Full wwPDB EM Validation Report ⓘ

Dec 26, 2024 – 02:49 AM EST

PDB ID	:	5IYA
EMDB ID	:	EMD-8135
Title	:	Human core-PIC in the closed state
Authors	:	He, Y.; Yan, C.; Fang, J.; Inouye, C.; Tjian, R.; Ivanov, I.; Nogales, E.
Deposited on	:	2016-03-24
Resolution	:	5.40 Å(reported)

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 ⓘ 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 ⓘ) were used in the production of this report:

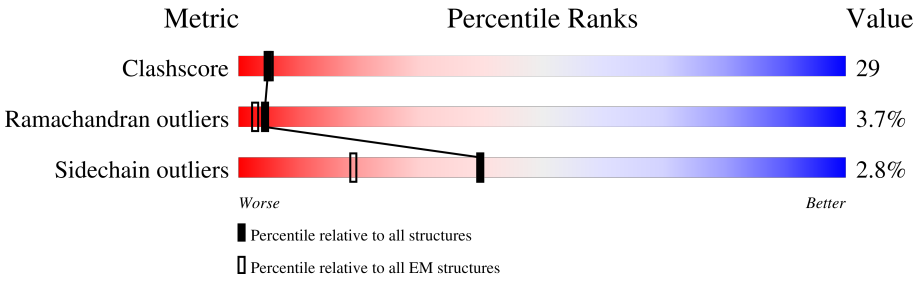
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance

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

The reported resolution of this entry is 5.40 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	A	1970	5% 41% 30% 26%
2	B	1174	50% 46%
3	C	275	47% 50%
4	D	142	5% 65% 25% 9%
5	E	210	52% 46%
6	F	127	6% 35% 31% 32%
7	G	172	5% 65% 32%
8	H	150	44% 47% 7%

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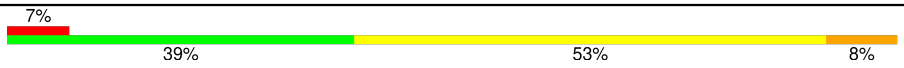
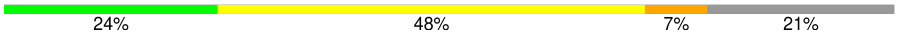
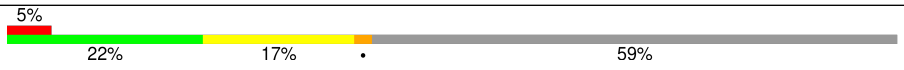
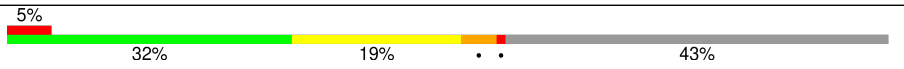
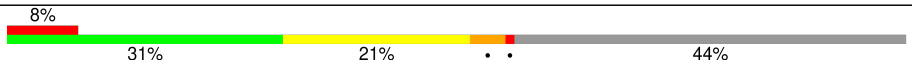
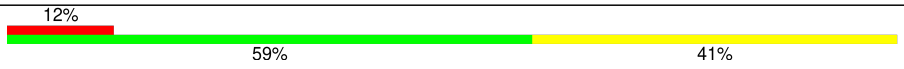
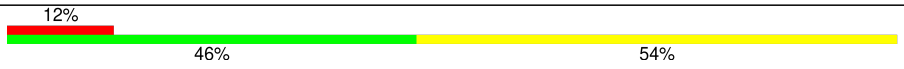
Mol	Chain	Length	Quality of chain
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	316	
14	N	376	
15	O	109	
16	P	339	
17	Q	439	
18	R	291	
19	S	517	
20	T	249	
21	U	301	
22	X	59	
23	Y	59	

2 Entry composition (i)

There are 25 unique types of molecules in this entry. The entry contains 46697 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 DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1454	11515	7234	2058	2150	73	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1165	9317	5878	1637	1738	64	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	275	2213	1386	380	440	7	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	129	1062	665	179	214	4	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	210	1723	1088	301	325	9	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	86	689	437	120	127	5	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	150	Total	C	N	O	S	0	0
			1205	764	196	239	6		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	125	Total	C	N	O	S	0	0
			1013	626	177	198	12		

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	117	Total	C	N	O	S	0	0
			937	604	154	177	2		

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			388	241	75	66	6		

- Molecule 13 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	260	Total	C	N	O	S	0	0
			2018	1265	360	376	17		

- Molecule 14 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	113	Total	C	N	O	S	0	0
			930	585	152	189	4		

- Molecule 15 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	99	Total	C	N	O	S	0	0
			806	510	142	151	3		

- Molecule 16 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	185	Total	C	N	O	S	0	0
			1462	946	257	252	7		

- Molecule 17 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	180	Total	C	N	O	S	0	0
			1484	938	262	273	11		

- Molecule 18 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	165	Total	C	N	O	S	0	0
			1357	865	235	253	4		

- Molecule 19 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	138	Total	C	N	O	S	0	0
			1137	719	207	208	3		

- Molecule 20 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	222	Total	C	N	O	S	0	0
			1788	1127	320	338	3		

- Molecule 21 is a protein called Transcription elongation factor A protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	170	Total	C	N	O	S	0	0
			1343	818	247	263	15		

- Molecule 22 is a DNA chain called SCP-X.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	59	Total	C	N	O	P	0	0
			1218	575	235	350	58		

- Molecule 23 is a DNA chain called SCP-Y.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	59	Total	C	N	O	P	0	0
			1195	568	215	354	58		

- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
24	A	1	Total	Mg	0
			1	1	
24	B	1	Total	Mg	0
			1	1	

- Molecule 25 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
25	A	2	Total	Zn	0
			2	2	
25	B	1	Total	Zn	0
			1	1	
25	C	1	Total	Zn	0
			1	1	
25	I	2	Total	Zn	0
			2	2	
25	J	1	Total	Zn	0
			1	1	
25	L	1	Total	Zn	0
			1	1	
25	M	1	Total	Zn	0
			1	1	
25	Q	1	Total	Zn	0
			1	1	

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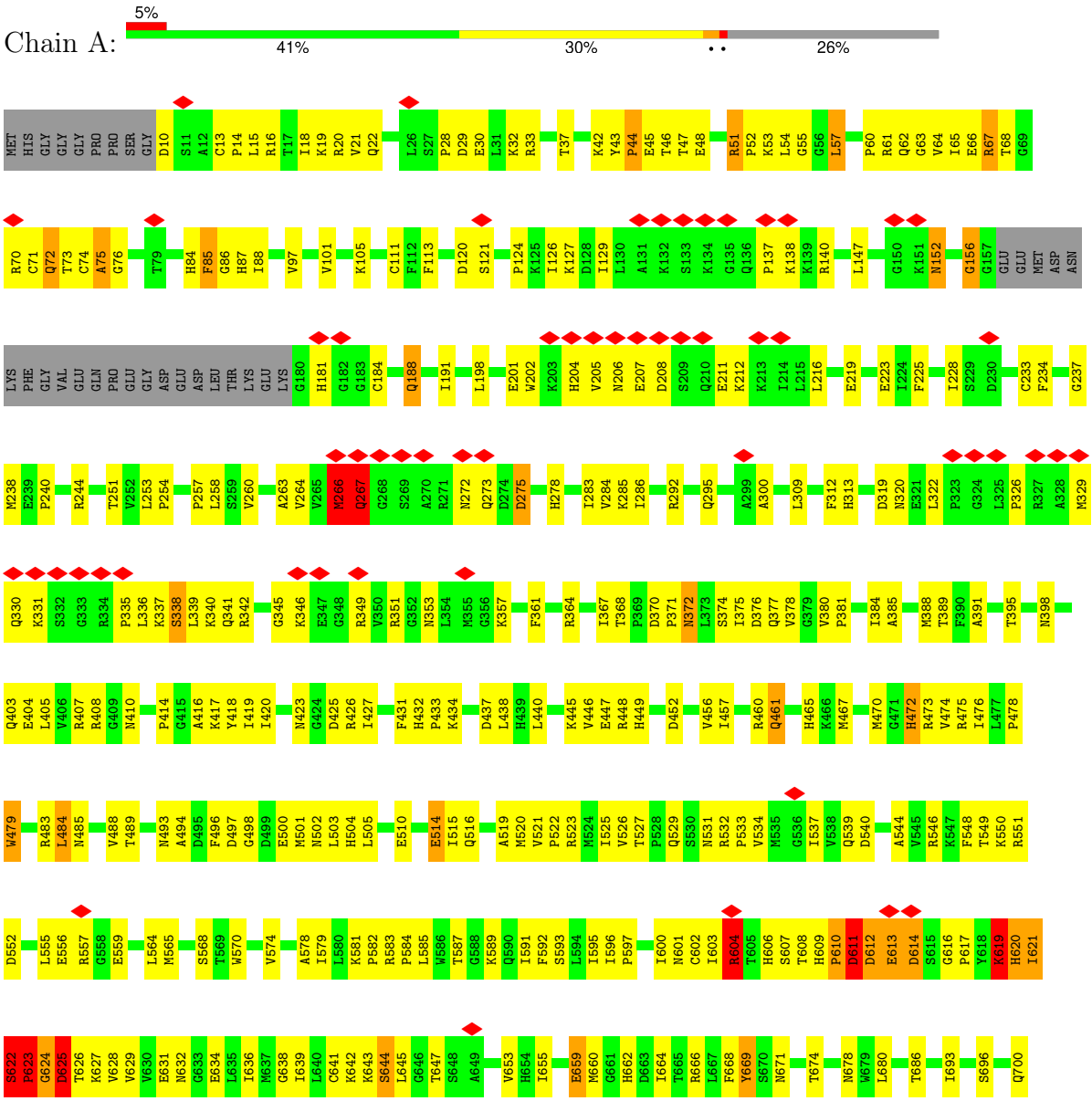
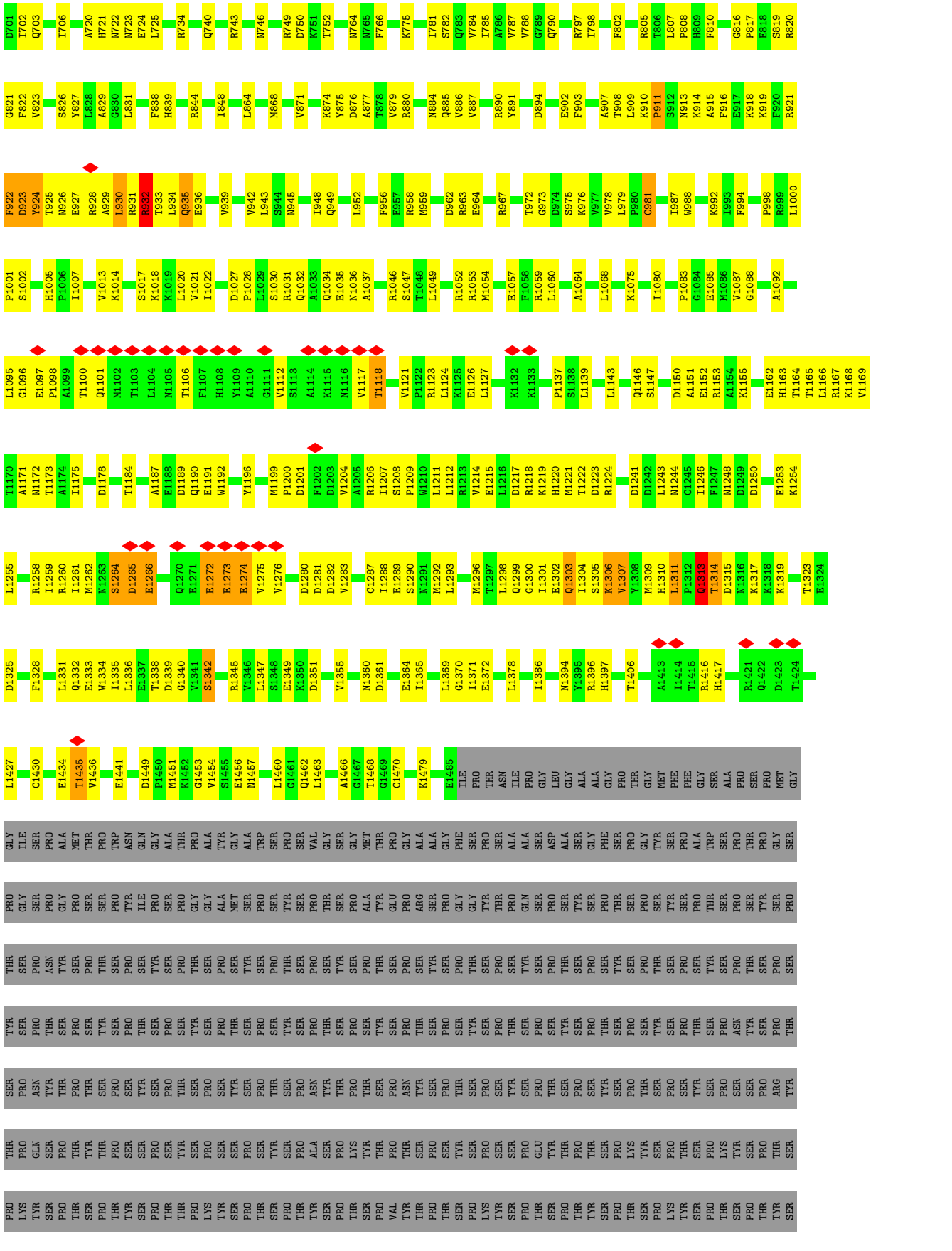
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
25	U	1	1	1	0

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: DNA-directed RNA polymerase II subunit RPB1




D701 I702 Q703 I706 A720 H721 N722 N723 E724 L725 R734 Q740 R743 N746 R749 D750 K751 T752 N764 N765 F766 K775 I781 S782 Q783 V784 I785 A786 V787 V788 G789 Q790 R797 I798 F802 R805 T806 L807 P808 H809 F810 G816 P817 E818 S819 R820
G821 F822 V823 S826 Y827 L828 A829 G830 L831 F838 H839 R844 I848 L864 M868 V871 K874 Y875 D876 A877 T878 V879 R880 N884 Q885 V886 V887 R890 Y891 D894 E902 F903 A907 T908 L909 K910 P911 S912 N913 K914 A915 F916 E917 K918 K919 F920 R921
F922 D923 Y924 T925 N926 E927 R928 A929 L930 R931 R932 T933 L934 Q935 E936 V939 V942 L943 S944 N945 I948 Q949 L952 F956 E957 R958 M959 D962 R963 E964 R967 T972 G973 D974 S975 K976 V977 V978 L979 P980 C981 I987 W988 K992 I993 F994 P998 R999 L1000
P1001 S1002 H1005 P1006 I1007 V1013 K1014 S1017 K1018 K1019 L1020 V1021 I1022 D1027 P1028 L1029 S1030 R1031 Q1032 A1033 Q1034 E1035 N1036 A1037 R1046 S1047 T1048 L1049 R1052 R1053 M1054 E1057 F1058 R1059 L1060 A1064 L1068 K1075 I1080 P1083 G1084 E1085 M1086 V1087 G1088 A1092
L1095 G1096 E1097 P1098 A1099 T1100 Q1101 M1102 T1103 L1104 N1105 T1106 F1107 H1108 Y1109 A1110 G1111 V1112 S1113 A1114 K1115 N1116 V1117 T1118 V1121 P1122 R1123 L1124 K1125 E1126 L1127 K1132 K1133 P1137 S1138 L1139 L1143 Q1146 S1147 D1150 A1151 E1152 R1153 A1154 K1155 E1162 H1163 T1164 T1165 L1166 R1167 K1168 V1169
T1170 A1171 N1172 T1173 A1174 I1175 D1178 T1184 A1187 E1188 D1189 Q1190 E1191 W1192 Y1196 M1199 P1200 D1201 F1202 D1203 V1204 A1205 R1206 I1207 S1208 P1209 W1210 L1211 L1212 R1213 V1214 E1215 L1216 D1217 R1218 K1219 H1220 M1221 T1222 D1223 R1224 D1241 D1242 L1243 N1244 C1245 I1246 F1247 N1248 D1249 D1250 E1253 K1254
L1255 R1258 I1259 R1260 I1261 M1262 N1263 S1264 D1265 E1266 Q1270 E1271 E1272 E1273 E1274 V1275 V1276 D1280 D1281 D1282 V1283 C1287 I1288 E1289 S1290 N1291 M1292 L1293 M1296 T1297 L1298 Q1299 G1300 I1301 E1302 Q1303 I1304 S1305 K1306 V1307 Y1308 M1309 H1310 L1311 P1312 Q1313 T1314 D1315 N1316 K1317 K1318 K1319 T1323 E1324
D1325 F1328 L1331 Q1332 E1333 W1334 I1335 L1336 E1337 T1338 D1339 G1340 V1341 S1342 R1345 V1346 L1347 S1348 E1349 K1350 D1351 V1355 N1360 D1361 E1364 I1365 L1369 G1370 I1371 E1372 L1378 I1386 N1394 Y1395 R1396 H1397 T1406 A1413 I1414 T1415 R1416 H1417 R1421 Q1422 D1423 T1424
L1427 C1430 E1434 T1435 V1436 E1441 D1449 P1450 M1451 K1452 G1453 V1454 S1455 E1456 N1457 L1460 G1461 Q1462 L1463 A1466 G1467 T1468 G1469 C1470 K1479 E1485 ILE PRO THR ASN ILE PRO GLY LEU GLY ALA ALA GLY PRO THR GLY MET PHE PHE GLY SER ALA PRO SER PRO MET GLY
GLY ILE SER PRO ALA MET THR PRO TRP ASN GLN GLY ALA THR PRO ALA TYR GLY ALA TYR SER VAL GLY SER GLY MET THR PRO GLY ALA ALA GLY PHE SER PRO SER ALA ALA SER ASP ALA SER ALA SER GLY PHE SER PRO GLY TYR SER PRO ALA TRP SER PRO THR PRO GLY SER
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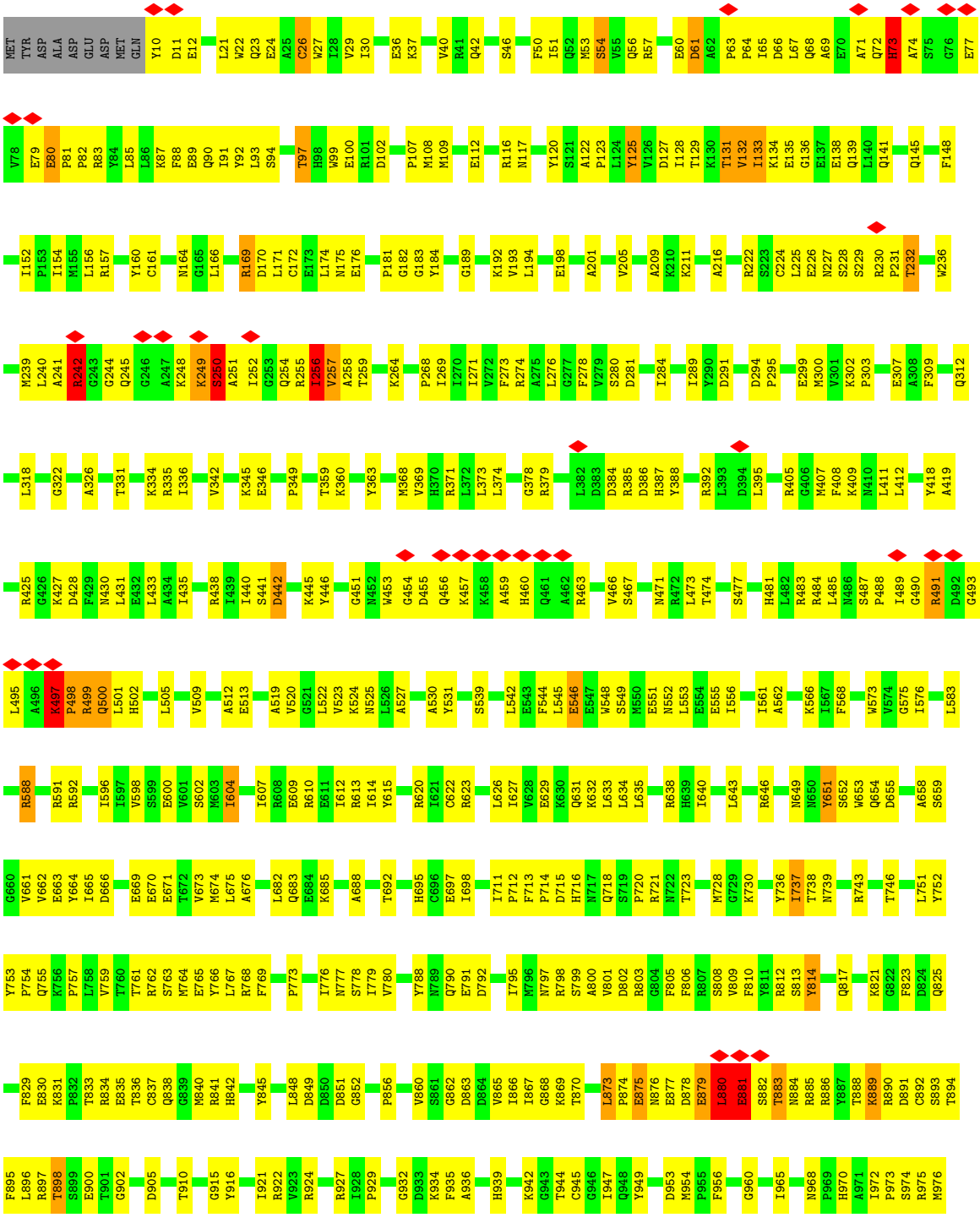
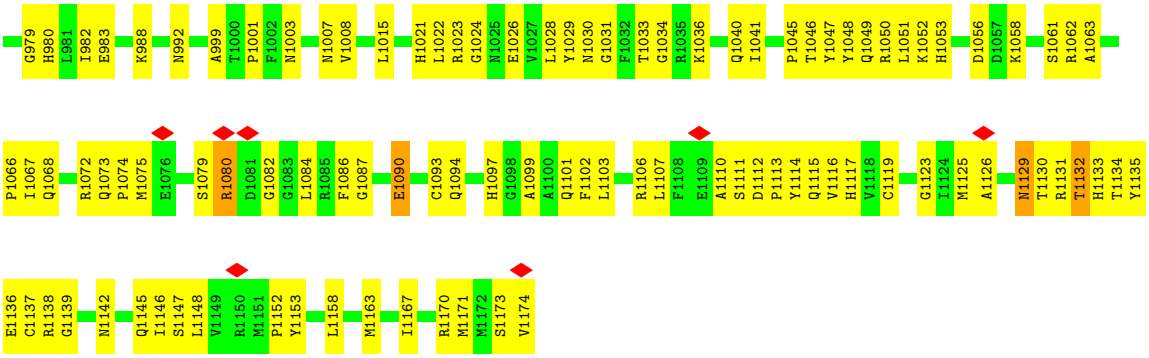
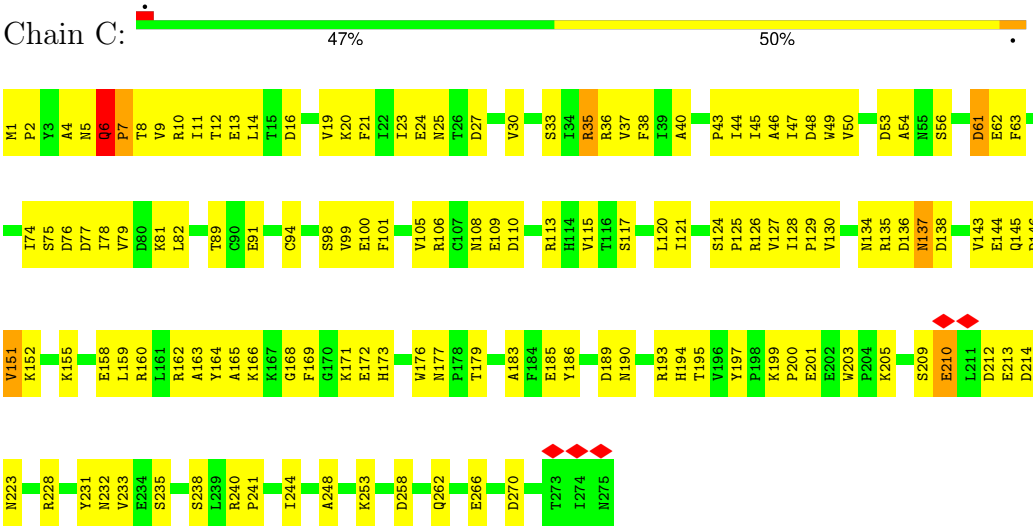
• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

Chain B:

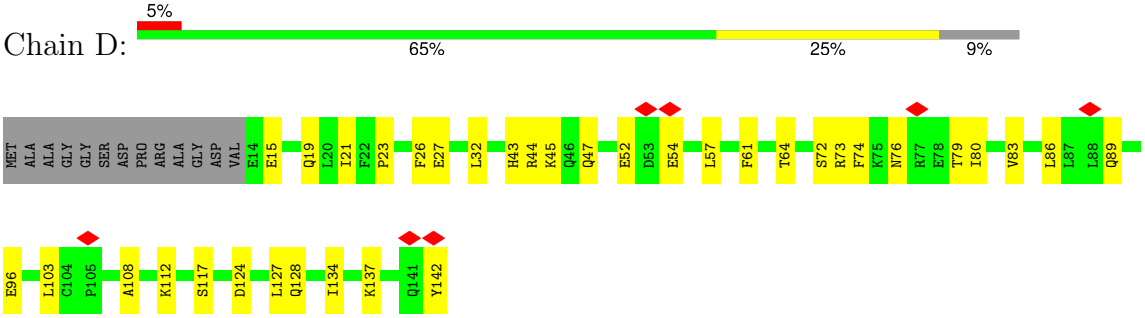




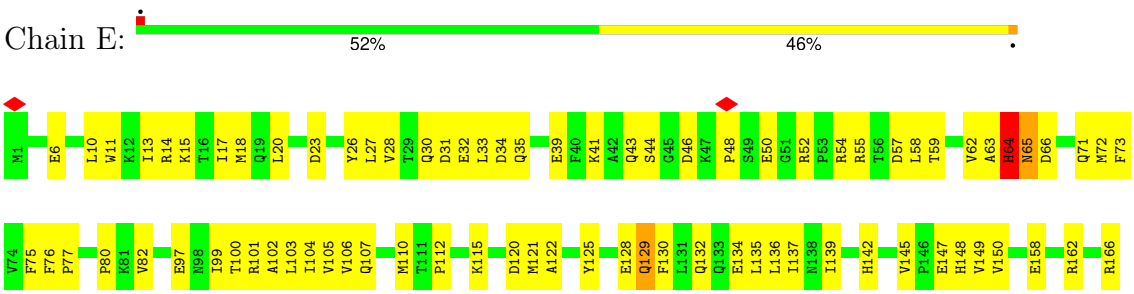
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

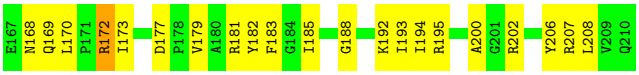


• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

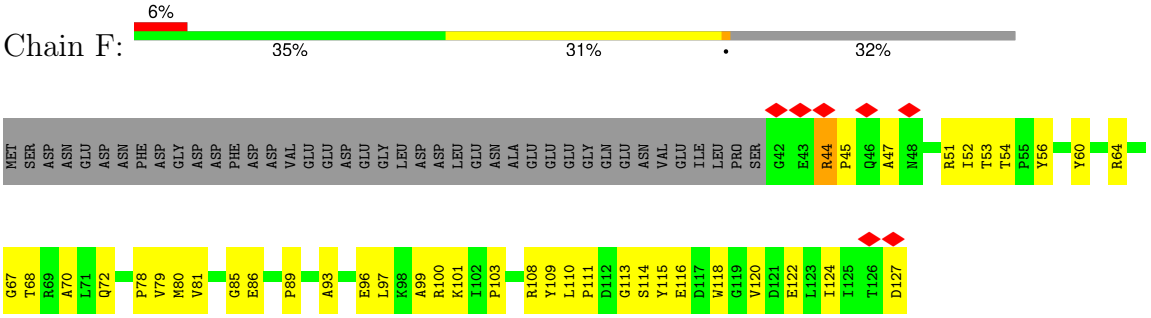


• Molecule 5: DNA-directed RNA polymerase II subunit RPB5

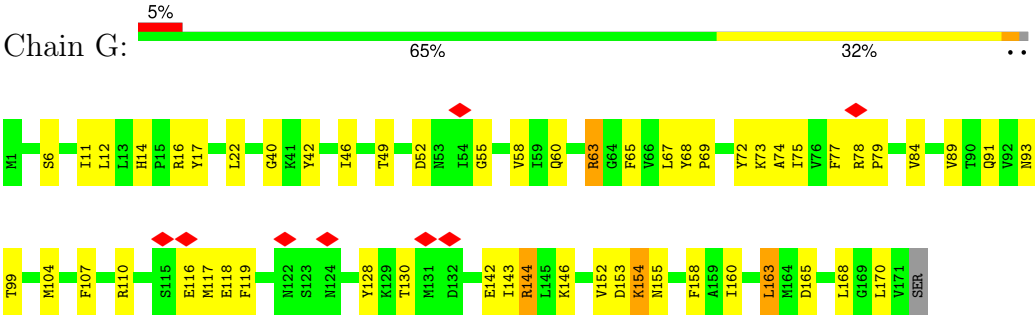




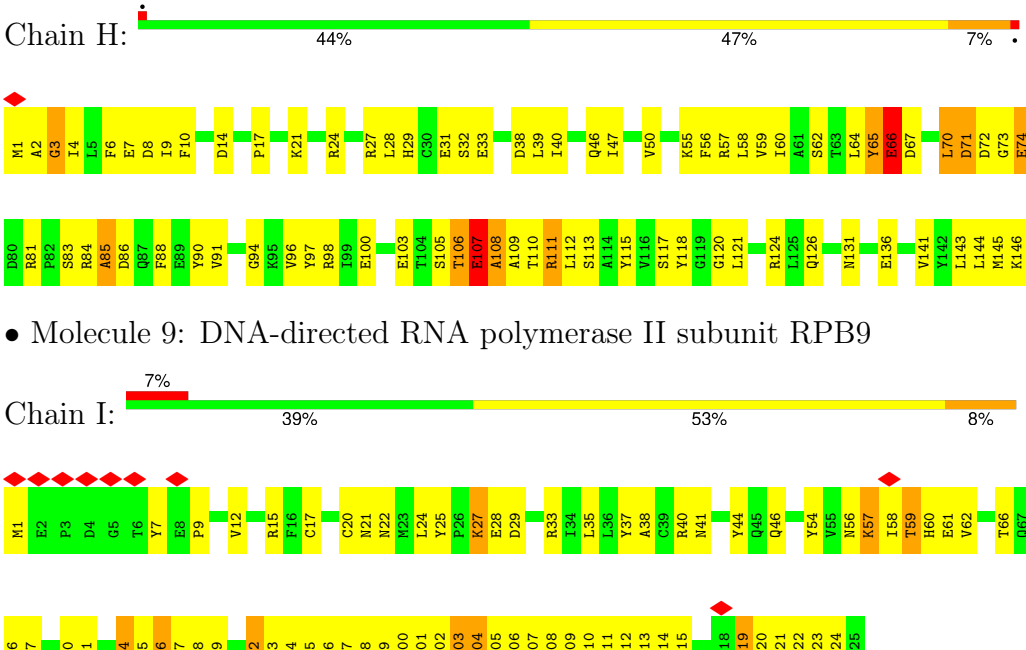
• Molecule 6: DNA-directed RNA polymerase II subunit RPB6



• Molecule 7: DNA-directed RNA polymerase II subunit RPB7



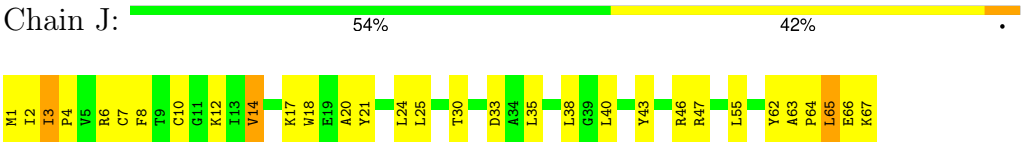
• Molecule 8: DNA-directed RNA polymerase II subunit RPB8



• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

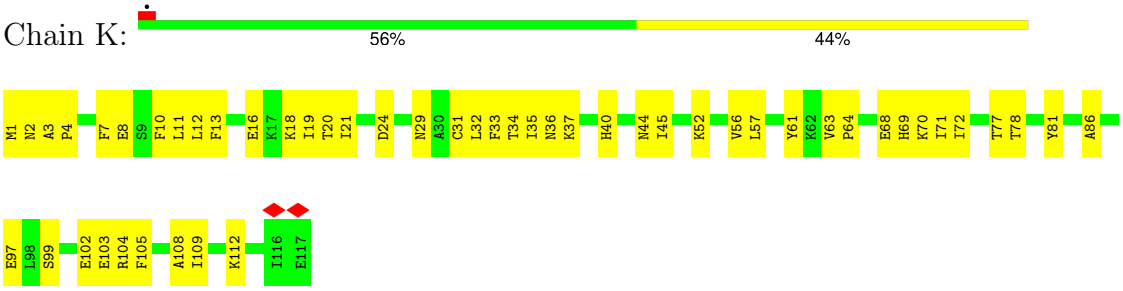
• Molecule 10: DNA-directed RNA polymerase II subunit RPB10

Chain J:



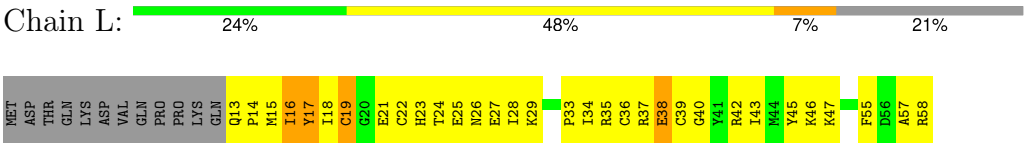
• Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a

Chain K:



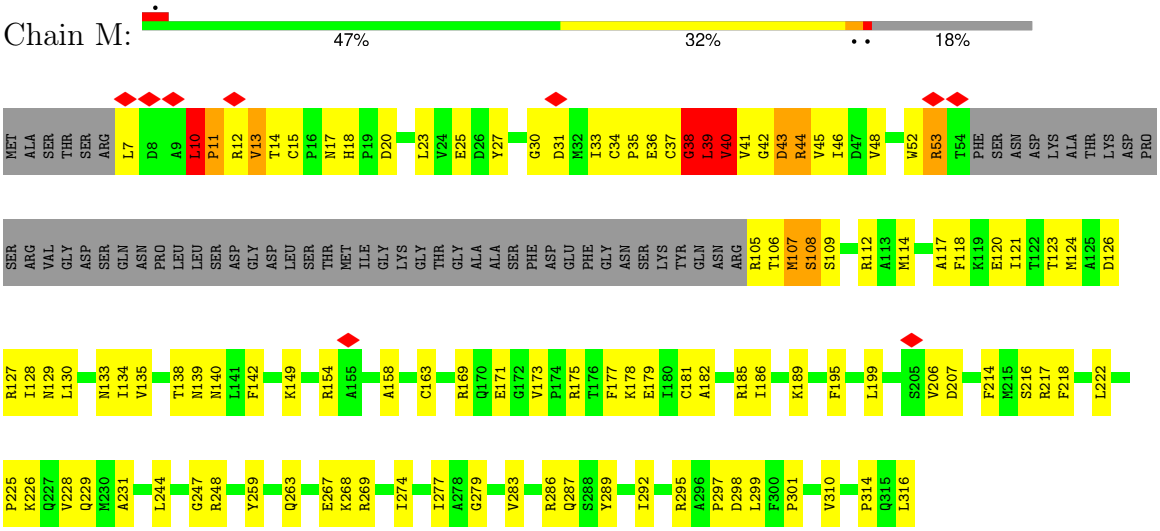
• Molecule 12: DNA-directed RNA polymerase II subunit RPB12

Chain L:



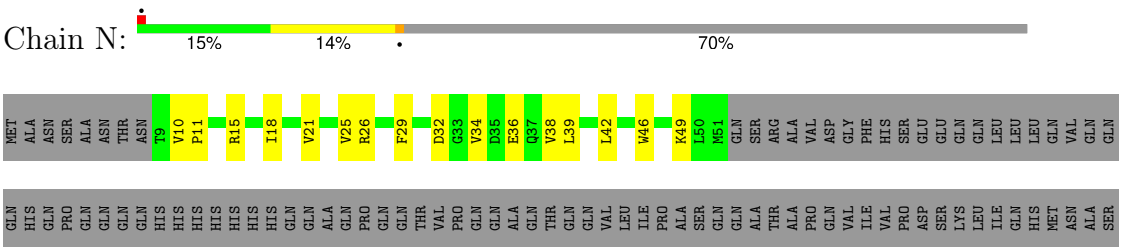
• Molecule 13: Transcription initiation factor IIB

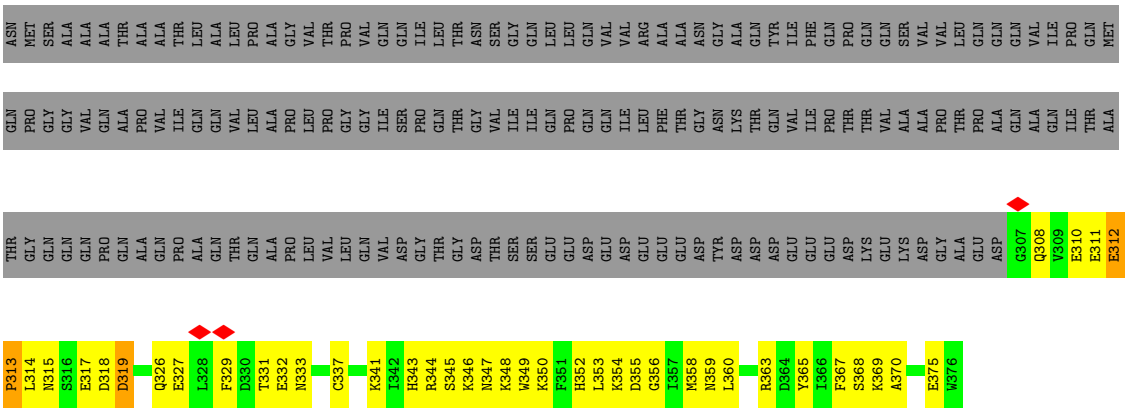
Chain M:



• Molecule 14: Transcription initiation factor IIA subunit 1

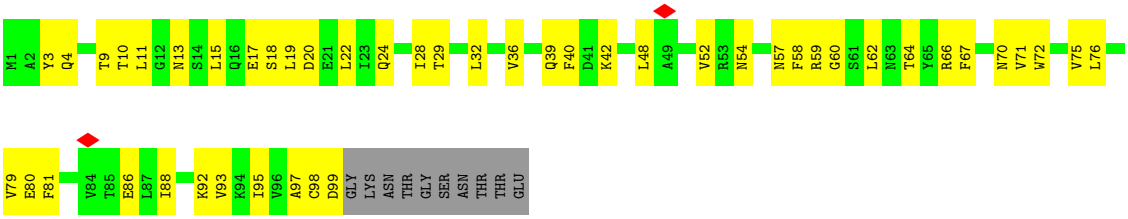
Chain N:





