Full wwPDB X-ray Structure Validation Report (i)

Mar 12, 2026 – 01:37 PM UTC

PDB ID	:	2YU9 / pdb_00002yu9
Title	:	RNA polymerase II elongation complex in 150 mm MG+2 with UTP
Authors	:	Wang, D.; Bushnell, D.A.; Westover, K.D.; Kaplan, C.D.; Kornberg, R.D.
Deposited on	:	2007-04-06
Resolution	:	3.40 Å(reported)

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

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

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

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

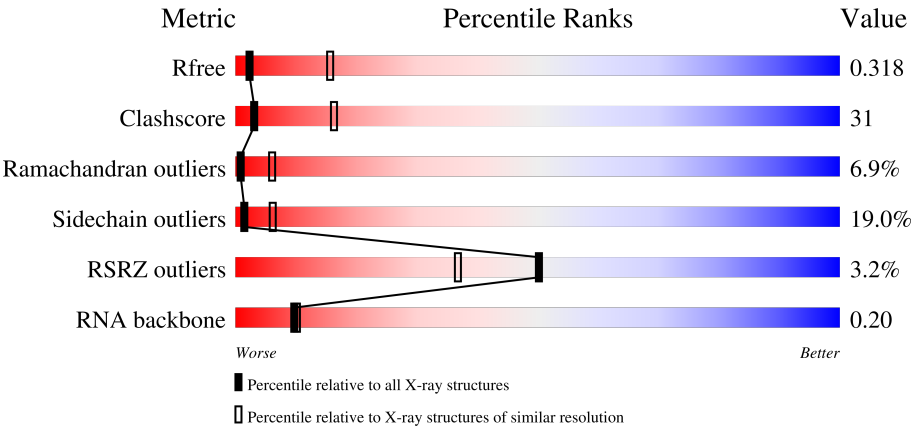
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)
RNA backbone	3983	1157 (3.80-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	R	10	50% 80% 20%
2	T	28	25% 39% 46% 14%
3	N	14	71% 29%
4	A	1733	3% 38% 31% 11% · 19%

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Mol	Chain	Length	Quality of chain
5	B	1224	4% 37% 40% 12% 8%
6	C	318	42% 32% 9% 16%
7	E	215	65% 28% 7%
8	F	155	29% 20% 6% 45%
9	H	146	58% 27% 6% 9%
10	I	122	3% 59% 27% 11%
11	J	70	20% 39% 30% 7%
12	K	120	49% 35% 11% 5%
13	L	70	37% 20% 9% 34%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	UTP	A	2003[A]	-	-	X	-

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 29530 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	R	10	216	98	45	64	9	0	0	0

- Molecule 2 is a DNA chain called 28-MER DNA template strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	T	28	566	271	104	164	27	0	0	0

- Molecule 3 is a DNA chain called 5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	N	14	284	137	49	85	13	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	A	1411	11094	6994	1945	2094	61	0	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	B	1121	8914	5643	1563	1653	55	0	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	85	Total	C	N	O	S	0	0	0
			688	439	116	130	3			

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 11 is a protein called DNA-directed RNA polymerases I/II/III subunit 10.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypep-

tide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

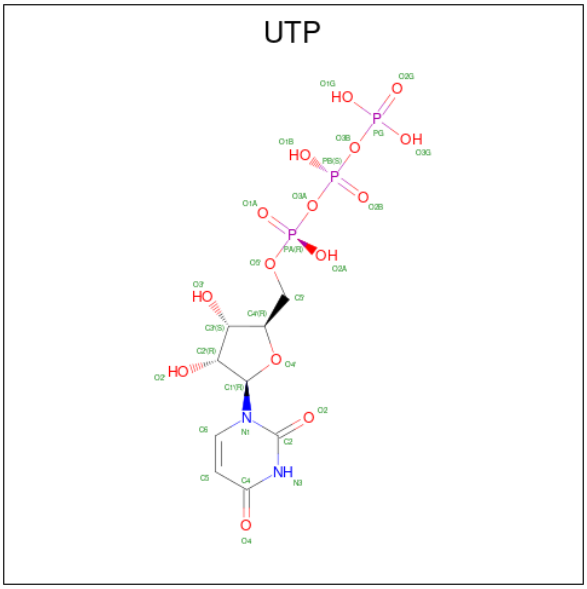
- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	2	Total	Zn	0	0
			2	2		
14	B	1	Total	Zn	0	0
			1	1		
14	C	1	Total	Zn	0	0
			1	1		
14	I	2	Total	Zn	0	0
			2	2		
14	J	1	Total	Zn	0	0
			1	1		
14	L	1	Total	Zn	0	0
			1	1		

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	2	Total	Mg	0	0
			2	2		

- Molecule 16 is URIDINE 5'-TRIPHOSPHATE (CCD ID: UTP) (formula: $C_9H_{15}N_2O_{15}P_3$).



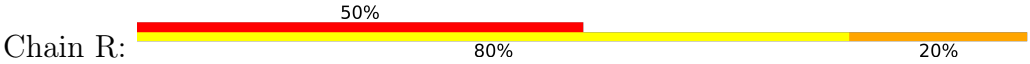
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	A	1	Total	C	N	O	P	0	1
			58	18	4	30	6		

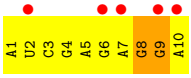
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*A)-3'

Chain R:



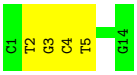


• Molecule 2: 28-MER DNA template strand

Chain T:

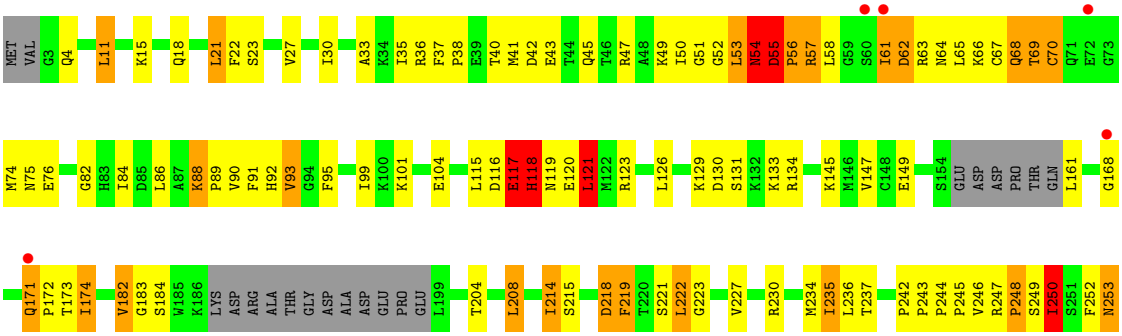
• Molecule 3: 5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*AP*G)-3'

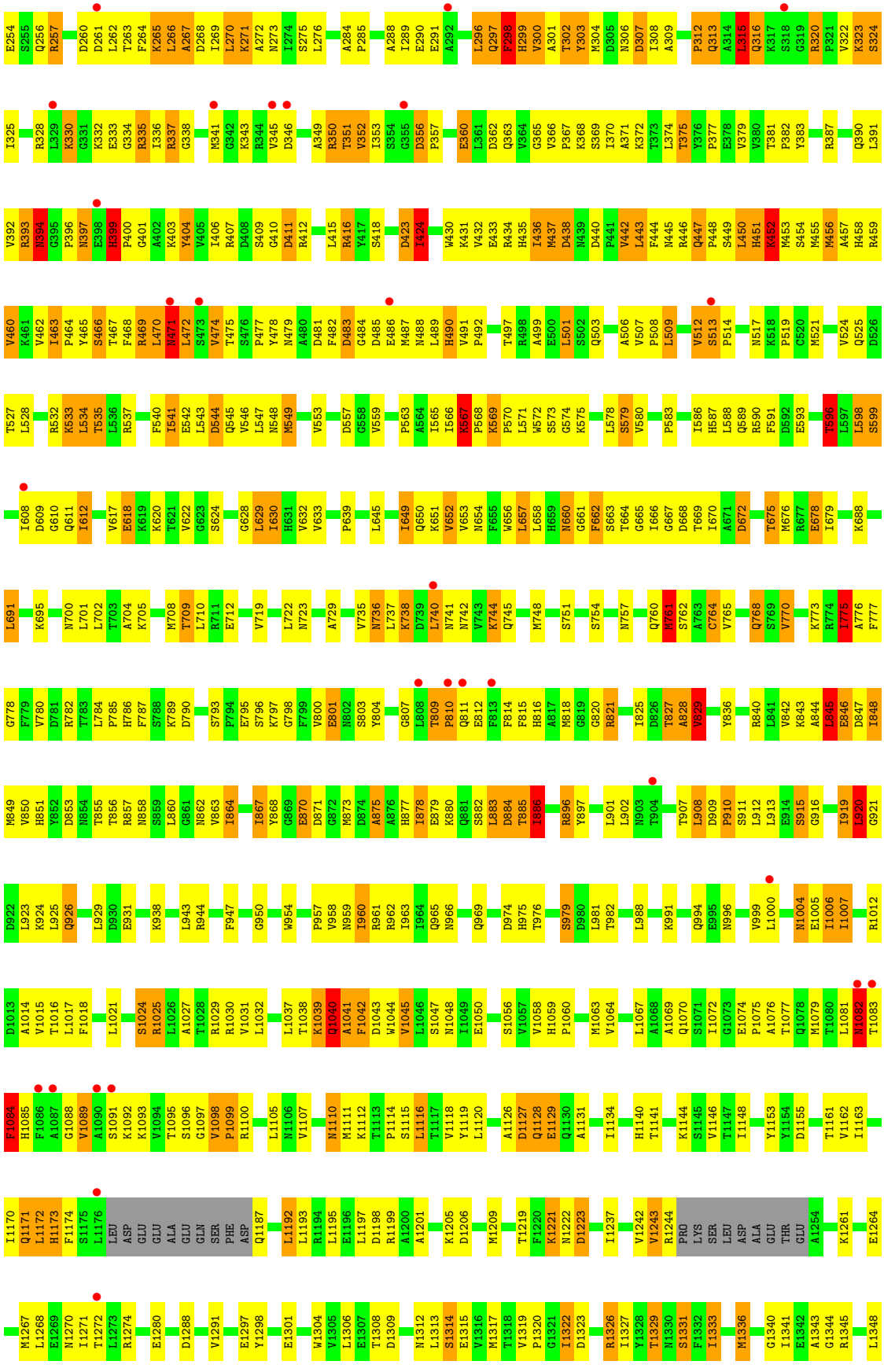
Chain N:

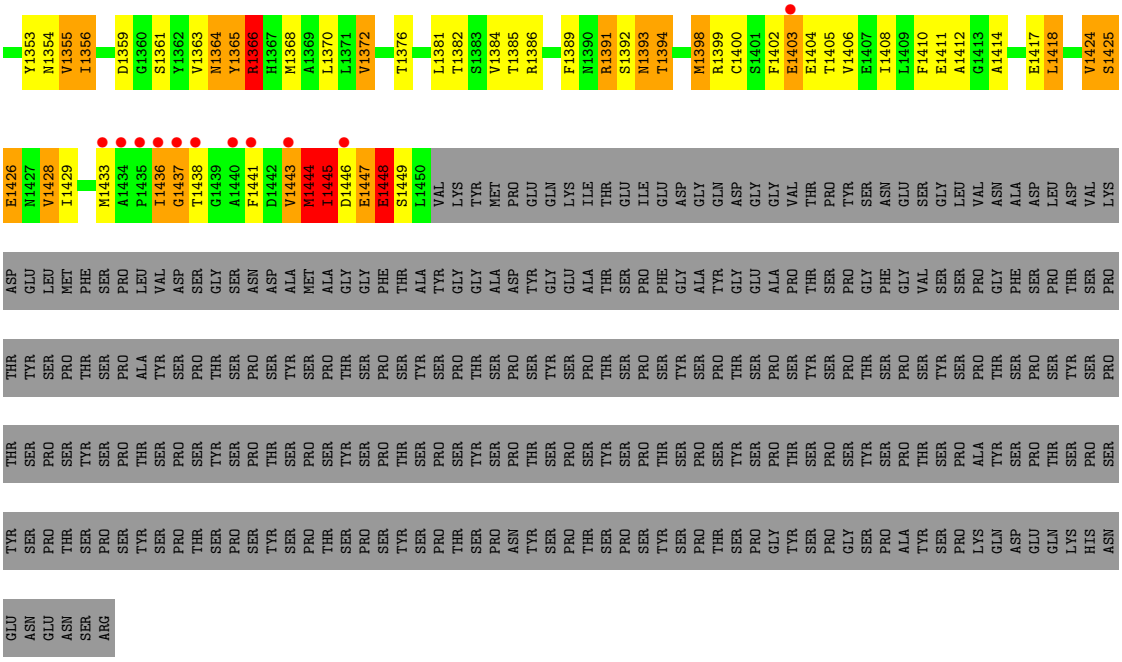


• Molecule 4: DNA-directed RNA polymerase II largest subunit

Chain A:

