Full wwPDB EM Validation Report ⓘ

May 12, 2024 – 06:32 am BST

PDB ID	:	6RI7
EMDB ID	:	EMD-4885
Title	:	Cryo-EM structure of E. coli RNA polymerase elongation complex bound to GreB transcription factor
Authors	:	Abdelkareem, M.; Saint-Andre, C.; Takacs, M.; Papai, G.; Crucifix, C.; Guo, X.; Ortiz, J.; Weixlbaumer, A.
Deposited on	:	2019-04-23
Resolution	:	3.90 Å(reported)
Based on initial model	:	6ALH

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:

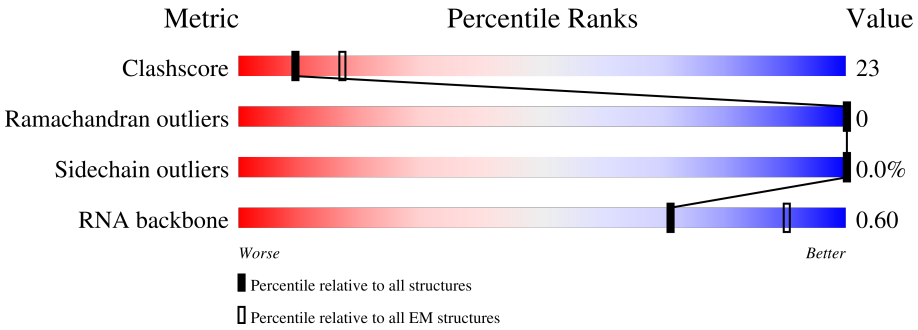
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.90 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	N	39	10% 44% 44%
2	T	39	5% 77% 18%
3	F	158	7% 54% 44%
3	G	158	65% 94% 5%
4	A	329	45% 24% 31%
4	B	329	43% 27% 30%
5	C	1342	5% 53% 46%

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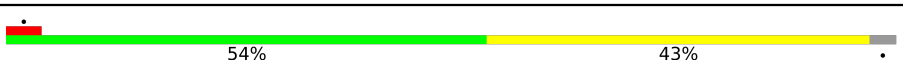
Mol	Chain	Length	Quality of chain
6	D	1407	
7	E	91	
8	R	14	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 28461 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 DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	N	22	Total	C	N	O	P	0	0
			454	215	88	129	22		

- Molecule 2 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	T	32	Total	C	N	O	P	0	0
			650	310	116	192	32		

- Molecule 3 is a protein called Transcription elongation factor GreB.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	156	Total	C	N	O	S	0	0
			1292	821	225	242	4		
3	G	156	Total	C	N	O		0	0
			771	459	156	156			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	228	Total	C	N	O	S	0	0
			1768	1102	312	348	6		
4	B	229	Total	C	N	O	S	0	0
			1772	1104	313	349	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	1319	Total	C	N	O	S	0	0
			10407	6530	1814	2020	43		

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	1358	Total	C	N	O	S	0	0
			10545	6620	1883	1992	50		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	73	Total	C	N	O	S	0	0
			582	355	111	115	1		

- Molecule 8 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	R	10	Total	C	N	O	P	0	0
			217	96	39	72	10		

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
9	D	2	Total	Zn	0
			2	2	

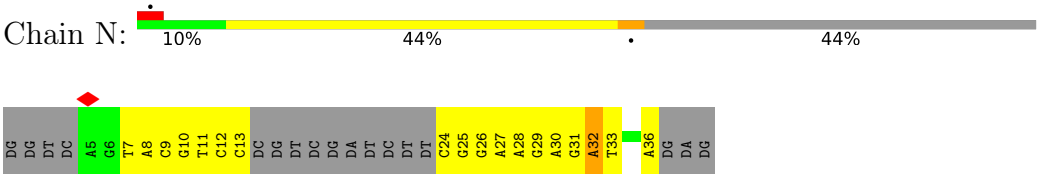
- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
10	D	1	Total	Mg	0
			1	1	

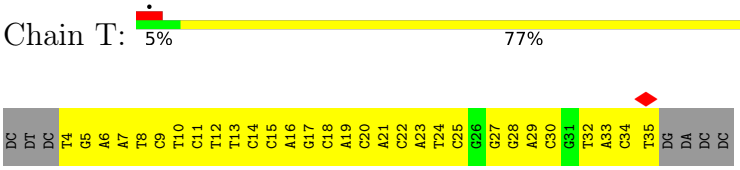
3 Residue-property plots (i)

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.

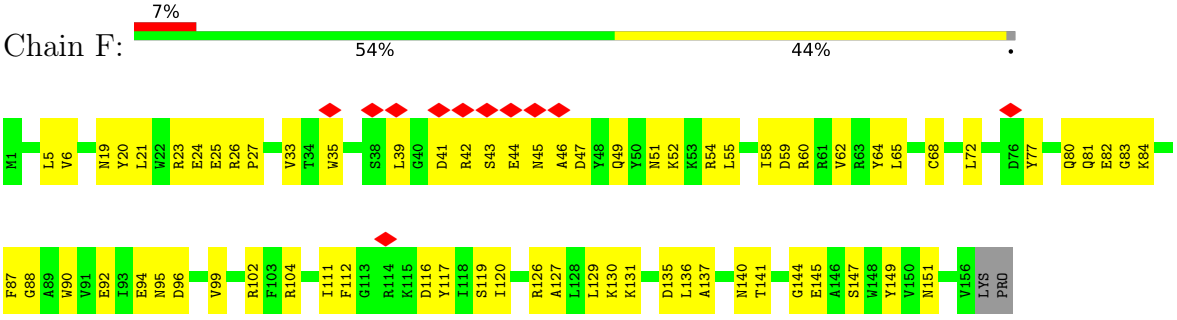
• Molecule 1: Non-template DNA



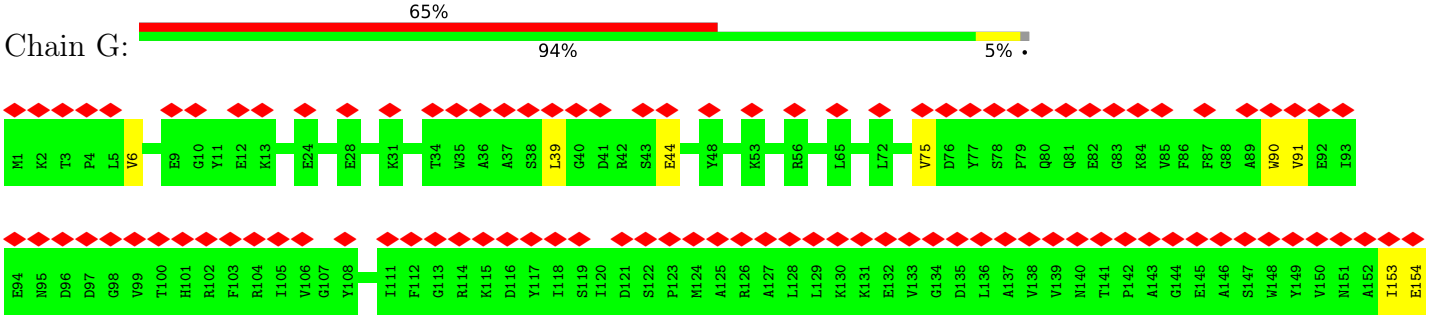
• Molecule 2: Template DNA



• Molecule 3: Transcription elongation factor GreB

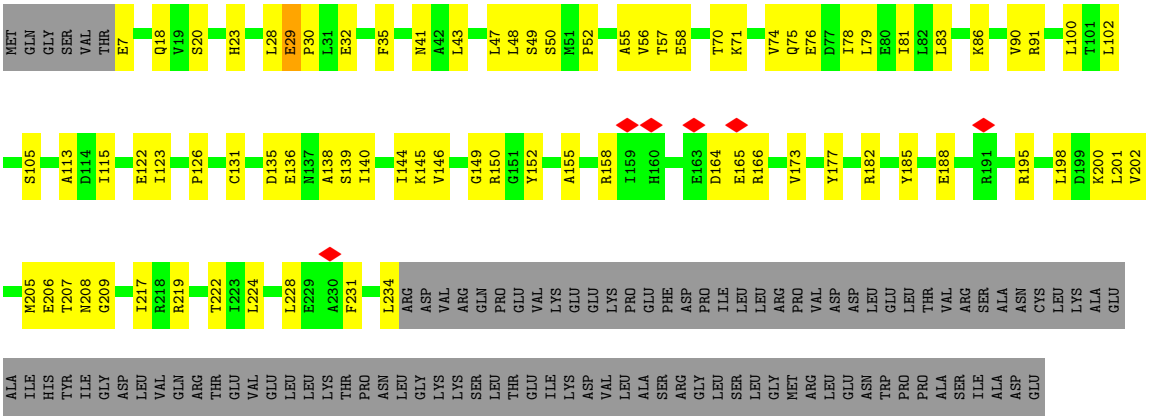


• Molecule 3: Transcription elongation factor GreB



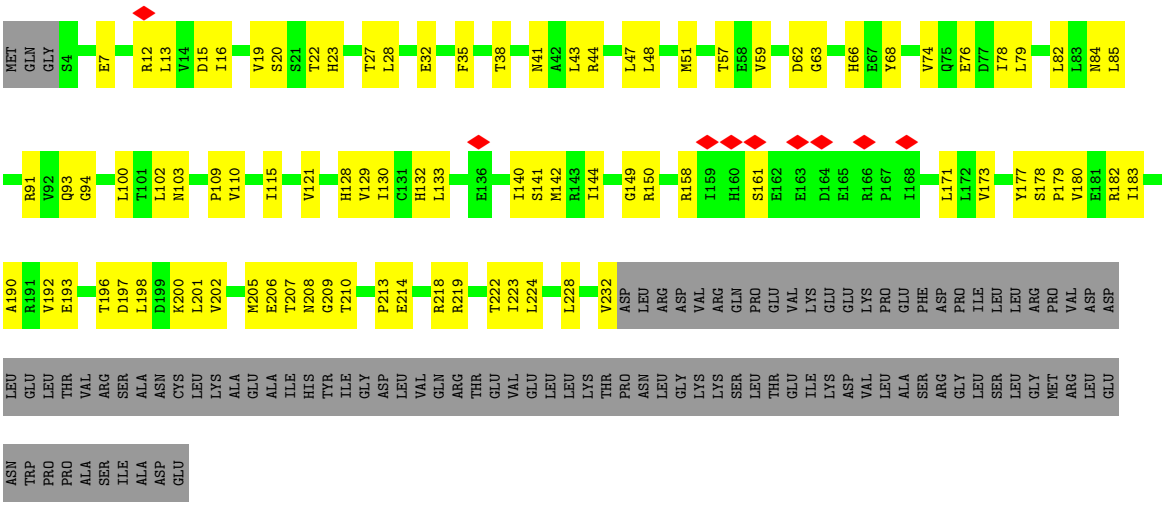
• Molecule 4: DNA-directed RNA polymerase subunit alpha

Chain A:



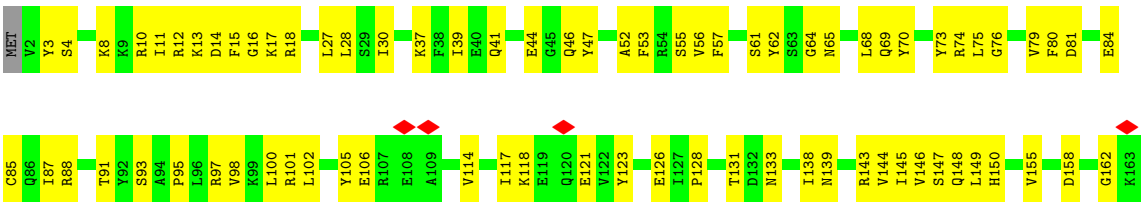
• Molecule 4: DNA-directed RNA polymerase subunit alpha

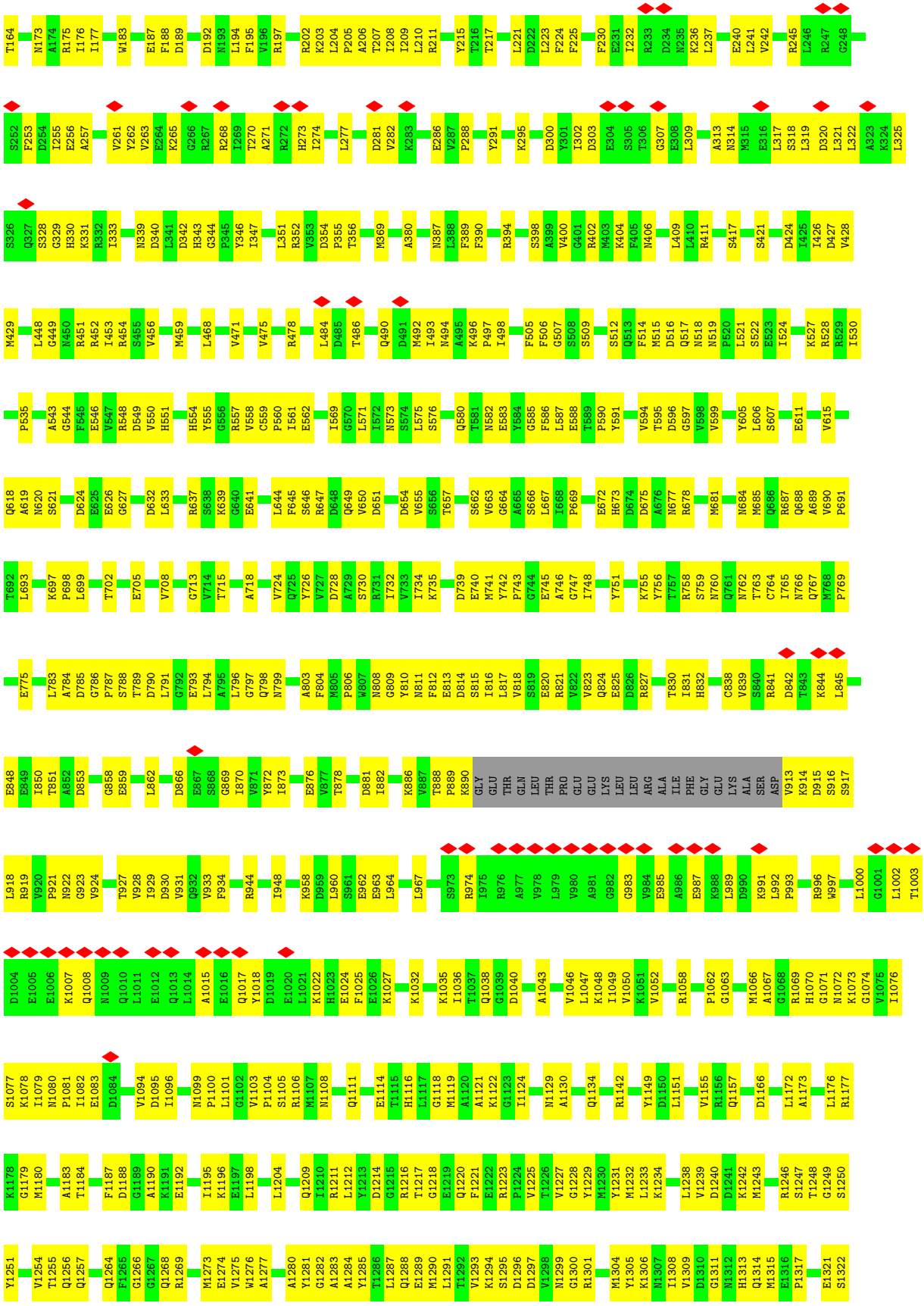
Chain B:

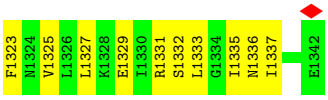


• Molecule 5: DNA-directed RNA polymerase subunit beta

Chain C:

