:419:ILE:HD13	3:0:634:ILE:HG12	1.97	0.45
3:0:659:MET:HA	3:0:662:ALA:HB3	1.98	0.45
5:2:51:VAL:HG13	5:2:109:ARG:HE	1.82	0.45
7:7:480:ARG:HG3	7:7:481:GLU:O	2.16	0.45
7:7:636:ARG:O	7:7:640:LEU:N	2.40	0.45
7:7:705:PHE:CZ	7:7:707:SER:HB2	2.51	0.45
12:A:55:ASP:O	12:A:58:LEU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:147:VAL:HA	12:A:170:THR:HA	1.98	0.45
12:A:275:SER:O	12:A:279:LEU:HB2	2.17	0.45
13:B:526:GLU:HG3	13:B:775:LYS:HZ3	1.80	0.45
14:C:27:LEU:HA	14:C:228:PHE:CZ	2.51	0.45
17:F:140:ASP:CG	17:F:142:SER:H	2.25	0.45
4:6:275:GLU:O	4:6:279:ALA:N	2.37	0.45
7:7:539:ASN:HD21	7:7:542:GLU:HB3	1.80	0.45
9:O:197:MET:HE3	9:O:197:MET:HB2	1.88	0.45
10:N:4:DA:H2"	10:N:5:DA:H8	1.80	0.45
10:N:10:DA:N3	10:N:11:DA:C6	2.84	0.45
12:A:315:LEU:HB2	24:M:96:ILE:HA	1.98	0.45
12:A:633:VAL:HG21	12:A:645:LEU:HD22	1.98	0.45
12:A:1359:ASP:OD2	12:A:1361:SER:OG	2.25	0.45
13:B:857:ARG:NH1	13:B:945:GLU:OE2	2.50	0.45
14:C:8:VAL:HG11	22:K:105:PHE:CD1	2.48	0.45
16:E:165:LEU:O	16:E:169:ARG:N	2.47	0.45
19:H:10:PHE:HD2	19:H:57:VAL:HG21	1.81	0.45
19:H:124:ARG:NH1	19:H:126:GLU:OE1	2.49	0.45
1:1:465:UNK:O	1:1:470:UNK:N	2.50	0.45
3:0:134:ARG:HH12	3:0:305:PRO:HD2	1.81	0.45
3:0:587:ARG:O	3:0:591:SER:N	2.35	0.45
5:2:387:LEU:C	5:2:390:GLY:H	2.23	0.45
5:2:466:GLN:CD	5:2:466:GLN:H	2.24	0.45
7:7:223:VAL:H	7:7:337:VAL:HA	1.82	0.45
7:7:593:PHE:O	7:7:597:TYR:N	2.22	0.45
7:7:616:GLN:HE21	7:7:628:TYR:HB2	1.80	0.45
7:7:664:LEU:O	7:7:692:ARG:HG3	2.16	0.45
9:O:157:ILE:HD13	9:O:160:ILE:HD11	1.98	0.45
10:N:7:DA:C2	10:N:8:DA:C4	3.04	0.45
12:A:253:ASN:HA	13:B:935:ARG:HH22	1.80	0.45
12:A:497:THR:HG22	13:B:1146:PHE:HA	1.98	0.45
12:A:698:GLN:HG2	20:I:99:LEU:HD21	1.97	0.45
12:A:1213:GLY:HA3	12:A:1228:TRP:CZ3	2.51	0.45
13:B:414:ALA:O	13:B:418:LYS:N	2.44	0.45
21:J:31:ASP:O	21:J:35:ALA:N	2.48	0.45
25:Q:141:ARG:HB3	25:Q:348:TYR:HB2	1.98	0.45
1:1:477:UNK:O	1:1:481:UNK:N	2.49	0.45
3:0:208:TYR:HD2	3:0:209:SER:O	1.99	0.45
3:0:594:ARG:NE	4:6:241:THR:O	2.34	0.45
5:2:380:ARG:HE	5:2:380:ARG:HB2	1.50	0.45
7:7:302:GLU:CD	7:7:321:GLU:HB3	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:397:ILE:HG21	7:7:428:CYS:SG	2.57	0.45
10:N:50:DG:C8	10:N:51:DT:C5	3.04	0.45
12:A:567:LYS:HB3	19:H:96:VAL:HB	1.99	0.45
12:A:828:ALA:O	12:A:831:THR:OG1	2.32	0.45
12:A:916:GLY:HA2	12:A:919:ILE:HB	1.98	0.45
12:A:1209:MET:HE2	12:A:1231:ASP:HA	1.99	0.45
13:B:649:LYS:NZ	13:B:736:THR:HG23	2.31	0.45
13:B:961:LEU:HD23	13:B:961:LEU:HA	1.79	0.45
14:C:260:LEU:O	14:C:263:THR:OG1	2.29	0.45
24:M:126:VAL:HG22	24:M:154:TYR:HE2	1.81	0.45
24:M:289:PHE:HD1	24:M:289:PHE:HA	1.68	0.45
2:4:194:ILE:HA	2:4:197:MET:HE2	1.98	0.45
5:2:352:ASN:ND2	5:2:373:MET:O	2.50	0.45
7:7:370:LEU:O	7:7:373:MET:HG3	2.16	0.45
7:7:564:GLU:CD	7:7:564:GLU:H	2.23	0.45
7:7:621:LYS:HE3	7:7:750:TYR:CD1	2.52	0.45
7:7:699:GLU:HG3	7:7:701:PHE:H	1.82	0.45
9:O:162:GLY:O	9:O:214:LEU:N	2.41	0.45
9:O:194:ILE:HD11	10:N:20:DT:H5"	1.97	0.45
12:A:14:VAL:HB	12:A:1430:LEU:HD13	1.99	0.45
12:A:254:GLU:O	12:A:257:ARG:NH2	2.46	0.45
13:B:399:ASP:OD1	13:B:509:ALA:N	2.49	0.45
13:B:423:LYS:HD3	13:B:423:LYS:HA	1.76	0.45
14:C:183:TRP:CE3	14:C:213:PRO:HD3	2.52	0.45
22:K:12:LEU:HD11	22:K:16:GLU:O	2.16	0.45
26:R:63:ARG:O	26:R:65:ASN:ND2	2.49	0.45
30:X:268:LEU:HA	30:X:268:LEU:HD23	1.74	0.45
2:4:194:ILE:HB	2:4:195:PRO:HD3	1.99	0.45
3:0:13:PRO:HA	3:0:92:TYR:CG	2.50	0.45
3:0:161:ASN:ND2	3:0:189:THR:O	2.49	0.45
5:2:47:ILE:O	5:2:51:VAL:HG23	2.16	0.45
7:7:540:TRP:HB3	7:7:544:SER:OG	2.16	0.45
7:7:565:PHE:CZ	7:7:583:MET:HG3	2.51	0.45
11:T:130:DA:H1'	11:T:131:DC:O4'	2.16	0.45
12:A:88:LYS:HD2	12:A:89:PRO:HD2	1.98	0.45
12:A:1079:MET:HE2	12:A:1097:GLY:HA2	1.99	0.45
12:A:1286:LYS:HB2	12:A:1304:TRP:CE3	2.51	0.45
13:B:91:SER:N	13:B:133:LYS:O	2.44	0.45
13:B:386:LEU:O	13:B:390:LEU:N	2.48	0.45
13:B:1165:ILE:HD13	13:B:1187:ASN:HB2	1.99	0.45
19:H:93:TYR:CG	19:H:143:LEU:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:I:103:CYS:HB3	20:I:108:HIS:N	2.32	0.45
24:M:157:CYS:C	24:M:159:ASP:H	2.24	0.45
24:M:157:CYS:HB3	24:M:210:MET:HE1	1.98	0.45
2:4:79:TYR:O	2:4:148:THR:OG1	2.34	0.45
2:4:214:LYS:HG2	2:4:237:HIS:CE1	2.52	0.45
3:0:156:CYS:C	3:0:158:TYR:H	2.25	0.45
3:0:212:TYR:O	3:0:221:ARG:NH2	2.49	0.45
3:0:301:ASP:HB2	3:0:305:PRO:HG3	1.98	0.45
3:0:325:ILE:HG12	3:0:334:PHE:CE2	2.52	0.45
3:0:722:ARG:H	3:0:722:ARG:HG3	1.47	0.45
5:2:47:ILE:HG23	5:2:100:LEU:HD21	1.97	0.45
5:2:371:VAL:HG22	7:7:117:ASP:O	2.17	0.45
7:7:240:ASP:O	7:7:244:MET:N	2.28	0.45
7:7:337:VAL:HG23	7:7:339:GLU:HG3	1.97	0.45
12:A:903:ASN:HD21	12:A:905:ASP:HB3	1.81	0.45
13:B:621:GLU:O	13:B:623:GLU:HG3	2.17	0.45
13:B:728:ARG:HH12	13:B:1048:THR:N	2.15	0.45
13:B:773:MET:HE1	13:B:985:GLY:HA2	1.98	0.45
13:B:1084:GLN:NE2	14:C:191:TYR:HA	2.31	0.45
15:D:40:HIS:NE2	18:G:6:ASP:OD1	2.50	0.45
16:E:48:ASP:OD1	16:E:51:GLY:N	2.48	0.45
19:H:79:TRP:O	19:H:80:ARG:HG3	2.17	0.45
24:M:173:ALA:HB3	24:M:203:PHE:HE1	1.82	0.45
25:Q:343:ARG:HD2	25:Q:343:ARG:HA	1.59	0.45
26:R:270:MET:N	26:R:270:MET:SD	2.89	0.45
29:W:108:ARG:HH12	29:W:109:LEU:HD22	1.82	0.45
3:0:92:TYR:HA	3:0:95:LYS:HB3	1.98	0.45
4:6:139:LYS:NZ	4:6:143:PRO:O	2.32	0.45
4:6:214:LEU:O	4:6:218:ARG:HB2	2.17	0.45
5:2:87:LEU:HD12	5:2:98:ILE:HG23	1.99	0.45
6:5:17:LYS:O	6:5:21:LEU:HG	2.17	0.45
12:A:61:ILE:H	12:A:65:LEU:HD12	1.82	0.45
12:A:708:MET:HB2	12:A:712:GLU:HB3	1.99	0.45
12:A:904:THR:HA	12:A:907:THR:HB	1.99	0.45
13:B:26:THR:OG1	13:B:27:ALA:N	2.49	0.45
13:B:680:THR:OG1	13:B:681:TRP:N	2.50	0.45
16:E:64:PRO:HB2	16:E:69:ILE:HD11	1.97	0.45
16:E:108:GLY:N	16:E:131:THR:O	2.43	0.45
16:E:117:THR:HG1	16:E:120:ALA:H	1.65	0.45
16:E:118:PRO:HA	16:E:121:MET:HB3	1.98	0.45
17:F:99:LEU:O	17:F:102:SER:OG	2.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:R:104:ILE:HG21	26:R:122:LEU:HD22	1.97	0.45
1:1:563:HIS:O	1:1:567:HIS:N	2.37	0.45
3:0:22:TYR:O	3:0:26:CYS:N	2.48	0.45
3:0:217:LYS:HE3	3:0:310:PRO:HA	1.98	0.45
3:0:238:HIS:CE1	3:0:462:THR:HB	2.51	0.45
3:0:259:ARG:HA	3:0:262:ARG:HE	1.80	0.45
3:0:425:ILE:HA	3:0:428:ALA:HB2	1.99	0.45
3:0:546:TYR:O	3:0:550:ILE:HG12	2.16	0.45
3:0:618:ARG:HD3	3:0:618:ARG:HA	1.75	0.45
4:6:132:CYS:HA	4:6:204:PRO:HB3	1.99	0.45
4:6:137:LEU:HG	4:6:204:PRO:HG2	1.98	0.45
7:7:485:ILE:O	7:7:511:LEU:N	2.50	0.45
8:3:65:LYS:O	8:3:67:LYS:N	2.50	0.45
10:N:8:DA:N3	10:N:9:DA:C5	2.85	0.45
12:A:414:ASP:OD1	12:A:415:LEU:N	2.50	0.45
12:A:731:ARG:HD3	12:A:731:ARG:HA	1.66	0.45
12:A:1277:GLU:O	12:A:1279:ILE:HG12	2.17	0.45
13:B:59:LEU:HD12	13:B:59:LEU:HA	1.79	0.45
13:B:649:LYS:HE2	13:B:711:GLU:O	2.17	0.45
13:B:791:THR:HG22	13:B:792:MET:HG3	1.98	0.45
13:B:832:GLY:O	13:B:835:GLN:NE2	2.39	0.45
13:B:1009:ASP:OD1	13:B:1009:ASP:N	2.49	0.45
24:M:27:CYS:HB3	24:M:29:VAL:HG13	1.99	0.45
26:R:75:MET:HA	26:R:78:ALA:HB3	1.99	0.45
27:U:269:ILE:HG21	28:V:106:ILE:HG21	1.99	0.45
29:W:183:ILE:HA	29:W:186:LEU:HB2	1.98	0.45
1:1:508:LYS:HG3	1:1:509:ILE:N	2.31	0.44
1:1:629:LYS:O	1:1:633:TYR:N	2.39	0.44
2:4:175:ARG:HH12	2:4:252:MET:C	2.24	0.44
3:0:249:SER:HB2	3:0:436:ARG:NH2	2.32	0.44
3:0:281:LYS:HA	3:0:284:ASP:HB3	1.99	0.44
3:0:553:MET:O	3:0:557:MET:N	2.39	0.44
3:0:568:LEU:O	3:0:597:ILE:N	2.42	0.44
3:0:705:ASP:N	3:0:705:ASP:OD1	2.50	0.44
4:6:322:MET:HE2	4:6:322:MET:HB3	1.73	0.44
5:2:368:ALA:HB3	5:2:370:PHE:HE1	1.81	0.44
7:7:492:VAL:HG12	7:7:493:VAL:HG22	1.99	0.44
9:O:179:HIS:HE1	9:O:237:PHE:CE2	2.35	0.44
10:N:32:DA:H1'	10:N:33:DA:C8	2.52	0.44
12:A:1121:GLU:HB3	12:A:1124:HIS:HB2	1.99	0.44
12:A:1208:THR:OG1	12:A:1231:ASP:OD2	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:332:ASP:O	13:B:336:ARG:HG2	2.18	0.44
13:B:704:ALA:HB2	13:B:738:PHE:CD1	2.52	0.44
14:C:61:GLU:HA	14:C:64:ALA:HB3	1.99	0.44
15:D:24:ALA:N	15:D:28:GLN:O	2.49	0.44
16:E:74:ASP:O	16:E:106:GLN:NE2	2.50	0.44
17:F:85:MET:HG3	17:F:89:GLU:HB2	1.99	0.44
18:G:48:VAL:HA	18:G:76:ALA:HA	1.99	0.44
18:G:61:ILE:HG12	18:G:68:ALA:HB2	1.99	0.44
22:K:12:LEU:HD12	22:K:13:GLY:H	1.82	0.44
25:Q:98:TYR:CB	26:R:96:ARG:HA	2.47	0.44
29:W:17:VAL:O	29:W:21:TYR:HB2	2.15	0.44
29:W:66:LEU:HA	29:W:94:ALA:HB2	1.99	0.44
29:W:169:GLN:OE1	29:W:173:ASN:ND2	2.50	0.44
1:1:339:LEU:HD11	3:0:610:ILE:HD11	1.99	0.44
3:0:378:SER:HA	3:0:403:ALA:HB1	1.98	0.44
3:0:539:VAL:HA	3:0:621:LEU:HB2	1.99	0.44
7:7:389:GLY:O	7:7:692:ARG:HA	2.17	0.44
7:7:631:THR:HG22	7:7:632:PRO:O	2.17	0.44
10:N:16:DC:O2	10:N:17:DG:N7	2.50	0.44
12:A:181:LEU:O	12:A:202:LEU:N	2.37	0.44
12:A:336:ILE:HG21	12:A:1401:SER:HA	1.99	0.44
12:A:1390:ASN:HA	12:A:1399:ARG:HD2	1.98	0.44
13:B:102:VAL:HG12	13:B:112:LEU:HB2	1.98	0.44
13:B:890:TYR:CE2	13:B:910:VAL:HG21	2.52	0.44
14:C:84:ARG:HD2	22:K:7:PHE:HB3	1.98	0.44
15:D:143:ASN:O	15:D:147:TYR:N	2.40	0.44
16:E:197:LYS:HE2	16:E:199:ILE:HD11	1.99	0.44
18:G:93:SER:HB3	18:G:100:GLU:HB3	1.98	0.44
25:Q:373:TYR:HB3	26:R:70:LEU:HD11	1.99	0.44
27:U:247:LEU:HD23	28:V:116:CYS:HB3	1.99	0.44
30:X:261:LYS:O	30:X:265:ASN:N	2.38	0.44
1:1:502:ARG:HA	1:1:502:ARG:HD2	1.77	0.44
2:4:50:ILE:HG21	2:4:181:CYS:SG	2.58	0.44
3:0:13:PRO:HA	3:0:92:TYR:CD1	2.53	0.44
3:0:298:ILE:HD12	3:0:298:ILE:HA	1.82	0.44
3:0:471:ARG:HH22	3:0:647:ARG:N	2.15	0.44
3:0:542:PRO:HB3	3:0:626:PRO:HA	1.99	0.44
4:6:403:CYS:HB3	4:6:408:SER:H	1.82	0.44
5:2:406:PRO:O	5:2:409:ARG:NH1	2.51	0.44
7:7:102:ALA:O	7:7:523:LYS:HB3	2.16	0.44
7:7:383:ILE:HG13	7:7:528:ASN:C	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:443:LYS:HA	7:7:469:ASP:HB3	1.99	0.44
9:O:214:LEU:HB2	9:O:223:ILE:HD12	1.98	0.44
12:A:151:ASP:OD1	12:A:152:VAL:N	2.50	0.44
12:A:1189:SER:N	12:A:1242:VAL:O	2.42	0.44
12:A:1212:VAL:O	12:A:1216:ILE:HG12	2.17	0.44
12:A:1334:ASP:O	12:A:1338:VAL:N	2.44	0.44
12:A:1397:LEU:HD23	12:A:1397:LEU:HA	1.88	0.44
13:B:135:ARG:HA	13:B:135:ARG:HD3	1.79	0.44
13:B:210:LYS:NZ	13:B:462:ALA:O	2.47	0.44
13:B:299:GLU:HG3	13:B:572:HIS:NE2	2.33	0.44
13:B:322:PHE:HZ	20:I:30:ARG:HB3	1.83	0.44
18:G:39:THR:O	18:G:43:GLY:N	2.48	0.44
19:H:101:ALA:HB2	19:H:116:TYR:CZ	2.52	0.44
3:0:143:ARG:HA	3:0:146:GLU:HG2	1.99	0.44
3:0:525:MET:O	3:0:528:GLU:HG2	2.18	0.44
4:6:136:MET:HE3	4:6:237:GLY:HA3	1.98	0.44
4:6:312:LYS:HA	4:6:312:LYS:HD3	1.77	0.44
5:2:118:GLN:O	5:2:122:GLY:N	2.50	0.44
5:2:473:LYS:HD2	5:2:473:LYS:HA	1.80	0.44
6:5:48:GLU:HB2	6:5:52:HIS:HE1	1.82	0.44
7:7:346:ASP:HA	7:7:508:HIS:CG	2.52	0.44
7:7:541:MET:HA	7:7:545:GLN:CD	2.42	0.44
7:7:694:LYS:HZ1	7:7:696:ARG:HH21	1.66	0.44
7:7:752:SER:OG	7:7:754:ARG:HG3	2.16	0.44
8:3:46:ILE:HD12	8:3:63:LEU:HD22	2.00	0.44
10:N:31:DC:H2"	10:N:32:DA:C8	2.52	0.44
12:A:445:ASN:HB2	12:A:455:MET:HG2	1.99	0.44
12:A:474:VAL:HA	12:A:521:MET:HE3	1.98	0.44
12:A:1286:LYS:HB2	12:A:1304:TRP:CZ3	2.53	0.44
13:B:333:PHE:HE1	13:B:337:ARG:HH21	1.65	0.44
19:H:26:ILE:HG13	19:H:42:ILE:HD12	1.99	0.44
26:R:276:ASN:HA	26:R:279:LYS:HE2	1.99	0.44
29:W:15:PHE:O	29:W:19:GLY:N	2.49	0.44
2:4:297:SER:C	2:4:299:ILE:H	2.24	0.44
4:6:231:GLU:HG2	4:6:260:ARG:O	2.17	0.44
7:7:363:ARG:HB3	7:7:548:HIS:HA	1.98	0.44
7:7:439:THR:HB	7:7:441:ASP:H	1.82	0.44
12:A:794:PRO:HB2	12:A:799:PHE:HB3	1.98	0.44
12:A:949:ASP:OD1	12:A:951:GLU:N	2.50	0.44
25:Q:30:ASN:O	25:Q:34:MET:N	2.40	0.44
1:1:373:ASP:HA	1:1:376:LYS:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:296:LEU:HD22	2:4:300:PRO:HG3	2.00	0.44
3:0:68:LYS:HZ2	3:0:204:ASN:HA	1.81	0.44
3:0:162:LEU:O	3:0:167:VAL:HG23	2.17	0.44
3:0:259:ARG:HB3	3:0:259:ARG:NH1	2.33	0.44
3:0:422:PRO:HG2	3:0:423:TYR:CD2	2.53	0.44
3:0:591:SER:O	4:6:272:ILE:HB	2.17	0.44
4:6:403:CYS:SG	4:6:437:CYS:HB3	2.57	0.44
5:2:29:PRO:O	5:2:33:LEU:N	2.45	0.44
5:2:69:ASN:OD1	5:2:69:ASN:N	2.50	0.44
6:5:48:GLU:O	6:5:52:HIS:ND1	2.51	0.44
7:7:411:CYS:CB	7:7:417:VAL:HG22	2.48	0.44
12:A:16:GLU:OE2	12:A:1418:LEU:HD21	2.18	0.44
12:A:339:ASN:ND2	13:B:1117:GLN:OE1	2.51	0.44
12:A:1115:SER:OG	12:A:1116:LEU:N	2.51	0.44
12:A:1342:GLU:HG3	16:E:198:ILE:HD13	2.00	0.44
12:A:1412:ALA:HA	12:A:1417:GLU:HG3	1.99	0.44
17:F:92:ARG:O	17:F:96:THR:OG1	2.31	0.44
18:G:26:LEU:HD23	18:G:26:LEU:HA	1.88	0.44
22:K:49:GLU:OE2	22:K:52:ASN:ND2	2.44	0.44
24:M:123:ASP:O	24:M:127:GLN:N	2.33	0.44
24:M:157:CYS:SG	24:M:158:HIS:N	2.88	0.44
28:V:81:LYS:HA	28:V:81:LYS:HD3	1.76	0.44
1:1:230:PRO:O	1:1:232:UNK:N	2.51	0.44
2:4:225:GLN:O	2:4:229:ASP:HB3	2.18	0.44
7:7:403:ILE:HG13	7:7:405:LYS:N	2.23	0.44
7:7:538:ALA:HB1	7:7:729:GLN:HB3	2.00	0.44
9:O:158:GLN:HB3	10:N:23:DA:C4'	2.42	0.44
12:A:224:PHE:CD2	12:A:231:PRO:HG3	2.53	0.44
12:A:376:TYR:CE1	12:A:498:ARG:HD2	2.53	0.44
12:A:563:PRO:HB3	12:A:572:TRP:CE2	2.53	0.44
12:A:1262:LYS:O	12:A:1266:THR:OG1	2.31	0.44
13:B:61:ASP:N	13:B:61:ASP:OD1	2.48	0.44
13:B:997:GLU:OE1	13:B:997:GLU:N	2.28	0.44
13:B:1065:GLN:OE1	13:B:1067:ARG:N	2.49	0.44
15:D:144:THR:O	15:D:148:LEU:HG	2.18	0.44
26:R:71:VAL:HA	26:R:222:CYS:O	2.17	0.44
29:W:116:ASN:O	29:W:165:ASN:HB2	2.16	0.44
30:X:274:LEU:HA	30:X:277:LYS:HB2	2.00	0.44
1:1:234:UNK:O	1:1:262:ASN:ND2	2.51	0.44
3:0:7:ASP:O	3:0:62:HIS:NE2	2.50	0.44
3:0:199:MET:HA	3:0:202:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:128:LEU:HD23	4:6:129:THR:N	2.33	0.44
4:6:141:LEU:HB2	4:6:144:ASN:O	2.16	0.44
4:6:165:PRO:HG2	4:6:375:HIS:HB3	2.00	0.44
5:2:273:LYS:HE2	5:2:277:MET:SD	2.57	0.44
5:2:367:LYS:HB2	5:2:375:LEU:HD23	2.00	0.44
7:7:579:LEU:HD13	7:7:766:LYS:HE3	1.99	0.44
9:O:169:PRO:HA	9:O:208:VAL:O	2.17	0.44
12:A:231:PRO:O	12:A:234:MET:HB3	2.18	0.44
12:A:590:ARG:HH21	12:A:621:THR:HG1	1.62	0.44
13:B:451:LYS:HG3	24:M:138:ASP:HB3	1.99	0.44
13:B:542:MET:HG2	13:B:747:MET:HB3	2.00	0.44
13:B:1006:ILE:HG23	21:J:45:CYS:HB3	1.99	0.44
22:K:77:THR:OG1	22:K:81:TYR:HB3	2.18	0.44
26:R:95:ILE:HG22	26:R:97:ILE:HG23	1.99	0.44
27:U:244:MET:HG2	27:U:267:VAL:HG22	2.00	0.44
3:0:338:LEU:O	3:0:342:LEU:HG	2.17	0.44
3:0:669:VAL:HG13	3:0:670:LEU:HG	2.00	0.44
7:7:354:ILE:HG12	7:7:452:LEU:HD21	2.00	0.44
7:7:383:ILE:HD13	7:7:383:ILE:HA	1.80	0.44
7:7:568:GLU:CD	7:7:580:LEU:HD13	2.43	0.44
7:7:642:ASN:CG	7:7:649:ILE:HD13	2.43	0.44
12:A:335:ARG:HA	12:A:335:ARG:HD3	1.75	0.44
12:A:1153:TYR:HB2	12:A:1192:LEU:HB3	2.00	0.44
12:A:1258:HIS:HA	12:A:1261:LYS:HD3	2.00	0.44
12:A:1329:THR:HG22	12:A:1331:SER:H	1.82	0.44
12:A:1409:LEU:O	12:A:1413:GLY:N	2.38	0.44
12:A:1428:VAL:HG13	13:B:1151:LEU:HD21	1.99	0.44
13:B:583:ASN:ND2	13:B:628:THR:H	2.15	0.44
15:D:55:ALA:O	15:D:59:ILE:HG12	2.18	0.44
18:G:25:TYR:O	18:G:29:LYS:HG2	2.18	0.44
20:I:8:ARG:NH1	20:I:8:ARG:HB2	2.33	0.44
24:M:87:LEU:HD13	24:M:130:PHE:CE2	2.52	0.44
29:W:34:PHE:CE1	30:X:201:THR:HA	2.52	0.44
3:0:486:THR:O	3:0:673:LYS:NZ	2.51	0.43
3:0:732:ASP:OD1	3:0:733:GLN:N	2.46	0.43
4:6:190:GLN:HA	4:6:193:ILE:HB	2.01	0.43
4:6:211:GLN:HB3	4:6:244:PRO:CD	2.42	0.43
7:7:594:LEU:HD22	7:7:706:TYR:CZ	2.53	0.43
7:7:715:GLU:HA	7:7:718:TYR:CD1	2.53	0.43
8:3:135:THR:O	8:3:139:LEU:N	2.37	0.43
9:O:105:ARG:HG2	9:O:112:THR:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:390:GLN:NE2	12:A:394:ASN:OD1	2.42	0.43
12:A:535:THR:HG21	12:A:617:VAL:HB	2.00	0.43
12:A:940:ARG:HH21	12:A:944:ARG:HH12	1.65	0.43
13:B:48:LEU:HD23	13:B:173:MET:SD	2.58	0.43
13:B:848:ARG:NH1	21:J:8:PHE:O	2.51	0.43
14:C:88:CYS:HB2	14:C:91:HIS:O	2.18	0.43
14:C:153:LEU:HD12	14:C:153:LEU:HA	1.81	0.43
16:E:29:PHE:C	16:E:30:ILE:HD12	2.42	0.43
16:E:180:ARG:NH2	16:E:192:ARG:H	2.16	0.43
18:G:21:ARG:HG3	18:G:25:TYR:CZ	2.53	0.43
24:M:163:LEU:HA	24:M:166:LYS:HG2	2.00	0.43
25:Q:126:LYS:H	25:Q:126:LYS:HE2	1.82	0.43
25:Q:138:ARG:O	25:Q:352:MET:HA	2.18	0.43
26:R:120:TYR:CG	26:R:226:PRO:HA	2.53	0.43
1:1:588:ASP:O	1:1:592:LYS:N	2.34	0.43
2:4:35:LYS:O	2:4:39:THR:N	2.34	0.43
3:0:243:VAL:O	3:0:247:SER:N	2.43	0.43
3:0:745:ILE:H	3:0:745:ILE:HG13	1.64	0.43
4:6:294:GLU:HA	4:6:297:LEU:HB3	2.00	0.43
5:2:148:HIS:O	5:2:153:THR:N	2.51	0.43
5:2:396:ILE:HG12	5:2:400:LEU:HG	1.99	0.43
9:O:94:TYR:O	28:V:71:PHE:HB3	2.17	0.43
12:A:41:MET:HG2	12:A:42:ASP:H	1.83	0.43
12:A:269:ILE:O	12:A:273:ASN:N	2.44	0.43
13:B:216:GLU:OE1	13:B:500:THR:OG1	2.35	0.43
13:B:989:THR:OG1	13:B:990:ILE:N	2.51	0.43
16:E:57:MET:HE2	16:E:57:MET:HB2	1.92	0.43
18:G:64:THR:C	18:G:66:GLY:H	2.26	0.43
26:R:64:SER:C	26:R:216:GLY:HA2	2.43	0.43
29:W:18:ARG:NH2	30:X:247:ASN:HA	2.33	0.43
29:W:149:CYS:HB2	29:W:156:LEU:HD21	2.00	0.43
30:X:274:LEU:HD12	30:X:277:LYS:HB2	2.00	0.43
1:1:189:LYS:HE3	1:1:189:LYS:HB3	1.78	0.43
4:6:234:ILE:HB	4:6:263:VAL:HB	1.99	0.43
5:2:31:THR:HG22	5:2:226:PHE:HD2	1.82	0.43
5:2:273:LYS:HG2	5:2:277:MET:HG2	2.00	0.43
5:2:346:LYS:NZ	5:2:376:GLY:O	2.39	0.43
6:5:23:ILE:O	6:5:27:MET:HG3	2.18	0.43
7:7:457:TYR:OH	7:7:488:ASP:N	2.31	0.43
7:7:550:ALA:O	7:7:702:ASN:HB2	2.18	0.43
7:7:608:PHE:N	7:7:671:ILE:O	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:471:ASN:ND2	12:A:650:GLN:OE1	2.39	0.43
12:A:664:THR:HG22	13:B:1014:PRO:HB3	2.00	0.43
12:A:752:LYS:HD3	12:A:752:LYS:HA	1.73	0.43
13:B:209:GLU:CD	13:B:485:ARG:HE	2.26	0.43
13:B:227:LYS:H	13:B:395:GLN:NE2	2.15	0.43
13:B:515:HIS:HB3	13:B:518:HIS:CD2	2.54	0.43