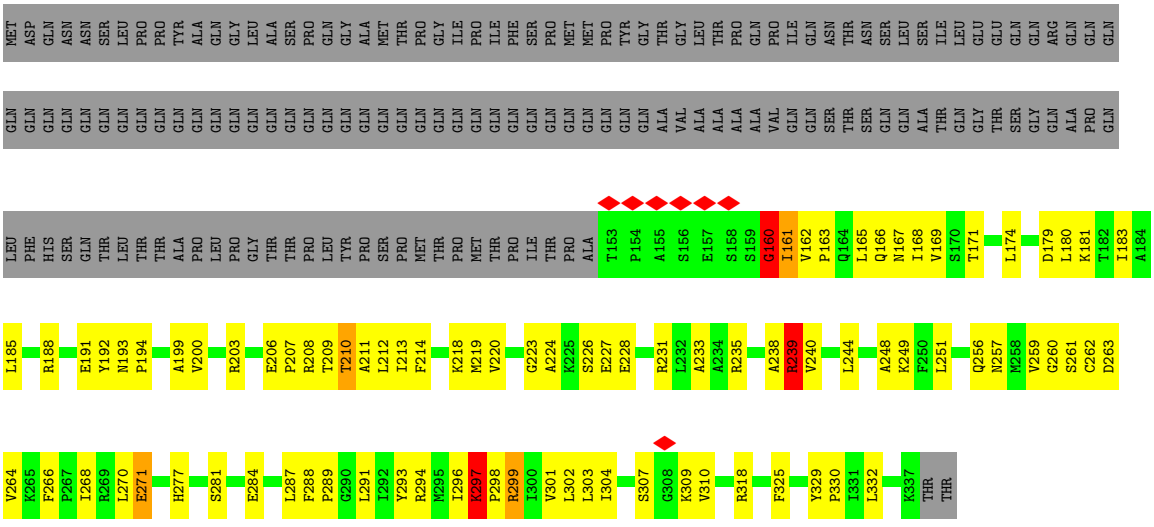
• Molecule 15: Transcription initiation factor IIA subunit 2

Chain O:



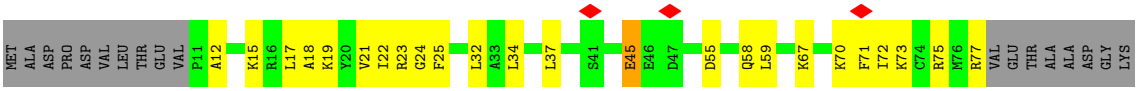
• Molecule 16: TATA-box-binding protein

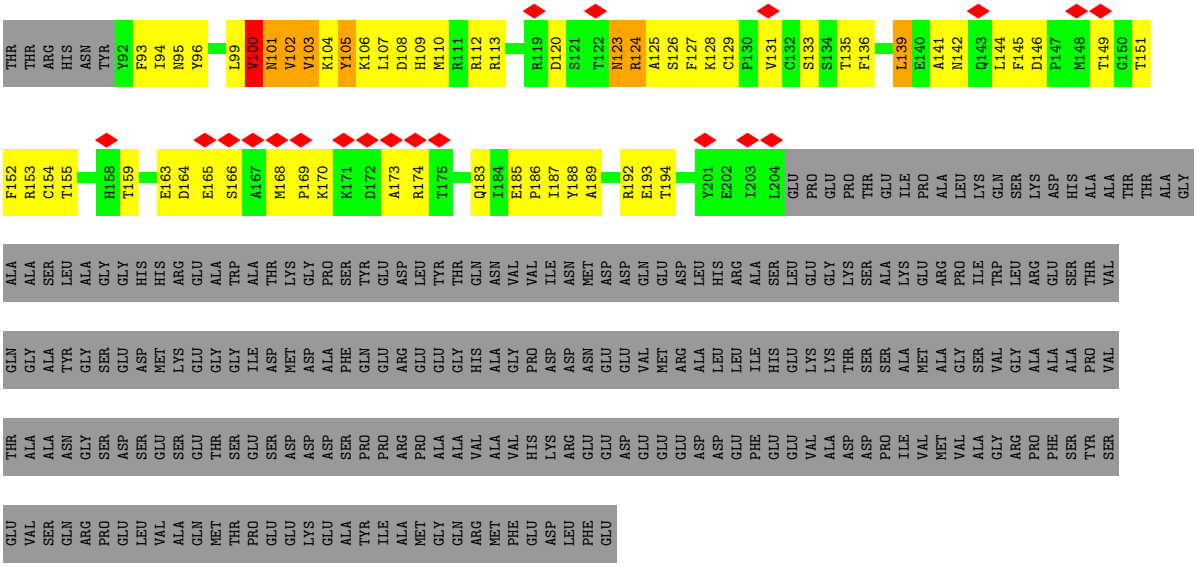
Chain P:



• Molecule 17: General transcription factor IIE subunit 1

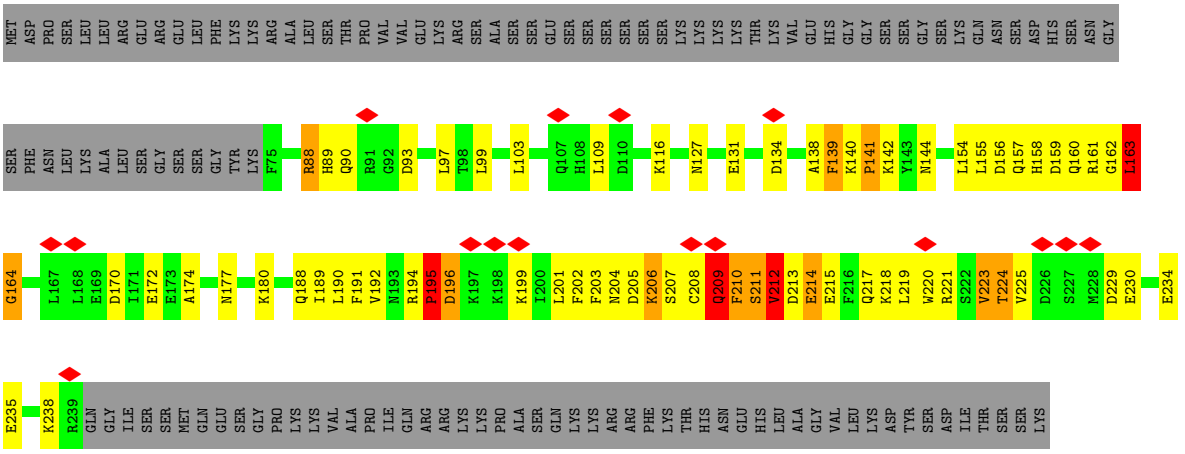
Chain Q:





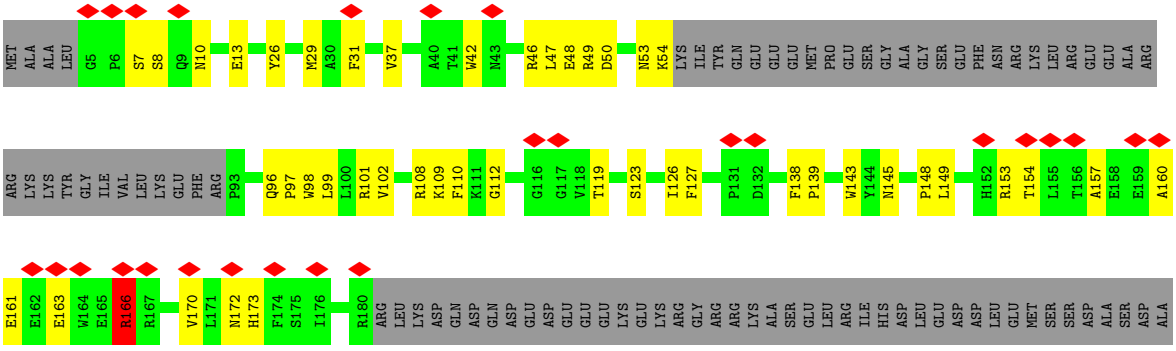
• Molecule 18: Transcription initiation factor IIE subunit beta

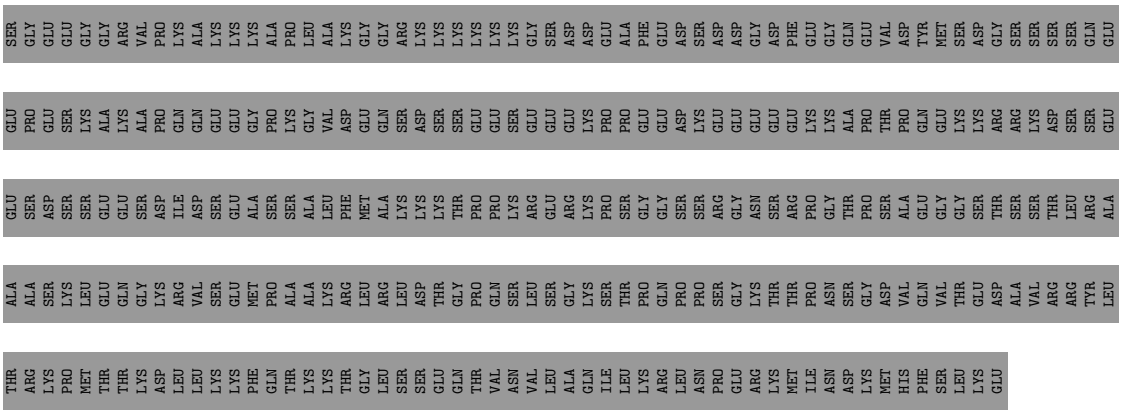
Chain R:



• Molecule 19: General transcription factor IIF subunit 1

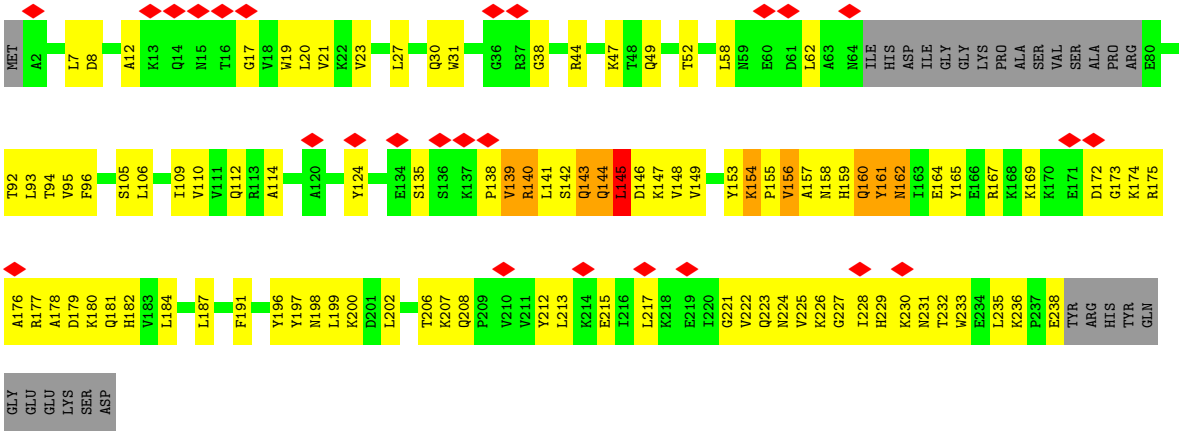
Chain S:





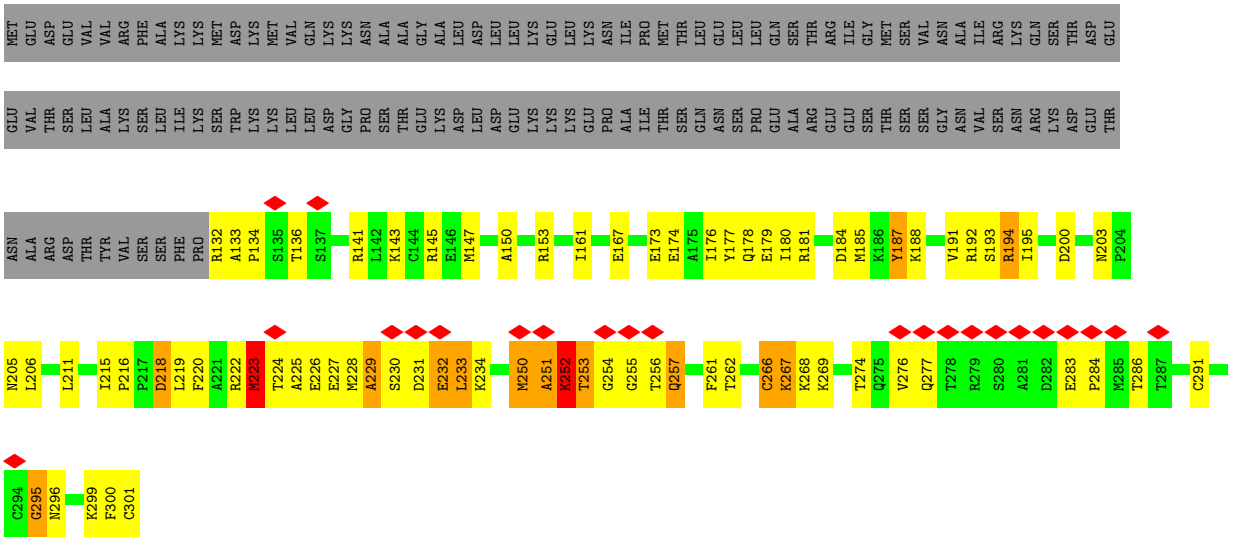
• Molecule 20: General transcription factor IIF subunit 2

Chain T:



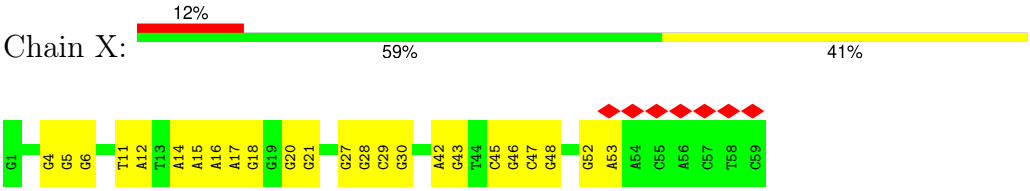
• Molecule 21: Transcription elongation factor A protein 1

Chain U:



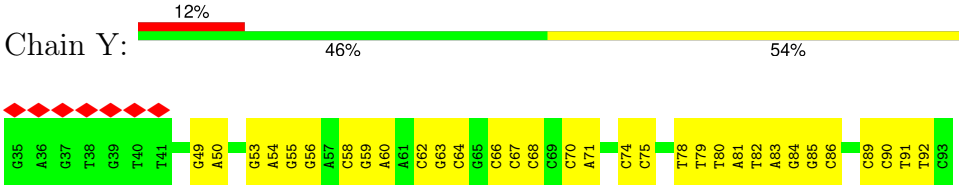
• Molecule 22: SCP-X

Chain X:



• Molecule 23: SCP-Y

Chain Y:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34728	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 ($e^-/Å^2$)	42	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	27500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.055	Depositor
Minimum map value	-0.029	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	503.03998, 503.03998, 503.03998	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	A	0.27	0/11727	0.59	9/15833 (0.1%)
2	B	0.29	1/9503 (0.0%)	0.62	6/12831 (0.0%)
3	C	0.27	0/2259	0.67	2/3073 (0.1%)
4	D	0.28	0/1077	0.51	0/1446
5	E	0.29	0/1753	0.63	2/2368 (0.1%)
6	F	0.25	0/700	0.51	0/946
7	G	0.27	0/1382	0.54	0/1874
8	H	0.27	0/1227	0.61	2/1654 (0.1%)
9	I	0.27	0/1038	0.90	2/1407 (0.1%)
10	J	0.26	0/542	0.55	0/730
11	K	0.26	0/956	0.52	0/1294
12	L	0.26	0/394	0.61	0/524
13	M	0.26	0/2049	0.74	4/2769 (0.1%)
14	N	0.31	0/945	0.58	1/1274 (0.1%)
15	O	0.26	0/816	0.54	0/1105
16	P	0.31	0/1489	0.65	3/2005 (0.1%)
17	Q	0.29	0/1507	0.60	2/2023 (0.1%)
18	R	0.42	0/1380	0.91	2/1854 (0.1%)
19	S	0.29	0/1166	0.53	1/1575 (0.1%)
20	T	0.26	0/1817	0.58	1/2445 (0.0%)
21	U	0.33	0/1358	0.69	2/1820 (0.1%)
22	X	0.55	0/1369	0.90	0/2114
23	Y	0.55	0/1337	0.93	0/2059
All	All	0.31	1/47791 (0.0%)	0.65	39/65023 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
3	C	0	1
17	Q	0	1
18	R	0	1
21	U	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1090	GLU	CD-OE1	7.40	1.33	1.25

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	84	HIS	C-N-CD	-24.01	67.78	120.60
18	R	194	ARG	C-N-CD	-22.48	71.14	120.60
13	M	10	LEU	C-N-CD	-20.59	75.30	120.60
3	C	6	GLN	C-N-CD	-20.16	76.26	120.60
2	B	497	LYS	C-N-CD	-20.03	76.53	120.60
1	A	622	SER	C-N-CD	-10.02	98.56	120.60
16	P	239	ARG	NE-CZ-NH1	9.25	124.92	120.30
1	A	1307	VAL	N-CA-C	9.09	135.55	111.00
2	B	242	ARG	N-CA-C	-8.46	88.15	111.00
13	M	38	GLY	N-CA-C	-8.24	92.49	113.10
1	A	1311	LEU	CB-CG-CD1	-8.12	97.20	111.00
16	P	239	ARG	NE-CZ-NH2	-7.93	116.34	120.30
1	A	266	MET	N-CA-C	-7.76	90.05	111.00
20	T	145	LEU	N-CA-C	-7.38	91.06	111.00
5	E	64	HIS	N-CA-C	6.88	129.58	111.00
2	B	133	ILE	N-CA-C	-6.68	92.96	111.00
13	M	37	CYS	C-N-CA	-6.48	108.70	122.30
18	R	195	PRO	N-CA-C	-6.44	95.36	112.10
21	U	232	GLU	N-CA-C	6.42	128.32	111.00
16	P	160	GLY	N-CA-C	6.27	128.78	113.10
13	M	43	ASP	N-CA-C	6.26	127.90	111.00
8	H	74	GLU	N-CA-C	-5.98	94.86	111.00
14	N	319	ASP	N-CA-C	5.92	126.99	111.00
1	A	622	SER	N-CA-C	-5.77	95.41	111.00
2	B	1090	GLU	OE1-CD-OE2	5.76	130.21	123.30
1	A	614	ASP	N-CA-C	5.63	126.19	111.00
17	Q	102	VAL	C-N-CA	-5.59	107.74	121.70
9	I	103	ARG	N-CA-C	-5.56	95.99	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	S	166	ARG	NE-CZ-NH1	5.50	123.05	120.30
21	U	232	GLU	C-N-CA	-5.44	108.11	121.70
17	Q	73	LYS	N-CA-C	-5.39	96.45	111.00
2	B	880	LEU	N-CA-C	5.37	125.50	111.00
1	A	514	GLU	OE1-CD-OE2	-5.35	116.88	123.30
2	B	546	GLU	CA-CB-CG	5.32	125.10	113.40
5	E	62	VAL	C-N-CA	-5.23	108.63	121.70
8	H	85	ALA	N-CA-C	-5.16	97.07	111.00
1	A	625	ASP	C-N-CA	-5.15	108.81	121.70
1	A	604	ARG	C-N-CA	-5.06	109.06	121.70
3	C	137	ASN	N-CA-C	-5.00	97.50	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	623	PRO	Mainchain
1	A	85	PHE	Peptide
3	C	210	GLU	Mainchain
17	Q	100	VAL	Mainchain
18	R	230	GLU	Mainchain
21	U	250	MET	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11515	0	11607	677	0
2	B	9317	0	9307	574	0
3	C	2213	0	2153	138	0
4	D	1062	0	1042	24	0
5	E	1723	0	1745	82	0
6	F	689	0	715	45	0
7	G	1351	0	1358	53	0
8	H	1205	0	1167	108	0
9	I	1013	0	931	81	0
10	J	533	0	553	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	937	0	959	46	0
12	L	388	0	393	65	0
13	M	2018	0	2060	136	0
14	N	930	0	888	64	0
15	O	806	0	818	51	0
16	P	1462	0	1548	117	0
17	Q	1484	0	1496	250	0
18	R	1357	0	1375	294	0
19	S	1137	0	1101	38	0
20	T	1788	0	1819	143	0
21	U	1343	0	1338	92	0
22	X	1218	0	661	25	0
23	Y	1195	0	663	30	0
24	A	1	0	0	0	0
24	B	1	0	0	0	0
25	A	2	0	0	0	0
25	B	1	0	0	0	0
25	C	1	0	0	0	0
25	I	2	0	0	0	0
25	J	1	0	0	0	0
25	L	1	0	0	0	0
25	M	1	0	0	0	0
25	Q	1	0	0	0	0
25	U	1	0	0	0	0
All	All	46697	0	45697	2635	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 29.