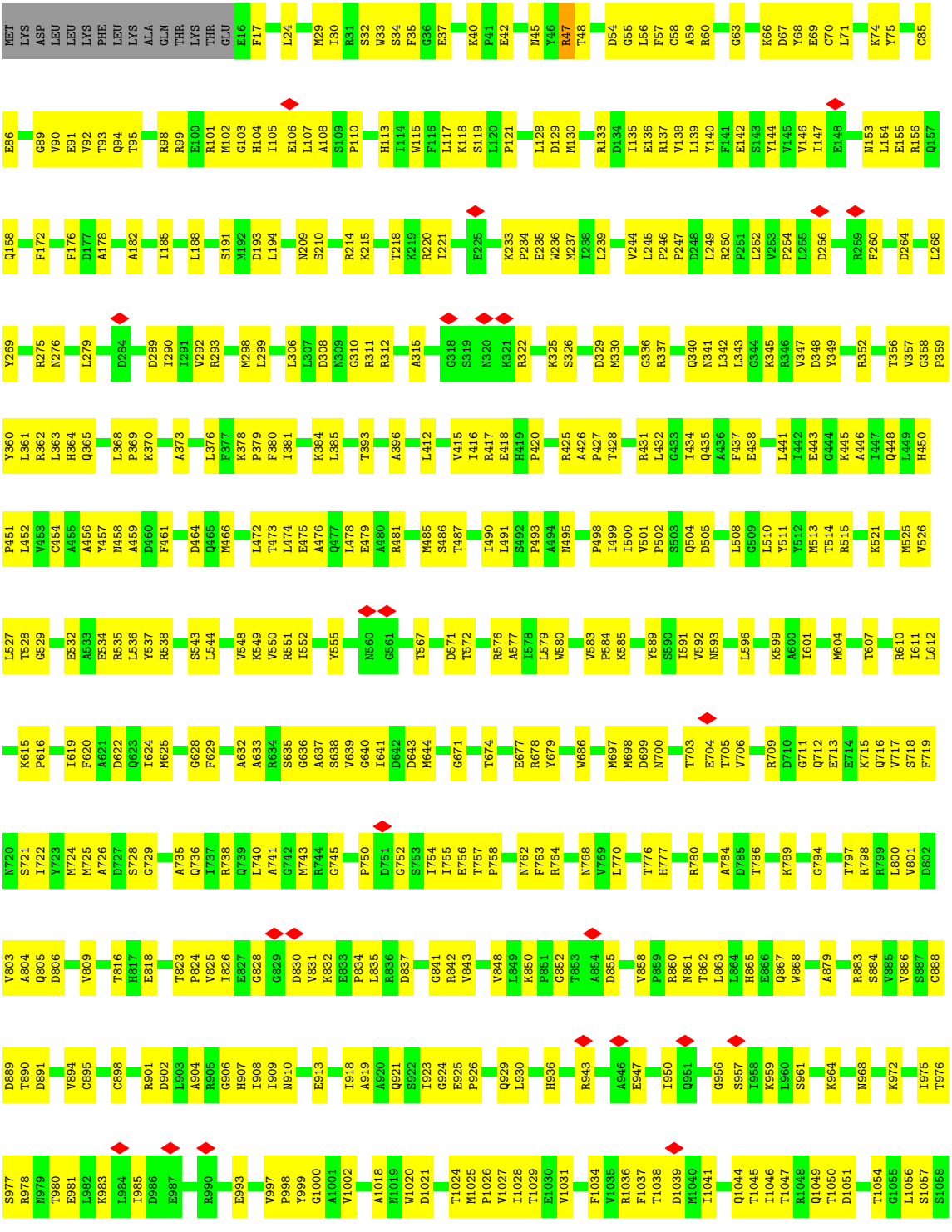


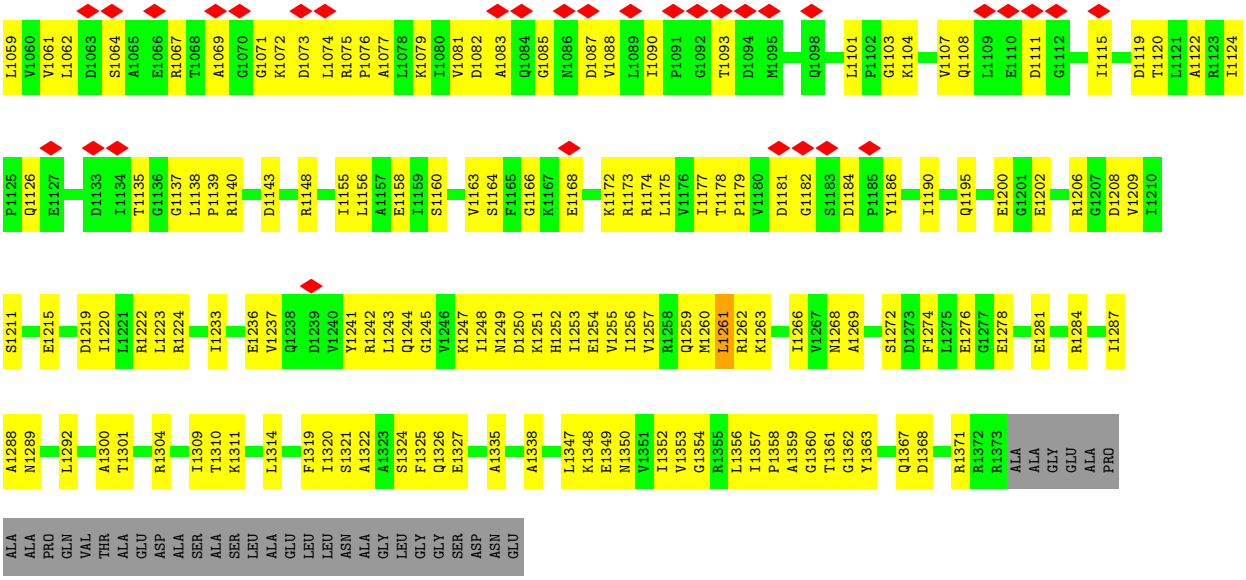

T164 N173 A174 R175 I176 I177 W183 E187 F188 D189 D192 N193 L194 F195 V196 R197 R202 K203 L204 P205 A206 T207 I208 I209 L210 R211 Y215 T216 T217 L221 D222 L223 F224 F225 F230 E231 I232 R233 D234 N235 K236 L237 E240 L241 V242 R245 L246 R247 G248
S252 F253 D254 I255 E256 A257 V261 Y262 V263 E264 K265 G266 R267 R268 I269 T270 A271 R272 H273 I274 L277 D281 V282 K283 E286 Y287 P288 Y291 K295 D300 Y301 T302 D303 E304 S305 T306 G307 E308 L309 A313 N314 M315 E316 L317 S318 L319 D320 L321 L322 A323 K324 L325
S326 Q327 S328 G329 H330 K331 R332 I333 N339 D340 L341 D342 H343 G344 P345 Y346 I347 L351 R352 V353 D354 P355 T356 M369 A380 N387 L388 F389 F390 R394 S398 A399 V400 G401 R402 M403 K404 F405 M406 L409 L410 R411 S417 S421 D424 I425 I426 D427 V428
M429 L448 G449 N450 R451 R452 I453 R454 S455 V456 M459 L468 V471 V475 R478 L484 D485 T486 Q490 D491 M492 I493 N494 A495 K496 P497 I498 F505 F506 G507 S508 S509 S512 Q513 F514 M515 D516 Q517 N518 N519 P520 L521 S522 E523 I524 K527 R528 R529 I530
P535 A543 G544 F545 E546 V547 R548 D549 V550 H551 H554 Y555 G556 R557 V558 C559 P560 I561 E562 I569 G570 L571 I572 N573 S574 L575 S576 Q580 T581 N582 E583 Y584 G585 F586 L587 E588 T589 P590 Y591 V594 T595 D596 G597 V598 V599 Y605 L606 S607 E611 V615
Q618 A619 N620 S621 D624 E625 E626 G627 D632 L633 R637 S638 K639 G640 E641 L644 F645 S646 R647 D648 Q649 V650 D651 D654 V655 S656 T657 S662 V663 G664 A665 S666 L667 I668 P669 E672 H673 D674 D675 A676 N677 R678 M681 N684 M685 Q686 R687 Q688 A689 V690 P691
T692 L693 K697 P698 L699 T702 E705 V708 G713 V714 T715 A718 V724 Q725 Y726 V727 D728 A729 S730 R731 I732 V733 I734 K735 D739 E740 M741 Y742 P743 G744 E745 A746 G747 I748 Y751 K755 Y756 T757 R758 S759 N760 Q761 N762 T763 C764 I765 N766 Q767 M768 P769
E775 L783 A784 D785 G786 P787 S788 T789 D790 L791 G792 E793 L794 A795 L796 G797 Q798 N799 A803 F804 M805 P806 W807 N808 G809 Y810 N811 F812 E813 D814 S815 I816 L817 V818 S819 E820 R821 V822 V823 Q824 E825 D826 R827 T830 I831 H832 C838 V839 S840 R841 D842 T843 K844 L845
E848 E849 I850 T851 A852 D853 G858 E859 L862 D866 E867 S868 G869 I870 V871 Y872 I873 E876 V877 T878 D881 I882 K886 V887 T888 P889 K890 GLY GLU THR GLN LEU THR PRO GLU GLU LYS LEU LEU ARG ALA ILE PHE GLY GLU LYS ALA SER ASP V913 K914 D915 S916 S917
L918 R919 V920 P921 N922 G923 V924 T927 V928 I929 D930 V931 Q932 V933 F934 R944 I948 K958 D959 L960 S961 E962 E963 L964 L967 S973 R974 I975 R976 A977 V978 L979 V980 A981 G982 G983 V984 E985 A986 E987 K988 L989 D990 K991 L992 P993 R996 W997 L1000 G1001 L1002 T1003
D1004 E1005 E1006 K1007 Q1008 N1009 Q1010 L1011 E1012 Q1013 L1014 A1015 E1016 Q1017 Y1018 D1019 E1020 L1021 K1022 H1023 E1024 F1025 E1026 K1027 K1032 K1035 I1036 T1037 Q1038 G1039 D1040 A1043 V1046 L1047 K1048 I1049 V1050 K1051 V1052 R1058 P1062 G1063 M1066 A1067 G1068 R1069 H1070 G1071 N1072 K1073 G1074 V1075 I1076
S1077 K1078 I1079 N1080 P1081 I1082 E1083 D1084 V1094 D1095 I1096 N1099 P1100 L1101 G1102 V1103 P1104 S1105 R1106 M1107 N1108 Q1111 E1114 T1115 H1116 L1117 G1118 M1119 A1120 A1121 K1122 G1123 I1124 N1129 A1130 Q1134 R1142 Y1149 D1150 L1151 V1155 R1156 Q1157 D1166 L1172 A1173 L1176 R1177
K1178 G1179 M1180 A1183 T1184 F1187 D1188 G1189 A1190 K1191 E1192 I1195 K1196 E1197 L1198 L1204 Q1209 I1210 R1211 L1212 Y1213 D1214 G1215 R1216 T1217 G1218 E1219 Q1220 F1221 E1222 R1223 P1224 V1225 T1226 V1227 G1228 Y1229 M1230 Y1231 M1232 L1233 K1234 L1238 V1239 D1240 D1241 K1242 M1243 R1246 S1247 T1248 G1249 S1250
Y1251 V1254 T1255 Q1256 Q1257 Q1264 F1265 G1266 G1267 Q1268 R1269 M1273 E1274 V1275 W1276 A1277 A1280 Y1281 G1282 A1283 A1284 Y1285 T1286 L1287 Q1288 E1289 M1290 L1291 T1292 V1293 K1294 S1295 D1296 D1297 V1298 N1299 G1300 R1301 M1304 Y1305 K1306 N1307 I1308 V1309 D1310 G1311 N1312 H1313 Q1314 M1315 E1316 P1317 E1321 S1322



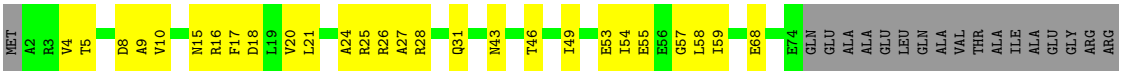
• Molecule 6: DNA-directed RNA polymerase subunit beta'

Chain D:





• Molecule 7: DNA-directed RNA polymerase subunit omega



• Molecule 8: RNA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	121680	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 ($e^-/Å^2$)	59	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.535	Depositor
Minimum map value	-1.180	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.107	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	299.232, 299.232, 299.232	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.039, 1.039, 1.039	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	N	1.00	0/509	1.05	1/781 (0.1%)
2	T	1.17	0/727	1.02	0/1118
3	F	0.36	0/1319	0.49	0/1780
3	G	0.25	0/770	0.45	0/1071
4	A	0.51	0/1790	0.57	0/2426
4	B	0.43	0/1794	0.58	0/2432
5	C	0.51	0/10573	0.57	0/14265
6	D	0.49	0/10706	0.58	0/14456
7	E	0.42	0/584	0.54	0/786
8	R	1.00	0/242	0.96	0/376
All	All	0.53	0/29014	0.60	1/39491 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	A	0	1
5	C	0	1
6	D	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	32	DA	O4'-C1'-N9	5.08	111.56	108.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	29	GLU	Peptide
5	C	1295	SER	Peptide
6	D	47	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	454	0	248	22	0
2	T	650	0	361	60	0
3	F	1292	0	1281	61	0
3	G	771	0	348	5	0
4	A	1768	0	1793	64	0
4	B	1772	0	1799	80	0
5	C	10407	0	10420	523	0
6	D	10545	0	10760	535	0
7	E	582	0	593	30	0
8	R	217	0	107	15	0
9	D	2	0	0	0	0
10	D	1	0	0	0	0
All	All	28461	0	27710	1267	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 23.