13:B:1155:SER:OG	13:B:1156:ASP:OD1	2.31	0.43
15:D:29:LEU:HD13	18:G:82:PHE:CZ	2.53	0.43
16:E:165:LEU:HD11	16:E:172:GLU:HG2	2.00	0.43
18:G:38:CYS:SG	18:G:39:THR:N	2.91	0.43
24:M:276:THR:HB	24:M:308:THR:HG21	2.00	0.43
25:Q:117:HIS:CG	25:Q:391:LYS:HB2	2.53	0.43
2:4:153:MET:HE3	2:4:153:MET:HB2	1.82	0.43
3:0:16:LYS:H	3:0:16:LYS:HG2	1.60	0.43
3:0:53:LEU:O	3:0:57:ILE:HG12	2.19	0.43
3:0:278:ASP:O	3:0:281:LYS:NZ	2.51	0.43
3:0:377:CYS:SG	3:0:407:THR:OG1	2.57	0.43
3:0:492:PHE:CZ	3:0:700:GLY:HA3	2.53	0.43
5:2:350:TYR:H	5:2:407:GLN:NE2	2.16	0.43
5:2:384:ARG:HG2	5:2:387:LEU:HD22	2.00	0.43
7:7:354:ILE:O	7:7:404:LYS:NZ	2.39	0.43
7:7:699:GLU:HB3	7:7:702:ASN:HD22	1.83	0.43
9:O:205:LEU:HD23	9:O:207:PHE:CZ	2.53	0.43
11:T:133:DT:H2'	11:T:134:DT:C6	2.53	0.43
11:T:150:DG:C2	11:T:151:DC:C2	3.06	0.43
12:A:91:PHE:HA	12:A:235:ILE:HA	1.99	0.43
12:A:465:TYR:CD1	13:B:976:ILE:HG13	2.53	0.43
12:A:1136:SER:HB2	12:A:1274:ARG:CZ	2.49	0.43
12:A:1199:ARG:O	12:A:1203:ASN:N	2.43	0.43
12:A:1224:LEU:O	12:A:1226:VAL:HG23	2.17	0.43
13:B:664:THR:HG23	13:B:678:GLU:HA	2.00	0.43
13:B:857:ARG:HH12	13:B:942:ARG:NH1	2.17	0.43
13:B:918:ILE:HD11	13:B:935:ARG:HB3	2.00	0.43
16:E:20:LYS:HB2	16:E:35:VAL:HG22	2.00	0.43
18:G:47:CYS:N	18:G:77:VAL:HG22	2.31	0.43
19:H:101:ALA:HB2	19:H:116:TYR:CE2	2.54	0.43
20:I:17:ARG:HA	20:I:17:ARG:HD2	1.61	0.43
25:Q:128:ASN:O	25:Q:128:ASN:ND2	2.51	0.43
26:R:126:LYS:O	26:R:220:HIS:ND1	2.46	0.43
27:U:258:TRP:HE1	27:U:285:TRP:HB2	1.83	0.43
1:1:212:THR:HB	1:1:213:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:487:UNK:N	2:4:55:GLU:OE2	2.51	0.43
3:0:71:TYR:HD1	3:0:72:CYS:N	2.16	0.43
4:6:136:MET:HA	4:6:145:ARG:HD2	1.99	0.43
4:6:262:LYS:HB2	4:6:287:PHE:CD2	2.49	0.43
4:6:363:CYS:HB3	4:6:368:LEU:H	1.83	0.43
4:6:377:ALA:HA	4:6:380:TYR:CG	2.54	0.43
7:7:324:GLU:O	7:7:328:LYS:N	2.52	0.43
12:A:332:LYS:HE2	12:A:332:LYS:HB2	1.85	0.43
12:A:913:LEU:HA	12:A:979:SER:N	2.33	0.43
12:A:951:GLU:O	12:A:954:TRP:NE1	2.52	0.43
13:B:285:ILE:HA	13:B:288:ALA:HB3	2.01	0.43
13:B:825:VAL:HA	13:B:1010:LEU:O	2.18	0.43
13:B:828:ALA:HB2	13:B:1085:ILE:HD12	2.00	0.43
22:K:107:THR:O	22:K:111:LEU:HG	2.18	0.43
26:R:63:ARG:NH1	26:R:66:ARG:HE	2.16	0.43
27:U:262:LEU:N	27:U:279:ALA:O	2.46	0.43
3:0:60:GLN:O	3:0:67:ARG:NH1	2.41	0.43
3:0:173:LYS:HE2	3:0:173:LYS:O	2.18	0.43
3:0:383:LEU:O	3:0:387:THR:HG23	2.18	0.43
3:0:540:PHE:HD1	3:0:602:ALA:HA	1.84	0.43
3:0:694:PRO:HG2	3:0:697:ILE:HB	2.01	0.43
4:6:272:ILE:HA	4:6:275:GLU:HB3	2.00	0.43
4:6:349:CYS:HB3	4:6:352:CYS:SG	2.58	0.43
4:6:403:CYS:SG	4:6:404:PHE:N	2.91	0.43
5:2:11:THR:HA	5:2:14:LEU:HB2	1.99	0.43
7:7:302:GLU:CG	7:7:322:SER:H	2.32	0.43
7:7:326:VAL:HA	7:7:329:ARG:HH21	1.83	0.43
7:7:348:ARG:O	7:7:405:LYS:HD3	2.18	0.43
10:N:7:DA:C4	10:N:8:DA:N7	2.86	0.43
10:N:35:DG:H2"	10:N:36:DT:H71	1.99	0.43
12:A:23:SER:O	12:A:27:VAL:HG23	2.18	0.43
12:A:140:THR:O	12:A:143:LYS:HG2	2.19	0.43
12:A:415:LEU:HD13	12:A:415:LEU:HA	1.83	0.43
13:B:856:PHE:HE1	13:B:969:ARG:HG3	1.83	0.43
13:B:879:ARG:HA	13:B:885:MET:SD	2.59	0.43
14:C:147:LEU:HD23	14:C:147:LEU:HA	1.80	0.43
15:D:162:ALA:O	15:D:166:LEU:N	2.47	0.43
23:L:53:HIS:C	23:L:54:ARG:HD2	2.43	0.43
29:W:97:ALA:HB1	30:X:268:LEU:HD22	2.00	0.43
1:1:229:GLY:HA2	1:1:230:PRO:HD3	1.83	0.43
3:0:304:GLU:N	3:0:305:PRO:HD3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:349:CYS:CB	4:6:352:CYS:SG	3.07	0.43
5:2:25:LEU:HD13	5:2:25:LEU:HA	1.80	0.43
7:7:416:SER:O	7:7:661:SER:OG	2.36	0.43
7:7:670:LEU:HD23	7:7:691:LEU:HD23	1.99	0.43
8:3:51:PRO:HB3	8:3:64:ARG:HD2	2.00	0.43
8:3:137:GLU:O	8:3:141:LYS:N	2.38	0.43
9:O:113:ALA:HB2	9:O:139:TYR:CE2	2.54	0.43
12:A:1171:GLN:HA	12:A:1174:PHE:HB2	2.01	0.43
13:B:486:TYR:CA	13:B:1096:ARG:HH22	2.30	0.43
13:B:883:LEU:HD13	13:B:931:TYR:CE1	2.54	0.43
13:B:910:VAL:HG13	13:B:938:SER:HB2	2.00	0.43
14:C:37:MET:HE3	14:C:176:ILE:HD12	2.00	0.43
16:E:115:ASN:N	16:E:115:ASN:OD1	2.50	0.43
20:I:28:GLU:HA	20:I:35:VAL:HG22	2.00	0.43
21:J:28:ASP:N	21:J:28:ASP:OD1	2.51	0.43
23:L:47:ARG:HH22	23:L:49:LYS:HA	1.83	0.43
24:M:92:LEU:HD23	24:M:92:LEU:HA	1.87	0.43
24:M:270:ALA:O	24:M:277:ILE:HG12	2.18	0.43
26:R:299:ILE:O	26:R:303:LEU:N	2.39	0.43
29:W:9:VAL:O	29:W:13:LEU:HG	2.19	0.43
29:W:9:VAL:HG22	29:W:189:ILE:HD13	2.00	0.43
1:1:185:LEU:HD13	1:1:210:TRP:CH2	2.53	0.43
1:1:370:UNK:C	1:1:372:VAL:H	2.30	0.43
3:0:114:LEU:HD22	3:0:192:PRO:HB2	2.00	0.43
3:0:119:GLU:HA	3:0:122:LYS:NZ	2.34	0.43
4:6:233:LEU:HD23	4:6:234:ILE:N	2.34	0.43
7:7:386:LEU:HB3	7:7:513:LEU:HB3	2.00	0.43
7:7:407:VAL:HG22	7:7:484:PHE:HB2	2.01	0.43
7:7:411:CYS:SG	7:7:420:TRP:HD1	2.41	0.43
7:7:539:ASN:ND2	7:7:542:GLU:HB3	2.34	0.43
7:7:679:SER:H	7:7:682:GLN:HG3	1.83	0.43
9:O:193:LEU:HB3	9:O:206:ILE:HB	2.00	0.43
10:N:35:DG:C2'	10:N:36:DT:H71	2.49	0.43
12:A:455:MET:HE1	13:B:1138:MET:HG2	2.01	0.43
12:A:1161:THR:H	12:A:1167:GLU:CD	2.26	0.43
12:A:1230:GLU:HB2	12:A:1233:ASP:OD1	2.18	0.43
13:B:499:ASN:OD1	13:B:500:THR:N	2.51	0.43
13:B:894:ASP:N	13:B:898:LEU:O	2.39	0.43
13:B:1138:MET:SD	13:B:1143:ALA:HB3	2.59	0.43
14:C:22:LEU:HD12	14:C:22:LEU:HA	1.87	0.43
16:E:78:LEU:HD21	16:E:109:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:K:37:LYS:N	22:K:69:ALA:O	2.52	0.43
27:U:255:LYS:N	27:U:255:LYS:HD2	2.34	0.43
1:1:255:LYS:O	1:1:259:ILE:HG12	2.19	0.43
2:4:85:TYR:HB3	2:4:88:PRO:HD2	2.00	0.43
2:4:192:GLN:O	2:4:196:ILE:HG13	2.19	0.43
3:0:49:THR:HA	3:0:52:LEU:HD12	2.01	0.43
3:0:245:ILE:HG13	3:0:638:ARG:CZ	2.49	0.43
3:0:436:ARG:HD2	3:0:437:PHE:H	1.83	0.43
3:0:502:ASP:OD1	3:0:502:ASP:N	2.51	0.43
4:6:138:GLU:OE2	4:6:140:ASP:HB2	2.18	0.43
4:6:159:GLU:HA	4:6:162:ASP:HB3	2.00	0.43
4:6:336:CYS:SG	4:6:337:SER:N	2.92	0.43
6:5:25:ALA:HA	6:5:29:ASP:HB2	2.01	0.43
6:5:44:PRO:HA	6:5:47:VAL:HG23	2.01	0.43
7:7:363:ARG:HB2	7:7:548:HIS:CE1	2.54	0.43
7:7:464:ARG:NH2	7:7:466:ARG:HH12	2.15	0.43
8:3:43:VAL:HG22	8:3:47:PHE:HD2	1.84	0.43
9:O:106:ILE:HG13	9:O:109:PRO:O	2.19	0.43
9:O:185:TYR:HB2	9:O:193:LEU:HD12	2.00	0.43
12:A:549:MET:HE3	12:A:656:TRP:HB2	2.01	0.43
12:A:1127:ASP:HB2	12:A:1130:GLN:HB3	2.00	0.43
13:B:259:TYR:HD1	13:B:259:TYR:HA	1.72	0.43
13:B:1037:LEU:HB3	13:B:1062:HIS:HD2	1.84	0.43
13:B:1201:LYS:HZ2	13:B:1205:GLN:CD	2.27	0.43
16:E:124:VAL:O	16:E:126:SER:N	2.51	0.43
19:H:33:GLN:HB3	19:H:35:GLN:OE1	2.18	0.43
24:M:267:LYS:HG3	24:M:268:GLU:H	1.84	0.43
26:R:104:ILE:HG13	26:R:124:LEU:HD21	2.01	0.43
30:X:133:GLU:O	30:X:137:LYS:N	2.42	0.43
2:4:276:CYS:O	2:4:280:GLY:N	2.31	0.43
3:0:169:ASP:CG	3:0:170:TYR:H	2.27	0.43
3:0:314:GLN:HB2	3:0:317:LEU:HD22	2.01	0.43
3:0:327:ARG:HB3	3:0:330:HIS:CG	2.53	0.43
3:0:441:ASP:HB3	3:0:444:ILE:HG12	2.00	0.43
3:0:446:ILE:O	3:0:449:VAL:HG22	2.19	0.43
3:0:473:LEU:HB2	3:0:475:PHE:CD1	2.54	0.43
3:0:535:ASP:OD1	3:0:535:ASP:N	2.52	0.43
4:6:128:LEU:HD21	4:6:235:VAL:HG23	2.01	0.43
4:6:178:LEU:O	4:6:180:GLN:NE2	2.52	0.43
5:2:438:VAL:O	5:2:442:ARG:N	2.35	0.43
5:2:492:PHE:CG	6:5:9:LEU:HD23	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:397:ILE:HG13	7:7:424:PHE:HE2	1.84	0.43
7:7:510:LYS:HB2	7:7:531:ILE:HG13	2.00	0.43
9:O:195:TYR:HD1	9:O:204:LEU:HD13	1.84	0.43
11:T:134:DT:H2"	11:T:135:DG:C8	2.54	0.43
12:A:143:LYS:HG3	12:A:144:THR:HG23	2.01	0.43
12:A:226:GLU:CD	12:A:226:GLU:H	2.26	0.43
12:A:579:SER:HB3	12:A:611:GLN:HA	2.01	0.43
12:A:592:ASP:N	12:A:595:THR:OG1	2.52	0.43
12:A:737:LEU:HD13	12:A:741:ASN:ND2	2.34	0.43
12:A:1155:ASP:OD2	12:A:1241:ARG:NH1	2.52	0.43
13:B:289:LEU:HA	13:B:289:LEU:HD23	1.79	0.43
15:D:47:LEU:HD21	18:G:3:PHE:CD2	2.54	0.43
16:E:50:MET:HE2	16:E:50:MET:HB2	1.86	0.43
18:G:83:LYS:HG3	18:G:150:CYS:SG	2.59	0.43
24:M:128:ALA:O	24:M:132:LYS:N	2.46	0.43
24:M:144:LYS:O	24:M:147:LYS:HB3	2.19	0.43
24:M:279:VAL:HG21	24:M:304:VAL:HG21	2.01	0.43
1:1:580:LYS:HA	1:1:583:TYR:HD2	1.84	0.42
2:4:123:GLU:HA	2:4:126:VAL:HB	2.01	0.42
3:0:318:THR:HG23	3:0:376:PHE:CE1	2.54	0.42
3:0:396:PHE:O	3:0:400:LYS:NZ	2.52	0.42
3:0:643:ARG:HG2	3:0:649:ARG:HA	2.01	0.42
4:6:138:GLU:CD	4:6:140:ASP:HB2	2.44	0.42
4:6:233:LEU:HA	4:6:262:LYS:O	2.18	0.42
5:2:154:PRO:HD2	5:2:355:LEU:HD23	2.01	0.42
5:2:370:PHE:HB2	5:2:373:MET:N	2.25	0.42
7:7:558:TRP:O	7:7:737:THR:OG1	2.29	0.42
12:A:707:GLY:HA2	12:A:1281:ARG:HD2	2.01	0.42
12:A:1452:LYS:H	12:A:1452:LYS:HG2	1.63	0.42
13:B:86:ARG:HG3	13:B:138:GLU:HG2	2.00	0.42
13:B:1076:HIS:O	14:C:31:ASN:ND2	2.50	0.42
16:E:64:PRO:HB3	16:E:75:MET:HE2	2.01	0.42
20:I:72:ASP:OD1	20:I:72:ASP:N	2.51	0.42
24:M:157:CYS:O	24:M:159:ASP:N	2.52	0.42
26:R:108:LEU:HD11	26:R:120:TYR:HB2	2.01	0.42
26:R:277:PHE:N	26:R:279:LYS:HE2	2.23	0.42
3:0:11:LEU:HG	3:0:96:GLU:OE1	2.19	0.42
3:0:135:ARG:HH21	3:0:393:VAL:HG23	1.85	0.42
4:6:350:PRO:HD2	4:6:370:LEU:HD22	2.01	0.42
7:7:625:PRO:HD2	7:7:649:ILE:HG23	2.00	0.42
9:O:95:ASN:HB3	9:O:98:ARG:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:88:LYS:HZ2	12:A:205:GLU:H	1.68	0.42
12:A:815:PHE:HA	12:A:818:MET:HE2	2.01	0.42
12:A:956:LEU:HD23	12:A:956:LEU:HA	1.88	0.42
12:A:1435:PRO:HA	12:A:1439:GLY:O	2.19	0.42
13:B:209:GLU:OE1	13:B:485:ARG:NE	2.52	0.42
15:D:144:THR:HG21	18:G:46:LEU:HD21	2.01	0.42
18:G:116:PRO:HD2	18:G:163:ILE:HG13	2.01	0.42
24:M:258:TYR:O	24:M:262:LYS:HG2	2.19	0.42
25:Q:98:TYR:HB2	26:R:96:ARG:HA	2.01	0.42
29:W:148:LEU:HD23	29:W:148:LEU:HA	1.89	0.42
1:1:195:PHE:CZ	1:1:199:VAL:HG21	2.54	0.42
3:0:69:ILE:C	3:0:70:ILE:HD12	2.44	0.42
3:0:162:LEU:O	3:0:167:VAL:N	2.46	0.42
3:0:280:GLN:CD	3:0:280:GLN:H	2.27	0.42
3:0:336:LYS:O	3:0:340:GLU:HG2	2.20	0.42
3:0:539:VAL:HG22	3:0:599:LEU:HA	2.01	0.42
4:6:148:MET:HE2	4:6:148:MET:HB3	1.88	0.42
4:6:211:GLN:HE22	4:6:246:ASP:C	2.28	0.42
4:6:404:PHE:HB3	4:6:435:GLU:O	2.20	0.42
5:2:56:GLU:CD	5:2:97:MET:HB3	2.45	0.42
5:2:247:ARG:O	5:2:251:GLN:N	2.36	0.42
5:2:433:LEU:HA	5:2:433:LEU:HD23	1.82	0.42
5:2:499:SER:HA	5:2:502:LEU:HD12	2.01	0.42
7:7:488:ASP:O	7:7:489:GLU:HG3	2.20	0.42
7:7:569:TYR:HA	7:7:577:ARG:NE	2.34	0.42
7:7:577:ARG:HG2	7:7:580:LEU:CB	2.49	0.42
10:N:9:DA:C1'	10:N:10:DA:H5'	2.46	0.42
10:N:28:DT:H1'	10:N:29:DT:H5'	2.01	0.42
12:A:29:ALA:HB1	13:B:1184:GLY:HA2	2.02	0.42
12:A:317:LYS:HB2	12:A:317:LYS:HE3	1.76	0.42
12:A:573:SER:O	12:A:576:GLN:HG3	2.18	0.42
13:B:639:ILE:HG12	13:B:691:GLU:HB2	2.01	0.42
13:B:773:MET:HB2	13:B:773:MET:HE3	1.82	0.42
13:B:1046:PRO:HB2	13:B:1047:PHE:CD1	2.54	0.42
14:C:6:PRO:HB3	14:C:25:VAL:HB	2.01	0.42
14:C:148:ARG:N	14:C:151:GLN:OE1	2.33	0.42
15:D:125:SER:O	15:D:129:LEU:N	2.44	0.42
18:G:2:PHE:CE1	18:G:79:PHE:HB2	2.54	0.42
18:G:38:CYS:C	18:G:155:SER:HA	2.44	0.42
19:H:91:ASP:OD1	19:H:91:ASP:N	2.52	0.42
21:J:17:LYS:HG3	21:J:39:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:M:129:ALA:O	24:M:133:ILE:HG12	2.19	0.42
25:Q:120:LYS:HE3	26:R:132:GLU:HB3	1.99	0.42
26:R:73:LEU:HD23	26:R:77:LEU:HD13	2.01	0.42
27:U:247:LEU:HD13	28:V:118:SER:HB3	2.01	0.42
27:U:269:ILE:HD13	28:V:108:VAL:HG11	2.01	0.42
1:1:221:ALA:O	1:1:225:SER:OG	2.36	0.42
3:0:74:ARG:NH2	3:0:236:GLU:HB3	2.31	0.42
3:0:83:LEU:HD21	3:0:107:GLY:N	2.35	0.42
3:0:516:PRO:HA	3:0:520:ARG:H	1.84	0.42
7:7:364:PRO:HD3	7:7:695:ARG:HD3	2.01	0.42
7:7:369:SER:O	7:7:372:LYS:HB2	2.19	0.42
7:7:723:GLN:HB2	7:7:733:PHE:CZ	2.54	0.42
10:N:6:DA:H2"	10:N:7:DA:H8	1.83	0.42
12:A:150:THR:HA	12:A:166:GLY:HA2	2.01	0.42
12:A:208:LEU:O	12:A:212:LYS:HG3	2.19	0.42
13:B:190:TYR:HD1	21:J:63:TYR:HE1	1.67	0.42
13:B:195:CYS:SG	13:B:197:PHE:HB2	2.59	0.42
13:B:703:ILE:HA	13:B:740:HIS:O	2.20	0.42
13:B:864:LYS:HG3	13:B:872:GLU:OE1	2.20	0.42
13:B:1204:PHE:CE2	13:B:1216:LEU:HD11	2.55	0.42
14:C:61:GLU:O	14:C:65:HIS:N	2.37	0.42
15:D:163:VAL:O	15:D:167:LEU:N	2.38	0.42
15:D:189:ASP:OD1	18:G:167:TYR:OH	2.28	0.42
20:I:78:CYS:SG	20:I:80:SER:OG	2.59	0.42
28:V:61:THR:HB	28:V:86:THR:HB	2.00	0.42
28:V:81:LYS:HA	28:V:109:ASP:O	2.19	0.42
29:W:144:ARG:HH12	29:W:146:GLU:HB2	1.84	0.42
29:W:183:ILE:O	29:W:187:LYS:N	2.37	0.42
1:1:205:PRO:HA	1:1:206:PRO:HD3	1.93	0.42
2:4:138:LYS:O	2:4:142:GLN:N	2.52	0.42
3:0:226:VAL:O	3:0:230:SER:OG	2.19	0.42
3:0:374:LEU:HB3	3:0:410:SER:HG	1.84	0.42
4:6:143:PRO:HB2	4:6:147:ALA:HB3	2.01	0.42
5:2:416:LEU:HA	5:2:432:VAL:HG21	2.00	0.42
9:O:70:ILE:O	9:O:124:THR:HA	2.19	0.42
12:A:290:GLU:O	12:A:294:SER:N	2.39	0.42
13:B:128:LEU:N	13:B:168:GLY:O	2.43	0.42
17:F:79:ARG:HB3	17:F:146:TRP:CZ2	2.55	0.42
17:F:113:GLY:O	17:F:115:THR:HG23	2.19	0.42
18:G:57:GLN:HG2	18:G:58:ARG:N	2.34	0.42
24:M:187:ARG:NH1	24:M:241:ARG:HD3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Q:129:PRO:HG2	25:Q:132:ASP:CG	2.45	0.42
26:R:314:SER:O	26:R:318:LEU:N	2.42	0.42
29:W:95:ILE:HD12	29:W:193:ARG:HH11	1.84	0.42
3:0:117:HIS:HE1	3:0:119:GLU:HB3	1.83	0.42
3:0:541:PHE:HA	3:0:623:ILE:HB	2.02	0.42
3:0:722:ARG:O	3:0:726:GLN:N	2.50	0.42
5:2:370:PHE:CE1	5:2:375:LEU:HB2	2.54	0.42
7:7:325:VAL:HG13	7:7:328:LYS:HD2	2.01	0.42
7:7:757:ARG:NH1	7:7:758:GLU:HA	2.33	0.42
9:O:161:VAL:HG13	9:O:215:THR:HB	2.02	0.42
12:A:1208:THR:HG22	12:A:1211:GLN:CD	2.44	0.42
12:A:1445:ILE:HG22	18:G:59:GLY:O	2.19	0.42
13:B:46:GLN:NE2	13:B:47:GLN:HG2	2.34	0.42
13:B:247:GLY:C	13:B:249:ARG:H	2.28	0.42
13:B:564:GLU:N	13:B:589:VAL:O	2.53	0.42
13:B:766:ARG:HD3	13:B:766:ARG:HA	1.73	0.42
13:B:1000:PRO:HB2	13:B:1072:MET:HE2	2.01	0.42
19:H:96:VAL:HG22	19:H:143:LEU:HG	2.00	0.42
22:K:6:ARG:O	22:K:9:LEU:HB2	2.19	0.42
30:X:272:ALA:C	30:X:275:PRO:HD2	2.44	0.42
1:1:546:LEU:O	1:1:550:CYS:N	2.40	0.42
2:4:30:ILE:HD13	2:4:179:LEU:HB2	2.02	0.42
3:0:133:CYS:HA	3:0:136:MET:HB3	2.00	0.42
3:0:245:ILE:HD11	3:0:441:ASP:C	2.45	0.42
3:0:402:ILE:O	3:0:406:ALA:N	2.36	0.42
3:0:442:ALA:O	3:0:446:ILE:HG12	2.20	0.42
3:0:671:ARG:N	3:0:675:ASP:OD2	2.53	0.42
5:2:36:TYR:HD2	5:2:37:ARG:HD3	1.85	0.42
5:2:71:LYS:HD2	5:2:72:LEU:N	2.35	0.42
5:2:75:GLN:HA	5:2:78:ILE:HG12	2.01	0.42
7:7:635:GLU:O	7:7:639:ILE:HG13	2.19	0.42
8:3:69:LYS:HB2	8:3:71:GLN:HE22	1.84	0.42
9:O:70:ILE:N	9:O:126:ALA:O	2.51	0.42
12:A:1139:GLU:O	12:A:1275:GLY:HA3	2.19	0.42
13:B:102:VAL:HG13	13:B:110:HIS:CD2	2.55	0.42
13:B:541:LEU:HD23	13:B:541:LEU:HA	1.83	0.42
13:B:649:LYS:HZ2	13:B:736:THR:HA	1.85	0.42
13:B:901:PRO:HD2	23:L:60:ARG:HA	2.02	0.42
14:C:59:ALA:HB3	14:C:62:PHE:HB2	2.01	0.42
16:E:124:VAL:HG13	16:E:132:ILE:HB	2.02	0.42
19:H:10:PHE:CG	19:H:28:ALA:HB1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Q:103:LEU:HB2	26:R:92:LEU:HD22	2.01	0.42
25:Q:118:LEU:HB3	25:Q:392:VAL:HG23	2.02	0.42
1:1:192:MET:HE2	1:1:192:MET:HB2	1.93	0.42
1:1:344:UNK:C	1:1:347:PRO:HD2	2.49	0.42
1:1:511:ALA:HB2	2:4:264:LYS:HD2	2.02	0.42
2:4:71:ASN:OD1	2:4:71:ASN:N	2.41	0.42
2:4:273:ARG:HB2	4:6:324:PHE:CE1	2.55	0.42
3:0:134:ARG:HH22	3:0:304:GLU:C	2.28	0.42
5:2:276:LEU:HG	5:2:280:SER:OG	2.20	0.42
5:2:350:TYR:O	5:2:372:ASN:HB2	2.20	0.42
5:2:350:TYR:N	5:2:407:GLN:OE1	2.47	0.42
7:7:399:ALA:O	7:7:402:THR:HB	2.20	0.42
7:7:612:VAL:HG13	7:7:613:TYR:H	1.84	0.42
10:N:15:DG:H2"	10:N:16:DC:H6	1.85	0.42
12:A:492:PRO:O	12:A:493:GLN:NE2	2.53	0.42
12:A:519:PRO:O	12:A:624:SER:HB2	2.20	0.42
12:A:565:ILE:O	12:A:570:PRO:HA	2.19	0.42
12:A:601:LYS:HB3	12:A:603:ASN:OD1	2.20	0.42
12:A:851:HIS:C	12:A:853:ASP:H	2.28	0.42
13:B:71:LEU:HD12	13:B:71:LEU:HA	1.85	0.42
13:B:329:THR:O	13:B:333:PHE:HB3	2.20	0.42
13:B:365:THR:HG23	13:B:374:LYS:HE2	2.00	0.42
13:B:685:LEU:HD23	13:B:690:VAL:HG13	2.00	0.42
13:B:840:ILE:HB	13:B:1011:ILE:HB	2.02	0.42
13:B:876:LYS:O	13:B:878:GLN:NE2	2.52	0.42
19:H:35:GLN:NE2	19:H:128:ASN:HD22	2.18	0.42
19:H:77:ARG:HD3	19:H:77:ARG:HA	1.88	0.42
25:Q:342:LEU:O	25:Q:346:GLU:HG3	2.20	0.42
29:W:12:LEU:HB2	29:W:185:SER:HB2	2.02	0.42
29:W:23:GLY:O	29:W:26:VAL:HG12	2.19	0.42
2:4:123:GLU:O	2:4:127:GLU:HG2	2.20	0.42
2:4:218:SER:HA	2:4:237:HIS:CD2	2.54	0.42
3:0:79:ILE:HG23	3:0:207:ILE:HB	2.02	0.42
3:0:408:LEU:HD22	3:0:412:TYR:HE2	1.85	0.42
3:0:495:MET:HE1	3:0:717:THR:HB	2.01	0.42
3:0:510:PHE:CG	3:0:511:GLU:N	2.88	0.42
4:6:269:GLN:HG3	4:6:288:TYR:HE2	1.85	0.42
5:2:414:GLU:OE2	7:7:169:HIS:N	2.52	0.42
7:7:715:GLU:O	7:7:719:SER:OG	2.37	0.42
8:3:134:ARG:O	8:3:138:GLU:N	2.38	0.42
12:A:983:ILE:H	12:A:983:ILE:HG12	1.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:1195:LEU:HD11	12:A:1238:ILE:HD12	2.01	0.42
12:A:1390:ASN:O	12:A:1399:ARG:HD2	2.19	0.42
13:B:190:TYR:HD1	21:J:63:TYR:CE1	2.38	0.42
16:E:23:VAL:HG22	16:E:28:TYR:HB2	2.01	0.42
16:E:39:LEU:O	16:E:43:LYS:HG3	2.20	0.42
24:M:252:VAL:O	24:M:255:SER:OG	2.31	0.42
26:R:134:VAL:O	26:R:215:VAL:N	2.42	0.42
1:1:184:LEU:HD13	1:1:220:PHE:CD1	2.55	0.42
3:0:28:ILE:HD11	3:0:56:THR:HG23	2.02	0.42
3:0:244:CYS:SG	3:0:446:ILE:HD11	2.59	0.42
3:0:257:LEU:O	3:0:261:THR:HG23	2.20	0.42
4:6:155:ASP:HA	4:6:158:HIS:CE1	2.54	0.42
4:6:209:SER:OG	4:6:242:THR:O	2.38	0.42
5:2:450:ARG:NH2	6:5:58:LEU:HB2	2.35	0.42
5:2:481:LEU:HD23	5:2:481:LEU:HA	1.89	0.42
6:5:6:LYS:H	6:5:6:LYS:HG3	1.52	0.42
7:7:437:VAL:HG13	7:7:454:VAL:HG13	2.02	0.42
7:7:646:ASN:ND2	7:7:648:GLN:OE1	2.48	0.42
9:O:109:PRO:HB2	9:O:111:THR:HG23	2.02	0.42
12:A:16:GLU:HG2	12:A:1418:LEU:HD11	2.02	0.42