All (2635) 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)
17:Q:110:MET:HB2	18:R:218:LYS:CG	1.11	1.56
2:B:239:MET:SD	2:B:256:ILE:HG23	1.45	1.53
17:Q:187:ILE:CD1	18:R:211:SER:CB	1.86	1.51
8:H:65:TYR:CE1	8:H:79:ASP:OD2	1.65	1.50
17:Q:110:MET:CE	18:R:213:ASP:CB	1.89	1.50
1:A:1310:HIS:N	21:U:252:LYS:HD2	1.24	1.48
16:P:209:THR:CG2	16:P:224:ALA:N	1.79	1.45
17:Q:187:ILE:CG1	18:R:211:SER:HB3	1.44	1.45
17:Q:110:MET:CE	18:R:213:ASP:HB3	0.98	1.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:209:THR:HG22	16:P:223:GLY:C	1.31	1.43
17:Q:187:ILE:CG1	18:R:211:SER:CB	1.92	1.43
17:Q:24:GLY:CA	18:R:210:PHE:CD2	1.89	1.43
18:R:155:LEU:CG	18:R:204:ASN:ND2	1.79	1.42
17:Q:23:ARG:NH1	18:R:207:SER:HB3	1.32	1.40
17:Q:187:ILE:HG23	18:R:212:VAL:CA	1.34	1.40
17:Q:110:MET:CB	18:R:218:LYS:CG	2.00	1.40
17:Q:23:ARG:NH2	18:R:206:LYS:CG	1.84	1.39
17:Q:110:MET:HE3	18:R:213:ASP:CB	1.46	1.39
2:B:239:MET:CE	2:B:256:ILE:HD13	1.50	1.39
2:B:132:VAL:CG2	2:B:141:GLN:HG3	1.51	1.38
13:M:178:LYS:O	20:T:154:LYS:CB	1.69	1.38
1:A:922:PHE:CE2	1:A:952:LEU:HD23	1.58	1.37
3:C:200:PRO:HG2	3:C:217:GLN:CG	1.54	1.36
17:Q:187:ILE:CD1	18:R:211:SER:HB3	0.89	1.36
16:P:209:THR:HG22	16:P:224:ALA:N	1.38	1.35
13:M:12:ARG:O	13:M:13:VAL:HG13	1.23	1.33
17:Q:110:MET:CB	18:R:218:LYS:HG3	1.55	1.32
18:R:223:VAL:O	18:R:224:THR:CG2	1.74	1.32
16:P:209:THR:HG22	16:P:223:GLY:CA	1.60	1.32
1:A:924:TYR:CD1	1:A:949:GLN:NE2	1.99	1.30
17:Q:110:MET:CG	18:R:218:LYS:HB2	1.59	1.30
13:M:179:GLU:CA	20:T:154:LYS:HG2	1.62	1.29
1:A:1307:VAL:CG2	1:A:1338:THR:HB	1.62	1.28
17:Q:110:MET:SD	18:R:213:ASP:HB3	1.72	1.28
1:A:1310:HIS:HB3	21:U:252:LYS:NZ	1.46	1.27
17:Q:110:MET:HB2	18:R:218:LYS:CB	1.63	1.27
18:R:195:PRO:HG2	18:R:199:LYS:CB	1.63	1.27
17:Q:70:LYS:HG3	18:R:225:VAL:O	1.09	1.26
17:Q:187:ILE:CG2	18:R:212:VAL:CA	2.08	1.25
17:Q:187:ILE:HD13	18:R:211:SER:CB	1.53	1.24
18:R:155:LEU:HG	18:R:204:ASN:ND2	0.93	1.24
17:Q:23:ARG:NH2	18:R:206:LYS:HG3	0.92	1.24
1:A:621:ILE:O	1:A:623:PRO:HD3	1.35	1.22
8:H:65:TYR:CZ	8:H:81:ARG:NH2	2.07	1.22
2:B:79:GLU:O	2:B:80:GLU:HG2	1.36	1.22
21:U:252:LYS:O	21:U:253:THR:HG23	1.39	1.21
2:B:79:GLU:O	2:B:80:GLU:CG	1.87	1.21
1:A:926:ASN:OD1	1:A:931:ARG:NE	1.74	1.21
12:L:15:MET:O	12:L:16:ILE:HG23	1.35	1.21
1:A:616:GLY:O	1:A:619:LYS:HB2	1.40	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:102:VAL:O	17:Q:103:VAL:C	1.79	1.20
21:U:218:ASP:O	21:U:222:ARG:HB2	1.41	1.19
13:M:179:GLU:HA	20:T:154:LYS:CG	1.71	1.19
18:R:210:PHE:O	18:R:212:VAL:CG1	1.90	1.19
17:Q:105:TYR:HB2	18:R:234:GLU:HG2	1.19	1.18
3:C:200:PRO:CG	3:C:217:GLN:HG3	1.72	1.18
2:B:881:GLU:C	2:B:883:THR:H	1.41	1.18
1:A:621:ILE:O	1:A:623:PRO:CD	1.92	1.18
18:R:202:PHE:O	18:R:203:PHE:CD1	1.97	1.17
8:H:65:TYR:HE1	8:H:79:ASP:OD2	0.91	1.16
17:Q:107:LEU:CA	18:R:218:LYS:HE3	1.75	1.16
17:Q:24:GLY:HA3	18:R:210:PHE:CD2	1.24	1.15
17:Q:105:TYR:HE1	17:Q:109:HIS:NE2	1.43	1.15
18:R:210:PHE:O	18:R:212:VAL:HG13	0.97	1.15
12:L:18:ILE:HD11	12:L:47:LYS:CE	1.75	1.15
2:B:873:LEU:CB	2:B:874:PRO:HD3	1.77	1.14
13:M:34:CYS:H	13:M:39:LEU:CB	1.51	1.14
16:P:297:LYS:HB3	16:P:298:PRO:HD3	1.23	1.14
17:Q:187:ILE:CG2	18:R:212:VAL:HA	1.70	1.14
3:C:136:ASP:HB2	3:C:145:GLN:OE1	1.46	1.14
17:Q:70:LYS:CG	18:R:225:VAL:O	1.94	1.14
18:R:212:VAL:HG23	18:R:213:ASP:N	1.58	1.14
17:Q:102:VAL:HB	17:Q:105:TYR:HB3	1.16	1.13
17:Q:23:ARG:HH11	18:R:207:SER:CB	1.61	1.13
1:A:1310:HIS:H	21:U:252:LYS:CD	1.62	1.13
16:P:209:THR:CG2	16:P:223:GLY:C	2.13	1.13
12:L:15:MET:O	12:L:16:ILE:CG2	1.97	1.13
1:A:1310:HIS:CB	21:U:252:LYS:HZ2	1.63	1.12
17:Q:25:PHE:CD2	18:R:215:GLU:CD	2.23	1.12
17:Q:105:TYR:CE1	17:Q:109:HIS:NE2	2.16	1.12
2:B:239:MET:HE3	2:B:256:ILE:HD13	1.18	1.12
12:L:15:MET:O	12:L:16:ILE:HG12	1.49	1.12
2:B:873:LEU:HB2	2:B:874:PRO:HD3	1.21	1.12
17:Q:109:HIS:HB3	18:R:221:ARG:HG2	1.22	1.12
14:N:318:ASP:HA	16:P:239:ARG:HD2	1.12	1.11
1:A:1307:VAL:HG22	1:A:1338:THR:CB	1.81	1.11
17:Q:112:ARG:CG	18:R:221:ARG:HH22	1.63	1.11
2:B:239:MET:SD	2:B:256:ILE:CG2	2.38	1.10
18:R:195:PRO:HG2	18:R:199:LYS:HB2	1.16	1.10
2:B:92:TYR:CB	20:T:145:LEU:HD22	1.82	1.10
16:P:206:GLU:HB2	16:P:207:PRO:HD3	1.30	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:23:ARG:HH21	18:R:206:LYS:CG	1.55	1.10
3:C:200:PRO:HB2	3:C:217:GLN:OE1	1.50	1.10
2:B:132:VAL:CG2	2:B:141:GLN:CG	2.30	1.10
16:P:209:THR:HG21	16:P:224:ALA:N	1.63	1.09
17:Q:23:ARG:NH1	18:R:207:SER:CB	2.14	1.09
1:A:922:PHE:CE2	1:A:952:LEU:CD2	2.35	1.09
1:A:924:TYR:CE1	1:A:949:GLN:NE2	2.20	1.09
1:A:1310:HIS:CA	21:U:252:LYS:HD2	1.83	1.09
17:Q:107:LEU:HA	18:R:218:LYS:HE3	1.15	1.09
17:Q:112:ARG:HG2	18:R:221:ARG:HH22	1.07	1.09
1:A:1310:HIS:CB	21:U:252:LYS:NZ	2.14	1.08
20:T:179:ASP:OD1	20:T:182:HIS:HB3	1.53	1.08
2:B:876:ASN:O	2:B:879:GLU:HG3	1.54	1.08
16:P:209:THR:HA	16:P:223:GLY:HA3	1.33	1.08
17:Q:110:MET:SD	18:R:218:LYS:HD2	1.93	1.08
18:R:190:LEU:CD1	18:R:205:ASP:HB2	1.83	1.08
2:B:876:ASN:O	2:B:879:GLU:CG	2.01	1.07
17:Q:187:ILE:HD11	18:R:211:SER:HB3	1.30	1.07
2:B:242:ARG:O	2:B:252:ILE:HG23	1.54	1.07
1:A:927:GLU:O	1:A:931:ARG:HG3	1.55	1.07
3:C:136:ASP:C	3:C:138:ASP:H	1.51	1.07
18:R:223:VAL:O	18:R:224:THR:HG23	0.89	1.07
2:B:79:GLU:O	2:B:80:GLU:CB	2.01	1.07
1:A:932:ARG:HB3	1:A:939:VAL:HG11	1.10	1.06
13:M:34:CYS:N	13:M:39:LEU:HB3	1.68	1.06
21:U:252:LYS:HA	21:U:252:LYS:HE3	1.36	1.06
17:Q:110:MET:HG3	18:R:218:LYS:HB2	1.15	1.06
1:A:1310:HIS:N	21:U:252:LYS:CD	2.18	1.05
1:A:1310:HIS:HB3	21:U:252:LYS:HG2	1.38	1.05
3:C:200:PRO:CG	3:C:217:GLN:CG	2.32	1.05
8:H:75:TYR:O	8:H:77:PRO:HD3	1.53	1.05
17:Q:110:MET:SD	18:R:213:ASP:CB	2.36	1.05
3:C:6:GLN:O	11:K:104:ARG:NH1	1.89	1.05
13:M:12:ARG:O	13:M:13:VAL:CG1	2.05	1.04
18:R:212:VAL:HG23	18:R:213:ASP:H	0.94	1.04
1:A:922:PHE:CZ	1:A:952:LEU:HD23	1.93	1.04
1:A:1304:ILE:HD12	1:A:1307:VAL:CG1	1.86	1.04
2:B:880:LEU:O	2:B:881:GLU:CB	2.03	1.04
16:P:161:ILE:HG21	16:P:263:ASP:O	1.58	1.04
1:A:1304:ILE:HD12	1:A:1307:VAL:HG11	1.38	1.04
17:Q:112:ARG:HB3	18:R:221:ARG:NH2	1.72	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:15:MET:O	12:L:16:ILE:CG1	2.05	1.03
12:L:18:ILE:HD11	12:L:47:LYS:HE3	1.35	1.03
17:Q:110:MET:SD	18:R:213:ASP:CG	2.37	1.03
3:C:5:ASN:C	3:C:7:PRO:HD3	1.74	1.03
13:M:178:LYS:O	20:T:154:LYS:HB3	0.86	1.03
16:P:160:GLY:O	16:P:161:ILE:HG12	1.56	1.03
1:A:932:ARG:CB	1:A:939:VAL:HG11	1.88	1.03
16:P:297:LYS:CB	16:P:298:PRO:CD	2.37	1.03
17:Q:24:GLY:HA2	18:R:210:PHE:CD2	1.88	1.03
1:A:330:GLN:HB3	13:M:107:MET:SD	1.97	1.02
1:A:923:ASP:C	1:A:925:THR:H	1.58	1.02
1:A:1307:VAL:HG22	1:A:1338:THR:HB	1.02	1.02
2:B:132:VAL:HG21	2:B:141:GLN:HG3	1.04	1.02
2:B:499:ARG:O	2:B:500:GLN:O	1.75	1.02
12:L:16:ILE:O	12:L:17:TYR:HB2	1.57	1.02
12:L:18:ILE:HD11	12:L:47:LYS:CD	1.88	1.01
16:P:209:THR:CG2	16:P:224:ALA:H	1.74	1.01
17:Q:110:MET:CB	18:R:218:LYS:CD	2.38	1.00
1:A:923:ASP:O	1:A:925:THR:N	1.94	1.00
1:A:1313:GLN:HG2	1:A:1333:GLU:HG2	1.43	1.00
17:Q:24:GLY:HA2	18:R:210:PHE:CG	1.96	1.00
21:U:232:GLU:O	21:U:233:LEU:HB2	1.58	1.00
1:A:927:GLU:O	1:A:931:ARG:CG	2.09	1.00
1:A:926:ASN:OD1	1:A:931:ARG:CD	2.10	1.00
1:A:622:SER:O	1:A:624:GLY:N	1.95	0.99
2:B:239:MET:CE	2:B:256:ILE:CD1	2.39	0.99
1:A:926:ASN:ND2	1:A:931:ARG:HD2	1.77	0.99
13:M:34:CYS:O	13:M:39:LEU:HB2	1.62	0.99
17:Q:109:HIS:HB3	18:R:221:ARG:CG	1.91	0.99
17:Q:102:VAL:O	17:Q:104:LYS:N	1.96	0.99
2:B:132:VAL:HG21	2:B:141:GLN:CG	1.90	0.99
17:Q:25:PHE:HD2	18:R:215:GLU:CD	1.61	0.99
8:H:85:ALA:O	8:H:144:LEU:CD2	2.10	0.98
13:M:43:ASP:O	13:M:44:ARG:C	1.97	0.98
13:M:34:CYS:H	13:M:39:LEU:HB3	0.83	0.98
18:R:208:CYS:O	18:R:209:GLN:O	1.81	0.98
17:Q:105:TYR:CE1	17:Q:109:HIS:CD2	2.50	0.98
17:Q:110:MET:CB	18:R:218:LYS:CB	2.34	0.98
21:U:218:ASP:O	21:U:222:ARG:CB	2.12	0.98
2:B:132:VAL:HG23	2:B:141:GLN:CG	1.93	0.98
2:B:242:ARG:O	2:B:252:ILE:CG2	2.12	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:VAL:HG22	2:B:141:GLN:O	1.63	0.97
3:C:217:GLN:O	3:C:218:ALA:CB	2.12	0.97
1:A:1307:VAL:HG23	1:A:1339:ASP:H	1.30	0.97
8:H:74:GLU:O	8:H:76:ASN:N	1.96	0.97
16:P:297:LYS:HB3	16:P:298:PRO:CD	1.93	0.97
2:B:880:LEU:O	2:B:881:GLU:HB2	1.14	0.97
17:Q:25:PHE:CE2	18:R:215:GLU:HG3	2.00	0.97
3:C:200:PRO:HG2	3:C:217:GLN:HG3	0.98	0.97
8:H:75:TYR:O	8:H:77:PRO:CD	2.12	0.97
1:A:611:ASP:CG	1:A:626:THR:OG1	2.02	0.96
5:E:64:HIS:O	5:E:65:ASN:O	1.83	0.96
18:R:127:ASN:HD21	18:R:140:LYS:CD	1.77	0.96
3:C:6:GLN:CG	3:C:25:ASN:ND2	2.28	0.96
18:R:190:LEU:HD12	18:R:205:ASP:HB2	1.43	0.96
3:C:200:PRO:CB	3:C:217:GLN:OE1	2.13	0.96
8:H:100:GLU:HB2	8:H:113:SER:HB2	1.48	0.96
17:Q:107:LEU:HA	18:R:218:LYS:CE	1.96	0.96
17:Q:109:HIS:O	18:R:221:ARG:HD3	1.65	0.96
2:B:881:GLU:C	2:B:883:THR:N	2.15	0.95
18:R:220:TRP:O	18:R:223:VAL:HG22	1.65	0.95
1:A:551:ARG:HG2	1:A:625:ASP:OD2	1.65	0.95
17:Q:109:HIS:O	18:R:221:ARG:NH1	1.99	0.95
17:Q:110:MET:CB	18:R:218:LYS:HD2	1.94	0.95
17:Q:32:LEU:HD11	18:R:203:PHE:CD2	2.00	0.95
1:A:621:ILE:O	1:A:623:PRO:N	1.99	0.95
17:Q:110:MET:CB	18:R:218:LYS:HB2	1.93	0.95
1:A:932:ARG:HB3	1:A:939:VAL:CG1	1.96	0.95
2:B:240:LEU:HG	2:B:255:ARG:O	1.67	0.95
9:I:99:SER:OG	9:I:105:GLU:HB2	1.67	0.95
2:B:92:TYR:HB3	20:T:145:LEU:CG	1.97	0.95
1:A:426:ARG:HB3	13:M:40:VAL:HG21	1.46	0.94
18:R:210:PHE:O	18:R:211:SER:C	2.04	0.94
18:R:223:VAL:C	18:R:224:THR:HG23	1.88	0.94
8:H:64:LEU:H	8:H:70:LEU:HD21	1.30	0.94
2:B:92:TYR:HB3	20:T:145:LEU:HD22	1.46	0.94
18:R:195:PRO:CG	18:R:199:LYS:CB	2.45	0.94
1:A:1310:HIS:HB3	21:U:252:LYS:HZ2	0.80	0.94
13:M:34:CYS:O	13:M:39:LEU:CD2	2.14	0.93
17:Q:110:MET:HE1	18:R:213:ASP:HB3	1.46	0.93
17:Q:102:VAL:HB	17:Q:105:TYR:CB	1.97	0.93
17:Q:102:VAL:CB	17:Q:105:TYR:HB3	1.98	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:712:PRO:HB3	2:B:999:ALA:HB1	1.51	0.93
12:L:15:MET:O	12:L:16:ILE:CB	2.15	0.93
2:B:132:VAL:HG23	2:B:141:GLN:HG3	1.47	0.93
17:Q:187:ILE:HG21	18:R:212:VAL:O	1.68	0.93
18:R:202:PHE:O	18:R:203:PHE:CG	2.21	0.93
8:H:65:TYR:CE2	8:H:81:ARG:NH2	2.29	0.92
1:A:924:TYR:HD1	1:A:949:GLN:NE2	1.48	0.92
17:Q:187:ILE:HB	18:R:211:SER:OG	1.70	0.92
18:R:155:LEU:CG	18:R:204:ASN:HD21	1.55	0.92
1:A:1313:GLN:C	1:A:1315:ASP:H	1.69	0.92
3:C:200:PRO:HG2	3:C:217:GLN:CD	1.89	0.92
17:Q:110:MET:CG	18:R:218:LYS:CB	2.47	0.92
13:M:178:LYS:C	20:T:154:LYS:CB	2.38	0.92
1:A:551:ARG:HH22	8:H:121:LEU:HA	1.34	0.91
1:A:612:ASP:HB3	1:A:617:PRO:HD3	1.50	0.91
17:Q:109:HIS:C	18:R:221:ARG:HD3	1.89	0.91
17:Q:23:ARG:CZ	18:R:206:LYS:HG3	1.99	0.91
18:R:213:ASP:O	18:R:215:GLU:N	2.03	0.91
17:Q:25:PHE:CD2	18:R:215:GLU:CG	2.53	0.91
17:Q:105:TYR:HE1	17:Q:109:HIS:HE2	0.93	0.91
17:Q:110:MET:HB2	18:R:218:LYS:CD	2.00	0.91
16:P:297:LYS:CB	16:P:298:PRO:HD3	1.98	0.91
17:Q:187:ILE:CB	18:R:211:SER:OG	2.19	0.91
2:B:92:TYR:HB3	20:T:145:LEU:CD2	2.01	0.91
2:B:92:TYR:HB3	20:T:145:LEU:HB2	1.51	0.91
12:L:25:GLU:HB2	12:L:27:GLU:HG2	1.53	0.90
18:R:212:VAL:CG2	18:R:213:ASP:H	1.83	0.90
17:Q:23:ARG:HH11	18:R:207:SER:HB3	0.75	0.90
1:A:922:PHE:HE2	1:A:952:LEU:CD2	1.79	0.90
5:E:64:HIS:O	5:E:65:ASN:C	2.07	0.90
17:Q:107:LEU:N	18:R:218:LYS:HE3	1.87	0.90
2:B:132:VAL:CG2	2:B:141:GLN:O	2.20	0.90
9:I:58:ILE:O	9:I:59:THR:OG1	1.88	0.90
13:M:178:LYS:C	20:T:154:LYS:HB3	1.90	0.90
18:R:162:GLY:C	18:R:164:GLY:H	1.66	0.90
8:H:65:TYR:CZ	8:H:79:ASP:OD2	2.24	0.90
5:E:63:ALA:O	5:E:64:HIS:HB2	1.70	0.89
17:Q:23:ARG:HH22	18:R:206:LYS:HG3	1.34	0.89
13:M:34:CYS:O	13:M:39:LEU:HD23	1.50	0.89
14:N:343:HIS:HB3	14:N:350:LYS:HB2	1.50	0.89
17:Q:113:ARG:NE	18:R:217:GLN:O	2.06	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:112:ARG:HG2	18:R:221:ARG:NH2	1.86	0.89
5:E:6:GLU:OE2	5:E:54:ARG:NH2	2.05	0.89
17:Q:112:ARG:CG	18:R:221:ARG:NH2	2.35	0.89
3:C:45:ILE:HG12	3:C:79:VAL:HB	1.55	0.89
3:C:6:GLN:HG3	3:C:25:ASN:ND2	1.87	0.89
17:Q:25:PHE:CD2	18:R:215:GLU:HG3	2.07	0.89
18:R:195:PRO:HG2	18:R:199:LYS:HB3	1.54	0.89
1:A:1310:HIS:CB	21:U:252:LYS:HG2	2.00	0.89
17:Q:112:ARG:CB	18:R:221:ARG:NH2	2.35	0.89
18:R:210:PHE:CG	18:R:212:VAL:HG11	2.08	0.89
1:A:608:THR:C	1:A:610:PRO:HD2	1.94	0.88
1:A:926:ASN:CG	1:A:931:ARG:HD2	1.93	0.88
17:Q:110:MET:HB3	18:R:218:LYS:HD2	1.55	0.88
20:T:179:ASP:C	20:T:181:GLN:H	1.73	0.88
1:A:923:ASP:C	1:A:925:THR:N	2.24	0.88
17:Q:187:ILE:HD13	18:R:211:SER:HB3	0.89	0.88
18:R:127:ASN:HD21	18:R:140:LYS:CE	1.85	0.88
17:Q:187:ILE:CG1	18:R:211:SER:OG	2.20	0.88
18:R:195:PRO:CG	18:R:199:LYS:HB3	2.03	0.88
8:H:17:PRO:HB3	8:H:27:ARG:HB3	1.53	0.88
17:Q:110:MET:HE1	18:R:213:ASP:CB	2.01	0.88
8:H:65:TYR:CD1	8:H:81:ARG:NE	2.40	0.88
2:B:873:LEU:HB2	2:B:874:PRO:CD	2.03	0.88
18:R:212:VAL:CG2	18:R:213:ASP:N	2.35	0.88
2:B:876:ASN:O	2:B:879:GLU:HG2	1.74	0.87
18:R:210:PHE:C	18:R:212:VAL:HG13	1.93	0.87
12:L:16:ILE:O	12:L:17:TYR:CB	2.22	0.87
17:Q:106:LYS:HG2	18:R:218:LYS:HE2	1.56	0.87
21:U:134:PRO:O	21:U:145:ARG:NH1	2.07	0.87
1:A:1287:CYS:HA	2:B:250:SER:HB2	1.56	0.87
2:B:239:MET:SD	2:B:256:ILE:CD1	2.62	0.87
2:B:92:TYR:HB3	20:T:145:LEU:CB	2.04	0.87
2:B:881:GLU:O	2:B:883:THR:N	2.07	0.87
3:C:136:ASP:C	3:C:138:ASP:N	2.24	0.87
3:C:217:GLN:O	3:C:218:ALA:HB3	1.72	0.87
12:L:18:ILE:HD11	12:L:47:LYS:HD3	1.55	0.87
9:I:103:ARG:HG2	9:I:105:GLU:OE1	1.72	0.87
18:R:158:HIS:CE1	18:R:206:LYS:HE2	2.10	0.87
16:P:209:THR:CG2	16:P:223:GLY:CA	2.50	0.86
1:A:922:PHE:CZ	1:A:952:LEU:CD2	2.56	0.86
3:C:200:PRO:HG3	3:C:217:GLN:HB3	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:105:TYR:CB	18:R:234:GLU:HG2	2.05	0.86
18:R:162:GLY:O	18:R:164:GLY:N	2.08	0.86
1:A:1307:VAL:HG23	1:A:1339:ASP:N	1.90	0.86
2:B:239:MET:SD	2:B:256:ILE:HD13	2.16	0.86
17:Q:109:HIS:O	18:R:221:ARG:CD	2.24	0.86
17:Q:24:GLY:CA	18:R:210:PHE:CG	2.52	0.86
17:Q:109:HIS:O	18:R:221:ARG:CZ	2.24	0.85
17:Q:110:MET:SD	18:R:213:ASP:OD1	2.34	0.85
17:Q:112:ARG:HB3	18:R:221:ARG:CZ	2.04	0.85
13:M:106:THR:C	13:M:108:SER:H	1.77	0.85
14:N:327:GLU:HB2	16:P:188:ARG:HH12	1.40	0.85
12:L:16:ILE:CG1	12:L:28:ILE:N	2.38	0.85
17:Q:110:MET:CE	18:R:213:ASP:CA	2.53	0.85
17:Q:187:ILE:HG23	18:R:212:VAL:C	1.97	0.85
20:T:154:LYS:HD2	20:T:154:LYS:H	1.40	0.85
1:A:620:HIS:C	1:A:621:ILE:HG12	1.96	0.85
19:S:102:VAL:HB	19:S:108:ARG:HB3	1.59	0.85
1:A:621:ILE:C	1:A:623:PRO:N	2.26	0.85
2:B:646:ARG:HD3	2:B:651:TYR:H	1.40	0.85
17:Q:187:ILE:CG2	18:R:212:VAL:O	2.25	0.84
21:U:252:LYS:O	21:U:253:THR:CG2	2.23	0.84
17:Q:187:ILE:CG2	18:R:212:VAL:C	2.45	0.84
13:M:179:GLU:HA	20:T:154:LYS:HG2	0.86	0.84
3:C:136:ASP:CB	3:C:145:GLN:OE1	2.26	0.84
5:E:63:ALA:O	5:E:64:HIS:CB	2.26	0.84
12:L:18:ILE:CD1	12:L:47:LYS:HD3	2.07	0.84
2:B:93:LEU:N	20:T:145:LEU:HD23	1.92	0.84
8:H:74:GLU:C	8:H:76:ASN:H	1.80	0.84
10:J:63:ALA:HB3	10:J:64:PRO:HD3	1.59	0.84
2:B:718:GLN:HG2	2:B:720:PRO:HD2	1.57	0.84
1:A:643:LYS:NZ	21:U:301:CYS:O	2.11	0.84
12:L:15:MET:C	12:L:16:ILE:HG12	1.95	0.83
16:P:289:PRO:HB3	23:Y:84:DG:H5'	1.57	0.83
1:A:1310:HIS:HB3	21:U:252:LYS:CG	2.08	0.83
2:B:24:GLU:OE1	2:B:762:ARG:NH1	2.11	0.83
9:I:103:ARG:O	9:I:105:GLU:N	2.11	0.83
1:A:551:ARG:CG	1:A:625:ASP:OD2	2.26	0.83
2:B:490:GLY:O	2:B:491:ARG:C	2.14	0.83
2:B:79:GLU:O	2:B:80:GLU:HB2	1.78	0.83
21:U:252:LYS:HA	21:U:252:LYS:CE	2.09	0.83
3:C:49:TRP:HB3	3:C:164:TYR:HB2	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:16:ILE:HG13	12:L:28:ILE:N	1.93	0.83
17:Q:110:MET:SD	18:R:218:LYS:CD	2.66	0.83
18:R:190:LEU:HD11	18:R:205:ASP:HB2	1.61	0.83
12:L:19:CYS:HB3	12:L:22:CYS:SG	2.19	0.83
1:A:611:ASP:CG	1:A:626:THR:HG1	1.82	0.82
18:R:210:PHE:CD2	18:R:212:VAL:HG11	2.14	0.82
5:E:147:GLU:HB3	5:E:194:ILE:HB	1.62	0.82
5:E:15:LYS:NZ	5:E:35:GLN:OE1	2.12	0.82
20:T:179:ASP:OD1	20:T:182:HIS:CB	2.27	0.82
13:M:107:MET:HE3	13:M:107:MET:H	1.44	0.82
1:A:426:ARG:HG2	13:M:40:VAL:HG11	1.62	0.82
20:T:175:ARG:HD2	20:T:207:LYS:HB3	1.60	0.82
1:A:549:THR:O	1:A:589:LYS:NZ	2.13	0.82
2:B:499:ARG:O	2:B:500:GLN:C	2.15	0.82
2:B:499:ARG:HB3	2:B:499:ARG:NH1	1.95	0.82
17:Q:110:MET:HB2	18:R:218:LYS:HG3	0.82	0.81
18:R:155:LEU:CD2	18:R:204:ASN:ND2	2.43	0.81
1:A:609:HIS:N	1:A:610:PRO:CD	2.43	0.81
14:N:318:ASP:CA	16:P:239:ARG:HD2	2.04	0.81
18:R:191:PHE:HB3	18:R:202:PHE:CE1	2.15	0.81
17:Q:112:ARG:CB	18:R:221:ARG:HH22	1.90	0.81
1:A:611:ASP:HB3	1:A:617:PRO:HG3	1.63	0.81
1:A:723:ASN:HB2	9:I:109:ARG:HB2	1.61	0.81
1:A:1209:PRO:HB3	9:I:33:ARG:HH12	1.44	0.81
1:A:1310:HIS:CA	21:U:252:LYS:CD	2.50	0.81
2:B:79:GLU:C	2:B:80:GLU:HG2	2.00	0.81
1:A:653:VAL:HG23	1:A:669:TYR:HE2	1.46	0.81
14:N:318:ASP:HA	16:P:239:ARG:CD	2.05	0.81
2:B:227:ASN:O	2:B:405:ARG:NH2	2.14	0.81
2:B:488:PRO:O	2:B:489:ILE:CG1	2.29	0.81
2:B:873:LEU:CB	2:B:874:PRO:CD	2.59	0.81
2:B:289:ILE:HG13	2:B:291:ASP:H	1.43	0.81
2:B:488:PRO:O	2:B:489:ILE:HG12	1.80	0.81
12:L:18:ILE:HA	12:L:25:GLU:HA	1.63	0.81
18:R:127:ASN:ND2	18:R:140:LYS:CD	2.44	0.81
18:R:210:PHE:O	18:R:212:VAL:N	2.13	0.81
21:U:250:MET:O	21:U:251:ALA:HB2	1.80	0.81
1:A:330:GLN:CB	13:M:107:MET:SD	2.68	0.80
10:J:67:LYS:HB2	12:L:23:HIS:HD2	1.47	0.80
16:P:297:LYS:HA	16:P:297:LYS:CE	2.09	0.80
17:Q:25:PHE:HD2	18:R:215:GLU:CG	1.90	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:67:LYS:HG3	12:L:23:HIS:HB3	1.63	0.80
2:B:72:GLN:O	2:B:73:HIS:O	1.99	0.80
8:H:40:ILE:HD12	8:H:124:ARG:HD3	1.61	0.80
16:P:206:GLU:CB	16:P:207:PRO:HD3	2.09	0.80
17:Q:105:TYR:HB2	18:R:234:GLU:CG	2.08	0.80
8:H:106:THR:O	8:H:108:ALA:N	2.12	0.80
17:Q:110:MET:HB3	18:R:218:LYS:CD	2.09	0.80
18:R:163:LEU:O	18:R:164:GLY:O	2.00	0.79
1:A:1313:GLN:C	1:A:1315:ASP:N	2.33	0.79
17:Q:106:LYS:HG2	18:R:218:LYS:HG2	1.64	0.79
10:J:64:PRO:O	10:J:66:GLU:N	2.12	0.79
2:B:623:ARG:NH2	2:B:697:GLU:OE2	2.15	0.79
13:M:43:ASP:O	13:M:45:VAL:N	2.14	0.79
17:Q:110:MET:HE3	18:R:213:ASP:CA	2.12	0.79
17:Q:71:PHE:HA	17:Q:100:VAL:HG22	1.65	0.79
17:Q:110:MET:HE3	18:R:213:ASP:HB3	0.80	0.79
13:M:178:LYS:HG2	20:T:156:VAL:HG12	1.64	0.79
1:A:926:ASN:CG	1:A:931:ARG:CD	2.51	0.79
2:B:216:ALA:HB2	2:B:241:ALA:HB2	1.65	0.79
10:J:17:LYS:HB3	10:J:38:LEU:HD22	1.65	0.78
1:A:1313:GLN:CG	1:A:1333:GLU:HG2	2.13	0.78
17:Q:104:LYS:HZ2	18:R:238:LYS:HD2	1.48	0.78
17:Q:187:ILE:HG12	18:R:211:SER:CB	1.50	0.78
1:A:30:GLU:HA	1:A:33:ARG:HB2	1.65	0.78
18:R:210:PHE:CG	18:R:212:VAL:CG1	2.67	0.78
18:R:195:PRO:CG	18:R:199:LYS:HB2	2.06	0.78
18:R:213:ASP:O	18:R:215:GLU:HB2	1.84	0.78
17:Q:106:LYS:NZ	18:R:219:LEU:HD13	1.99	0.77
20:T:221:GLY:HA2	20:T:236:LYS:HG3	1.67	0.77
18:R:155:LEU:CB	18:R:204:ASN:HD21	1.97	0.77
1:A:921:ARG:O	1:A:1052:ARG:NH1	2.17	0.77
9:I:105:GLU:HG3	9:I:107:ALA:HB3	1.67	0.77
1:A:537:ILE:HB	1:A:645:LEU:HD21	1.67	0.77
18:R:155:LEU:CG	18:R:204:ASN:HD22	1.72	0.77
17:Q:32:LEU:CD1	18:R:203:PHE:CD2	2.67	0.77
1:A:1307:VAL:HG21	1:A:1338:THR:HB	1.64	0.76
17:Q:102:VAL:C	17:Q:104:LYS:N	2.38	0.76
3:C:5:ASN:O	3:C:7:PRO:HD3	1.83	0.76
18:R:162:GLY:C	18:R:164:GLY:N	2.39	0.76
1:A:609:HIS:O	1:A:610:PRO:O	2.04	0.76
2:B:1072:ARG:HH21	2:B:1113:PRO:HG2	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:130:VAL:O	3:C:134:ASN:ND2	2.19	0.76
8:H:65:TYR:O	8:H:66:GLU:HB2	1.86	0.76
17:Q:187:ILE:HG23	18:R:212:VAL:HA	0.76	0.76
9:I:73:SER:O	9:I:80:ARG:NH2	2.17	0.76
18:R:191:PHE:HB3	18:R:202:PHE:CD1	2.20	0.76
1:A:137:PRO:HB3	1:A:237:GLY:HA3	1.68	0.76
2:B:239:MET:HE1	2:B:256:ILE:HD13	1.63	0.76
19:S:50:ASP:HB3	19:S:97:PRO:HG2	1.66	0.76
1:A:1169:VAL:HG21	1:A:1298:LEU:HD22	1.66	0.76
1:A:884:ASN:ND2	6:F:111:PRO:O	2.18	0.76
8:H:85:ALA:O	8:H:144:LEU:HD23	1.85	0.76
16:P:297:LYS:HB2	16:P:298:PRO:HD2	1.68	0.76
17:Q:107:LEU:N	18:R:218:LYS:CE	2.49	0.75
12:L:40:GLY:O	12:L:42:ARG:NH1	2.19	0.75
17:Q:70:LYS:CG	18:R:225:VAL:HG12	2.16	0.75
21:U:173:GLU:OE2	21:U:187:TYR:OH	2.04	0.75
1:A:1206:ARG:HD3	1:A:1265:ASP:HA	1.69	0.75
1:A:1307:VAL:CG2	1:A:1338:THR:CB	2.50	0.75
2:B:754:PRO:HB2	2:B:773:PRO:HG2	1.69	0.75
17:Q:102:VAL:HB	17:Q:105:TYR:CD2	2.21	0.75
1:A:1208:SER:HB2	1:A:1261:ILE:HG12	1.69	0.75
18:R:210:PHE:HB2	18:R:212:VAL:CG1	2.16	0.75
2:B:92:TYR:C	20:T:145:LEU:HD22	2.06	0.74
2:B:93:LEU:C	20:T:145:LEU:HD23	2.07	0.74
2:B:133:ILE:CG2	2:B:139:GLN:HE22	2.00	0.74
2:B:817:GLN:HE21	2:B:916:TYR:HB2	1.52	0.74
1:A:611:ASP:OD2	1:A:617:PRO:HB3	1.87	0.74
21:U:232:GLU:O	21:U:233:LEU:CB	2.28	0.74
1:A:374:SER:OG	1:A:666:ARG:NH2	2.20	0.74
1:A:609:HIS:N	1:A:610:PRO:HD2	2.03	0.74
1:A:700:GLN:OE1	1:A:703:GLN:NE2	2.20	0.74
1:A:1310:HIS:CE1	1:A:1334:TRP:HE3	2.06	0.74
2:B:134:LYS:HD3	2:B:138:GLU:HB2	1.68	0.74
3:C:100:GLU:OE2	3:C:162:ARG:NH2	2.20	0.74
18:R:154:LEU:HD23	18:R:162:GLY:O	1.86	0.74
20:T:47:LYS:HG2	20:T:52:THR:HG23	1.69	0.74
1:A:539:GLN:HE21	2:B:970:HIS:HB2	1.52	0.74
2:B:239:MET:SD	2:B:256:ILE:HD12	2.27	0.74
2:B:894:THR:HA	13:M:52:TRP:CH2	2.23	0.74
2:B:924:ARG:NH1	3:C:62:GLU:OE1	2.19	0.74
3:C:12:THR:H	3:C:21:PHE:HA	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:189:LYS:NZ	22:X:12:DA:OP2	2.20	0.74
1:A:1304:ILE:O	1:A:1307:VAL:HB	1.86	0.74
2:B:806:PHE:O	2:B:1050:ARG:NH1	2.21	0.74
18:R:195:PRO:O	18:R:196:ASP:CB	2.34	0.74
1:A:1310:HIS:CB	21:U:252:LYS:HZ3	1.99	0.74
17:Q:107:LEU:CA	18:R:218:LYS:CE	2.61	0.74
1:A:958:ARG:NH1	1:A:962:ASP:OD1	2.21	0.74
17:Q:106:LYS:C	18:R:218:LYS:HE3	2.08	0.74
20:T:231:ASN:HB2	23:Y:68:DC:H5"	1.68	0.74
17:Q:70:LYS:HG3	18:R:225:VAL:C	2.05	0.74
1:A:631:GLU:HG3	1:A:636:ILE:HD11	1.70	0.73
12:L:18:ILE:CD1	12:L:47:LYS:CD	2.66	0.73
17:Q:106:LYS:C	18:R:218:LYS:CE	2.57	0.73
1:A:922:PHE:HZ	1:A:952:LEU:HG	1.53	0.73
17:Q:110:MET:HE1	18:R:213:ASP:CA	2.16	0.73
1:A:611:ASP:O	1:A:612:ASP:HB2	1.87	0.73
13:M:179:GLU:N	20:T:154:LYS:HG2	2.03	0.73
2:B:132:VAL:HG23	2:B:141:GLN:HG2	1.71	0.73
3:C:200:PRO:HG3	3:C:217:GLN:CB	2.19	0.73
1:A:1304:ILE:HD12	1:A:1307:VAL:HG12	1.69	0.73
3:C:101:PHE:HB2	3:C:163:ALA:HB3	1.71	0.73
20:T:139:VAL:O	20:T:140:ARG:CB	2.37	0.73
2:B:93:LEU:N	20:T:145:LEU:CD2	2.51	0.73
2:B:759:VAL:HG12	2:B:999:ALA:HB2	1.71	0.73
3:C:200:PRO:HG2	3:C:217:GLN:OE1	1.89	0.73
8:H:110:THR:O	8:H:111:ARG:CB	2.37	0.73
3:C:200:PRO:CG	3:C:217:GLN:OE1	2.36	0.73
1:A:831:LEU:HB2	2:B:715:ASP:HB2	1.70	0.72
2:B:133:ILE:HG23	2:B:139:GLN:NE2	2.03	0.72
18:R:158:HIS:CE1	18:R:206:LYS:CE	2.71	0.72
2:B:1119:CYS:HB2	2:B:1137:CYS:SG	2.28	0.72
8:H:65:TYR:CE1	8:H:81:ARG:NH2	2.52	0.72
1:A:1310:HIS:CB	21:U:252:LYS:CG	2.65	0.72
2:B:100:GLU:OE2	2:B:116:ARG:NH1	2.22	0.72
12:L:37:ARG:O	12:L:39:CYS:N	2.22	0.72
17:Q:144:LEU:O	17:Q:153:ARG:N	2.23	0.72
19:S:126:ILE:HB	19:S:138:PHE:HB2	1.70	0.72
20:T:179:ASP:C	20:T:181:GLN:N	2.41	0.72
2:B:92:TYR:HB3	20:T:145:LEU:HD13	1.71	0.72
1:A:257:PRO:HD2	1:A:260:VAL:HB	1.71	0.72
2:B:57:ARG:NH1	2:B:60:GLU:OE1	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:105:GLU:HG3	9:I:107:ALA:CB	2.19	0.72
14:N:26:ARG:NE	14:N:36:GLU:OE1	2.21	0.72
17:Q:32:LEU:HD13	18:R:203:PHE:CE2	2.24	0.72
1:A:616:GLY:O	1:A:619:LYS:CB	2.30	0.72
2:B:252:ILE:HG13	2:B:255:ARG:HD2	1.70	0.72
21:U:218:ASP:HB2	21:U:222:ARG:HH21	1.54	0.72
2:B:92:TYR:CB	20:T:145:LEU:HB2	2.19	0.72
8:H:111:ARG:NE	8:H:126:GLN:OE1	2.21	0.72
9:I:94:ALA:HA	9:I:114:CYS:HA	1.72	0.72
17:Q:70:LYS:HG3	18:R:225:VAL:HG12	1.71	0.72
2:B:109:MET:HE1	2:B:174:LEU:HB3	1.72	0.72
1:A:1163:HIS:HA	1:A:1300:GLY:HA3	1.70	0.72
2:B:205:VAL:O	2:B:371:ARG:NH1	2.23	0.72
2:B:878:ASP:O	2:B:879:GLU:O	2.07	0.72
14:N:311:GLU:HB3	16:P:251:LEU:HD23	1.72	0.72
2:B:92:TYR:HB3	20:T:145:LEU:CD1	2.19	0.71
6:F:56:TYR:O	6:F:108:ARG:NH2	2.22	0.71
16:P:209:THR:O	16:P:210:THR:HB	1.89	0.71
1:A:922:PHE:HE2	1:A:952:LEU:HD23	1.27	0.71
1:A:1211:LEU:HD11	1:A:1258:ARG:HB2	1.71	0.71
1:A:1310:HIS:HB2	21:U:252:LYS:HZ3	1.56	0.71
12:L:17:TYR:O	12:L:26:ASN:N	2.20	0.71
1:A:734:ARG:NH2	9:I:104:ALA:O	2.23	0.71
1:A:1310:HIS:H	21:U:252:LYS:HD2	0.89	0.71
2:B:1129:ASN:HA	2:B:1135:TYR:HA	1.71	0.71
1:A:608:THR:CB	1:A:610:PRO:HD2	2.19	0.71
1:A:790:GLN:NE2	1:A:820:ARG:O	2.22	0.71
1:A:1303:GLN:HE22	1:A:1342:SER:HB3	1.55	0.71
1:A:546:ARG:HG3	1:A:639:ILE:HD11	1.72	0.71
1:A:1457:ASN:OD1	1:A:1462:GLN:NE2	2.22	0.71
9:I:99:SER:OG	9:I:105:GLU:CB	2.37	0.71
16:P:209:THR:CA	16:P:223:GLY:HA3	2.17	0.71
1:A:790:GLN:HA	1:A:822:PHE:HA	1.71	0.71
7:G:110:ARG:NH2	7:G:118:GLU:OE2	2.24	0.71
1:A:582:PRO:HD2	8:H:47:ILE:HD12	1.72	0.71
2:B:743:ARG:O	2:B:922:ARG:NH1	2.24	0.71
2:B:849:ASP:OD2	12:L:29:LYS:NZ	2.23	0.71
14:N:326:GLN:O	15:O:92:LYS:NZ	2.22	0.71
21:U:251:ALA:O	21:U:252:LYS:HB2	1.90	0.71
21:U:286:THR:HG21	21:U:299:LYS:HB3	1.72	0.71
2:B:803:ARG:NH1	10:J:8:PHE:O	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1067:ILE:HG22	2:B:1068:GLN:H	1.55	0.70
17:Q:67:LYS:HG3	17:Q:72:ILE:HD11	1.73	0.70
20:T:176:ALA:O	20:T:208:GLN:NE2	2.24	0.70
18:R:154:LEU:CD2	18:R:162:GLY:O	2.39	0.70
15:O:79:VAL:HG21	15:O:93:VAL:HG12	1.73	0.70
13:M:106:THR:C	13:M:108:SER:N	2.44	0.70
16:P:271:GLU:OE1	16:P:271:GLU:N	2.23	0.70
3:C:47:ILE:HA	3:C:165:ALA:HA	1.73	0.70
17:Q:102:VAL:CB	17:Q:105:TYR:HD2	2.04	0.70
2:B:216:ALA:N	2:B:239:MET:O	2.25	0.70
13:M:297:PRO:HB3	13:M:310:VAL:HG21	1.73	0.70
1:A:121:SER:HA	1:A:126:ILE:HG21	1.73	0.70
2:B:983:GLU:OE2	2:B:1047:TYR:N	2.19	0.70
9:I:105:GLU:CG	9:I:107:ALA:HB3	2.22	0.70
3:C:10:ARG:NH2	3:C:24:GLU:OE2	2.23	0.70
14:N:353:LEU:HB2	14:N:370:ALA:HB3	1.74	0.70
1:A:266:MET:O	1:A:267:GLN:HB2	1.90	0.69
1:A:1309:MET:SD	21:U:252:LYS:HD3	2.32	0.69
13:M:286:ARG:HG3	13:M:316:LEU:HG	1.74	0.69
13:M:34:CYS:N	13:M:39:LEU:CB	2.22	0.69
18:R:90:GLN:NE2	18:R:172:GLU:OE2	2.25	0.69
17:Q:25:PHE:HA	18:R:215:GLU:OE1	1.93	0.69
21:U:252:LYS:HE3	21:U:252:LYS:CA	2.18	0.69
1:A:1451:MET:HE1	1:A:1460:LEU:HD22	1.74	0.69
2:B:777:ASN:O	10:J:47:ARG:NH1	2.25	0.69
5:E:80:PRO:HA	5:E:107:GLN:HB2	1.73	0.69
8:H:64:LEU:C	8:H:66:GLU:H	1.94	0.69
8:H:113:SER:OG	8:H:126:GLN:NE2	2.26	0.69
14:N:344:ARG:NH2	23:Y:78:DT:OP1	2.24	0.69
1:A:1310:HIS:HB3	21:U:252:LYS:CE	2.23	0.69
1:A:1310:HIS:HB2	21:U:252:LYS:NZ	2.06	0.69
2:B:427:LYS:HE3	20:T:164:GLU:HG2	1.74	0.69
3:C:6:GLN:HG2	3:C:25:ASN:ND2	2.06	0.69
8:H:17:PRO:HG3	8:H:27:ARG:H	1.58	0.69
16:P:209:THR:HG21	16:P:224:ALA:H	1.38	0.69
17:Q:106:LYS:CG	18:R:218:LYS:HE2	2.22	0.69
17:Q:108:ASP:OD2	18:R:234:GLU:OE2	2.10	0.69
19:S:157:ALA:HA	19:S:161:GLU:HB2	1.75	0.69
20:T:145:LEU:HD11	20:T:148:VAL:HG22	1.75	0.69
1:A:529:GLN:HE22	1:A:1097:GLU:HB3	1.55	0.69
16:P:307:SER:OG	23:Y:83:DA:OP1	2.09	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:158:HIS:CE1	18:R:206:LYS:HZ3	2.11	0.69
2:B:634:LEU:HD23	2:B:661:VAL:HA	1.75	0.69
2:B:133:ILE:CG2	2:B:139:GLN:NE2	2.55	0.68
3:C:136:ASP:O	3:C:138:ASP:N	2.22	0.68
17:Q:113:ARG:CD	18:R:217:GLN:O	2.41	0.68
20:T:179:ASP:O	20:T:181:GLN:N	2.26	0.68
1:A:475:ARG:NH2	11:K:68:GLU:OE2	2.26	0.68
1:A:551:ARG:CD	1:A:625:ASP:OD2	2.41	0.68
2:B:92:TYR:HB2	20:T:145:LEU:HD22	1.71	0.68
2:B:245:GLN:HE21	2:B:252:ILE:HD12	1.58	0.68
5:E:15:LYS:NZ	5:E:33:LEU:O	2.27	0.68
13:M:38:GLY:O	13:M:39:LEU:HB2	1.93	0.68
16:P:209:THR:HG21	16:P:224:ALA:CA	2.23	0.68
2:B:36:GLU:OE1	2:B:652:SER:OG	2.11	0.68
13:M:34:CYS:C	13:M:39:LEU:HB2	2.12	0.68
17:Q:32:LEU:CD1	18:R:203:PHE:CE2	2.76	0.68
2:B:360:LYS:HG3	2:B:553:LEU:HD23	1.74	0.68
6:F:47:ALA:HB1	6:F:51:ARG:HE	1.58	0.68
10:J:3:ILE:HG21	10:J:18:TRP:HB2	1.74	0.68
20:T:8:ASP:HB3	20:T:105:SER:HA	1.75	0.68
1:A:1287:CYS:HA	2:B:250:SER:CB	2.23	0.68
12:L:22:CYS:HB3	12:L:39:CYS:HB2	1.75	0.68
14:N:375:GLU:OE1	15:O:59:ARG:NH2	2.26	0.68
20:T:177:ARG:O	20:T:179:ASP:N	2.26	0.68
2:B:93:LEU:CA	20:T:145:LEU:HD23	2.23	0.68
2:B:201:ALA:O	2:B:222:ARG:NH2	2.26	0.68
1:A:67:ARG:HH22	13:M:48:VAL:HG23	1.59	0.68
1:A:71:CYS:H	1:A:75:ALA:HA	1.58	0.68
1:A:601:ASN:HD21	1:A:632:ASN:H	1.42	0.68
2:B:894:THR:HA	13:M:52:TRP:HH2	1.56	0.68
17:Q:110:MET:CG	18:R:218:LYS:HD2	2.24	0.68
21:U:250:MET:O	21:U:251:ALA:CB	2.41	0.68
1:A:844:ARG:NH2	2:B:500:GLN:O	2.26	0.68
3:C:253:LYS:NZ	11:K:102:GLU:OE1	2.27	0.68
13:M:134:ILE:HG12	13:M:171:GLU:HG3	1.76	0.68
16:P:163:PRO:HA	16:P:262:CYS:HB3	1.75	0.68
1:A:420:ILE:N	1:A:445:LYS:O	2.24	0.68
11:K:44:ASN:OD1	11:K:45:ILE:N	2.27	0.68
2:B:830:GLU:OE2	2:B:870:THR:OG1	2.11	0.68
14:N:353:LEU:N	14:N:370:ALA:O	2.17	0.68
17:Q:109:HIS:O	18:R:221:ARG:NE	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:213:ASP:C	18:R:215:GLU:N	2.45	0.68
1:A:653:VAL:HG23	1:A:669:TYR:CE2	2.27	0.67
2:B:87:LYS:HB3	2:B:129:THR:HB	1.76	0.67
2:B:1106:ARG:HA	2:B:1110:ALA:HB3	1.77	0.67
5:E:170:LEU:HD23	5:E:208:LEU:HB2	1.76	0.67
18:R:158:HIS:CE1	18:R:206:LYS:NZ	2.61	0.67
21:U:206:LEU:HD11	21:U:228:MET:HB3	1.76	0.67
1:A:826:SER:H	1:A:829:ALA:HB3	1.59	0.67
17:Q:105:TYR:CD1	17:Q:109:HIS:CD2	2.83	0.67
17:Q:187:ILE:HD13	18:R:211:SER:HB2	1.68	0.67
18:R:127:ASN:ND2	18:R:140:LYS:HD2	2.08	0.67
1:A:22:GLN:HB3	2:B:1170:ARG:HG3	1.77	0.67
1:A:620:HIS:O	1:A:621:ILE:HG12	1.95	0.67
3:C:53:ASP:HB3	3:C:160:ARG:HB3	1.76	0.67
7:G:93:ASN:OD1	7:G:94:LYS:N	2.26	0.67
7:G:99:THR:HG21	7:G:143:ILE:HD11	1.76	0.67
7:G:153:ASP:O	7:G:155:ASN:N	2.27	0.67
1:A:551:ARG:HD3	1:A:625:ASP:CG	2.15	0.67
1:A:552:ASP:HB3	8:H:24:ARG:HD3	1.76	0.67
1:A:65:ILE:HD12	1:A:263:ALA:HB3	1.76	0.67
1:A:1310:HIS:H	21:U:252:LYS:CE	2.07	0.67
2:B:483:ARG:NH2	2:B:527:ALA:O	2.27	0.67
5:E:64:HIS:C	5:E:65:ASN:O	2.32	0.67
18:R:210:PHE:CB	18:R:212:VAL:CG1	2.73	0.67
1:A:874:LYS:HG3	1:A:880:ARG:HD2	1.77	0.67
1:A:1314:THR:OG1	1:A:1332:GLN:NE2	2.28	0.67
8:H:85:ALA:HB1	8:H:144:LEU:HD22	1.77	0.67
19:S:49:ARG:NH1	19:S:96:GLN:O	2.25	0.67
19:S:166:ARG:HH11	19:S:166:ARG:HG3	1.59	0.67
1:A:1196:TYR:CD2	1:A:1246:ILE:HD11	2.29	0.67
18:R:220:TRP:O	18:R:223:VAL:CG2	2.42	0.67
21:U:180:ILE:HG21	21:U:187:TYR:HB2	1.76	0.67
1:A:43:TYR:HD1	1:A:45:GLU:HG2	1.59	0.67
2:B:63:PRO:HB3	2:B:408:PHE:HZ	1.59	0.67
2:B:133:ILE:HG22	2:B:139:GLN:HE22	1.60	0.67
18:R:89:HIS:CE1	18:R:139:PHE:HE2	2.13	0.67
1:A:1273:GLU:O	1:A:1274:GLU:C	2.32	0.67
8:H:85:ALA:HB3	8:H:144:LEU:HD21	1.76	0.67
17:Q:109:HIS:CB	18:R:221:ARG:HG2	2.13	0.67
8:H:75:TYR:O	8:H:77:PRO:N	2.27	0.67
17:Q:187:ILE:HG12	18:R:211:SER:OG	1.85	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:190:LEU:HD12	18:R:205:ASP:CB	2.22	0.67
1:A:418:TYR:O	1:A:447:GLU:N	2.28	0.66
1:A:885:GLN:NE2	5:E:168:ASN:OD1	2.22	0.66
2:B:501:LEU:HD11	2:B:505:LEU:HD22	1.77	0.66
10:J:21:TYR:HB2	10:J:38:LEU:HD11	1.77	0.66
12:L:25:GLU:CB	12:L:27:GLU:HG2	2.25	0.66
2:B:892:CYS:HA	13:M:52:TRP:HE1	1.58	0.66
1:A:642:LYS:HD3	21:U:284:PRO:HD3	1.77	0.66
1:A:1323:THR:HG23	1:A:1325:ASP:H	1.59	0.66
2:B:842:HIS:HE1	13:M:27:TYR:HB3	1.61	0.66
17:Q:70:LYS:CG	18:R:225:VAL:C	2.63	0.66
3:C:50:VAL:HB	12:L:55:PHE:HB2	1.77	0.66
8:H:85:ALA:CB	8:H:144:LEU:HD22	2.26	0.66
14:N:46:TRP:HZ2	15:O:11:LEU:HD12	1.60	0.66
12:L:34:ILE:HG13	12:L:42:ARG:HD2	1.78	0.66
16:P:179:ASP:OD1	16:P:181:LYS:NZ	2.29	0.66
16:P:293:TYR:HD2	16:P:302:LEU:HD13	1.61	0.66
1:A:619:LYS:O	1:A:620:HIS:HB2	1.94	0.66
3:C:67:ARG:NH1	3:C:150:ILE:O	2.28	0.66
13:M:107:MET:HE3	13:M:107:MET:N	2.10	0.66
1:A:1272:GLU:O	1:A:1274:GLU:N	2.28	0.66
2:B:848:LEU:HD21	2:B:868:GLY:HA3	1.77	0.66
3:C:99:VAL:HG13	3:C:124:SER:HB2	1.77	0.66
10:J:64:PRO:C	10:J:66:GLU:H	1.98	0.66
1:A:426:ARG:CB	13:M:40:VAL:HG21	1.94	0.66
1:A:782:SER:O	1:A:787:VAL:N	2.29	0.66
2:B:1029:TYR:OH	3:C:185:GLU:OE1	2.13	0.66
18:R:191:PHE:CB	18:R:202:PHE:CD1	2.79	0.66
1:A:361:PHE:H	2:B:1063:ALA:HA	1.61	0.66
13:M:124:MET:HA	13:M:127:ARG:NH2	2.11	0.66
3:C:200:PRO:CG	3:C:217:GLN:CB	2.74	0.65
3:C:214:ASP:OD2	3:C:216:SER:OG	2.12	0.65
10:J:63:ALA:N	10:J:64:PRO:CD	2.59	0.65
18:R:140:LYS:NZ	20:T:238:GLU:OE2	2.30	0.65
18:R:191:PHE:CB	18:R:202:PHE:CE1	2.79	0.65
1:A:923:ASP:HB3	1:A:925:THR:OG1	1.96	0.65
2:B:92:TYR:CB	20:T:145:LEU:HD13	2.27	0.65
2:B:935:PHE:HE2	2:B:945:CYS:HB2	1.62	0.65
20:T:164:GLU:OE2	20:T:167:ARG:NH2	2.29	0.65
1:A:784:VAL:HG23	1:A:785:ILE:HG13	1.78	0.65
1:A:1172:ASN:O	1:A:1215:GLU:N	2.19	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:5:ASN:C	3:C:7:PRO:CD	2.60	0.65
12:L:18:ILE:CD1	12:L:47:LYS:HE3	2.19	0.65
22:X:17:DA:H2"	22:X:18:DG:C8	2.31	0.65
1:A:275:ASP:HB2	1:A:342:ARG:NH2	2.10	0.65
1:A:551:ARG:HD3	1:A:625:ASP:OD2	1.96	0.65
1:A:434:LYS:HB2	1:A:437:ASP:HB3	1.79	0.65
1:A:1117:VAL:O	1:A:1118:THR:C	2.34	0.65
1:A:1304:ILE:CD1	1:A:1307:VAL:HG11	2.22	0.65
1:A:1290:SER:HB3	2:B:250:SER:O	1.97	0.65
17:Q:23:ARG:NH2	18:R:206:LYS:CB	2.60	0.65
2:B:65:ILE:HG21	2:B:412:LEU:HD11	1.76	0.65
2:B:102:ASP:O	13:M:217:ARG:NE	2.27	0.65
16:P:209:THR:CG2	16:P:224:ALA:CA	2.73	0.65
1:A:1146:GLN:O	1:A:1150:ASP:N	2.27	0.64
1:A:1147:SER:OG	1:A:1351:ASP:OD2	2.15	0.64
2:B:93:LEU:HD12	2:B:123:PRO:O	1.98	0.64
16:P:209:THR:HG22	16:P:223:GLY:HA3	1.71	0.64
1:A:113:PHE:CE1	18:R:229:ASP:N	2.62	0.64
1:A:924:TYR:HD1	1:A:949:GLN:HE22	1.15	0.64
7:G:91:GLN:HB2	7:G:98:PHE:HD2	1.63	0.64
8:H:74:GLU:C	8:H:76:ASN:N	2.40	0.64
11:K:77:THR:OG1	11:K:81:TYR:O	2.14	0.64
1:A:370:ASP:HB2	1:A:483:ARG:HB3	1.80	0.64
2:B:499:ARG:HB3	2:B:499:ARG:CZ	2.27	0.64
2:B:714:PRO:HD2	2:B:1001:PRO:HB3	1.77	0.64
1:A:1253:GLU:HG2	1:A:1254:LYS:HG2	1.79	0.64
1:A:1310:HIS:HE1	1:A:1334:TRP:HA	1.61	0.64
3:C:13:GLU:O	3:C:20:LYS:N	2.30	0.64
17:Q:106:LYS:HG2	18:R:218:LYS:CE	2.27	0.64
19:S:126:ILE:N	19:S:138:PHE:O	2.23	0.64
1:A:1244:ASN:HB3	1:A:1260:ARG:HB2	1.79	0.64
17:Q:105:TYR:CD1	17:Q:109:HIS:NE2	2.66	0.64
3:C:258:ASP:OD2	11:K:18:LYS:NZ	2.31	0.64
9:I:103:ARG:C	9:I:105:GLU:H	2.00	0.64
12:L:15:MET:C	12:L:16:ILE:HG23	2.15	0.64
16:P:160:GLY:C	16:P:161:ILE:HG12	2.17	0.64
11:K:29:ASN:ND2	11:K:78:THR:O	2.30	0.64
17:Q:110:MET:HE1	18:R:213:ASP:HA	1.79	0.64
18:R:161:ARG:NE	18:R:203:PHE:CE1	2.60	0.64
20:T:158:ASN:HB3	20:T:161:TYR:HB3	1.79	0.64
2:B:646:ARG:HD3	2:B:651:TYR:N	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:874:PRO:O	2:B:876:ASN:N	2.27	0.64
13:M:106:THR:HB	13:M:109:SER:OG	1.96	0.64
20:T:179:ASP:CG	20:T:182:HIS:HB3	2.18	0.64
1:A:1250:ASP:HA	1:A:1255:LEU:HD21	1.78	0.64
1:A:1288:ILE:O	1:A:1292:MET:N	2.27	0.64
8:H:10:PHE:N	8:H:56:PHE:O	2.28	0.64
1:A:629:VAL:HG13	1:A:636:ILE:HB	1.81	0.63
1:A:1310:HIS:HB3	21:U:252:LYS:CD	2.28	0.63
1:A:1036:ASN:HB2	5:E:202:ARG:HB3	1.78	0.63
2:B:1107:LEU:O	2:B:1111:SER:OG	2.15	0.63
16:P:166:GLN:HG3	23:Y:81:DA:H5"	1.80	0.63
17:Q:17:LEU:HD13	17:Q:194:THR:HB	1.80	0.63
2:B:829:PHE:HE1	2:B:869:LYS:HD3	1.63	0.63
9:I:103:ARG:C	9:I:105:GLU:N	2.51	0.63
14:N:368:SER:N	15:O:54:ASN:O	2.25	0.63
2:B:692:THR:HB	9:I:76:PRO:HB2	1.79	0.63
2:B:840:MET:O	2:B:842:HIS:N	2.31	0.63
12:L:26:ASN:HA	12:L:37:ARG:HH12	1.63	0.63
18:R:155:LEU:CB	18:R:204:ASN:ND2	2.59	0.63
1:A:514:GLU:OE2	2:B:1101:GLN:HB2	1.99	0.63
1:A:622:SER:C	1:A:624:GLY:N	2.51	0.63
14:N:333:ASN:HB3	14:N:359:ASN:O	1.99	0.63
1:A:619:LYS:O	1:A:620:HIS:CB	2.46	0.63
5:E:27:LEU:HD12	5:E:64:HIS:CD2	2.33	0.63
11:K:18:LYS:O	11:K:36:ASN:N	2.23	0.63
17:Q:102:VAL:HB	17:Q:105:TYR:HD2	1.62	0.63
1:A:485:ASN:HB3	1:A:488:VAL:HG23	1.79	0.63
1:A:497:ASP:HB2	2:B:942:LYS:HE3	1.80	0.63
1:A:1313:GLN:HG2	1:A:1333:GLU:CG	2.26	0.63
17:Q:25:PHE:HD2	18:R:215:GLU:OE2	1.80	0.63
17:Q:109:HIS:HB3	18:R:221:ARG:CD	2.28	0.63
2:B:765:GLU:O	2:B:768:ARG:NH1	2.31	0.62
2:B:1087:GLY:N	2:B:1090:GLU:OE1	2.28	0.62
13:M:297:PRO:HA	13:M:310:VAL:HG11	1.82	0.62
1:A:191:ILE:HD12	1:A:216:LEU:HD11	1.81	0.62
2:B:779:ILE:HA	2:B:1045:PRO:HA	1.80	0.62
2:B:956:PHE:O	2:B:1029:TYR:N	2.23	0.62
9:I:92:LYS:NZ	9:I:93:GLU:OE2	2.32	0.62
10:J:40:LEU:O	10:J:46:ARG:NE	2.32	0.62
2:B:513:GLU:O	2:B:525:ASN:ND2	2.32	0.62
3:C:47:ILE:HG21	3:C:68:LEU:HD23	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:129:PRO:HG2	3:C:134:ASN:HD22	1.63	0.62
8:H:84:ARG:O	8:H:86:ASP:N	2.31	0.62
17:Q:113:ARG:HB2	18:R:221:ARG:HD2	1.81	0.62
1:A:939:VAL:HA	1:A:942:VAL:HG22	1.81	0.62
1:A:1208:SER:O	1:A:1260:ARG:NH1	2.31	0.62
8:H:85:ALA:O	8:H:144:LEU:HD22	1.99	0.62
9:I:58:ILE:O	9:I:59:THR:CB	2.47	0.62
1:A:43:TYR:CD1	1:A:45:GLU:HG2	2.34	0.62
1:A:1290:SER:CB	2:B:250:SER:O	2.48	0.62
13:M:173:VAL:HB	13:M:175:ARG:HH12	1.64	0.62
17:Q:113:ARG:HE	18:R:217:GLN:HB3	1.64	0.62
1:A:1080:ILE:HD13	6:F:54:THR:HG21	1.82	0.62
3:C:35:ARG:HA	3:C:38:PHE:CD2	2.35	0.62
2:B:322:GLY:HA3	2:B:335:ARG:HB3	1.81	0.62
2:B:838:GLN:OE1	2:B:886:ARG:NH1	2.33	0.62
1:A:948:ILE:HG13	1:A:1007:ILE:HD11	1.81	0.62
2:B:831:LYS:NZ	2:B:845:TYR:O	2.27	0.62
9:I:95:VAL:N	9:I:113:VAL:O	2.24	0.62
2:B:808:SER:OG	2:B:1050:ARG:NH1	2.33	0.62
3:C:56:SER:OG	3:C:158:GLU:N	2.33	0.62
17:Q:22:ILE:HG22	17:Q:34:LEU:HD13	1.81	0.62
17:Q:102:VAL:O	17:Q:105:TYR:N	2.33	0.62
2:B:226:GLU:OE1	2:B:227:ASN:ND2	2.33	0.62
2:B:801:VAL:HA	2:B:805:PHE:HB3	1.81	0.62
3:C:110:ASP:HA	3:C:155:LYS:HD2	1.82	0.62
5:E:107:GLN:HG2	5:E:132:GLN:NE2	2.15	0.62
6:F:78:PRO:HD3	7:G:16:ARG:HA	1.82	0.62
14:N:34:VAL:HG11	15:O:28:ILE:HG22	1.82	0.62
18:R:190:LEU:CD1	18:R:205:ASP:CB	2.72	0.62
1:A:934:LEU:O	1:A:936:GLU:N	2.30	0.61
12:L:16:ILE:HG13	12:L:28:ILE:H	1.64	0.61
17:Q:110:MET:CA	18:R:218:LYS:HG3	2.29	0.61
20:T:31:TRP:HD1	20:T:62:LEU:HD21	1.64	0.61
1:A:1204:VAL:HA	1:A:1207:ILE:HG23	1.81	0.61
2:B:194:LEU:HD11	2:B:466:VAL:HG12	1.81	0.61
5:E:149:VAL:HB	5:E:192:LYS:HB3	1.80	0.61
8:H:9:ILE:O	8:H:33:GLU:HG2	1.99	0.61
1:A:931:ARG:O	1:A:933:THR:N	2.32	0.61
1:A:1272:GLU:C	1:A:1274:GLU:H	2.03	0.61
20:T:177:ARG:NH2	20:T:212:TYR:HB2	2.15	0.61
1:A:621:ILE:O	1:A:621:ILE:HG22	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:LYS:O	2:B:129:THR:N	2.23	0.61
3:C:1:MET:HG3	3:C:2:PRO:HD2	1.82	0.61
6:F:100:ARG:HB2	6:F:120:VAL:HG12	1.83	0.61
8:H:65:TYR:CE1	8:H:81:ARG:NE	2.67	0.61
8:H:96:VAL:HB	8:H:136:GLU:HA	1.83	0.61
16:P:297:LYS:HB2	16:P:298:PRO:CD	2.21	0.61
1:A:208:ASP:OD2	1:A:212:LYS:NZ	2.33	0.61
2:B:788:TYR:HB2	2:B:795:ILE:HD11	1.81	0.61
8:H:85:ALA:HB3	8:H:144:LEU:CD2	2.31	0.61
9:I:87:GLN:HE21	9:I:121:HIS:HB3	1.65	0.61
12:L:18:ILE:O	12:L:45:TYR:HB3	2.00	0.61
15:O:59:ARG:O	15:O:80:GLU:N	2.32	0.61
1:A:85:PHE:CD1	1:A:257:PRO:HD3	2.36	0.61
2:B:50:PHE:HA	2:B:54:SER:HB2	1.83	0.61
7:G:58:VAL:HB	7:G:67:LEU:HB3	1.82	0.61
16:P:192:TYR:HB2	16:P:200:VAL:HG22	1.83	0.61
1:A:72:GLN:HE22	1:A:84:HIS:CD2	2.18	0.61
1:A:784:VAL:HA	1:A:827:TYR:HB2	1.83	0.61
1:A:922:PHE:HZ	1:A:952:LEU:CG	2.13	0.61
1:A:1290:SER:OG	2:B:250:SER:O	2.19	0.61
5:E:104:ILE:O	5:E:129:GLN:NE2	2.33	0.61
13:M:34:CYS:O	13:M:39:LEU:CB	2.44	0.61
18:R:142:LYS:HE2	18:R:144:ASN:HB3	1.83	0.61
20:T:20:LEU:O	20:T:114:ALA:N	2.34	0.61
1:A:275:ASP:HA	1:A:278:HIS:ND1	2.16	0.61
1:A:926:ASN:HD21	1:A:931:ARG:HD2	1.62	0.61
5:E:63:ALA:O	5:E:64:HIS:CG	2.54	0.61
13:M:40:VAL:C	13:M:42:GLY:H	2.04	0.61
21:U:251:ALA:O	21:U:252:LYS:CB	2.49	0.61
1:A:693:ILE:HG13	2:B:1023:ARG:HE	1.63	0.61
1:A:1347:LEU:HB3	5:E:137:ILE:HG12	1.82	0.61
2:B:67:LEU:HD22	2:B:419:ALA:HB1	1.83	0.61
2:B:405:ARG:O	2:B:409:LYS:HG3	2.00	0.61
7:G:11:ILE:O	7:G:68:TYR:N	2.25	0.61
1:A:18:ILE:HG21	2:B:1171:MET:HG3	1.83	0.61
1:A:622:SER:C	1:A:624:GLY:H	2.04	0.61
2:B:713:PHE:HB3	2:B:716:HIS:ND1	2.15	0.61
5:E:48:PRO:HD2	5:E:52:ARG:HD2	1.82	0.61
8:H:105:SER:O	8:H:106:THR:CB	2.48	0.61
17:Q:106:LYS:HZ3	18:R:219:LEU:HD13	1.64	0.61
1:A:426:ARG:CG	13:M:40:VAL:HG11	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:ASP:CB	1:A:617:PRO:HG3	2.29	0.60
1:A:1248:ASN:ND2	1:A:1254:LYS:O	2.28	0.60
2:B:37:LYS:HE2	2:B:653:TRP:CD1	2.36	0.60
14:N:341:LYS:HB3	14:N:352:HIS:HB2	1.80	0.60
16:P:161:ILE:O	16:P:161:ILE:HG22	1.99	0.60
17:Q:25:PHE:HE2	18:R:215:GLU:HG3	1.61	0.60
1:A:935:GLN:HA	1:A:1001:PRO:HA	1.81	0.60
2:B:225:LEU:HD13	2:B:228:SER:HB2	1.83	0.60
8:H:31:GLU:HA	8:H:38:ASP:HA	1.82	0.60
8:H:103:GLU:HG2	8:H:109:ALA:HB2	1.83	0.60
12:L:15:MET:HG3	12:L:47:LYS:HB2	1.83	0.60
18:R:127:ASN:HD21	18:R:140:LYS:HE2	1.64	0.60