All (1267) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:12:DC:O2	2:T:28:DG:N2	1.96	0.98
5:C:888:THR:O	5:C:913:VAL:HA	1.64	0.97
1:N:10:DG:N2	2:T:30:DC:O2	2.00	0.92
1:N:10:DG:N1	2:T:30:DC:N3	2.17	0.91
4:A:7:GLU:HB3	4:B:150:ARG:HH12	1.34	0.90
4:A:207:THR:HG22	4:A:209:GLY:H	1.37	0.90
4:B:59:VAL:O	4:B:171:LEU:HB2	1.72	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:101:ARG:HE	5:C:118:LYS:HD3	1.39	0.86
5:C:985:GLU:O	5:C:989:LEU:HB2	1.76	0.86
6:D:824:PRO:HD3	6:D:835:LEU:HD12	1.57	0.84
1:N:13:DC:O2	2:T:27:DG:N2	2.11	0.83
4:A:56:VAL:HA	4:A:146:VAL:HG22	1.61	0.82
6:D:591:ILE:HG23	6:D:592:VAL:HG13	1.59	0.82
5:C:133:ASN:O	5:C:527:LYS:NZ	2.11	0.82
6:D:1027:VAL:HB	6:D:1122:ALA:H	1.45	0.82
6:D:1350:ASN:HD22	6:D:1358:PRO:HD3	1.43	0.81
5:C:1246:ARG:HH21	5:C:1249:GLY:H	1.28	0.80
6:D:129:ASP:OD2	6:D:220:ARG:NH1	2.14	0.80
6:D:555:TYR:HE2	6:D:585:LYS:HD2	1.47	0.80
6:D:393:THR:HG23	6:D:396:ALA:H	1.47	0.79
6:D:1166:GLY:HA3	6:D:1174:ARG:HD2	1.65	0.79
6:D:144:TYR:OH	6:D:293:ARG:NH2	2.15	0.78
5:C:1246:ARG:NH2	5:C:1250:SER:O	2.17	0.78
5:C:17:LYS:N	5:C:1188:ASP:OD2	2.15	0.78
6:D:425:ARG:NH1	6:D:458:ASN:O	2.16	0.78
5:C:741:MET:SD	5:C:974:ARG:NH1	2.56	0.78
6:D:245:LEU:O	6:D:250:ARG:NH1	2.17	0.78
5:C:12:ARG:HD3	5:C:1183:ALA:HB2	1.66	0.78
6:D:959:LYS:HB3	6:D:983:LYS:HB2	1.66	0.78
5:C:131:THR:HG22	5:C:133:ASN:H	1.45	0.78
6:D:741:ALA:O	6:D:762:ASN:ND2	2.17	0.77
4:A:166:ARG:NH2	5:C:876:GLU:OE1	2.17	0.77
1:N:29:DG:N2	2:T:11:DC:O2	2.16	0.77
5:C:515:MET:HE3	5:C:517:GLN:HB2	1.67	0.77
6:D:709:ARG:NH2	6:D:712:GLN:OE1	2.17	0.77
6:D:308:ASP:OD2	6:D:311:ARG:NE	2.18	0.76
5:C:69:GLN:HE21	5:C:101:ARG:HD2	1.50	0.76
6:D:1241:TYR:O	6:D:1245:GLY:N	2.19	0.76
5:C:1314:GLN:HA	7:E:28:ARG:HH22	1.51	0.76
6:D:113:HIS:CE1	6:D:115:TRP:HB2	2.20	0.76
5:C:591:TYR:OH	5:C:637:ARG:NH2	2.18	0.76
5:C:230:PHE:HB2	5:C:333:ILE:HB	1.68	0.75
4:B:23:HIS:ND1	4:B:206:GLU:OE2	2.19	0.75
5:C:490:GLN:HA	5:C:493:ILE:HG22	1.68	0.75
5:C:1311:GLY:O	7:E:31:GLN:NE2	2.19	0.75
5:C:992:LEU:HD13	5:C:996:ARG:HB2	1.68	0.75
6:D:1172:LYS:HA	6:D:1190:ILE:O	1.85	0.75
6:D:961:SER:HB2	6:D:981:GLU:HB3	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:883:ARG:NH2	6:D:898:CYS:SG	2.59	0.74
5:C:143:ARG:NH2	5:C:512:SER:O	2.21	0.74
4:A:74:VAL:HG22	4:A:76:GLU:H	1.51	0.74
6:D:1061:VAL:O	6:D:1104:LYS:N	2.21	0.74
4:B:74:VAL:HG12	4:B:76:GLU:H	1.51	0.74
4:B:93:GLN:HG3	4:B:94:GLY:H	1.52	0.74
4:A:29:GLU:HG3	4:A:30:PRO:HD3	1.69	0.73
3:F:52:LYS:NZ	6:D:1244:GLN:OE1	2.21	0.73
5:C:747:GLY:O	5:C:974:ARG:NH2	2.20	0.73
5:C:1287:LEU:HD22	6:D:1357:ILE:HD11	1.70	0.73
6:D:490:ILE:HG13	6:D:491:LEU:HG	1.70	0.73
6:D:67:ASP:OD1	6:D:95:THR:N	2.22	0.73
5:C:12:ARG:NH2	5:C:793:GLU:OE1	2.16	0.73
5:C:549:ASP:OD1	5:C:550:VAL:N	2.21	0.72
4:B:103:ASN:HA	4:B:140:ILE:O	1.88	0.72
4:B:182:ARG:NH1	6:D:534:GLU:OE1	2.22	0.72
1:N:29:DG:H2"	1:N:30:DA:C8	2.25	0.72
5:C:143:ARG:NH2	5:C:507:GLY:O	2.21	0.72
5:C:557:ARG:NH2	5:C:607:SER:O	2.22	0.72
5:C:1142:ARG:NH2	5:C:1166:ASP:OD1	2.22	0.72
5:C:672:GLU:N	5:C:672:GLU:OE1	2.22	0.72
6:D:343:LEU:HD21	6:D:1348:LYS:HG3	1.72	0.71
5:C:915:ASP:OD2	5:C:919:ARG:NH2	2.23	0.71
4:B:205:MET:HE2	4:B:213:PRO:HB3	1.71	0.71
5:C:811:ASN:HA	5:C:815:SER:HB2	1.73	0.70
6:D:357:VAL:HG22	6:D:461:PHE:CE2	2.26	0.70
3:F:44:GLU:OE1	5:C:678:ARG:NH2	2.20	0.70
6:D:1049:GLN:O	6:D:1057:SER:HA	1.91	0.70
5:C:318:SER:OG	5:C:320:ASP:OD1	2.08	0.70
5:C:453:ILE:HD12	5:C:587:LEU:HD21	1.74	0.70
5:C:1066:MET:HE1	5:C:1076:ILE:HD12	1.72	0.70
8:R:7:G:H2'	8:R:8:A:H8	1.56	0.70
4:B:22:THR:OG1	4:B:207:THR:N	2.25	0.69
5:C:590:PRO:HB2	5:C:655:VAL:HG21	1.73	0.69
2:T:7:DA:H2'	2:T:8:DT:C6	2.28	0.69
6:D:1069:ALA:HA	6:D:1072:LYS:HE2	1.74	0.69
6:D:584:PRO:HD3	6:D:620:PHE:CD1	2.28	0.69
5:C:915:ASP:OD1	5:C:917:SER:N	2.24	0.69
5:C:797:GLY:N	5:C:1231:TYR:OH	2.25	0.69
5:C:1118:GLY:O	5:C:1121:ALA:N	2.26	0.69
6:D:491:LEU:HB2	6:D:904:ALA:HA	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:18:DC:H2'	2:T:19:DA:C8	2.28	0.68
4:B:208:ASN:OD1	4:B:209:GLY:N	2.26	0.68
6:D:515:ARG:NH2	6:D:718:SER:O	2.26	0.68
6:D:591:ILE:HD11	6:D:604:MET:HA	1.73	0.68
6:D:528:THR:N	6:D:532:GLU:OE2	2.26	0.68
5:C:839:VAL:HG12	5:C:1049:ILE:HA	1.76	0.68
6:D:529:GLY:O	6:D:532:GLU:HG2	1.93	0.68
2:T:22:DC:H2'	2:T:23:DA:H8	1.59	0.68
5:C:1329:GLU:O	5:C:1332:SER:OG	2.07	0.68
4:A:7:GLU:HB3	4:B:150:ARG:NH1	2.08	0.68
6:D:357:VAL:HG22	6:D:461:PHE:HE2	1.59	0.68
6:D:1350:ASN:O	6:D:1354:GLY:N	2.26	0.68
4:A:28:LEU:HD22	4:A:201:LEU:HD23	1.74	0.68
5:C:1223:ARG:NH2	6:D:719:PHE:O	2.27	0.68
4:A:100:LEU:HD23	4:A:115:ILE:HG21	1.77	0.67
6:D:841:GLY:HA2	6:D:901:ARG:HD3	1.76	0.67
4:A:102:LEU:HD12	4:A:115:ILE:HG12	1.76	0.67
5:C:1122:LYS:NZ	5:C:1229:TYR:OH	2.23	0.67
5:C:10:ARG:NH1	5:C:697:LYS:HD3	2.10	0.67
3:F:42:ARG:HB2	3:F:45:ASN:HB2	1.75	0.67
5:C:288:PRO:HG2	5:C:291:TYR:HB2	1.77	0.67
5:C:211:ARG:NH2	5:C:217:THR:OG1	2.23	0.67
6:D:37:GLU:OE2	6:D:106:GLU:N	2.23	0.67
1:N:24:DC:N3	2:T:16:DA:N1	2.42	0.67
4:B:23:HIS:HA	4:B:206:GLU:HG2	1.77	0.67
5:C:1297:ASP:CG	5:C:1300:GLY:H	1.98	0.67
5:C:302:ILE:HG22	5:C:309:LEU:HA	1.75	0.66
6:D:576:ARG:HD3	6:D:593:ASN:HA	1.76	0.66
6:D:718:SER:OG	6:D:719:PHE:N	2.29	0.66
6:D:93:THR:HG22	6:D:94:GLN:H	1.60	0.66
5:C:551:HIS:H	5:C:554:HIS:CE1	2.13	0.66
5:C:148:GLN:NE2	5:C:535:PRO:O	2.22	0.66
5:C:1223:ARG:NH2	6:D:721:SER:OG	2.29	0.66
4:B:192:VAL:HG12	4:B:193:GLU:H	1.60	0.66
2:T:18:DC:H2'	2:T:19:DA:H8	1.60	0.66
6:D:1143:ASP:OD1	6:D:1148:ARG:NH1	2.27	0.66
5:C:3:TYR:OH	5:C:1157:GLN:OE1	2.13	0.66
5:C:1274:GLU:N	5:C:1274:GLU:OE1	2.29	0.66
6:D:91:GLU:OE1	6:D:101:ARG:NH2	2.28	0.66
6:D:1360:GLY:O	6:D:1363:TYR:N	2.29	0.66
5:C:544:GLY:O	5:C:548:ARG:NH1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:883:ARG:NH2	6:D:895:CYS:SG	2.69	0.66
6:D:513:MET:HE3	6:D:579:LEU:HB2	1.77	0.66
5:C:559:CYS:SG	5:C:562:GLU:N	2.64	0.65
5:C:985:GLU:O	5:C:989:LEU:CB	2.43	0.65
6:D:555:TYR:CE2	6:D:585:LYS:HD2	2.30	0.65
6:D:674:THR:N	6:D:677:GLU:OE2	2.21	0.65
1:N:10:DG:H2'	1:N:11:DT:C6	2.31	0.65
5:C:618:GLN:NE2	6:D:770:LEU:H	1.95	0.65
6:D:1038:THR:OG1	6:D:1079:LYS:N	2.29	0.65
5:C:812:PHE:CD2	5:C:813:GLU:HG2	2.32	0.65
6:D:678:ARG:NH1	6:D:756:GLU:OE1	2.30	0.65
6:D:936:HIS:N	6:D:1135:THR:O	2.27	0.65
4:B:79:LEU:HA	4:B:82:LEU:HD12	1.79	0.65
5:C:411:ARG:NH2	5:C:427:ASP:OD2	2.25	0.65
5:C:582:ASN:OD1	5:C:583:GLU:N	2.29	0.65
6:D:610:ARG:HG3	6:D:611:ILE:HG13	1.79	0.65
4:A:18:GLN:NE2	4:A:20:SER:O	2.30	0.65
4:A:57:THR:HG22	4:A:58:GLU:HG3	1.78	0.65
5:C:97:ARG:HB3	5:C:121:GLU:HB2	1.79	0.65
5:C:611:GLU:OE2	5:C:637:ARG:NH2	2.30	0.65
5:C:1106:ARG:O	5:C:1108:ASN:N	2.29	0.65
3:F:33:VAL:HG12	3:F:51:ASN:HB3	1.78	0.65
5:C:255:ILE:HB	5:C:263:VAL:HB	1.79	0.65
5:C:204:LEU:HD13	5:C:208:ILE:HD13	1.79	0.64
5:C:1254:VAL:HG13	5:C:1255:THR:H	1.62	0.64
6:D:843:VAL:HG22	6:D:863:LEU:HA	1.78	0.64
6:D:1155:ILE:N	6:D:1211:SER:OG	2.28	0.64
8:R:7:G:H2'	8:R:8:A:C8	2.33	0.64
4:A:75:GLN:HG3	4:A:76:GLU:HG3	1.79	0.64
5:C:81:ASP:O	5:C:85:CYS:HB2	1.98	0.64
6:D:322:ARG:NH1	8:R:8:A:O2'	2.27	0.64
6:D:527:LEU:HB2	6:D:550:VAL:HG12	1.79	0.64
4:B:100:LEU:HD21	4:B:121:VAL:HG11	1.79	0.64
6:D:113:HIS:HD2	6:D:239:LEU:HD11	1.62	0.64
6:D:1249:ASN:OD1	6:D:1250:ASP:N	2.31	0.64
5:C:810:TYR:CE2	5:C:1078:LYS:HD3	2.33	0.64
5:C:821:ARG:NH1	5:C:824:GLN:OE1	2.30	0.64
5:C:915:ASP:OD1	5:C:916:SER:N	2.30	0.64
6:D:155:GLU:HB2	6:D:158:GLN:HB2	1.80	0.64
5:C:95:PRO:HA	5:C:126:GLU:HG2	1.80	0.63
5:C:1290:MET:HA	5:C:1294:LYS:HD2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:882:ILE:HG13	5:C:919:ARG:HG2	1.79	0.63
3:F:42:ARG:NH2	3:F:44:GLU:OE2	2.31	0.63
5:C:1094:VAL:HG22	5:C:1095:ASP:H	1.61	0.63
3:F:21:LEU:HD23	3:F:58:ILE:HG13	1.79	0.63
6:D:1173:ARG:HG3	6:D:1174:ARG:H	1.60	0.63
5:C:1083:GLU:OE1	5:C:1083:GLU:N	2.26	0.63
7:E:15:ASN:HD22	7:E:18:ASP:CG	2.01	0.63
4:B:35:PHE:HA	4:B:38:THR:HG22	1.79	0.63
5:C:1291:LEU:HD22	6:D:345:LYS:HE3	1.81	0.63
6:D:491:LEU:HD23	6:D:498:PRO:HA	1.80	0.63
6:D:1061:VAL:HG12	6:D:1103:GLY:HA2	1.81	0.63
5:C:933:VAL:HG22	5:C:1050:VAL:HG22	1.80	0.63
5:C:1072:ASN:ND2	5:C:1111:GLN:OE1	2.31	0.63
5:C:1275:VAL:HG13	5:C:1287:LEU:HD11	1.81	0.63
6:D:888:CYS:SG	6:D:890:THR:OG1	2.50	0.63
1:N:7:DT:H2"	1:N:8:DA:N7	2.13	0.63
5:C:842:ASP:HB2	5:C:1047:LEU:HD21	1.80	0.63
6:D:425:ARG:HG2	6:D:426:ALA:H	1.63	0.63
1:N:32:DA:C8	1:N:33:DT:H72	2.34	0.62
5:C:866:ASP:OD1	5:C:869:GLY:N	2.32	0.62
6:D:56:LEU:HB3	6:D:250:ARG:HH21	1.64	0.62
4:B:214:GLU:OE2	4:B:218:ARG:NE	2.32	0.62
5:C:685:MET:SD	5:C:1073:LYS:HG2	2.39	0.62
5:C:1257:GLN:HE22	6:D:341:ASN:HB3	1.64	0.62
5:C:339:ASN:OD1	5:C:340:ASP:N	2.29	0.62
5:C:509:SER:HB3	5:C:512:SER:H	1.64	0.62
5:C:785:ASP:OD2	5:C:791:LEU:N	2.33	0.62
5:C:1214:ASP:O	5:C:1218:GLY:N	2.28	0.62
4:B:27:THR:HG22	4:B:202:VAL:HG22	1.80	0.62
6:D:156:ARG:NH2	6:D:191:SER:OG	2.32	0.62
6:D:1158:GLU:HG3	6:D:1186:TYR:CZ	2.34	0.62
4:A:182:ARG:HB3	4:A:206:GLU:HB3	1.82	0.62
5:C:406:ASN:HB3	5:C:411:ARG:HB2	1.82	0.62
5:C:766:ASN:OD1	5:C:767:GLN:N	2.32	0.62
5:C:1276:TRP:CZ2	6:D:801:VAL:HG21	2.34	0.62
6:D:527:LEU:HD21	6:D:536:LEU:HD12	1.81	0.62
5:C:560:PRO:HB2	6:D:776:THR:HG21	1.80	0.62
6:D:269:TYR:HE1	6:D:306:LEU:HD11	1.65	0.62
6:D:638:SER:OG	6:D:639:VAL:N	2.30	0.62
3:F:52:LYS:HA	3:F:55:LEU:HD12	1.81	0.62
5:C:65:ASN:O	5:C:105:TYR:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:6:VAL:O	3:G:75:VAL:N	2.30	0.62
4:B:19:VAL:HB	4:B:23:HIS:HB3	1.80	0.61
5:C:1073:LYS:NZ	8:R:14:G:OP1	2.27	0.61
3:F:129:LEU:HG	3:F:130:LYS:HG3	1.80	0.61
5:C:506:PHE:O	5:C:512:SER:OG	2.15	0.61
5:C:1192:GLU:OE2	6:D:764:ARG:NE	2.22	0.61
6:D:834:PRO:HG2	6:D:837:ASP:HB2	1.83	0.61
5:C:144:VAL:HG23	5:C:515:MET:HB2	1.82	0.61
2:T:5:DG:OP2	2:T:5:DG:H2'	2.01	0.61
5:C:596:ASP:OD1	5:C:597:GLY:N	2.33	0.61
5:C:739:ASP:OD1	5:C:740:GLU:N	2.31	0.61
6:D:956:GLY:HA3	6:D:985:ILE:O	2.00	0.61
5:C:380:ALA:HB2	3:G:39:LEU:HA	1.82	0.61
6:D:362:ARG:O	6:D:364:HIS:N	2.33	0.61
6:D:1036:ARG:HE	6:D:1081:VAL:HG11	1.65	0.61
6:D:1268:ASN:N	6:D:1301:THR:OG1	2.34	0.61
2:T:14:DC:OP1	6:D:311:ARG:NH1	2.25	0.61
5:C:1306:LYS:O	5:C:1309:VAL:HG22	2.00	0.61
6:D:901:ARG:HH21	6:D:906:GLY:HA2	1.64	0.61
6:D:964:LYS:HB3	6:D:977:SER:HB3	1.83	0.61
6:D:29:MET:O	6:D:32:SER:OG	2.18	0.61
6:D:1027:VAL:HG21	6:D:1122:ALA:HB3	1.80	0.61
5:C:922:ASN:OD1	5:C:923:GLY:N	2.33	0.61
5:C:983:GLY:HA3	5:C:1002:LEU:HA	1.83	0.61
8:R:10:G:H2'	8:R:11:U:H6	1.65	0.61
4:B:28:LEU:HD12	4:B:201:LEU:HD23	1.83	0.61
5:C:320:ASP:OD1	5:C:321:LEU:N	2.34	0.61
6:D:825:VAL:HG23	6:D:832:LYS:HB2	1.82	0.61
2:T:8:DT:OP2	2:T:8:DT:H6	1.83	0.60
4:A:231:PHE:CE1	4:B:28:LEU:HD11	2.36	0.60
5:C:10:ARG:NH1	5:C:790:ASP:OD2	2.30	0.60
5:C:759:SER:HB3	5:C:763:THR:O	2.00	0.60
5:C:1083:GLU:CD	5:C:1083:GLU:H	2.03	0.60
5:C:101:ARG:HA	5:C:118:LYS:HG2	1.83	0.60
5:C:678:ARG:NH1	5:C:681:MET:SD	2.74	0.60
6:D:800:LEU:O	6:D:803:VAL:HG12	2.00	0.60
8:R:10:G:H2'	8:R:11:U:C6	2.36	0.60
5:C:88:ARG:NE	5:C:1040:ASP:OD2	2.27	0.60
6:D:55:GLY:H	6:D:58:CYS:HB2	1.66	0.60
6:D:1077:ALA:HA	6:D:1101:LEU:HG	1.82	0.60
5:C:207:THR:HA	5:C:210:LEU:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:253:PHE:HA	5:C:265:LYS:HG3	1.83	0.60
6:D:218:THR:HA	6:D:221:ILE:HG22	1.82	0.60
6:D:510:LEU:HD22	6:D:601:ILE:HD12	1.84	0.60
6:D:950:ILE:HG13	6:D:1020:TRP:CH2	2.36	0.60
5:C:619:ALA:N	5:C:654:ASP:OD2	2.34	0.60
6:D:85:CYS:HB3	6:D:90:VAL:H	1.65	0.60
6:D:431:ARG:HD3	6:D:493:PRO:HG3	1.83	0.60
6:D:58:CYS:SG	6:D:60:ARG:HG2	2.41	0.60
6:D:514:THR:HG21	6:D:596:LEU:HD12	1.84	0.60
5:C:914:LYS:HG2	5:C:915:ASP:H	1.67	0.60
6:D:632:ALA:O	6:D:635:SER:OG	2.16	0.60
4:B:183:ILE:HG22	4:B:205:MET:HG3	1.83	0.60
5:C:1273:MET:HG2	5:C:1276:TRP:CZ3	2.36	0.60
6:D:119:SER:OG	6:D:121:PRO:O	2.19	0.60
4:B:44:ARG:CZ	6:D:538:ARG:HD2	2.30	0.60
5:C:211:ARG:HH22	5:C:217:THR:HG1	1.49	0.60
5:C:806:PRO:HA	5:C:811:ASN:HD21	1.67	0.60
5:C:866:ASP:OD1	5:C:870:ILE:N	2.28	0.60
3:F:120:ILE:O	3:F:126:ARG:NH1	2.34	0.59
6:D:37:GLU:HB2	6:D:104:HIS:NE2	2.17	0.59
6:D:848:VAL:HB	6:D:858:VAL:HG22	1.83	0.59
5:C:814:ASP:OD2	5:C:1106:ARG:NH2	2.35	0.59
6:D:59:ALA:HA	6:D:63:GLY:H	1.68	0.59
6:D:1311:LYS:O	6:D:1314:LEU:N	2.35	0.59
6:D:1350:ASN:HA	6:D:1353:VAL:HG12	1.84	0.59
3:F:90:TRP:CD2	3:F:104:ARG:HB2	2.38	0.59
3:F:95:ASN:OD1	3:F:96:ASP:N	2.35	0.59
4:B:32:GLU:HB3	4:B:35:PHE:CD2	2.38	0.59
4:B:196:THR:HG23	6:D:443:GLU:HG3	1.83	0.59
5:C:128:PRO:HG2	5:C:506:PHE:CD2	2.37	0.59
5:C:528:ARG:NH2	5:C:576:SER:O	2.35	0.59
6:D:842:ARG:NH1	6:D:1254:GLU:OE2	2.36	0.59
4:A:28:LEU:HB2	4:A:201:LEU:HB3	1.84	0.59
3:F:136:LEU:HG	3:F:149:TYR:CE1	2.38	0.59
5:C:580:GLN:NE2	5:C:605:TYR:OH	2.36	0.59
6:D:362:ARG:O	6:D:365:GLN:HG2	2.02	0.59
6:D:431:ARG:N	6:D:921:GLN:OE1	2.35	0.59
6:D:947:GLU:O	6:D:1020:TRP:NE1	2.35	0.59
5:C:825:GLU:OE1	5:C:827:ARG:NH1	2.36	0.58
5:C:851:THR:HG23	5:C:853:ASP:H	1.68	0.58
6:D:235:GLU:OE1	6:D:235:GLU:N	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:425:ARG:HG2	6:D:426:ALA:N	2.17	0.58
6:D:426:ALA:O	6:D:428:THR:N	2.36	0.58
6:D:1079:LYS:NZ	6:D:1087:ASP:OD1	2.26	0.58
7:E:15:ASN:ND2	7:E:18:ASP:H	2.01	0.58
5:C:1313:HIS:CD2	7:E:31:GLN:HE22	2.20	0.58
6:D:641:ILE:HD11	6:D:764:ARG:HG3	1.85	0.58
6:D:1064:SER:O	6:D:1072:LYS:NZ	2.29	0.58
2:T:20:DC:O3'	6:D:352:ARG:NH2	2.35	0.58
4:A:78:ILE:HA	4:A:81:ILE:HD12	1.84	0.58
5:C:339:ASN:HB3	5:C:343:HIS:H	1.68	0.58
5:C:514:PHE:CE2	5:C:760:ASN:HB3	2.39	0.58
6:D:1160:SER:HB2	6:D:1206:ARG:H	1.68	0.58
4:A:43:LEU:HD13	4:A:217:ILE:HD11	1.85	0.58
5:C:594:VAL:HG11	5:C:650:VAL:HG23	1.84	0.58
6:D:45:ASN:ND2	6:D:48:THR:OG1	2.30	0.58
6:D:755:ILE:HG22	6:D:757:THR:H	1.68	0.58
6:D:70:CYS:SG	6:D:71:LEU:N	2.76	0.58
6:D:185:ILE:HA	6:D:188:LEU:HD12	1.84	0.58
5:C:145:ILE:HB	5:C:456:VAL:HG22	1.85	0.58
5:C:271:ALA:HA	5:C:274:ILE:HD12	1.85	0.58
5:C:688:GLN:NE2	8:R:12:G:O3'	2.35	0.58
5:C:176:ILE:HD11	5:C:428:VAL:HG21	1.86	0.58
5:C:1018:TYR:O	5:C:1022:LYS:HG2	2.04	0.58
6:D:709:ARG:HH12	6:D:713:GLU:H	1.51	0.58
6:D:1335:ALA:O	6:D:1338:ALA:N	2.36	0.58