12:A:1364:ASN:HD21	12:A:1366:ARG:HD2	1.85	0.42
13:B:304:ASP:OD1	13:B:306:ASN:N	2.53	0.42
14:C:183:TRP:CD2	14:C:213:PRO:HD3	2.55	0.42
24:M:124:ASN:O	24:M:127:GLN:HG2	2.20	0.42
24:M:206:THR:O	24:M:209:ILE:HG12	2.19	0.42
25:Q:134:HIS:CD2	25:Q:135:LEU:H	2.38	0.42
27:U:257:ARG:HE	27:U:257:ARG:HB3	1.58	0.42
2:4:210:ILE:O	2:4:233:GLY:HA3	2.20	0.41
3:0:467:ASP:C	3:0:470:PRO:HD2	2.45	0.41
3:0:586:TYR:CE1	3:0:598:LEU:HB2	2.55	0.41
5:2:243:SER:O	5:2:247:ARG:N	2.42	0.41
5:2:249:MET:O	5:2:253:MET:N	2.33	0.41
5:2:347:ILE:HG22	5:2:373:MET:HE1	2.01	0.41
5:2:370:PHE:N	5:2:370:PHE:CD1	2.88	0.41
7:7:310:ILE:HG12	7:7:338:LEU:HB3	2.02	0.41
7:7:383:ILE:HG13	7:7:528:ASN:CA	2.50	0.41
7:7:410:LEU:HD13	7:7:485:ILE:HG23	2.02	0.41
7:7:493:VAL:HG12	7:7:494:PRO:HD2	2.02	0.41
9:O:73:THR:HG23	9:O:158:GLN:HG3	2.01	0.41
12:A:66:LYS:HG3	12:A:72:GLU:HA	2.02	0.41
12:A:150:THR:O	12:A:164:ARG:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:914:GLU:OE1	12:A:978:PRO:HB2	2.20	0.41
12:A:1116:LEU:N	12:A:1308:THR:O	2.53	0.41
14:C:35:ARG:HH21	22:K:41:THR:H	1.66	0.41
14:C:112:ASN:ND2	21:J:19:GLU:OE2	2.53	0.41
16:E:177:ARG:O	16:E:212:ARG:NH1	2.53	0.41
19:H:111:LEU:HD22	19:H:111:LEU:H	1.85	0.41
19:H:134:ASN:OD1	19:H:134:ASN:N	2.36	0.41
19:H:142:LEU:C	19:H:143:LEU:HD12	2.44	0.41
25:Q:103:LEU:HD12	26:R:92:LEU:HA	2.01	0.41
26:R:124:LEU:HD13	26:R:127:LYS:HE3	2.00	0.41
27:U:244:MET:HB2	28:V:113:ILE:HA	2.02	0.41
27:U:263:LYS:HG3	27:U:277:GLN:O	2.20	0.41
29:W:65:ARG:HH11	29:W:93:HIS:CG	2.37	0.41
2:4:161:ASN:HA	2:4:164:SER:HB3	2.01	0.41
3:0:312:LEU:O	3:0:314:GLN:N	2.52	0.41
3:0:347:LYS:HE2	3:0:347:LYS:HB2	1.86	0.41
3:0:372:LYS:HE2	3:0:376:PHE:CZ	2.55	0.41
4:6:264:LEU:HD22	4:6:300:LEU:HD13	2.01	0.41
5:2:141:ASN:O	5:2:145:THR:N	2.36	0.41
5:2:408:MET:HG3	5:2:411:LEU:HB3	2.02	0.41
7:7:467:SER:O	7:7:471:GLN:NE2	2.52	0.41
7:7:472:LYS:O	7:7:476:PHE:N	2.44	0.41
7:7:476:PHE:CE1	7:7:480:ARG:HB2	2.55	0.41
7:7:526:ASP:HB2	7:7:529:PHE:CD2	2.56	0.41
7:7:723:GLN:O	7:7:726:LEU:HB2	2.20	0.41
8:3:43:VAL:HG22	8:3:47:PHE:CD2	2.54	0.41
12:A:412:ARG:O	24:M:51:VAL:HG12	2.20	0.41
12:A:417:TYR:CE2	24:M:35:VAL:HG21	2.52	0.41
12:A:445:ASN:OD1	12:A:446:ARG:N	2.53	0.41
12:A:1157:ASP:CG	12:A:1160:SER:H	2.28	0.41
12:A:1364:ASN:ND2	12:A:1366:ARG:HD2	2.35	0.41
13:B:199:MET:HE2	13:B:492:LEU:HD21	2.00	0.41
13:B:269:ILE:O	13:B:282:ILE:HG23	2.20	0.41
13:B:451:LYS:HA	13:B:451:LYS:HD2	1.85	0.41
13:B:637:LEU:HD23	13:B:637:LEU:HA	1.78	0.41
13:B:1167:GLY:O	13:B:1215:ARG:HA	2.20	0.41
15:D:47:LEU:HD21	18:G:3:PHE:CE2	2.55	0.41
16:E:108:GLY:O	16:E:132:ILE:HA	2.20	0.41
19:H:130:ARG:H	19:H:130:ARG:HD2	1.85	0.41
20:I:93:LYS:HE2	20:I:93:LYS:HB3	1.86	0.41
22:K:77:THR:HG23	22:K:83:PRO:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:W:126:ILE:H	29:W:126:ILE:HD12	1.85	0.41
30:X:259:PHE:O	30:X:262:MET:HG2	2.20	0.41
1:1:263:TYR:HB2	1:1:266:VAL:HG12	2.01	0.41
3:0:48:LYS:HE3	3:0:48:LYS:HB3	1.95	0.41
3:0:77:SER:HA	3:0:80:GLU:CD	2.45	0.41
3:0:421:GLU:HB2	3:0:434:ILE:HG12	2.02	0.41
4:6:362:VAL:HG13	4:6:368:LEU:C	2.45	0.41
5:2:346:LYS:HE2	5:2:377:GLN:HB2	2.01	0.41
5:2:431:GLN:CD	5:2:435:PRO:HD2	2.45	0.41
7:7:363:ARG:HD3	7:7:548:HIS:CD2	2.54	0.41
7:7:374:PHE:HA	7:7:379:ALA:HA	2.01	0.41
10:N:13:DG:C4	10:N:14:DC:C4	3.08	0.41
12:A:170:THR:HG23	12:A:185:TRP:HD1	1.85	0.41
12:A:353:ILE:HG21	12:A:487:MET:SD	2.61	0.41
12:A:592:ASP:C	12:A:595:THR:HG1	2.27	0.41
12:A:1020:CYS:N	12:A:1023:ARG:HH21	2.19	0.41
13:B:60:GLN:OE1	13:B:95:ILE:HG22	2.21	0.41
13:B:345:LYS:HD3	13:B:348:ARG:NH1	2.36	0.41
13:B:837:ASP:N	13:B:837:ASP:OD1	2.53	0.41
20:I:17:ARG:O	20:I:25:LEU:HD12	2.20	0.41
24:M:185:VAL:HG12	24:M:186:ALA:H	1.85	0.41
26:R:63:ARG:HE	26:R:63:ARG:HB2	1.52	0.41
1:1:270:TYR:HE2	1:1:284:TRP:HE1	1.69	0.41
2:4:259:ARG:N	2:4:260:PRO:HD3	2.36	0.41
2:4:287:PHE:CE1	4:6:321:LYS:HB2	2.54	0.41
3:0:117:HIS:ND1	3:0:120:VAL:HG23	2.35	0.41
3:0:156:CYS:O	3:0:157:GLU:HB3	2.19	0.41
3:0:555:GLN:HA	3:0:560:LEU:HD22	2.02	0.41
3:0:651:ASN:OD1	3:0:651:ASN:N	2.52	0.41
5:2:450:ARG:HH21	6:5:58:LEU:HB2	1.84	0.41
7:7:389:GLY:HA3	7:7:689:ARG:O	2.20	0.41
7:7:676:HIS:HD2	7:7:714:GLN:HE22	1.67	0.41
10:N:40:DG:H2"	10:N:41:DA:N7	2.35	0.41
12:A:434:ARG:NH1	12:A:440:ASP:OD2	2.42	0.41
12:A:1027:ALA:O	12:A:1031:VAL:HG23	2.20	0.41
12:A:1194:ARG:HE	12:A:1237:ILE:HD12	1.84	0.41
13:B:106:ASP:OD1	13:B:108:VAL:HG12	2.20	0.41
13:B:343:ILE:C	13:B:348:ARG:HH12	2.28	0.41
13:B:614:SER:OG	13:B:697:GLU:OE1	2.20	0.41
13:B:649:LYS:HZ3	13:B:736:THR:HG23	1.85	0.41
18:G:116:PRO:HD3	18:G:164:LYS:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:H:89:LEU:HB3	19:H:143:LEU:HD21	2.02	0.41
20:I:61:ASP:O	20:I:64:SER:OG	2.37	0.41
1:1:235:UNK:O	1:1:239:PRO:HD2	2.20	0.41
2:4:65:LEU:O	5:2:37:ARG:NH2	2.53	0.41
2:4:275:SER:HB2	2:4:281:ARG:C	2.45	0.41
3:0:48:LYS:O	3:0:52:LEU:N	2.42	0.41
3:0:140:GLN:O	3:0:144:LYS:HG3	2.20	0.41
4:6:374:THR:O	4:6:378:ARG:HG2	2.20	0.41
12:A:149:GLU:O	12:A:166:GLY:HA2	2.20	0.41
12:A:450:LEU:HD12	12:A:451:HIS:HD2	1.85	0.41
12:A:576:GLN:HG3	12:A:576:GLN:H	1.57	0.41
12:A:687:LYS:HE2	12:A:794:PRO:HG2	2.03	0.41
13:B:570:VAL:HB	13:B:573:GLN:OE1	2.20	0.41
13:B:1038:SER:O	21:J:33:GLY:HA3	2.20	0.41
16:E:41:ASP:HA	16:E:44:ALA:HB3	2.02	0.41
19:H:83:GLN:HA	22:K:54:ARG:NH1	2.34	0.41
25:Q:121:PHE:HB2	26:R:131:ASN:HB3	2.02	0.41
25:Q:378:VAL:HA	25:Q:384:PHE:HD1	1.85	0.41
29:W:147:PHE:HB2	29:W:156:LEU:HB2	2.02	0.41
1:1:596:LEU:O	1:1:600:VAL:N	2.38	0.41
2:4:177:LEU:HD12	2:4:211:ASP:O	2.20	0.41
3:0:77:SER:O	3:0:80:GLU:HG2	2.21	0.41
3:0:117:HIS:CD2	3:0:156:CYS:HA	2.55	0.41
3:0:307:VAL:H	3:0:382:SER:HB3	1.86	0.41
3:0:609:GLY:N	3:0:668:ARG:HH12	2.19	0.41
3:0:633:ARG:HB2	3:0:636:LYS:HB2	2.02	0.41
4:6:138:GLU:OE2	4:6:145:ARG:NH2	2.51	0.41
4:6:362:VAL:HA	4:6:369:MET:HA	2.02	0.41
5:2:276:LEU:O	5:2:280:SER:N	2.53	0.41
7:7:302:GLU:HG3	7:7:322:SER:N	2.36	0.41
7:7:440:SER:HA	7:7:470:SER:H	1.85	0.41
7:7:489:GLU:OE1	7:7:491:HIS:HE1	2.04	0.41
7:7:519:ARG:CG	7:7:522:ASP:HB2	2.51	0.41
8:3:131:GLU:O	8:3:135:THR:N	2.37	0.41
12:A:134:ARG:HH12	12:A:221:SER:HA	1.85	0.41
12:A:230:ARG:HB2	12:A:233:TRP:CE2	2.56	0.41
12:A:412:ARG:HB3	24:M:51:VAL:HG11	2.03	0.41
13:B:357:GLN:NE2	13:B:358:LYS:HG3	2.35	0.41
24:M:294:THR:O	24:M:296:ALA:N	2.54	0.41
25:Q:123:SER:HB3	25:Q:361:TRP:CH2	2.54	0.41
26:R:261:VAL:O	26:R:264:SER:OG	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:U:244:MET:HE2	28:V:111:LEU:HD22	2.03	0.41
1:1:375:LEU:HD21	3:0:551:VAL:HG11	2.03	0.41
2:4:32:ILE:HG12	2:4:77:ALA:HB1	2.02	0.41
2:4:160:VAL:O	2:4:164:SER:N	2.34	0.41
3:0:537:MET:N	3:0:586:TYR:OH	2.52	0.41
4:6:196:LEU:HA	4:6:199:ILE:HB	2.02	0.41
4:6:274:LYS:HD2	4:6:285:GLU:HG2	2.02	0.41
5:2:10:VAL:O	5:2:14:LEU:HD13	2.20	0.41
7:7:373:MET:HE2	7:7:382:GLY:H	1.86	0.41
9:O:139:TYR:O	9:O:143:ILE:HG12	2.20	0.41
12:A:943:LEU:HD23	12:A:943:LEU:HA	1.85	0.41
12:A:1111:MET:HE2	12:A:1111:MET:HB3	1.86	0.41
12:A:1373:ASP:O	12:A:1377:THR:HG23	2.21	0.41
13:B:737:THR:OG1	13:B:737:THR:O	2.38	0.41
13:B:830:TYR:CZ	13:B:1000:PRO:HD3	2.56	0.41
21:J:44:TYR:HA	21:J:47:ARG:CB	2.51	0.41
24:M:30:TYR:CG	24:M:31:PRO:HD2	2.56	0.41
24:M:185:VAL:HA	24:M:237:THR:HG21	2.02	0.41
25:Q:138:ARG:HG2	26:R:58:ASP:N	2.36	0.41
29:W:74:GLU:H	29:W:83:GLU:HA	1.86	0.41
29:W:134:LEU:HD23	29:W:134:LEU:HA	1.86	0.41
2:4:212:VAL:O	2:4:235:TYR:HA	2.21	0.41
3:0:140:GLN:HG2	3:0:143:ARG:HE	1.86	0.41
3:0:498:THR:O	3:0:506:ILE:HG12	2.20	0.41
3:0:704:ALA:O	3:0:708:LEU:HD21	2.21	0.41
4:6:198:SER:O	4:6:202:GLN:N	2.53	0.41
4:6:281:ASN:O	4:6:284:ASP:N	2.42	0.41
4:6:451:CYS:HB3	4:6:454:CYS:HB2	2.02	0.41
5:2:87:LEU:HD23	5:2:87:LEU:H	1.85	0.41
7:7:439:THR:HB	7:7:442:ASN:H	1.86	0.41
7:7:576:LYS:HE2	7:7:766:LYS:C	2.46	0.41
12:A:532:ARG:HD3	12:A:749:ALA:HB2	2.02	0.41
13:B:799:PRO:CB	13:B:818:PRO:HG2	2.51	0.41
14:C:241:ASP:HB3	22:K:109:TRP:CE2	2.55	0.41
16:E:39:LEU:O	16:E:42:PHE:HB3	2.21	0.41
16:E:46:TYR:CE2	16:E:58:MET:HA	2.56	0.41
16:E:46:TYR:CD2	16:E:58:MET:HG2	2.56	0.41
16:E:178:ILE:HG23	16:E:214:CYS:HA	2.03	0.41
21:J:43:ARG:NE	21:J:45:CYS:SG	2.89	0.41
22:K:13:GLY:H	22:K:37:LYS:NZ	2.19	0.41
24:M:126:VAL:HG22	24:M:154:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:R:94:LYS:HE2	26:R:94:LYS:HB2	1.95	0.41
1:1:171:LYS:HA	1:1:214:ILE:HD12	2.02	0.41
2:4:293:LEU:HG	4:6:380:TYR:HE1	1.85	0.41
2:4:303:ASN:HB2	2:4:311:GLN:HG2	2.02	0.41
3:0:101:GLU:HG3	3:0:173:LYS:HZ1	1.86	0.41
3:0:106:LEU:HD22	3:0:176:PHE:HB2	2.02	0.41
3:0:111:ARG:HG3	3:0:193:TYR:CG	2.55	0.41
3:0:158:TYR:HA	3:0:161:ASN:ND2	2.36	0.41
3:0:210:TYR:HE1	3:0:234:PHE:CD1	2.39	0.41
3:0:239:ASN:HA	3:0:242:ASN:HD21	1.86	0.41
3:0:264:ALA:HB1	3:0:336:LYS:HE2	2.03	0.41
4:6:116:THR:N	4:6:117:PRO:HD3	2.35	0.41
4:6:120:ARG:HB3	4:6:309:PRO:HD3	2.03	0.41
4:6:211:GLN:HB2	4:6:243:ASP:CG	2.46	0.41
5:2:349:SER:OG	5:2:374:VAL:HG23	2.21	0.41
5:2:366:LEU:HD13	5:2:374:VAL:HG12	2.01	0.41
6:5:5:ARG:NH1	6:5:33:GLU:OE2	2.44	0.41
6:5:14:PRO:HA	6:5:17:LYS:HD2	2.02	0.41
7:7:230:ASN:O	7:7:345:ASN:HB3	2.21	0.41
7:7:366:GLN:CG	7:7:548:HIS:HE1	2.32	0.41
7:7:421:ARG:NH2	7:7:432:PRO:HG3	2.34	0.41
7:7:497:MET:HE2	7:7:497:MET:HB2	1.87	0.41
7:7:530:LEU:HD13	7:7:530:LEU:HA	1.97	0.41
7:7:668:THR:HG23	7:7:702:ASN:C	2.46	0.41
7:7:679:SER:H	7:7:682:GLN:CG	2.34	0.41
9:O:73:THR:HG22	9:O:122:VAL:HG22	2.02	0.41
10:N:11:DA:C4	10:N:12:DG:C5	3.09	0.41
12:A:416:ARG:HG3	12:A:417:TYR:CD1	2.56	0.41
12:A:1340:GLY:HA2	16:E:183:PRO:HD2	2.03	0.41
12:A:1363:VAL:HB	12:A:1368:MET:HE2	2.03	0.41
12:A:1408:ILE:HD13	12:A:1408:ILE:HA	1.88	0.41
13:B:276:ILE:HA	13:B:338:GLY:HA3	2.02	0.41
13:B:328:GLU:OE1	13:B:328:GLU:N	2.33	0.41
13:B:435:THR:O	13:B:439:ALA:N	2.53	0.41
13:B:603:LEU:O	13:B:608:ASP:N	2.54	0.41
13:B:773:MET:SD	13:B:987:LYS:HB3	2.60	0.41
13:B:1174:LYS:HB2	13:B:1179:GLN:HB2	2.02	0.41
13:B:1175:LEU:HA	13:B:1178:ASN:HA	2.03	0.41
15:D:209:ARG:HE	15:D:210:ILE:HG12	1.86	0.41
18:G:22:MET:O	18:G:26:LEU:N	2.42	0.41
18:G:38:CYS:HA	18:G:44:TYR:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:G:115:MET:HE3	18:G:119:LEU:HD23	2.03	0.41
18:G:151:ILE:HD13	18:G:151:ILE:HA	1.95	0.41
20:I:10:CYS:SG	20:I:32:CYS:HB3	2.61	0.41
21:J:20:SER:O	21:J:24:LEU:HG	2.21	0.41
22:K:10:PHE:HA	22:K:37:LYS:HB3	2.01	0.41
22:K:60:ALA:O	22:K:73:LEU:HD12	2.21	0.41
25:Q:110:ASP:HB2	25:Q:114:MET:HE3	2.02	0.41
27:U:252:THR:HG23	27:U:257:ARG:HH12	1.86	0.41
27:U:254:THR:O	27:U:256:ALA:N	2.54	0.41
27:U:257:ARG:HG2	27:U:283:ALA:O	2.21	0.41
29:W:56:PRO:HA	29:W:59:ALA:HB3	2.03	0.41
29:W:67:ILE:HA	29:W:89:VAL:HA	2.03	0.41
1:1:280:GLU:HB3	1:1:284:TRP:CD2	2.56	0.41
3:0:2:LYS:HA	3:0:10:VAL:O	2.19	0.41
3:0:69:ILE:HG23	3:0:231:ILE:HG23	2.03	0.41
3:0:584:GLU:O	3:0:588:LYS:N	2.39	0.41
4:6:278:LYS:N	4:6:285:GLU:OE1	2.54	0.41
4:6:299:GLU:HA	4:6:302:ASN:OD1	2.20	0.41
4:6:326:THR:HG23	4:6:348:PHE:HB2	2.03	0.41
4:6:338:CYS:HB3	4:6:364:PRO:HG3	2.02	0.41
5:2:39:LEU:HB3	5:2:43:ALA:HB3	2.02	0.41
6:5:30:ILE:H	6:5:30:ILE:HG12	1.60	0.41
7:7:401:CYS:O	7:7:404:LYS:HD3	2.20	0.41
7:7:596:GLN:HG3	7:7:600:ARG:NH2	2.35	0.41
8:3:39:CYS:O	8:3:43:VAL:HG12	2.21	0.41
9:O:91:ASN:O	9:O:104:MET:HG3	2.20	0.41
12:A:456:MET:HG2	12:A:510:GLN:HG3	2.02	0.41
12:A:567:LYS:O	19:H:95:TYR:HA	2.21	0.41
12:A:768:GLN:OE1	12:A:816:HIS:HA	2.21	0.41
12:A:872:GLY:O	12:A:1058:VAL:HG12	2.21	0.41
12:A:1191:TRP:CE3	12:A:1191:TRP:HA	2.56	0.41
13:B:293:PRO:HG2	13:B:296:GLU:HB2	2.02	0.41
13:B:599:THR:O	13:B:603:LEU:HG	2.21	0.41
15:D:67:ARG:HA	15:D:70:PHE:HB3	2.03	0.41
16:E:67:GLU:OE1	16:E:68:SER:OG	2.38	0.41
18:G:65:ASP:O	18:G:67:SER:N	2.54	0.41
20:I:59:VAL:O	20:I:62:ILE:HG22	2.21	0.41
20:I:75:CYS:SG	20:I:108:HIS:HB3	2.61	0.41
21:J:44:TYR:HA	21:J:47:ARG:HB2	2.03	0.41
21:J:52:THR:OG1	21:J:52:THR:O	2.39	0.41
22:K:61:TYR:HB3	22:K:73:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Q:101:PHE:HB3	25:Q:383:SER:HA	2.03	0.41
29:W:159:ASP:OD1	29:W:160:ASP:N	2.53	0.41
2:4:175:ARG:HD3	2:4:255:ASP:HB2	2.02	0.40
2:4:176:LEU:HD23	2:4:176:LEU:H	1.86	0.40
3:0:4:TYR:OH	3:0:9:PRO:HG3	2.21	0.40
3:0:589:ALA:HB3	3:0:596:ALA:HB2	2.02	0.40
5:2:19:GLN:HG3	5:2:85:HIS:CD2	2.57	0.40
6:5:16:ILE:O	6:5:19:LEU:HB2	2.19	0.40
7:7:234:VAL:O	7:7:315:SER:HA	2.21	0.40
7:7:310:ILE:HD11	7:7:338:LEU:HD23	2.03	0.40
7:7:409:VAL:HG13	7:7:486:ILE:HD12	2.03	0.40
9:O:101:ALA:HB2	9:O:116:PHE:CE2	2.56	0.40
12:A:761:MET:HA	12:A:804:TYR:HB2	2.03	0.40
12:A:870:GLU:OE1	16:E:202:SER:HB2	2.21	0.40
12:A:1124:HIS:HB3	12:A:1130:GLN:HG2	2.03	0.40
12:A:1132:LYS:HD3	12:A:1132:LYS:HA	1.90	0.40
13:B:555:ILE:H	13:B:555:ILE:HG13	1.37	0.40
13:B:865:LYS:NZ	13:B:871:THR:HG23	2.36	0.40
14:C:78:GLU:H	14:C:78:GLU:CD	2.21	0.40
18:G:115:MET:HG2	18:G:163:ILE:HG12	2.04	0.40
19:H:10:PHE:CD1	19:H:28:ALA:HB1	2.56	0.40
19:H:104:PHE:CE2	19:H:137:GLN:HG2	2.56	0.40
20:I:111:THR:HG23	20:I:113:ASP:H	1.86	0.40
1:1:517:UNK:O	1:1:519:UNK:N	2.54	0.40
2:4:192:GLN:O	2:4:195:PRO:HD2	2.21	0.40
2:4:205:LYS:HA	2:4:205:LYS:HD2	1.95	0.40
3:0:57:ILE:O	3:0:61:MET:HG2	2.21	0.40
3:0:192:PRO:HA	3:0:195:ILE:HB	2.03	0.40
3:0:703:ASP:HA	3:0:706:LEU:HD23	2.03	0.40
3:0:735:GLY:O	3:0:739:TRP:N	2.49	0.40
4:6:232:VAL:O	4:6:261:VAL:HG13	2.21	0.40
4:6:261:VAL:HB	4:6:280:THR:HG21	2.02	0.40
4:6:266:LEU:O	4:6:268:ALA:N	2.50	0.40
4:6:270:VAL:HB	4:6:273:CYS:HB2	2.02	0.40
4:6:280:THR:OG1	4:6:281:ASN:ND2	2.54	0.40
5:2:349:SER:HA	5:2:407:GLN:NE2	2.37	0.40
5:2:370:PHE:HA	7:7:116:HIS:C	2.47	0.40
12:A:811:GLN:H	12:A:811:GLN:CD	2.25	0.40
13:B:87:LYS:O	13:B:137:TYR:N	2.33	0.40
13:B:249:ARG:N	13:B:249:ARG:HD2	2.36	0.40
13:B:628:THR:C	13:B:632:ARG:HH21	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:925:LEU:HD12	13:B:928:ARG:HH22	1.86	0.40
13:B:1074:ASN:CG	13:B:1076:HIS:H	2.29	0.40
18:G:37:SER:O	18:G:45:ILE:N	2.48	0.40
27:U:262:LEU:HB2	27:U:279:ALA:HB3	2.04	0.40
29:W:52:THR:HG23	29:W:53:GLU:HG3	2.03	0.40
1:1:387:MET:C	1:1:389:LEU:H	2.30	0.40
3:0:224:ASN:HA	3:0:227:SER:OG	2.21	0.40
3:0:337:ARG:HD2	8:3:82:VAL:HA	2.04	0.40
3:0:341:TYR:CD1	3:0:366:LEU:HD12	2.56	0.40
3:0:351:VAL:N	3:0:422:PRO:HD3	2.37	0.40
3:0:661:HIS:HA	3:0:664:GLN:HE21	1.85	0.40
4:6:193:ILE:HD13	4:6:193:ILE:HA	1.93	0.40
5:2:217:ASP:O	5:2:221:VAL:HG23	2.22	0.40
6:5:53:GLU:HA	6:5:56:ARG:CB	2.50	0.40
7:7:370:LEU:HD23	7:7:370:LEU:HA	1.95	0.40
10:N:41:DA:H2"	10:N:42:DA:C8	2.56	0.40
12:A:1235:LYS:O	12:A:1237:ILE:HG12	2.22	0.40
13:B:280:ILE:HG23	13:B:284:ILE:HD12	2.03	0.40
13:B:483:LEU:HD12	13:B:484:ASN:H	1.86	0.40
13:B:579:ARG:NH2	13:B:623:GLU:OE2	2.34	0.40
18:G:14:HIS:HD1	18:G:16:SER:H	1.68	0.40
20:I:58:VAL:HA	20:I:62:ILE:HG21	2.02	0.40
24:M:132:LYS:O	24:M:136:LEU:N	2.53	0.40
24:M:179:GLY:O	24:M:183:ALA:N	2.50	0.40
29:W:124:CYS:SG	29:W:154:GLU:HB2	2.62	0.40
29:W:190:ASP:HA	29:W:193:ARG:CZ	2.52	0.40
1:1:473:UNK:O	1:1:477:UNK:N	2.54	0.40
2:4:176:LEU:HG	2:4:210:ILE:HG13	2.04	0.40
2:4:273:ARG:HG2	4:6:373:SER:HB3	2.03	0.40
3:0:159:HIS:O	3:0:162:LEU:HB3	2.21	0.40
3:0:374:LEU:HD23	3:0:410:SER:HB2	2.03	0.40
3:0:419:ILE:O	3:0:436:ARG:N	2.55	0.40
4:6:127:ILE:HG13	4:6:170:GLY:N	2.28	0.40
5:2:31:THR:HA	5:2:226:PHE:CD2	2.56	0.40
5:2:81:MET:HB3	5:2:81:MET:HE2	1.77	0.40
5:2:408:MET:HE2	5:2:408:MET:HB2	1.95	0.40
7:7:342:ASP:HB2	7:7:345:ASN:CG	2.47	0.40
7:7:634:GLN:OE1	7:7:635:GLU:N	2.54	0.40
12:A:411:ASP:OD1	12:A:412:ARG:N	2.54	0.40
12:A:596:THR:HG22	12:A:598:LEU:H	1.86	0.40
12:A:857:ARG:HD3	12:A:861:GLY:HA2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:1135:ARG:NH2	12:A:1139:GLU:OE1	2.54	0.40
12:A:1383:SER:O	12:A:1388:GLY:HA3	2.21	0.40
15:D:188:ALA:HA	15:D:207:LEU:HD13	2.03	0.40
17:F:93:ILE:HD13	17:F:93:ILE:HA	1.81	0.40
19:H:16:ASP:HB3	19:H:25:ARG:HB2	2.04	0.40
23:L:53:HIS:C	23:L:54:ARG:HH11	2.29	0.40
24:M:30:TYR:CD1	24:M:31:PRO:HD2	2.57	0.40
24:M:214:LEU:O	24:M:218:SER:OG	2.28	0.40
2:4:272:PHE:HD1	2:4:272:PHE:HA	1.74	0.40
3:0:216:PRO:HA	3:0:219:ALA:HB3	2.04	0.40
3:0:377:CYS:SG	3:0:406:ALA:HB3	2.62	0.40
3:0:539:VAL:O	3:0:600:SER:N	2.51	0.40
3:0:629:TYR:HE1	3:0:633:ARG:HA	1.87	0.40
3:0:747:HIS:HD2	3:0:751:ARG:HH11	1.70	0.40
4:6:133:SER:HB2	4:6:206:GLY:O	2.22	0.40
4:6:319:LEU:H	4:6:319:LEU:HD12	1.86	0.40
7:7:102:ALA:N	7:7:332:GLU:OE2	2.55	0.40
7:7:165:SER:C	7:7:172:GLU:H	2.28	0.40
7:7:303:ARG:HG2	7:7:506:ALA:HA	2.03	0.40
7:7:561:MET:HG2	7:7:566:TYR:CE1	2.56	0.40
7:7:593:PHE:HA	7:7:745:ILE:HG21	2.03	0.40
12:A:601:LYS:HE2	12:A:603:ASN:HD21	1.87	0.40
12:A:726:ARG:HD3	12:A:766:GLY:HA3	2.02	0.40
13:B:313:MET:HE2	13:B:313:MET:HB3	1.98	0.40
13:B:566:LEU:HB2	13:B:588:GLY:HA2	2.03	0.40
13:B:648:HIS:HD2	13:B:712:PRO:HA	1.87	0.40
13:B:1177:HIS:HB2	13:B:1179:GLN:HG3	2.03	0.40
15:D:47:LEU:HD22	15:D:49:ALA:HB2	2.03	0.40
16:E:37:LEU:HA	16:E:38:PRO:HD3	1.95	0.40
22:K:94:ILE:HA	22:K:94:ILE:HD13	1.87	0.40
24:M:315:ILE:HG13	24:M:316:LEU:HD22	2.03	0.40
26:R:135:PHE:HA	26:R:214:ILE:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