23:Y:59:DG:H2"	23:Y:60:DA:C8	2.36	0.60
1:A:47:THR:O	1:A:48:GLU:CB	2.48	0.60
1:A:1306:LYS:O	1:A:1307:VAL:HG12	2.00	0.60
2:B:91:ILE:HG22	20:T:142:SER:OG	2.02	0.60
4:D:103:LEU:HD22	7:G:144:ARG:HH12	1.64	0.60
8:H:64:LEU:C	8:H:66:GLU:N	2.55	0.60
17:Q:108:ASP:HB2	18:R:234:GLU:OE2	1.99	0.60
1:A:620:HIS:O	1:A:621:ILE:CB	2.47	0.60
1:A:628:VAL:HA	1:A:638:GLY:HA3	1.83	0.60
2:B:568:PHE:O	2:B:614:ILE:N	2.34	0.60
2:B:600:GLU:O	2:B:620:ARG:NH2	2.30	0.60
6:F:96:GLU:O	6:F:100:ARG:N	2.34	0.60
9:I:22:ASN:OD1	9:I:41:ASN:ND2	2.35	0.60
14:N:308:GLN:NE2	14:N:310:GLU:O	2.28	0.60
15:O:86:GLU:HG3	15:O:88:ILE:HD11	1.83	0.60
20:T:224:ASN:HB3	20:T:226:LYS:HG2	1.82	0.60
20:T:228:ILE:HD12	20:T:230:LYS:HD3	1.83	0.60
1:A:1143:LEU:HB3	1:A:1147:SER:HB2	1.83	0.60
16:P:209:THR:HG22	16:P:223:GLY:N	2.08	0.60
1:A:1112:VAL:HA	21:U:254:GLY:HA3	1.83	0.60
12:L:22:CYS:SG	12:L:24:THR:OG1	2.56	0.60
20:T:20:LEU:N	20:T:112:GLN:O	2.28	0.60
2:B:655:ASP:O	2:B:659:SER:N	2.35	0.60
2:B:737:ILE:HD11	2:B:743:ARG:HG3	1.83	0.60
4:D:108:ALA:N	4:D:128:GLN:OE1	2.32	0.60
8:H:98:ARG:HD3	8:H:115:TYR:HD2	1.66	0.60
19:S:47:LEU:HD22	20:T:7:LEU:HD22	1.84	0.60
1:A:47:THR:O	1:A:48:GLU:HB2	2.02	0.60
2:B:117:ASN:HA	2:B:189:GLY:HA3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:162:VAL:O	16:P:162:VAL:HG23	2.02	0.60
18:R:155:LEU:HG	18:R:204:ASN:HD22	0.77	0.60
4:D:26:PHE:HZ	7:G:42:TYR:HA	1.66	0.60
11:K:20:THR:N	11:K:34:THR:O	2.28	0.60
1:A:1212:LEU:HD23	1:A:1259:ILE:HD11	1.83	0.59
14:N:318:ASP:OD1	16:P:239:ARG:HD2	2.01	0.59
17:Q:70:LYS:HB2	18:R:225:VAL:HG12	1.83	0.59
20:T:155:PRO:O	20:T:157:ALA:N	2.27	0.59
1:A:1394:ASN:HB3	1:A:1397:HIS:ND1	2.17	0.59
3:C:146:ASP:O	3:C:148:ILE:N	2.36	0.59
21:U:256:THR:O	21:U:257:GLN:O	2.20	0.59
1:A:593:SER:HB3	1:A:634:GLU:HA	1.84	0.59
2:B:56:GLN:O	2:B:60:GLU:N	2.30	0.59
3:C:106:ARG:NE	3:C:108:ASN:OD1	2.35	0.59
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.84	0.59
8:H:14:ASP:HB3	8:H:29:HIS:HB2	1.85	0.59
19:S:102:VAL:O	19:S:108:ARG:N	2.35	0.59
1:A:544:ALA:HB2	1:A:680:LEU:HD13	1.83	0.59
1:A:1028:PRO:O	1:A:1032:GLN:N	2.34	0.59
1:A:1310:HIS:CB	21:U:252:LYS:CD	2.81	0.59
13:M:178:LYS:C	20:T:154:LYS:HB2	2.21	0.59
17:Q:106:LYS:C	18:R:218:LYS:HE2	2.21	0.59
19:S:126:ILE:O	19:S:138:PHE:N	2.35	0.59
2:B:240:LEU:HD23	2:B:257:VAL:CG1	2.33	0.59
11:K:21:ILE:HG23	11:K:33:PHE:CE1	2.38	0.59
1:A:816:GLY:O	1:A:819:SER:OG	2.14	0.59
2:B:175:ASN:O	2:B:739:ASN:ND2	2.32	0.59
20:T:222:VAL:HG22	20:T:223:GLN:H	1.67	0.59
1:A:880:ARG:NH1	1:A:884:ASN:O	2.35	0.59
2:B:92:TYR:C	20:T:145:LEU:CD2	2.70	0.59
2:B:873:LEU:HB3	2:B:874:PRO:HD3	1.80	0.59
2:B:897:ARG:NH1	2:B:1079:SER:OG	2.35	0.59
6:F:44:ARG:H	6:F:45:PRO:HD2	1.67	0.59
9:I:119:CYS:SG	9:I:120:GLY:N	2.76	0.59
1:A:686:THR:HG21	2:B:1041:ILE:HG13	1.84	0.59
3:C:217:GLN:O	3:C:218:ALA:HB2	1.99	0.59
6:F:51:ARG:NH1	6:F:122:GLU:OE1	2.34	0.59
9:I:112:TYR:N	9:I:123:TRP:O	2.34	0.59
14:N:21:VAL:HG11	15:O:40:PHE:HD1	1.68	0.59
1:A:1168:LYS:HG3	1:A:1220:HIS:CE1	2.37	0.59
2:B:240:LEU:CG	2:B:255:ARG:O	2.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:556:ILE:HD12	2:B:561:ILE:HG21	1.84	0.59
8:H:3:GLY:N	8:H:67:ASP:OD1	2.34	0.59
17:Q:102:VAL:HB	17:Q:105:TYR:CG	2.37	0.59
1:A:479:TRP:N	11:K:2:ASN:O	2.35	0.59
1:A:611:ASP:O	1:A:612:ASP:CB	2.50	0.59
1:A:1264:SER:O	1:A:1266:GLU:N	2.33	0.59
17:Q:131:VAL:HG21	17:Q:159:THR:HG21	1.85	0.59
2:B:1022:LEU:HD12	2:B:1023:ARG:HG2	1.85	0.58
5:E:13:ILE:HG22	5:E:136:LEU:HA	1.85	0.58
13:M:182:ALA:HB2	20:T:154:LYS:HA	1.84	0.58
17:Q:102:VAL:CG2	17:Q:105:TYR:HD2	2.16	0.58
2:B:63:PRO:HB3	2:B:408:PHE:CZ	2.38	0.58
2:B:542:LEU:HA	2:B:545:LEU:HD12	1.85	0.58
2:B:1115:GLN:HB2	2:B:1148:LEU:HD11	1.84	0.58
17:Q:106:LYS:HG2	18:R:218:LYS:CG	2.32	0.58
2:B:866:ILE:H	2:B:895:PHE:HA	1.67	0.58
2:B:1036:LYS:HB2	3:C:194:HIS:HB3	1.85	0.58
20:T:139:VAL:O	20:T:140:ARG:HB2	2.02	0.58
1:A:565:MET:HG2	11:K:61:TYR:C	2.24	0.58
2:B:430:ASN:HB2	20:T:159:HIS:HE1	1.67	0.58
2:B:573:TRP:CZ2	2:B:576:ILE:HG23	2.38	0.58
17:Q:104:LYS:NZ	18:R:238:LYS:HD2	2.18	0.58
1:A:73:THR:OG1	2:B:1130:THR:OG1	2.14	0.58
1:A:286:ILE:HD13	1:A:313:HIS:CD2	2.38	0.58
1:A:381:PRO:HB3	11:K:2:ASN:HD21	1.68	0.58
2:B:88:PHE:CD2	2:B:128:ILE:HG12	2.37	0.58
2:B:548:TRP:CD1	2:B:583:LEU:HD13	2.38	0.58
8:H:85:ALA:CB	8:H:144:LEU:CD2	2.82	0.58
10:J:63:ALA:H	10:J:64:PRO:CD	2.16	0.58
14:N:49:LYS:NZ	15:O:17:GLU:OE1	2.25	0.58
1:A:330:GLN:CG	13:M:107:MET:SD	2.91	0.58
2:B:171:LEU:HD22	2:B:176:GLU:HG2	1.84	0.58
10:J:12:LYS:HE2	10:J:40:LEU:HA	1.86	0.58
12:L:18:ILE:O	12:L:18:ILE:HG22	2.03	0.58
20:T:154:LYS:HD2	20:T:154:LYS:N	2.17	0.58
1:A:47:THR:HG23	1:A:53:LYS:HA	1.86	0.58
1:A:1223:ASP:OD2	1:A:1224:ARG:NE	2.36	0.58
2:B:718:GLN:NE2	2:B:975:ARG:O	2.32	0.58
2:B:755:GLN:HB2	2:B:776:ILE:HA	1.85	0.58
7:G:6:SER:HA	7:G:73:LYS:HA	1.85	0.58
8:H:110:THR:O	8:H:111:ARG:HB3	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:143:LYS:NZ	21:U:147:MET:SD	2.75	0.58
1:A:423:ASN:ND2	1:A:425:ASP:OD2	2.31	0.58
1:A:922:PHE:CZ	1:A:952:LEU:CG	2.87	0.58
2:B:897:ARG:HD2	2:B:1079:SER:HA	1.85	0.58
17:Q:25:PHE:HB3	18:R:215:GLU:OE2	2.04	0.58
1:A:555:LEU:HD22	1:A:591:ILE:HG13	1.84	0.58
1:A:607:SER:HB2	1:A:641:CYS:SG	2.44	0.58
1:A:797:ARG:HB3	1:A:820:ARG:HB3	1.85	0.58
1:A:1187:ALA:HA	1:A:1190:GLN:HB2	1.84	0.58
2:B:936:ALA:HB2	2:B:1051:LEU:HD11	1.86	0.58
7:G:98:PHE:HZ	17:Q:152:PHE:CE1	2.22	0.58
9:I:98:GLN:NE2	9:I:108:MET:HG3	2.18	0.58
11:K:11:LEU:O	11:K:37:LYS:NZ	2.36	0.58
16:P:160:GLY:O	16:P:161:ILE:CG1	2.43	0.58
21:U:200:ASP:OD2	21:U:203:ASN:ND2	2.30	0.58
2:B:224:CYS:HB2	2:B:230:ARG:HA	1.86	0.58
7:G:78:ARG:NH1	7:G:79:PRO:O	2.37	0.58
16:P:209:THR:O	16:P:210:THR:CB	2.51	0.58
17:Q:113:ARG:HE	18:R:217:GLN:C	2.06	0.58
19:S:112:GLY:HA2	19:S:145:ASN:O	2.04	0.58
1:A:1164:THR:N	1:A:1299:GLN:O	2.35	0.57
3:C:77:ASP:HB2	3:C:128:ILE:HG22	1.85	0.57
17:Q:106:LYS:HZ1	18:R:219:LEU:HD13	1.68	0.57
4:D:23:PRO:O	4:D:27:GLU:N	2.35	0.57
5:E:44:SER:OG	5:E:46:ASP:HB2	2.04	0.57
10:J:64:PRO:C	10:J:66:GLU:N	2.55	0.57
16:P:180:LEU:HB3	16:P:200:VAL:HG23	1.86	0.57
17:Q:32:LEU:HD13	18:R:161:ARG:NH2	2.19	0.57
18:R:213:ASP:O	18:R:215:GLU:CB	2.52	0.57
19:S:31:PHE:HB2	20:T:92:THR:HB	1.86	0.57
1:A:44:PRO:HG3	1:A:284:VAL:HB	1.85	0.57
2:B:257:VAL:HG23	2:B:257:VAL:O	2.03	0.57
2:B:552:ASN:OD1	2:B:553:LEU:N	2.37	0.57
14:N:314:LEU:HD11	16:P:238:ALA:HB1	1.86	0.57
1:A:1037:ALA:HA	5:E:200:ALA:HB1	1.86	0.57
2:B:1072:ARG:HE	2:B:1113:PRO:HD2	1.68	0.57
13:M:295:ARG:HG2	13:M:299:LEU:HG	1.86	0.57
20:T:12:ALA:HA	20:T:109:ILE:HD11	1.85	0.57
5:E:110:MET:HB2	5:E:115:LYS:HE3	1.87	0.57
11:K:7:PHE:HA	11:K:10:PHE:CE2	2.39	0.57
17:Q:25:PHE:CD2	18:R:215:GLU:OE2	2.56	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1307:VAL:CG2	1:A:1339:ASP:N	2.65	0.57
2:B:411:LEU:HD12	2:B:440:ILE:HD11	1.86	0.57
3:C:193:ARG:NH2	3:C:218:ALA:O	2.38	0.57
16:P:296:ILE:O	16:P:297:LYS:C	2.42	0.57
1:A:66:GLU:O	1:A:68:THR:N	2.38	0.57
1:A:426:ARG:HB3	13:M:40:VAL:CG2	2.28	0.57
2:B:240:LEU:CD2	2:B:257:VAL:HG11	2.34	0.57
10:J:43:TYR:HA	10:J:46:ARG:HB2	1.86	0.57
14:N:354:LYS:HA	14:N:369:LYS:HA	1.86	0.57
16:P:301:VAL:HG11	22:X:14:DA:H5"	1.85	0.57
17:Q:23:ARG:CZ	18:R:207:SER:CB	2.76	0.57
1:A:21:VAL:HB	1:A:1449:ASP:HB3	1.87	0.57
1:A:642:LYS:HZ3	21:U:283:GLU:HA	1.69	0.57
2:B:823:PHE:HD1	13:M:140:ASN:HB3	1.69	0.57
2:B:1114:TYR:CE1	2:B:1153:TYR:HD2	2.22	0.57
18:R:210:PHE:CB	18:R:212:VAL:HG13	2.34	0.57
21:U:230:SER:O	21:U:231:ASP:HB3	2.05	0.57
5:E:148:HIS:HB2	5:E:183:PHE:CZ	2.40	0.57
17:Q:129:CYS:SG	17:Q:159:THR:OG1	2.62	0.57
18:R:195:PRO:O	18:R:196:ASP:HB3	2.02	0.57
18:R:195:PRO:O	18:R:199:LYS:HD2	2.04	0.57
19:S:8:SER:HB3	20:T:49:GLN:HA	1.86	0.57
1:A:922:PHE:HE2	1:A:952:LEU:HD21	1.68	0.57
1:A:1313:GLN:CB	1:A:1333:GLU:HG2	2.35	0.57
1:A:1313:GLN:HB2	1:A:1333:GLU:HG2	1.85	0.57
2:B:490:GLY:O	2:B:491:ARG:O	2.23	0.57
16:P:293:TYR:HB3	16:P:302:LEU:HB2	1.87	0.57
1:A:202:TRP:HB2	1:A:212:LYS:HE2	1.88	0.56
2:B:488:PRO:O	2:B:489:ILE:HG13	2.04	0.56
3:C:136:ASP:HB2	3:C:145:GLN:CD	2.22	0.56
3:C:205:LYS:HB3	3:C:209:SER:OG	2.05	0.56
12:L:18:ILE:HB	12:L:45:TYR:HD2	1.70	0.56
13:M:173:VAL:O	13:M:175:ARG:NH1	2.38	0.56
15:O:66:ARG:HD3	16:P:185:LEU:HA	1.87	0.56
15:O:66:ARG:NE	16:P:185:LEU:O	2.37	0.56
1:A:275:ASP:HB2	1:A:342:ARG:HH22	1.70	0.56
3:C:101:PHE:N	3:C:163:ALA:O	2.27	0.56
3:C:115:VAL:O	3:C:150:ILE:N	2.36	0.56
17:Q:187:ILE:HG21	18:R:212:VAL:C	2.19	0.56
2:B:92:TYR:CA	20:T:145:LEU:HD22	2.33	0.56
2:B:239:MET:HE1	2:B:256:ILE:CD1	2.28	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:803:ARG:HD3	10:J:8:PHE:HA	1.88	0.56
8:H:7:GLU:HG3	8:H:59:VAL:HG22	1.87	0.56
12:L:33:PRO:HG2	12:L:35:ARG:HG2	1.87	0.56
13:M:169:ARG:NH1	13:M:207:ASP:O	2.37	0.56
13:M:214:PHE:HB3	13:M:218:PHE:CE2	2.40	0.56
13:M:279:GLY:HA2	20:T:153:TYR:CE1	2.40	0.56
17:Q:128:LYS:NZ	17:Q:133:SER:O	2.37	0.56
18:R:155:LEU:CD2	18:R:204:ASN:HD21	2.11	0.56
1:A:620:HIS:O	1:A:621:ILE:CG1	2.53	0.56
1:A:891:TYR:CZ	1:A:1087:VAL:HG21	2.41	0.56
1:A:1246:ILE:HG23	1:A:1258:ARG:HG3	1.86	0.56
3:C:6:GLN:CG	3:C:25:ASN:HD22	2.18	0.56
3:C:48:ASP:HB3	3:C:166:LYS:HD2	1.86	0.56
17:Q:70:LYS:CB	18:R:225:VAL:HG12	2.36	0.56
1:A:924:TYR:HE1	1:A:949:GLN:NE2	1.93	0.56
1:A:1196:TYR:HD2	1:A:1246:ILE:HD11	1.68	0.56
4:D:15:GLU:HG2	4:D:23:PRO:HD3	1.87	0.56
10:J:63:ALA:H	10:J:64:PRO:HD2	1.71	0.56
1:A:181:HIS:ND1	1:A:181:HIS:O	2.38	0.56
1:A:357:LYS:O	2:B:1086:PHE:N	2.36	0.56
1:A:375:ILE:HD11	1:A:666:ARG:HE	1.68	0.56
2:B:876:ASN:OD1	2:B:879:GLU:CD	2.43	0.56
12:L:25:GLU:HB2	12:L:27:GLU:CG	2.33	0.56
1:A:740:GLN:O	1:A:743:ARG:HG2	2.05	0.56
2:B:225:LEU:H	2:B:231:PRO:HD2	1.71	0.56
2:B:626:LEU:HD22	2:B:633:LEU:HD11	1.87	0.56
2:B:829:PHE:CE1	2:B:869:LYS:HD3	2.40	0.56
20:T:138:PRO:C	20:T:140:ARG:H	2.09	0.56
1:A:329:MET:HE1	1:A:335:PRO:HA	1.87	0.56
1:A:686:THR:HG21	2:B:1041:ILE:HA	1.88	0.56
8:H:107:GLU:O	8:H:108:ALA:C	2.44	0.56
13:M:179:GLU:HG2	20:T:154:LYS:HE3	1.88	0.56
17:Q:104:LYS:HZ1	18:R:238:LYS:HE3	1.70	0.56
17:Q:113:ARG:HE	18:R:217:GLN:CA	2.18	0.56
19:S:166:ARG:HH11	19:S:166:ARG:CG	2.19	0.56
6:F:79:VAL:HG12	6:F:81:VAL:H	1.71	0.56
7:G:63:ARG:NH2	7:G:65:PHE:O	2.38	0.56
2:B:156:LEU:HB2	2:B:183:GLY:H	1.71	0.56
2:B:591:ARG:HA	2:B:596:ILE:HB	1.88	0.56
2:B:633:LEU:HG	2:B:635:LEU:H	1.71	0.56
3:C:63:PHE:O	3:C:67:ARG:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:205:LYS:NZ	3:C:213:GLU:OE2	2.34	0.56
1:A:47:THR:HA	1:A:54:LEU:HG	1.87	0.55
1:A:85:PHE:HD1	1:A:257:PRO:HD3	1.70	0.55
1:A:1209:PRO:HB3	9:I:33:ARG:NH1	2.19	0.55
1:A:1307:VAL:HG22	1:A:1307:VAL:O	2.06	0.55
2:B:485:LEU:HB2	2:B:524:LYS:HB2	1.88	0.55
2:B:676:ALA:N	2:B:695:HIS:O	2.33	0.55
2:B:814:TYR:N	2:B:921:ILE:O	2.32	0.55
5:E:30:GLN:O	5:E:34:ASP:N	2.34	0.55
13:M:214:PHE:O	13:M:218:PHE:HD2	1.89	0.55
14:N:318:ASP:OD1	16:P:239:ARG:CD	2.50	0.55
9:I:59:THR:O	9:I:59:THR:HG22	2.05	0.55
17:Q:141:ALA:HB1	17:Q:152:PHE:CE1	2.40	0.55
17:Q:187:ILE:C	18:R:212:VAL:HA	2.26	0.55
1:A:364:ARG:NH1	1:A:461:GLN:OE1	2.39	0.55
1:A:372:ASN:O	1:A:372:ASN:ND2	2.38	0.55
2:B:268:PRO:HB2	2:B:271:ILE:HG12	1.88	0.55
2:B:837:CYS:HB2	2:B:889:LYS:HD2	1.88	0.55
13:M:17:ASN:OD1	13:M:18:HIS:ND1	2.39	0.55
17:Q:102:VAL:HG21	17:Q:105:TYR:HD2	1.71	0.55
4:D:79:THR:HG23	4:D:137:LYS:HG2	1.89	0.55
20:T:217:LEU:HB3	20:T:233:TRP:CE3	2.40	0.55
1:A:43:TYR:CD2	1:A:44:PRO:HD2	2.42	0.55
1:A:408:ARG:NH1	1:A:414:PRO:HB2	2.21	0.55
1:A:922:PHE:N	1:A:922:PHE:CD1	2.74	0.55
5:E:54:ARG:O	5:E:58:LEU:N	2.35	0.55
9:I:68:ILE:HG23	9:I:122:ARG:HD2	1.88	0.55
15:O:67:PHE:HB2	15:O:72:TRP:CE3	2.41	0.55
16:P:288:PHE:CD1	16:P:289:PRO:HD2	2.42	0.55
1:A:46:THR:HA	1:A:57:LEU:HD13	1.89	0.55
1:A:489:THR:O	1:A:493:ASN:N	2.39	0.55
1:A:516:GLN:HA	1:A:520:MET:HG2	1.89	0.55
1:A:1280:ASP:HB3	1:A:1283:VAL:HG22	1.87	0.55
2:B:248:LYS:C	2:B:249:LYS:HG2	2.27	0.55
14:N:360:LEU:HD11	15:O:81:PHE:CD2	2.41	0.55
1:A:65:ILE:HG22	1:A:66:GLU:H	1.72	0.55
1:A:1313:GLN:O	1:A:1315:ASP:N	2.39	0.55
2:B:566:LYS:HA	2:B:576:ILE:HG22	1.89	0.55
2:B:934:LYS:HG2	2:B:1051:LEU:HD12	1.88	0.55
14:N:332:GLU:HB2	15:O:93:VAL:HA	1.88	0.55
16:P:171:THR:HG23	16:P:256:GLN:HG3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:270:LEU:HD22	16:P:291:LEU:HD13	1.89	0.55
18:R:88:ARG:NH1	18:R:97:LEU:HD23	2.22	0.55
19:S:119:THR:HG22	19:S:123:SER:HA	1.89	0.55
20:T:138:PRO:O	20:T:140:ARG:N	2.40	0.55
1:A:910:LYS:HD2	1:A:911:PRO:HD2	1.88	0.55
2:B:829:PHE:HD1	2:B:869:LYS:HB3	1.72	0.55
17:Q:113:ARG:NE	18:R:217:GLN:HB3	2.21	0.55
20:T:31:TRP:CD1	20:T:62:LEU:HD21	2.41	0.55
1:A:21:VAL:HG21	1:A:1427:LEU:HD11	1.88	0.55
1:A:880:ARG:HG2	1:A:886:VAL:HA	1.88	0.55
1:A:935:GLN:O	1:A:1002:SER:N	2.40	0.55
1:A:1150:ASP:OD2	1:A:1153:ARG:N	2.39	0.55
21:U:266:CYS:O	21:U:268:LYS:N	2.32	0.55
1:A:43:TYR:CG	1:A:44:PRO:HD2	2.41	0.55
1:A:426:ARG:NE	1:A:447:GLU:OE2	2.33	0.55
1:A:928:ARG:O	1:A:930:LEU:N	2.40	0.55
1:A:1027:ASP:OD2	5:E:162:ARG:NE	2.25	0.55
2:B:810:PHE:HB2	2:B:927:ARG:HG2	1.89	0.55
2:B:1040:GLN:NE2	3:C:195:THR:OG1	2.40	0.55
6:F:81:VAL:HG12	6:F:101:LYS:HD3	1.88	0.55
7:G:98:PHE:HE2	17:Q:145:PHE:CG	2.25	0.55
19:S:127:PHE:HB2	20:T:19:TRP:HB2	1.88	0.55
20:T:145:LEU:O	20:T:146:ASP:HB3	2.07	0.55
1:A:613:GLU:HG3	21:U:261:PHE:HD1	1.72	0.54
2:B:751:LEU:HD11	2:B:806:PHE:HA	1.89	0.54
5:E:149:VAL:O	5:E:192:LYS:N	2.23	0.54
8:H:84:ARG:C	8:H:86:ASP:N	2.60	0.54
17:Q:24:GLY:HA2	18:R:210:PHE:CD1	2.41	0.54
17:Q:106:LYS:CB	18:R:218:LYS:HE2	2.37	0.54
1:A:515:ILE:HG23	1:A:519:ALA:HB3	1.89	0.54
1:A:608:THR:HB	1:A:610:PRO:CD	2.36	0.54
1:A:1463:LEU:HD21	6:F:64:ARG:HH22	1.71	0.54
2:B:248:LYS:O	2:B:249:LYS:HG2	2.07	0.54
2:B:552:ASN:HB3	2:B:555:GLU:HB3	1.89	0.54
2:B:1094:GLN:HA	2:B:1097:HIS:HB2	1.88	0.54
1:A:608:THR:HG21	1:A:639:ILE:HG23	1.89	0.54
1:A:1121:VAL:HA	1:A:1124:LEU:HB3	1.89	0.54
2:B:953:ASP:HA	3:C:36:ARG:HH12	1.72	0.54
5:E:10:LEU:HB3	5:E:58:LEU:HD11	1.89	0.54
5:E:73:PHE:O	5:E:103:LEU:N	2.28	0.54
10:J:67:LYS:HB2	12:L:23:HIS:CD2	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:360:LEU:HB2	14:N:365:TYR:HE2	1.72	0.54
16:P:214:PHE:HD2	16:P:218:LYS:HB2	1.73	0.54
17:Q:110:MET:HE3	18:R:213:ASP:C	2.27	0.54
1:A:320:ASN:HB2	1:A:336:LEU:HD23	1.90	0.54
1:A:622:SER:O	1:A:624:GLY:CA	2.55	0.54
1:A:926:ASN:OD1	1:A:931:ARG:CG	2.56	0.54
1:A:1146:GLN:HG2	1:A:1150:ASP:HB2	1.88	0.54
2:B:568:PHE:N	2:B:612:ILE:O	2.33	0.54
2:B:836:THR:HG22	2:B:885:ARG:HB3	1.90	0.54
3:C:125:PRO:O	3:C:127:VAL:N	2.40	0.54
5:E:105:VAL:HG12	5:E:132:GLN:HG3	1.88	0.54
10:J:14:VAL:HG23	10:J:17:LYS:HB2	1.90	0.54
15:O:28:ILE:HB	15:O:32:LEU:HD23	1.88	0.54
1:A:1307:VAL:O	1:A:1307:VAL:HG13	2.08	0.54
2:B:240:LEU:HD23	2:B:257:VAL:CG2	2.37	0.54
3:C:68:LEU:HD12	3:C:71:ILE:HD12	1.90	0.54
1:A:902:GLU:O	1:A:979:LEU:N	2.34	0.54
1:A:936:GLU:HB2	1:A:939:VAL:HG23	1.89	0.54
1:A:1273:GLU:O	1:A:1273:GLU:HG3	2.07	0.54
2:B:512:ALA:HA	2:B:723:THR:HG22	1.89	0.54
8:H:8:ASP:OD1	8:H:9:ILE:N	2.41	0.54
9:I:110:LEU:O	9:I:124:THR:OG1	2.26	0.54
13:M:267:GLU:OE1	13:M:269:ARG:NH2	2.41	0.54
18:R:103:LEU:HB3	18:R:109:LEU:HA	1.90	0.54
2:B:440:ILE:H	2:B:440:ILE:HD12	1.71	0.54
2:B:778:SER:O	2:B:1046:THR:N	2.37	0.54
3:C:23:ILE:HB	3:C:231:TYR:HE2	1.72	0.54
14:N:38:VAL:HG13	15:O:22:LEU:HD22	1.88	0.54
17:Q:23:ARG:CZ	18:R:206:LYS:CG	2.71	0.54
19:S:110:PHE:CD1	19:S:148:PRO:HA	2.42	0.54
20:T:30:GLN:HG2	20:T:62:LEU:HG	1.89	0.54
1:A:927:GLU:O	1:A:931:ARG:CB	2.56	0.54
2:B:573:TRP:CZ3	2:B:575:GLY:HA2	2.43	0.54
16:P:165:LEU:HA	16:P:260:GLY:HA2	1.89	0.54
16:P:297:LYS:HA	16:P:297:LYS:NZ	2.22	0.54
1:A:46:THR:HG23	1:A:57:LEU:HD22	1.88	0.54
1:A:378:VAL:O	1:A:475:ARG:N	2.41	0.54
2:B:1135:TYR:HB2	2:B:1146:ILE:HG13	1.90	0.54
3:C:46:ALA:HB3	3:C:176:TRP:NE1	2.23	0.54
5:E:166:ARG:HB2	5:E:169:GLN:HG3	1.90	0.54
5:E:172:ARG:O	5:E:207:ARG:NE	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:25:GLU:O	12:L:37:ARG:NH2	2.39	0.54
1:A:43:TYR:OH	1:A:285:LYS:HE2	2.06	0.54
1:A:330:GLN:HG2	13:M:107:MET:SD	2.48	0.54
1:A:526:VAL:HA	1:A:533:PRO:HA	1.88	0.54
2:B:670:GLU:HA	2:B:673:VAL:HG22	1.90	0.54
2:B:868:GLY:HA2	2:B:893:SER:HB2	1.89	0.54
2:B:1117:HIS:HA	2:B:1147:SER:O	2.07	0.54
3:C:44:ILE:N	3:C:168:GLY:O	2.31	0.54
3:C:177:ASN:ND2	3:C:179:THR:O	2.41	0.54
11:K:35:ILE:HB	11:K:71:ILE:HG13	1.89	0.54
14:N:32:ASP:OD1	15:O:29:THR:OG1	2.23	0.54
17:Q:102:VAL:CB	17:Q:105:TYR:CD2	2.85	0.54
19:S:48:GLU:O	19:S:99:LEU:N	2.38	0.54
21:U:205:ASN:HB3	21:U:231:ASP:OD2	2.08	0.54
2:B:132:VAL:HG23	2:B:141:GLN:O	2.07	0.53
8:H:6:PHE:HB3	8:H:60:ILE:HB	1.90	0.53
9:I:17:CYS:N	9:I:22:ASN:O	2.35	0.53
15:O:71:VAL:HG22	15:O:98:CYS:HA	1.90	0.53
23:Y:74:DC:H2"	23:Y:75:DC:H6	1.73	0.53
1:A:871:VAL:HG23	1:A:1088:GLY:HA3	1.90	0.53
1:A:1005:HIS:CE1	1:A:1007:ILE:HB	2.43	0.53
2:B:813:SER:HA	2:B:922:ARG:HA	1.88	0.53
18:R:195:PRO:O	18:R:196:ASP:HB2	2.07	0.53
18:R:225:VAL:O	18:R:225:VAL:HG12	2.08	0.53
20:T:30:GLN:NE2	20:T:62:LEU:O	2.28	0.53
21:U:132:ARG:N	21:U:167:GLU:OE2	2.41	0.53
1:A:608:THR:HB	1:A:610:PRO:HD2	1.87	0.53
1:A:875:TYR:HA	1:A:1083:PRO:HB2	1.91	0.53
2:B:752:TYR:HE1	2:B:809:VAL:HG23	1.72	0.53
4:D:112:LYS:HE2	4:D:124:ASP:OD2	2.09	0.53
18:R:210:PHE:CG	18:R:212:VAL:HG13	2.43	0.53
1:A:1307:VAL:HG22	1:A:1338:THR:CA	2.38	0.53
2:B:309:PHE:HE2	9:I:25:TYR:HE2	1.57	0.53
2:B:935:PHE:CE2	2:B:945:CYS:HB2	2.42	0.53
13:M:225:PRO:HG2	13:M:228:VAL:HG23	1.90	0.53
17:Q:34:LEU:HA	17:Q:37:LEU:HD12	1.91	0.53
1:A:579:ILE:O	1:A:584:PRO:HA	2.08	0.53
1:A:602:CYS:HB2	1:A:655:ILE:HD11	1.91	0.53
1:A:910:LYS:O	1:A:963:ARG:NH2	2.37	0.53
2:B:51:ILE:HD12	2:B:160:TYR:CE2	2.44	0.53
3:C:74:ILE:HG13	3:C:76:ASP:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:88:PHE:HD1	8:H:146:LYS:HD2	1.73	0.53
16:P:325:PHE:CZ	16:P:329:TYR:HD2	2.26	0.53
17:Q:77:ARG:N	17:Q:93:PHE:O	2.35	0.53
18:R:191:PHE:CB	18:R:202:PHE:HD1	2.22	0.53
2:B:471:ASN:OD1	2:B:473:LEU:HG	2.08	0.53
2:B:956:PHE:HB2	2:B:960:GLY:HA2	1.90	0.53
9:I:84:HIS:HB3	9:I:92:LYS:HB3	1.91	0.53
17:Q:109:HIS:C	18:R:221:ARG:CD	2.70	0.53
1:A:225:PHE:HA	1:A:228:ILE:HG12	1.91	0.53
2:B:591:ARG:NH2	2:B:669:GLU:OE1	2.42	0.53
4:D:26:PHE:CZ	7:G:42:TYR:HA	2.44	0.53
1:A:272:ASN:ND2	1:A:278:HIS:HD2	2.07	0.53
1:A:579:ILE:HB	1:A:585:LEU:HB2	1.91	0.53
1:A:1123:ARG:NH1	1:A:1126:GLU:OE1	2.40	0.53
1:A:1314:THR:O	1:A:1314:THR:HG22	2.09	0.53
2:B:71:ALA:HA	2:B:81:PRO:HB3	1.90	0.53
2:B:152:ILE:HG23	2:B:154:ILE:HD11	1.90	0.53
2:B:182:GLY:HA2	2:B:184:TYR:CE1	2.44	0.53
2:B:623:ARG:O	2:B:665:ILE:N	2.37	0.53
2:B:792:ASP:OD1	2:B:975:ARG:NH2	2.42	0.53
4:D:73:ARG:NH1	4:D:103:LEU:O	2.41	0.53
7:G:119:PHE:HB2	7:G:128:TYR:HE1	1.73	0.53
18:R:213:ASP:O	18:R:215:GLU:CA	2.56	0.53
1:A:1219:LYS:O	1:A:1222:THR:OG1	2.22	0.53
3:C:63:PHE:HE2	10:J:2:ILE:HG21	1.73	0.53
7:G:119:PHE:HB2	7:G:128:TYR:CE1	2.44	0.53
8:H:24:ARG:HG2	8:H:46:GLN:HE22	1.73	0.53
1:A:124:PRO:HA	1:A:127:LYS:HB2	1.91	0.53
1:A:152:ASN:O	1:A:152:ASN:ND2	2.41	0.53
1:A:1307:VAL:O	1:A:1338:THR:HG22	2.08	0.53
2:B:753:TYR:CZ	10:J:4:PRO:HB3	2.44	0.53
1:A:620:HIS:O	1:A:621:ILE:HB	2.09	0.52
2:B:455:ASP:O	2:B:457:LYS:N	2.37	0.52
2:B:1068:GLN:N	2:B:1073:GLN:O	2.43	0.52
3:C:14:LEU:HD23	11:K:112:LYS:HE2	1.91	0.52
3:C:19:VAL:HG12	3:C:233:VAL:HB	1.90	0.52
3:C:101:PHE:O	3:C:163:ALA:N	2.28	0.52
10:J:63:ALA:N	10:J:64:PRO:HD2	2.24	0.52
20:T:94:THR:HG22	20:T:109:ILE:HG23	1.91	0.52
1:A:410:ASN:OD1	1:A:417:LYS:NZ	2.35	0.52
1:A:914:LYS:O	1:A:918:LYS:N	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:GLU:HA	2:B:27:TRP:HD1	1.74	0.52
2:B:240:LEU:HD13	2:B:242:ARG:NE	2.24	0.52
8:H:28:LEU:HD11	8:H:50:VAL:HG21	1.91	0.52
8:H:65:TYR:OH	8:H:79:ASP:OD2	2.27	0.52
15:O:9:THR:O	15:O:13:ASN:N	2.30	0.52
16:P:161:ILE:HG13	16:P:329:TYR:CE2	2.44	0.52
18:R:202:PHE:C	18:R:203:PHE:CG	2.83	0.52
19:S:46:ARG:HB2	19:S:101:ARG:HB2	1.91	0.52
1:A:641:CYS:SG	1:A:644:SER:OG	2.52	0.52
1:A:998:PRO:HA	1:A:1059:ARG:NE	2.24	0.52
2:B:83:ARG:O	2:B:134:LYS:HA	2.08	0.52
2:B:1021:HIS:CE1	2:B:1023:ARG:HB2	2.44	0.52
7:G:22:LEU:HD21	7:G:68:TYR:CE2	2.45	0.52
14:N:360:LEU:HD11	15:O:81:PHE:HD2	1.73	0.52
17:Q:71:PHE:HD1	17:Q:72:ILE:HG23	1.74	0.52
20:T:143:GLN:O	20:T:144:GLN:HB2	2.09	0.52
1:A:403:GLN:HG3	1:A:440:LEU:HD21	1.92	0.52
2:B:566:LYS:NZ	2:B:609:GLU:O	2.43	0.52
2:B:1026:GLU:N	2:B:1041:ILE:O	2.39	0.52
8:H:40:ILE:HB	8:H:124:ARG:HG2	1.91	0.52
9:I:66:THR:HA	9:I:122:ARG:NH2	2.25	0.52
18:R:195:PRO:HB2	18:R:199:LYS:HD3	1.90	0.52
21:U:194:ARG:HD2	21:U:220:PHE:CE2	2.44	0.52
1:A:457:ILE:HG21	2:B:1102:PHE:CZ	2.44	0.52
1:A:568:SER:N	1:A:671:ASN:OD1	2.29	0.52
6:F:56:TYR:HE1	6:F:124:ILE:HD12	1.74	0.52
14:N:15:ARG:HA	14:N:18:ILE:HD12	1.91	0.52
17:Q:106:LYS:CG	18:R:218:LYS:HG2	2.37	0.52
18:R:140:LYS:H	18:R:141:PRO:HD2	1.74	0.52
23:Y:62:DC:H1'	23:Y:63:DG:H5'	1.90	0.52
2:B:780:VAL:HG13	2:B:965:ILE:HB	1.90	0.52
13:M:214:PHE:HB3	13:M:218:PHE:HE2	1.75	0.52
18:R:195:PRO:HB2	18:R:199:LYS:CD	2.39	0.52
1:A:876:ASP:HA	6:F:52:ILE:HD13	1.92	0.52
1:A:1243:LEU:HD11	1:A:1259:ILE:HD12	1.91	0.52
2:B:40:VAL:HA	2:B:42:GLN:HE22	1.75	0.52
2:B:613:ARG:HD3	2:B:615:TYR:HE2	1.74	0.52
17:Q:110:MET:SD	18:R:218:LYS:HB2	2.49	0.52
1:A:879:VAL:O	1:A:887:VAL:N	2.29	0.52
1:A:1416:ARG:NH2	1:A:1434:GLU:OE2	2.43	0.52
2:B:544:PHE:O	2:B:548:TRP:N	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:34:CYS:C	13:M:39:LEU:CB	2.74	0.52
13:M:127:ARG:HG3	13:M:127:ARG:HH21	1.74	0.52
17:Q:72:ILE:HD12	17:Q:96:TYR:CD1	2.45	0.52
21:U:230:SER:O	21:U:231:ASP:CB	2.56	0.52
1:A:817:PRO:HB2	1:A:822:PHE:HB3	1.92	0.52
1:A:1309:MET:SD	21:U:252:LYS:CD	2.98	0.52
2:B:249:LYS:O	2:B:251:ALA:N	2.42	0.52
2:B:273:PHE:HA	2:B:276:LEU:HD12	1.92	0.52
13:M:23:LEU:HD21	13:M:41:VAL:HG21	1.92	0.52
14:N:25:VAL:HB	15:O:36:VAL:HG22	1.91	0.52
17:Q:18:ALA:HA	17:Q:21:VAL:HG22	1.90	0.52
1:A:138:LYS:HE3	1:A:1441:GLU:HG3	1.91	0.52
1:A:381:PRO:HB3	11:K:2:ASN:ND2	2.25	0.52
1:A:433:PRO:HD3	13:M:35:PRO:O	2.10	0.52
2:B:711:ILE:HD12	2:B:939:HIS:HA	1.90	0.52
2:B:867:ILE:O	2:B:894:THR:N	2.43	0.52
3:C:100:GLU:N	3:C:124:SER:OG	2.43	0.52
14:N:312:GLU:O	14:N:314:LEU:N	2.37	0.52
1:A:405:LEU:HD23	1:A:448:ARG:HB2	1.92	0.51
1:A:529:GLN:NE2	1:A:1098:PRO:HD3	2.25	0.51
1:A:600:ILE:HD12	1:A:659:GLU:HB2	1.92	0.51
1:A:674:THR:O	1:A:678:ASN:ND2	2.42	0.51
1:A:1139:LEU:N	1:A:1338:THR:O	2.42	0.51
2:B:21:LEU:HD21	2:B:635:LEU:HD23	1.91	0.51
2:B:222:ARG:HB3	2:B:232:THR:O	2.09	0.51
2:B:551:GLU:OE1	2:B:551:GLU:N	2.42	0.51
2:B:934:LYS:HE3	2:B:1053:HIS:CG	2.44	0.51
7:G:12:LEU:HG	7:G:63:ARG:NH1	2.26	0.51
8:H:64:LEU:O	8:H:66:GLU:N	2.33	0.51
8:H:75:TYR:C	8:H:77:PRO:HD3	2.26	0.51
13:M:218:PHE:HD1	13:M:277:ILE:HG22	1.74	0.51
14:N:42:LEU:HD11	15:O:15:LEU:HD12	1.91	0.51
14:N:317:GLU:OE2	16:P:235:ARG:HD2	2.10	0.51
20:T:184:LEU:HA	20:T:187:LEU:HD12	1.92	0.51
1:A:1453:GLY:O	1:A:1457:ASN:ND2	2.44	0.51
2:B:345:LYS:O	2:B:349:PRO:HG3	2.10	0.51
8:H:70:LEU:O	8:H:72:ASP:N	2.38	0.51
9:I:88:LYS:HD2	9:I:121:HIS:CE1	2.45	0.51
1:A:611:ASP:HB3	1:A:617:PRO:CG	2.37	0.51
1:A:1162:GLU:OE2	1:A:1224:ARG:NH1	2.42	0.51
1:A:1162:GLU:HG3	1:A:1306:LYS:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:842:HIS:ND1	13:M:25:GLU:O	2.43	0.51
2:B:1137:CYS:HB3	2:B:1142:ASN:HB3	1.91	0.51
8:H:10:PHE:CE1	8:H:32:SER:HB2	2.46	0.51
9:I:86:CYS:HB3	9:I:89:CYS:SG	2.50	0.51
11:K:19:ILE:HA	11:K:35:ILE:HA	1.92	0.51
13:M:231:ALA:HA	13:M:301:PRO:HG3	1.93	0.51
14:N:356:GLY:HA3	14:N:367:PHE:CZ	2.46	0.51
14:N:358:MET:HB2	14:N:365:TYR:HB2	1.92	0.51
15:O:3:TYR:OH	15:O:99:ASP:O	2.24	0.51
17:Q:113:ARG:HE	18:R:217:GLN:CB	2.23	0.51
23:Y:70:DC:H2"	23:Y:71:DA:H8	1.76	0.51
1:A:21:VAL:HG23	1:A:1451:MET:SD	2.51	0.51
1:A:1175:ILE:HB	9:I:54:TYR:HB3	1.93	0.51
2:B:108:MET:SD	2:B:120:TYR:HA	2.51	0.51
2:B:133:ILE:C	2:B:135:GLU:H	2.14	0.51
2:B:258:ALA:HB2	2:B:269:ILE:HG22	1.93	0.51
2:B:331:THR:HG21	2:B:334:LYS:HE2	1.92	0.51
3:C:151:VAL:HG22	3:C:152:LYS:H	1.75	0.51
4:D:72:SER:O	4:D:142:TYR:OH	2.23	0.51
13:M:124:MET:HA	13:M:127:ARG:HH22	1.76	0.51
14:N:312:GLU:HB2	14:N:313:PRO:HD3	1.93	0.51
16:P:207:PRO:HB3	16:P:233:ALA:HB2	1.93	0.51
20:T:206:THR:HG21	20:T:213:LEU:HD13	1.92	0.51
2:B:125:TYR:HE1	2:B:148:PHE:HB2	1.76	0.51
5:E:99:ILE:HD11	5:E:102:ALA:HB2	1.93	0.51
16:P:167:ASN:HB2	23:Y:80:DT:C4'	2.40	0.51
16:P:199:ALA:HB2	16:P:214:PHE:HD1	1.75	0.51
17:Q:146:ASP:HB3	17:Q:149:THR:HG22	1.90	0.51
1:A:551:ARG:HH12	8:H:120:GLY:C	2.14	0.51
1:A:574:VAL:O	8:H:73:GLY:O	2.29	0.51
1:A:611:ASP:OD2	1:A:617:PRO:CB	2.57	0.51
1:A:696:SER:O	1:A:700:GLN:N	2.36	0.51
1:A:1127:LEU:HD21	1:A:1378:LEU:HD11	1.93	0.51
13:M:263:GLN:HA	13:M:268:LYS:HG2	1.92	0.51
18:R:213:ASP:O	18:R:214:GLU:C	2.47	0.51
1:A:1117:VAL:O	1:A:1117:VAL:HG12	2.11	0.51
1:A:1204:VAL:O	1:A:1207:ILE:HG12	2.11	0.51
1:A:1435:THR:OG1	1:A:1436:VAL:N	2.42	0.51
2:B:1079:SER:O	13:M:53:ARG:NH2	2.44	0.51
3:C:20:LYS:HE2	3:C:232:ASN:ND2	2.25	0.51
13:M:40:VAL:C	13:M:42:GLY:N	2.64	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:167:ASN:HB3	16:P:259:VAL:HB	1.92	0.51
16:P:206:GLU:CB	16:P:207:PRO:CD	2.87	0.51
18:R:103:LEU:HD12	18:R:116:LYS:HE3	1.92	0.51
22:X:47:DC:H2"	22:X:48:DG:C8	2.46	0.51
3:C:43:PRO:HA	3:C:169:PHE:HB3	1.91	0.51
5:E:103:LEU:HA	5:E:128:GLU:HB2	1.93	0.51
8:H:17:PRO:CB	8:H:27:ARG:HB3	2.35	0.51
8:H:65:TYR:CE1	8:H:81:ARG:CZ	2.93	0.51
13:M:38:GLY:O	13:M:39:LEU:CB	2.59	0.51
16:P:277:HIS:O	16:P:281:SER:N	2.42	0.51
1:A:456:VAL:HG21	1:A:503:LEU:HD11	1.92	0.51
1:A:583:ARG:NH2	3:C:223:ASN:OD1	2.34	0.51
1:A:987:ILE:HG12	1:A:1068:LEU:HD21	1.91	0.51
2:B:85:LEU:HB3	2:B:131:THR:O	2.10	0.51
2:B:1062:ARG:NH1	2:B:1066:PRO:O	2.43	0.51
3:C:101:PHE:HB3	3:C:120:LEU:HD11	1.92	0.51
4:D:86:LEU:O	4:D:89:GLN:HG2	2.10	0.51
8:H:64:LEU:O	8:H:83:SER:O	2.29	0.51
17:Q:23:ARG:HH21	18:R:206:LYS:HG3	0.69	0.51
17:Q:183:GLN:O	17:Q:186:PRO:HD2	2.11	0.51
21:U:276:VAL:HG22	21:U:277:GLN:H	1.76	0.51
1:A:478:PRO:HB3	11:K:4:PRO:CD	2.41	0.51
2:B:278:PHE:HZ	2:B:359:THR:HG23	1.76	0.51
2:B:519:ALA:HB1	2:B:523:VAL:HG23	1.93	0.51
8:H:75:TYR:CD2	8:H:77:PRO:HG3	2.45	0.51
20:T:27:LEU:HD11	20:T:58:LEU:HD21	1.93	0.51
1:A:564:LEU:HD22	1:A:570:TRP:CE2	2.45	0.50
1:A:909:LEU:HB2	1:A:975:SER:OG	2.11	0.50
2:B:264:LYS:HE3	2:B:326:ALA:HA	1.93	0.50
2:B:425:ARG:HH11	2:B:425:ARG:HG3	1.75	0.50
12:L:38:GLU:O	13:M:226:LYS:NZ	2.43	0.50
19:S:31:PHE:O	20:T:92:THR:N	2.44	0.50
22:X:52:DG:H2"	22:X:53:DA:C8	2.46	0.50
1:A:426:ARG:H	13:M:40:VAL:CG2	2.24	0.50
1:A:722:ASN:HB2	1:A:724:GLU:HG2	1.93	0.50
2:B:797:ASN:ND2	2:B:954:MET:SD	2.85	0.50
1:A:721:HIS:HA	9:I:108:MET:O	2.11	0.50
2:B:761:THR:H	2:B:764:MET:HE3	1.76	0.50
2:B:1028:LEU:HD13	2:B:1041:ILE:HB	1.94	0.50
5:E:59:THR:HG23	5:E:75:PHE:HA	1.92	0.50
5:E:150:VAL:HG12	5:E:185:ILE:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:70:ALA:HB1	6:F:89:PRO:HB2	1.94	0.50
16:P:167:ASN:O	16:P:259:VAL:N	2.41	0.50
16:P:297:LYS:HA	16:P:297:LYS:HE2	1.89	0.50
17:Q:187:ILE:HB	18:R:211:SER:HG	1.69	0.50
1:A:500:GLU:OE2	2:B:1058:LYS:HB3	2.12	0.50
1:A:1317:LYS:HB2	21:U:295:GLY:HA3	1.93	0.50
2:B:568:PHE:CZ	2:B:573:TRP:HD1	2.28	0.50
7:G:11:ILE:HB	7:G:68:TYR:HB2	1.93	0.50
9:I:62:VAL:HA	9:I:103:ARG:NH2	2.26	0.50
13:M:289:TYR:OH	13:M:314:PRO:O	2.17	0.50
1:A:292:ARG:NH1	1:A:295:GLN:OE1	2.45	0.50
2:B:713:PHE:CD1	2:B:1001:PRO:HA	2.46	0.50
2:B:884:ASN:OD1	2:B:885:ARG:N	2.44	0.50
2:B:988:LYS:O	2:B:992:ASN:ND2	2.43	0.50
2:B:1094:GLN:HG2	2:B:1103:LEU:HB2	1.93	0.50
4:D:76:ASN:HB3	4:D:79:THR:HB	1.92	0.50
5:E:54:ARG:HA	5:E:57:ASP:HB2	1.93	0.50
8:H:98:ARG:HB3	8:H:115:TYR:HB2	1.93	0.50
17:Q:108:ASP:CB	18:R:234:GLU:OE2	2.59	0.50
20:T:93:LEU:HB2	20:T:110:VAL:HB	1.93	0.50
2:B:1123:GLY:HA3	2:B:1170:ARG:HB2	1.93	0.50
3:C:11:ILE:HG12	11:K:108:ALA:HB1	1.93	0.50
3:C:172:GLU:HG2	12:L:58:ARG:HH22	1.77	0.50
6:F:44:ARG:HD3	6:F:113:GLY:O	2.12	0.50
13:M:279:GLY:CA	20:T:153:TYR:HE1	2.25	0.50
14:N:333:ASN:HB3	14:N:360:LEU:HA	1.93	0.50
16:P:291:LEU:N	16:P:304:ILE:O	2.31	0.50
20:T:159:HIS:CG	20:T:160:GLN:N	2.79	0.50
1:A:233:CYS:O	1:A:238:MET:N	2.45	0.50
1:A:371:PRO:HD2	2:B:788:TYR:CE1	2.46	0.50
1:A:489:THR:HG23	1:A:494:ALA:HB3	1.92	0.50
1:A:595:ILE:HG22	1:A:668:PHE:CE1	2.46	0.50
2:B:205:VAL:HG21	2:B:368:MET:HG3	1.92	0.50
7:G:12:LEU:HG	7:G:63:ARG:HH11	1.77	0.50
11:K:12:LEU:HD21	11:K:18:LYS:HA	1.92	0.50
13:M:222:LEU:HD22	13:M:269:ARG:HG3	1.94	0.50
17:Q:120:ASP:HB3	17:Q:174:ARG:HG3	1.94	0.50
18:R:163:LEU:C	18:R:164:GLY:O	2.49	0.50
21:U:188:LYS:O	21:U:192:ARG:HG3	2.11	0.50
1:A:432:HIS:CE1	1:A:438:LEU:HB2	2.47	0.50
2:B:1030:ASN:ND2	2:B:1033:THR:OG1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:65:ASN:OD1	5:E:66:ASP:N	2.44	0.50
18:R:223:VAL:C	18:R:224:THR:CG2	2.60	0.50
1:A:16:ARG:HD2	2:B:1147:SER:HB3	1.93	0.50
1:A:516:GLN:O	1:A:523:ARG:NH1	2.41	0.50
1:A:764:ASN:OD1	1:A:766:PHE:N	2.36	0.50
2:B:157:ARG:HB2	2:B:181:PRO:O	2.12	0.50
2:B:240:LEU:CD2	2:B:257:VAL:CG1	2.90	0.50
2:B:242:ARG:C	2:B:244:GLY:H	2.15	0.50
2:B:591:ARG:HG2	2:B:598:VAL:HG12	1.93	0.50
2:B:1072:ARG:HD3	2:B:1112:ASP:OD1	2.12	0.50
2:B:1075:MET:HB2	2:B:1082:GLY:HA2	1.94	0.50
17:Q:113:ARG:HD3	18:R:217:GLN:O	2.10	0.50
20:T:229:HIS:CD2	22:X:28:DG:H21	2.30	0.50
2:B:10:TYR:CE2	2:B:12:GLU:HB3	2.47	0.49
2:B:36:GLU:OE1	2:B:654:GLN:N	2.34	0.49
2:B:1066:PRO:HD3	13:M:30:GLY:HA3	1.94	0.49
4:D:19:GLN:HB2	4:D:21:ILE:HG12	1.93	0.49
7:G:55:GLY:N	7:G:69:PRO:O	2.35	0.49
13:M:118:PHE:HE1	13:M:142:PHE:HB3	1.77	0.49
1:A:286:ILE:HD13	1:A:313:HIS:HD2	1.77	0.49
1:A:380:VAL:N	1:A:475:ARG:O	2.37	0.49
1:A:510:GLU:HA	6:F:67:GLY:HA3	1.94	0.49
5:E:52:ARG:HG2	5:E:54:ARG:NH1	2.28	0.49
7:G:93:ASN:HD21	17:Q:151:THR:HA	1.76	0.49
14:N:310:GLU:HB3	14:N:313:PRO:HD2	1.94	0.49
14:N:345:SER:N	14:N:348:LYS:O	2.43	0.49
16:P:293:TYR:CD2	16:P:302:LEU:HD13	2.44	0.49
18:R:88:ARG:NH2	18:R:93:ASP:HB3	2.27	0.49
18:R:191:PHE:CB	18:R:202:PHE:HE1	2.23	0.49
20:T:144:GLN:O	20:T:145:LEU:CB	2.60	0.49
1:A:33:ARG:O	2:B:1138:ARG:HG2	2.11	0.49
1:A:389:THR:HG22	1:A:449:HIS:HA	1.95	0.49
2:B:166:LEU:HB3	2:B:170:ASP:HB2	1.94	0.49
5:E:14:ARG:O	5:E:18:MET:HG2	2.12	0.49
10:J:7:CYS:HB3	10:J:10:CYS:SG	2.52	0.49
18:R:177:ASN:HD21	18:R:202:PHE:HE2	1.60	0.49
1:A:1272:GLU:C	1:A:1274:GLU:N	2.66	0.49
2:B:240:LEU:HD23	2:B:257:VAL:HG11	1.95	0.49
2:B:342:VAL:HG13	2:B:346:GLU:HB2	1.94	0.49
6:F:45:PRO:HD3	6:F:115:TYR:CZ	2.48	0.49
9:I:28:GLU:OE2	9:I:33:ARG:NH1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:88:LYS:HD2	9:I:121:HIS:HE1	1.77	0.49
12:L:19:CYS:HB2	12:L:36:CYS:SG	2.53	0.49
13:M:105:ARG:NH1	23:Y:64:DC:OP1	2.45	0.49
17:Q:106:LYS:O	18:R:218:LYS:HE3	2.12	0.49
20:T:162:ASN:O	20:T:165:TYR:HB3	2.13	0.49
1:A:16:ARG:N	2:B:1148:LEU:O	2.32	0.49
1:A:456:VAL:O	1:A:472:HIS:N	2.35	0.49
1:A:527:THR:N	1:A:532:ARG:O	2.36	0.49
1:A:926:ASN:OD1	1:A:927:GLU:N	2.45	0.49
2:B:89:GLU:OE2	20:T:140:ARG:NH1	2.46	0.49
2:B:92:TYR:CG	20:T:145:LEU:HD13	2.48	0.49
2:B:1142:ASN:ND2	2:B:1145:GLN:HG2	2.28	0.49
3:C:94:CYS:O	3:C:98:SER:N	2.46	0.49
11:K:109:ILE:HA	11:K:112:LYS:NZ	2.27	0.49
1:A:97:VAL:HG21	1:A:322:LEU:HD11	1.95	0.49
1:A:364:ARG:HG3	1:A:501:MET:O	2.12	0.49
1:A:581:LYS:HB2	8:H:91:VAL:H	1.78	0.49
1:A:1169:VAL:HG22	1:A:1220:HIS:NE2	2.28	0.49
1:A:1309:MET:O	1:A:1336:LEU:HA	2.13	0.49
1:A:1319:LYS:HE3	1:A:1331:LEU:HD23	1.95	0.49
13:M:169:ARG:HD3	13:M:207:ASP:H	1.77	0.49
15:O:11:LEU:HG	15:O:40:PHE:HZ	1.77	0.49
1:A:525:ILE:O	1:A:534:VAL:N	2.36	0.49
1:A:1143:LEU:HB3	1:A:1147:SER:CB	2.42	0.49
1:A:1223:ASP:OD2	1:A:1224:ARG:NH2	2.45	0.49
1:A:1372:GLU:CD	5:E:195:ARG:HH21	2.15	0.49
2:B:89:GLU:HG3	2:B:90:GLN:H	1.77	0.49
2:B:763:SER:HA	2:B:766:TYR:CD2	2.47	0.49
3:C:27:ASP:HB3	3:C:30:VAL:HG23	1.95	0.49
11:K:81:TYR:HE2	11:K:86:ALA:HB2	1.78	0.49
1:A:540:ASP:HB3	1:A:680:LEU:HD21	1.94	0.49
1:A:781:ILE:HA	1:A:784:VAL:HG22	1.95	0.49
1:A:802:PHE:HZ	2:B:670:GLU:O	1.96	0.49
2:B:915:GLY:HA3	13:M:133:ASN:OD1	2.13	0.49
7:G:95:VAL:HG11	17:Q:127:PHE:CZ	2.48	0.49
12:L:14:PRO:O	12:L:27:GLU:OE1	2.30	0.49
1:A:432:HIS:HE2	1:A:438:LEU:HD13	1.77	0.49
1:A:821:GLY:HA2	1:A:838:PHE:CD2	2.48	0.49
2:B:798:ARG:O	2:B:801:VAL:HB	2.13	0.49
2:B:835:GLU:OE1	2:B:835:GLU:N	2.46	0.49
2:B:936:ALA:O	2:B:1049:GLN:N	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:44:ARG:HD2	4:D:47:GLN:OE1	2.12	0.49
8:H:62:SER:HA	8:H:141:VAL:HA	1.93	0.49
11:K:56:VAL:HA	11:K:77:THR:HG22	1.95	0.49
1:A:987:ILE:HG23	1:A:1060:LEU:HD11	1.95	0.49
2:B:418:TYR:OH	2:B:433:LEU:HD23	2.13	0.49
2:B:956:PHE:HD2	2:B:960:GLY:HA2	1.77	0.49
8:H:105:SER:HB2	8:H:108:ALA:HB2	1.93	0.49
20:T:155:PRO:C	20:T:157:ALA:H	2.14	0.49
1:A:903:PHE:HA	1:A:978:VAL:HA	1.95	0.48
1:A:1031:ARG:HA	1:A:1034:GLN:HB3	1.94	0.48
1:A:1189:ASP:HA	1:A:1192:TRP:HD1	1.77	0.48
1:A:1310:HIS:CE1	1:A:1334:TRP:HA	2.47	0.48
2:B:573:TRP:HZ2	2:B:576:ILE:HG23	1.78	0.48
2:B:867:ILE:HB	2:B:894:THR:HB	1.94	0.48
3:C:210:GLU:O	3:C:213:GLU:HB2	2.13	0.48
8:H:105:SER:O	8:H:106:THR:HB	2.12	0.48
13:M:117:ALA:O	13:M:121:ILE:N	2.46	0.48
21:U:218:ASP:O	21:U:222:ARG:HB3	2.10	0.48
1:A:604:ARG:HA	1:A:604:ARG:HD3	1.58	0.48
1:A:1372:GLU:OE1	5:E:193:ILE:HG21	2.13	0.48
3:C:45:ILE:CG1	3:C:79:VAL:HB	2.36	0.48
3:C:266:GLU:O	3:C:270:ASP:HB2	2.13	0.48
5:E:149:VAL:HB	5:E:192:LYS:HE2	1.94	0.48
9:I:57:LYS:HE2	9:I:60:HIS:CE1	2.48	0.48
1:A:642:LYS:NZ	21:U:283:GLU:HA	2.29	0.48
1:A:1220:HIS:HA	1:A:1223:ASP:HB3	1.93	0.48
1:A:1304:ILE:HG22	1:A:1340:GLY:HA3	1.95	0.48
2:B:57:ARG:O	2:B:61:ASP:N	2.46	0.48
2:B:209:ALA:HB1	2:B:211:LYS:HG3	1.96	0.48
2:B:294:ASP:OD2	2:B:379:ARG:NH2	2.44	0.48
2:B:932:GLY:N	2:B:945:CYS:O	2.37	0.48
2:B:1003:ASN:ND2	2:B:1007:ASN:OD1	2.42	0.48
2:B:1068:GLN:O	2:B:1072:ARG:N	2.45	0.48
3:C:134:ASN:OD1	3:C:135:ARG:N	2.46	0.48
5:E:28:VAL:HG13	5:E:32:GLU:OE1	2.13	0.48
9:I:103:ARG:O	9:I:104:ALA:C	2.52	0.48
13:M:295:ARG:NH2	13:M:298:ASP:OD2	2.45	0.48
21:U:225:ALA:HB3	21:U:228:MET:HG2	1.94	0.48
1:A:65:ILE:HD11	1:A:258:LEU:HB2	1.96	0.48
1:A:1117:VAL:O	1:A:1118:THR:O	2.30	0.48
2:B:26:CYS:O	2:B:29:VAL:HB	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:837:CYS:HB3	2:B:840:MET:HE3	1.96	0.48
2:B:848:LEU:HD23	2:B:852:GLY:HA2	1.95	0.48
3:C:105:VAL:HG12	3:C:159:LEU:HB3	1.95	0.48
3:C:262:GLN:O	3:C:266:GLU:HG2	2.14	0.48
13:M:178:LYS:O	20:T:154:LYS:HB2	1.94	0.48
16:P:299:ARG:HA	16:P:299:ARG:HD2	1.47	0.48
17:Q:71:PHE:HA	17:Q:100:VAL:CG2	2.40	0.48
17:Q:124:ARG:HG2	17:Q:126:SER:H	1.76	0.48
1:A:616:GLY:HA2	1:A:619:LYS:HD3	1.96	0.48
2:B:562:ALA:O	2:B:610:ARG:NH2	2.38	0.48
14:N:345:SER:O	14:N:347:ASN:N	2.43	0.48
21:U:145:ARG:NE	21:U:173:GLU:OE1	2.34	0.48
22:X:4:DG:H2"	22:X:5:DG:C8	2.49	0.48
1:A:14:PRO:HG2	1:A:16:ARG:NH1	2.29	0.48
1:A:140:ARG:NH1	1:A:234:PHE:O	2.47	0.48
1:A:156:GLY:HA2	1:A:181:HIS:CE1	2.49	0.48
1:A:426:ARG:N	13:M:40:VAL:CG2	2.77	0.48
1:A:660:MET:HB3	1:A:664:ILE:HB	1.94	0.48
1:A:798:ILE:O	1:A:820:ARG:NE	2.46	0.48
1:A:981:CYS:SG	1:A:1075:LYS:HB3	2.54	0.48
2:B:1163:MET:HA	2:B:1167:ILE:O	2.13	0.48
11:K:40:HIS:CE1	11:K:63:VAL:H	2.31	0.48
17:Q:123:ASN:O	17:Q:123:ASN:ND2	2.45	0.48
19:S:49:ARG:HB3	19:S:96:GLN:HB3	1.96	0.48
22:X:15:DA:H2"	22:X:16:DA:C8	2.49	0.48
1:A:345:GLY:O	1:A:351:ARG:HB3	2.13	0.48
1:A:1191:GLU:HG2	9:I:1:MET:SD	2.54	0.48
4:D:124:ASP:HA	4:D:127:LEU:HB3	1.96	0.48
5:E:39:GLU:O	5:E:43:GLN:N	2.40	0.48
5:E:41:LYS:O	5:E:46:ASP:N	2.42	0.48
6:F:108:ARG:HB2	6:F:116:GLU:HG3	1.96	0.48
7:G:97:LEU:HD13	7:G:128:TYR:CD2	2.48	0.48
12:L:22:CYS:HB3	12:L:39:CYS:CB	2.40	0.48
18:R:170:ASP:OD1	18:R:180:LYS:NZ	2.34	0.48
1:A:253:LEU:HD12	1:A:254:PRO:HD2	1.96	0.48
1:A:817:PRO:HB2	1:A:822:PHE:CB	2.42	0.48
2:B:97:THR:HG22	2:B:107:PRO:HA	1.95	0.48
2:B:133:ILE:HG23	2:B:139:GLN:HE21	1.79	0.48
2:B:675:LEU:HD21	2:B:697:GLU:OE2	2.13	0.48
5:E:106:VAL:HG23	5:E:129:GLN:HE22	1.78	0.48
6:F:86:GLU:N	6:F:86:GLU:OE1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:38:GLU:HG2	12:L:39:CYS:N	2.27	0.48
17:Q:166:SER:OG	17:Q:170:LYS:HB3	2.13	0.48
19:S:127:PHE:HB2	20:T:19:TRP:CB	2.43	0.48
23:Y:89:DC:H2"	23:Y:90:DC:C5	2.49	0.48
1:A:71:CYS:O	1:A:75:ALA:N	2.47	0.48
1:A:426:ARG:H	13:M:40:VAL:HG21	1.79	0.48
1:A:921:ARG:HB2	1:A:956:PHE:CZ	2.48	0.48
2:B:1029:TYR:CE1	2:B:1036:LYS:HG2	2.48	0.48
7:G:14:HIS:HB3	7:G:17:TYR:CD2	2.49	0.48
13:M:244:LEU:HD11	13:M:295:ARG:HD3	1.95	0.48
16:P:169:VAL:HB	16:P:257:ASN:HB3	1.96	0.48
17:Q:105:TYR:HD1	18:R:234:GLU:OE1	1.97	0.48
22:X:14:DA:H2"	22:X:15:DA:H8	1.79	0.48
1:A:775:LYS:HB3	2:B:974:SER:HB3	1.95	0.48
1:A:927:GLU:O	1:A:931:ARG:HB2	2.14	0.48
2:B:198:GLU:O	2:B:488:PRO:HD3	2.14	0.48
2:B:1130:THR:HB	2:B:1134:THR:N	2.28	0.48
7:G:97:LEU:HD13	7:G:128:TYR:HD2	1.79	0.48
9:I:25:TYR:N	9:I:38:ALA:O	2.40	0.48
14:N:317:GLU:C	16:P:239:ARG:HG3	2.34	0.48
15:O:76:LEU:HD13	15:O:95:ILE:HD12	1.95	0.48
21:U:174:GLU:O	21:U:178:GLN:N	2.42	0.48
1:A:198:LEU:HB3	1:A:216:LEU:HD12	1.95	0.47
1:A:702:ILE:HG23	1:A:752:THR:HB	1.96	0.47
1:A:913:ASN:OD1	1:A:967:ARG:NH2	2.47	0.47
1:A:959:MET:HE1	1:A:1047:SER:HA	1.95	0.47
1:A:1430:CYS:HB2	1:A:1435:THR:HA	1.96	0.47
2:B:10:TYR:HE2	2:B:12:GLU:HB3	1.79	0.47
2:B:438:ARG:HA	2:B:441:SER:HB2	1.96	0.47
3:C:33:SER:O	3:C:37:VAL:HG23	2.14	0.47
6:F:45:PRO:HA	6:F:115:TYR:O	2.14	0.47
10:J:30:THR:HG22	10:J:33:ASP:H	1.78	0.47
12:L:16:ILE:O	12:L:17:TYR:CG	2.67	0.47
17:Q:55:ASP:HB3	17:Q:58:GLN:HB2	1.96	0.47
17:Q:187:ILE:HD11	18:R:211:SER:N	2.29	0.47
2:B:956:PHE:CD2	2:B:960:GLY:HA2	2.49	0.47
2:B:1040:GLN:HG2	3:C:203:TRP:CZ2	2.48	0.47
17:Q:110:MET:HB3	18:R:218:LYS:CG	2.24	0.47
18:R:192:VAL:HG12	18:R:201:LEU:O	2.14	0.47
1:A:101:VAL:O	1:A:105:LYS:HG3	2.14	0.47
1:A:465:HIS:CE1	1:A:467:MET:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:388:TYR:HE1	2:B:502:HIS:HB3	1.80	0.47
3:C:16:ASP:HA	3:C:240:ARG:HG3	1.96	0.47
9:I:105:GLU:HG3	9:I:107:ALA:HB2	1.96	0.47
17:Q:126:SER:HB2	17:Q:136:PHE:O	2.14	0.47
1:A:111:CYS:HA	1:A:188:GLN:NE2	2.29	0.47
1:A:376:ASP:OD2	1:A:473:ARG:NE	2.47	0.47
1:A:478:PRO:HB3	11:K:4:PRO:HD2	1.96	0.47
1:A:592:PHE:CE2	1:A:596:ILE:HD11	2.49	0.47
2:B:242:ARG:HH21	2:B:252:ILE:HD11	1.80	0.47
2:B:309:PHE:HE2	9:I:25:TYR:CE2	2.32	0.47
2:B:780:VAL:HG21	2:B:1048:TYR:CE2	2.50	0.47
3:C:109:GLU:OE1	3:C:109:GLU:N	2.37	0.47
9:I:102:ALA:C	9:I:104:ALA:H	2.16	0.47
15:O:64:THR:OG1	15:O:75:VAL:HB	2.14	0.47
2:B:936:ALA:HA	2:B:942:LYS:HA	1.95	0.47
2:B:1028:LEU:HB2	2:B:1041:ILE:HD13	1.95	0.47
5:E:173:ILE:N	5:E:208:LEU:O	2.41	0.47
7:G:52:ASP:H	7:G:72:TYR:HA	1.79	0.47
16:P:180:LEU:HA	16:P:183:ILE:HD12	1.97	0.47
17:Q:154:CYS:SG	17:Q:155:THR:N	2.88	0.47
1:A:204:HIS:CD2	1:A:207:GLU:HG2	2.50	0.47
1:A:868:MET:HB2	1:A:1092:ALA:HB2	1.95	0.47
2:B:273:PHE:CD1	2:B:284:ILE:HG23	2.49	0.47
2:B:626:LEU:HG	2:B:698:ILE:HD13	1.95	0.47
6:F:52:ILE:HG21	6:F:110:LEU:HD21	1.97	0.47
6:F:99:ALA:O	6:F:100:ARG:HG2	2.14	0.47
18:R:213:ASP:C	18:R:215:GLU:H	2.14	0.47
1:A:391:ALA:HB2	1:A:447:GLU:HG2	1.97	0.47
1:A:597:PRO:HB2	1:A:660:MET:HE3	1.95	0.47
3:C:169:PHE:HZ	11:K:10:PHE:CZ	2.32	0.47
5:E:20:LEU:HD12	5:E:182:TYR:CE1	2.49	0.47
6:F:80:MET:HG3	6:F:103:PRO:HD3	1.97	0.47
8:H:112:LEU:HB3	8:H:131:ASN:HD21	1.80	0.47
9:I:96:PHE:HD2	9:I:110:LEU:HD22	1.79	0.47
11:K:35:ILE:HB	11:K:71:ILE:CG1	2.44	0.47
18:R:208:CYS:C	18:R:209:GLN:O	2.48	0.47
2:B:274:ARG:NH2	2:B:312:GLN:OE1	2.45	0.47
2:B:604:ILE:O	2:B:613:ARG:N	2.44	0.47
3:C:24:GLU:HG2	3:C:228:ARG:HA	1.97	0.47
12:L:25:GLU:O	12:L:37:ARG:NH1	2.47	0.47