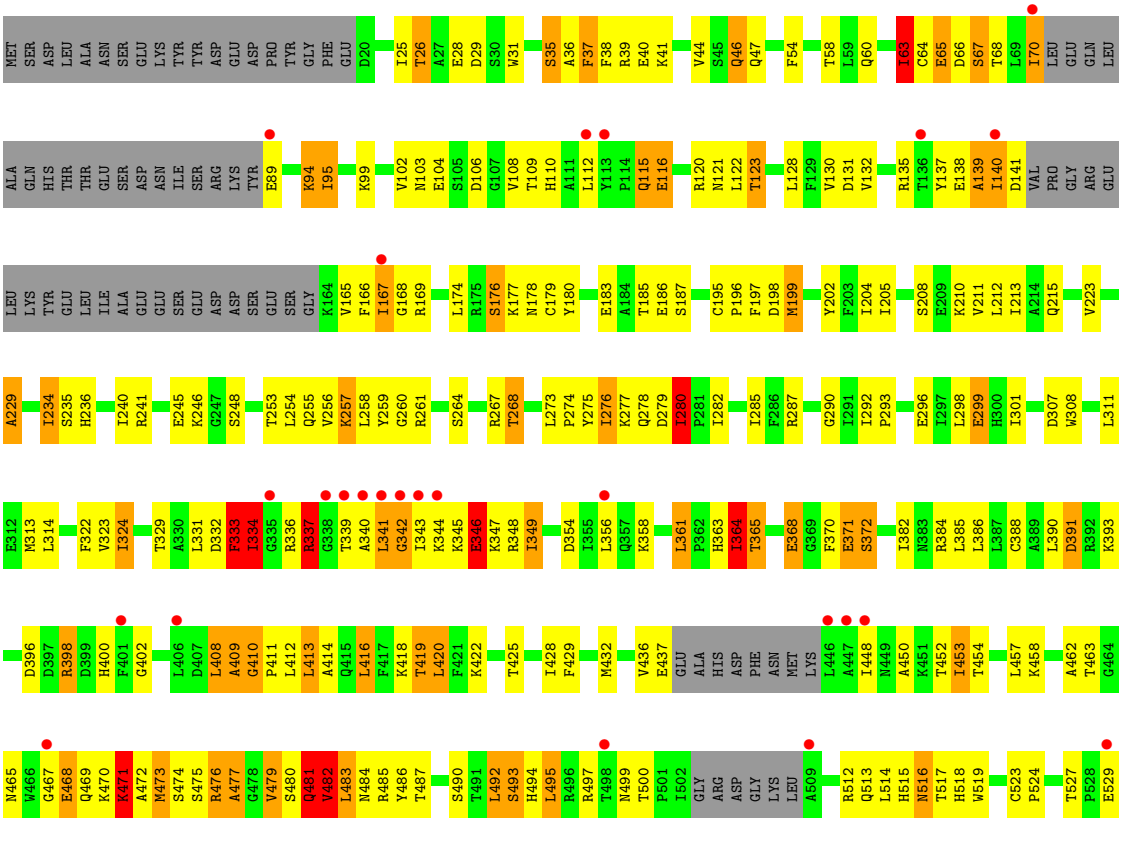


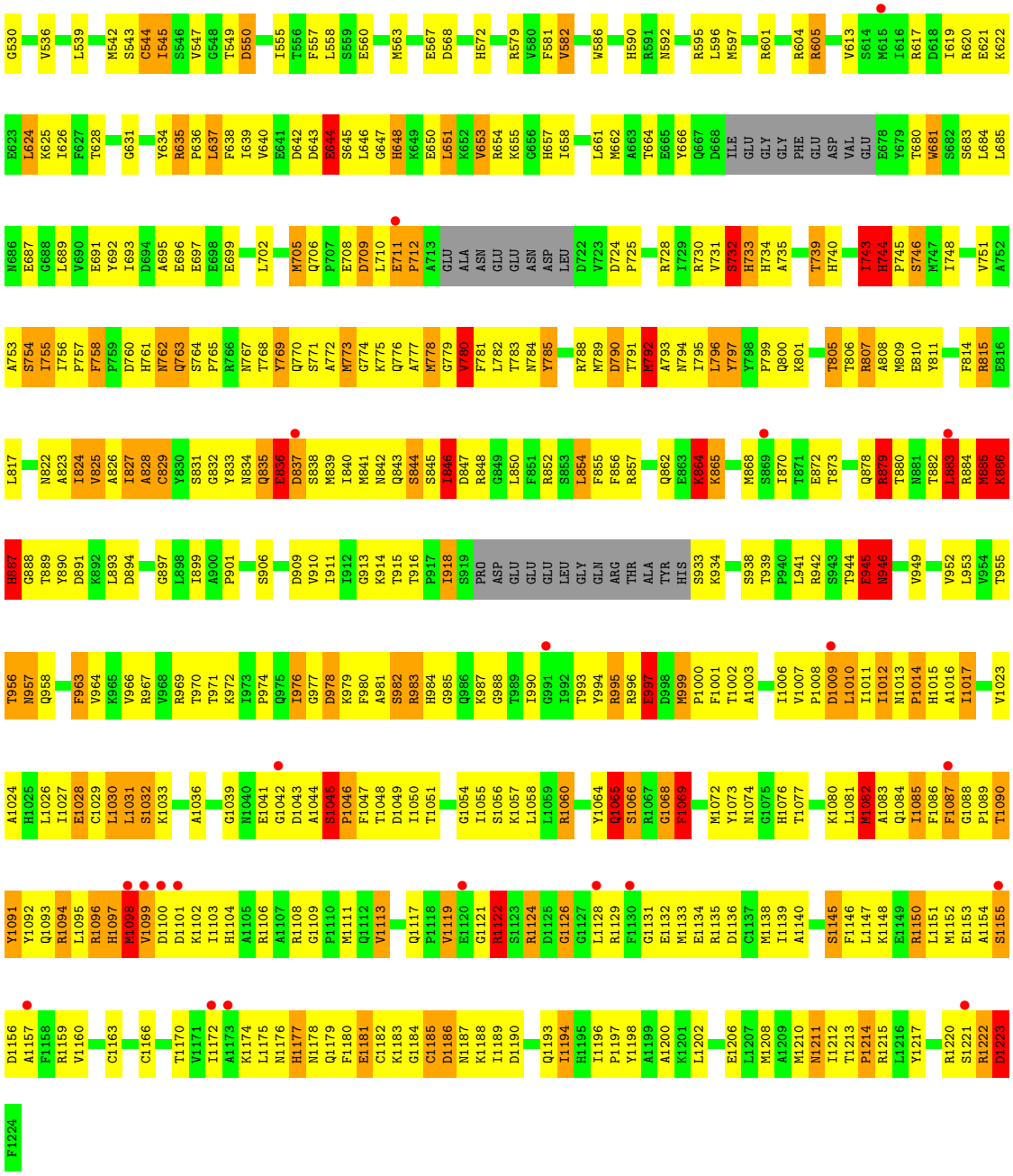

E254 S255 Q256 R257 D260 D261 L262 T263 F264 K265 L266 A267 D268 I269 L270 K271 A272 N273 I274 S275 L276 A284 P285 A288 I289 E290 E291 A292 L296 Q297 F298 H299 V300 A301 T302 Y303 M304 D305 N306 D307 I308 A309 P312 Q313 A314 L315 Q316 K317 S318 G319 R320 P321 V322 K323 S324
I325 R328 L329 K330 G331 K332 E333 G334 R335 I336 R337 G338 M341 G342 K343 R344 V345 D346 A349 R350 T351 V352 I353 S354 G355 D356 P357 E360 L361 D362 Q363 V364 G365 V366 P367 K368 S369 I370 A371 K372 T373 L374 T375 Y376 P377 E378 V379 V380 T381 P382 Y383 R387 Q390 L391
V392 R393 N394 G395 P396 N397 E398 H399 P400 G401 A402 K403 Y404 V405 I406 R407 D408 S409 G410 D411 R412 L415 R416 Y417 S418 D423 I424 W430 K431 V432 E433 R434 H435 I436 M437 D438 N439 D440 P441 V442 L443 F444 N445 R446 Q447 P448 S449 L450 H451 K452 M453 S454 M455 M456 A457 H458 R459
V460 K461 V462 I463 P464 Y465 S466 T467 F468 R469 L470 N471 L472 S473 T474 T475 S476 P477 Y478 N479 A480 D481 F482 D483 G484 D485 E486 M487 N488 L489 H490 V491 P492 T497 R498 A499 E500 L501 S502 Q503 A506 V507 P508 L509 V512 S513 P514 N517 K518 P519 C520 M521 V524 Q525 D526
T527 L528 R532 K533 L534 T535 L536 R537 F540 I541 E542 L543 D544 Q545 V546 L547 N548 M549 V553 D557 G558 V559 P563 A564 I565 I566 K567 P568 K569 P570 L571 W572 S573 G574 K575 L578 S579 V580 P583 I586 H587 L588 Q589 R590 F591 D592 E593 T596 L597 L598 S599
I608 D609 G610 Q611 I612 V617 E618 K619 K620 T621 V622 G623 S624 G628 L629 I630 H631 V632 V633 P639 L645 I649 Q650 K651 V652 V653 N654 F655 W656 L657 L658 H659 N660 G661 F662 S663 T664 G665 I666 G667 D668 T669 I670 A671 D672 T675 M676 R677 E678 I679 K688
L691 K695 N700 L701 L702 T703 A704 K705 M708 T709 L710 R711 E712 V719 L722 N723 A729 V735 N736 L737 K738 D739 L740 N741 N742 V743 K744 Q745 M748 S751 S754 N757 Q760 N761 S762 A763 C764 V765 Q768 S769 V770 K773 R774 I775 A776 F777
G778 F779 V780 D781 R782 T783 L784 P785 H786 F787 S788 K789 D790 S793 P794 E795 S796 K797 G798 F799 V800 E801 N802 S803 Y804 G807 L808 T809 P810 Q811 E812 F813 F814 F815 H816 A817 M818 G819 G820 R821 I825 D826 T827 A828 V829 Y836 R840 L841 V842 K843 A844 L845 E846 D847 I848
M849 V850 H851 Y852 D853 N854 T855 T856 R857 N858 S859 L860 G861 N862 V863 I864 I867 Y868 G869 E870 D871 G872 M873 D874 A875 A876 H877 I878 E879 K880 Q881 S882 L883 D884 T885 I886 R896 Y897 L901 L902 N903 T904 T907 L908 D909 P910 S911 L912 L913 E914 S915 G916 I919 L920 G921
D922 L923 K924 L925 Q926 L929 D930 E931 K938 L943 R944 F947 G950 W954 P957 V958 N959 I960 R961 R962 I963 I964 Q965 N966 Q969 D974 H975 T976 S979 D980 L981 T982 L988 K991 Q994 E995 N996 V999 L1000 N1004 E1005 I1006 I1007 R1012
D1013 A1014 V1015 T1016 L1017 F1018 L1021 S1024 R1025 L1026 A1027 T1028 R1029 R1030 V1031 L1032 L1037 T1038 K1039 Q1040 A1041 F1042 D1043 W1044 V1045 L1046 S1047 N1048 I1049 E1050 S1056 V1057 V1058 H1059 P1060 M1063 V1064 L1067 A1068 A1069 Q1070 S1071 I1072 G1073 E1074 P1075 A1076 T1077 Q1078 M1079 T1080 L1081 N1082 T1083
F1084 H1085 F1086 A1087 G1088 V1089 A1090 S1091 K1092 K1093 V1094 T1095 S1096 G1097 V1098 P1099 R1100 L1105 N1106 V1107 N1110 M1111 K1112 T1113 P1114 S1115 L1116 T1117 V1118 Y1119 L1120 A1126 D1127 Q1128 E1129 Q1130 A1131 I1134 H1140 T1141 K1144 S1145 V1146 T1147 I1148 Y1153 Y1154 D1155 T1161 V1162 I1163
I1170 Q1171 L1172 H1173 F1174 S1175 L1176 LEU ASP GLU GLU ALA GLU GLN SER PHE ASP Q1187 L1192 L1193 R1194 L1195 E1196 L1197 D1198 R1199 A1200 A1201 K1205 D1206 M1209 T1219 F1220 K1221 N1222 D1223 I1237 V1242 V1243 R1244 PRO LYS SER LEU ASP ALA GLU THR GLU A1254 K1261 E1264
M1267 L1268 E1269 N1270 I1271 T1272 L1273 R1274 E1280 D1288 V1291 E1297 Y1298 E1301 W1304 V1305 L1306 E1307 T1308 D1309 N1312 L1313 S1314 E1315 V1316 M1317 T1318 V1319 P1320 G1321 I1322 D1323 R1326 I1327 Y1328 T1329 N1330 S1331 F1332 I1333 M1336 G1340 I1341 E1342 A1343 G1344 R1345 L1348