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	1	256/542 (47%)	236 (92%)	18 (7%)	2 (1%)	16	52
2	4	279/338 (82%)	237 (85%)	42 (15%)	0	100	100
3	0	752/778 (97%)	677 (90%)	75 (10%)	0	100	100
4	6	336/461 (73%)	297 (88%)	37 (11%)	2 (1%)	21	57
5	2	456/513 (89%)	406 (89%)	50 (11%)	0	100	100
6	5	64/72 (89%)	54 (84%)	10 (16%)	0	100	100
7	7	630/843 (75%)	541 (86%)	89 (14%)	0	100	100
8	3	136/321 (42%)	122 (90%)	14 (10%)	0	100	100
9	O	178/240 (74%)	173 (97%)	5 (3%)	0	100	100
12	A	1386/1733 (80%)	1269 (92%)	115 (8%)	2 (0%)	48	81
13	B	1133/1224 (93%)	1057 (93%)	74 (6%)	2 (0%)	43	75
14	C	260/318 (82%)	243 (94%)	17 (6%)	0	100	100
15	D	153/221 (69%)	142 (93%)	11 (7%)	0	100	100
16	E	211/215 (98%)	205 (97%)	6 (3%)	0	100	100
17	F	81/155 (52%)	78 (96%)	3 (4%)	0	100	100
18	G	169/171 (99%)	156 (92%)	13 (8%)	0	100	100
19	H	132/146 (90%)	118 (89%)	13 (10%)	1 (1%)	16	52
20	I	114/122 (93%)	101 (89%)	13 (11%)	0	100	100
21	J	63/70 (90%)	54 (86%)	9 (14%)	0	100	100
22	K	110/120 (92%)	105 (96%)	5 (4%)	0	100	100
23	L	43/70 (61%)	33 (77%)	10 (23%)	0	100	100
24	M	273/345 (79%)	243 (89%)	30 (11%)	0	100	100
25	Q	140/735 (19%)	130 (93%)	10 (7%)	0	100	100
26	R	176/400 (44%)	167 (95%)	9 (5%)	0	100	100
27	U	42/286 (15%)	38 (90%)	4 (10%)	0	100	100
28	V	46/122 (38%)	44 (96%)	2 (4%)	0	100	100
29	W	189/482 (39%)	183 (97%)	6 (3%)	0	100	100
30	X	152/328 (46%)	139 (91%)	12 (8%)	1 (1%)	18	54
All	All	7960/11371 (70%)	7248 (91%)	702 (9%)	10 (0%)	49	81