7:E:58:LEU:HD12	7:E:59:ILE:HG12	1.85	0.58
5:C:718:ALA:HB2	5:C:783:LEU:HD11	1.86	0.58
6:D:368:LEU:HD22	6:D:373:ALA:HB2	1.86	0.58
6:D:475:GLU:OE2	7:E:28:ARG:NE	2.37	0.58
6:D:85:CYS:SG	6:D:86:GLU:N	2.76	0.57
6:D:435:GLN:OE1	6:D:486:SER:OG	2.19	0.57
6:D:842:ARG:HH21	6:D:1251:LYS:HG3	1.69	0.57
7:E:46:THR:HA	7:E:49:ILE:HD12	1.86	0.57
5:C:1297:ASP:OD1	5:C:1299:ASN:N	2.37	0.57
5:C:735:LYS:HA	5:C:748:ILE:HG22	1.86	0.57
6:D:1368:ASP:OD1	6:D:1371:ARG:NH2	2.36	0.57
4:B:19:VAL:HG12	4:B:20:SER:H	1.69	0.57
6:D:1281:GLU:HG3	6:D:1284:ARG:H	1.68	0.57
5:C:11:ILE:HG23	5:C:1149:TYR:OH	2.04	0.57
6:D:902:ASP:HB2	6:D:909:ILE:HD13	1.86	0.57
2:T:32:DT:H2"	2:T:33:DA:C5	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:1308:ILE:HD12	6:D:380:PHE:HE1	1.70	0.57
6:D:950:ILE:HG13	6:D:1020:TRP:HH2	1.69	0.57
5:C:859:GLU:HA	5:C:862:LEU:HB2	1.86	0.57
6:D:1024:THR:HG23	6:D:1124:ILE:H	1.70	0.57
5:C:521:LEU:HD12	5:C:794:LEU:HD21	1.86	0.57
5:C:732:ILE:HD11	5:C:769:PRO:HB3	1.85	0.57
6:D:113:HIS:HE1	6:D:115:TRP:HB2	1.65	0.57
2:T:14:DC:H2"	2:T:15:DC:OP2	2.05	0.56
4:B:84:ASN:HD21	6:D:551:ARG:HH22	1.51	0.56
5:C:68:LEU:HD11	5:C:100:LEU:HB3	1.86	0.56
5:C:325:LEU:O	5:C:328:SER:OG	2.19	0.56
5:C:404:LYS:NZ	5:C:449:GLY:O	2.31	0.56
6:D:452:LEU:HG	6:D:625:MET:HE3	1.86	0.56
6:D:644:MET:SD	6:D:740:LEU:HD23	2.45	0.56
2:T:19:DA:OP1	5:C:1269:ARG:NE	2.35	0.56
5:C:468:LEU:HA	5:C:471:VAL:HG12	1.87	0.56
5:C:1103:VAL:HG22	5:C:1111:GLN:HE21	1.69	0.56
6:D:310:GLY:HA2	6:D:315:ALA:HB2	1.86	0.56
6:D:1082:ASP:OD1	6:D:1085:GLY:N	2.37	0.56
7:E:25:ARG:NH2	7:E:68:GLU:OE1	2.38	0.56
3:F:77:TYR:OH	3:F:80:GLN:HB3	2.05	0.56
4:A:91:ARG:HB3	4:A:122:GLU:HB3	1.87	0.56
4:B:59:VAL:HG22	4:B:144:ILE:HA	1.85	0.56
5:C:1077:SER:OG	5:C:1078:LYS:N	2.37	0.56
5:C:1234:LYS:HE2	5:C:1238:LEU:HD11	1.86	0.56
6:D:209:ASN:HA	6:D:214:ARG:HH21	1.69	0.56
6:D:786:THR:HA	6:D:789:LYS:HE2	1.87	0.56
5:C:675:ASP:OD2	5:C:677:ASN:N	2.31	0.56
4:A:105:SER:HB3	4:A:139:SER:HB2	1.88	0.56
6:D:373:ALA:O	6:D:376:LEU:N	2.38	0.56
6:D:961:SER:O	6:D:980:THR:HA	2.04	0.56
5:C:1239:VAL:O	5:C:1242:LYS:N	2.38	0.56
7:E:31:GLN:HB2	7:E:46:THR:HG21	1.88	0.56
5:C:931:VAL:HG22	5:C:1052:VAL:HG22	1.87	0.56
3:F:135:ASP:OD1	3:F:136:LEU:N	2.36	0.56
4:A:135:ASP:OD1	4:A:136:GLU:N	2.38	0.56
6:D:830:ASP:OD1	6:D:831:VAL:N	2.38	0.56
5:C:97:ARG:HD3	5:C:123:TYR:HB3	1.87	0.56
5:C:1209:GLN:HA	5:C:1225:VAL:O	2.05	0.56
5:C:1282:GLY:HA3	7:E:17:PHE:CZ	2.41	0.56
6:D:1269:ALA:O	6:D:1272:SER:OG	2.14	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:921:PRO:O	5:C:924:VAL:HG22	2.06	0.55
6:D:1045:THR:HG22	6:D:1067:ARG:HD3	1.88	0.55
3:F:68:CYS:HA	3:F:72:LEU:HD13	1.89	0.55
4:B:44:ARG:HG3	4:B:183:ILE:HD11	1.88	0.55
5:C:818:VAL:HG22	5:C:1096:ILE:HG12	1.88	0.55
6:D:842:ARG:HH21	6:D:1251:LYS:CG	2.19	0.55
7:E:26:ARG:NE	7:E:53:GLU:OE1	2.37	0.55
2:T:19:DA:H5"	5:C:1269:ARG:HD3	1.88	0.55
4:B:15:ASP:OD1	4:B:16:ILE:N	2.39	0.55
5:C:667:LEU:HA	5:C:702:THR:HG21	1.88	0.55
6:D:615:LYS:HB2	6:D:616:PRO:HD3	1.88	0.55
2:T:22:DC:H2'	2:T:23:DA:C8	2.39	0.55
6:D:425:ARG:HD2	6:D:459:ALA:HB2	1.88	0.55
5:C:786:GLY:N	5:C:789:THR:OG1	2.40	0.55
5:C:256:GLU:HA	5:C:261:VAL:HA	1.89	0.55
5:C:387:ASN:HD21	5:C:394:ARG:HH11	1.53	0.55
5:C:498:ILE:HD12	5:C:498:ILE:H	1.72	0.55
5:C:1176:LEU:O	5:C:1179:GLY:N	2.22	0.55
6:D:1069:ALA:HA	6:D:1072:LYS:HB2	1.87	0.55
5:C:850:ILE:HG13	5:C:1048:LYS:HD3	1.88	0.55
6:D:37:GLU:HB2	6:D:104:HIS:CE1	2.42	0.55
6:D:384:LYS:HG3	6:D:415:VAL:HG12	1.88	0.55
6:D:798:ARG:O	6:D:801:VAL:HG22	2.07	0.55
2:T:7:DA:H8	2:T:7:DA:OP2	1.89	0.55
5:C:300:ASP:OD1	5:C:313:ALA:N	2.38	0.54
5:C:657:THR:OG1	5:C:1187:PHE:HB2	2.08	0.54
5:C:698:PRO:HG3	5:C:1231:TYR:CZ	2.42	0.54
5:C:1246:ARG:NH2	5:C:1249:GLY:H	2.00	0.54
6:D:289:ASP:HA	6:D:292:VAL:HG22	1.88	0.54
3:F:60:ARG:NH1	6:D:752:GLY:O	2.41	0.54
5:C:128:PRO:HG2	5:C:506:PHE:HD2	1.72	0.54
5:C:718:ALA:HA	5:C:751:TYR:CE2	2.42	0.54
5:C:1062:PRO:HB3	5:C:1077:SER:O	2.07	0.54
6:D:349:TYR:HE1	6:D:379:PRO:HG2	1.72	0.54
5:C:295:LYS:HB2	5:C:317:LEU:HD12	1.90	0.54
5:C:810:TYR:CD1	6:D:359:PRO:HD2	2.43	0.54
5:C:1071:GLY:O	5:C:1073:LYS:N	2.40	0.54
6:D:549:LYS:HG2	6:D:571:ASP:OD1	2.07	0.54
6:D:1168:GLU:HA	6:D:1173:ARG:HB2	1.89	0.54
6:D:1219:ASP:HA	6:D:1222:ARG:HG2	1.89	0.54
5:C:620:ASN:HD21	6:D:768:ASN:HB2	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:759:SER:HG	5:C:763:THR:H	1.54	0.54
5:C:74:ARG:HH21	5:C:121:GLU:CD	2.10	0.54
5:C:79:VAL:HG23	5:C:80:PHE:CD2	2.43	0.54
5:C:302:ILE:HD13	5:C:307:GLY:HA2	1.90	0.54
5:C:69:GLN:NE2	5:C:101:ARG:HD2	2.19	0.54
5:C:155:VAL:HA	5:C:175:ARG:O	2.08	0.54
6:D:1025:MET:HB3	6:D:1124:ILE:HD12	1.89	0.54
6:D:1350:ASN:ND2	6:D:1358:PRO:HD3	2.19	0.54
4:B:62:ASP:OD1	4:B:63:GLY:N	2.41	0.54
5:C:519:ASN:HD22	5:C:689:ALA:HB3	1.72	0.54
5:C:964:LEU:HD12	5:C:967:LEU:HD23	1.90	0.54
6:D:342:LEU:HD23	6:D:1352:ILE:HG23	1.89	0.54
5:C:13:LYS:HB2	5:C:1149:TYR:CE1	2.42	0.54
2:T:5:DG:OP2	2:T:5:DG:H8	1.91	0.54
6:D:269:TYR:CE1	6:D:306:LEU:HD11	2.42	0.54
2:T:23:DA:H2'	2:T:24:DT:C6	2.43	0.53
4:B:109:PRO:HA	4:B:132:HIS:CD2	2.43	0.53
5:C:1129:ASN:OD1	5:C:1177:ARG:NH2	2.41	0.53
6:D:107:LEU:HD23	6:D:276:ASN:ND2	2.23	0.53
5:C:690:VAL:HG12	5:C:1234:LYS:O	2.08	0.53
5:C:1225:VAL:HB	6:D:638:SER:HB2	1.90	0.53
5:C:590:PRO:HG3	5:C:605:TYR:HE1	1.73	0.53
5:C:838:CYS:HB2	5:C:918:LEU:HD22	1.90	0.53
6:D:1164:SER:HA	6:D:1200:GLU:HG2	1.90	0.53
8:R:12:G:H2'	8:R:13:U:H6	1.73	0.53
5:C:1212:LEU:HD13	5:C:1225:VAL:HG22	1.89	0.53
5:C:1247:SER:OG	5:C:1248:THR:N	2.41	0.53
6:D:1322:ALA:O	6:D:1325:PHE:N	2.36	0.53
5:C:93:SER:HA	5:C:128:PRO:HA	1.90	0.53
5:C:672:GLU:HG2	5:C:673:HIS:N	2.23	0.53
3:F:6:VAL:HG21	3:F:72:LEU:HB3	1.91	0.53
3:F:20:TYR:HD2	3:F:21:LEU:HD12	1.72	0.53
4:B:47:LEU:HD23	4:B:183:ILE:HD13	1.91	0.53
6:D:1208:ASP:OD1	6:D:1209:VAL:N	2.41	0.53
3:F:92:GLU:HG2	3:F:102:ARG:HB2	1.91	0.53
5:C:1276:TRP:CE2	6:D:801:VAL:HG21	2.42	0.53
3:G:91:VAL:HA	3:G:153:ILE:HA	1.90	0.53
5:C:632:ASP:O	5:C:647:ARG:N	2.42	0.53
2:T:20:DC:H4'	6:D:352:ARG:HH22	1.73	0.53
5:C:61:SER:OG	5:C:64:GLY:N	2.41	0.53
5:C:339:ASN:ND2	5:C:342:ASP:H	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:550:VAL:HG23	5:C:554:HIS:ND1	2.24	0.53
6:D:425:ARG:HG2	6:D:427:PRO:HD2	1.90	0.53
6:D:709:ARG:NH1	6:D:713:GLU:H	2.06	0.53
6:D:968:ASN:OD1	6:D:972:LYS:N	2.41	0.53
1:N:27:DA:P	6:D:1148:ARG:HE	2.32	0.53
4:A:55:ALA:O	4:A:146:VAL:HG13	2.08	0.53
5:C:987:GLU:HG2	5:C:991:LYS:HE3	1.91	0.53
8:R:6:C:H2'	8:R:7:G:C8	2.43	0.53
6:D:473:THR:HG23	6:D:476:ALA:H	1.72	0.52
1:N:10:DG:O6	2:T:30:DC:N4	2.30	0.52
5:C:494:ASN:O	5:C:497:PRO:HD2	2.09	0.52
5:C:1122:LYS:HG2	5:C:1229:TYR:CZ	2.44	0.52
5:C:1173:ALA:O	5:C:1176:LEU:N	2.41	0.52
5:C:1192:GLU:HA	5:C:1195:ILE:HD12	1.91	0.52
6:D:481:ARG:HG3	6:D:485:MET:HE3	1.91	0.52
3:F:47:ASP:H	6:D:736:GLN:HE21	1.57	0.52
3:F:82:GLU:HG2	3:F:83:GLY:H	1.74	0.52
5:C:189:ASP:O	5:C:192:ASP:N	2.39	0.52
5:C:1255:THR:O	5:C:1257:GLN:N	2.42	0.52
5:C:1336:ASN:OD1	5:C:1337:ILE:N	2.42	0.52
6:D:805:GLN:CD	6:D:1348:LYS:HB2	2.30	0.52
6:D:943:ARG:O	6:D:947:GLU:HG2	2.09	0.52
1:N:25:DG:H2'	1:N:26:DG:C8	2.44	0.52
4:B:84:ASN:ND2	6:D:551:ARG:HH22	2.08	0.52
4:B:219:ARG:O	4:B:223:ILE:HG12	2.09	0.52
5:C:10:ARG:NH1	5:C:791:LEU:HD12	2.24	0.52
5:C:1296:ASP:CG	5:C:1322:SER:H	2.12	0.52
6:D:511:TYR:HE2	6:D:515:ARG:HH11	1.56	0.52
6:D:1252:HIS:O	6:D:1255:VAL:HG12	2.09	0.52
2:T:6:DA:H2"	2:T:7:DA:C8	2.44	0.52
5:C:759:SER:OG	5:C:762:ASN:N	2.43	0.52
6:D:552:ILE:O	6:D:567:THR:OG1	2.16	0.52
3:F:64:TYR:HD2	3:F:65:LEU:HD12	1.74	0.52
5:C:387:ASN:HD21	5:C:394:ARG:NH1	2.07	0.52
5:C:878:THR:N	5:C:881:ASP:OD2	2.43	0.52
6:D:264:ASP:OD2	6:D:325:LYS:N	2.33	0.52
6:D:577:ALA:O	6:D:580:TRP:N	2.42	0.52
6:D:865:HIS:CD2	6:D:867:GLN:H	2.27	0.52
6:D:1233:ILE:O	6:D:1237:VAL:HG12	2.09	0.52
6:D:495:ASN:HD22	6:D:1247:LYS:HB2	1.75	0.52
2:T:34:DC:H2'	2:T:35:DT:C6	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:451:PRO:HB2	6:D:625:MET:HE1	1.90	0.52
6:D:956:GLY:CA	6:D:985:ILE:O	2.58	0.52
6:D:1263:LYS:HA	6:D:1281:GLU:HA	1.90	0.52
3:F:59:ASP:HA	3:F:62:VAL:HG12	1.91	0.52
4:A:195:ARG:HE	4:A:198:LEU:HD11	1.75	0.52
5:C:1284:ALA:HB3	6:D:1361:THR:HB	1.91	0.52
6:D:420:PRO:HA	6:D:437:PHE:O	2.10	0.52
6:D:1029:THR:N	6:D:1119:ASP:O	2.40	0.52
3:F:43:SER:O	3:F:49:GLN:NE2	2.42	0.51
6:D:361:LEU:HA	6:D:365:GLN:HE21	1.74	0.51
6:D:452:LEU:HG	6:D:625:MET:CE	2.40	0.51
2:T:20:DC:H2'	2:T:21:DA:C8	2.45	0.51
6:D:193:ASP:OD1	6:D:194:LEU:N	2.43	0.51
6:D:888:CYS:SG	6:D:889:ASP:N	2.83	0.51
3:F:119:SER:OG	3:F:120:ILE:N	2.43	0.51
5:C:796:LEU:N	5:C:1231:TYR:OH	2.43	0.51
5:C:1325:VAL:HG13	6:D:249:LEU:HD13	1.91	0.51
2:T:10:DT:OP2	2:T:10:DT:H2'	2.11	0.51
2:T:20:DC:C3'	6:D:352:ARG:HH22	2.24	0.51
4:A:150:ARG:NH1	4:B:7:GLU:O	2.27	0.51
4:A:231:PHE:HE2	4:B:43:LEU:HD21	1.76	0.51
4:B:110:VAL:HG12	4:B:130:ILE:HD12	1.91	0.51
5:C:560:PRO:O	6:D:780:ARG:NH2	2.44	0.51
6:D:349:TYR:CD2	6:D:472:LEU:HD11	2.46	0.51
3:F:35:TRP:HB3	6:D:599:LYS:NZ	2.25	0.51
4:A:79:LEU:HD21	5:C:693:LEU:HD11	1.93	0.51
5:C:558:VAL:HG11	5:C:573:ASN:HB3	1.92	0.51
5:C:1280:ALA:HB1	6:D:918:ILE:HG22	1.92	0.51
6:D:110:PRO:HB2	6:D:182:ALA:HB1	1.92	0.51
6:D:607:THR:HA	6:D:610:ARG:HG2	1.91	0.51
6:D:921:GLN:O	6:D:924:GLY:N	2.43	0.51
6:D:1107:VAL:HG22	6:D:1122:ALA:HB2	1.92	0.51
2:T:25:DC:OP1	5:C:139:ASN:ND2	2.43	0.51
5:C:702:THR:N	5:C:705:GLU:OE2	2.33	0.51
5:C:1116:HIS:CE1	6:D:641:ILE:HG22	2.46	0.51
5:C:1239:VAL:HG13	5:C:1240:ASP:N	2.25	0.51
6:D:57:PHE:HB3	6:D:98:ARG:HH12	1.74	0.51
6:D:1036:ARG:NE	6:D:1081:VAL:HG11	2.26	0.51
3:F:84:LYS:HD3	3:F:130:LYS:HG2	1.92	0.51
4:B:190:ALA:HB2	4:B:200:LYS:HB2	1.92	0.51
5:C:257:ALA:HB1	5:C:282:VAL:HG11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:960:LEU:HB3	5:C:1025:PHE:CE1	2.46	0.51
5:C:1002:LEU:HD22	5:C:1008:GLN:HB2	1.93	0.51
7:E:17:PHE:O	7:E:20:VAL:N	2.44	0.51
5:C:177:ILE:HG12	5:C:183:TRP:CD1	2.46	0.51
5:C:389:PHE:HB2	5:C:390:PHE:CE2	2.46	0.51
5:C:1002:LEU:HD21	5:C:1007:LYS:HB2	1.93	0.51
2:T:5:DG:H2"	2:T:6:DA:N7	2.26	0.51
4:A:58:GLU:HB2	4:A:145:LYS:HB3	1.92	0.51
6:D:640:GLY:O	6:D:643:ASP:HB2	2.10	0.51
5:C:633:LEU:HA	5:C:645:PHE:O	2.11	0.50
5:C:804:PHE:HB3	5:C:1100:PRO:HG3	1.92	0.50
6:D:697:MET:HE1	6:D:741:ALA:HB3	1.93	0.50
4:A:149:GLY:HA3	4:A:177:TYR:CZ	2.46	0.50
5:C:1256:GLN:NE2	6:D:99:ARG:HH22	2.09	0.50
6:D:537:TYR:CE1	6:D:544:LEU:HD13	2.46	0.50
2:T:6:DA:H2"	2:T:7:DA:H8	1.75	0.50
4:B:41:ASN:ND2	5:C:1216:ARG:O	2.43	0.50
6:D:147:ILE:HG12	6:D:178:ALA:HA	1.93	0.50
6:D:526:VAL:C	6:D:527:LEU:HD12	2.31	0.50
6:D:555:TYR:HD2	6:D:585:LYS:HB3	1.76	0.50
6:D:572:THR:OG1	6:D:576:ARG:HD2	2.12	0.50
6:D:743:MET:HG3	6:D:745:GLY:H	1.76	0.50
5:C:1043:ALA:O	5:C:1046:VAL:HG12	2.12	0.50
5:C:101:ARG:HH21	5:C:118:LYS:NZ	2.10	0.50
5:C:1256:GLN:HE21	6:D:99:ARG:HH22	1.57	0.50
6:D:252:LEU:HD11	6:D:260:PHE:HB3	1.93	0.50
6:D:709:ARG:NH1	6:D:712:GLN:H	2.09	0.50
6:D:709:ARG:CZ	6:D:712:GLN:H	2.24	0.50
6:D:726:ALA:O	6:D:729:GLY:N	2.35	0.50
2:T:13:DT:C4	2:T:14:DC:N4	2.80	0.50
3:F:87:PHE:CD1	3:F:120:ILE:HD12	2.47	0.50
4:A:231:PHE:CE2	4:B:43:LEU:HD21	2.46	0.50
5:C:84:GLU:HA	5:C:87:ILE:HD12	1.93	0.50
5:C:402:ARG:HH21	5:C:417:SER:C	2.14	0.50
5:C:809:GLY:O	5:C:811:ASN:N	2.44	0.50
6:D:826:ILE:HG22	6:D:828:GLY:H	1.76	0.50
4:A:23:HIS:HB2	4:A:205:MET:O	2.12	0.50
5:C:914:LYS:HG2	5:C:915:ASP:N	2.27	0.50
5:C:1239:VAL:HG13	5:C:1240:ASP:H	1.77	0.50
6:D:93:THR:HG22	6:D:94:GLN:N	2.25	0.50
6:D:349:TYR:CE2	6:D:472:LEU:HD11	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:1242:ARG:O	6:D:1245:GLY:N	2.44	0.50
7:E:9:ALA:N	7:E:55:GLU:OE2	2.42	0.50
5:C:1035:LYS:O	5:C:1038:GLN:HG2	2.11	0.50
5:C:41:GLN:NE2	5:C:73:TYR:O	2.45	0.49
5:C:88:ARG:HA	5:C:934:PHE:CZ	2.46	0.49
5:C:724:VAL:HB	5:C:775:GLU:H	1.77	0.49
5:C:1082:ILE:H	5:C:1082:ILE:HD12	1.75	0.49
5:C:1220:GLN:HG2	5:C:1221:PHE:O	2.11	0.49
6:D:233:LYS:O	6:D:236:TRP:HB2	2.11	0.49
6:D:826:ILE:HG22	6:D:828:GLY:N	2.27	0.49
6:D:1051:ASP:HB3	6:D:1054:THR:OG1	2.11	0.49
5:C:11:ILE:HG22	5:C:1172:LEU:HD11	1.93	0.49
5:C:870:ILE:HD13	5:C:944:ARG:HD3	1.93	0.49
5:C:1323:PHE:CZ	5:C:1327:LEU:HD11	2.47	0.49
6:D:1050:THR:HA	6:D:1057:SER:HA	1.94	0.49
6:D:1309:ILE:HG13	6:D:1310:THR:N	2.26	0.49
3:F:47:ASP:N	6:D:736:GLN:HE21	2.10	0.49
4:B:102:LEU:HD13	4:B:115:ILE:HA	1.94	0.49
5:C:699:LEU:HG	5:C:799:ASN:HD22	1.78	0.49
5:C:798:GLN:OE1	5:C:827:ARG:HB2	2.12	0.49
5:C:886:LYS:HG2	5:C:916:SER:HB2	1.94	0.49
6:D:74:LYS:HG2	6:D:75:TYR:CD1	2.48	0.49
6:D:416:ILE:O	6:D:418:GLU:N	2.46	0.49
6:D:705:THR:OG1	6:D:718:SER:HA	2.12	0.49
6:D:735:ALA:O	6:D:738:ARG:HB3	2.13	0.49
6:D:1269:ALA:HB1	6:D:1272:SER:HB2	1.93	0.49
5:C:1254:VAL:HG13	5:C:1255:THR:N	2.26	0.49
5:C:1283:ALA:HA	6:D:479:GLU:OE1	2.11	0.49
6:D:919:ALA:HA	6:D:1252:HIS:ND1	2.27	0.49
6:D:1061:VAL:O	6:D:1104:LYS:CA	2.59	0.49
6:D:1357:ILE:O	6:D:1362:GLY:HA3	2.12	0.49
4:A:71:LYS:HE2	4:A:140:ILE:HG22	1.93	0.49
5:C:98:VAL:O	5:C:121:GLU:HA	2.12	0.49
5:C:742:TYR:HB3	5:C:743:PRO:HD2	1.94	0.49
5:C:1288:GLN:NE2	5:C:1317:PRO:HB3	2.28	0.49
6:D:95:THR:O	6:D:98:ARG:HB3	2.11	0.49
6:D:113:HIS:CD2	6:D:239:LEU:HD11	2.44	0.49
6:D:1178:THR:HA	6:D:1184:ASP:HB3	1.93	0.49
3:F:95:ASN:HB3	3:F:99:VAL:H	1.78	0.49
5:C:215:TYR:HE2	5:C:426:ILE:HD11	1.77	0.49
6:D:957:SER:HB3	6:D:985:ILE:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:1046:ILE:HD12	6:D:1059:LEU:HD22	1.94	0.49
2:T:9:DC:C6	2:T:10:DT:H72	2.47	0.49
3:F:25:GLU:OE2	3:F:54:ARG:NH2	2.46	0.49
5:C:678:ARG:HG3	5:C:1106:ARG:HB3	1.94	0.49
5:C:821:ARG:O	5:C:824:GLN:HB2	2.13	0.49
6:D:1026:PRO:HB2	6:D:1028:ILE:HG23	1.95	0.49
5:C:205:PRO:O	5:C:208:ILE:HG22	2.13	0.49
5:C:742:TYR:H	5:C:746:ALA:HB2	1.78	0.49
5:C:1069:ARG:NH2	5:C:1114:GLU:OE2	2.39	0.49
5:C:1105:SER:HA	6:D:736:GLN:OE1	2.13	0.49
6:D:140:TYR:OH	6:D:312:ARG:HG2	2.12	0.49
6:D:1138:LEU:HB3	6:D:1139:PRO:HD3	1.94	0.49
6:D:1266:ILE:HB	6:D:1276:GLU:O	2.12	0.49
3:G:90:TRP:N	3:G:154:GLU:O	2.46	0.49
5:C:10:ARG:HH11	5:C:697:LYS:HD3	1.77	0.49
5:C:624:ASP:O	5:C:626:GLU:N	2.46	0.49