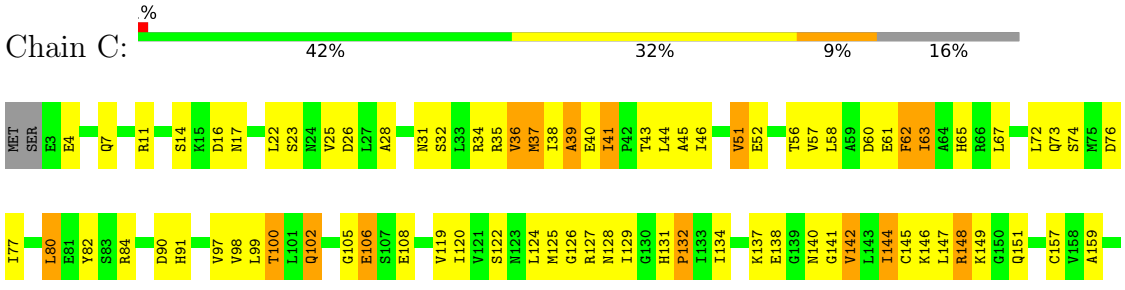
• Molecule 5: DNA-directed RNA polymerase II 140 kDa polypeptide

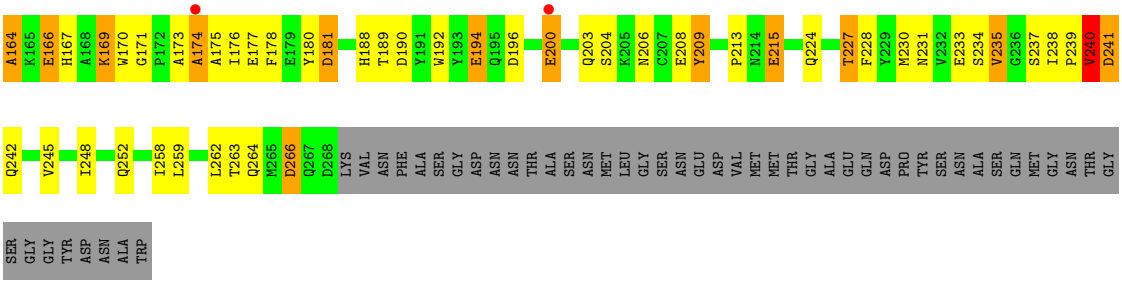
Chain B:



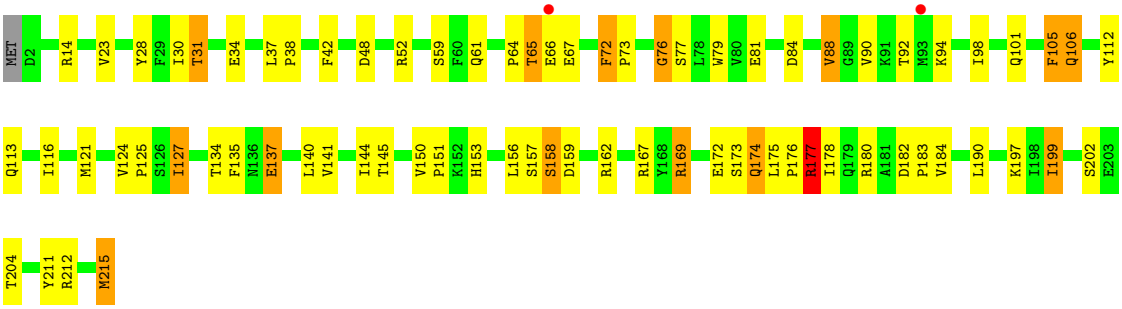


• Molecule 6: DNA-directed RNA polymerase II 45 kDa polypeptide

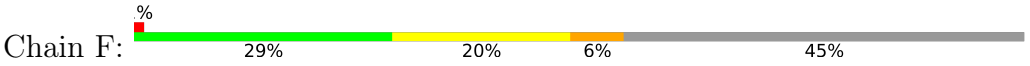


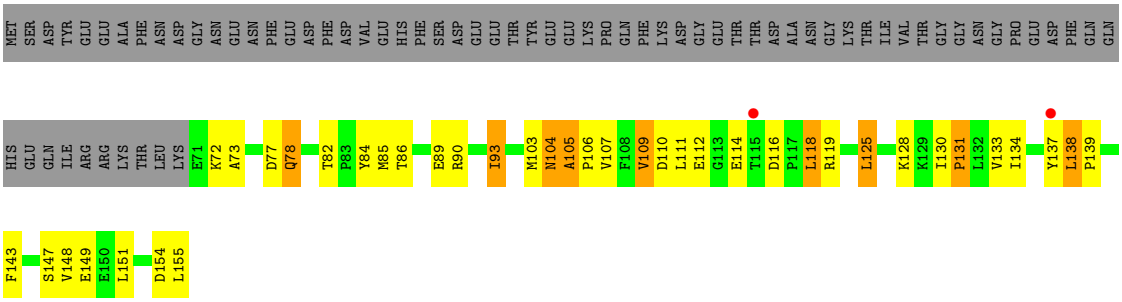


• Molecule 7: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

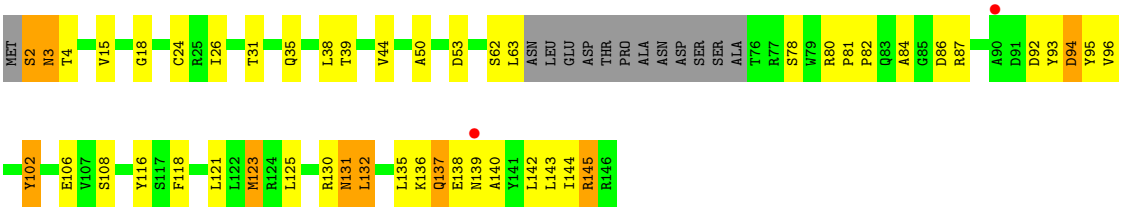


• Molecule 8: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide

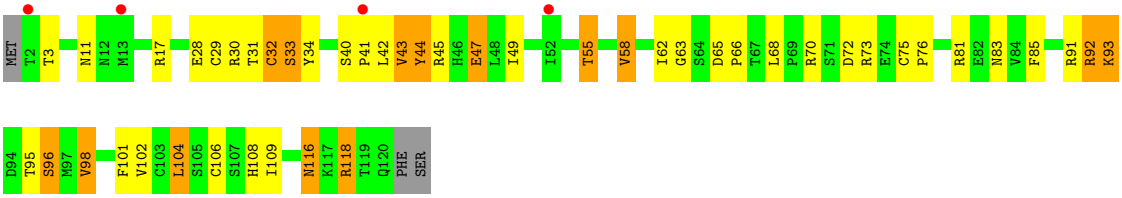




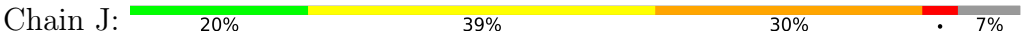
• Molecule 9: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide

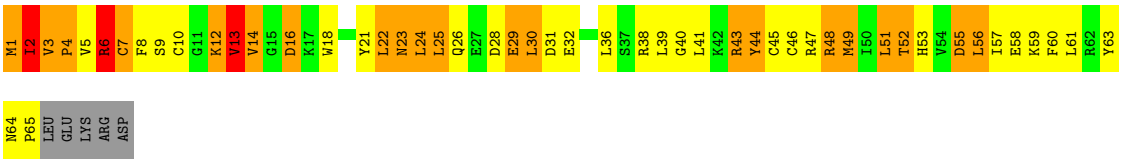


• Molecule 10: DNA-directed RNA polymerase II subunit 9

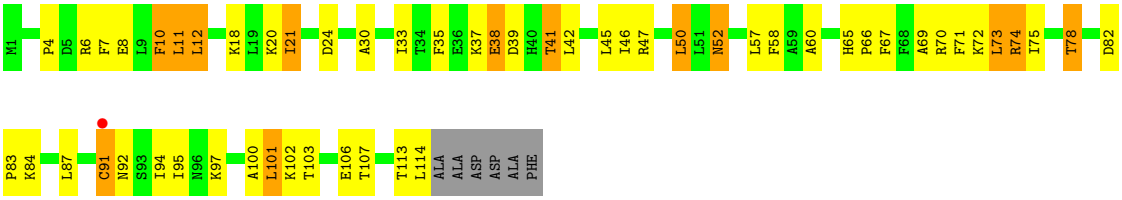


• Molecule 11: DNA-directed RNA polymerases I/II/III subunit 10

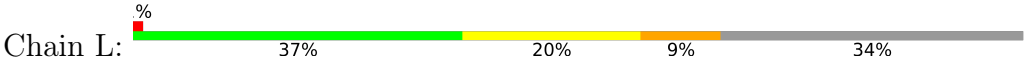


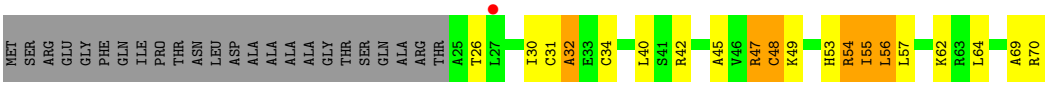


• Molecule 12: DNA-directed RNA polymerase II 13.6 kDa polypeptide



• Molecule 13: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	170.61Å 222.73Å 196.16Å 90.00° 101.87° 90.00°	Depositor
Resolution (Å)	19.98 – 3.40 19.98 – 3.40	Depositor EDS
% Data completeness (in resolution range)	90.0 (19.98-3.40) 89.5 (19.98-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 3.44Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.283 , 0.344 0.271 , 0.318	Depositor DCC
R_{free} test set	2609 reflections (2.67%)	wwPDB-VP
Wilson B-factor (Å^2)	101.5	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 125.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	29530	wwPDB-VP
Average B, all atoms (Å^2)	146.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	R	0.42	0/243	0.77	0/378
2	T	0.44	1/634 (0.2%)	1.07	6/975 (0.6%)
3	N	0.43	0/317	1.01	0/488
4	A	0.63	0/11292	0.96	21/15267 (0.1%)
5	B	0.67	1/9087 (0.0%)	0.96	12/12253 (0.1%)
6	C	0.69	0/2133	0.99	3/2891 (0.1%)
7	E	0.55	0/1788	0.95	3/2406 (0.1%)
8	F	0.58	0/700	0.98	3/945 (0.3%)
9	H	0.60	1/1086 (0.1%)	0.91	1/1470 (0.1%)
10	I	0.57	0/989	0.93	5/1331 (0.4%)
11	J	0.56	0/541	0.90	0/727
12	K	0.62	0/937	0.93	0/1265
13	L	0.85	0/365	1.17	4/485 (0.8%)
All	All	0.63	3/30112 (0.0%)	0.96	58/40881 (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
4	A	0	18
5	B	0	20
6	C	0	1
9	H	0	1
11	J	0	4
All	All	0	44

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	18	DA	O3'-P	5.92	1.70	1.61
9	H	102	TYR	CA-C	5.92	1.55	1.52
5	B	799	PRO	CA-C	5.23	1.58	1.52