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	6	411	PRO
13	B	364	ILE
1	1	230	PRO
4	6	425	SER
13	B	363	HIS
12	A	464	PRO
19	H	110	ASP
12	A	465	TYR
30	X	272	ALA
1	1	239	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 PDB entries followed by that with respect to all EM entries.

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	1	169/395 (43%)	151 (89%)	18 (11%)	6	24
2	4	198/298 (66%)	169 (85%)	29 (15%)	3	16
3	0	686/707 (97%)	601 (88%)	85 (12%)	4	20
4	6	247/406 (61%)	201 (81%)	46 (19%)	1	11
5	2	258/468 (55%)	212 (82%)	46 (18%)	2	12
6	5	53/66 (80%)	40 (76%)	13 (24%)	1	5
7	7	414/737 (56%)	316 (76%)	98 (24%)	1	5
8	3	53/303 (18%)	49 (92%)	4 (8%)	12	36
9	O	152/205 (74%)	145 (95%)	7 (5%)	24	47
12	A	1221/1520 (80%)	1085 (89%)	136 (11%)	6	23
13	B	995/1061 (94%)	890 (89%)	105 (11%)	6	24
14	C	230/274 (84%)	208 (90%)	22 (10%)	8	28
15	D	139/200 (70%)	120 (86%)	19 (14%)	3	17
16	E	195/197 (99%)	174 (89%)	21 (11%)	6	24
17	F	73/137 (53%)	67 (92%)	6 (8%)	10	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	G	152/152 (100%)	140 (92%)	12 (8%)	11	35
19	H	119/128 (93%)	102 (86%)	17 (14%)	3	17
20	I	110/116 (95%)	101 (92%)	9 (8%)	10	34
21	J	60/65 (92%)	52 (87%)	8 (13%)	4	18
22	K	97/102 (95%)	87 (90%)	10 (10%)	7	25
23	L	40/57 (70%)	31 (78%)	9 (22%)	1	6
24	M	245/299 (82%)	216 (88%)	29 (12%)	5	21
25	Q	109/641 (17%)	101 (93%)	8 (7%)	13	37
26	R	107/363 (30%)	97 (91%)	10 (9%)	8	29
27	U	40/260 (15%)	39 (98%)	1 (2%)	42	62
28	V	47/108 (44%)	43 (92%)	4 (8%)	10	33
29	W	155/429 (36%)	148 (96%)	7 (4%)	24	47
30	X	62/295 (21%)	61 (98%)	1 (2%)	55	70
All	All	6426/9989 (64%)	5646 (88%)	780 (12%)	7	21