5:C:997:TRP:CD1	5:C:1000:LEU:HD21	2.48	0.49
4:B:15:ASP:HB3	4:B:27:THR:OG1	2.13	0.49
5:C:223:LEU:HD21	5:C:426:ILE:HG23	1.94	0.49
5:C:1124:ILE:HG21	5:C:1180:MET:SD	2.53	0.49
5:C:1285:TYR:HD2	6:D:475:GLU:HB3	1.76	0.49
6:D:485:MET:O	6:D:487:THR:N	2.46	0.49
6:D:501:VAL:HG22	6:D:502:PRO:O	2.13	0.49
6:D:580:TRP:CZ3	6:D:589:TYR:HA	2.47	0.49
6:D:1163:VAL:HG12	6:D:1202:GLU:O	2.12	0.49
6:D:1272:SER:HB3	6:D:1274:PHE:HD2	1.76	0.49
5:C:562:GLU:OE1	5:C:662:SER:OG	2.22	0.48
6:D:254:PRO:HA	6:D:260:PHE:CD1	2.48	0.48
6:D:336:GLY:O	6:D:340:GLN:CB	2.61	0.48
6:D:432:LEU:O	6:D:434:ILE:N	2.45	0.48
6:D:750:PRO:HD3	6:D:777:HIS:CD2	2.48	0.48
6:D:968:ASN:ND2	6:D:972:LYS:HB2	2.28	0.48
2:T:29:DA:H2"	2:T:30:DC:C6	2.48	0.48
3:F:51:ASN:O	3:F:55:LEU:HG	2.13	0.48
5:C:18:ARG:HE	5:C:620:ASN:HA	1.78	0.48
5:C:148:GLN:OE1	5:C:454:ARG:NH1	2.46	0.48
5:C:594:VAL:HG12	5:C:595:THR:O	2.13	0.48
5:C:747:GLY:HA2	5:C:974:ARG:HE	1.78	0.48
5:C:1264:GLN:O	5:C:1266:GLY:N	2.45	0.48
6:D:1126:GLN:HE21	6:D:1195:GLN:HE21	1.59	0.48
3:F:141:THR:N	3:F:144:GLY:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:810:TYR:CE1	6:D:359:PRO:HD2	2.48	0.48
4:A:49:SER:OG	4:A:50:SER:N	2.46	0.48
6:D:722:ILE:HA	6:D:725:MET:HE3	1.95	0.48
5:C:232:ILE:HG12	5:C:237:LEU:HG	1.96	0.48
5:C:1314:GLN:HB2	7:E:28:ARG:HH12	1.77	0.48
6:D:725:MET:O	6:D:728:SER:OG	2.31	0.48
6:D:1284:ARG:O	6:D:1287:ILE:HG13	2.13	0.48
6:D:1349:GLU:OE1	6:D:1349:GLU:N	2.37	0.48
6:D:1357:ILE:HG22	6:D:1359:ALA:H	1.77	0.48
5:C:39:ILE:HD11	5:C:75:LEU:HD22	1.94	0.48
6:D:805:GLN:O	6:D:1347:LEU:HB2	2.13	0.48
1:N:36:DA:H2	2:T:4:DT:H3	1.60	0.48
5:C:30:ILE:HD12	5:C:30:ILE:H	1.79	0.48
5:C:575:LEU:HD23	5:C:576:SER:O	2.14	0.48
5:C:870:ILE:HB	5:C:944:ARG:HD3	1.96	0.48
5:C:886:LYS:O	5:C:916:SER:N	2.40	0.48
5:C:1293:VAL:HG11	5:C:1304:MET:HG2	1.96	0.48
6:D:805:GLN:OE1	6:D:1348:LYS:HB2	2.13	0.48
5:C:459:MET:HB3	5:C:505:PHE:CZ	2.49	0.48
5:C:848:GLU:HG2	5:C:889:PRO:HD3	1.96	0.48
5:C:1211:ARG:C	5:C:1212:LEU:HD12	2.33	0.48
5:C:1211:ARG:O	5:C:1212:LEU:HD12	2.14	0.48
6:D:369:PRO:HG3	6:D:446:ALA:O	2.14	0.48
1:N:9:DC:C2	1:N:10:DG:C8	3.02	0.48
4:B:158:ARG:HA	4:B:161:SER:OG	2.13	0.48
5:C:18:ARG:HH21	5:C:620:ASN:C	2.17	0.48
6:D:495:ASN:ND2	6:D:1247:LYS:O	2.47	0.48
6:D:611:ILE:HG22	6:D:612:LEU:HD12	1.94	0.48
6:D:865:HIS:CE1	6:D:868:TRP:HD1	2.31	0.48
5:C:662:SER:O	5:C:666:SER:N	2.30	0.48
6:D:823:THR:HG22	6:D:879:ALA:HB2	1.95	0.48
6:D:850:LYS:HG2	6:D:852:GLY:H	1.79	0.48
3:F:26:ARG:NH2	6:D:1243:LEU:O	2.46	0.47
5:C:195:PHE:CD1	5:C:203:LYS:HG2	2.49	0.47
5:C:688:GLN:HE22	8:R:13:U:H5'	1.78	0.47
6:D:45:ASN:C	6:D:47:ARG:H	2.18	0.47
6:D:136:GLU:O	6:D:139:LEU:N	2.47	0.47
6:D:336:GLY:O	6:D:340:GLN:HB3	2.14	0.47
6:D:555:TYR:HB2	6:D:585:LYS:O	2.14	0.47
6:D:1056:LEU:HD13	6:D:1108:GLN:HE22	1.79	0.47
5:C:673:HIS:ND1	6:D:763:PHE:O	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:130:MET:HB3	6:D:135:ILE:HD11	1.95	0.47
6:D:341:ASN:C	6:D:342:LEU:HD12	2.34	0.47
6:D:709:ARG:HG3	6:D:711:GLY:H	1.78	0.47
6:D:1158:GLU:HG3	6:D:1186:TYR:CE2	2.49	0.47
5:C:319:LEU:HA	5:C:322:LEU:HD12	1.96	0.47
5:C:1067:ALA:HB2	5:C:1073:LYS:HA	1.96	0.47
5:C:1331:ARG:HG3	6:D:33:TRP:CH2	2.50	0.47
6:D:907:HIS:ND1	6:D:908:ILE:O	2.46	0.47
6:D:1029:THR:HG23	6:D:1119:ASP:O	2.14	0.47
4:A:152:TYR:CE1	5:C:824:GLN:HG2	2.49	0.47
4:B:47:LEU:HD23	4:B:183:ILE:HG21	1.96	0.47
5:C:52:ALA:O	5:C:55:SER:OG	2.22	0.47
5:C:530:ILE:HB	5:C:573:ASN:O	2.14	0.47
5:C:605:TYR:C	5:C:606:LEU:HD12	2.33	0.47
5:C:873:ILE:HG13	5:C:944:ARG:HH22	1.80	0.47
5:C:1285:TYR:CD2	6:D:475:GLU:HB3	2.49	0.47
5:C:1289:GLU:OE2	6:D:472:LEU:HB2	2.15	0.47
6:D:68:TYR:OH	6:D:94:GLN:HG3	2.14	0.47
6:D:450:HIS:HE1	6:D:452:LEU:HG	1.80	0.47
1:N:24:DC:N3	2:T:16:DA:C2	2.83	0.47
4:B:192:VAL:HG12	4:B:193:GLU:N	2.26	0.47
5:C:519:ASN:O	5:C:522:SER:N	2.47	0.47
5:C:558:VAL:CG1	5:C:573:ASN:HB3	2.44	0.47
5:C:599:VAL:H	5:C:627:GLY:CA	2.28	0.47
6:D:741:ALA:C	6:D:762:ASN:HD22	2.15	0.47
8:R:9:U:H2'	8:R:10:G:H8	1.79	0.47
8:R:12:G:H2'	8:R:13:U:C6	2.49	0.47
4:A:57:THR:HG23	4:A:158:ARG:NH1	2.29	0.47
4:A:208:ASN:OD1	4:A:209:GLY:N	2.48	0.47
5:C:1103:VAL:HB	5:C:1104:PRO:HD3	1.96	0.47
6:D:40:LYS:HB3	6:D:42:GLU:OE1	2.14	0.47
6:D:697:MET:HG3	6:D:698:MET:N	2.29	0.47
1:N:29:DG:N2	2:T:11:DC:C2	2.83	0.47
3:F:140:ASN:HA	3:F:145:GLU:HA	1.97	0.47
5:C:257:ALA:HB3	5:C:262:TYR:CE2	2.50	0.47
5:C:715:THR:OG1	5:C:784:ALA:O	2.28	0.47
6:D:45:ASN:ND2	6:D:48:THR:H	2.13	0.47
6:D:215:LYS:O	6:D:218:THR:HG22	2.14	0.47
6:D:347:VAL:HG12	6:D:348:ASP:O	2.14	0.47
6:D:1090:ILE:HB	6:D:1093:THR:OG1	2.15	0.47
6:D:1181:ASP:OD1	6:D:1182:GLY:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:1261:LEU:HD12	6:D:1304:ARG:HH21	1.79	0.47
7:E:54:ILE:HD13	7:E:59:ILE:HB	1.97	0.47
4:A:144:ILE:HG22	4:A:146:VAL:HG23	1.97	0.47
5:C:355:PRO:HG2	5:C:356:THR:HG23	1.97	0.47
5:C:421:SER:OG	5:C:424:ASP:N	2.40	0.47
6:D:983:LYS:HA	6:D:993:GLU:O	2.14	0.47
7:E:10:VAL:HG21	7:E:16:ARG:HH11	1.80	0.47
7:E:54:ILE:O	7:E:57:GLY:N	2.42	0.47
5:C:15:PHE:CG	5:C:1190:ALA:HB2	2.49	0.47
5:C:102:LEU:HD23	5:C:117:ILE:HD11	1.97	0.47
5:C:591:TYR:HD2	5:C:606:LEU:HD13	1.80	0.47
5:C:684:ASN:OD1	5:C:687:ARG:NH2	2.48	0.47
5:C:845:LEU:HD21	5:C:890:LYS:HA	1.97	0.47
5:C:960:LEU:O	5:C:963:GLU:HB2	2.14	0.47
3:F:26:ARG:NH1	3:F:55:LEU:HD22	2.30	0.47
4:B:59:VAL:HG21	4:B:85:LEU:HD13	1.96	0.47
5:C:1116:HIS:HE1	6:D:641:ILE:H	1.63	0.47
5:C:1214:ASP:HB3	5:C:1217:THR:OG1	2.14	0.47
6:D:30:ILE:O	6:D:33:TRP:HB2	2.16	0.47
4:A:135:ASP:HB3	4:A:138:ALA:HB3	1.96	0.46
5:C:133:ASN:CG	5:C:713:GLY:HA3	2.36	0.46
6:D:816:THR:HB	6:D:818:GLU:OE1	2.15	0.46
7:E:8:ASP:HB2	7:E:55:GLU:CD	2.35	0.46
3:F:77:TYR:HE2	3:F:81:GLN:H	1.63	0.46
4:B:78:ILE:O	4:B:82:LEU:HG	2.16	0.46
5:C:620:ASN:HD21	6:D:768:ASN:CB	2.28	0.46
5:C:702:THR:C	5:C:1183:ALA:HB1	2.36	0.46
5:C:1296:ASP:OD1	5:C:1321:GLU:HB3	2.14	0.46
6:D:1041:ILE:HG22	6:D:1044:GLN:HB2	1.97	0.46
6:D:805:GLN:OE1	6:D:1348:LYS:HE3	2.16	0.46
6:D:818:GLU:OE1	6:D:818:GLU:N	2.48	0.46
6:D:1073:ASP:HA	6:D:1075:ARG:HH12	1.80	0.46
1:N:24:DC:H42	2:T:16:DA:H61	1.63	0.46
4:A:152:TYR:CE1	5:C:824:GLN:HA	2.50	0.46
5:C:13:LYS:HD3	5:C:14:ASP:N	2.29	0.46
5:C:471:VAL:O	5:C:475:VAL:HG23	2.16	0.46
5:C:615:VAL:HG21	5:C:645:PHE:HD2	1.80	0.46
6:D:275:ARG:HG2	6:D:299:LEU:HA	1.98	0.46
6:D:508:LEU:HD21	6:D:637:ALA:HB3	1.97	0.46
5:C:929:ILE:HG13	5:C:930:ASP:N	2.30	0.46
5:C:1305:TYR:O	5:C:1309:VAL:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:1047:THR:HB	6:D:1062:LEU:HD11	1.98	0.46
2:T:5:DG:H2"	2:T:6:DA:C8	2.50	0.46
2:T:21:DA:H2'	2:T:22:DC:C6	2.51	0.46
4:A:188:GLU:OE2	4:A:200:LYS:HD2	2.15	0.46
4:B:180:VAL:HA	4:B:207:THR:HA	1.96	0.46
5:C:702:THR:HA	5:C:1184:THR:H	1.80	0.46
5:C:803:ALA:CB	5:C:1227:VAL:HG12	2.46	0.46
5:C:812:PHE:HD2	5:C:813:GLU:HG2	1.80	0.46
5:C:1246:ARG:HH21	5:C:1249:GLY:N	2.04	0.46
6:D:135:ILE:O	6:D:138:VAL:HB	2.16	0.46
6:D:136:GLU:OE2	6:D:312:ARG:NH2	2.45	0.46
5:C:206:ALA:O	5:C:209:ILE:HG22	2.16	0.46
5:C:669:PRO:HG3	5:C:1069:ARG:NH2	2.30	0.46
5:C:1032:LYS:HE2	5:C:1036:ILE:HD11	1.97	0.46
5:C:1058:ARG:HE	5:C:1240:ASP:CG	2.19	0.46
5:C:1288:GLN:HG3	6:D:1356:LEU:HD23	1.98	0.46
6:D:330:MET:O	6:D:337:ARG:HG2	2.15	0.46
6:D:521:LYS:O	6:D:543:SER:N	2.35	0.46
6:D:1143:ASP:OD1	6:D:1148:ARG:HD2	2.15	0.46
4:A:113:ALA:HB2	4:A:126:PRO:HB3	1.98	0.46
5:C:448:LEU:HD11	5:C:554:HIS:HA	1.98	0.46
5:C:590:PRO:HG3	5:C:605:TYR:CE1	2.51	0.46
5:C:639:LYS:O	5:C:641:GLU:HG2	2.15	0.46
5:C:1151:LEU:HD21	5:C:1198:LEU:HD13	1.97	0.46
5:C:1232:MET:C	5:C:1233:LEU:HD12	2.35	0.46
5:C:1281:TYR:CZ	6:D:431:ARG:HG2	2.51	0.46
6:D:290:ILE:HD12	6:D:290:ILE:H	1.79	0.46
3:F:26:ARG:HB3	3:F:27:PRO:HD3	1.97	0.46
3:F:111:ILE:O	3:F:112:PHE:CD1	2.69	0.46
4:B:79:LEU:O	4:B:82:LEU:HB2	2.16	0.46
5:C:726:TYR:CE2	5:C:728:ASP:HB2	2.51	0.46
5:C:1119:MET:HG3	5:C:1204:LEU:HD13	1.97	0.46
6:D:1140:ARG:HH21	6:D:1236:GLU:CD	2.18	0.46
4:A:155:ALA:O	4:A:158:ARG:N	2.49	0.46
6:D:146:VAL:HB	6:D:156:ARG:O	2.15	0.46
6:D:709:ARG:CG	6:D:711:GLY:H	2.29	0.46
6:D:805:GLN:HG2	6:D:1347:LEU:HB2	1.98	0.46
1:N:30:DA:H2"	1:N:31:DG:C8	2.51	0.45
3:F:87:PHE:CG	3:F:88:GLY:N	2.83	0.45
4:A:83:LEU:O	4:A:86:LYS:HB3	2.16	0.45
4:B:179:PRO:O	4:B:208:ASN:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:70:TYR:HA	5:C:100:LEU:HD23	1.98	0.45
5:C:204:LEU:HB3	5:C:208:ILE:HG21	1.96	0.45
5:C:615:VAL:HG13	5:C:650:VAL:HA	1.98	0.45
6:D:709:ARG:NH1	6:D:713:GLU:O	2.49	0.45
6:D:901:ARG:NH2	6:D:906:GLY:HA2	2.30	0.45
2:T:20:DC:C4'	6:D:352:ARG:HH22	2.29	0.45
3:F:141:THR:HG22	6:D:671:GLY:HA3	1.98	0.45
5:C:1063:GLY:H	5:C:1076:ILE:HG23	1.81	0.45
6:D:1363:TYR:OH	6:D:1367:GLN:NE2	2.49	0.45
3:F:94:GLU:OE2	3:F:151:ASN:ND2	2.49	0.45
4:A:32:GLU:HB2	4:A:35:PHE:CD2	2.51	0.45
5:C:202:ARG:HH21	5:C:369:MET:HA	1.81	0.45
5:C:1293:VAL:HG23	5:C:1315:MET:HE3	1.98	0.45
6:D:865:HIS:CE1	6:D:868:TRP:CD1	3.05	0.45
4:A:47:LEU:HD23	4:A:47:LEU:HA	1.77	0.45
4:B:149:GLY:HA3	4:B:177:TYR:CZ	2.51	0.45
5:C:207:THR:HG1	5:C:354:ASP:CG	2.19	0.45
5:C:242:VAL:O	5:C:245:ARG:HB2	2.16	0.45
5:C:559:CYS:SG	5:C:561:ILE:N	2.77	0.45
5:C:886:LYS:NZ	5:C:916:SER:HB3	2.30	0.45
6:D:1039:ASP:HB3	6:D:1077:ALA:HB3	1.98	0.45
5:C:409:LEU:HD23	5:C:409:LEU:HA	1.80	0.45
5:C:1277:ALA:O	5:C:1280:ALA:N	2.50	0.45
6:D:526:VAL:HG12	6:D:549:LYS:HB2	1.99	0.45
6:D:537:TYR:CE1	6:D:544:LEU:HB2	2.52	0.45
4:B:47:LEU:HD11	4:B:180:VAL:HG11	1.99	0.45
4:B:51:MET:O	4:B:150:ARG:HA	2.17	0.45
5:C:223:LEU:HD11	5:C:426:ILE:HG21	1.98	0.45
6:D:90:VAL:HG12	6:D:91:GLU:O	2.16	0.45
6:D:137:ARG:HG2	6:D:142:GLU:OE2	2.16	0.45
6:D:432:LEU:HD22	6:D:435:GLN:HE21	1.82	0.45
6:D:454:CYS:O	6:D:457:TYR:N	2.50	0.45
6:D:1039:ASP:O	6:D:1076:PRO:HA	2.17	0.45
6:D:1251:LYS:O	6:D:1254:GLU:HB2	2.17	0.45
2:T:15:DC:H5'	2:T:15:DC:C6	2.52	0.45
5:C:162:GLY:O	5:C:164:THR:N	2.49	0.45
5:C:569:ILE:C	5:C:571:LEU:H	2.20	0.45
5:C:1081:PRO:HB2	5:C:1083:GLU:OE1	2.17	0.45
6:D:128:LEU:HD13	6:D:128:LEU:O	2.16	0.45
6:D:1326:GLN:O	6:D:1327:GLU:HB3	2.17	0.45
3:F:46:ALA:HA	3:F:49:GLN:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:90:TRP:CE2	3:F:104:ARG:HB2	2.51	0.45
5:C:1308:ILE:HD12	6:D:380:PHE:CE1	2.52	0.45
6:D:341:ASN:O	6:D:345:LYS:HE2	2.16	0.45
6:D:794:GLY:O	6:D:797:THR:OG1	2.24	0.45
6:D:918:ILE:HG13	6:D:919:ALA:N	2.32	0.45
6:D:1155:ILE:C	6:D:1156:LEU:HD12	2.38	0.45
4:B:102:LEU:HB3	4:B:142:MET:SD	2.57	0.45
5:C:37:LYS:HD2	5:C:47:TYR:CE1	2.52	0.45
5:C:232:ILE:HB	5:C:331:LYS:HA	1.99	0.45
5:C:580:GLN:HB2	5:C:588:GLU:HG3	1.98	0.45
5:C:1069:ARG:CZ	5:C:1231:TYR:HD2	2.30	0.45
5:C:1094:VAL:HG22	5:C:1095:ASP:N	2.31	0.45
5:C:1101:LEU:HD12	6:D:505:ASP:OD1	2.17	0.45
6:D:1036:ARG:HA	6:D:1111:ASP:OD1	2.16	0.45
6:D:1163:VAL:HG22	6:D:1164:SER:H	1.82	0.45
6:D:1173:ARG:HG3	6:D:1174:ARG:N	2.31	0.45
4:A:48:LEU:HD23	4:A:48:LEU:HA	1.76	0.45
5:C:344:GLY:HA3	5:C:346:TYR:CE2	2.52	0.45
6:D:59:ALA:HB1	6:D:90:VAL:HG11	1.98	0.45
6:D:362:ARG:N	6:D:365:GLN:HE21	2.14	0.45
6:D:850:LYS:HB3	6:D:855:ASP:HB2	1.98	0.45
6:D:1036:ARG:HG3	6:D:1081:VAL:HG21	1.99	0.45
6:D:1215:GLU:OE2	6:D:1224:ARG:NH1	2.50	0.45
7:E:21:LEU:HD23	7:E:21:LEU:HA	1.81	0.45
2:T:14:DC:C2	2:T:15:DC:C4	3.05	0.44
2:T:17:DG:H2'	2:T:18:DC:C6	2.52	0.44
4:A:57:THR:O	4:A:173:VAL:HG22	2.17	0.44
5:C:521:LEU:HD13	5:C:796:LEU:HD21	1.98	0.44
5:C:633:LEU:HD13	5:C:644:LEU:HD23	1.99	0.44
6:D:74:LYS:HG2	6:D:75:TYR:CE1	2.52	0.44
6:D:358:GLY:N	6:D:359:PRO:HD3	2.32	0.44
6:D:1028:ILE:HA	6:D:1120:THR:HA	1.99	0.44
6:D:1034:PHE:CD2	6:D:1083:ALA:HA	2.51	0.44
2:T:27:DG:H2"	2:T:28:DG:O5'	2.16	0.44
5:C:12:ARG:HH21	5:C:793:GLU:CD	2.15	0.44
5:C:236:LYS:HB3	5:C:286:GLU:HG3	1.99	0.44
5:C:599:VAL:H	5:C:627:GLY:HA3	1.82	0.44
6:D:103:GLY:O	6:D:244:VAL:N	2.42	0.44
6:D:890:THR:HG22	6:D:891:ASP:N	2.33	0.44
4:B:133:LEU:HD21	4:B:140:ILE:HG12	1.99	0.44
5:C:303:ASP:O	5:C:307:GLY:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:516:ASP:O	5:C:518:ASN:N	2.44	0.44
5:C:832:HIS:HE1	5:C:1238:LEU:HD22	1.82	0.44
6:D:17:PHE:HZ	6:D:1353:VAL:HG21	1.82	0.44
6:D:268:LEU:HD23	6:D:268:LEU:HA	1.81	0.44
6:D:356:THR:OG1	6:D:357:VAL:N	2.51	0.44
6:D:438:GLU:OE2	6:D:481:ARG:NH2	2.36	0.44
6:D:452:LEU:HD13	6:D:500:ILE:HG22	1.99	0.44
6:D:475:GLU:HG3	7:E:24:ALA:HB1	1.99	0.44
6:D:719:PHE:HD1	6:D:724:MET:HE1	1.83	0.44
6:D:1237:VAL:CG1	6:D:1253:ILE:HD13	2.47	0.44
5:C:225:PHE:HE2	5:C:347:ILE:HB	1.83	0.44
5:C:619:ALA:O	5:C:621:SER:N	2.50	0.44
5:C:817:LEU:HD11	5:C:1080:ASN:HD22	1.82	0.44
6:D:210:SER:O	6:D:214:ARG:HG3	2.18	0.44
6:D:356:THR:HG23	6:D:448:GLN:HG2	1.99	0.44
6:D:583:VAL:HA	6:D:620:PHE:HE1	1.81	0.44
3:F:116:ASP:OD1	3:F:116:ASP:N	2.51	0.44
5:C:582:ASN:HB3	5:C:586:PHE:H	1.80	0.44
5:C:632:ASP:HA	5:C:647:ARG:HB2	2.00	0.44
5:C:1015:ALA:O	5:C:1018:TYR:HB3	2.18	0.44
5:C:1268:GLN:NE2	6:D:352:ARG:HB2	2.32	0.44
6:D:926:PRO:HG2	6:D:1248:ILE:HD11	1.99	0.44
3:F:39:LEU:HD13	3:F:41:ASP:OD2	2.17	0.44
5:C:76:GLY:O	5:C:95:PRO:HD2	2.18	0.44
5:C:808:ASN:H	6:D:633:ALA:HB2	1.83	0.44
6:D:102:MET:HG2	6:D:246:PRO:HG3	2.00	0.44
6:D:103:GLY:C	6:D:244:VAL:HG22	2.37	0.44
6:D:108:ALA:HB3	6:D:279:LEU:HD22	2.00	0.44
6:D:275:ARG:CZ	6:D:298:MET:HB3	2.48	0.44
6:D:909:ILE:HD11	6:D:913:GLU:HB3	1.99	0.44
4:B:103:ASN:OD1	4:B:141:SER:HA	2.17	0.44
5:C:217:THR:O	5:C:221:LEU:HG	2.17	0.44
5:C:1024:GLU:O	5:C:1027:LYS:HG2	2.18	0.44
6:D:68:TYR:HA	6:D:92:VAL:CG2	2.47	0.44
6:D:153:ASN:C	6:D:154:LEU:HD12	2.38	0.44
6:D:1347:LEU:HG	6:D:1357:ILE:HG23	1.99	0.44
5:C:232:ILE:HA	5:C:237:LEU:HG	1.99	0.44
5:C:448:LEU:HD23	5:C:451:ARG:HD2	1.98	0.44
6:D:245:LEU:HD12	6:D:246:PRO:HD2	1.98	0.44
6:D:352:ARG:HG3	6:D:466:MET:O	2.18	0.44
6:D:700:ASN:O	6:D:704:GLU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:976:THR:O	6:D:999:TYR:HE1	2.01	0.44
7:E:4:VAL:HG13	7:E:5:THR:HG23	1.99	0.44
4:B:228:LEU:HA	4:B:228:LEU:HD23	1.75	0.44
5:C:546:GLU:OE1	5:C:546:GLU:N	2.43	0.44
5:C:944:ARG:NE	5:C:948:ILE:HD11	2.33	0.44
5:C:1250:SER:OG	5:C:1251:TYR:N	2.51	0.44
5:C:1297:ASP:O	5:C:1301:ARG:HB2	2.17	0.44