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1170	ILE	N-CA-C	8.02	118.12	110.42
4	A	88	LYS	CA-C-N	8.00	128.06	119.90
4	A	88	LYS	C-N-CA	8.00	128.06	119.90
5	B	1085	ILE	CB-CA-C	-7.45	101.92	110.41
4	A	553	VAL	CA-C-N	7.21	126.83	119.19
4	A	553	VAL	C-N-CA	7.21	126.83	119.19
2	T	19	DT	P-O3'-C3'	-6.97	109.75	120.20
8	F	105	ALA	CA-C-N	6.97	128.55	119.84
8	F	105	ALA	C-N-CA	6.97	128.55	119.84
2	T	18	DA	P-O3'-C3'	6.68	130.22	120.20
5	B	899	ILE	CB-CA-C	-6.55	104.12	111.45
2	T	25	DC	C1'-O4'-C4'	-6.54	99.89	109.70
13	L	47	ARG	N-CA-C	6.49	117.61	108.00
4	A	1088	GLY	N-CA-C	-6.44	104.70	112.49
4	A	793	SER	CA-C-N	6.34	125.84	119.24
4	A	793	SER	C-N-CA	6.34	125.84	119.24
4	A	399	HIS	CA-C-N	-6.30	111.96	119.84
4	A	399	HIS	C-N-CA	-6.30	111.96	119.84
2	T	25	DC	O4'-C1'-N1	6.15	117.62	108.40
4	A	356	ASP	CA-C-N	6.11	126.90	120.12
4	A	356	ASP	C-N-CA	6.11	126.90	120.12
5	B	234	ILE	N-CA-C	5.91	116.62	107.99
10	I	68	LEU	CA-C-N	5.91	126.72	120.11
10	I	68	LEU	C-N-CA	5.91	126.72	120.11
2	T	19	DT	O3'-P-O5'	5.83	112.75	104.00
4	A	524	VAL	N-CA-C	5.82	116.55	108.23
10	I	43	VAL	CB-CA-C	-5.74	106.01	111.06
13	L	45	ALA	N-CA-C	5.73	116.48	108.00
4	A	845	LEU	N-CA-C	-5.68	106.15	114.39
13	L	32	ALA	N-CA-C	5.64	117.42	111.28
6	C	51	VAL	N-CA-C	5.58	116.20	108.84
5	B	810	GLU	N-CA-C	5.56	118.86	111.75
7	E	202	SER	N-CA-C	5.48	117.59	108.99
5	B	550	ASP	CA-C-N	5.44	125.09	119.05
5	B	550	ASP	C-N-CA	5.44	125.09	119.05
4	A	1016	THR	N-CA-C	5.42	117.63	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	H	102	TYR	N-CA-C	5.42	116.75	108.30
10	I	93	LYS	N-CA-C	5.37	118.62	111.75
5	B	1039	GLY	N-CA-C	-5.37	108.23	115.21
7	E	177	ARG	N-CA-C	5.36	117.97	109.50
5	B	828	ALA	N-CA-C	5.34	117.61	108.90
5	B	743	ILE	CB-CA-C	-5.29	105.00	112.14
2	T	6	DG	P-O3'-C3'	5.29	128.13	120.20
5	B	280	ILE	N-CA-C	5.29	113.65	107.89
13	L	40	LEU	N-CA-C	5.26	117.97	109.40
10	I	72	ASP	N-CA-C	5.22	117.57	110.88
4	A	456	MET	N-CA-C	5.20	117.30	109.23
7	E	90	VAL	N-CA-C	-5.19	108.78	113.71
8	F	109	VAL	N-CA-C	5.19	115.04	107.88
6	C	105	GLY	N-CA-C	-5.18	104.52	112.85
5	B	854	LEU	N-CA-C	5.13	118.47	110.32
5	B	739	THR	N-CA-C	-5.12	108.79	114.62
4	A	437	MET	N-CA-C	5.08	117.39	109.52
4	A	397	ASN	N-CA-C	5.08	119.09	112.13
4	A	596	THR	N-CA-C	5.05	116.92	110.61
6	C	108	GLU	N-CA-C	-5.04	105.97	111.82
4	A	236	LEU	N-CA-C	5.03	116.89	107.99
4	A	411	ASP	N-CA-C	5.00	117.36	110.35

There are no chirality outliers.

All (44) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	1039	LYS	Peptide
4	A	1040	GLN	Peptide
4	A	1082	ASN	Peptide
4	A	117	GLU	Peptide
4	A	1444	MET	Peptide
4	A	1445	ILE	Peptide
4	A	1447	GLU	Peptide
4	A	218	ASP	Peptide
4	A	222	LEU	Peptide
4	A	298	PHE	Peptide
4	A	330	LYS	Peptide
4	A	467	THR	Peptide
4	A	471	ASN	Peptide
4	A	53	LEU	Peptide
4	A	54	ASN	Peptide

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Mol	Chain	Res	Type	Group
4	A	882	SER	Peptide
4	A	883	LEU	Peptide
4	A	920	LEU	Peptide
5	B	1009	ASP	Peptide
5	B	1068	GLY	Peptide
5	B	1098	MET	Peptide
5	B	1177	HIS	Peptide
5	B	1222	ARG	Peptide
5	B	333	PHE	Peptide
5	B	334	ILE	Peptide
5	B	337	ARG	Peptide
5	B	342	GLY	Peptide
5	B	36	ALA	Peptide
5	B	368	GLU	Peptide
5	B	481	GLN	Peptide
5	B	744	HIS	Peptide
5	B	763	GLN	Peptide
5	B	836	GLU	Peptide
5	B	883	LEU	Peptide
5	B	886	LYS	Peptide
5	B	887	HIS	Peptide
5	B	945	GLU	Peptide
5	B	985	GLY	Peptide
6	C	39	ALA	Peptide
9	H	2	SER	Peptide
11	J	1	MET	Peptide
11	J	24	LEU	Peptide
11	J	39	LEU	Peptide
11	J	4	PRO	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	R	216	0	109	59	0
2	T	566	0	316	44	0
3	N	284	0	161	3	0
4	A	11094	0	11178	715	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	8914	0	8953	770	0
6	C	2095	0	2051	124	0
7	E	1752	0	1776	52	0
8	F	688	0	707	25	0
9	H	1068	0	1040	39	0
10	I	971	0	927	30	0
11	J	532	0	542	123	0
12	K	919	0	929	43	0
13	L	363	0	386	10	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	2	0	0	0	0
16	A	58	0	22	12	0
All	All	29530	0	29097	1844	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 31.