All (780) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	180	LEU
1	1	214	ILE
1	1	257	LEU
1	1	263	TYR
1	1	276	LYS
1	1	280	GLU
1	1	287	PHE
1	1	340	ASP
1	1	348	VAL
1	1	381	LEU
1	1	508	LYS
1	1	553	LEU
1	1	556	THR
1	1	563	HIS
1	1	564	PHE
1	1	583	TYR
1	1	585	HIS
1	1	593	LEU
2	4	30	ILE

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Mol	Chain	Res	Type
2	4	43	GLU
2	4	61	LEU
2	4	79	TYR
2	4	125	LEU
2	4	129	ILE
2	4	131	LYS
2	4	132	LEU
2	4	134	GLU
2	4	137	LYS
2	4	149	LEU
2	4	161	ASN
2	4	162	ARG
2	4	175	ARG
2	4	180	THR
2	4	229	ASP
2	4	236	LEU
2	4	239	GLU
2	4	244	LEU
2	4	245	ILE
2	4	246	GLN
2	4	253	PHE
2	4	254	ILE
2	4	258	LEU
2	4	259	ARG
2	4	262	ILE
2	4	273	ARG
2	4	287	PHE
2	4	288	ILE
3	0	14	TYR
3	0	28	ILE
3	0	32	LEU
3	0	34	VAL
3	0	39	ILE
3	0	48	LYS
3	0	54	SER
3	0	66	HIS
3	0	80	GLU
3	0	85	GLU
3	0	109	THR
3	0	111	ARG
3	0	113	ASN
3	0	115	CYS

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Mol	Chain	Res	Type
3	0	116	LEU
3	0	131	GLU
3	0	133	CYS
3	0	138	ASN
3	0	148	ASP
3	0	155	LEU
3	0	162	LEU
3	0	163	TYR
3	0	165	ILE
3	0	175	VAL
3	0	190	LEU
3	0	206	ILE
3	0	207	ILE
3	0	213	LEU
3	0	222	VAL
3	0	226	VAL
3	0	231	ILE
3	0	232	VAL
3	0	248	LEU
3	0	250	LEU
3	0	251	ASP
3	0	253	THR
3	0	255	ASP
3	0	284	ASP
3	0	290	VAL
3	0	298	ILE
3	0	312	LEU
3	0	318	THR
3	0	338	LEU
3	0	344	THR
3	0	350	HIS
3	0	351	VAL
3	0	352	ILE
3	0	355	THR
3	0	383	LEU
3	0	401	ASP
3	0	411	THR
3	0	430	VAL
3	0	435	MET
3	0	447	LYS
3	0	449	VAL
3	0	453	PHE

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Mol	Chain	Res	Type
3	0	456	VAL
3	0	458	ILE
3	0	477	THR
3	0	487	LEU
3	0	506	ILE
3	0	520	ARG
3	0	531	LYS
3	0	535	ASP
3	0	539	VAL
3	0	545	LEU
3	0	560	LEU
3	0	572	GLU
3	0	599	LEU
3	0	614	HIS
3	0	615	GLN
3	0	627	PHE
3	0	639	LEU
3	0	649	ARG
3	0	651	ASN
3	0	654	LEU
3	0	657	ASP
3	0	674	ASP
3	0	705	ASP
3	0	710	THR
3	0	711	ASP
3	0	722	ARG
3	0	742	GLU
3	0	745	ILE
3	0	754	GLN
4	6	115	ILE
4	6	119	GLN
4	6	120	ARG
4	6	134	GLU
4	6	136	MET
4	6	138	GLU
4	6	146	HIS
4	6	148	MET
4	6	149	ILE
4	6	150	ILE
4	6	154	ILE
4	6	155	ASP
4	6	158	HIS

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Mol	Chain	Res	Type
4	6	164	ASN
4	6	166	ILE
4	6	185	VAL
4	6	194	ASP
4	6	202	GLN
4	6	210	LEU
4	6	214	LEU
4	6	222	LEU
4	6	227	HIS
4	6	241	THR
4	6	247	ILE
4	6	262	LYS
4	6	263	VAL
4	6	274	LYS
4	6	284	ASP
4	6	291	LEU
4	6	293	ASP
4	6	297	LEU
4	6	303	GLU
4	6	305	VAL
4	6	308	LEU
4	6	310	VAL
4	6	320	VAL
4	6	326	THR
4	6	363	CYS
4	6	368	LEU
4	6	372	LEU
4	6	375	HIS
4	6	384	MET
4	6	386	LEU
4	6	406	CYS
4	6	448	LEU
4	6	449	HIS
5	2	11	THR
5	2	14	LEU
5	2	16	GLU
5	2	17	ILE
5	2	22	GLN
5	2	25	LEU
5	2	28	SER
5	2	42	LEU
5	2	48	MET

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Mol	Chain	Res	Type
5	2	55	ASN
5	2	56	GLU
5	2	59	LEU
5	2	60	LEU
5	2	61	ASP
5	2	63	ASP
5	2	71	LYS
5	2	74	PHE
5	2	99	ASN
5	2	112	LEU
5	2	208	LEU
5	2	222	LEU
5	2	278	LEU
5	2	286	ARG
5	2	348	TYR
5	2	349	SER
5	2	352	ASN
5	2	371	VAL
5	2	374	VAL
5	2	380	ARG
5	2	396	ILE
5	2	413	GLU
5	2	414	GLU
5	2	425	ASN
5	2	432	VAL
5	2	450	ARG
5	2	457	SER
5	2	464	THR
5	2	470	LEU
5	2	474	TYR
5	2	476	GLN
5	2	481	LEU
5	2	484	LYS
5	2	486	ASP
5	2	487	LYS
5	2	491	PHE
5	2	493	ILE
6	5	5	ARG
6	5	6	LYS
6	5	20	ILE
6	5	24	ASP
6	5	26	LYS

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Mol	Chain	Res	Type
6	5	30	ILE
6	5	36	ASP
6	5	42	VAL
6	5	46	LYS
6	5	48	GLU
6	5	50	VAL
6	5	54	LEU
6	5	58	LEU
7	7	302	GLU
7	7	307	ASP
7	7	309	ASP
7	7	315	SER
7	7	320	ASN
7	7	325	VAL
7	7	332	GLU
7	7	342	ASP
7	7	343	PHE
7	7	348	ARG
7	7	349	ASN
7	7	351	ASP
7	7	355	ASP
7	7	356	LEU
7	7	357	LYS
7	7	361	GLN
7	7	362	ILE
7	7	363	ARG
7	7	365	TYR
7	7	380	ARG
7	7	383	ILE
7	7	384	ILE
7	7	385	VAL
7	7	386	LEU
7	7	393	THR
7	7	395	VAL
7	7	403	ILE
7	7	411	CYS
7	7	419	GLN
7	7	420	TRP
7	7	421	ARG
7	7	427	TRP
7	7	428	CYS
7	7	431	GLN

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Mol	Chain	Res	Type
7	7	433	GLU
7	7	435	CYS
7	7	437	VAL
7	7	440	SER
7	7	444	GLU
7	7	445	MET
7	7	447	GLN
7	7	452	LEU
7	7	453	VAL
7	7	456	THR
7	7	464	ARG
7	7	469	ASP
7	7	472	LYS
7	7	475	ASP
7	7	484	PHE
7	7	489	GLU
7	7	491	HIS
7	7	492	VAL
7	7	493	VAL
7	7	497	MET
7	7	501	VAL
7	7	508	HIS
7	7	510	LYS
7	7	514	THR
7	7	518	VAL
7	7	524	ILE
7	7	530	LEU
7	7	534	LYS
7	7	535	LEU
7	7	545	GLN
7	7	552	VAL
7	7	564	GLU
7	7	566	TYR
7	7	571	ARG
7	7	576	LYS
7	7	578	MET
7	7	579	LEU
7	7	587	LYS
7	7	601	ARG
7	7	605	ILE
7	7	612	VAL
7	7	620	LEU

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Mol	Chain	Res	Type
7	7	626	PHE
7	7	634	GLN
7	7	637	MET
7	7	638	ASN
7	7	641	GLN
7	7	645	TYR
7	7	663	ASP
7	7	664	LEU
7	7	666	GLU
7	7	669	CYS
7	7	671	ILE
7	7	691	LEU
7	7	692	ARG
7	7	698	ASP
7	7	712	ASP
7	7	716	MET
7	7	719	SER
7	7	722	ARG
7	7	723	GLN
7	7	726	LEU
7	7	729	GLN
7	7	760	LEU
8	3	34	CYS
8	3	36	HIS
8	3	53	GLN
8	3	63	LEU
9	O	153	THR
9	O	159	ASN
9	O	173	GLU
9	O	188	GLU
9	O	214	LEU
9	O	215	THR
9	O	234	LEU
12	A	23	SER
12	A	25	GLU
12	A	47	ARG
12	A	53	LEU
12	A	54	ASN
12	A	55	ASP
12	A	61	ILE
12	A	62	ASP
12	A	69	THR

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Mol	Chain	Res	Type
12	A	75	ASN
12	A	76	GLU
12	A	77	CYS
12	A	81	PHE
12	A	84	ILE
12	A	91	PHE
12	A	106	VAL
12	A	124	GLN
12	A	141	LEU
12	A	147	VAL
12	A	167	CYS
12	A	174	ILE
12	A	175	ARG
12	A	177	ASP
12	A	182	VAL
12	A	199	LEU
12	A	201	VAL
12	A	203	SER
12	A	232	GLU
12	A	235	ILE
12	A	239	LEU
12	A	256	GLN
12	A	268	ASP
12	A	279	LEU
12	A	289	ILE
12	A	299	HIS
12	A	308	ILE
12	A	346	ASP
12	A	351	THR
12	A	379	VAL
12	A	420	ARG
12	A	438	ASP
12	A	450	LEU
12	A	465	TYR
12	A	470	LEU
12	A	474	VAL
12	A	486	GLU
12	A	489	LEU
12	A	501	LEU
12	A	505	CYS
12	A	523	ILE
12	A	524	VAL

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Mol	Chain	Res	Type
12	A	525	GLN
12	A	526	ASP
12	A	529	CYS
12	A	538	ASP
12	A	544	ASP
12	A	546	VAL
12	A	566	ILE
12	A	576	GLN
12	A	577	ILE
12	A	592	ASP
12	A	598	LEU
12	A	603	ASN
12	A	622	VAL
12	A	640	GLN
12	A	666	ILE
12	A	672	ASP
12	A	690	VAL
12	A	691	LEU
12	A	694	THR
12	A	709	THR
12	A	712	GLU
12	A	717	ASN
12	A	758	ILE
12	A	765	VAL
12	A	770	VAL
12	A	790	ASP
12	A	795	GLU
12	A	801	GLU
12	A	848	ILE
12	A	862	ASN
12	A	867	ILE
12	A	884	ASP
12	A	889	SER
12	A	890	ASP
12	A	900	ASP
12	A	909	ASP
12	A	919	ILE
12	A	931	GLU
12	A	949	ASP
12	A	953	ASN
12	A	961	ARG
12	A	979	SER

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Mol	Chain	Res	Type
12	A	982	THR
12	A	983	ILE
12	A	1038	THR
12	A	1107	VAL
12	A	1113	THR
12	A	1128	GLN
12	A	1130	GLN
12	A	1135	ARG
12	A	1138	ILE
12	A	1144	LYS
12	A	1163	ILE
12	A	1165	GLU
12	A	1171	GLN
12	A	1174	PHE
12	A	1195	LEU
12	A	1197	LEU
12	A	1206	ASP
12	A	1209	MET
12	A	1211	GLN
12	A	1220	PHE
12	A	1231	ASP
12	A	1242	VAL
12	A	1243	VAL
12	A	1256	GLU
12	A	1266	THR
12	A	1272	THR
12	A	1295	THR
12	A	1305	VAL
12	A	1327	ILE
12	A	1330	ASN
12	A	1334	ASP
12	A	1350	LYS
12	A	1359	ASP
12	A	1377	THR
12	A	1382	THR
12	A	1393	ASN
12	A	1400	CYS
12	A	1404	GLU
12	A	1406	VAL
12	A	1407	GLU
12	A	1424	VAL
12	A	1448	GLU