14:N:332:GLU:HB3	15:O:92:LYS:HE2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:161:TYR:O	20:T:164:GLU:HB3	2.15	0.47
2:B:1036:LYS:HB2	3:C:194:HIS:CB	2.43	0.47
12:L:26:ASN:HA	12:L:37:ARG:NH1	2.26	0.47
16:P:167:ASN:ND2	23:Y:79:DT:H1'	2.30	0.47
18:R:210:PHE:O	18:R:212:VAL:CB	2.61	0.47
19:S:10:ASN:O	20:T:47:LYS:HB2	2.15	0.47
19:S:42:TRP:CD1	19:S:102:VAL:HG11	2.50	0.47
21:U:184:ASP:O	21:U:188:LYS:HG3	2.15	0.47
1:A:609:HIS:N	1:A:610:PRO:HD3	2.29	0.47
1:A:1307:VAL:CG2	1:A:1338:THR:CA	2.93	0.47
1:A:1468:THR:O	6:F:64:ARG:NH2	2.42	0.47
2:B:46:SER:HB2	2:B:395:LEU:HD23	1.95	0.47
2:B:499:ARG:HB3	2:B:499:ARG:HH11	1.75	0.47
2:B:539:SER:HA	2:B:542:LEU:HB3	1.97	0.47
2:B:685:LYS:HA	2:B:688:ALA:HB2	1.97	0.47
6:F:108:ARG:HB2	6:F:116:GLU:CG	2.45	0.47
8:H:65:TYR:CE1	8:H:79:ASP:CG	2.71	0.47
15:O:4:GLN:OE1	15:O:4:GLN:N	2.43	0.47
1:A:601:ASN:ND2	1:A:632:ASN:H	2.09	0.46
3:C:8:THR:H	3:C:25:ASN:HB3	1.79	0.46
5:E:188:GLY:HA2	5:E:208:LEU:HD21	1.97	0.46
12:L:18:ILE:N	12:L:45:TYR:O	2.47	0.46
13:M:39:LEU:CD1	13:M:41:VAL:HG13	2.45	0.46
13:M:48:VAL:O	13:M:52:TRP:N	2.48	0.46
17:Q:104:LYS:NZ	18:R:238:LYS:CE	2.78	0.46
17:Q:188:TYR:CD2	17:Q:192:ARG:HB2	2.49	0.46
1:A:922:PHE:CE2	1:A:952:LEU:HD21	2.39	0.46
2:B:255:ARG:HG2	2:B:307:GLU:OE2	2.15	0.46
2:B:551:GLU:HB3	2:B:556:ILE:HD13	1.96	0.46
10:J:67:LYS:NZ	12:L:23:HIS:O	2.47	0.46
11:K:99:SER:O	11:K:103:GLU:HG3	2.15	0.46
17:Q:25:PHE:CB	18:R:215:GLU:OE2	2.63	0.46
1:A:60:PRO:HG2	1:A:62:GLN:HB3	1.97	0.46
1:A:74:CYS:HA	2:B:1129:ASN:O	2.15	0.46
1:A:452:ASP:HA	1:A:474:VAL:HG23	1.97	0.46
1:A:1290:SER:OG	2:B:250:SER:C	2.53	0.46
1:A:1371:ILE:HD11	1:A:1406:THR:HG22	1.98	0.46
2:B:455:ASP:C	2:B:457:LYS:H	2.18	0.46
2:B:1061:SER:HA	2:B:1084:LEU:HD11	1.96	0.46
2:B:1132:THR:HG23	2:B:1133:HIS:CD2	2.50	0.46
9:I:12:VAL:HG11	9:I:15:ARG:NH2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:10:LEU:H	13:M:11:PRO:HD3	1.34	0.46
13:M:15:CYS:HB2	13:M:18:HIS:O	2.16	0.46
17:Q:106:LYS:HG2	18:R:218:LYS:CD	2.45	0.46
21:U:291:CYS:N	21:U:296:ASN:O	2.36	0.46
23:Y:66:DC:H2"	23:Y:67:DC:C6	2.50	0.46
1:A:662:HIS:NE2	6:F:127:ASP:OD2	2.28	0.46
2:B:172:CYS:HB2	10:J:62:TYR:CG	2.51	0.46
2:B:386:ASP:HB3	2:B:502:HIS:HD2	1.80	0.46
2:B:1114:TYR:CD1	2:B:1153:TYR:HB2	2.50	0.46
3:C:53:ASP:N	3:C:160:ARG:O	2.48	0.46
7:G:95:VAL:HG11	17:Q:127:PHE:HZ	1.79	0.46
8:H:50:VAL:HG13	8:H:56:PHE:CZ	2.51	0.46
14:N:32:ASP:HB3	14:N:34:VAL:HG23	1.98	0.46
14:N:349:TRP:HH2	16:P:191:GLU:OE2	1.98	0.46
17:Q:104:LYS:HZ2	18:R:238:LYS:CD	2.25	0.46
17:Q:105:TYR:HA	18:R:234:GLU:CD	2.35	0.46
18:R:140:LYS:HB2	18:R:141:PRO:HD3	1.96	0.46
22:X:12:DA:N6	23:Y:82:DT:H3	2.14	0.46
1:A:18:ILE:HD11	1:A:1460:LEU:CD2	2.46	0.46
1:A:76:GLY:HA3	2:B:1131:ARG:NH2	2.31	0.46
1:A:619:LYS:O	1:A:620:HIS:CG	2.69	0.46
2:B:249:LYS:HE3	2:B:249:LYS:HB3	1.41	0.46
2:B:752:TYR:HE1	2:B:809:VAL:CG2	2.29	0.46
3:C:4:ALA:HB1	11:K:97:GLU:OE1	2.14	0.46
6:F:56:TYR:HD1	6:F:124:ILE:HB	1.81	0.46
13:M:118:PHE:CE1	13:M:142:PHE:HB3	2.51	0.46
16:P:289:PRO:HB2	23:Y:83:DA:H4'	1.97	0.46
19:S:26:TYR:HB2	19:S:139:PRO:O	2.16	0.46
20:T:228:ILE:HA	22:X:30:DG:H5"	1.97	0.46
1:A:520:MET:HB3	1:A:522:PRO:HD2	1.97	0.46
1:A:994:PHE:CZ	1:A:1064:ALA:HA	2.50	0.46
2:B:1130:THR:N	2:B:1134:THR:O	2.48	0.46
3:C:14:LEU:HB3	3:C:19:VAL:HG23	1.98	0.46
5:E:71:GLN:O	5:E:100:THR:OG1	2.25	0.46
8:H:110:THR:O	8:H:111:ARG:HB2	2.13	0.46
10:J:35:LEU:HB3	10:J:46:ARG:HD2	1.98	0.46
14:N:343:HIS:O	14:N:350:LYS:N	2.36	0.46
16:P:268:ILE:HD13	16:P:332:LEU:HG	1.98	0.46
17:Q:110:MET:O	17:Q:113:ARG:HB3	2.16	0.46
23:Y:89:DC:H2"	23:Y:90:DC:C6	2.51	0.46
1:A:357:LYS:HE3	2:B:1073:GLN:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ILE:O	1:A:388:MET:N	2.43	0.46
1:A:432:HIS:NE2	1:A:438:LEU:HD13	2.31	0.46
1:A:788:VAL:HB	1:A:823:VAL:HB	1.98	0.46
1:A:848:ILE:HD13	2:B:499:ARG:HG3	1.97	0.46
1:A:1274:GLU:HG3	1:A:1276:VAL:HG23	1.97	0.46
2:B:242:ARG:O	2:B:244:GLY:N	2.49	0.46
2:B:425:ARG:HD3	2:B:427:LYS:HD2	1.98	0.46
2:B:1066:PRO:HB2	2:B:1075:MET:HG3	1.98	0.46
3:C:54:ALA:HB3	3:C:160:ARG:HB2	1.97	0.46
5:E:122:ALA:HB3	5:E:125:TYR:HB3	1.98	0.46
13:M:279:GLY:HA2	20:T:153:TYR:HE1	1.81	0.46
17:Q:185:GLU:O	17:Q:189:ALA:N	2.48	0.46
19:S:109:LYS:HD2	19:S:149:LEU:HD23	1.97	0.46
1:A:63:GLY:HA3	1:A:258:LEU:HD23	1.98	0.46
1:A:364:ARG:HB2	1:A:502:ASN:OD1	2.16	0.46
1:A:408:ARG:HH11	1:A:414:PRO:HB2	1.79	0.46
1:A:527:THR:HG22	1:A:532:ARG:O	2.16	0.46
1:A:611:ASP:CB	1:A:626:THR:OG1	2.64	0.46
2:B:573:TRP:CH2	2:B:575:GLY:HA2	2.51	0.46
2:B:910:THR:HB	12:L:43:ILE:HD13	1.98	0.46
6:F:116:GLU:HG3	6:F:118:TRP:HE1	1.81	0.46
16:P:209:THR:HG21	16:P:224:ALA:CB	2.46	0.46
18:R:190:LEU:O	18:R:203:PHE:N	2.49	0.46
20:T:172:ASP:OD1	20:T:173:GLY:N	2.48	0.46
1:A:557:ARG:HD2	8:H:75:TYR:CE2	2.49	0.46
1:A:1274:GLU:O	1:A:1276:VAL:N	2.49	0.46
1:A:1310:HIS:CG	21:U:252:LYS:HG2	2.50	0.46
2:B:26:CYS:O	2:B:30:ILE:HG13	2.15	0.46
2:B:63:PRO:HG2	2:B:64:PRO:HD3	1.97	0.46
2:B:240:LEU:HD13	2:B:242:ARG:HD3	1.97	0.46
2:B:1093:CYS:O	2:B:1097:HIS:N	2.49	0.46
3:C:117:SER:HB2	3:C:130:VAL:HG11	1.98	0.46
8:H:107:GLU:OE1	8:H:107:GLU:HA	2.15	0.46
9:I:73:SER:HB2	9:I:115:THR:OG1	2.15	0.46
9:I:81:THR:HG22	9:I:94:ALA:O	2.16	0.46
12:L:17:TYR:O	12:L:25:GLU:HA	2.15	0.46
13:M:268:LYS:O	13:M:269:ARG:NH1	2.37	0.46
20:T:30:GLN:O	20:T:62:LEU:HD11	2.16	0.46
1:A:930:LEU:HD11	8:H:107:GLU:OE2	2.16	0.46
1:A:1030:SER:O	1:A:1034:GLN:N	2.41	0.46
2:B:29:VAL:HG22	2:B:643:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:451:GLY:HA2	2:B:467:SER:HB3	1.97	0.46
2:B:520:VAL:C	2:B:522:LEU:H	2.20	0.46
2:B:1062:ARG:NH2	2:B:1074:PRO:HB3	2.31	0.46
8:H:117:SER:HA	8:H:121:LEU:O	2.16	0.46
9:I:56:ASN:CG	9:I:57:LYS:H	2.20	0.46
12:L:25:GLU:CG	12:L:27:GLU:HG2	2.46	0.46
13:M:185:ARG:HA	20:T:158:ASN:HB2	1.98	0.46
20:T:177:ARG:HH21	20:T:212:TYR:HB2	1.81	0.46
20:T:197:TYR:HB2	20:T:202:LEU:HD21	1.98	0.46
20:T:198:ASN:HD21	20:T:200:LYS:HZ3	1.64	0.46
22:X:42:DA:H2"	22:X:43:DG:H8	1.81	0.46
1:A:721:HIS:O	9:I:109:ARG:HA	2.16	0.45
2:B:876:ASN:OD1	2:B:879:GLU:OE2	2.34	0.45
1:A:909:LEU:HD13	1:A:973:GLY:HA2	1.98	0.45
1:A:1036:ASN:OD1	1:A:1037:ALA:N	2.49	0.45
2:B:89:GLU:HB3	2:B:127:ASP:HB3	1.98	0.45
2:B:175:ASN:HA	10:J:62:TYR:CD2	2.51	0.45
2:B:295:PRO:O	2:B:299:GLU:HG2	2.16	0.45
2:B:834:ARG:HA	2:B:840:MET:SD	2.55	0.45
2:B:939:HIS:CD2	2:B:980:HIS:HA	2.50	0.45
3:C:212:ASP:O	3:C:213:GLU:C	2.50	0.45
5:E:72:MET:HG3	5:E:101:ARG:HB2	1.97	0.45
7:G:165:ASP:HB2	7:G:168:LEU:HD11	1.98	0.45
8:H:2:ALA:O	8:H:4:ILE:N	2.50	0.45
17:Q:12:ALA:O	17:Q:15:LYS:HB2	2.15	0.45
20:T:146:ASP:OD2	20:T:147:LYS:HG2	2.16	0.45
1:A:51:ARG:H	1:A:52:PRO:HD2	1.81	0.45
1:A:75:ALA:C	2:B:1131:ARG:HH21	2.19	0.45
1:A:452:ASP:CG	1:A:476:ILE:HG12	2.36	0.45
1:A:1085:GLU:OE1	6:F:60:TYR:OH	2.28	0.45
2:B:93:LEU:H	20:T:145:LEU:HB3	1.81	0.45
8:H:10:PHE:CE2	8:H:58:LEU:HD13	2.52	0.45
9:I:25:TYR:HD2	9:I:40:ARG:HG3	1.81	0.45
17:Q:18:ALA:O	17:Q:22:ILE:HG23	2.15	0.45
20:T:139:VAL:O	20:T:140:ARG:HB3	2.11	0.45
21:U:136:THR:OG1	21:U:141:ARG:NH1	2.49	0.45
1:A:385:ALA:HB2	1:A:476:ILE:HD12	1.98	0.45
1:A:478:PRO:HB2	1:A:479:TRP:CE3	2.52	0.45
1:A:1137:PRO:HA	1:A:1360:ASN:HD21	1.80	0.45
2:B:125:TYR:HE2	20:T:148:VAL:O	1.99	0.45
3:C:11:ILE:HA	3:C:21:PHE:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:116:GLU:O	7:G:130:THR:HA	2.16	0.45
13:M:39:LEU:HD12	13:M:41:VAL:HG13	1.99	0.45
20:T:198:ASN:OD1	20:T:199:LEU:N	2.50	0.45
21:U:133:ALA:HB2	21:U:167:GLU:HG3	1.98	0.45
23:Y:53:DG:H2"	23:Y:54:DA:C8	2.51	0.45
1:A:956:PHE:HA	1:A:959:MET:HB2	1.99	0.45
1:A:1301:ILE:O	1:A:1304:ILE:HG12	2.16	0.45
2:B:128:ILE:HB	2:B:145:GLN:HB2	1.99	0.45
2:B:369:VAL:O	2:B:373:LEU:N	2.41	0.45
2:B:384:ASP:OD2	2:B:387:HIS:N	2.49	0.45
2:B:631:GLN:O	2:B:683:GLN:HG2	2.16	0.45
2:B:845:TYR:OH	2:B:891:ASP:OD1	2.33	0.45
2:B:1029:TYR:CD1	2:B:1036:LYS:HG2	2.51	0.45
11:K:64:PRO:HD2	11:K:70:LYS:O	2.16	0.45
13:M:123:THR:O	13:M:127:ARG:NH2	2.50	0.45
16:P:209:THR:CG2	16:P:223:GLY:HA3	2.36	0.45
16:P:264:VAL:HG23	16:P:266:PHE:H	1.81	0.45
16:P:297:LYS:CE	16:P:297:LYS:CA	2.89	0.45
17:Q:70:LYS:HB2	18:R:225:VAL:CG1	2.47	0.45
1:A:431:PHE:HD2	13:M:33:ILE:HG21	1.82	0.45
1:A:514:GLU:OE1	2:B:1099:ALA:HB1	2.17	0.45
2:B:68:GLN:HA	2:B:83:ARG:HA	1.98	0.45
2:B:201:ALA:HA	2:B:392:ARG:HG2	1.98	0.45
2:B:881:GLU:HA	2:B:883:THR:OG1	2.16	0.45
6:F:44:ARG:HB3	6:F:114:SER:HA	1.97	0.45
8:H:57:ARG:O	8:H:145:MET:HA	2.17	0.45
8:H:98:ARG:HD3	8:H:115:TYR:CD2	2.48	0.45
18:R:202:PHE:O	18:R:203:PHE:CE1	2.64	0.45
21:U:299:LYS:HB2	21:U:301:CYS:O	2.17	0.45
1:A:84:HIS:N	1:A:257:PRO:HB3	2.32	0.45
1:A:548:PHE:HE2	1:A:592:PHE:HB2	1.81	0.45
1:A:1178:ASP:OD1	1:A:1184:THR:HA	2.16	0.45
2:B:281:ASP:CG	9:I:22:ASN:HD22	2.20	0.45
2:B:795:ILE:HG12	2:B:947:ILE:HG22	1.99	0.45
7:G:46:ILE:HD11	7:G:77:PHE:HB2	1.99	0.45
7:G:107:PHE:O	7:G:160:ILE:HG13	2.17	0.45
10:J:3:ILE:HD13	10:J:18:TRP:CB	2.47	0.45
13:M:177:PHE:O	13:M:181:CYS:N	2.38	0.45
14:N:25:VAL:HG11	15:O:36:VAL:HG13	1.99	0.45
16:P:329:TYR:N	16:P:330:PRO:HD2	2.32	0.45
1:A:1310:HIS:NE2	1:A:1334:TRP:HE3	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:193:VAL:HG11	2:B:481:HIS:CD2	2.52	0.45
2:B:640:ILE:HA	2:B:643:LEU:HD12	1.98	0.45
5:E:134:GLU:CD	5:E:181:ARG:HH12	2.20	0.45
7:G:60:GLN:HB2	7:G:63:ARG:NE	2.32	0.45
18:R:156:ASP:O	18:R:158:HIS:N	2.50	0.45
19:S:172:ASN:OD1	19:S:173:HIS:N	2.50	0.45
20:T:23:VAL:HG21	20:T:31:TRP:CZ3	2.52	0.45
1:A:1479:LYS:HD3	6:F:103:PRO:HA	1.99	0.45
2:B:66:ASP:HB3	2:B:85:LEU:HD13	1.99	0.45
2:B:738:THR:OG1	10:J:62:TYR:OH	2.23	0.45
2:B:780:VAL:HG21	2:B:1048:TYR:HE2	1.80	0.45
12:L:18:ILE:O	12:L:19:CYS:C	2.54	0.45
17:Q:145:PHE:HA	17:Q:152:PHE:HA	1.98	0.45
20:T:95:VAL:O	20:T:106:LEU:HD12	2.17	0.45
1:A:902:GLU:N	1:A:979:LEU:O	2.48	0.45
1:A:909:LEU:HD22	1:A:1328:PHE:CZ	2.51	0.45
1:A:926:ASN:OD1	1:A:931:ARG:HG3	2.17	0.45
2:B:939:HIS:HE2	2:B:983:GLU:HB2	1.82	0.45
11:K:105:PHE:O	11:K:109:ILE:HG12	2.16	0.45
18:R:155:LEU:HD11	18:R:203:PHE:HA	1.98	0.45
19:S:29:MET:HB2	20:T:96:PHE:CD1	2.52	0.45
20:T:138:PRO:O	20:T:141:LEU:HG	2.17	0.45
22:X:11:DT:H2"	22:X:12:DA:C8	2.52	0.45
1:A:404:GLU:OE1	1:A:407:ARG:HD2	2.17	0.44
1:A:579:ILE:HD12	1:A:585:LEU:HD12	1.99	0.44
1:A:972:THR:O	1:A:1317:LYS:HD3	2.17	0.44
1:A:1241:ASP:O	1:A:1262:MET:HG3	2.17	0.44
1:A:1361:ASP:OD2	1:A:1364:GLU:HG2	2.16	0.44
2:B:254:GLN:NE2	2:B:300:MET:SD	2.74	0.44
2:B:626:LEU:HA	2:B:662:VAL:HG12	1.98	0.44
3:C:6:GLN:HG2	3:C:25:ASN:HD21	1.77	0.44
3:C:37:VAL:HG12	3:C:248:ALA:HB1	1.99	0.44
4:D:83:VAL:HG13	4:D:134:ILE:HG12	1.99	0.44
12:L:13:GLN:O	12:L:29:LYS:HD3	2.17	0.44
20:T:145:LEU:HD11	20:T:148:VAL:CG2	2.46	0.44
20:T:165:TYR:O	20:T:169:LYS:HG2	2.17	0.44
22:X:14:DA:H2"	22:X:15:DA:C8	2.52	0.44
1:A:47:THR:C	1:A:48:GLU:HG2	2.38	0.44
1:A:431:PHE:HB2	13:M:33:ILE:HG21	1.99	0.44
1:A:556:GLU:HG3	1:A:559:GLU:H	1.82	0.44
1:A:894:ASP:OD1	1:A:1396:ARG:NH2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1022:ILE:HG12	1:A:1034:GLN:OE1	2.17	0.44
2:B:385:ARG:HD2	2:B:497:LYS:HE3	1.99	0.44
2:B:856:PRO:HD3	12:L:46:LYS:HD3	1.99	0.44
2:B:862:GLY:O	2:B:898:THR:HA	2.18	0.44
2:B:1117:HIS:CE1	2:B:1148:LEU:HD13	2.52	0.44
3:C:189:ASP:OD2	3:C:212:ASP:HB3	2.17	0.44
16:P:212:LEU:O	16:P:219:MET:HA	2.18	0.44
17:Q:23:ARG:CZ	18:R:207:SER:H	2.30	0.44
17:Q:187:ILE:HG21	18:R:212:VAL:CA	2.20	0.44
17:Q:187:ILE:O	18:R:212:VAL:HG12	2.17	0.44
20:T:199:LEU:HD13	20:T:233:TRP:NE1	2.32	0.44
20:T:227:GLY:C	22:X:30:DG:H5"	2.38	0.44
21:U:229:ALA:HB1	21:U:234:LYS:HB3	1.99	0.44
1:A:361:PHE:N	2:B:1062:ARG:O	2.50	0.44
1:A:395:THR:OG1	1:A:398:ASN:OD1	2.31	0.44
2:B:21:LEU:HD23	2:B:633:LEU:HD23	2.00	0.44
2:B:240:LEU:HD22	2:B:242:ARG:NH1	2.33	0.44
2:B:629:GLU:N	2:B:632:LYS:O	2.42	0.44
2:B:674:MET:HB2	9:I:77:THR:HG22	1.98	0.44
5:E:26:TYR:HD1	5:E:65:ASN:H	1.63	0.44
8:H:76:ASN:OD1	8:H:78:THR:OG1	2.33	0.44
16:P:309:LYS:HD2	23:Y:82:DT:H3'	2.00	0.44
21:U:177:TYR:CE1	21:U:181:ARG:HA	2.52	0.44
2:B:93:LEU:HD23	2:B:160:TYR:CE2	2.52	0.44
2:B:99:TRP:HB2	13:M:129:ASN:ND2	2.32	0.44
2:B:905:ASP:OD2	2:B:922:ARG:NE	2.44	0.44
3:C:200:PRO:CG	3:C:217:GLN:CD	2.68	0.44
5:E:192:LYS:HA	5:E:206:TYR:HD1	1.82	0.44
8:H:71:ASP:OD1	8:H:71:ASP:N	2.50	0.44
12:L:15:MET:HA	12:L:27:GLU:OE1	2.16	0.44
14:N:29:PHE:CE1	15:O:36:VAL:HG21	2.52	0.44
17:Q:55:ASP:O	17:Q:59:LEU:N	2.42	0.44
17:Q:135:THR:HG23	17:Q:164:ASP:OD1	2.18	0.44
21:U:223:MET:HB3	21:U:224:THR:H	1.58	0.44
1:A:578:ALA:N	1:A:585:LEU:O	2.51	0.44
1:A:926:ASN:ND2	1:A:931:ARG:CD	2.64	0.44
1:A:931:ARG:C	1:A:933:THR:H	2.19	0.44
2:B:83:ARG:HB3	2:B:133:ILE:O	2.17	0.44
2:B:134:LYS:HG3	2:B:136:GLY:H	1.83	0.44
2:B:627:ILE:HA	2:B:695:HIS:CD2	2.53	0.44
2:B:888:THR:O	2:B:890:ARG:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:888:THR:O	2:B:890:ARG:N	2.50	0.44
2:B:1056:ASP:OD1	2:B:1056:ASP:N	2.51	0.44
5:E:71:GLN:NE2	5:E:97:GLU:HG3	2.32	0.44
5:E:104:ILE:HG23	5:E:129:GLN:NE2	2.32	0.44
6:F:53:THR:HB	6:F:108:ARG:HH11	1.83	0.44
7:G:60:GLN:HB2	7:G:63:ARG:HE	1.82	0.44
8:H:94:GLY:HA3	8:H:118:TYR:HA	1.98	0.44
20:T:223:GLN:HB3	20:T:233:TRP:CE3	2.52	0.44
1:A:283:ILE:HA	1:A:286:ILE:HG12	2.00	0.44
1:A:607:SER:O	21:U:301:CYS:HA	2.17	0.44
1:A:1031:ARG:O	1:A:1035:GLU:N	2.42	0.44
2:B:11:ASP:HB2	2:B:638:ARG:HD3	2.00	0.44
9:I:17:CYS:O	9:I:21:ASN:N	2.46	0.44
9:I:96:PHE:HA	9:I:111:TYR:O	2.18	0.44
13:M:11:PRO:HB2	13:M:12:ARG:H	1.60	0.44
13:M:138:THR:HG23	13:M:163:CYS:HB3	1.99	0.44
15:O:64:THR:HG22	16:P:188:ARG:HB3	2.00	0.44
16:P:294:ARG:HH21	16:P:294:ARG:HG3	1.82	0.44
18:R:154:LEU:HD21	18:R:162:GLY:O	2.15	0.44
19:S:143:TRP:NE1	19:S:145:ASN:OD1	2.37	0.44
1:A:1199:MET:O	1:A:1201:ASP:N	2.51	0.44
2:B:169:ARG:HA	2:B:172:CYS:SG	2.57	0.44
2:B:655:ASP:HA	2:B:658:ALA:HB3	2.00	0.44
3:C:101:PHE:HA	3:C:121:ILE:O	2.18	0.44
4:D:44:ARG:HB2	4:D:61:PHE:CZ	2.53	0.44
7:G:84:VAL:HG12	7:G:144:ARG:HD3	1.98	0.44
8:H:39:LEU:HA	8:H:124:ARG:O	2.17	0.44
8:H:75:TYR:O	8:H:75:TYR:CG	2.70	0.44
14:N:337:CYS:O	15:O:97:ALA:HA	2.17	0.44
16:P:174:LEU:O	16:P:249:LYS:N	2.51	0.44
20:T:17:GLY:HA2	20:T:109:ILE:O	2.17	0.44
20:T:223:GLN:HB3	20:T:233:TRP:CD2	2.52	0.44
21:U:225:ALA:CB	21:U:228:MET:HG2	2.48	0.44
23:Y:49:DG:H2"	23:Y:50:DA:C8	2.53	0.44
1:A:349:ARG:O	1:A:353:ASN:HB2	2.17	0.44
1:A:1313:GLN:OE1	1:A:1335:ILE:HD13	2.18	0.44
2:B:663:GLU:OE2	2:B:695:HIS:NE2	2.50	0.44
10:J:63:ALA:CB	10:J:64:PRO:HD3	2.32	0.44
16:P:167:ASN:HB2	23:Y:80:DT:H4'	2.00	0.44
1:A:64:VAL:HB	1:A:70:ARG:O	2.18	0.44
1:A:129:ILE:CD1	1:A:140:ARG:HA	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:875:TYR:HE1	1:A:1470:CYS:SG	2.40	0.44
2:B:37:LYS:HE2	2:B:653:TRP:HD1	1.80	0.44
3:C:74:ILE:HG22	3:C:129:PRO:O	2.17	0.44
3:C:241:PRO:HA	3:C:244:ILE:HD12	2.00	0.44
6:F:68:THR:O	6:F:72:GLN:HG3	2.17	0.44
9:I:97:PHE:O	9:I:111:TYR:N	2.47	0.44
9:I:97:PHE:HD1	9:I:98:GLN:O	2.00	0.44
18:R:160:GLN:C	18:R:162:GLY:H	2.21	0.44
19:S:47:LEU:HG	19:S:98:TRP:CE3	2.53	0.44
20:T:225:VAL:HG23	20:T:227:GLY:H	1.83	0.44
21:U:176:ILE:HG22	21:U:187:TYR:CD2	2.53	0.44
1:A:43:TYR:O	1:A:45:GLU:N	2.51	0.43
1:A:367:ILE:HD13	1:A:494:ALA:HB1	1.99	0.43
1:A:1014:LYS:O	1:A:1018:LYS:HG3	2.18	0.43
2:B:198:GLU:OE1	2:B:487:SER:OG	2.33	0.43
2:B:280:SER:HB3	9:I:21:ASN:HB2	1.99	0.43
2:B:318:LEU:HD13	2:B:336:ILE:HG23	1.99	0.43
2:B:746:THR:O	2:B:812:ARG:HA	2.18	0.43
2:B:1030:ASN:OD1	2:B:1031:GLY:N	2.51	0.43
5:E:192:LYS:HG3	5:E:206:TYR:CE1	2.53	0.43
14:N:327:GLU:OE1	16:P:188:ARG:NH1	2.51	0.43
15:O:48:LEU:HD23	15:O:52:VAL:HG21	2.00	0.43
17:Q:45:GLU:OE1	17:Q:94:ILE:N	2.43	0.43
18:R:127:ASN:ND2	18:R:140:LYS:HD3	2.31	0.43
20:T:229:HIS:ND1	22:X:29:DC:O4’	2.51	0.43
21:U:150:ALA:HA	21:U:153:ARG:NH1	2.33	0.43
23:Y:55:DG:H2”	23:Y:56:DG:C8	2.53	0.43
1:A:908:THR:C	1:A:910:LYS:H	2.21	0.43
1:A:1369:LEU:HD23	5:E:139:ILE:HB	2.00	0.43
2:B:249:LYS:C	2:B:251:ALA:H	2.21	0.43
2:B:309:PHE:CD2	9:I:40:ARG:HD2	2.54	0.43
2:B:845:TYR:CE2	2:B:865:VAL:HG11	2.53	0.43
6:F:51:ARG:HD3	6:F:118:TRP:CZ2	2.53	0.43
7:G:49:THR:H	7:G:74:ALA:HA	1.82	0.43
8:H:50:VAL:HG13	8:H:56:PHE:HZ	1.83	0.43
13:M:178:LYS:O	20:T:154:LYS:CG	2.57	0.43
19:S:46:ARG:N	19:S:101:ARG:O	2.38	0.43
20:T:196:TYR:HD1	20:T:232:THR:HG21	1.83	0.43
20:T:198:ASN:HD21	20:T:200:LYS:HE2	1.83	0.43
21:U:216:PRO:HD2	21:U:219:LEU:HD23	1.99	0.43
22:X:16:DA:H2”	22:X:17:DA:N7	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:LYS:HE2	13:M:107:MET:HG3	1.99	0.43
2:B:431:LEU:O	2:B:435:ILE:HG12	2.17	0.43
2:B:602:SER:O	2:B:614:ILE:HG23	2.19	0.43
2:B:979:GLY:HA2	2:B:982:ILE:HD12	2.00	0.43
8:H:1:MET:HA	8:H:66:GLU:OE2	2.17	0.43
8:H:56:PHE:CE1	8:H:148:LEU:HA	2.54	0.43
14:N:363:ARG:NH2	15:O:86:GLU:OE2	2.51	0.43
17:Q:123:ASN:O	17:Q:125:ALA:N	2.50	0.43
18:R:163:LEU:O	18:R:164:GLY:C	2.56	0.43
20:T:141:LEU:HD13	20:T:143:GLN:NE2	2.32	0.43
21:U:266:CYS:O	21:U:267:LYS:HG2	2.18	0.43
1:A:20:ARG:HE	2:B:1174:VAL:C	2.22	0.43
1:A:137:PRO:HB3	1:A:237:GLY:CA	2.45	0.43
1:A:219:GLU:O	1:A:223:GLU:HG2	2.18	0.43
1:A:367:ILE:CD1	1:A:494:ALA:HB1	2.47	0.43
1:A:457:ILE:CG2	1:A:504:HIS:HB2	2.48	0.43
1:A:1184:THR:HG22	1:A:1190:GLN:HA	2.00	0.43
2:B:891:ASP:OD1	2:B:893:SER:OG	2.36	0.43
2:B:970:HIS:C	2:B:973:PRO:HD2	2.39	0.43
11:K:109:ILE:HA	11:K:112:LYS:HZ3	1.83	0.43
13:M:179:GLU:HG2	20:T:154:LYS:CE	2.48	0.43
15:O:57:ASN:OD1	15:O:58:PHE:N	2.51	0.43
16:P:174:LEU:HD22	16:P:248:ALA:HB1	2.00	0.43
1:A:28:PRO:HB3	1:A:251:THR:OG1	2.18	0.43
1:A:312:PHE:HE2	1:A:326:PRO:HB2	1.82	0.43
1:A:456:VAL:HG12	1:A:505:LEU:HD13	2.00	0.43
1:A:910:LYS:HB3	1:A:963:ARG:HH12	1.83	0.43
1:A:1151:ALA:HB2	1:A:1334:TRP:CZ2	2.53	0.43
1:A:1167:ARG:HA	1:A:1293:LEU:HD22	2.01	0.43
1:A:1345:ARG:O	1:A:1349:GLU:HG2	2.19	0.43
2:B:68:GLN:HG3	2:B:82:PRO:O	2.19	0.43
2:B:161:CYS:O	2:B:164:ASN:ND2	2.51	0.43
2:B:682:LEU:HD23	2:B:682:LEU:HA	1.82	0.43
4:D:96:GLU:OE2	4:D:117:SER:OG	2.22	0.43
17:Q:32:LEU:HD11	18:R:203:PHE:HD2	1.68	0.43
20:T:191:PHE:CD2	20:T:235:LEU:HG	2.54	0.43
1:A:391:ALA:HA	1:A:446:VAL:O	2.19	0.43
1:A:907:ALA:H	1:A:975:SER:HB3	1.82	0.43
1:A:1013:VAL:HG22	1:A:1049:LEU:HD23	2.00	0.43
2:B:360:LYS:HA	2:B:363:TYR:HD2	1.82	0.43
2:B:454:GLY:HA3	2:B:459:ALA:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:76:PHE:HA	5:E:77:PRO:HD2	1.82	0.43
5:E:112:PRO:HA	5:E:115:LYS:HD2	2.00	0.43
13:M:182:ALA:HB2	20:T:154:LYS:HG3	2.01	0.43
15:O:20:ASP:OD1	15:O:24:GLN:NE2	2.52	0.43
15:O:60:GLY:O	15:O:76:LEU:HD23	2.18	0.43
16:P:297:LYS:HE2	16:P:297:LYS:CA	2.48	0.43
18:R:210:PHE:CB	18:R:212:VAL:HG11	2.46	0.43
21:U:276:VAL:HG13	21:U:277:GLN:HG3	2.00	0.43
1:A:264:VAL:O	1:A:266:MET:HG3	2.19	0.43
1:A:1018:LYS:O	1:A:1021:VAL:HG23	2.18	0.43
1:A:1301:ILE:HD13	1:A:1342:SER:OG	2.19	0.43
2:B:442:ASP:HA	2:B:445:LYS:HD2	1.99	0.43
2:B:736:TYR:CD2	2:B:737:ILE:HG12	2.54	0.43
2:B:1036:LYS:HG3	3:C:186:TYR:OH	2.18	0.43
3:C:173:HIS:HB3	3:C:176:TRP:CE3	2.53	0.43
3:C:235:SER:HB2	3:C:241:PRO:HG3	1.99	0.43
4:D:74:PHE:CD2	4:D:80:ILE:HG12	2.54	0.43
7:G:94:LYS:O	7:G:110:ARG:HD2	2.18	0.43
10:J:21:TYR:CZ	10:J:25:LEU:HD21	2.54	0.43
14:N:46:TRP:CZ2	15:O:11:LEU:HD12	2.48	0.43
14:N:332:GLU:HB3	15:O:92:LYS:CE	2.49	0.43
15:O:64:THR:HG21	16:P:188:ARG:CZ	2.49	0.43
16:P:303:LEU:O	16:P:310:VAL:HA	2.18	0.43
17:Q:19:LYS:O	17:Q:22:ILE:HG13	2.19	0.43
17:Q:34:LEU:HD23	17:Q:37:LEU:HD12	2.00	0.43
21:U:262:THR:HA	21:U:269:LYS:HG2	2.00	0.43
1:A:19:LYS:N	2:B:1173:SER:HA	2.34	0.43
1:A:877:ALA:O	1:A:890:ARG:HA	2.19	0.43
1:A:967:ARG:HH11	1:A:967:ARG:HG3	1.84	0.43
1:A:1027:ASP:OD1	1:A:1027:ASP:N	2.52	0.43
1:A:1209:PRO:CB	9:I:33:ARG:HH12	2.23	0.43
1:A:1365:ILE:O	1:A:1370:GLY:N	2.46	0.43
2:B:240:LEU:HD23	2:B:257:VAL:HG21	2.00	0.43
2:B:588:ARG:O	2:B:592:ARG:N	2.41	0.43
2:B:654:GLN:O	2:B:658:ALA:N	2.39	0.43
2:B:777:ASN:O	10:J:47:ARG:HD2	2.19	0.43
8:H:90:TYR:O	8:H:144:LEU:HA	2.18	0.43
8:H:106:THR:C	8:H:108:ALA:N	2.71	0.43
13:M:169:ARG:HD3	13:M:206:VAL:HB	2.00	0.43
14:N:337:CYS:SG	14:N:353:LEU:HD13	2.58	0.43
15:O:60:GLY:HA3	15:O:79:VAL:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:209:THR:HG21	16:P:224:ALA:HB2	2.00	0.43
17:Q:22:ILE:HG21	17:Q:34:LEU:HB3	2.00	0.43
17:Q:104:LYS:NZ	18:R:238:LYS:HE3	2.34	0.43
19:S:53:ASN:HB2	19:S:96:GLN:OE1	2.19	0.43
20:T:21:VAL:HA	20:T:114:ALA:O	2.18	0.43
21:U:184:ASP:OD1	21:U:185:MET:N	2.52	0.43
1:A:805:ARG:NH2	2:B:671:GLU:O	2.52	0.43
1:A:945:ASN:HB3	1:A:948:ILE:HG22	2.00	0.43
2:B:79:GLU:HA	2:B:79:GLU:OE2	2.18	0.43
2:B:874:PRO:C	2:B:876:ASN:H	2.17	0.43
3:C:11:ILE:HA	3:C:21:PHE:HB2	2.01	0.43
10:J:20:ALA:O	10:J:24:LEU:HG	2.19	0.43
16:P:165:LEU:HD13	16:P:318:ARG:HG3	2.00	0.43
19:S:127:PHE:CB	20:T:19:TRP:HB2	2.48	0.43
1:A:18:ILE:HD13	2:B:1171:MET:HB2	2.00	0.43
1:A:460:ARG:HA	1:A:501:MET:SD	2.59	0.43
1:A:1372:GLU:HG3	5:E:148:HIS:HE1	1.84	0.43
10:J:1:MET:SD	10:J:55:LEU:N	2.81	0.43
13:M:14:THR:N	13:M:20:ASP:HB3	2.34	0.43
13:M:18:HIS:NE2	13:M:36:GLU:OE2	2.52	0.43
16:P:161:ILE:HG13	16:P:329:TYR:HE2	1.83	0.43
1:A:368:THR:O	1:A:483:ARG:HA	2.19	0.42
1:A:601:ASN:HB2	1:A:988:TRP:CZ3	2.54	0.42
1:A:807:LEU:HB2	1:A:810:PHE:CD2	2.54	0.42
1:A:874:LYS:HD2	6:F:111:PRO:HB3	2.01	0.42
1:A:875:TYR:HA	1:A:1083:PRO:CB	2.49	0.42
1:A:1166:LEU:HD12	1:A:1296:MET:SD	2.59	0.42
1:A:1317:LYS:HE2	21:U:295:GLY:HA3	2.00	0.42
2:B:23:GLN:OE1	2:B:23:GLN:N	2.51	0.42
2:B:72:GLN:C	2:B:73:HIS:O	2.57	0.42
2:B:805:PHE:O	2:B:929:PRO:HG2	2.19	0.42
2:B:838:GLN:HE21	2:B:890:ARG:HD3	1.84	0.42
3:C:9:VAL:HG11	11:K:105:PHE:HA	1.99	0.42
3:C:151:VAL:HG22	3:C:152:LYS:N	2.34	0.42
5:E:58:LEU:HB3	5:E:76:PHE:CD2	2.54	0.42
8:H:66:GLU:O	8:H:67:ASP:OD1	2.36	0.42
20:T:212:TYR:O	20:T:215:GLU:HB2	2.19	0.42
23:Y:58:DC:H2"	23:Y:59:DG:H5'	2.00	0.42
1:A:364:ARG:NH2	1:A:500:GLU:O	2.52	0.42
1:A:880:ARG:HH12	5:E:169:GLN:CD	2.22	0.42
1:A:1175:ILE:HG12	1:A:1212:LEU:HD13	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1470:CYS:O	6:F:109:TYR:HD2	2.02	0.42
2:B:860:VAL:HG12	2:B:902:GLY:C	2.38	0.42
2:B:1030:ASN:HB3	2:B:1034:GLY:N	2.34	0.42
2:B:1102:PHE:O	2:B:1106:ARG:HG2	2.19	0.42
2:B:1130:THR:HB	2:B:1134:THR:H	1.84	0.42
5:E:82:VAL:HG23	5:E:106:VAL:HG13	2.00	0.42
8:H:9:ILE:HA	8:H:57:ARG:HA	2.01	0.42
13:M:12:ARG:C	13:M:13:VAL:HG13	2.20	0.42
18:R:195:PRO:HG3	18:R:199:LYS:HB3	1.98	0.42
20:T:200:LYS:NZ	23:Y:68:DC:OP1	2.51	0.42
1:A:64:VAL:HG21	1:A:68:THR:HG23	2.00	0.42
1:A:88:ILE:HD13	1:A:284:VAL:HG22	2.01	0.42
1:A:319:ASP:O	1:A:322:LEU:HG	2.19	0.42
1:A:540:ASP:OD2	2:B:968:ASN:ND2	2.53	0.42
1:A:826:SER:OG	1:A:829:ALA:N	2.47	0.42
2:B:53:MET:O	2:B:57:ARG:N	2.50	0.42
2:B:65:ILE:CG2	2:B:412:LEU:HD11	2.44	0.42
2:B:757:PRO:HD3	2:B:769:PHE:CE2	2.54	0.42
6:F:45:PRO:HB3	6:F:115:TYR:CE1	2.54	0.42
8:H:75:TYR:O	8:H:76:ASN:C	2.57	0.42
10:J:20:ALA:O	10:J:24:LEU:N	2.45	0.42
11:K:13:PHE:HB2	11:K:16:GLU:HG3	2.01	0.42
17:Q:187:ILE:HD11	18:R:211:SER:CB	2.09	0.42
1:A:609:HIS:HB2	21:U:300:PHE:CZ	2.54	0.42
2:B:69:ALA:N	2:B:82:PRO:O	2.46	0.42
2:B:94:SER:O	2:B:122:ALA:HB1	2.19	0.42
2:B:728:MET:HE2	2:B:942:LYS:HE2	2.01	0.42
2:B:1028:LEU:HD13	2:B:1041:ILE:HD13	2.02	0.42
3:C:40:ALA:HB1	3:C:171:LYS:HB2	2.00	0.42
9:I:98:GLN:HB2	9:I:100:HIS:CE1	2.55	0.42
10:J:35:LEU:HB3	10:J:46:ARG:CD	2.49	0.42
12:L:17:TYR:HB2	12:L:26:ASN:HB3	2.02	0.42
16:P:261:SER:HB3	23:Y:81:DA:H4'	2.02	0.42
16:P:284:GLU:HB3	16:P:287:LEU:HB3	2.01	0.42
1:A:10:ASP:N	2:B:1132:THR:HA	2.34	0.42
1:A:484:LEU:HD21	1:A:496:PHE:HE1	1.83	0.42
1:A:775:LYS:CB	2:B:974:SER:HB3	2.50	0.42
1:A:909:LEU:HD22	1:A:1328:PHE:CE2	2.55	0.42
1:A:1310:HIS:CE1	1:A:1334:TRP:CE3	2.96	0.42
2:B:527:ALA:HB3	2:B:530:ALA:HB2	2.00	0.42
2:B:862:GLY:N	2:B:900:GLU:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:55:ARG:HH11	5:E:107:GLN:HE22	1.68	0.42
5:E:130:PHE:HB3	5:E:135:LEU:HD11	2.01	0.42
8:H:24:ARG:HG2	8:H:46:GLN:NE2	2.33	0.42
9:I:37:TYR:N	9:I:46:GLN:O	2.35	0.42
11:K:24:ASP:H	11:K:31:CYS:HA	1.84	0.42
11:K:37:LYS:HA	11:K:69:HIS:HB3	2.01	0.42
11:K:57:LEU:H	11:K:77:THR:HA	1.84	0.42
13:M:158:ALA:HA	13:M:186:ILE:HG13	2.01	0.42
14:N:329:PHE:HB3	14:N:331:THR:HG23	2.01	0.42
17:Q:106:LYS:O	18:R:218:LYS:CE	2.66	0.42
19:S:13:GLU:HG3	20:T:44:ARG:HA	2.00	0.42
1:A:903:PHE:CZ	1:A:976:LYS:HB3	2.55	0.42
2:B:240:LEU:HD13	2:B:242:ARG:CD	2.50	0.42
2:B:896:LEU:HD21	2:B:900:GLU:HB2	2.00	0.42
2:B:972:ILE:O	2:B:976:MET:N	2.51	0.42
2:B:1116:VAL:HG11	2:B:1125:MET:SD	2.59	0.42
3:C:61:ASP:OD1	3:C:61:ASP:N	2.52	0.42
3:C:75:SER:N	3:C:238:SER:O	2.42	0.42
13:M:135:VAL:HG12	13:M:139:ASN:ND2	2.34	0.42
13:M:214:PHE:HA	13:M:217:ARG:NH1	2.34	0.42
16:P:227:GLU:HG2	16:P:228:GLU:H	1.85	0.42
1:A:606:HIS:HB3	1:A:627:LYS:HA	2.01	0.42
1:A:611:ASP:CG	1:A:617:PRO:HG3	2.40	0.42
1:A:908:THR:O	1:A:963:ARG:NH1	2.53	0.42
1:A:931:ARG:C	1:A:933:THR:N	2.73	0.42
1:A:939:VAL:O	1:A:943:LEU:HG	2.19	0.42
2:B:1015:LEU:HD21	2:B:1024:GLY:HA2	2.01	0.42
3:C:5:ASN:O	3:C:7:PRO:CD	2.62	0.42
4:D:32:LEU:HD11	7:G:75:ILE:HG22	2.02	0.42
5:E:177:ASP:OD2	5:E:179:VAL:HB	2.19	0.42
7:G:55:GLY:HA3	7:G:69:PRO:HB2	2.00	0.42
14:N:38:VAL:CG1	15:O:22:LEU:HD22	2.49	0.42
17:Q:112:ARG:HB3	18:R:221:ARG:NH1	2.31	0.42
1:A:72:GLN:HG2	1:A:74:CYS:H	1.83	0.42
1:A:371:PRO:HD2	2:B:788:TYR:CD1	2.53	0.42
1:A:1151:ALA:C	1:A:1155:LYS:HZ3	2.22	0.42
1:A:1217:ASP:OD2	1:A:1220:HIS:N	2.53	0.42
1:A:1460:LEU:O	2:B:1152:PRO:HD3	2.20	0.42
2:B:411:LEU:HD12	2:B:440:ILE:CD1	2.49	0.42
2:B:442:ASP:OD1	2:B:445:LYS:HD2	2.19	0.42
7:G:158:PHE:CZ	17:Q:139:LEU:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:99:LEU:O	17:Q:101:ASN:ND2	2.52	0.42
20:T:174:LYS:HE3	22:X:20:DG:H1'	2.02	0.42
21:U:215:ILE:HG22	21:U:220:PHE:HB2	2.01	0.42
21:U:218:ASP:C	21:U:218:ASP:OD1	2.58	0.42
1:A:13:CYS:HB2	2:B:1135:TYR:CE2	2.55	0.42
1:A:71:CYS:N	1:A:75:ALA:HA	2.31	0.42
1:A:1096:GLY:O	1:A:1100:THR:HG23	2.20	0.42
1:A:1302:GLU:O	1:A:1303:GLN:HB3	2.20	0.42
2:B:487:SER:C	2:B:489:ILE:H	2.24	0.42
2:B:800:ALA:O	2:B:805:PHE:HB2	2.20	0.42
2:B:837:CYS:SG	2:B:838:GLN:N	2.93	0.42
2:B:849:ASP:HB3	2:B:851:ASP:OD1	2.20	0.42
2:B:934:LYS:HA	2:B:944:THR:HG22	2.01	0.42
3:C:81:LYS:HG3	3:C:82:LEU:HD12	2.01	0.42
5:E:31:ASP:O	5:E:35:GLN:N	2.53	0.42
8:H:75:TYR:CE2	8:H:77:PRO:CG	3.03	0.42
9:I:57:LYS:HE2	9:I:60:HIS:NE2	2.35	0.42
9:I:61:GLU:O	9:I:103:ARG:NH1	2.53	0.42
12:L:21:GLU:OE1	12:L:21:GLU:N	2.53	0.42
15:O:42:LYS:HE3	15:O:42:LYS:HB3	1.75	0.42
16:P:168:ILE:HG13	16:P:226:SER:C	2.40	0.42
16:P:209:THR:HG22	16:P:224:ALA:H	1.47	0.42
17:Q:187:ILE:O	18:R:212:VAL:HA	2.19	0.42
21:U:191:VAL:O	21:U:195:ILE:N	2.46	0.42
1:A:606:HIS:HB3	1:A:628:VAL:H	1.85	0.42
1:A:632:ASN:OD1	1:A:992:LYS:NZ	2.52	0.42
1:A:1454:VAL:HG11	1:A:1466:ALA:HB3	2.02	0.42
2:B:497:LYS:H	2:B:498:PRO:HD3	1.04	0.42
2:B:1080:ARG:HG2	13:M:53:ARG:CZ	2.50	0.42
5:E:158:GLU:OE2	5:E:162:ARG:NH2	2.53	0.42
8:H:75:TYR:CE2	8:H:77:PRO:HG3	2.55	0.42
16:P:231:ARG:O	16:P:235:ARG:HG3	2.20	0.42
22:X:27:DG:H2"	22:X:28:DG:C8	2.55	0.42
1:A:419:ILE:O	1:A:426:ARG:HA	2.19	0.41
1:A:1171:ALA:O	9:I:57:LYS:HD3	2.20	0.41
2:B:67:LEU:CD2	2:B:419:ALA:HB1	2.48	0.41
2:B:109:MET:HB3	2:B:112:GLU:HB2	2.02	0.41
2:B:374:LEU:O	2:B:378:GLY:N	2.51	0.41
2:B:499:ARG:C	2:B:500:GLN:O	2.53	0.41
2:B:552:ASN:O	2:B:556:ILE:HG12	2.19	0.41
3:C:6:GLN:HG3	3:C:25:ASN:CG	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:6:GLN:HB2	11:K:104:ARG:HH12	1.85	0.41
4:D:52:GLU:O	4:D:54:GLU:N	2.52	0.41
8:H:88:PHE:CD1	8:H:146:LYS:HD2	2.52	0.41
9:I:7:TYR:CZ	9:I:9:PRO:HG3	2.55	0.41
13:M:283:VAL:O	13:M:287:GLN:HG2	2.20	0.41
15:O:18:SER:O	15:O:22:LEU:HG	2.20	0.41
18:R:131:GLU:HB3	18:R:138:ALA:HB3	2.01	0.41
18:R:188:GLN:HG3	18:R:189:ILE:HG13	2.01	0.41
19:S:37:VAL:HG11	19:S:42:TRP:CZ2	2.55	0.41
21:U:286:THR:CG2	21:U:299:LYS:HB3	2.47	0.41
1:A:204:HIS:O	1:A:206:ASN:N	2.43	0.41
1:A:275:ASP:N	1:A:275:ASP:OD1	2.52	0.41
1:A:378:VAL:N	1:A:473:ARG:O	2.52	0.41
1:A:427:ILE:HG23	13:M:38:GLY:CA	2.50	0.41
1:A:963:ARG:HG2	1:A:967:ARG:NH1	2.35	0.41
1:A:1304:ILE:O	1:A:1306:LYS:N	2.54	0.41
2:B:473:LEU:HD22	2:B:1052:LYS:HD3	2.02	0.41
2:B:798:ARG:N	2:B:949:TYR:O	2.48	0.41
3:C:20:LYS:HA	3:C:232:ASN:HA	2.00	0.41
7:G:63:ARG:HH22	7:G:67:LEU:N	2.18	0.41
11:K:1:MET:SD	11:K:3:ALA:HB3	2.59	0.41
16:P:227:GLU:HG2	16:P:228:GLU:N	2.35	0.41
18:R:155:LEU:HB3	18:R:204:ASN:HD21	1.80	0.41
22:X:45:DC:H2"	22:X:46:DG:C8	2.56	0.41
23:Y:85:DG:C2	23:Y:86:DC:C2	3.09	0.41
1:A:349:ARG:HB3	2:B:1158:LEU:HD12	2.02	0.41
1:A:611:ASP:OD2	1:A:617:PRO:HG3	2.19	0.41
1:A:1167:ARG:HE	1:A:1293:LEU:HB3	1.86	0.41
2:B:109:MET:CE	2:B:174:LEU:HB3	2.48	0.41
2:B:453:TRP:HB3	2:B:463:ARG:CB	2.49	0.41
2:B:531:TYR:HD2	2:B:622:CYS:SG	2.44	0.41
2:B:836:THR:C	2:B:886:ARG:HA	2.41	0.41
7:G:40:GLY:HA2	7:G:152:VAL:HG11	2.03	0.41
7:G:79:PRO:HG3	7:G:104:MET:SD	2.60	0.41
7:G:146:LYS:HD3	7:G:165:ASP:OD2	2.21	0.41
7:G:154:LYS:HG3	7:G:155:ASN:H	1.86	0.41
8:H:105:SER:HB2	8:H:108:ALA:CB	2.50	0.41
9:I:102:ALA:C	9:I:104:ALA:N	2.72	0.41
13:M:154:ARG:HD3	13:M:154:ARG:HA	1.88	0.41
15:O:62:LEU:HA	15:O:76:LEU:HG	2.02	0.41
17:Q:113:ARG:HB2	18:R:221:ARG:CD	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:23:VAL:HG13	20:T:27:LEU:HD23	2.01	0.41
1:A:202:TRP:O	1:A:211:GLU:HA	2.21	0.41
1:A:419:ILE:HA	1:A:446:VAL:HA	2.02	0.41
1:A:504:HIS:HB3	2:B:1106:ARG:NH2	2.35	0.41
1:A:1173:THR:HB	9:I:56:ASN:CB	2.49	0.41
1:A:1207:ILE:HD12	1:A:1260:ARG:CB	2.51	0.41
1:A:1456:GLU:HG2	1:A:1457:ASN:N	2.35	0.41
2:B:166:LEU:HB3	2:B:170:ASP:CB	2.50	0.41
2:B:258:ALA:HB2	2:B:269:ILE:CG2	2.49	0.41
2:B:302:LYS:HB3	2:B:303:PRO:HD3	2.02	0.41
2:B:505:LEU:HG	2:B:509:VAL:HB	2.03	0.41
2:B:720:PRO:HG2	2:B:721:ARG:NH1	2.35	0.41
2:B:865:VAL:HA	2:B:895:PHE:HB3	2.02	0.41
5:E:41:LYS:HA	5:E:46:ASP:HB3	2.02	0.41
7:G:142:GLU:O	7:G:170:LEU:HA	2.20	0.41
9:I:101:SER:HB2	9:I:102:ALA:H	1.59	0.41
14:N:25:VAL:HG12	15:O:39:GLN:HB3	2.02	0.41
20:T:177:ARG:NH1	22:X:20:DG:OP2	2.54	0.41
21:U:161:ILE:HG21	21:U:211:LEU:HB3	2.01	0.41
21:U:193:SER:OG	21:U:194:ARG:NH1	2.53	0.41
1:A:374:SER:HB3	1:A:377:GLN:HG3	2.02	0.41
1:A:478:PRO:HB3	11:K:4:PRO:HD3	2.02	0.41
1:A:546:ARG:CG	1:A:639:ILE:HD11	2.47	0.41
1:A:1355:VAL:HA	5:E:142:HIS:HA	2.02	0.41
2:B:799:SER:O	2:B:802:ASP:HB2	2.21	0.41
2:B:833:THR:O	2:B:840:MET:HE3	2.20	0.41
2:B:1040:GLN:NE2	3:C:197:TYR:H	2.18	0.41
2:B:1126:ALA:HB3	2:B:1137:CYS:SG	2.61	0.41
6:F:53:THR:HB	6:F:108:ARG:NH1	2.36	0.41
7:G:117:MET:HE1	7:G:163:LEU:HD22	2.03	0.41
13:M:216:SER:HA	13:M:229:GLN:NE2	2.35	0.41
14:N:10:VAL:HB	14:N:11:PRO:HD3	2.02	0.41
1:A:37:THR:OG1	1:A:86:GLY:HA3	2.20	0.41
1:A:375:ILE:HG12	1:A:666:ARG:HB2	2.03	0.41
2:B:669:GLU:O	2:B:673:VAL:HG13	2.21	0.41
2:B:1130:THR:C	2:B:1132:THR:H	2.21	0.41
3:C:190:ASN:ND2	3:C:195:THR:O	2.50	0.41
9:I:69:ILE:O	9:I:72:VAL:HG22	2.21	0.41
12:L:38:GLU:HG2	12:L:39:CYS:H	1.86	0.41
13:M:248:ARG:NH2	23:Y:85:DG:OP2	2.51	0.41
17:Q:21:VAL:O	17:Q:25:PHE:HD1	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:208:CYS:O	18:R:209:GLN:C	2.55	0.41
20:T:174:LYS:HB3	22:X:20:DG:H4'	2.02	0.41
20:T:202:LEU:HD11	20:T:233:TRP:HB2	2.03	0.41
1:A:61:ARG:O	1:A:72:GLN:HB3	2.19	0.41
1:A:201:GLU:HA	1:A:212:LYS:O	2.21	0.41
1:A:916:PHE:CD1	1:A:963:ARG:HD2	2.55	0.41
1:A:1080:ILE:CD1	6:F:54:THR:HG21	2.50	0.41
2:B:764:MET:HG2	2:B:767:LEU:HD12	2.01	0.41
2:B:790:GLN:HA	2:B:968:ASN:HD22	1.86	0.41
3:C:1:MET:SD	11:K:52:LYS:HE3	2.61	0.41
4:D:23:PRO:HG2	4:D:26:PHE:HB2	2.03	0.41
6:F:93:ALA:O	6:F:97:LEU:N	2.52	0.41
8:H:39:LEU:HD12	8:H:124:ARG:O	2.21	0.41
13:M:118:PHE:HA	13:M:121:ILE:HB	2.03	0.41
13:M:279:GLY:CA	20:T:153:TYR:CE1	3.01	0.41
14:N:315:ASN:C	14:N:317:GLU:H	2.23	0.41
16:P:180:LEU:HD12	16:P:183:ILE:HD12	2.02	0.41
17:Q:75:ARG:N	17:Q:95:ASN:O	2.41	0.41
20:T:227:GLY:O	22:X:30:DG:H5"	2.21	0.41
22:X:6:DG:N2	23:Y:89:DC:O2	2.54	0.41
1:A:120:ASP:OD1	1:A:121:SER:N	2.51	0.41
1:A:1000:LEU:HD12	1:A:1001:PRO:HD2	2.02	0.41
1:A:1175:ILE:H	9:I:54:TYR:HB3	1.86	0.41
2:B:22:TRP:HD1	2:B:24:GLU:HB2	1.86	0.41
2:B:63:PRO:HB2	2:B:88:PHE:CD1	2.56	0.41
2:B:194:LEU:HD13	2:B:467:SER:HB2	2.03	0.41
2:B:471:ASN:HD22	2:B:730:LYS:HE3	1.85	0.41
3:C:190:ASN:ND2	3:C:193:ARG:HA	2.36	0.41
3:C:199:LYS:NZ	3:C:201:GLU:OE1	2.46	0.41
4:D:45:LYS:HD2	4:D:45:LYS:HA	1.74	0.41
14:N:39:LEU:HD12	14:N:42:LEU:HD23	2.01	0.41
14:N:314:LEU:HD12	16:P:248:ALA:O	2.21	0.41
15:O:19:LEU:HD23	15:O:22:LEU:HD12	2.03	0.41
18:R:140:LYS:N	18:R:141:PRO:HD2	2.35	0.41
1:A:42:LYS:HD3	1:A:55:GLY:H	1.86	0.41
1:A:65:ILE:HG22	1:A:66:GLU:N	2.34	0.41
1:A:266:MET:O	1:A:267:GLN:CB	2.60	0.41
1:A:338:SER:O	1:A:342:ARG:HG3	2.21	0.41
1:A:608:THR:OG1	1:A:610:PRO:HD2	2.20	0.41
1:A:702:ILE:O	1:A:706:ILE:HG12	2.21	0.41
1:A:1053:ARG:NE	1:A:1057:GLU:OE1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1306:LYS:HB2	1:A:1306:LYS:HE3	1.57	0.41
1:A:1479:LYS:HB3	6:F:103:PRO:HB3	2.02	0.41
2:B:68:GLN:OE1	2:B:135:GLU:HG3	2.21	0.41
2:B:92:TYR:O	2:B:125:TYR:N	2.30	0.41
2:B:198:GLU:CD	2:B:524:LYS:HZ2	2.23	0.41
2:B:236:TRP:HB2	2:B:259:THR:HB	2.03	0.41
2:B:821:LYS:N	2:B:825:GLN:O	2.39	0.41
2:B:1137:CYS:HB3	2:B:1142:ASN:CB	2.51	0.41
9:I:29:ASP:O	9:I:33:ARG:N	2.53	0.41
11:K:32:LEU:HD21	11:K:72:ILE:HB	2.03	0.41
13:M:218:PHE:CD1	13:M:277:ILE:HG22	2.55	0.41
14:N:39:LEU:O	14:N:42:LEU:HB3	2.21	0.41
15:O:70:ASN:HB3	15:O:99:ASP:HB3	2.02	0.41
16:P:193:ASN:HA	16:P:194:PRO:HD2	1.92	0.41
16:P:200:VAL:HG12	16:P:213:ILE:HD13	2.02	0.41
17:Q:170:LYS:HG3	17:Q:173:ALA:H	1.86	0.41
19:S:54:LYS:HE2	19:S:54:LYS:HB2	1.84	0.41
20:T:198:ASN:O	20:T:202:LEU:HG	2.21	0.41
21:U:232:GLU:OE1	21:U:232:GLU:HA	2.20	0.41
1:A:63:GLY:HA2	1:A:71:CYS:SG	2.61	0.41
1:A:470:MET:SD	1:A:521:VAL:HG23	2.61	0.41
1:A:549:THR:OG1	1:A:639:ILE:HG13	2.20	0.41
1:A:720:ALA:HB2	1:A:725:LEU:HD13	2.02	0.41
1:A:915:ALA:O	1:A:919:LYS:N	2.45	0.41
1:A:1165:THR:O	1:A:1169:VAL:HG23	2.21	0.41
2:B:192:LYS:HE3	2:B:192:LYS:HB3	1.87	0.41
2:B:602:SER:OG	2:B:620:ARG:NH1	2.54	0.41
5:E:17:ILE:O	5:E:20:LEU:HB3	2.21	0.41
5:E:142:HIS:HB3	5:E:145:VAL:HG23	2.02	0.41
9:I:24:LEU:HD11	9:I:44:TYR:HE2	1.86	0.41
9:I:84:HIS:CD2	9:I:84:HIS:H	2.39	0.41
10:J:3:ILE:HD13	10:J:18:TRP:HB2	2.02	0.41
13:M:128:ILE:HG13	13:M:130:LEU:HG	2.02	0.41
13:M:259:TYR:HD1	13:M:274:ILE:HD12	1.86	0.41
16:P:240:VAL:O	16:P:244:LEU:HG	2.20	0.41
17:Q:23:ARG:CZ	18:R:207:SER:N	2.84	0.41
17:Q:129:CYS:HB2	17:Q:154:CYS:HB2	2.02	0.41
19:S:49:ARG:HD2	19:S:96:GLN:HB2	2.03	0.41
23:Y:91:DT:H2"	23:Y:92:DT:C6	2.56	0.41
1:A:15:LEU:HA	2:B:1148:LEU:HB3	2.02	0.40
1:A:33:ARG:HB3	2:B:1139:GLY:HA2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:ILE:O	1:A:445:LYS:N	2.39	0.40
1:A:432:HIS:CG	1:A:433:PRO:HD2	2.56	0.40
1:A:452:ASP:OD1	1:A:476:ILE:HG12	2.21	0.40
1:A:620:HIS:C	1:A:621:ILE:CG1	2.69	0.40
1:A:864:LEU:HD22	1:A:1095:LEU:HD23	2.02	0.40
1:A:922:PHE:CZ	1:A:952:LEU:HG	2.42	0.40
1:A:1017:SER:HA	1:A:1020:LEU:HG	2.03	0.40
1:A:1054:MET:O	1:A:1059:ARG:N	2.54	0.40
1:A:1218:ARG:HA	1:A:1221:MET:HG2	2.03	0.40
2:B:481:HIS:HA	2:B:484:ARG:NH1	2.36	0.40
2:B:761:THR:H	2:B:764:MET:CE	2.33	0.40
2:B:1123:GLY:HA3	2:B:1171:MET:H	1.85	0.40
3:C:47:ILE:HG22	12:L:57:ALA:HB2	2.03	0.40
4:D:64:THR:HG21	7:G:46:ILE:HG23	2.02	0.40
5:E:11:TRP:CZ2	5:E:15:LYS:HE3	2.56	0.40
5:E:120:ASP:O	5:E:122:ALA:N	2.54	0.40
7:G:11:ILE:N	7:G:68:TYR:O	2.49	0.40
9:I:80:ARG:HE	9:I:115:THR:HG21	1.85	0.40
11:K:81:TYR:CE2	11:K:86:ALA:HB2	2.55	0.40
16:P:281:SER:HG	16:P:293:TYR:HD1	1.68	0.40
17:Q:37:LEU:HD13	17:Q:71:PHE:CE1	2.55	0.40
19:S:48:GLU:OE1	19:S:101:ARG:NH2	2.55	0.40
20:T:154:LYS:HA	20:T:155:PRO:HD3	1.97	0.40
20:T:231:ASN:CB	23:Y:68:DC:H5”	2.44	0.40
1:A:746:ASN:HA	1:A:749:ARG:HE	1.86	0.40
1:A:1173:THR:HB	9:I:56:ASN:HB3	2.02	0.40
2:B:88:PHE:CE2	2:B:128:ILE:HG12	2.56	0.40
2:B:607:ILE:HG21	9:I:72:VAL:N	2.36	0.40
7:G:89:VAL:HA	7:G:99:THR:HA	2.03	0.40
7:G:163:LEU:O	7:G:163:LEU:HD23	2.21	0.40
8:H:97:TYR:CZ	8:H:115:TYR:HB3	2.56	0.40
12:L:34:ILE:HD12	12:L:42:ARG:HB3	2.03	0.40
13:M:178:LYS:C	20:T:154:LYS:CG	2.87	0.40
13:M:195:PHE:CZ	13:M:199:LEU:HD11	2.56	0.40
14:N:332:GLU:HA	15:O:92:LYS:O	2.21	0.40
21:U:191:VAL:O	21:U:195:ILE:HG13	2.22	0.40
1:A:32:LYS:HG2	1:A:87:HIS:NE2	2.36	0.40
1:A:240:PRO:HB3	1:A:244:ARG:HH11	1.87	0.40
1:A:309:LEU:HG	1:A:313:HIS:CD2	2.57	0.40
1:A:312:PHE:CE2	1:A:326:PRO:HB2	2.55	0.40
1:A:337:LYS:O	1:A:341:GLN:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:LYS:HG3	1:A:1436:VAL:HG21	2.03	0.40
1:A:404:GLU:OE1	1:A:407:ARG:NH1	2.45	0.40
1:A:550:LYS:HG2	1:A:552:ASP:H	1.86	0.40
1:A:587:THR:O	1:A:591:ILE:HG12	2.21	0.40
1:A:808:PRO:HG2	2:B:675:LEU:HD23	2.03	0.40
1:A:962:ASP:OD2	1:A:1046:ARG:HD2	2.21	0.40
1:A:1173:THR:HA	1:A:1214:VAL:HA	2.03	0.40
2:B:474:THR:H	2:B:477:SER:HB2	1.85	0.40
2:B:875:GLU:OE1	2:B:875:GLU:HA	2.21	0.40
3:C:19:VAL:CG1	3:C:233:VAL:HB	2.51	0.40
5:E:82:VAL:HG21	5:E:106:VAL:HG22	2.03	0.40
6:F:44:ARG:H	6:F:45:PRO:CD	2.34	0.40
6:F:110:LEU:N	6:F:114:SER:O	2.55	0.40
11:K:35:ILE:N	11:K:35:ILE:HD12	2.36	0.40
13:M:289:TYR:HA	13:M:292:ILE:HG12	2.03	0.40
16:P:203:ARG:HG3	16:P:203:ARG:HH21	1.87	0.40
1:A:336:LEU:HG	1:A:338:SER:H	1.86	0.40
1:A:416:ALA:HA	1:A:448:ARG:HA	2.03	0.40
1:A:420:ILE:HB	1:A:445:LYS:HB2	2.03	0.40
1:A:790:GLN:OE1	1:A:822:PHE:HB2	2.22	0.40
1:A:802:PHE:CZ	1:A:808:PRO:HB3	2.57	0.40
2:B:249:LYS:C	2:B:251:ALA:N	2.75	0.40
2:B:834:ARG:HD2	2:B:840:MET:SD	2.61	0.40
2:B:874:PRO:HB3	2:B:877:GLU:HB3	2.04	0.40
2:B:1080:ARG:HG2	13:M:53:ARG:NH1	2.36	0.40
3:C:7:PRO:O	3:C:8:THR:C	2.59	0.40
5:E:172:ARG:NE	5:E:208:LEU:HD22	2.36	0.40
8:H:91:VAL:HA	8:H:143:LEU:O	2.21	0.40
8:H:111:ARG:HG3	8:H:126:GLN:HE22	1.85	0.40
9:I:27:LYS:O	9:I:35:LEU:HD12	2.22	0.40
17:Q:124:ARG:HD3	17:Q:168:MET:SD	2.61	0.40
22:X:20:DG:H1'	22:X:21:DG:H5'	2.02	0.40
1:A:18:ILE:CD1	2:B:1171:MET:HB2	2.51	0.40
2:B:225:LEU:O	2:B:230:ARG:HG2	2.20	0.40
2:B:1068:GLN:HA	13:M:46:ILE:HG21	2.03	0.40
5:E:192:LYS:HG3	5:E:206:TYR:HE1	1.87	0.40
6:F:99:ALA:HB1	6:F:101:LYS:HG3	2.01	0.40
8:H:111:ARG:HG3	8:H:126:GLN:OE1	2.22	0.40
9:I:27:LYS:HE3	9:I:38:ALA:HB2	2.03	0.40
15:O:64:THR:CG2	16:P:188:ARG:HB3	2.52	0.40
16:P:207:PRO:HB3	16:P:233:ALA:CB	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:211:ALA:HA	16:P:220:VAL:O	2.21	0.40
17:Q:187:ILE:CD1	18:R:211:SER:CA	2.80	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	A	1450/1970 (74%)	1297 (89%)	100 (7%)	53 (4%)	2 19
2	B	1163/1174 (99%)	1044 (90%)	82 (7%)	37 (3%)	3 21
3	C	273/275 (99%)	244 (89%)	17 (6%)	12 (4%)	2 17
4	D	127/142 (89%)	118 (93%)	8 (6%)	1 (1%)	16 54
5	E	208/210 (99%)	198 (95%)	7 (3%)	3 (1%)	9 39
6	F	84/127 (66%)	78 (93%)	4 (5%)	2 (2%)	5 26
7	G	169/172 (98%)	158 (94%)	10 (6%)	1 (1%)	22 60
8	H	148/150 (99%)	121 (82%)	15 (10%)	12 (8%)	1 9
9	I	123/125 (98%)	102 (83%)	12 (10%)	9 (7%)	1 10
10	J	65/67 (97%)	53 (82%)	8 (12%)	4 (6%)	1 12
11	K	115/117 (98%)	112 (97%)	3 (3%)	0	100 100
12	L	44/58 (76%)	36 (82%)	4 (9%)	4 (9%)	0 8
13	M	256/316 (81%)	235 (92%)	11 (4%)	10 (4%)	2 18
14	N	109/376 (29%)	99 (91%)	6 (6%)	4 (4%)	2 19
15	O	97/109 (89%)	90 (93%)	7 (7%)	0	100 100
16	P	183/339 (54%)	167 (91%)	12 (7%)	4 (2%)	5 28
17	Q	176/439 (40%)	159 (90%)	11 (6%)	6 (3%)	3 20
18	R	163/291 (56%)	129 (79%)	20 (12%)	14 (9%)	0 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
19	S	134/517 (26%)	123 (92%)	7 (5%)	4 (3%)	3 22
20	T	218/249 (88%)	191 (88%)	17 (8%)	10 (5%)	2 16
21	U	168/301 (56%)	135 (80%)	20 (12%)	13 (8%)	1 9
All	All	5473/7524 (73%)	4889 (89%)	381 (7%)	203 (4%)	4 19