All (1844) 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)
16:A:2003[A]:UTP:C6	16:A:2003[A]:UTP:H5'2	1.44	1.52
9:H:2:SER:CB	9:H:3:ASN:HB2	1.35	1.50
4:A:1444:MET:CG	4:A:1445:ILE:HG13	1.49	1.42
9:H:2:SER:HB2	9:H:3:ASN:CB	1.52	1.40
4:A:1040:GLN:N	4:A:1041:ALA:HB3	1.43	1.31
4:A:116:ASP:CB	4:A:117:GLU:HB2	1.61	1.30
5:B:140:ILE:CG2	5:B:141:ASP:HB2	1.62	1.29
4:A:1040:GLN:H	4:A:1041:ALA:CB	1.55	1.20
4:A:1447:GLU:HA	4:A:1448:GLU:CG	1.72	1.20
5:B:886:LYS:HB3	5:B:887:HIS:CA	1.71	1.20
5:B:1097:HIS:O	5:B:1098:MET:HG3	1.40	1.19
5:B:140:ILE:HB	5:B:141:ASP:CB	1.73	1.19
5:B:333:PHE:CB	5:B:334:ILE:HG12	1.74	1.18
5:B:1031:LEU:HD12	5:B:1031:LEU:O	1.42	1.17
4:A:298:PHE:HA	4:A:299:HIS:O	1.40	1.15
4:A:665:GLY:HA2	5:B:1086:PHE:HD1	1.08	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:647:GLY:HA3	5:B:648:HIS:HB2	1.21	1.13
5:B:980:PHE:CE2	5:B:1094:ARG:HG2	1.82	1.13
4:A:920:LEU:HD22	4:A:921:GLY:H	1.07	1.13
1:R:6:G:H2'	1:R:7:A:H8	1.00	1.12
10:I:118:ARG:HG2	10:I:118:ARG:HH11	1.09	1.12
16:A:2003[A]:UTP:C6	16:A:2003[A]:UTP:C5'	2.31	1.12
5:B:333:PHE:N	5:B:334:ILE:HB	1.63	1.12
4:A:737:LEU:HA	4:A:738:LYS:HB2	1.24	1.12
5:B:647:GLY:HA3	5:B:648:HIS:CB	1.80	1.11
4:A:1004:ASN:HB2	4:A:1007:ILE:HD13	1.23	1.10
4:A:1172:LEU:HA	4:A:1173:HIS:HB2	1.18	1.09
4:A:1444:MET:HG3	4:A:1445:ILE:CG1	1.81	1.09
4:A:116:ASP:HB3	4:A:117:GLU:CB	1.83	1.09
4:A:1447:GLU:HA	4:A:1448:GLU:CB	1.80	1.09
5:B:341:LEU:HD13	5:B:343:ILE:HB	1.27	1.09
6:C:189:THR:HG22	6:C:190:ASP:H	1.17	1.09
5:B:980:PHE:HE2	5:B:1094:ARG:HG2	0.92	1.08
4:A:55:ASP:H	4:A:56:PRO:HD2	1.13	1.08
5:B:807:ARG:HG3	5:B:807:ARG:HH11	1.13	1.07
5:B:829:CYS:SG	5:B:1014:PRO:HG2	1.95	1.06
5:B:887:HIS:HB3	5:B:888:GLY:O	1.55	1.06
5:B:955:THR:HG22	5:B:956:THR:H	1.15	1.06
1:R:6:G:H2'	1:R:7:A:C8	1.88	1.06
5:B:337:ARG:HD3	5:B:339:THR:HG23	1.10	1.05
11:J:7:CYS:CA	11:J:49:MET:HE3	1.84	1.05
5:B:140:ILE:HB	5:B:141:ASP:HB3	1.33	1.04
5:B:140:ILE:HG22	5:B:141:ASP:HB2	1.07	1.04
5:B:1012:ILE:HG13	5:B:1013:ASN:N	1.72	1.04
5:B:341:LEU:CD1	5:B:343:ILE:HB	1.87	1.03
4:A:630:ILE:H	4:A:630:ILE:HD12	1.17	1.03
5:B:140:ILE:CB	5:B:141:ASP:CB	2.36	1.03
11:J:5:VAL:HG12	11:J:6:ARG:H	1.24	1.02
11:J:48:ARG:HH12	11:J:49:MET:HE1	1.19	1.02
16:A:2003[A]:UTP:O3A	16:A:2003[A]:UTP:H4'	1.57	1.02
5:B:828:ALA:HB2	5:B:1085:ILE:HG21	1.39	1.02
5:B:886:LYS:HB3	5:B:887:HIS:HA	1.05	1.02
5:B:778:MET:CE	5:B:1094:ARG:HD2	1.88	1.02
5:B:886:LYS:CB	5:B:887:HIS:HA	1.90	1.02
4:A:1172:LEU:HA	4:A:1173:HIS:CB	1.88	1.01
4:A:53:LEU:HG	4:A:54:ASN:H	1.24	1.01
5:B:140:ILE:CG2	5:B:141:ASP:CB	2.37	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:920:LEU:HD22	4:A:921:GLY:N	1.74	1.01
9:H:2:SER:CA	9:H:3:ASN:HB2	1.84	1.01
4:A:343:LYS:NZ	5:B:1197:PRO:HB3	1.76	1.00
5:B:1013:ASN:OD1	5:B:1015:HIS:HD2	1.44	1.00
4:A:1446:ASP:O	4:A:1447:GLU:HG3	1.60	1.00
5:B:708:GLU:O	5:B:712:PRO:HD3	1.61	1.00
11:J:44:TYR:HA	11:J:47:ARG:HB2	1.42	1.00
4:A:351:THR:HG23	5:B:1103:ILE:HG13	1.41	1.00
5:B:1012:ILE:HG13	5:B:1013:ASN:H	1.25	1.00
6:C:142:VAL:H	11:J:16:ASP:HB3	1.25	0.99
5:B:140:ILE:HB	5:B:141:ASP:C	1.87	0.99
4:A:343:LYS:HZ3	5:B:1197:PRO:HB3	1.25	0.99
4:A:1444:MET:HG3	4:A:1445:ILE:HG13	1.02	0.99
1:R:8:G:N2	2:T:22:DT:C2	2.30	0.99
4:A:116:ASP:HB3	4:A:117:GLU:HB2	0.99	0.99
4:A:1007:ILE:HD12	4:A:1007:ILE:H	1.21	0.99
5:B:140:ILE:H	5:B:141:ASP:C	1.69	0.99
5:B:1010:LEU:HD21	5:B:1092:TYR:CD1	1.97	0.98
16:A:2003[A]:UTP:H5'2	16:A:2003[A]:UTP:N1	1.76	0.98
5:B:333:PHE:HB2	5:B:334:ILE:HG12	1.45	0.98
4:A:1394:THR:HG21	4:A:1398:MET:HE2	1.46	0.98
4:A:1348:LEU:HD23	4:A:1372:VAL:HG22	1.44	0.97
4:A:1444:MET:HG2	4:A:1445:ILE:N	1.78	0.97
4:A:1447:GLU:HA	4:A:1448:GLU:HG3	1.42	0.97
4:A:1447:GLU:CA	4:A:1448:GLU:HB3	1.95	0.97
1:R:8:G:C2	2:T:22:DT:N3	2.33	0.96
5:B:337:ARG:CD	5:B:339:THR:HG23	1.95	0.96
5:B:757:PRO:HG2	5:B:1028:GLU:OE2	1.64	0.96
4:A:665:GLY:HA2	5:B:1086:PHE:CD1	2.01	0.95
4:A:116:ASP:CA	4:A:117:GLU:HB2	1.95	0.95
11:J:5:VAL:O	11:J:6:ARG:O	1.85	0.95
1:R:5:A:H5"	5:B:476:ARG:NH1	1.82	0.95
11:J:44:TYR:HD2	11:J:44:TYR:N	1.63	0.95
4:A:416:ARG:HG2	4:A:416:ARG:HH11	1.30	0.95
4:A:1172:LEU:CA	4:A:1173:HIS:HB2	1.97	0.95
4:A:828:ALA:HB2	5:B:530:GLY:HA2	1.49	0.94
4:A:737:LEU:HA	4:A:738:LYS:CB	1.97	0.94
4:A:1063:MET:HG3	4:A:1436:ILE:HG23	1.49	0.94
5:B:337:ARG:HD3	5:B:339:THR:CG2	1.97	0.94
1:R:8:G:N1	2:T:22:DT:C4	2.35	0.94
4:A:1444:MET:HB2	4:A:1445:ILE:HG23	1.46	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:999:MET:HG3	5:B:1000:PRO:HD2	1.50	0.94
5:B:340:ALA:O	5:B:342:GLY:HA2	1.67	0.93
1:R:5:A:C2	1:R:6:G:C5	2.56	0.93
5:B:840:ILE:HG22	5:B:841:MET:H	1.32	0.93
4:A:667:GLY:HA2	4:A:670:ILE:HG12	1.51	0.92
5:B:333:PHE:HB3	5:B:334:ILE:HG12	1.48	0.92
5:B:341:LEU:HB2	5:B:342:GLY:HA2	1.51	0.92
5:B:976:ILE:HG23	5:B:977:GLY:H	1.32	0.92
11:J:48:ARG:NH1	11:J:49:MET:HE1	1.82	0.92
4:A:1063:MET:CG	4:A:1436:ILE:HG23	2.00	0.92
4:A:737:LEU:CA	4:A:738:LYS:HB2	2.00	0.92
11:J:7:CYS:CB	11:J:49:MET:HE3	1.99	0.91
4:A:351:THR:HG23	5:B:1103:ILE:CG1	2.01	0.91
5:B:952:VAL:HG22	5:B:966:VAL:HG22	1.52	0.91
1:R:5:A:C2	1:R:6:G:C4	2.58	0.91
4:A:351:THR:HG22	4:A:352:VAL:H	1.35	0.91
4:A:567:LYS:HB3	9:H:96:VAL:H	1.36	0.91
5:B:199:MET:N	5:B:199:MET:SD	2.42	0.90
8:F:93:ILE:HD11	8:F:134:ILE:HD11	1.52	0.90
11:J:7:CYS:HA	11:J:49:MET:HE3	1.53	0.90
5:B:211:VAL:HG21	5:B:483:LEU:HD13	1.54	0.90
5:B:345:LYS:HA	5:B:347:LYS:H	1.35	0.89
5:B:140:ILE:HB	5:B:141:ASP:CA	2.02	0.89
5:B:705:MET:HA	5:B:705:MET:HE3	1.52	0.89
5:B:828:ALA:HB2	5:B:1085:ILE:CG2	2.02	0.88
4:A:416:ARG:HH11	4:A:416:ARG:CG	1.87	0.88
4:A:1004:ASN:HB2	4:A:1007:ILE:CD1	2.03	0.88
6:C:37:MET:O	6:C:41:ILE:HD11	1.73	0.88
4:A:55:ASP:N	4:A:56:PRO:HD2	1.88	0.88
5:B:340:ALA:O	5:B:341:LEU:HB2	1.72	0.88
5:B:1069:PHE:H	5:B:1069:PHE:HD1	1.21	0.88
4:A:374:LEU:CB	4:A:436:ILE:HD13	2.03	0.88
5:B:978:ASP:HA	5:B:1098:MET:HB3	1.54	0.87
4:A:393:ARG:O	4:A:394:ASN:HB2	1.73	0.87
4:A:1197:LEU:HD13	4:A:1209:MET:HE1	1.57	0.87
4:A:1444:MET:CG	4:A:1445:ILE:CG1	2.43	0.87
11:J:36:LEU:HB2	11:J:47:ARG:HH21	1.40	0.87
5:B:945:GLU:O	5:B:946:ASN:HB3	1.75	0.87
5:B:1106:ARG:CZ	5:B:1109:GLY:H	1.86	0.87
4:A:1444:MET:HB2	4:A:1445:ILE:CG2	2.05	0.86
5:B:331:LEU:O	5:B:334:ILE:HG21	1.76	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:846:ILE:HG12	5:B:974:PRO:HG2	1.57	0.86
5:B:785:TYR:CD1	5:B:795:ILE:HG12	2.09	0.86
5:B:957:ASN:HD22	5:B:958:GLN:N	1.73	0.86
4:A:57:ARG:O	4:A:68:GLN:HG2	1.76	0.86
11:J:7:CYS:HB2	11:J:49:MET:CE	2.05	0.85
5:B:983:ARG:HD2	5:B:1091:TYR:HD2	1.41	0.85
4:A:1447:GLU:CA	4:A:1448:GLU:CB	2.48	0.85
5:B:778:MET:HE3	5:B:1094:ARG:HD2	1.56	0.85
4:A:90:VAL:HA	4:A:204:THR:HG21	1.57	0.85
5:B:211:VAL:CG2	5:B:483:LEU:HD13	2.05	0.85
4:A:662:PHE:CD1	4:A:663:SER:N	2.45	0.85
5:B:1013:ASN:OD1	5:B:1015:HIS:CD2	2.30	0.85
4:A:133:LYS:HE3	4:A:1391:ARG:HH12	1.42	0.85
1:R:7:A:C2'	1:R:8:G:H5'	2.07	0.85
4:A:1007:ILE:HD12	4:A:1007:ILE:N	1.92	0.84
4:A:665:GLY:CA	5:B:1086:PHE:HD1	1.90	0.84
4:A:208:LEU:HD23	4:A:235:ILE:HD11	1.59	0.84
4:A:351:THR:CG2	5:B:1103:ILE:CG1	2.56	0.84
4:A:1444:MET:CB	4:A:1445:ILE:HG13	2.07	0.84
4:A:1364:ASN:HD22	4:A:1364:ASN:C	1.86	0.84
6:C:45:ALA:HA	6:C:72:LEU:HD12	1.58	0.84
4:A:787:PHE:CE1	4:A:796:SER:HA	2.12	0.83
4:A:1433:MET:HE2	5:B:1145:SER:HB3	1.60	0.83
4:A:1007:ILE:H	4:A:1007:ILE:CD1	1.91	0.83
11:J:44:TYR:HD2	11:J:44:TYR:H	0.86	0.83
5:B:211:VAL:O	5:B:480:SER:HA	1.79	0.83
5:B:516:ASN:HD22	5:B:516:ASN:H	1.24	0.83