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Mol	Chain	Res	Type
12	A	1450	LEU
13	B	25	ILE
13	B	26	THR
13	B	35	SER
13	B	58	THR
13	B	61	ASP
13	B	86	ARG
13	B	91	SER
13	B	101	MET
13	B	102	VAL
13	B	183	GLU
13	B	185	THR
13	B	222	ILE
13	B	223	VAL
13	B	240	ILE
13	B	244	LEU
13	B	245	GLU
13	B	253	THR
13	B	259	TYR
13	B	269	ILE
13	B	272	THR
13	B	282	ILE
13	B	294	ASP
13	B	317	CYS
13	B	333	PHE
13	B	357	GLN
13	B	363	HIS
13	B	364	ILE
13	B	391	ASP
13	B	399	ASP
13	B	420	LEU
13	B	428	ILE
13	B	461	LEU
13	B	476	ARG
13	B	479	VAL
13	B	487	THR
13	B	502	ILE
13	B	513	GLN
13	B	527	THR
13	B	555	ILE
13	B	570	VAL
13	B	591	ARG

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Mol	Chain	Res	Type
13	B	595	ARG
13	B	598	GLU
13	B	610	ASN
13	B	612	GLU
13	B	624	LEU
13	B	644	GLU
13	B	650	GLU
13	B	654	ARG
13	B	657	HIS
13	B	680	THR
13	B	690	VAL
13	B	691	GLU
13	B	697	GLU
13	B	734	HIS
13	B	755	ILE
13	B	786	ASN
13	B	790	ASP
13	B	795	ILE
13	B	805	THR
13	B	806	THR
13	B	861	ASP
13	B	864	LYS
13	B	880	THR
13	B	889	THR
13	B	898	LEU
13	B	916	THR
13	B	918	ILE
13	B	955	THR
13	B	956	THR
13	B	959	ASP
13	B	964	VAL
13	B	967	ARG
13	B	971	THR
13	B	982	SER
13	B	986	GLN
13	B	989	THR
13	B	993	THR
13	B	996	ARG
13	B	1002	THR
13	B	1009	ASP
13	B	1022	THR
13	B	1049	ASP

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Mol	Chain	Res	Type
13	B	1051	THR
13	B	1058	LEU
13	B	1074	ASN
13	B	1080	LYS
13	B	1081	LEU
13	B	1093	GLN
13	B	1098	MET
13	B	1103	ILE
13	B	1115	THR
13	B	1119	VAL
13	B	1133	MET
13	B	1138	MET
13	B	1145	SER
13	B	1149	GLU
13	B	1152	MET
13	B	1153	GLU
13	B	1163	CYS
13	B	1166	CYS
13	B	1177	HIS
13	B	1192	TYR
13	B	1215	ARG
13	B	1222	ARG
14	C	8	VAL
14	C	10	ILE
14	C	12	GLU
14	C	50	GLU
14	C	72	LEU
14	C	82	TYR
14	C	91	HIS
14	C	95	CYS
14	C	99	LEU
14	C	106	GLU
14	C	110	THR
14	C	112	ASN
14	C	115	SER
14	C	163	ILE
14	C	165	LYS
14	C	176	ILE
14	C	196	ASP
14	C	211	ASP
14	C	214	ASN
14	C	215	GLU

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Mol	Chain	Res	Type
14	C	219	PHE
14	C	240	VAL
15	D	38	ILE
15	D	52	LEU
15	D	58	VAL
15	D	61	GLU
15	D	68	ARG
15	D	122	GLU
15	D	124	GLU
15	D	131	GLU
15	D	137	ASN
15	D	142	LYS
15	D	160	VAL
15	D	172	LEU
15	D	173	HIS
15	D	175	PHE
15	D	177	VAL
15	D	187	THR
15	D	207	LEU
15	D	209	ARG
15	D	220	LEU
16	E	8	ASN
16	E	11	ARG
16	E	30	ILE
16	E	31	THR
16	E	33	GLU
16	E	34	GLU
16	E	39	LEU
16	E	50	MET
16	E	67	GLU
16	E	81	GLU
16	E	84	ASP
16	E	92	THR
16	E	93	MET
16	E	107	THR
16	E	117	THR
16	E	131	THR
16	E	134	THR
16	E	145	THR
16	E	182	ASP
16	E	207	ARG
16	E	213	ILE

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Mol	Chain	Res	Type
17	F	82	THR
17	F	86	THR
17	F	100	GLN
17	F	110	ASP
17	F	111	LEU
17	F	133	VAL
18	G	5	LYS
18	G	6	ASP
18	G	17	PHE
18	G	33	GLU
18	G	39	THR
18	G	49	LEU
18	G	58	ARG
18	G	77	VAL
18	G	101	VAL
18	G	134	GLU
18	G	138	THR
18	G	148	GLU
19	H	10	PHE
19	H	13	SER
19	H	14	GLU
19	H	16	ASP
19	H	23	VAL
19	H	25	ARG
19	H	41	ASP
19	H	42	ILE
19	H	44	VAL
19	H	46	LEU
19	H	58	THR
19	H	110	ASP
19	H	112	ILE
19	H	131	ASN
19	H	133	ASN
19	H	134	ASN
19	H	135	LEU
20	I	4	PHE
20	I	5	ARG
20	I	8	ARG
20	I	37	GLU
20	I	60	GLN
20	I	67	THR
20	I	89	GLN

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Mol	Chain	Res	Type
20	I	108	HIS
20	I	115	LYS
21	J	2	ILE
21	J	5	VAL
21	J	7	CYS
21	J	10	CYS
21	J	28	ASP
21	J	31	ASP
21	J	39	LEU
21	J	57	ILE
22	K	5	ASP
22	K	10	PHE
22	K	11	LEU
22	K	16	GLU
22	K	19	LEU
22	K	32	VAL
22	K	38	GLU
22	K	75	ILE
22	K	77	THR
22	K	92	ASN
23	L	26	THR
23	L	31	CYS
23	L	37	LYS
23	L	46	VAL
23	L	53	HIS
23	L	54	ARG
23	L	58	LYS
23	L	60	ARG
23	L	65	VAL
24	M	23	THR
24	M	48	CYS
24	M	51	VAL
24	M	52	LEU
24	M	54	ASP
24	M	87	LEU
24	M	101	THR
24	M	102	THR
24	M	104	MET
24	M	105	ARG
24	M	125	GLU
24	M	152	GLU
24	M	156	LEU

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Mol	Chain	Res	Type
24	M	166	LYS
24	M	168	MET
24	M	185	VAL
24	M	197	HIS
24	M	198	VAL
24	M	200	THR
24	M	234	GLN
24	M	236	LEU
24	M	242	PHE
24	M	243	CYS
24	M	264	LYS
24	M	277	ILE
24	M	287	LEU
24	M	289	PHE
24	M	319	HIS
24	M	321	ASP
25	Q	114	MET
25	Q	116	THR
25	Q	120	LYS
25	Q	126	LYS
25	Q	132	ASP
25	Q	140	HIS
25	Q	346	GLU
25	Q	359	ASN
26	R	63	ARG
26	R	76	PHE
26	R	118	HIS
26	R	123	GLU
26	R	128	VAL
26	R	129	VAL
26	R	132	GLU
26	R	225	MET
26	R	256	ASP
26	R	280	VAL
27	U	255	LYS
28	V	74	ASP
28	V	85	VAL
28	V	108	VAL
28	V	112	ARG
29	W	12	LEU
29	W	17	VAL
29	W	133	GLN

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Mol	Chain	Res	Type
29	W	139	LEU
29	W	141	ASN
29	W	143	ASP
29	W	152	CYS
30	X	218	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	379	ASN
1	1	621	ASN
3	0	23	ASN
3	0	37	ASN
3	0	60	GLN
3	0	88	ASN
3	0	291	GLN
3	0	294	HIS
3	0	664	GLN
4	6	151	GLN
4	6	188	ASN
4	6	211	GLN
4	6	449	HIS
5	2	85	HIS
5	2	372	ASN
5	2	395	GLN
5	2	498	ASN
6	5	52	HIS
7	7	347	HIS
7	7	366	GLN
7	7	592	GLN
7	7	676	HIS
7	7	682	GLN
7	7	697	ASN
7	7	761	GLN
12	A	4	GLN
12	A	109	HIS
12	A	256	GLN
12	A	451	HIS
12	A	700	ASN
12	A	741	ASN
12	A	935	GLN
12	A	953	ASN

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Mol	Chain	Res	Type
12	A	965	GLN
12	A	996	ASN
12	A	1040	GLN
12	A	1124	HIS
12	A	1187	GLN
12	A	1218	GLN
12	A	1330	ASN
12	A	1364	ASN
12	A	1427	ASN
13	B	60	GLN
13	B	73	GLN
13	B	110	HIS
13	B	350	GLN
13	B	363	HIS
13	B	395	GLN
13	B	443	ASN
13	B	449	ASN
13	B	518	HIS
13	B	794	ASN
13	B	1040	ASN
13	B	1062	HIS
14	C	65	HIS
14	C	135	GLN
14	C	252	GLN
15	D	34	GLN
16	E	5	ASN
16	E	63	ASN
16	E	114	ASN
19	H	11	GLN
19	H	83	GLN
19	H	128	ASN
20	I	89	GLN
20	I	90	GLN
22	K	29	ASN
22	K	40	HIS
22	K	110	ASN
23	L	53	HIS
24	M	114	GLN
24	M	127	GLN
24	M	212	ASN
24	M	303	GLN
26	R	65	ASN

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Mol	Chain	Res	Type
30	X	199	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 20 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
32	SF4	0	801	3	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	SF4	0	801	3	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	0	801	SF4	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	393:UNK	C	465:UNK	N	84.64
1	1	355:UNK	C	368:UNK	N	13.08
1	1	519:UNK	C	537:GLU	N	12.00

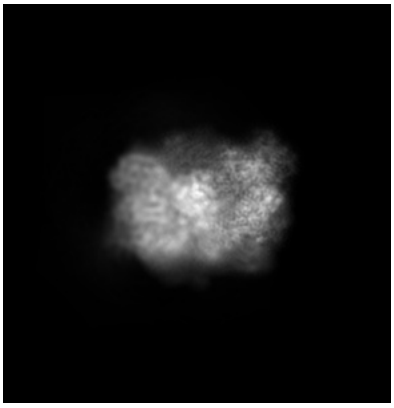
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-23905. These allow visual inspection of the internal detail of the map and identification of artifacts.

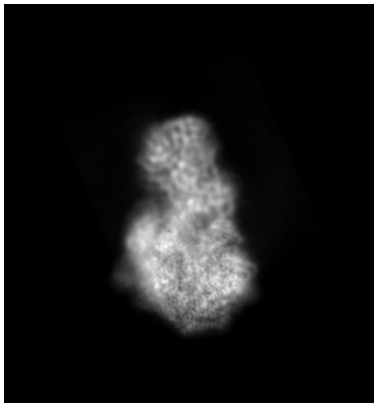
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

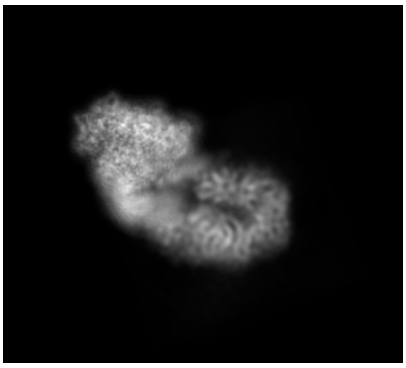
6.1.1 Primary map



X



Y

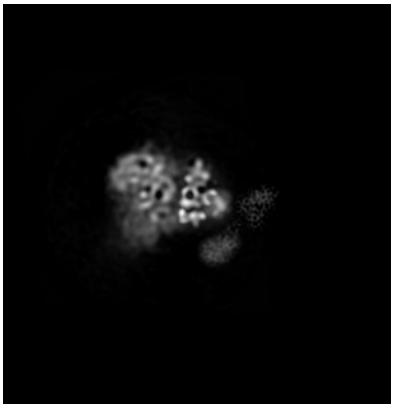


Z

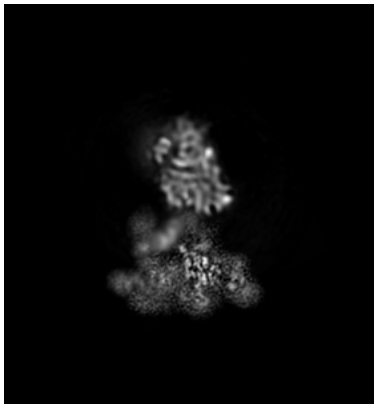
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

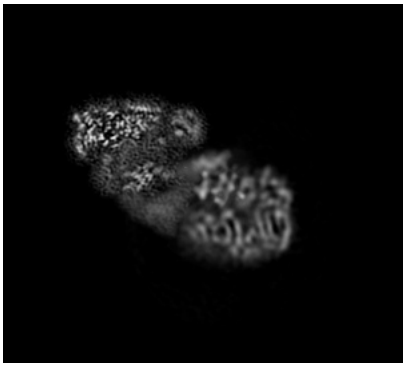
6.2.1 Primary map



X Index: 214



Y Index: 191

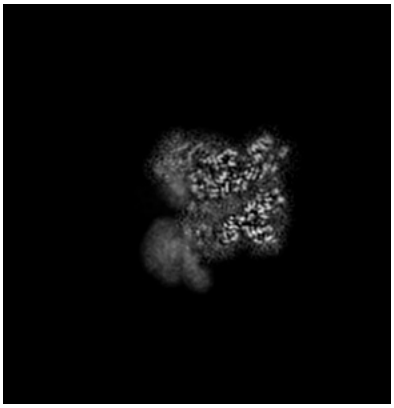


Z Index: 198

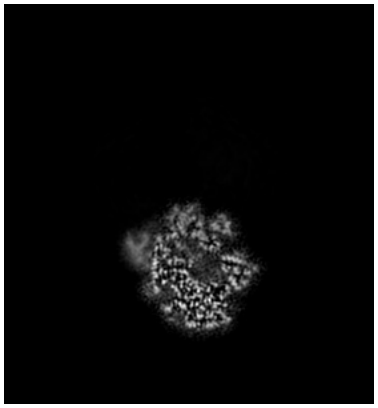
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

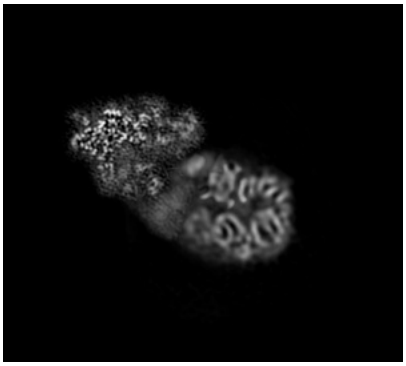
6.3.1 Primary map



X Index: 131



Y Index: 252

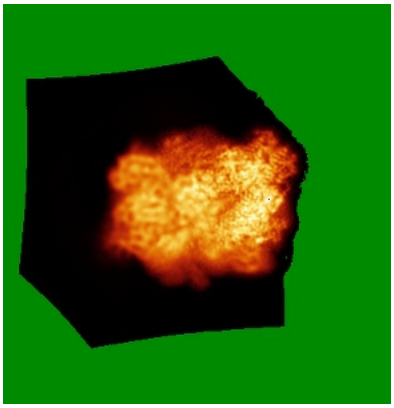


Z Index: 192

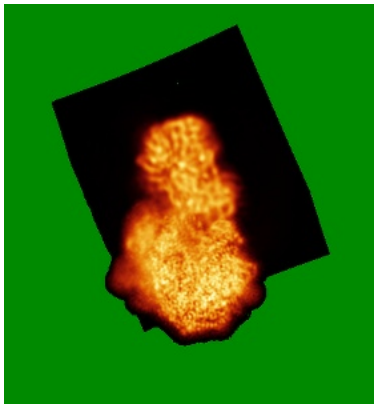
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

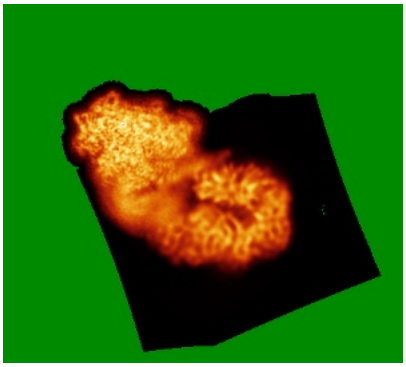
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0135. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

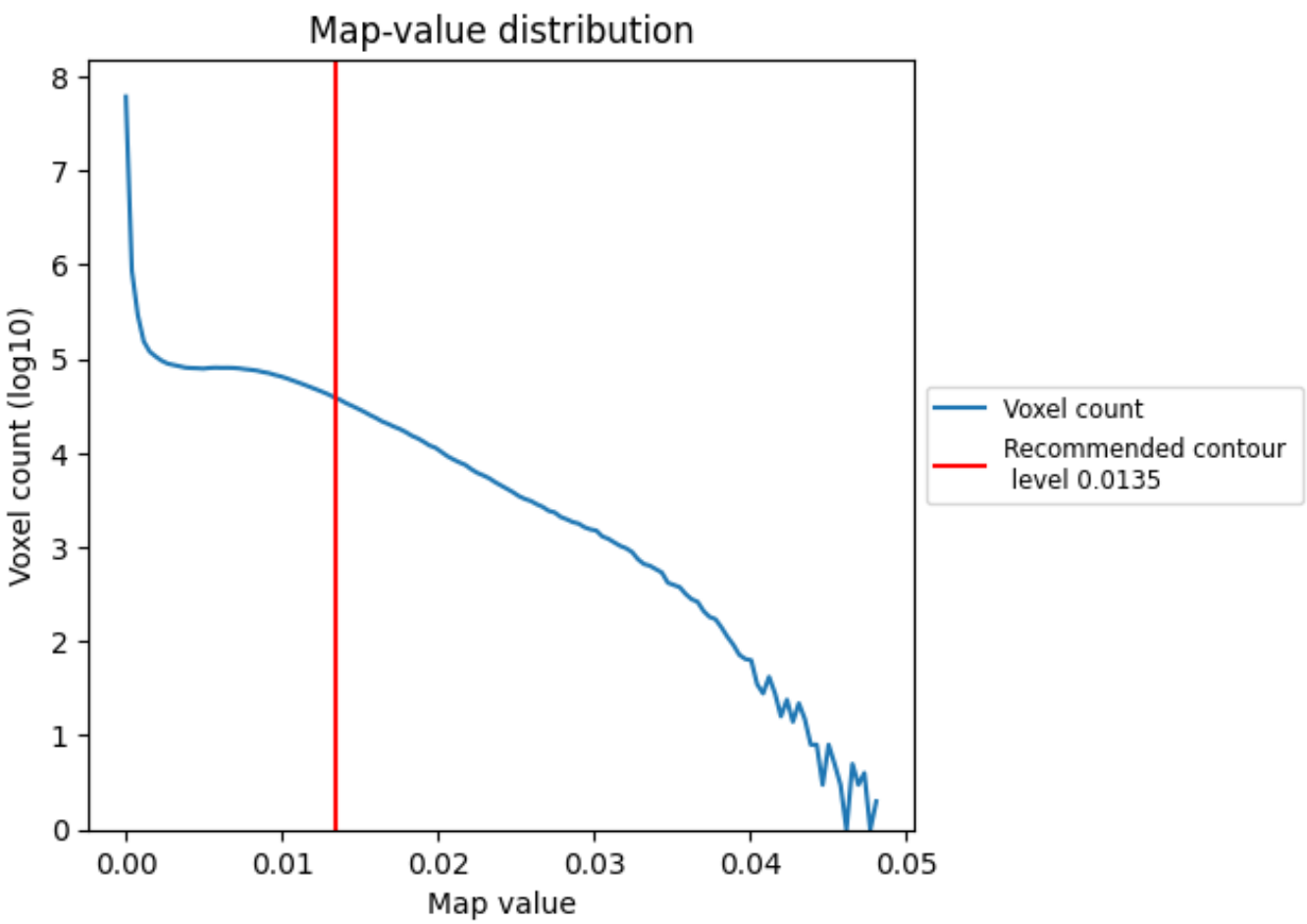
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