6:D:85:CYS:O	6:D:89:GLY:HA2	2.18	0.44
6:D:363:LEU:N	6:D:622:ASP:OD2	2.44	0.44
2:T:17:DG:H2'	2:T:18:DC:H6	1.83	0.43
5:C:452:ARG:HG3	5:C:585:GLY:O	2.18	0.43
5:C:521:LEU:O	5:C:524:ILE:HG22	2.17	0.43
5:C:691:PRO:HA	5:C:788:SER:OG	2.18	0.43
5:C:708:VAL:HG11	5:C:794:LEU:HD22	1.98	0.43
5:C:964:LEU:HD22	5:C:1025:PHE:CG	2.53	0.43
5:C:993:PRO:HG2	5:C:996:ARG:HG2	1.99	0.43
6:D:37:GLU:HG3	6:D:105:ILE:HA	2.00	0.43
6:D:185:ILE:O	6:D:188:LEU:HB2	2.17	0.43
6:D:635:SER:OG	6:D:636:GLY:N	2.50	0.43
5:C:27:LEU:O	5:C:528:ARG:NH1	2.52	0.43
5:C:106:GLU:HA	5:C:114:VAL:HG23	1.99	0.43
5:C:210:LEU:HD21	5:C:429:MET:SD	2.58	0.43
5:C:277:LEU:O	5:C:281:ASP:N	2.48	0.43
6:D:450:HIS:CE1	6:D:452:LEU:H	2.36	0.43
6:D:577:ALA:O	6:D:580:TRP:HB3	2.19	0.43
6:D:975:ILE:H	6:D:1000:GLY:HA2	1.84	0.43
6:D:1067:ARG:NH1	6:D:1072:LYS:O	2.50	0.43
2:T:10:DT:H4'	2:T:11:DC:OP1	2.18	0.43
2:T:15:DC:H1'	2:T:16:DA:H5'	2.00	0.43
5:C:263:VAL:HG22	5:C:273:HIS:CE1	2.54	0.43
6:D:431:ARG:CD	6:D:493:PRO:HG3	2.47	0.43
6:D:640:GLY:N	6:D:643:ASP:OD2	2.44	0.43
6:D:1025:MET:HB3	6:D:1124:ILE:HB	2.00	0.43
6:D:1223:LEU:HD23	6:D:1223:LEU:HA	1.83	0.43
3:F:19:ASN:O	3:F:23:ARG:HB3	2.19	0.43
3:F:77:TYR:CZ	3:F:81:GLN:OE1	2.71	0.43
4:A:224:LEU:HD22	4:B:228:LEU:CD1	2.48	0.43
4:B:57:THR:O	4:B:173:VAL:HB	2.17	0.43
5:C:796:LEU:N	5:C:796:LEU:HD12	2.34	0.43
5:C:927:THR:HG22	5:C:928:VAL:H	1.83	0.43
6:D:252:LEU:HA	6:D:252:LEU:HD12	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:25:DC:P	5:C:139:ASN:HD22	2.42	0.43
4:B:219:ARG:O	4:B:222:THR:OG1	2.28	0.43
4:B:224:LEU:HA	4:B:224:LEU:HD23	1.75	0.43
5:C:550:VAL:HG23	5:C:554:HIS:CG	2.53	0.43
5:C:697:LYS:HG3	5:C:697:LYS:O	2.19	0.43
5:C:1223:ARG:HH22	6:D:721:SER:N	2.17	0.43
5:C:1314:GLN:HA	7:E:28:ARG:NH2	2.28	0.43
6:D:1172:LYS:HA	6:D:1190:ILE:C	2.37	0.43
2:T:13:DT:C5	2:T:14:DC:N4	2.86	0.43
3:F:112:PHE:O	3:F:117:TYR:HB3	2.19	0.43
4:A:224:LEU:HD23	4:A:228:LEU:HD13	2.01	0.43
5:C:81:ASP:O	5:C:85:CYS:CB	2.66	0.43
5:C:146:VAL:HG12	5:C:147:SER:N	2.34	0.43
5:C:591:TYR:HH	5:C:637:ARG:NH2	2.15	0.43
6:D:133:ARG:O	6:D:137:ARG:HG3	2.18	0.43
6:D:358:GLY:O	6:D:360:TYR:N	2.46	0.43
6:D:1222:ARG:HG3	6:D:1223:LEU:HG	2.00	0.43
4:A:41:ASN:ND2	5:C:1218:GLY:HA3	2.34	0.43
4:A:185:TYR:HA	4:A:202:VAL:O	2.19	0.43
5:C:256:GLU:HB3	5:C:261:VAL:HG22	2.00	0.43
5:C:1130:ALA:O	5:C:1134:GLN:HG2	2.18	0.43
6:D:481:ARG:HA	6:D:485:MET:HE3	2.00	0.43
6:D:1261:LEU:HD12	6:D:1261:LEU:O	2.19	0.43
3:F:24:GLU:C	3:F:27:PRO:HD2	2.39	0.43
5:C:832:HIS:CE1	5:C:1238:LEU:HD22	2.54	0.43
6:D:679:TYR:OH	6:D:754:ILE:O	2.14	0.43
6:D:842:ARG:HG2	6:D:843:VAL:H	1.84	0.43
6:D:1175:LEU:HD12	6:D:1175:LEU:HA	1.89	0.43
6:D:1319:PHE:CZ	6:D:1320:ILE:HG13	2.54	0.43
2:T:27:DG:H3'	2:T:27:DG:OP1	2.19	0.43
2:T:29:DA:H2"	2:T:30:DC:H6	1.83	0.43
5:C:145:ILE:HG22	5:C:146:VAL:O	2.19	0.43
5:C:217:THR:HG23	5:C:351:LEU:HD21	1.99	0.43
5:C:240:GLU:C	5:C:241:LEU:HD12	2.38	0.43
5:C:764:CYS:HB2	5:C:831:ILE:HG22	2.00	0.43
5:C:848:GLU:HG2	5:C:889:PRO:CD	2.49	0.43
6:D:475:GLU:OE1	6:D:475:GLU:N	2.33	0.43
6:D:843:VAL:HG13	6:D:862:THR:O	2.18	0.43
6:D:1357:ILE:C	6:D:1359:ALA:H	2.21	0.43
4:B:19:VAL:HG21	4:B:23:HIS:HD2	1.83	0.43
5:C:1118:GLY:O	5:C:1119:MET:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:1294:LYS:HB3	6:D:347:VAL:HG13	2.00	0.43
6:D:37:GLU:CD	6:D:106:GLU:H	2.16	0.43
6:D:1156:LEU:HG	6:D:1209:VAL:HA	2.01	0.43
1:N:28:DA:H2"	1:N:29:DG:N7	2.34	0.42
5:C:91:THR:HG22	5:C:138:ILE:O	2.18	0.42
5:C:133:ASN:OD1	5:C:713:GLY:HA3	2.19	0.42
5:C:705:GLU:H	5:C:705:GLU:CD	2.17	0.42
5:C:1101:LEU:HD21	6:D:508:LEU:HD22	2.01	0.42
6:D:370:LYS:NZ	6:D:443:GLU:OE2	2.29	0.42
6:D:432:LEU:HD13	6:D:456:ALA:HB1	2.00	0.42
6:D:909:ILE:HG13	6:D:910:ASN:O	2.18	0.42
6:D:980:THR:HB	6:D:997:VAL:HB	2.00	0.42
6:D:1029:THR:HG21	6:D:1115:ILE:HD13	2.00	0.42
6:D:1276:GLU:O	6:D:1278:GLU:N	2.52	0.42
1:N:24:DC:C4	1:N:25:DG:C6	3.07	0.42
4:B:19:VAL:HG12	4:B:20:SER:N	2.35	0.42
5:C:18:ARG:HG2	5:C:1188:ASP:OD1	2.19	0.42
5:C:453:ILE:CD1	5:C:587:LEU:HD21	2.46	0.42
5:C:569:ILE:HD12	6:D:784:ALA:HA	2.02	0.42
5:C:1333:LEU:C	5:C:1335:ILE:H	2.23	0.42
6:D:326:SER:H	6:D:329:ASP:HB2	1.84	0.42
6:D:499:ILE:HD12	6:D:499:ILE:HA	1.87	0.42
6:D:860:ARG:HG3	6:D:861:ASN:CG	2.40	0.42
2:T:14:DC:N3	2:T:15:DC:N4	2.67	0.42
4:A:195:ARG:HG2	4:A:198:LEU:HD13	2.00	0.42
5:C:745:GLU:OE1	5:C:1017:GLN:HG3	2.18	0.42
5:C:1002:LEU:HD23	5:C:1003:THR:N	2.34	0.42
5:C:1314:GLN:HG3	7:E:28:ARG:HH22	1.84	0.42
6:D:417:ARG:NH1	7:E:43:ASN:HB2	2.34	0.42
6:D:441:LEU:HD12	6:D:441:LEU:N	2.34	0.42
6:D:525:MET:O	6:D:548:VAL:HG23	2.20	0.42
6:D:611:ILE:C	6:D:612:LEU:HD12	2.40	0.42
6:D:716:GLN:HG3	6:D:717:VAL:O	2.19	0.42
2:T:20:DC:C4'	6:D:352:ARG:HH12	2.32	0.42
4:B:178:SER:HB2	4:B:180:VAL:HG22	2.01	0.42
5:C:816:ILE:HD12	5:C:1074:GLY:HA3	2.00	0.42
6:D:432:LEU:HD22	6:D:435:GLN:NE2	2.35	0.42
6:D:628:GLY:O	6:D:629:PHE:C	2.57	0.42
6:D:1289:ASN:HA	6:D:1292:LEU:HB2	2.00	0.42
6:D:1348:LYS:O	6:D:1352:ILE:HG12	2.19	0.42
3:F:77:TYR:OH	3:F:81:GLN:OE1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:77:TYR:CZ	3:F:80:GLN:HB3	2.53	0.42
4:B:12:ARG:HH11	4:B:13:LEU:HB3	1.84	0.42
5:C:329:GLY:O	5:C:331:LYS:NZ	2.49	0.42
5:C:421:SER:N	5:C:424:ASP:OD2	2.52	0.42
5:C:468:LEU:HA	5:C:468:LEU:HD23	1.77	0.42
5:C:724:VAL:HA	5:C:734:ILE:HD12	2.00	0.42
5:C:1314:GLN:HG3	7:E:28:ARG:NH2	2.34	0.42
5:C:1333:LEU:HD13	6:D:115:TRP:CH2	2.55	0.42
6:D:24:LEU:HD23	6:D:24:LEU:HA	1.85	0.42
6:D:107:LEU:HA	6:D:276:ASN:HD21	1.84	0.42
6:D:478:LEU:HA	6:D:478:LEU:HD23	1.81	0.42
6:D:722:ILE:HA	6:D:725:MET:CE	2.50	0.42
6:D:1257:VAL:HA	6:D:1260:MET:SD	2.59	0.42
6:D:1259:GLN:HE22	6:D:1262:ARG:HD3	1.83	0.42
2:T:29:DA:P	5:C:496:LYS:HZ3	2.43	0.42
3:F:41:ASP:OD1	6:D:929:GLN:NE2	2.52	0.42
4:B:149:GLY:HA3	4:B:177:TYR:CE2	2.55	0.42
5:C:204:LEU:HA	5:C:204:LEU:HD23	1.81	0.42
5:C:514:PHE:CZ	5:C:760:ASN:HB3	2.54	0.42
5:C:830:THR:OG1	5:C:831:ILE:N	2.52	0.42
5:C:858:GLY:O	5:C:862:LEU:HG	2.19	0.42
5:C:1246:ARG:HE	5:C:1249:GLY:N	2.18	0.42
6:D:117:LEU:HD13	6:D:118:LYS:HG3	2.01	0.42
6:D:378:LYS:HA	6:D:381:ILE:HD12	2.02	0.42
6:D:697:MET:SD	6:D:738:ARG:HA	2.59	0.42
3:F:47:ASP:O	3:F:51:ASN:ND2	2.51	0.42
4:A:29:GLU:HG3	4:A:30:PRO:CD	2.44	0.42
5:C:803:ALA:HB2	5:C:1227:VAL:HG12	2.02	0.42
5:C:812:PHE:HA	6:D:505:ASP:OD2	2.19	0.42
5:C:888:THR:HG23	5:C:916:SER:OG	2.18	0.42
5:C:918:LEU:HA	5:C:918:LEU:HD12	1.83	0.42
5:C:1192:GLU:O	5:C:1196:LYS:HG2	2.20	0.42
5:C:1297:ASP:OD2	5:C:1300:GLY:N	2.41	0.42
6:D:234:PRO:O	6:D:237:MET:N	2.33	0.42
6:D:1002:VAL:O	6:D:1018:ALA:HA	2.20	0.42
6:D:1061:VAL:O	6:D:1104:LYS:HA	2.19	0.42
6:D:1256:ILE:O	6:D:1260:MET:HG3	2.20	0.42
4:A:164:ASP:OD1	4:A:165:GLU:N	2.49	0.42
5:C:150:HIS:CE1	5:C:454:ARG:HE	2.37	0.42
5:C:841:ARG:NH2	6:D:256:ASP:O	2.52	0.42
6:D:66:LYS:HE2	6:D:69:GLU:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:85:CYS:C	6:D:89:GLY:HA2	2.39	0.42
6:D:247:PRO:HA	6:D:250:ARG:CZ	2.49	0.42
8:R:9:U:H2'	8:R:10:G:C8	2.54	0.42
4:B:66:HIS:CD2	4:B:68:TYR:H	2.38	0.42
5:C:27:LEU:HA	5:C:27:LEU:HD23	1.76	0.42
5:C:149:LEU:HA	5:C:452:ARG:O	2.20	0.42
5:C:150:HIS:CE1	5:C:454:ARG:NE	2.87	0.42
5:C:689:ALA:HB2	5:C:1233:LEU:HD23	2.02	0.42
5:C:728:ASP:O	5:C:730:SER:N	2.53	0.42
6:D:54:ASP:N	6:D:58:CYS:SG	2.92	0.42
6:D:620:PHE:O	6:D:624:ILE:HG12	2.19	0.42
6:D:1256:ILE:HD12	6:D:1256:ILE:HG23	1.85	0.42
3:F:127:ALA:O	3:F:131:LYS:HE2	2.20	0.42
5:C:718:ALA:HA	5:C:751:TYR:HE2	1.83	0.42
5:C:742:TYR:HB2	5:C:746:ALA:HB2	2.02	0.42
5:C:809:GLY:HA3	6:D:629:PHE:CD2	2.55	0.42
5:C:1070:HIS:O	5:C:1108:ASN:ND2	2.53	0.42
5:C:1313:HIS:HB2	6:D:474:LEU:HB2	2.02	0.42
6:D:583:VAL:HA	6:D:620:PHE:CE1	2.54	0.42
4:A:7:GLU:OE1	4:B:150:ARG:NH2	2.53	0.41
5:C:57:PHE:HD2	5:C:70:TYR:HB2	1.85	0.41
5:C:232:ILE:HD12	5:C:330:HIS:O	2.19	0.41
6:D:67:ASP:HB3	6:D:68:TYR:HD2	1.85	0.41
6:D:616:PRO:HA	6:D:619:ILE:HG22	2.01	0.41
4:B:35:PHE:O	4:B:38:THR:HG22	2.20	0.41
5:C:4:SER:O	5:C:8:LYS:HG3	2.20	0.41
5:C:314:ASN:HD21	5:C:352:ARG:HG3	1.83	0.41
5:C:646:SER:HB3	5:C:649:GLN:HG3	2.02	0.41
5:C:756:TYR:CZ	5:C:766:ASN:ND2	2.88	0.41
6:D:644:MET:O	6:D:764:ARG:NH1	2.53	0.41
6:D:1031:VAL:HG21	6:D:1088:VAL:HG11	2.02	0.41
6:D:1137:GLY:O	6:D:1140:ARG:HB3	2.20	0.41
6:D:1220:ILE:HD13	6:D:1220:ILE:HA	1.93	0.41
6:D:1237:VAL:HG11	6:D:1253:ILE:HG21	2.02	0.41
6:D:1272:SER:OG	6:D:1300:ALA:HB2	2.20	0.41
6:D:1321:SER:OG	6:D:1349:GLU:OE2	2.38	0.41
3:F:68:CYS:CA	3:F:72:LEU:HD13	2.50	0.41
4:A:23:HIS:HB3	4:A:206:GLU:OE1	2.20	0.41
5:C:188:PHE:CZ	5:C:194:LEU:HD13	2.54	0.41
5:C:224:PHE:CD1	5:C:347:ILE:HG13	2.54	0.41
5:C:1099:ASN:OD1	5:C:1101:LEU:N	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:699:ASP:O	6:D:703:THR:HG22	2.20	0.41
6:D:978:ARG:HG2	6:D:999:TYR:CD1	2.54	0.41
3:F:5:LEU:HD21	3:F:87:PHE:CD2	2.56	0.41
3:F:46:ALA:HB3	6:D:736:GLN:HG2	2.02	0.41
3:F:136:LEU:HG	3:F:149:TYR:HE1	1.83	0.41
4:B:44:ARG:HA	4:B:183:ILE:HD11	2.01	0.41
5:C:62:TYR:CE1	3:G:44:GLU:HA	2.56	0.41
5:C:268:ARG:CZ	5:C:270:THR:HG22	2.50	0.41
5:C:484:LEU:O	5:C:486:THR:N	2.53	0.41
5:C:958:LYS:O	5:C:962:GLU:HG2	2.20	0.41
6:D:1067:ARG:HD2	6:D:1072:LYS:HA	2.03	0.41
5:C:398:SER:OG	5:C:400:VAL:HB	2.20	0.41
5:C:546:GLU:O	5:C:549:ASP:N	2.53	0.41
5:C:813:GLU:HA	6:D:504:GLN:NE2	2.36	0.41
6:D:34:SER:OG	6:D:35:PHE:N	2.53	0.41
6:D:474:LEU:HD21	7:E:27:ALA:HB1	2.01	0.41
7:E:15:ASN:O	7:E:16:ARG:HB3	2.20	0.41
5:C:27:LEU:HD13	5:C:663:VAL:HG11	2.03	0.41
5:C:149:LEU:HD21	5:C:451:ARG:HD3	2.03	0.41
5:C:667:LEU:HA	5:C:667:LEU:HD23	1.80	0.41
5:C:758:ARG:HG2	5:C:759:SER:O	2.20	0.41
5:C:927:THR:HG22	5:C:928:VAL:N	2.35	0.41
5:C:1079:ILE:HA	5:C:1079:ILE:HD12	1.75	0.41
5:C:1291:LEU:HD23	5:C:1291:LEU:HA	1.71	0.41
6:D:804:ALA:C	6:D:806:ASP:H	2.23	0.41
4:A:79:LEU:HD21	5:C:693:LEU:HD21	2.02	0.41
5:C:44:GLU:O	5:C:46:GLN:HG3	2.20	0.41
5:C:351:LEU:HA	5:C:354:ASP:OD2	2.21	0.41
5:C:741:MET:HG3	5:C:746:ALA:HB3	2.03	0.41
6:D:107:LEU:HA	6:D:276:ASN:ND2	2.35	0.41
6:D:432:LEU:HD23	6:D:432:LEU:HA	1.81	0.41
6:D:479:GLU:OE2	7:E:20:VAL:HG11	2.21	0.41
6:D:495:ASN:ND2	6:D:1247:LYS:HB2	2.33	0.41
6:D:1164:SER:O	6:D:1175:LEU:HD12	2.20	0.41
6:D:1321:SER:O	6:D:1324:SER:N	2.53	0.41
1:N:8:DA:C5	1:N:9:DC:C4	3.09	0.41
4:B:197:ASP:N	4:B:197:ASP:OD1	2.54	0.41
5:C:53:PHE:HA	5:C:56:VAL:HG12	2.02	0.41
5:C:74:ARG:NH2	5:C:121:GLU:OE2	2.48	0.41
5:C:543:ALA:HB3	5:C:548:ARG:NH2	2.35	0.41
5:C:615:VAL:N	5:C:651:ASP:OD2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:1243:MET:SD	6:D:445:LYS:HB3	2.60	0.41
6:D:185:ILE:HD13	6:D:188:LEU:HD12	2.03	0.41
6:D:686:TRP:CD2	6:D:758:PRO:HG2	2.56	0.41
6:D:706:VAL:HG12	6:D:715:LYS:HA	2.01	0.41
6:D:1179:PRO:HB2	6:D:1182:GLY:N	2.36	0.41
2:T:27:DG:H1'	2:T:28:DG:O4'	2.21	0.41
3:F:137:ALA:O	3:F:147:SER:HA	2.21	0.41
4:A:74:VAL:HG21	4:A:131:CYS:HB2	2.03	0.41
4:A:222:THR:OG1	4:B:232:VAL:HG11	2.20	0.41
4:B:128:HIS:ND1	4:B:129:VAL:O	2.53	0.41
5:C:187:GLU:OE2	5:C:197:ARG:NH2	2.54	0.41
6:D:809:VAL:HA	6:D:894:VAL:O	2.21	0.41
6:D:998:PRO:HG2	6:D:1020:TRP:CZ2	2.55	0.41
6:D:1071:GLY:HA3	6:D:1074:LEU:HD12	2.03	0.41
6:D:1177:ILE:O	6:D:1184:ASP:HB2	2.21	0.41
6:D:1287:ILE:HD12	6:D:1288:ALA:N	2.36	0.41
8:R:11:U:H2'	8:R:12:G:C8	2.56	0.41
4:A:52:PRO:HD3	4:A:219:ARG:HD2	2.03	0.41
4:A:228:LEU:HD21	4:B:224:LEU:HD12	2.04	0.41
5:C:765:ILE:HG13	5:C:787:PRO:HG3	2.03	0.41
5:C:1119:MET:SD	5:C:1228:GLY:HA2	2.61	0.41
6:D:139:LEU:HD23	6:D:139:LEU:HA	1.80	0.41
6:D:343:LEU:HD11	6:D:1348:LYS:HE2	2.03	0.41
6:D:884:SER:HB3	6:D:886:VAL:HG12	2.03	0.41
6:D:925:GLU:HB3	6:D:926:PRO:HD3	2.03	0.41
6:D:1037:PHE:CZ	6:D:1111:ASP:HB2	2.56	0.41
6:D:1292:LEU:HD23	6:D:1292:LEU:HA	1.89	0.41
2:T:15:DC:H6	2:T:15:DC:H2'	1.79	0.40
4:A:71:LYS:CE	4:A:140:ILE:HG22	2.51	0.40
5:C:478:ARG:HD2	5:C:492:MET:HG2	2.03	0.40
5:C:618:GLN:HA	5:C:654:ASP:OD2	2.21	0.40
5:C:786:GLY:O	5:C:789:THR:OG1	2.29	0.40
6:D:930:LEU:HA	6:D:930:LEU:HD23	1.90	0.40
4:B:66:HIS:CD2	4:B:68:TYR:HB2	2.56	0.40
5:C:10:ARG:CZ	5:C:791:LEU:HD12	2.51	0.40
5:C:16:GLY:O	5:C:1155:VAL:HA	2.22	0.40
5:C:158:ASP:HB3	5:C:173:ASN:OD1	2.20	0.40
5:C:208:ILE:HG23	5:C:209:ILE:N	2.36	0.40
5:C:844:LYS:HE2	6:D:48:THR:HG22	2.03	0.40
6:D:349:TYR:CD1	6:D:472:LEU:HD21	2.56	0.40
6:D:364:HIS:CG	7:E:4:VAL:HG23	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:385:LEU:HA	6:D:385:LEU:HD23	1.91	0.40
6:D:528:THR:HG23	6:D:529:GLY:N	2.35	0.40
6:D:1249:ASN:HD21	6:D:1251:LYS:NZ	2.19	0.40
4:A:90:VAL:HG23	4:A:123:ILE:HD13	2.02	0.40
4:A:234:LEU:HD23	4:B:214:GLU:HG2	2.03	0.40
4:B:91:ARG:HH21	4:B:210:THR:HA	1.86	0.40
4:B:198:LEU:HD23	4:B:198:LEU:HA	1.82	0.40
5:C:663:VAL:HG23	5:C:664:GLY:N	2.37	0.40
5:C:685:MET:SD	5:C:1073:LYS:HE2	2.61	0.40
6:D:59:ALA:O	6:D:63:GLY:N	2.54	0.40
6:D:172:PHE:HB2	6:D:176:PHE:HB2	2.03	0.40
6:D:188:LEU:O	6:D:191:SER:OG	2.24	0.40
6:D:923:ILE:O	6:D:926:PRO:HD2	2.20	0.40
6:D:1021:ASP:OD2	6:D:1024:THR:OG1	2.30	0.40
2:T:7:DA:H2'	2:T:8:DT:C5	2.56	0.40
2:T:12:DT:H1'	2:T:13:DT:C5	2.56	0.40
5:C:268:ARG:NH2	5:C:270:THR:HA	2.37	0.40
5:C:820:GLU:HA	5:C:823:VAL:HG12	2.02	0.40
5:C:866:ASP:HA	5:C:872:TYR:CZ	2.56	0.40
5:C:1032:LYS:HD2	5:C:1035:LYS:HD2	2.03	0.40
3:F:111:ILE:O	3:F:111:ILE:HD12	2.21	0.40
4:A:70:THR:CG2	5:C:755:LYS:HE2	2.51	0.40
4:B:48:LEU:HD11	6:D:535:ARG:HG3	2.03	0.40
5:C:28:LEU:HD23	5:C:28:LEU:HA	1.92	0.40
5:C:555:TYR:CE2	5:C:637:ARG:CZ	3.04	0.40
5:C:678:ARG:NH2	5:C:1106:ARG:HE	2.19	0.40
5:C:724:VAL:HA	5:C:734:ILE:CD1	2.52	0.40
6:D:42:GLU:OE1	6:D:42:GLU:N	2.51	0.40
6:D:412:LEU:O	6:D:415:VAL:HG22	2.20	0.40
6:D:464:ASP:OD1	8:R:14:G:O2'	2.23	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	
3	F	154/158 (98%)	136 (88%)	18 (12%)	0	100	100
3	G	154/158 (98%)	138 (90%)	16 (10%)	0	100	100
4	A	226/329 (69%)	201 (89%)	25 (11%)	0	100	100
4	B	227/329 (69%)	198 (87%)	29 (13%)	0	100	100
5	C	1315/1342 (98%)	1103 (84%)	212 (16%)	0	100	100
6	D	1356/1407 (96%)	1159 (86%)	197 (14%)	0	100	100
7	E	71/91 (78%)	64 (90%)	7 (10%)	0	100	100
All	All	3503/3814 (92%)	2999 (86%)	504 (14%)	0	100	100