5:B:637:LEU:CD1	5:B:740:HIS:HB3	2.09	0.83
4:A:446:ARG:HB2	4:A:487:MET:HE3	1.59	0.83
5:B:807:ARG:HG3	5:B:807:ARG:NH1	1.87	0.83
5:B:839:MET:HE3	5:B:1010:LEU:HD11	1.61	0.83
5:B:886:LYS:HB2	5:B:890:TYR:HE1	1.43	0.83
6:C:189:THR:HG22	6:C:190:ASP:N	1.94	0.83
5:B:333:PHE:N	5:B:334:ILE:CB	2.42	0.82
4:A:1444:MET:CB	4:A:1445:ILE:HG23	2.09	0.82
5:B:955:THR:HG22	5:B:956:THR:N	1.93	0.82
4:A:55:ASP:H	4:A:56:PRO:CD	1.93	0.82
4:A:828:ALA:CB	5:B:530:GLY:HA2	2.08	0.82
5:B:467:GLY:O	5:B:468:GLU:HB3	1.79	0.82
4:A:253:ASN:HD22	4:A:253:ASN:H	1.26	0.82
4:A:451:HIS:C	4:A:453:MET:H	1.87	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:140:ILE:N	5:B:141:ASP:C	2.36	0.82
5:B:103:ASN:HD22	5:B:169:ARG:HH22	1.26	0.82
5:B:778:MET:HE2	5:B:1094:ARG:HD2	1.62	0.82
11:J:48:ARG:NH1	11:J:49:MET:CE	2.42	0.81
5:B:805:THR:HG21	5:B:815:ARG:HH21	1.42	0.81
5:B:834:ASN:ND2	5:B:1013:ASN:HD22	1.78	0.81
5:B:1001:PHE:CE2	5:B:1073:TYR:HB2	2.16	0.81
9:H:137:GLN:C	9:H:139:ASN:H	1.89	0.81
5:B:343:ILE:HG13	5:B:344:LYS:H	1.44	0.81
4:A:351:THR:CG2	5:B:1103:ILE:HG13	2.11	0.81
4:A:1025:ARG:CG	4:A:1025:ARG:HH11	1.93	0.81
1:R:5:A:H5"	5:B:476:ARG:HH12	1.44	0.81
5:B:1106:ARG:NH2	5:B:1109:GLY:H	1.79	0.80
5:B:843:GLN:HB2	5:B:993:THR:HB	1.63	0.80
10:I:96:SER:HB2	10:I:98:VAL:HG23	1.64	0.80
4:A:1444:MET:CA	4:A:1445:ILE:HG23	2.12	0.80
16:A:2003[A]:UTP:O3A	16:A:2003[A]:UTP:C4'	2.30	0.80
5:B:978:ASP:OD1	5:B:978:ASP:N	2.14	0.80
5:B:708:GLU:O	5:B:712:PRO:CD	2.30	0.79
13:L:48:CYS:SG	13:L:49:LYS:N	2.55	0.79
4:A:406:ILE:HB	4:A:431:LYS:HB2	1.64	0.79
4:A:1444:MET:HA	4:A:1445:ILE:HG23	1.63	0.79
5:B:333:PHE:CB	5:B:334:ILE:CG1	2.60	0.79
11:J:25:LEU:HD12	11:J:25:LEU:N	1.97	0.79
4:A:343:LYS:HZ1	5:B:1197:PRO:CG	1.94	0.79
4:A:1444:MET:HG2	4:A:1445:ILE:H	1.44	0.78
12:K:21:ILE:HG22	12:K:33:ILE:HG12	1.63	0.78
5:B:1084:GLN:HE21	6:C:189:THR:CG2	1.97	0.78
4:A:1444:MET:HB2	4:A:1445:ILE:CG1	2.13	0.78
5:B:887:HIS:CB	5:B:888:GLY:O	2.32	0.78
11:J:7:CYS:CB	11:J:49:MET:CE	2.61	0.78
2:T:15:DA:H2"	2:T:16:DC:O5'	1.84	0.78
1:R:7:A:H2'	1:R:8:G:H5'	1.65	0.78
5:B:345:LYS:HA	5:B:346:GLU:HB3	1.64	0.78
5:B:710:LEU:O	5:B:711:GLU:HB3	1.84	0.78
9:H:2:SER:HB2	9:H:3:ASN:HB2	0.79	0.78
5:B:1033:LYS:HB2	5:B:1089:PRO:HD2	1.65	0.78
6:C:32:SER:O	6:C:36:VAL:HG12	1.83	0.78
5:B:801:LYS:O	11:J:52:THR:HG22	1.84	0.78
9:H:2:SER:CB	9:H:3:ASN:CB	2.30	0.78
4:A:1219:THR:HG21	4:A:1271:ILE:HD11	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:333:PHE:HB3	5:B:334:ILE:CG1	2.13	0.77
5:B:999:MET:HE3	5:B:1011:ILE:HD11	1.66	0.77
5:B:41:LYS:HE2	5:B:544:CYS:SG	2.25	0.77
4:A:416:ARG:HG2	4:A:416:ARG:NH1	1.98	0.77
6:C:57:VAL:HG11	11:J:60:PHE:HB2	1.65	0.77
11:J:41:LEU:O	11:J:47:ARG:CD	2.33	0.77
4:A:667:GLY:HA2	4:A:670:ILE:CG1	2.14	0.76
6:C:124:LEU:C	6:C:126:GLY:H	1.91	0.76
4:A:374:LEU:HB3	4:A:436:ILE:HD13	1.66	0.76
10:I:118:ARG:HG2	10:I:118:ARG:NH1	1.90	0.76
5:B:140:ILE:CB	5:B:141:ASP:HB2	2.10	0.76
4:A:315:LEU:HD12	4:A:316:GLN:H	1.51	0.76
4:A:709:THR:HB	4:A:712:GLU:H	1.46	0.76
5:B:710:LEU:O	5:B:711:GLU:CB	2.33	0.76
5:B:844:SER:O	5:B:847:ASP:HB2	1.86	0.76
4:A:423:ASP:CG	4:A:424:ILE:H	1.93	0.76
4:A:1441:PHE:CZ	8:F:89:GLU:HA	2.22	0.75
4:A:775:ILE:HG13	4:A:798:GLY:HA3	1.69	0.75
4:A:1171:GLN:HB3	4:A:1172:LEU:HB2	1.69	0.75
4:A:1118:VAL:CG2	4:A:1306:LEU:HB2	2.15	0.75
5:B:337:ARG:HB3	5:B:340:ALA:N	2.01	0.75
7:E:31:THR:HG23	7:E:34:GLU:HB2	1.68	0.75
11:J:8:PHE:H	11:J:49:MET:CE	2.00	0.75
5:B:647:GLY:CA	5:B:648:HIS:CB	2.63	0.75
11:J:41:LEU:O	11:J:47:ARG:HD2	1.87	0.75
11:J:2:ILE:HG23	11:J:2:ILE:O	1.85	0.75
4:A:920:LEU:HD13	4:A:920:LEU:C	2.12	0.75
5:B:341:LEU:HD13	5:B:343:ILE:CB	2.13	0.75
12:K:46:ILE:O	12:K:50:LEU:HB2	1.86	0.75
4:A:360:GLU:H	4:A:360:GLU:CD	1.94	0.75
4:A:343:LYS:NZ	5:B:1197:PRO:CB	2.49	0.75
5:B:711:GLU:H	5:B:712:PRO:CD	1.99	0.74
5:B:824:ILE:HD11	11:J:48:ARG:NH2	2.02	0.74
5:B:785:TYR:CE1	5:B:795:ILE:HG12	2.22	0.74
5:B:280:ILE:HB	5:B:285:ILE:HD11	1.69	0.74
5:B:953:LEU:HD11	13:L:55:ILE:HG22	1.69	0.74
4:A:1025:ARG:HH11	4:A:1025:ARG:HG2	1.49	0.74
4:A:609:ASP:O	4:A:611:GLN:N	2.20	0.74
5:B:653:VAL:HG12	5:B:689:LEU:HD13	1.70	0.74
6:C:189:THR:CG2	6:C:190:ASP:H	1.99	0.73
6:C:234:SER:HB3	6:C:240:VAL:HG13	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:298:PHE:HA	4:A:299:HIS:C	2.12	0.73
5:B:840:ILE:HG22	5:B:841:MET:N	1.99	0.73
5:B:807:ARG:HH11	5:B:807:ARG:CG	1.96	0.73
4:A:374:LEU:HB2	4:A:436:ILE:HD13	1.69	0.73
4:A:506:ALA:O	4:A:509:LEU:HG	1.87	0.73
5:B:340:ALA:C	5:B:342:GLY:HA2	2.13	0.73
5:B:344:LYS:O	5:B:346:GLU:HB3	1.89	0.73
7:E:88:VAL:HG21	7:E:112:TYR:HB2	1.70	0.73
9:H:50:ALA:O	9:H:53:ASP:HB2	1.87	0.73
4:A:346:ASP:HB2	5:B:1154:ALA:HB1	1.71	0.73
4:A:351:THR:CG2	5:B:1103:ILE:HG12	2.17	0.73
5:B:345:LYS:CA	5:B:346:GLU:CB	2.67	0.73
4:A:1410:PHE:HD2	5:B:1212:ILE:HD11	1.53	0.73
5:B:140:ILE:CB	5:B:141:ASP:C	2.60	0.73
5:B:212:LEU:HD13	5:B:409:ALA:HA	1.71	0.73
4:A:134:ARG:HD3	4:A:221:SER:O	1.88	0.73
4:A:479:ASN:ND2	16:A:2003[B]:UTP:O3'	2.22	0.73
4:A:1059:HIS:HE1	8:F:155:LEU:HD21	1.52	0.73
5:B:886:LYS:HB2	5:B:890:TYR:CE1	2.23	0.73
4:A:567:LYS:HB2	4:A:568:PRO:HD2	1.69	0.72
4:A:1171:GLN:H	4:A:1172:LEU:CB	2.02	0.72
5:B:422:LYS:HA	5:B:425:THR:HG22	1.71	0.72
10:I:118:ARG:HH11	10:I:118:ARG:CG	1.95	0.72
11:J:5:VAL:HG12	11:J:6:ARG:N	2.03	0.72
11:J:44:TYR:HA	11:J:47:ARG:CB	2.18	0.72
4:A:466:SER:HB2	5:B:1103:ILE:HD13	1.70	0.72
5:B:260:GLY:O	5:B:267:ARG:NH1	2.22	0.72
5:B:337:ARG:HB2	5:B:340:ALA:HB2	1.71	0.72
4:A:1243:VAL:HG13	4:A:1244:ARG:HG3	1.71	0.72
5:B:140:ILE:CB	5:B:141:ASP:HB3	2.08	0.72
4:A:1444:MET:CB	4:A:1445:ILE:CG1	2.68	0.72
11:J:7:CYS:HB2	11:J:49:MET:HE2	1.71	0.72
11:J:36:LEU:HB2	11:J:47:ARG:NH2	2.04	0.72
4:A:54:ASN:HD22	4:A:54:ASN:N	1.88	0.72
4:A:827:THR:C	4:A:829:VAL:H	1.97	0.72
5:B:333:PHE:CA	5:B:334:ILE:HB	2.15	0.72
5:B:778:MET:O	5:B:796:LEU:HD12	1.90	0.71
9:H:93:TYR:CD2	9:H:145:ARG:HB3	2.25	0.71
11:J:53:HIS:HE1	11:J:55:ASP:OD1	1.72	0.71
2:T:19:DT:C4	2:T:20:DC:C4	2.77	0.71
5:B:322:PHE:CZ	10:I:30:ARG:HG3	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1072:MET:HE3	5:B:1085:ILE:HD12	1.72	0.71
9:H:38:LEU:HD12	9:H:125:LEU:HD13	1.72	0.71
4:A:483:ASP:HB2	5:B:987:LYS:HE3	1.72	0.71
4:A:1082:ASN:HA	4:A:1097:GLY:HA3	1.72	0.71
5:B:999:MET:CG	5:B:1000:PRO:HD2	2.18	0.71
4:A:338:GLY:HA2	5:B:1129:ARG:HH22	1.54	0.71
4:A:387:ARG:O	4:A:391:LEU:HD13	1.89	0.71
5:B:322:PHE:HZ	10:I:30:ARG:HG3	1.54	0.71
5:B:846:ILE:CG1	5:B:974:PRO:HG2	2.21	0.71
5:B:1222:ARG:O	5:B:1223:ASP:HB2	1.90	0.71
11:J:57:ILE:O	11:J:61:LEU:HD12	1.91	0.71
5:B:299:GLU:OE1	5:B:572:HIS:HB3	1.90	0.71
5:B:486:TYR:HE2	5:B:776:GLN:O	1.73	0.71
4:A:99:ILE:HD11	4:A:234:MET:HB3	1.73	0.71
4:A:244:PRO:HB2	4:A:245:PRO:HD3	1.71	0.71
5:B:333:PHE:H	5:B:334:ILE:CG1	2.03	0.71
4:A:853:ASP:OD1	4:A:855:THR:HG22	1.89	0.71
5:B:103:ASN:HD22	5:B:169:ARG:NH2	1.89	0.70
5:B:198:ASP:OD1	5:B:485:ARG:NH2	2.22	0.70
5:B:333:PHE:HB3	5:B:334:ILE:CA	2.21	0.70
5:B:340:ALA:O	5:B:341:LEU:CB	2.39	0.70
6:C:144:ILE:HG22	6:C:145:CYS:HB3	1.71	0.70
2:T:15:DA:H2'	2:T:15:DA:N3	2.04	0.70
1:R:2:U:H2'	1:R:3:C:C6	2.26	0.70
1:R:10:A:C2	2:T:19:DT:N3	2.58	0.70
5:B:1031:LEU:O	5:B:1031:LEU:CD1	2.31	0.70
5:B:1166:CYS:HB3	5:B:1185:CYS:SG	2.32	0.70
5:B:287:ARG:NH1	5:B:324:ILE:O	2.23	0.70
5:B:834:ASN:HD21	5:B:1013:ASN:HD22	1.35	0.70
1:R:8:G:C2	2:T:22:DT:C2	2.77	0.70
5:B:345:LYS:HA	5:B:346:GLU:CB	2.20	0.70
5:B:886:LYS:HB3	5:B:887:HIS:C	2.17	0.70
11:J:14:VAL:HG21	11:J:49:MET:HG2	1.73	0.70