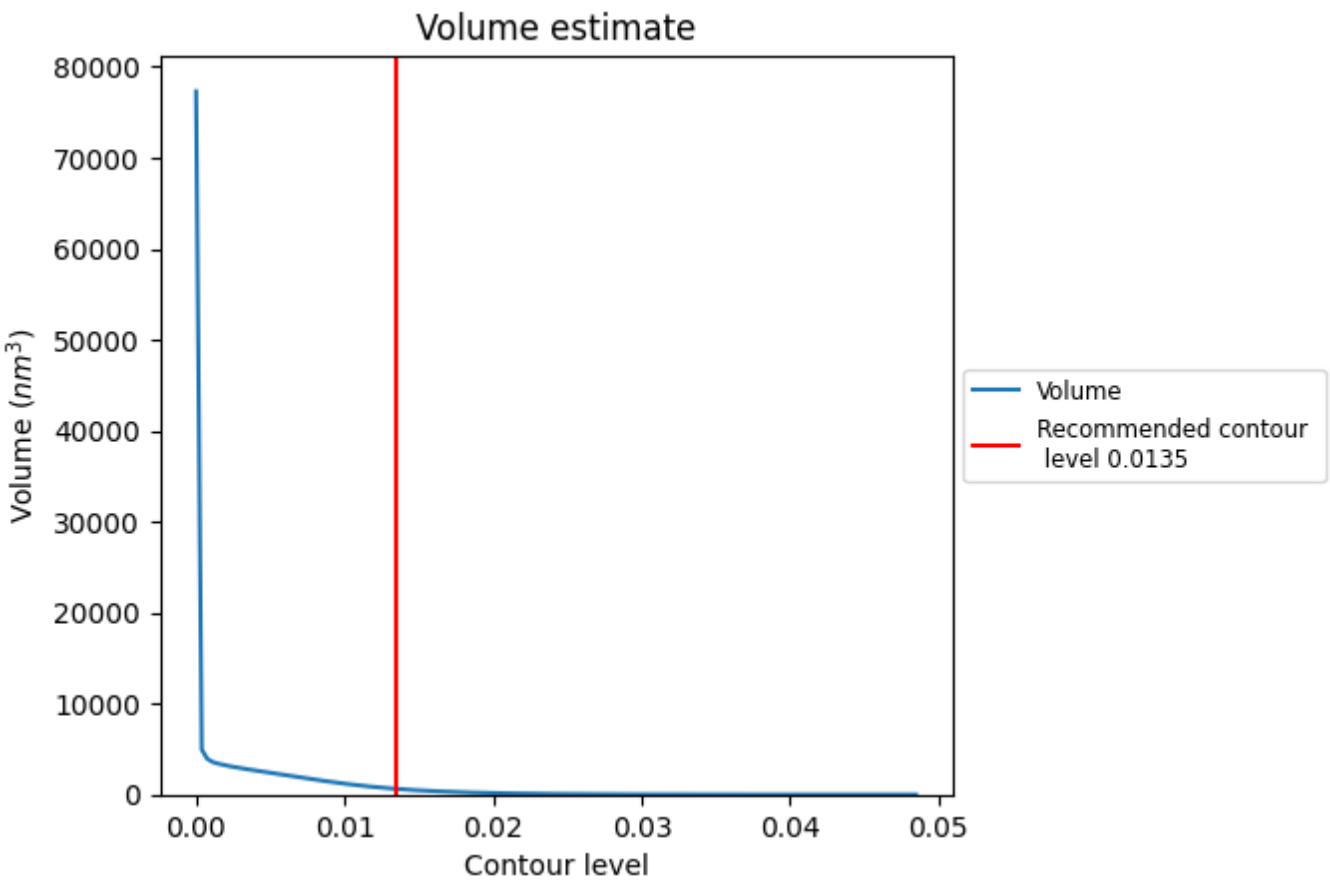
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate (i)



The volume at the recommended contour level is 626 nm^3; this corresponds to an approximate mass of 565 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

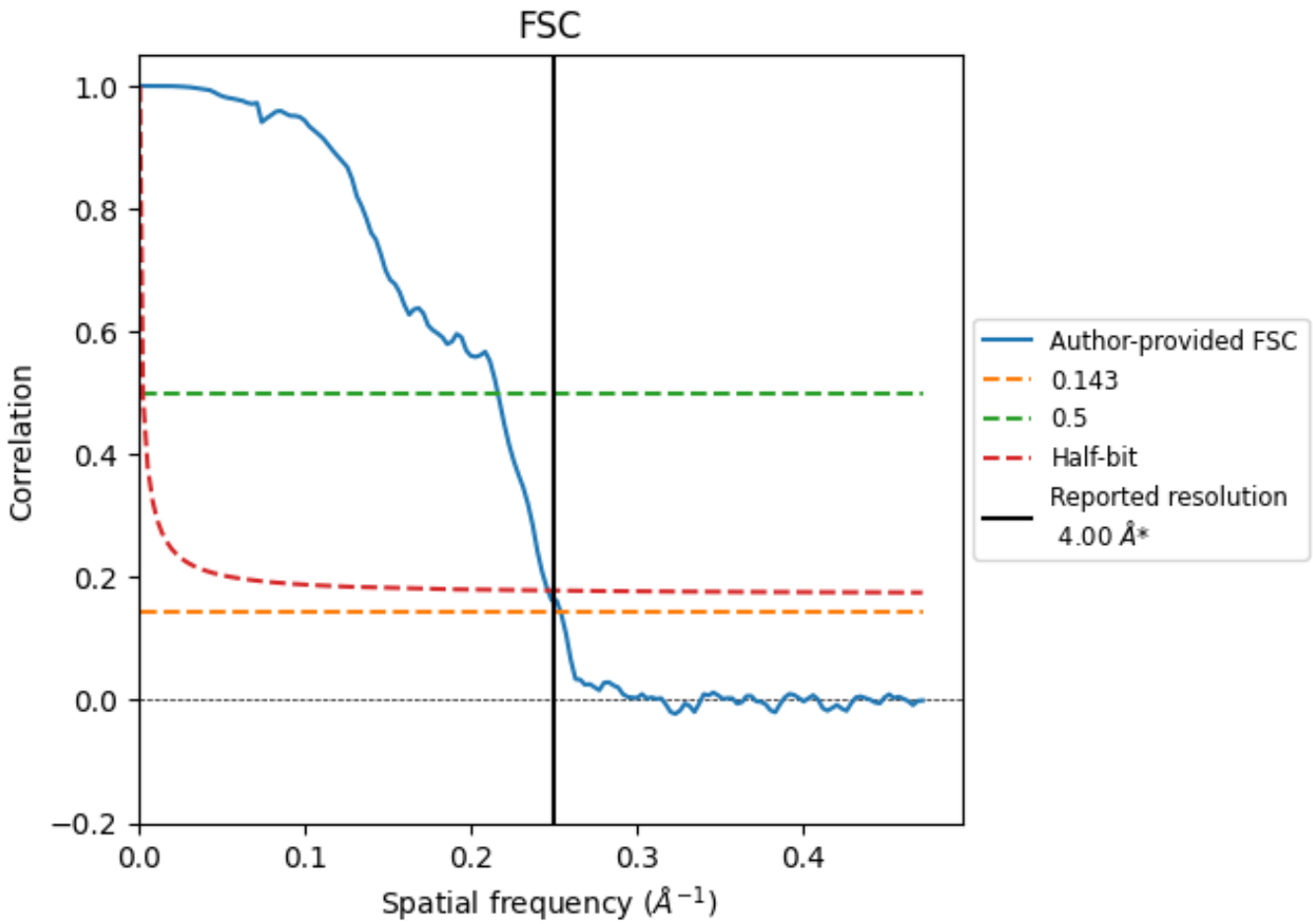
7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.250 Å^{-1}

8.2 Resolution estimates (i)

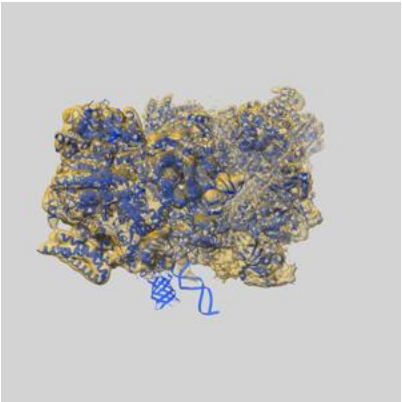
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.94	4.63	4.06
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

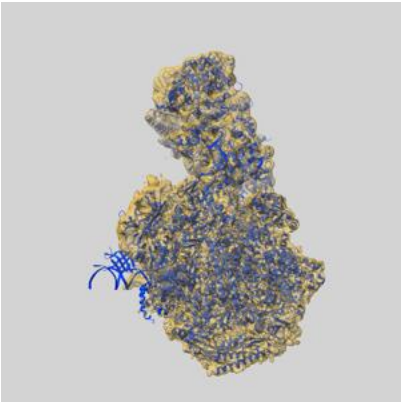
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-23905 and PDB model 7ML1. Per-residue inclusion information can be found in section 3 on page 11.

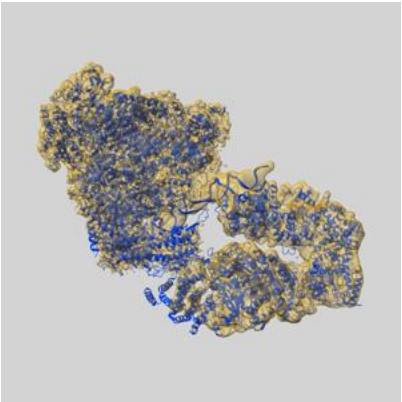
9.1 Map-model overlay (i)



X



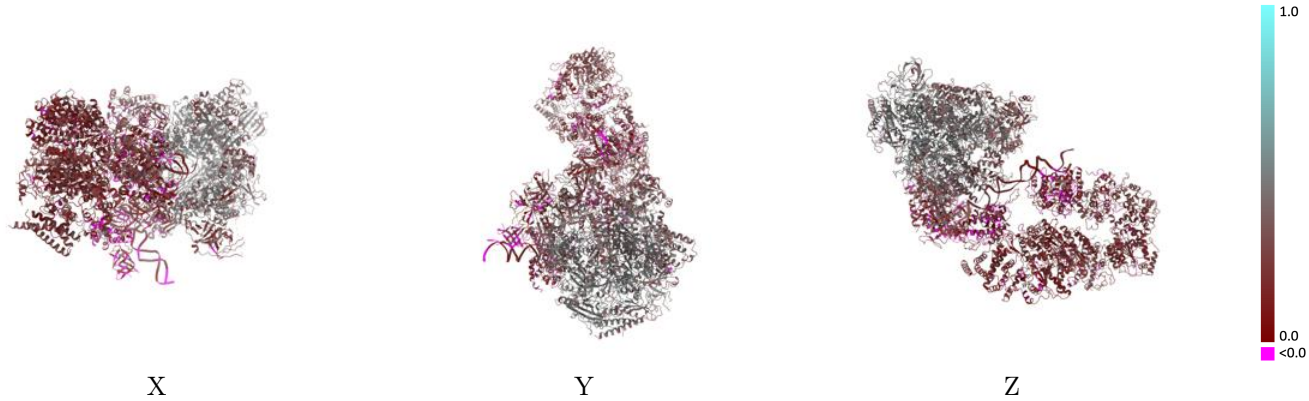
Y



Z

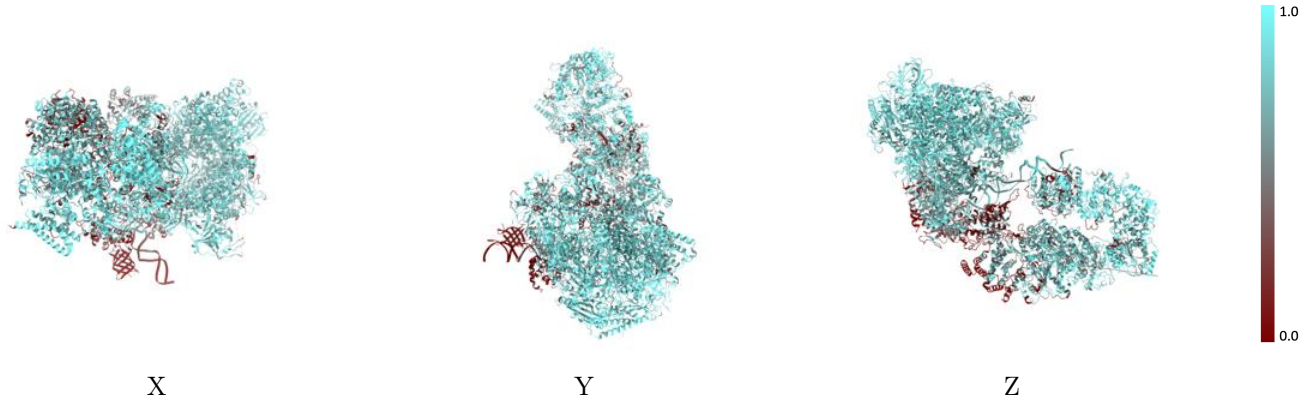
The images above show the 3D surface view of the map at the recommended contour level 0.0135 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



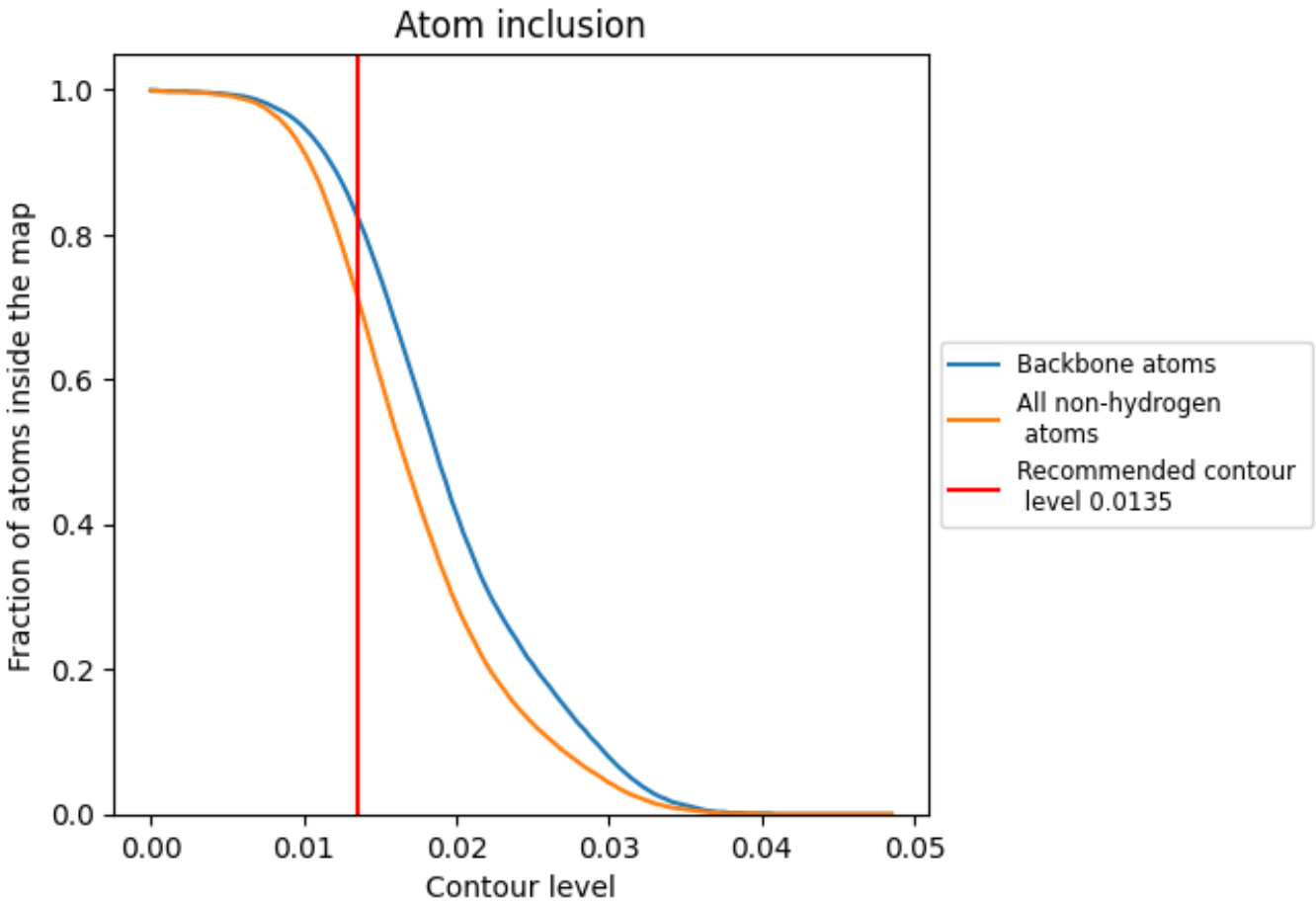
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0135).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0135) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7160	0.2910
0	0.6340	0.1760
1	0.6450	0.2160
2	0.8020	0.1990
3	0.0820	0.1450
4	0.7700	0.1940
5	0.7150	0.1830
6	0.7740	0.2030
7	0.7140	0.1470
A	0.8460	0.4220
B	0.8510	0.4330
C	0.8900	0.4570
D	0.5210	0.2800
E	0.8380	0.4000
F	0.8800	0.4500
G	0.7240	0.3180
H	0.8460	0.4070
I	0.7490	0.3410
J	0.8670	0.4430
K	0.7820	0.3930
L	0.8010	0.3570
M	0.3860	0.2450
N	0.6130	0.1410
O	0.3700	0.0900
Q	0.7420	0.2460
R	0.6120	0.2190
T	0.6550	0.1440
U	0.0060	0.0650
V	0.0180	0.0760
W	0.4290	0.1480
X	0.4160	0.1520