All (203) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	ARG
1	A	205	VAL
1	A	531	ASN
1	A	610	PRO
1	A	619	LYS
1	A	621	ILE
1	A	622	SER
1	A	623	PRO
1	A	911	PRO
1	A	924	TYR
1	A	929	ALA
1	A	932	ARG
1	A	1273	GLU
1	A	1303	GLN
2	B	61	ASP
2	B	73	HIS
2	B	80	GLU
2	B	232	THR
2	B	250	SER
2	B	491	ARG
2	B	498	PRO
2	B	500	GLN
2	B	549	SER
2	B	841	ARG
2	B	879	GLU
3	C	7	PRO
3	C	89	THR
3	C	126	ARG
3	C	147	ASP
3	C	218	ALA
5	E	64	HIS
5	E	65	ASN
7	G	154	LYS

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Mol	Chain	Res	Type
8	H	75	TYR
8	H	108	ALA
8	H	111	ARG
9	I	59	THR
9	I	85	PRO
9	I	86	CYS
9	I	104	ALA
9	I	106	ASP
12	L	16	ILE
12	L	38	GLU
13	M	11	PRO
13	M	13	VAL
13	M	40	VAL
13	M	44	ARG
16	P	160	GLY
16	P	161	ILE
18	R	134	ASP
18	R	163	LEU
18	R	195	PRO
18	R	196	ASP
18	R	209	GLN
18	R	211	SER
18	R	214	GLU
18	R	224	THR
20	T	139	VAL
20	T	140	ARG
20	T	156	VAL
21	U	223	MET
21	U	257	GLN
1	A	44	PRO
1	A	267	GLN
1	A	273	GLN
1	A	346	LYS
1	A	612	ASP
1	A	620	HIS
1	A	624	GLY
1	A	930	LEU
1	A	935	GLN
1	A	1101	GLN
1	A	1118	THR
1	A	1264	SER
1	A	1275	VAL