There are no Ramachandran outliers to report.

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	
3	F	137/139 (99%)	137 (100%)	0	100	100
4	A	196/286 (68%)	196 (100%)	0	100	100
4	B	197/286 (69%)	197 (100%)	0	100	100
5	C	1138/1157 (98%)	1138 (100%)	0	100	100
6	D	1134/1168 (97%)	1133 (100%)	1 (0%)	93	97
7	E	63/75 (84%)	63 (100%)	0	100	100
All	All	2865/3111 (92%)	2864 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	D	1261	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38)

such sidechains are listed below:

Mol	Chain	Res	Type
4	A	18	GLN
4	A	41	ASN
4	A	75	GLN
4	B	66	HIS
4	B	84	ASN
4	B	132	HIS
5	C	69	GLN
5	C	150	HIS
5	C	387	ASN
5	C	437	ASN
5	C	580	GLN
5	C	618	GLN
5	C	688	GLN
5	C	799	ASN
5	C	808	ASN
5	C	1116	HIS
5	C	1256	GLN
5	C	1257	GLN
5	C	1268	GLN
5	C	1313	HIS
6	D	45	ASN
6	D	232	ASN
6	D	341	ASN
6	D	365	GLN
6	D	450	HIS
6	D	488	ASN
6	D	865	HIS
6	D	875	ASN
6	D	936	HIS
6	D	951	GLN
6	D	1049	GLN
6	D	1108	GLN
6	D	1195	GLN
6	D	1279	GLN
6	D	1326	GLN
6	D	1350	ASN
6	D	1367	GLN
7	E	15	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	R	9/14 (64%)	3 (33%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	R	6	C
8	R	8	A
8	R	14	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

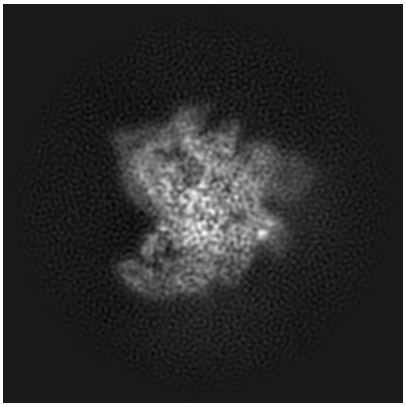
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4885. These allow visual inspection of the internal detail of the map and identification of artifacts.

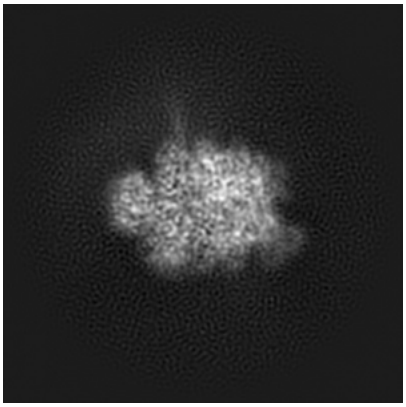
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

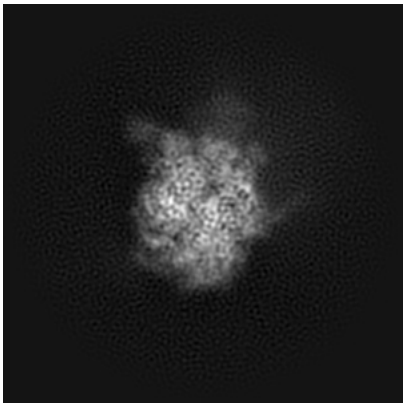
6.1.1 Primary map



X



Y

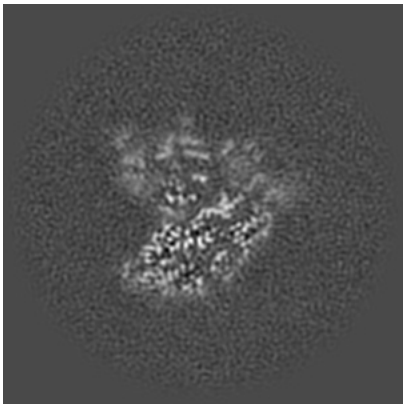


Z

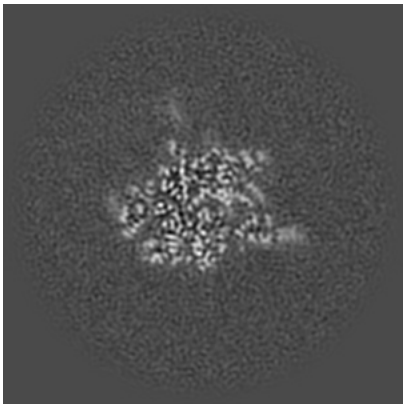
The images above show the map projected in three orthogonal directions.

6.2 Central slices

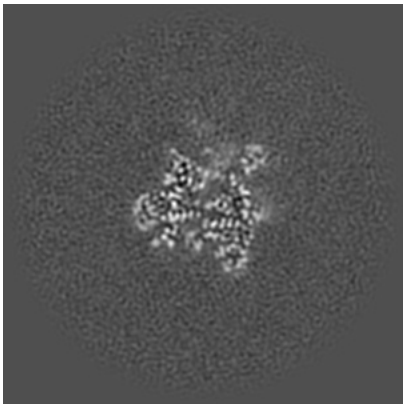
6.2.1 Primary map



X Index: 144



Y Index: 144

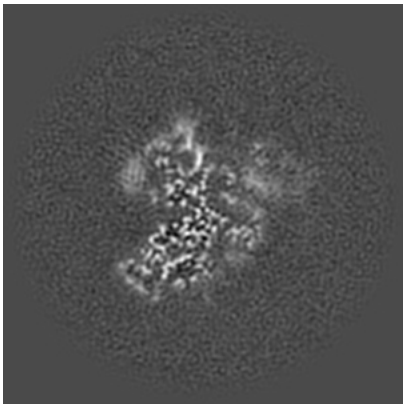


Z Index: 144

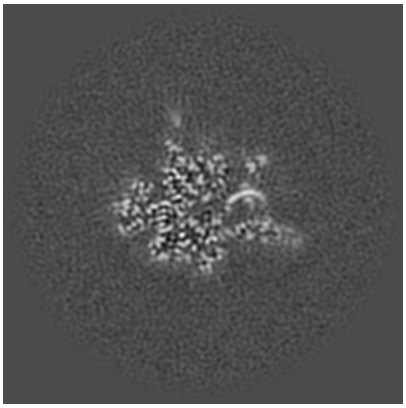
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

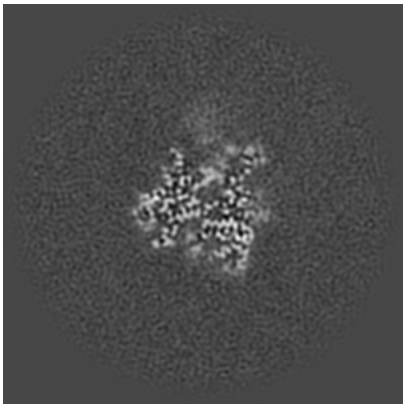
6.3.1 Primary map



X Index: 152



Y Index: 141

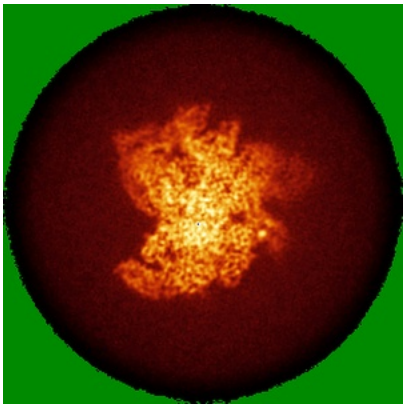


Z Index: 146

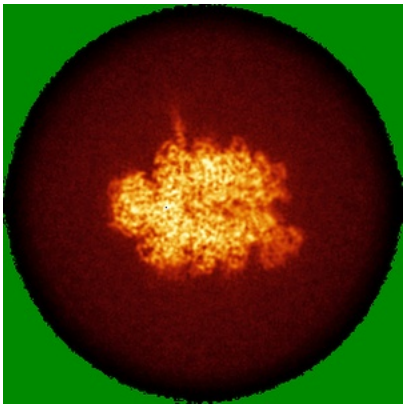
The images above show the largest variance slices of the map in three orthogonal directions.