4:A:117:GLU:H	4:A:118:HIS:CB	2.05	0.69
1:R:6:G:C4	1:R:7:A:N7	2.61	0.69
4:A:1410:PHE:HZ	5:B:1210:MET:HE3	1.57	0.69
6:C:45:ALA:HA	6:C:72:LEU:CD1	2.21	0.69
4:A:719:VAL:HG12	4:A:723:ASN:ND2	2.07	0.69
5:B:490:SER:HB3	5:B:775:LYS:HG2	1.74	0.69
11:J:2:ILE:O	11:J:2:ILE:CG2	2.40	0.69
4:A:399:HIS:HB3	4:A:400:PRO:HD3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:337:ARG:HB3	5:B:340:ALA:H	1.56	0.69
4:A:535:THR:HG21	4:A:617:VAL:H	1.56	0.69
5:B:806:THR:HG22	5:B:808:ALA:H	1.58	0.69
4:A:37:PHE:HB2	4:A:52:GLY:HA3	1.74	0.69
4:A:53:LEU:CG	4:A:54:ASN:H	2.04	0.69
4:A:54:ASN:H	4:A:54:ASN:HD22	1.38	0.69
4:A:1040:GLN:N	4:A:1041:ALA:CB	2.30	0.69
5:B:711:GLU:N	5:B:712:PRO:HD3	2.08	0.69
4:A:343:LYS:HZ1	5:B:1197:PRO:CB	2.06	0.69
5:B:211:VAL:HG21	5:B:483:LEU:CD1	2.22	0.69
5:B:793:ALA:HB3	5:B:856:PHE:HB2	1.73	0.69
4:A:860:LEU:HD12	4:A:862:ASN:HD21	1.57	0.68
4:A:404:TYR:HD2	4:A:412:ARG:HD3	1.55	0.68
5:B:1082:MET:HA	6:C:189:THR:HA	1.75	0.68
11:J:8:PHE:N	11:J:49:MET:HE3	2.07	0.68
5:B:345:LYS:HA	5:B:347:LYS:N	2.06	0.68
5:B:1154:ALA:O	5:B:1155:SER:HB3	1.92	0.68
4:A:490:HIS:HB3	5:B:1150:ARG:NH1	2.09	0.68
5:B:755:ILE:HD12	5:B:814:PHE:CD1	2.28	0.68
5:B:778:MET:O	5:B:796:LEU:CD1	2.42	0.68
5:B:955:THR:CG2	5:B:956:THR:H	1.98	0.68
4:A:575:LYS:HD3	4:A:612:ILE:HD11	1.76	0.68
5:B:779:GLY:HA2	5:B:796:LEU:HD12	1.74	0.68
5:B:887:HIS:HB3	5:B:888:GLY:C	2.19	0.68
8:F:77:ASP:O	8:F:78:GLN:HB2	1.93	0.68
6:C:164:ALA:HA	6:C:167:HIS:O	1.93	0.68
7:E:176:PRO:HG2	7:E:211:TYR:O	1.93	0.68
2:T:19:DT:C4	2:T:20:DC:N4	2.61	0.68
4:A:1063:MET:HG3	4:A:1436:ILE:CG2	2.21	0.68
5:B:978:ASP:HA	5:B:1098:MET:CB	2.24	0.68
4:A:38:PRO:HB3	4:A:270:LEU:HB3	1.76	0.68
6:C:238:ILE:HG23	6:C:242:GLN:HB2	1.76	0.68
4:A:351:THR:HG21	5:B:1103:ILE:HG12	1.74	0.68
5:B:757:PRO:O	5:B:758:PHE:HB2	1.94	0.68
5:B:955:THR:HG23	13:L:54:ARG:O	1.94	0.68
4:A:68:GLN:O	4:A:70:CYS:N	2.25	0.67
4:A:471:ASN:C	4:A:471:ASN:OD1	2.37	0.67
4:A:884:ASP:O	4:A:886:ILE:N	2.26	0.67
6:C:238:ILE:CG2	6:C:242:GLN:HB2	2.24	0.67
5:B:471:LYS:HD2	5:B:471:LYS:C	2.19	0.67
5:B:822:ASN:ND2	11:J:52:THR:HG21	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:18:DA:H2"	2:T:19:DT:H5'	1.74	0.67
5:B:822:ASN:HD22	11:J:52:THR:HG21	1.59	0.67
4:A:704:ALA:H	4:A:705:LYS:HA	1.58	0.67
4:A:1364:ASN:ND2	4:A:1366:ARG:HG2	2.10	0.67
11:J:5:VAL:O	11:J:6:ARG:C	2.36	0.67
5:B:475:SER:C	5:B:477:ALA:H	2.03	0.67
1:R:8:G:N2	2:T:22:DT:N3	2.38	0.67
1:R:8:G:C2	2:T:22:DT:C4	2.79	0.67
4:A:272:ALA:HA	4:A:275:SER:HB3	1.77	0.67
4:A:451:HIS:C	4:A:453:MET:N	2.45	0.67
6:C:37:MET:HA	6:C:41:ILE:HD11	1.77	0.67
4:A:53:LEU:HG	4:A:54:ASN:N	2.03	0.67
4:A:848:ILE:HD13	4:A:858:ASN:HB3	1.77	0.67
4:A:1446:ASP:C	4:A:1447:GLU:HG3	2.19	0.67
16:A:2003[A]:UTP:H4'	16:A:2003[A]:UTP:PB	2.34	0.67
5:B:794:ASN:O	5:B:795:ILE:HD12	1.94	0.67
5:B:983:ARG:HD2	5:B:1091:TYR:CD2	2.27	0.67
5:B:1064:TYR:O	5:B:1065:GLN:C	2.38	0.67
11:J:8:PHE:H	11:J:49:MET:HE3	1.58	0.67
4:A:775:ILE:HG23	4:A:818:MET:HE1	1.77	0.67
5:B:805:THR:HG21	5:B:815:ARG:NH2	2.09	0.67
4:A:53:LEU:HG	4:A:54:ASN:HD22	1.60	0.66
4:A:565:ILE:HG23	4:A:567:LYS:HE3	1.76	0.66
4:A:1096:SER:HA	4:A:1100:ARG:HB2	1.77	0.66
5:B:174:LEU:HD13	5:B:202:TYR:CE1	2.30	0.66
5:B:711:GLU:N	5:B:712:PRO:CD	2.57	0.66
5:B:773:MET:HE2	5:B:981:ALA:HB1	1.77	0.66
5:B:773:MET:O	5:B:775:LYS:N	2.25	0.66
4:A:365:GLY:O	4:A:468:PHE:HA	1.95	0.66
11:J:14:VAL:HG21	11:J:49:MET:CG	2.25	0.66
5:B:308:TRP:HA	5:B:311:LEU:HD12	1.77	0.66
4:A:404:TYR:N	4:A:404:TYR:HD1	1.94	0.66
4:A:1040:GLN:H	4:A:1041:ALA:HB3	0.62	0.66
4:A:579:SER:HB3	4:A:611:GLN:HA	1.77	0.66
4:A:1118:VAL:HG22	4:A:1306:LEU:HB2	1.78	0.66
4:A:1171:GLN:N	4:A:1172:LEU:HB2	2.11	0.66
5:B:1152:MET:HB2	5:B:1153:GLU:OE2	1.96	0.66
1:R:8:G:N2	2:T:21:DC:O2	2.29	0.66
4:A:55:ASP:N	4:A:56:PRO:CD	2.53	0.66
5:B:840:ILE:CG2	5:B:841:MET:H	2.06	0.66
5:B:120:ARG:HB2	5:B:122:LEU:HG	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:957:ASN:ND2	5:B:958:GLN:H	1.94	0.66
5:B:957:ASN:ND2	5:B:958:GLN:N	2.44	0.66
5:B:1023:VAL:HA	5:B:1026:LEU:HD12	1.77	0.66
1:R:5:A:H2'	1:R:6:G:C8	2.31	0.66
4:A:1410:PHE:CZ	5:B:1210:MET:HE3	2.31	0.66
5:B:911:ILE:HD11	5:B:941:LEU:HA	1.77	0.66
4:A:1444:MET:HG2	4:A:1445:ILE:HG13	1.65	0.66
4:A:104:GLU:HG3	4:A:174:ILE:HD12	1.79	0.65
4:A:1171:GLN:CB	4:A:1172:LEU:HB2	2.25	0.65
11:J:25:LEU:HD12	11:J:25:LEU:H	1.59	0.65
4:A:1376:THR:HG22	7:E:212:ARG:HH22	1.60	0.65
5:B:115:GLN:OE1	5:B:115:GLN:HA	1.97	0.65
5:B:120:ARG:HG2	5:B:955:THR:HG21	1.77	0.65
5:B:313:MET:HE2	5:B:390:LEU:HG	1.78	0.65
5:B:976:ILE:HG23	5:B:977:GLY:N	2.08	0.65
4:A:827:THR:O	4:A:829:VAL:N	2.28	0.65
4:A:875:ALA:HA	4:A:878:ILE:HD13	1.78	0.65
5:B:25:ILE:HG23	5:B:29:ASP:HB2	1.78	0.65
5:B:624:LEU:C	5:B:624:LEU:CD1	2.69	0.65
8:F:147:SER:C	8:F:149:GLU:H	2.02	0.65
12:K:102:LYS:O	12:K:106:GLU:HG2	1.96	0.65
4:A:117:GLU:H	4:A:118:HIS:CA	2.09	0.65
4:A:436:ILE:HD11	4:A:491:VAL:HG11	1.78	0.65
5:B:1041:GLU:HG2	5:B:1042:GLY:O	1.96	0.65
5:B:1068:GLY:O	5:B:1069:PHE:O	2.13	0.65
4:A:1448:GLU:HG3	4:A:1449:SER:N	2.10	0.65
5:B:848:ARG:HD2	11:J:8:PHE:HA	1.76	0.65
5:B:855:PHE:HD1	5:B:856:PHE:N	1.95	0.65
5:B:882:THR:O	5:B:883:LEU:C	2.39	0.65
5:B:1087:PHE:HD2	5:B:1087:PHE:C	2.05	0.65
6:C:164:ALA:HB2	6:C:171:GLY:CA	2.27	0.65
4:A:587:HIS:CE1	4:A:969:GLN:HG3	2.32	0.65
4:A:1171:GLN:N	4:A:1172:LEU:CB	2.59	0.65
5:B:346:GLU:H	5:B:349:ILE:HD13	1.61	0.65
5:B:1099:VAL:C	5:B:1101:ASP:H	2.05	0.65
11:J:44:TYR:N	11:J:44:TYR:CD2	2.38	0.65
5:B:915:THR:HB	5:B:934:LYS:HB3	1.79	0.65
4:A:214:ILE:HG22	4:A:215:SER:H	1.62	0.65
16:A:2003[A]:UTP:O2	16:A:2003[A]:UTP:H2'	1.97	0.65
6:C:262:LEU:HD11	12:K:87:LEU:HD23	1.79	0.65
9:H:2:SER:N	9:H:3:ASN:O	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:22:DT:H2'	2:T:23:DC:H6	1.61	0.65
4:A:299:HIS:O	4:A:301:ALA:N	2.30	0.65
4:A:323:LYS:HG2	4:A:324:SER:N	2.12	0.64
5:B:708:GLU:O	5:B:710:LEU:N	2.30	0.64
5:B:845:SER:O	5:B:847:ASP:N	2.30	0.64
5:B:1055:ILE:O	5:B:1058:LEU:N	2.30	0.64
4:A:214:ILE:HG22	4:A:215:SER:N	2.11	0.64
5:B:278:GLN:HG2	5:B:279:ASP:H	1.61	0.64
5:B:341:LEU:HB2	5:B:342:GLY:CA	2.24	0.64
5:B:773:MET:CE	5:B:981:ALA:CB	2.75	0.64
4:A:22:PHE:HB2	5:B:1211:ASN:OD1	1.98	0.64
5:B:710:LEU:HD11	5:B:732:SER:O	1.96	0.64
1:R:9:G:P	5:B:776:GLN:HE22	2.21	0.64
4:A:744:LYS:O	4:A:748:MET:HB2	1.97	0.64
1:R:5:A:C5'	5:B:476:ARG:NH1	2.59	0.64
4:A:1443:VAL:O	4:A:1444:MET:HB3	1.97	0.64
5:B:710:LEU:O	5:B:711:GLU:HG2	1.97	0.64
5:B:957:ASN:HD22	5:B:958:GLN:H	1.46	0.64
4:A:691:LEU:CD1	4:A:695:LYS:HD3	2.28	0.64
4:A:1219:THR:HG21	4:A:1271:ILE:CD1	2.27	0.64
4:A:1364:ASN:C	4:A:1364:ASN:ND2	2.53	0.64
1:R:7:A:O2'	1:R:8:G:H5'	1.98	0.64
5:B:483:LEU:HG	5:B:484:ASN:H	1.63	0.64
5:B:705:MET:HA	5:B:705:MET:CE	2.26	0.64
5:B:834:ASN:HB3	5:B:840:ILE:CD1	2.26	0.64
5:B:836:GLU:O	5:B:838:SER:N	2.30	0.64
11:J:12:LYS:O	11:J:14:VAL:N	2.31	0.64
4:A:868:TYR:CE1	4:A:1064:VAL:HG11	2.31	0.64
5:B:709:ASP:O	5:B:710:LEU:HD22	1.96	0.64
5:B:494:HIS:HA	5:B:497:ARG:HE	1.63	0.64
5:B:1097:HIS:O	5:B:1098:MET:CG	2.32	0.64
4:A:117:GLU:H	4:A:118:HIS:C	2.06	0.63
5:B:102:VAL:HG21	5:B:122:LEU:HD13	1.80	0.63
5:B:1012:ILE:CG1	5:B:1013:ASN:H	1.98	0.63
5:B:1106:ARG:HD2	5:B:1126:GLY:O	1.98	0.63
6:C:167:HIS:CD2	6:C:169:LYS:HG2	2.33	0.63
11:J:36:LEU:CB	11:J:47:ARG:HH21	2.10	0.63
5:B:333:PHE:CA	5:B:334:ILE:CB	2.75	0.63
5:B:979:LYS:HE3	5:B:987:LYS:HD2	1.81	0.63
7:E:177:ARG:HG2	7:E:215:MET:SD	2.38	0.63