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Mol	Chain	Res	Type
1	A	1282	ASP
1	A	1435	THR
2	B	257	VAL
2	B	428	ASP
2	B	460	HIS
2	B	649	ASN
2	B	791	GLU
2	B	875	GLU
2	B	881	GLU
2	B	882	SER
2	B	883	THR
2	B	889	LYS
3	C	91	GLU
3	C	143	VAL
4	D	57	LEU
5	E	121	MET
8	H	3	GLY
8	H	21	LYS
8	H	66	GLU
8	H	107	GLU
9	I	57	LYS
10	J	14	VAL
10	J	65	LEU
12	L	17	TYR
17	Q	103	VAL
17	Q	169	PRO
18	R	157	GLN
18	R	164	GLY
20	T	145	LEU
20	T	178	ALA
20	T	180	LYS
21	U	227	GLU
21	U	233	LEU
21	U	251	ALA
21	U	252	LYS
21	U	253	THR
21	U	267	LYS
1	A	156	GLY
1	A	338	SER
1	A	611	ASP
1	A	1200	PRO
1	A	1274	GLU

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Mol	Chain	Res	Type
1	A	1305	SER
1	A	1313	GLN
1	A	1314	THR
1	A	1417	HIS
2	B	229	SER
2	B	456	GLN
2	B	497	LYS
2	B	651	TYR
2	B	863	ASP
2	B	898	THR
2	B	1129	ASN
2	B	1132	THR
3	C	144	GLU
8	H	65	TYR
8	H	106	THR
9	I	92	LYS
9	I	119	CYS
13	M	10	LEU
14	N	346	LYS
17	Q	163	GLU
18	R	139	PHE
18	R	212	VAL
19	S	170	VAL
20	T	124	TYR
20	T	144	GLN
21	U	226	GLU
1	A	72	GLN
1	A	184	CYS
1	A	266	MET
1	A	461	GLN
1	A	479	TRP
1	A	981	CYS
2	B	74	ALA
2	B	256	ILE
2	B	495	LEU
2	B	873	LEU
2	B	1136	GLU
3	C	137	ASN
6	F	85	GLY
8	H	70	LEU
8	H	76	ASN
9	I	20	CYS