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

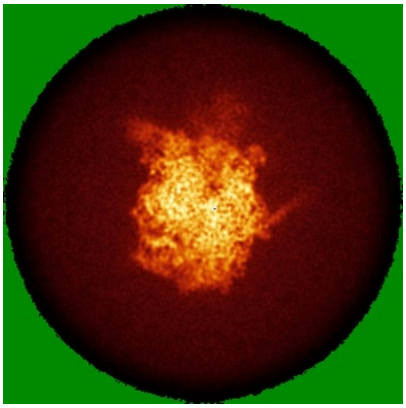
6.4.1 Primary map



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

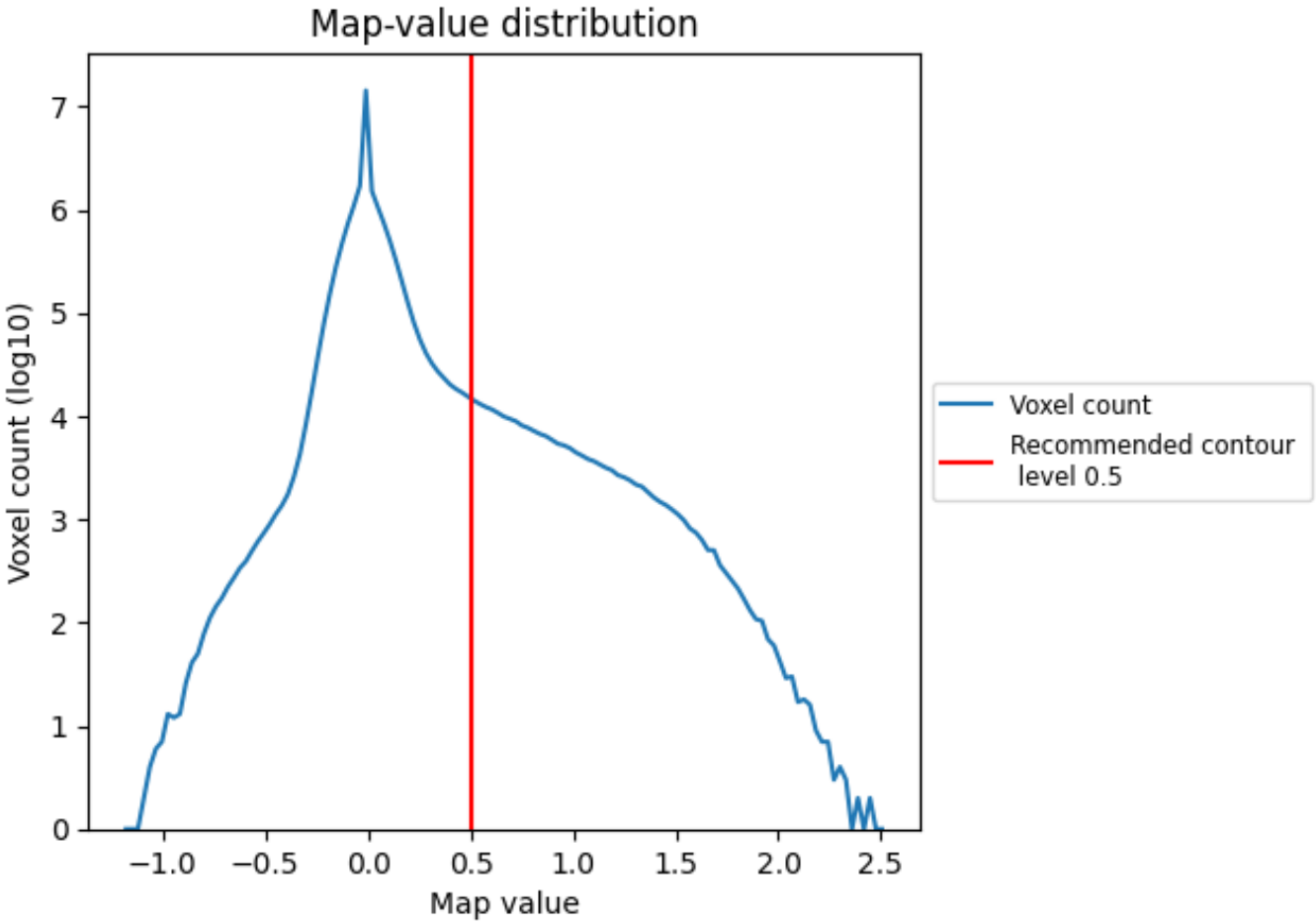
6.6 Mask visualisation (i)

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

7 Map analysis

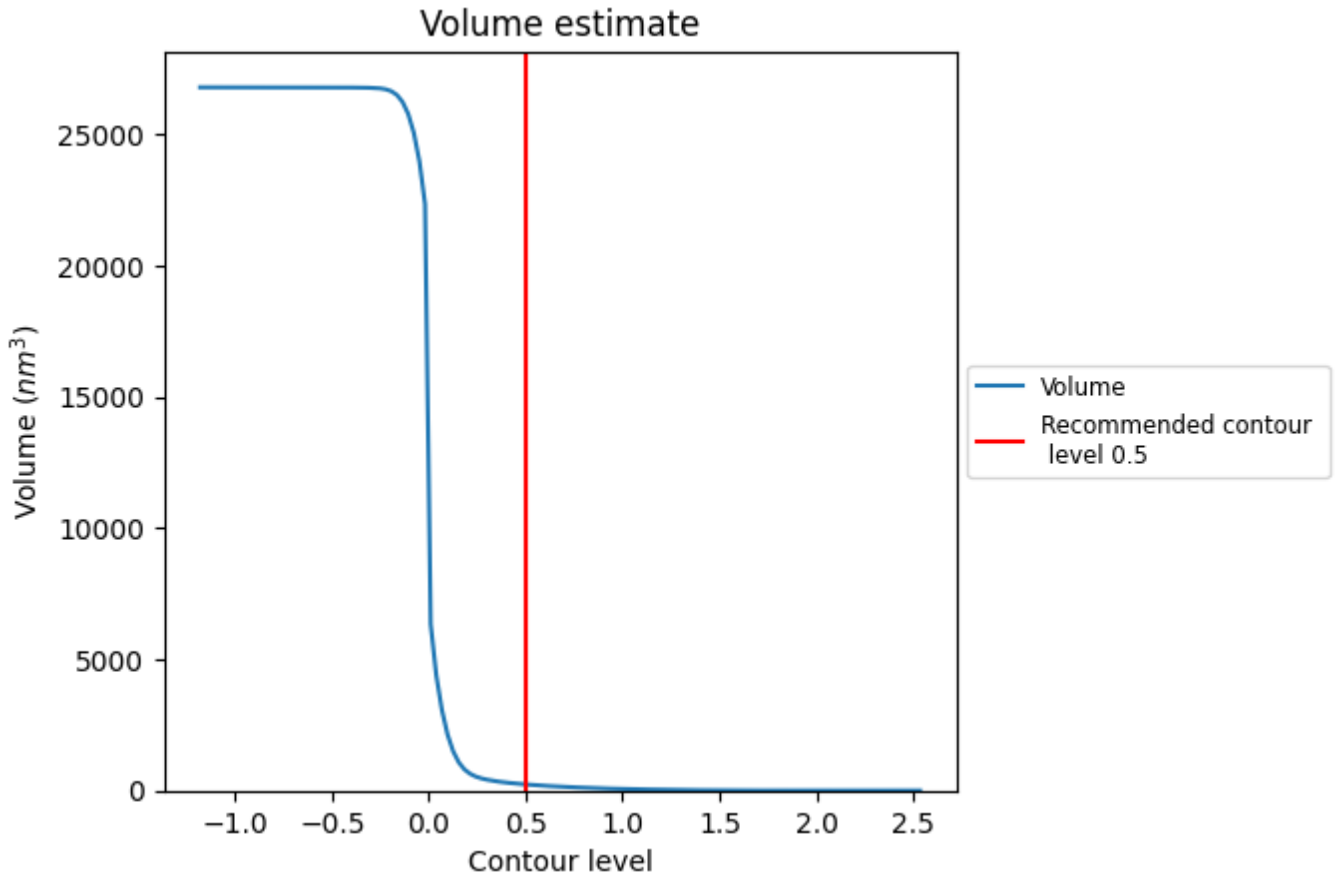
This section contains the results of statistical analysis of the map.

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.

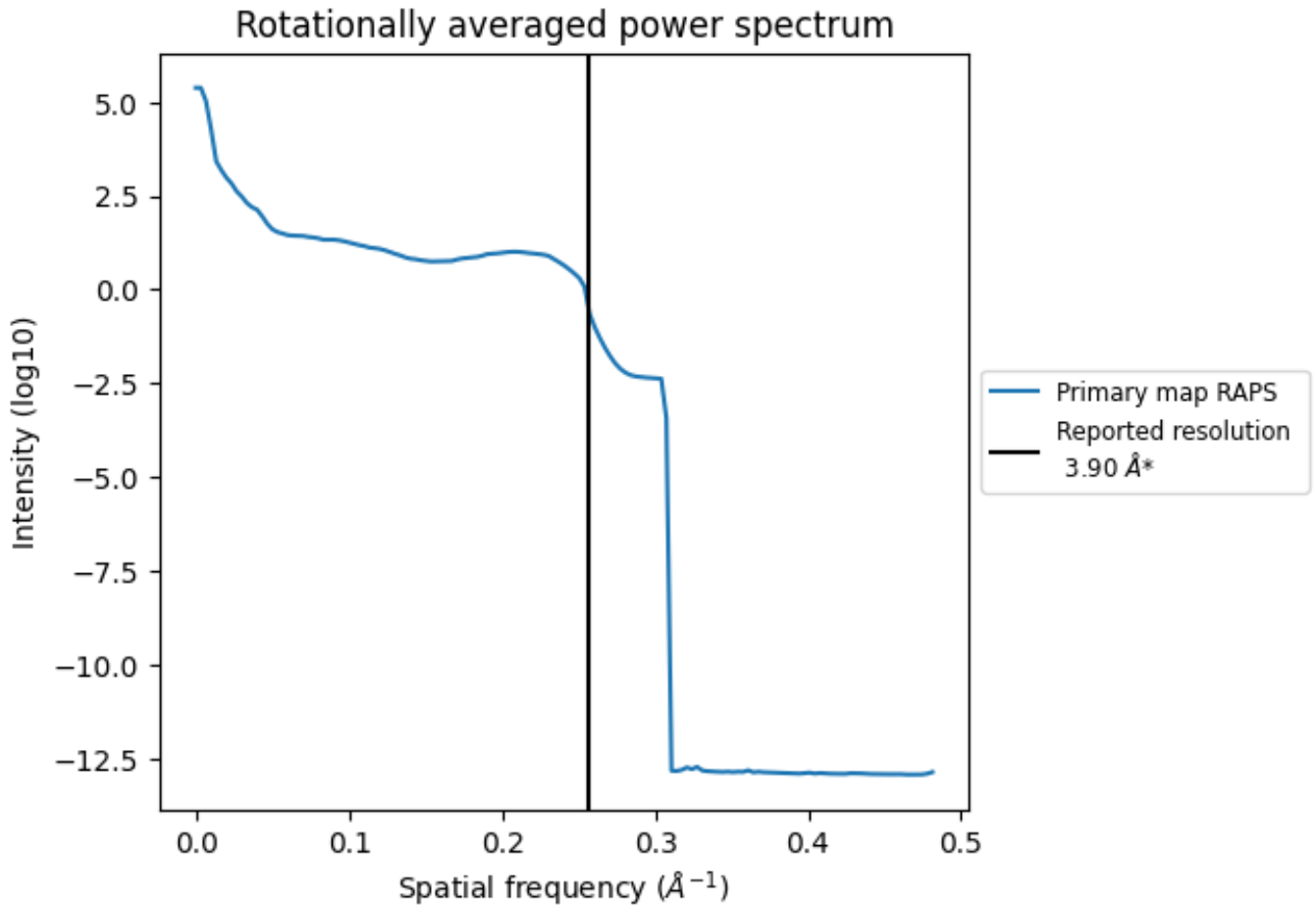
7.2 Volume estimate



The volume at the recommended contour level is 234 nm^3; this corresponds to an approximate mass of 211 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 0.256 $Å^{-1}$

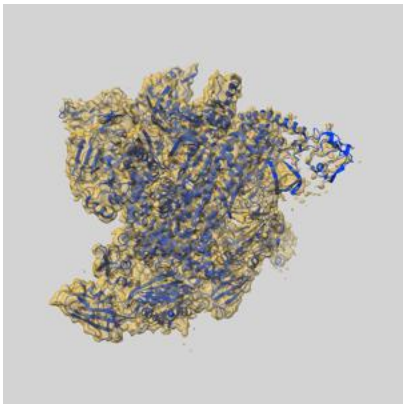
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

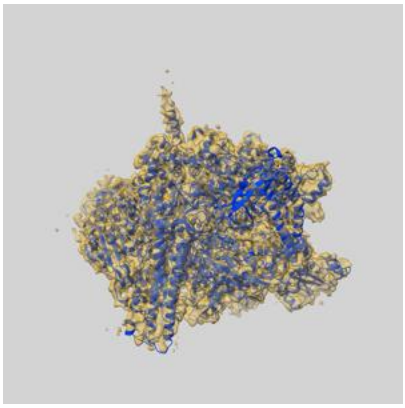
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4885 and PDB model 6RI7. Per-residue inclusion information can be found in section 3 on page 6.

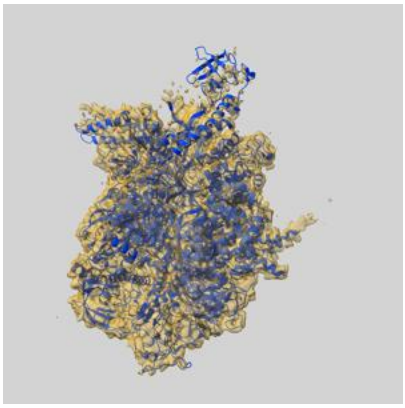
9.1 Map-model overlay



X



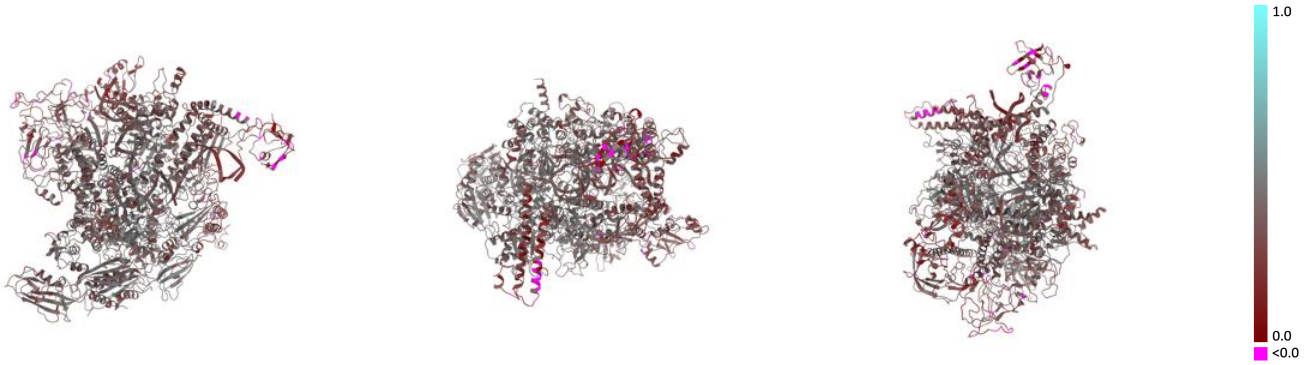
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 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.

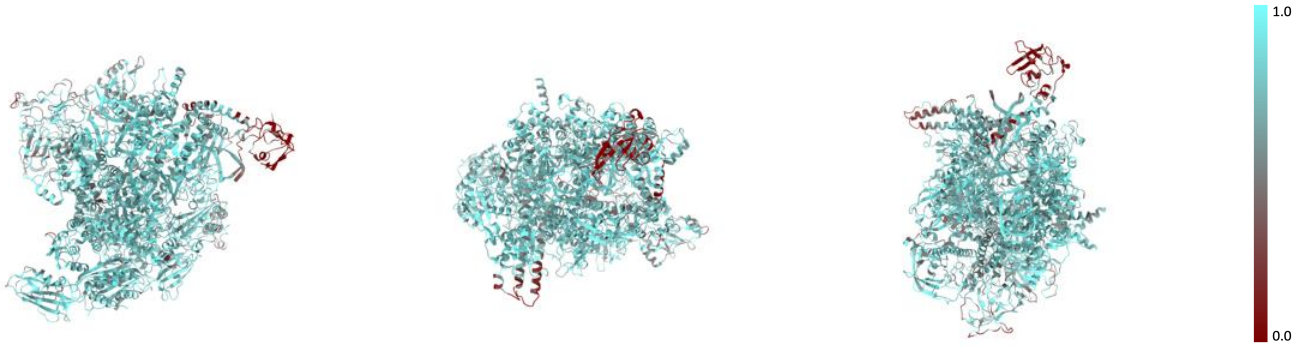
9.2 Q-score mapped to coordinate model (i)



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.

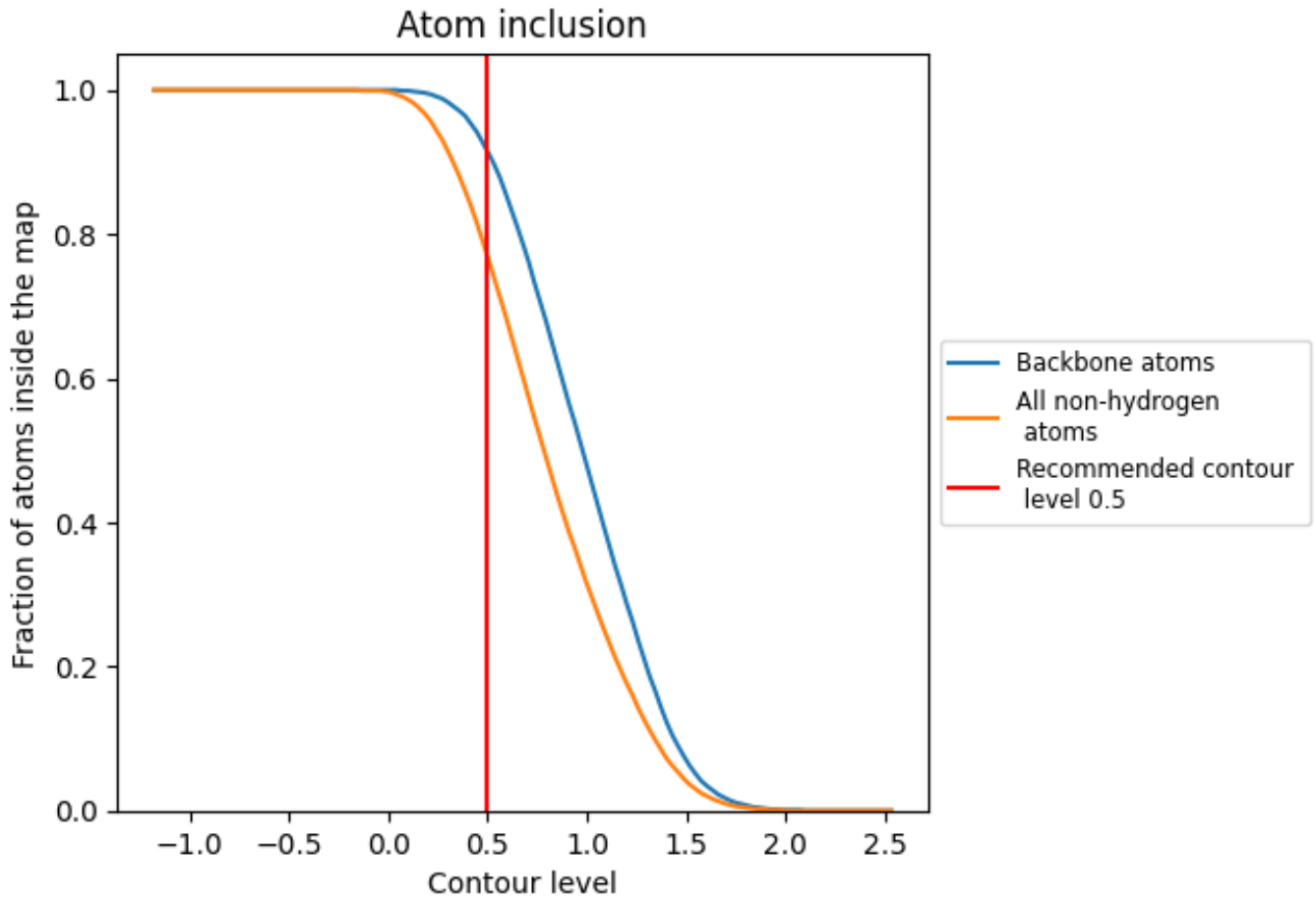
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 77% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7690	0.3690
A	0.8040	0.4150
B	0.7780	0.3800
C	0.7690	0.3720
D	0.7820	0.3730
E	0.7810	0.3650
F	0.7330	0.3410
G	0.3320	0.2530
N	0.8810	0.2870
R	0.9120	0.3970
T	0.8980	0.3540