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Mol	Chain	Res	Type
10	J	3	ILE
13	M	149	LYS
14	N	355	ASP
16	P	210	THR
17	Q	124	ARG
17	Q	165	GLU
18	R	141	PRO
20	T	38	GLY
20	T	135	SER
1	A	75	ALA
1	A	300	ALA
1	A	1106	THR
1	A	1266	GLU
1	A	1342	SER
3	C	151	VAL
8	H	71	ASP
10	J	6	ARG
13	M	39	LEU
13	M	108	SER
16	P	297	LYS
18	R	174	ALA
19	S	153	ARG
19	S	154	THR
19	S	160	ALA
21	U	229	ALA
21	U	266	CYS
21	U	295	GLY
1	A	1265	ASP
1	A	1281	ASP
2	B	737	ILE
6	F	44	ARG
12	L	19	CYS
13	M	247	GLY
14	N	312	GLU
13	M	38	GLY
1	A	51	ARG
1	A	498	GLY
2	B	493	GLY
21	U	255	GLY
3	C	6	GLN
3	C	78	ILE
17	Q	100	VAL

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Mol	Chain	Res	Type
2	B	1008	VAL
14	N	313	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	A	1279/1748 (73%)	1243 (97%)	36 (3%)	38	58
2	B	1020/1028 (99%)	994 (98%)	26 (2%)	42	61
3	C	252/252 (100%)	247 (98%)	5 (2%)	50	68
4	D	119/126 (94%)	118 (99%)	1 (1%)	79	85
5	E	192/192 (100%)	187 (97%)	5 (3%)	41	60
6	F	74/111 (67%)	74 (100%)	0	100	100
7	G	152/153 (99%)	149 (98%)	3 (2%)	50	68
8	H	131/131 (100%)	128 (98%)	3 (2%)	45	64
9	I	112/112 (100%)	109 (97%)	3 (3%)	40	59
10	J	56/56 (100%)	55 (98%)	1 (2%)	54	71
11	K	106/106 (100%)	105 (99%)	1 (1%)	75	83
12	L	43/55 (78%)	43 (100%)	0	100	100
13	M	222/268 (83%)	211 (95%)	11 (5%)	20	41
14	N	105/324 (32%)	104 (99%)	1 (1%)	73	81
15	O	90/98 (92%)	89 (99%)	1 (1%)	70	80
16	P	159/293 (54%)	154 (97%)	5 (3%)	35	54
17	Q	164/373 (44%)	157 (96%)	7 (4%)	25	46
18	R	150/261 (58%)	140 (93%)	10 (7%)	13	34
19	S	121/448 (27%)	118 (98%)	3 (2%)	42	61
20	T	196/218 (90%)	189 (96%)	7 (4%)	30	50
21	U	148/266 (56%)	141 (95%)	7 (5%)	22	44
All	All	4891/6619 (74%)	4755 (97%)	136 (3%)	40	58

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ASP
1	A	57	LEU
1	A	147	LEU
1	A	152	ASN
1	A	188	GLN
1	A	266	MET
1	A	267	GLN
1	A	275	ASP
1	A	339	LEU
1	A	372	ASN
1	A	472	HIS
1	A	484	LEU
1	A	603	ILE
1	A	604	ARG
1	A	611	ASP
1	A	613	GLU
1	A	614	ASP
1	A	619	LYS
1	A	625	ASP
1	A	644	SER
1	A	647	THR
1	A	659	GLU
1	A	669	TYR
1	A	750	ASP
1	A	839	HIS
1	A	922	PHE
1	A	923	ASP
1	A	932	ARG
1	A	964	GLU
1	A	1152	GLU
1	A	1272	GLU
1	A	1289	GLU
1	A	1306	LYS
1	A	1311	LEU
1	A	1313	GLN
1	A	1386	ILE
2	B	26	CYS
2	B	54	SER
2	B	73	HIS
2	B	77	GLU
2	B	97	THR
2	B	125	TYR

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Mol	Chain	Res	Type
2	B	131	THR
2	B	132	VAL
2	B	169	ARG
2	B	242	ARG
2	B	249	LYS
2	B	250	SER
2	B	256	ILE
2	B	407	MET
2	B	442	ASP
2	B	446	TYR
2	B	499	ARG
2	B	546	GLU
2	B	588	ARG
2	B	604	ILE
2	B	664	TYR
2	B	666	ASP
2	B	814	TYR
2	B	880	LEU
2	B	881	GLU
2	B	1080	ARG
3	C	35	ARG
3	C	61	ASP
3	C	113	ARG
3	C	215	GLU
3	C	217	GLN
4	D	43	HIS
5	E	23	ASP
5	E	50	GLU
5	E	64	HIS
5	E	129	GLN
5	E	172	ARG
7	G	63	ARG
7	G	144	ARG
7	G	163	LEU
8	H	55	LYS
8	H	66	GLU
8	H	107	GLU
9	I	27	LYS
9	I	71	ASP
9	I	72	VAL
10	J	65	LEU
11	K	8	GLU

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Mol	Chain	Res	Type
13	M	7	LEU
13	M	10	LEU
13	M	31	ASP
13	M	39	LEU
13	M	40	VAL
13	M	53	ARG
13	M	107	MET
13	M	112	ARG
13	M	114	MET
13	M	120	GLU
13	M	126	ASP
14	N	319	ASP
15	O	10	THR
16	P	208	ARG
16	P	239	ARG
16	P	271	GLU
16	P	297	LYS
16	P	299	ARG
17	Q	45	GLU
17	Q	101	ASN
17	Q	105	TYR
17	Q	123	ASN
17	Q	139	LEU
17	Q	142	ASN
17	Q	193	GLU
18	R	88	ARG
18	R	99	LEU
18	R	159	ASP
18	R	163	LEU
18	R	206	LYS
18	R	209	GLN
18	R	210	PHE
18	R	212	VAL
18	R	223	VAL
18	R	235	GLU
19	S	7	SER
19	S	163	GLU
19	S	166	ARG
20	T	143	GLN
20	T	145	LEU
20	T	149	VAL
20	T	154	LYS

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Mol	Chain	Res	Type
20	T	160	GLN
20	T	161	TYR
20	T	162	ASN
21	U	179	GLU
21	U	187	TYR
21	U	194	ARG
21	U	218	ASP
21	U	223	MET
21	U	252	LYS
21	U	274	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	516	GLN
1	A	529	GLN
1	A	539	GLN
1	A	700	GLN
1	A	703	GLN
1	A	1310	HIS
1	A	1332	GLN
2	B	98	HIS
2	B	227	ASN
2	B	245	GLN
2	B	452	ASN
2	B	817	GLN
2	B	970	HIS
2	B	1003	ASN
2	B	1007	ASN
2	B	1040	GLN
2	B	1101	GLN
2	B	1117	HIS
2	B	1160	GLN
3	C	5	ASN
3	C	6	GLN
3	C	25	ASN
3	C	137	ASN
5	E	64	HIS
5	E	71	GLN
5	E	129	GLN
5	E	132	GLN
9	I	87	GLN

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Mol	Chain	Res	Type
9	I	98	GLN
9	I	121	HIS
12	L	23	HIS
16	P	229	GLN
18	R	177	ASN
18	R	204	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 13 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

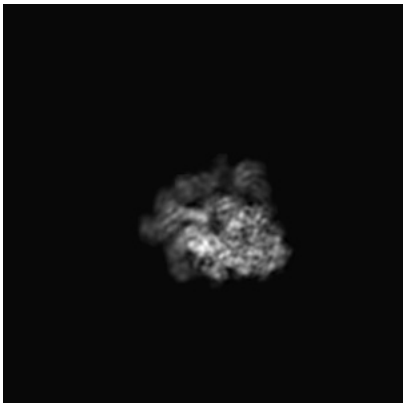
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8135. These allow visual inspection of the internal detail of the map and identification of artifacts.

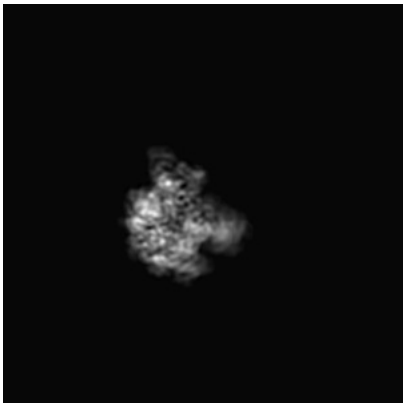
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

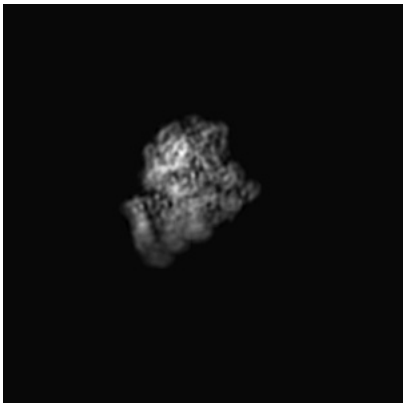
6.1.1 Primary map



X



Y



Z

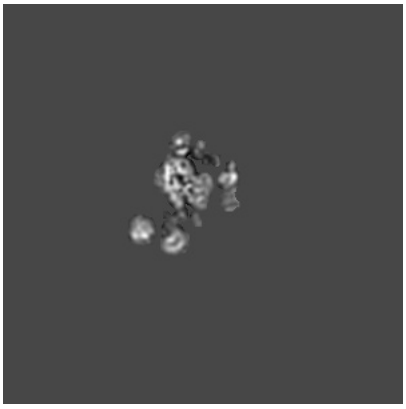
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map

X Index: 192

Y Index: 192

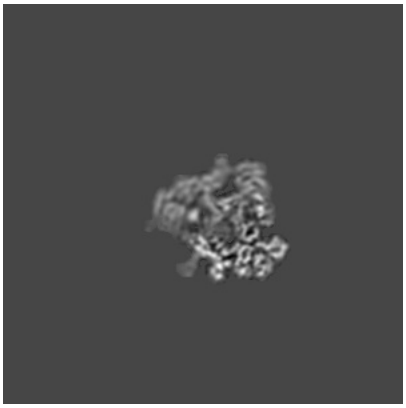


Z Index: 192

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: 165

Y Index: 227

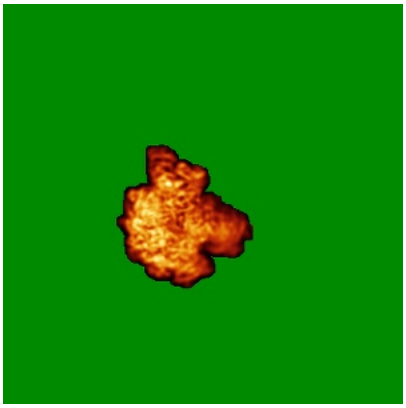
Z Index: 151

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

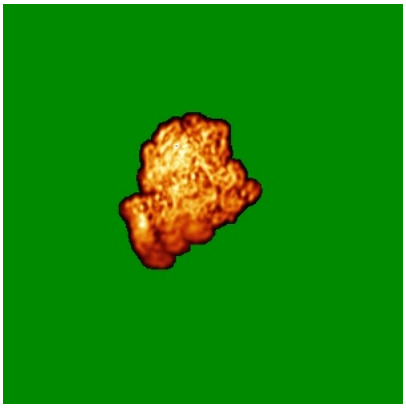
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map

X



Y

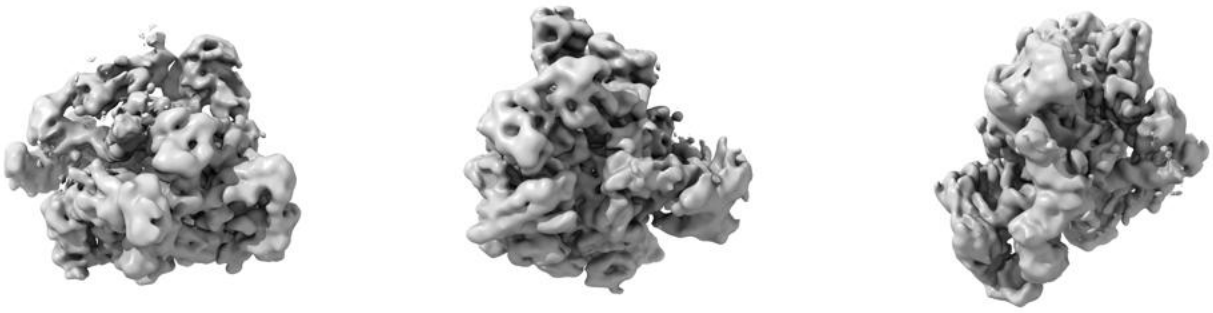


Z

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 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

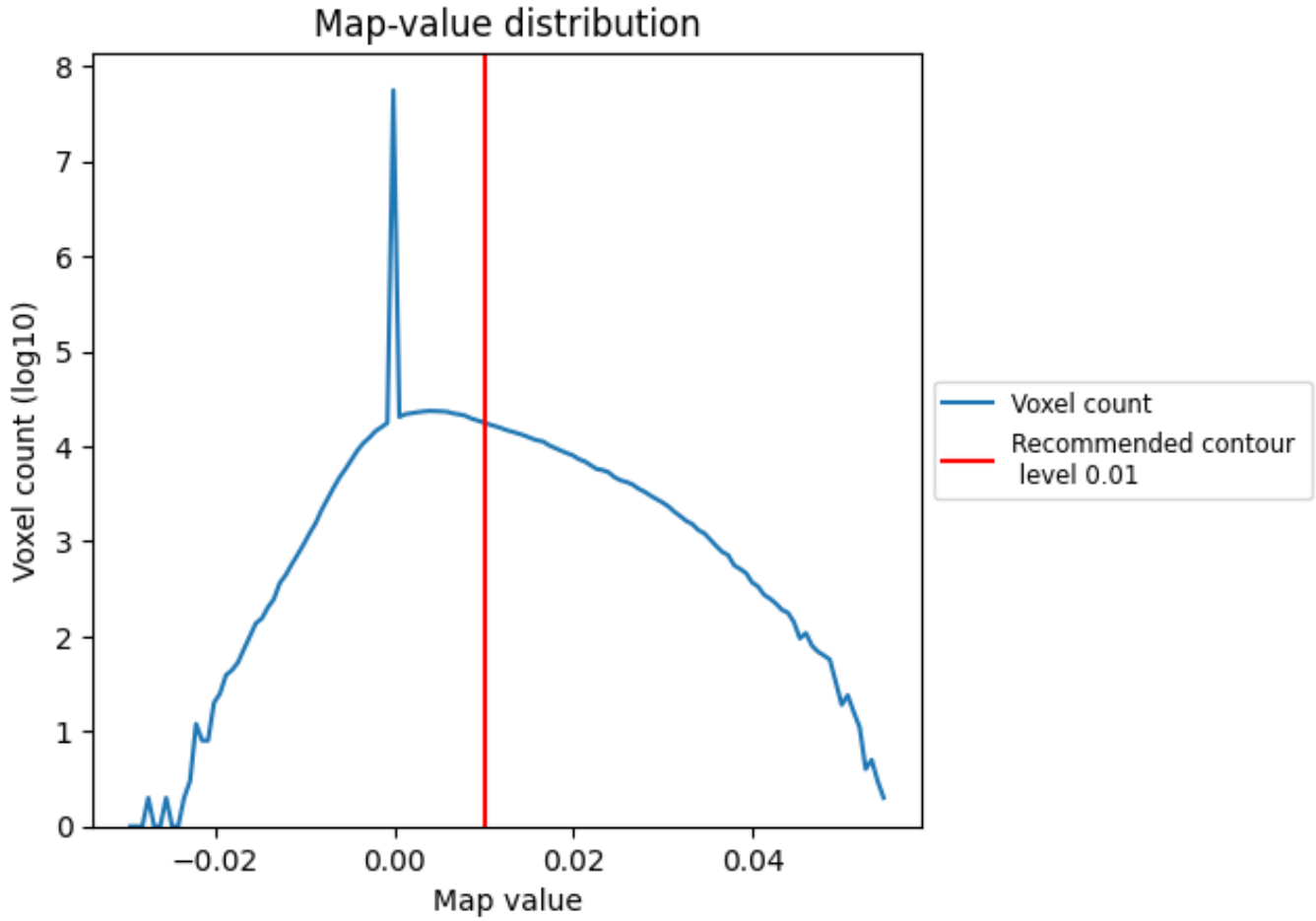
6.6 Mask visualisation (i)

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

7 Map analysis

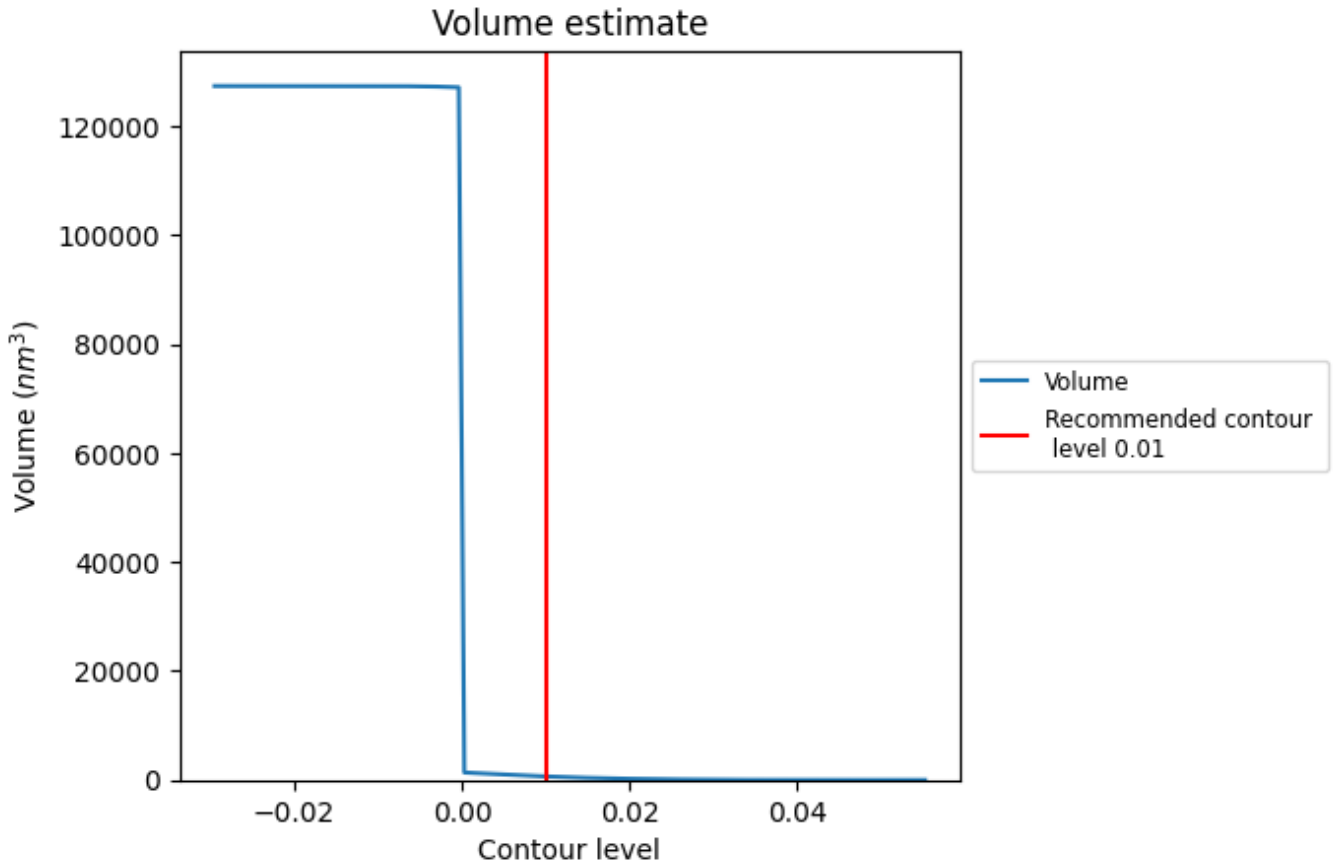
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

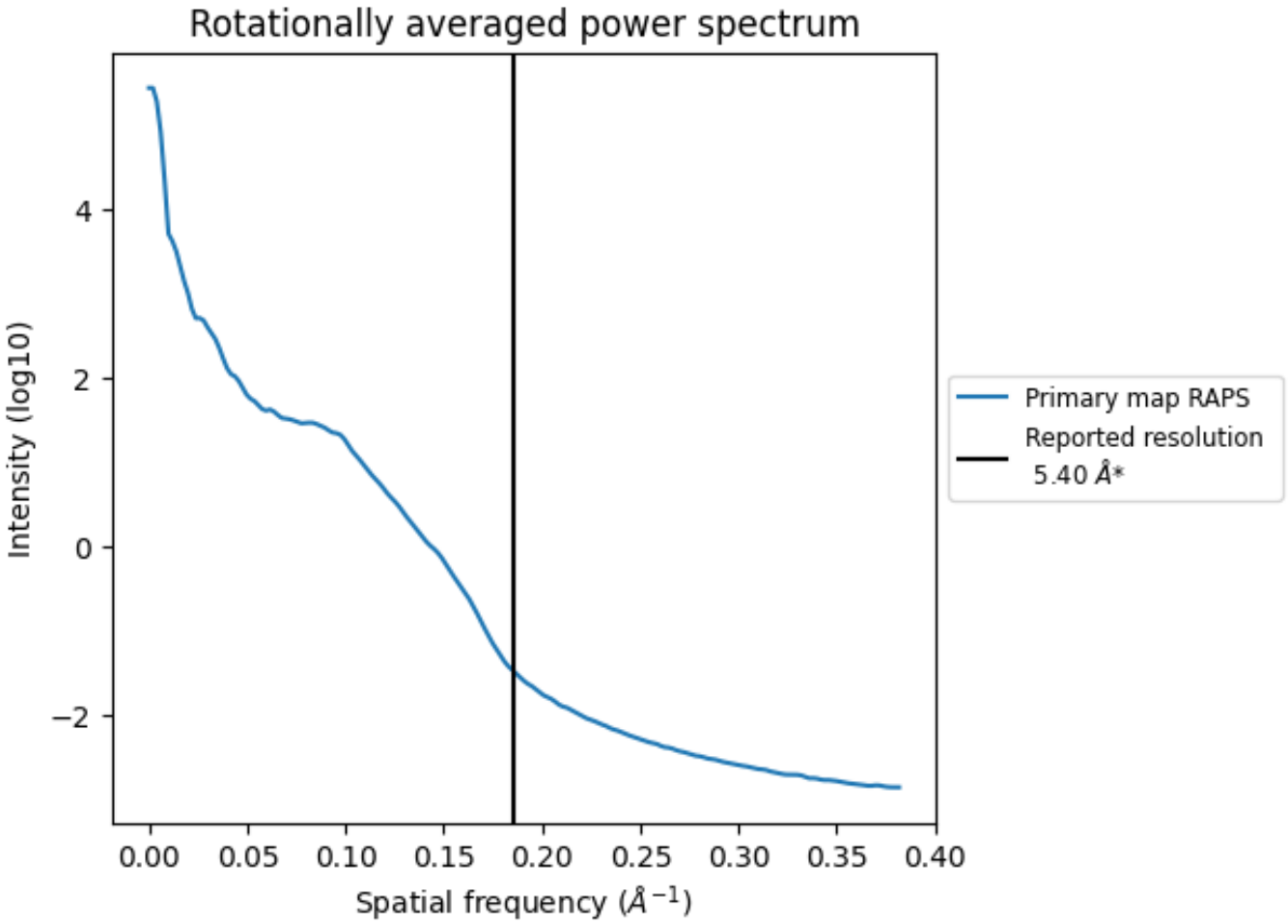
7.2 Volume estimate



The volume at the recommended contour level is 650 nm^3; this corresponds to an approximate mass of 587 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)

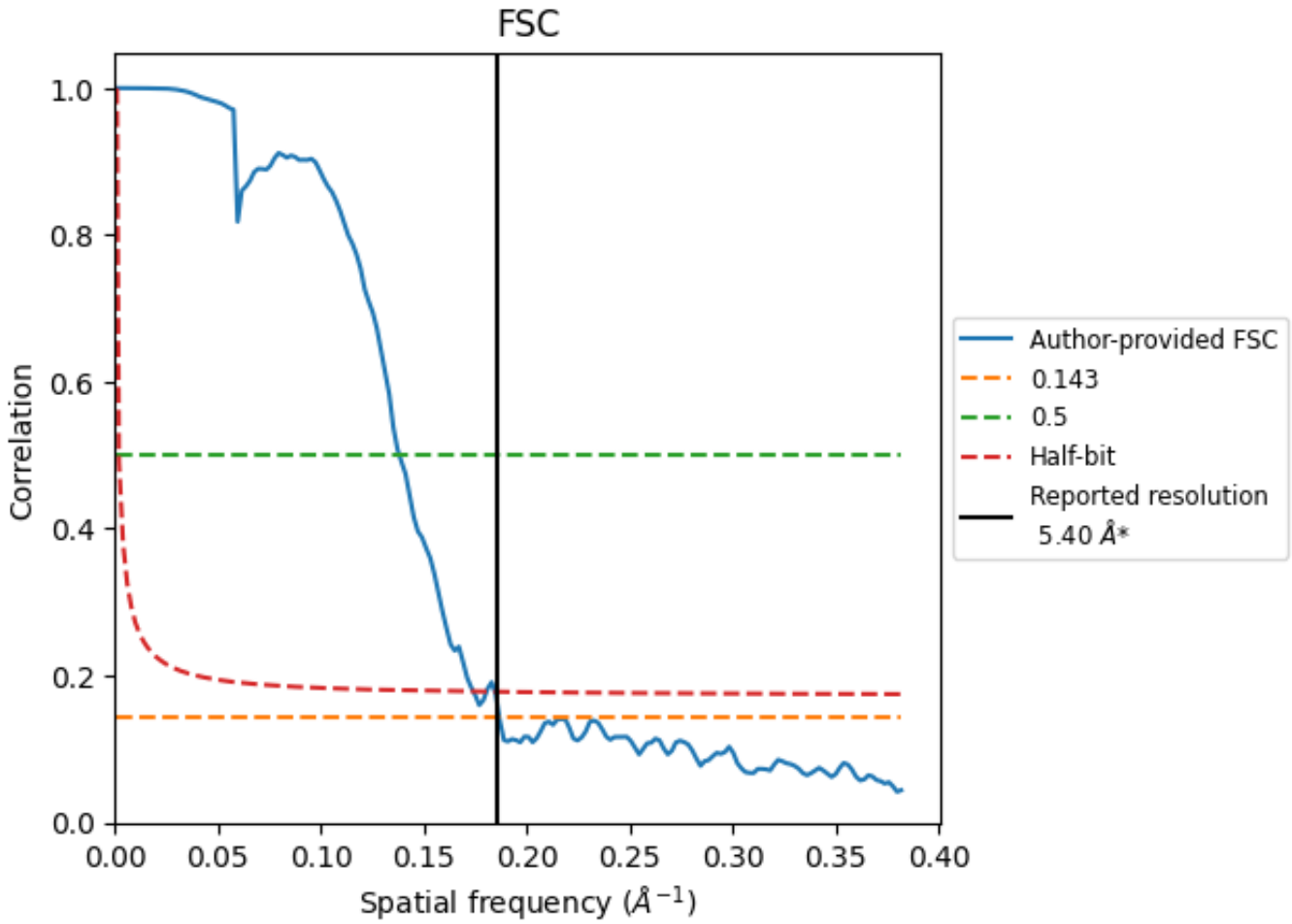


*Reported resolution corresponds to spatial frequency of 0.185 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.185 Å^{-1}

8.2 Resolution estimates (i)

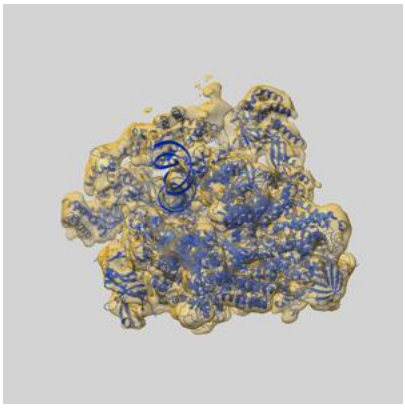
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.40	-	-
Author-provided FSC curve	5.36	7.24	5.74
Unmasked-calculated*	-	-	-

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

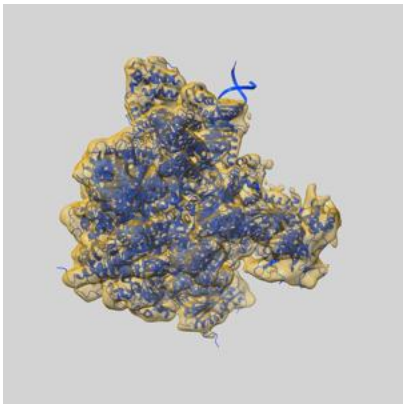
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8135 and PDB model 5IYA. Per-residue inclusion information can be found in section 3 on page 9.

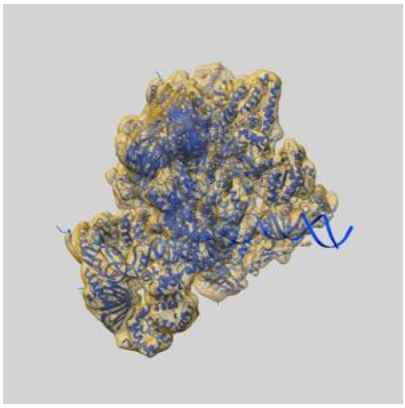
9.1 Map-model overlay



X



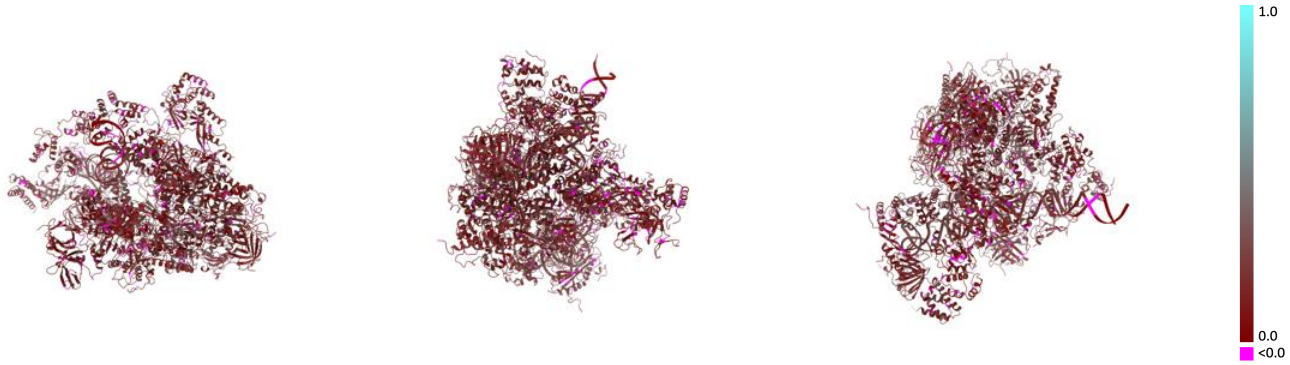
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

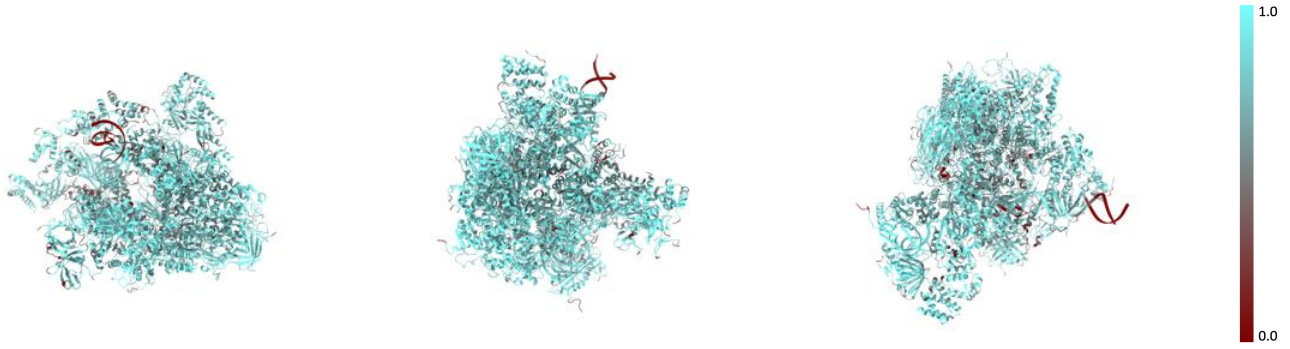
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

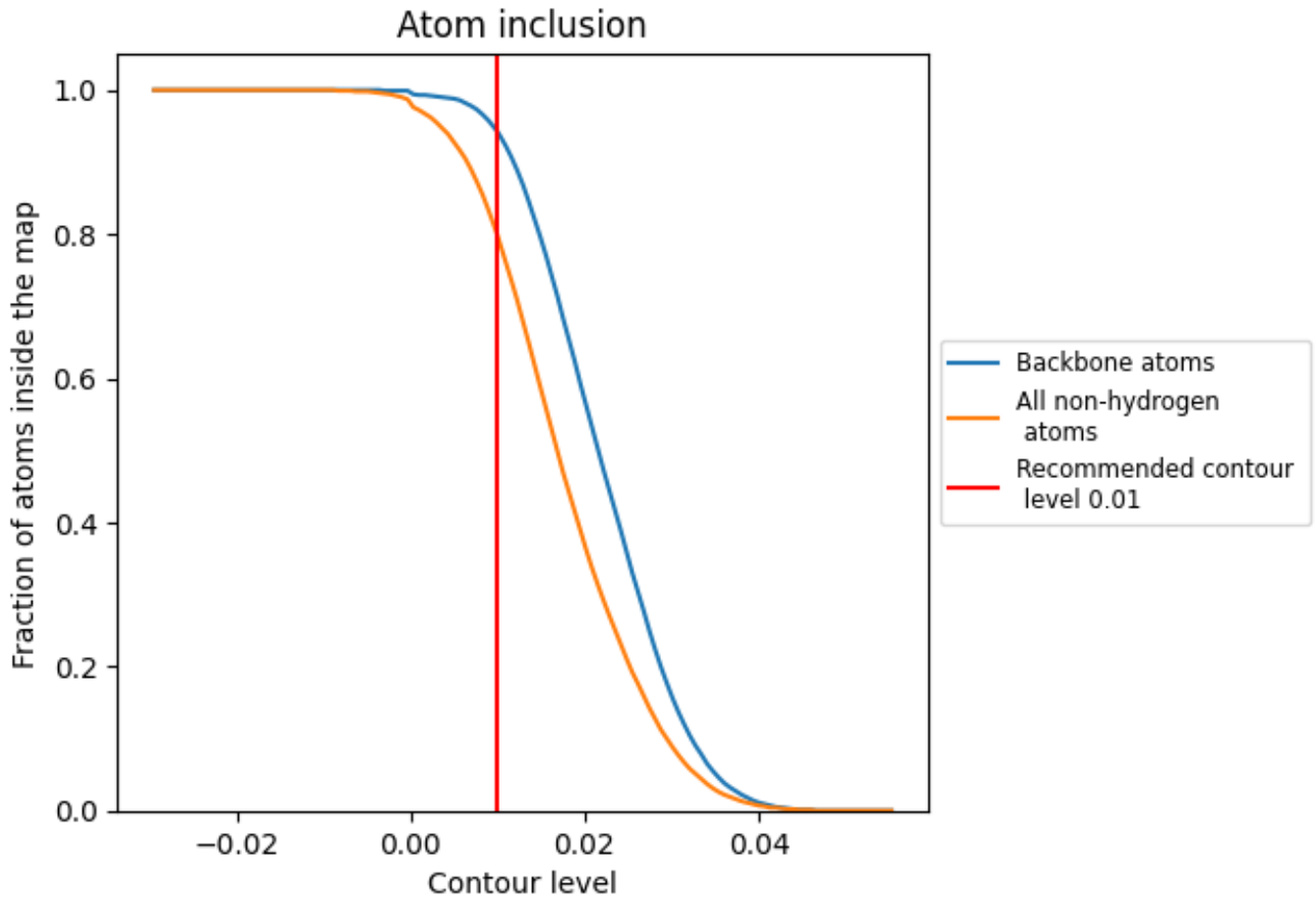
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7980	0.1690
A	0.7650	0.1720
B	0.7900	0.1810
C	0.8780	0.1910
D	0.7930	0.1480
E	0.8420	0.1770
F	0.7900	0.1630
G	0.8390	0.1380
H	0.8700	0.1770
I	0.8450	0.1800
J	0.8870	0.1640
K	0.8600	0.1900
L	0.8950	0.1890
M	0.7960	0.1750
N	0.8260	0.1660
O	0.8350	0.1590
P	0.8750	0.1480
Q	0.7520	0.1240
R	0.7790	0.1320
S	0.7240	0.1330
T	0.7640	0.1470
U	0.7460	0.1550
X	0.8020	0.2060
Y	0.7960	0.1850