11:J:64:ASN:N	11:J:65:PRO:CD	2.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:782:ARG:NH1	4:A:785:PRO:HA	2.13	0.63
5:B:140:ILE:CA	5:B:141:ASP:C	2.71	0.63
5:B:708:GLU:C	5:B:710:LEU:H	2.07	0.63
4:A:901:LEU:HG	4:A:926:GLN:HE21	1.63	0.63
16:A:2003[A]:UTP:H5'2	16:A:2003[A]:UTP:C5	2.27	0.63
1:R:4:G:H2'	1:R:5:A:H8	1.64	0.63
4:A:469:ARG:NH1	4:A:469:ARG:HB3	2.12	0.63
4:A:1171:GLN:H	4:A:1172:LEU:CA	2.11	0.63
5:B:332:ASP:C	5:B:334:ILE:HB	2.24	0.63
4:A:565:ILE:HG12	4:A:567:LYS:HZ1	1.64	0.63
5:B:843:GLN:NE2	5:B:847:ASP:OD1	2.32	0.63
4:A:1041:ALA:O	4:A:1043:ASP:N	2.31	0.63
1:R:5:A:H2	1:R:6:G:C4	2.13	0.63
4:A:404:TYR:N	4:A:404:TYR:CD1	2.65	0.63
5:B:654:ARG:H	5:B:657:HIS:HD2	1.45	0.63
4:A:253:ASN:HD22	4:A:253:ASN:N	1.94	0.62
5:B:475:SER:O	5:B:477:ALA:N	2.31	0.62
6:C:235:VAL:HG12	11:J:13:VAL:HG22	1.80	0.62
13:L:32:ALA:HB3	13:L:55:ILE:HD12	1.81	0.62
4:A:1004:ASN:ND2	7:E:167:ARG:HD2	2.13	0.62
5:B:882:THR:O	5:B:884:ARG:N	2.32	0.62
6:C:180:TYR:OH	6:C:188:HIS:CD2	2.52	0.62
4:A:447:GLN:HA	4:A:448:PRO:C	2.24	0.62
5:B:1072:MET:CE	5:B:1085:ILE:HB	2.28	0.62
4:A:466:SER:HB2	5:B:1103:ILE:CD1	2.29	0.62
5:B:516:ASN:H	5:B:516:ASN:ND2	1.97	0.62
5:B:1036:ALA:O	11:J:47:ARG:NH1	2.33	0.62
5:B:1119:VAL:O	5:B:1126:GLY:HA2	1.99	0.62
4:A:41:MET:HB2	4:A:49:LYS:HA	1.82	0.62
4:A:1040:GLN:CA	4:A:1041:ALA:HB3	2.28	0.62
11:J:1:MET:N	11:J:56:LEU:H	1.98	0.62
5:B:773:MET:C	5:B:775:LYS:H	2.06	0.62
1:R:8:G:N1	2:T:22:DT:O4	2.33	0.62
5:B:684:LEU:HD22	5:B:689:LEU:HD12	1.82	0.62
5:B:901:PRO:HA	5:B:949:VAL:HG12	1.82	0.62
5:B:976:ILE:O	5:B:990:ILE:HB	2.00	0.62
5:B:1208:MET:O	5:B:1211:ASN:N	2.31	0.62
11:J:64:ASN:O	11:J:65:PRO:C	2.43	0.62
4:A:370:ILE:C	4:A:372:LYS:H	2.07	0.62
5:B:276:ILE:HD13	5:B:277:LYS:H	1.64	0.62
5:B:1087:PHE:C	5:B:1087:PHE:CD2	2.78	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:630:ILE:H	4:A:630:ILE:CD1	1.97	0.61
5:B:463:THR:HB	5:B:465:ASN:HD22	1.65	0.61
5:B:1015:HIS:C	5:B:1017:ILE:H	2.08	0.61
11:J:1:MET:N	11:J:57:ILE:H	1.98	0.61
4:A:1091:SER:C	4:A:1093:LYS:H	2.08	0.61
5:B:282:ILE:HG21	5:B:382:ILE:HD11	1.82	0.61
5:B:979:LYS:CE	5:B:987:LYS:HD2	2.30	0.61
6:C:44:LEU:HD22	6:C:129:ILE:HG23	1.81	0.61
5:B:54:PHE:HA	5:B:58:THR:HB	1.82	0.61
5:B:638:PHE:CE1	5:B:743:ILE:HA	2.35	0.61
5:B:1044:ALA:O	5:B:1045:SER:O	2.19	0.61
6:C:16:ASP:C	6:C:17:ASN:HD22	2.08	0.61
11:J:3:VAL:HG11	11:J:18:TRP:HB2	1.83	0.61
5:B:773:MET:HE2	5:B:981:ALA:CB	2.31	0.61
5:B:848:ARG:NH1	11:J:8:PHE:O	2.32	0.61
4:A:351:THR:HG21	5:B:1103:ILE:CG1	2.30	0.61
9:H:116:TYR:HB2	9:H:123:MET:HB3	1.83	0.61
4:A:913:LEU:HG	4:A:915:SER:H	1.65	0.61
5:B:555:ILE:HD11	5:B:582:VAL:HG11	1.82	0.61
5:B:797:TYR:HD2	5:B:852:ARG:CB	2.14	0.61
4:A:56:PRO:C	4:A:57:ARG:HG3	2.25	0.61
5:B:1184:GLY:C	5:B:1186:ASP:H	2.09	0.61
4:A:117:GLU:C	4:A:118:HIS:O	2.44	0.60
2:T:10:DA:H61	3:N:5:DT:H3	1.49	0.60
16:A:2003[A]:UTP:C5'	16:A:2003[A]:UTP:N1	2.56	0.60
5:B:334:ILE:HG23	5:B:334:ILE:O	2.01	0.60
5:B:792:MET:HE2	5:B:855:PHE:HZ	1.65	0.60
5:B:792:MET:HE2	5:B:855:PHE:CZ	2.36	0.60
5:B:834:ASN:HB3	5:B:840:ILE:HD12	1.83	0.60
12:K:6:ARG:O	12:K:8:GLU:N	2.33	0.60
1:R:8:G:C2'	1:R:9:G:O5'	2.49	0.60
4:A:458:HIS:CE1	4:A:507:VAL:HG21	2.36	0.60
5:B:523:CYS:SG	5:B:524:PRO:HD2	2.41	0.60
5:B:640:VAL:HG22	5:B:651:LEU:HD22	1.81	0.60
6:C:56:THR:HG22	6:C:57:VAL:N	2.16	0.60
1:R:6:G:N3	1:R:7:A:C8	2.70	0.60
4:A:567:LYS:CB	4:A:568:PRO:HD2	2.32	0.60
4:A:1447:GLU:N	4:A:1448:GLU:HB3	2.15	0.60
4:A:471:ASN:OD1	4:A:472:LEU:N	2.34	0.60
4:A:768:GLN:NE2	4:A:816:HIS:ND1	2.48	0.60
1:R:8:G:N2	2:T:22:DT:N1	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:658:LEU:HD13	5:B:831:SER:HA	1.83	0.60
5:B:95:ILE:HD12	5:B:130:VAL:HG12	1.83	0.60
11:J:7:CYS:C	11:J:49:MET:HE3	2.26	0.60
4:A:320:ARG:CZ	4:A:320:ARG:H	2.14	0.60
4:A:662:PHE:CE1	4:A:663:SER:O	2.55	0.60
4:A:800:VAL:HG22	4:A:812:GLU:HB3	1.84	0.60
5:B:845:SER:C	5:B:847:ASP:H	2.10	0.60
4:A:343:LYS:NZ	5:B:1197:PRO:CG	2.65	0.60
4:A:350:ARG:HH11	4:A:350:ARG:HG3	1.67	0.60
4:A:836:TYR:CZ	4:A:840:ARG:HD2	2.36	0.60
4:A:1400:CYS:O	4:A:1405:THR:HG23	2.02	0.60
5:B:1074:ASN:OD1	5:B:1076:HIS:N	2.35	0.60
6:C:233:GLU:OE1	11:J:43:ARG:NH2	2.30	0.60
4:A:446:ARG:HB2	4:A:487:MET:CE	2.31	0.60
6:C:7:GLN:HB2	6:C:23:SER:HB2	1.83	0.60
4:A:341:MET:HE3	5:B:1135:ARG:NE	2.17	0.60
4:A:1333:ILE:O	4:A:1333:ILE:HD13	2.02	0.60
5:B:773:MET:CE	5:B:981:ALA:HB1	2.32	0.60
5:B:840:ILE:HG21	5:B:994:TYR:HD1	1.67	0.60
10:I:44:TYR:HD2	10:I:44:TYR:C	2.09	0.60
2:T:19:DT:H2'	2:T:20:DC:C6	2.37	0.59
4:A:492:PRO:HB3	4:A:497:THR:HG22	1.84	0.59
1:R:9:G:OP1	5:B:776:GLN:NE2	2.35	0.59
4:A:381:THR:HG22	4:A:382:PRO:HD2	1.83	0.59
4:A:528:LEU:HD23	4:A:751:SER:HA	1.83	0.59
4:A:868:TYR:HE1	4:A:1064:VAL:HG11	1.65	0.59
5:B:132:VAL:HG23	5:B:165:VAL:HG21	1.83	0.59
5:B:333:PHE:N	5:B:334:ILE:CG1	2.63	0.59
5:B:789:MET:HE1	5:B:967:ARG:HB2	1.85	0.59
4:A:629:LEU:HD22	4:A:633:VAL:CG2	2.32	0.59
5:B:839:MET:HE3	5:B:1010:LEU:CD1	2.32	0.59
5:B:862:GLN:HB3	5:B:963:PHE:HB2	1.83	0.59
5:B:999:MET:HE2	5:B:1008:PRO:O	2.03	0.59
5:B:1177:HIS:O	5:B:1179:GLN:N	2.36	0.59
5:B:1194:ILE:H	5:B:1194:ILE:HD13	1.67	0.59
11:J:3:VAL:HG22	11:J:4:PRO:HD2	1.84	0.59
4:A:335:ARG:HD2	5:B:1202:LEU:HD12	1.83	0.59
4:A:668:ASP:CG	4:A:742:ASN:HD22	2.10	0.59
5:B:1069:PHE:CD1	5:B:1069:PHE:N	2.66	0.59
6:C:208:GLU:HB3	6:C:209:TYR:CD1	2.36	0.59
7:E:88:VAL:HG21	7:E:112:TYR:CB	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:7:A:C2	1:R:8:G:C4	2.90	0.59
5:B:334:ILE:O	5:B:334:ILE:CG2	2.51	0.59
5:B:773:MET:HE3	5:B:981:ALA:HB2	1.84	0.59
5:B:1010:LEU:CD2	5:B:1092:TYR:CD1	2.80	0.59
1:R:6:G:O2'	1:R:7:A:H5'	2.02	0.59
4:A:780:VAL:HG12	5:B:699:GLU:OE2	2.02	0.59
5:B:781:PHE:CE2	5:B:785:TYR:HB2	2.38	0.59
5:B:845:SER:C	5:B:847:ASP:N	2.60	0.59
5:B:710:LEU:O	5:B:711:GLU:CG	2.50	0.59
5:B:1082:MET:HG2	6:C:188:HIS:O	2.03	0.59
4:A:453:MET:HG3	4:A:456:MET:CE	2.33	0.59
4:A:700:ASN:HD22	10:I:116:ASN:HD21	1.50	0.59
4:A:700:ASN:ND2	10:I:116:ASN:HD21	2.00	0.59
4:A:451:HIS:O	4:A:453:MET:N	2.35	0.58
5:B:341:LEU:CD1	5:B:343:ILE:CB	2.73	0.58
10:I:44:TYR:C	10:I:44:TYR:CD2	2.81	0.58
4:A:387:ARG:O	4:A:387:ARG:HG2	2.02	0.58
4:A:399:HIS:O	4:A:401:GLY:N	2.36	0.58
4:A:663:SER:HB2	5:B:1085:ILE:HG23	1.84	0.58
9:H:93:TYR:HD2	9:H:145:ARG:HB3	1.68	0.58
5:B:855:PHE:O	5:B:969:ARG:HA	2.02	0.58
6:C:100:THR:O	6:C:119:VAL:HG12	2.04	0.58
5:B:408:LEU:O	5:B:410:GLY:N	2.36	0.58
5:B:815:ARG:HB3	5:B:815:ARG:CZ	2.34	0.58
5:B:1166:CYS:CB	5:B:1185:CYS:SG	2.92	0.58
10:I:40:SER:C	10:I:42:LEU:H	2.12	0.58
10:I:73:ARG:O	10:I:81:ARG:HG2	2.03	0.58
11:J:28:ASP:O	11:J:30:LEU:HD12	2.04	0.58
4:A:399:HIS:O	4:A:400:PRO:C	2.41	0.58
4:A:541:ILE:HG22	4:A:545:GLN:HE22	1.68	0.58
4:A:871:ASP:OD1	4:A:1366:ARG:NH2	2.37	0.58
4:A:901:LEU:H	4:A:926:GLN:NE2	2.02	0.58
4:A:1436:ILE:O	4:A:1438:THR:N	2.36	0.58
5:B:25:ILE:HG23	5:B:29:ASP:CB	2.33	0.58
10:I:58:VAL:HA	10:I:62:ILE:HD12	1.85	0.58
4:A:298:PHE:CG	4:A:298:PHE:O	2.57	0.58
4:A:981:LEU:HD21	4:A:1039:LYS:HA	1.84	0.58
4:A:1171:GLN:CA	4:A:1172:LEU:HB2	2.33	0.58
6:C:142:VAL:N	11:J:16:ASP:HB3	2.08	0.58
4:A:392:VAL:HG13	4:A:415:LEU:HD22	1.86	0.58
4:A:1064:VAL:HG12	4:A:1370:LEU:HD22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1084:PHE:CZ	4:A:1093:LYS:HA	2.39	0.58
5:B:653:VAL:HG13	5:B:689:LEU:HB3	1.85	0.58
11:J:22:LEU:O	11:J:26:GLN:HB2	2.03	0.58
11:J:24:LEU:HD12	11:J:24:LEU:N	2.19	0.58
4:A:269:ILE:HG22	4:A:299:HIS:HB2	1.86	0.58
4:A:963:ILE:HG22	4:A:1045:VAL:HG22	1.84	0.58
6:C:84:ARG:HD3	12:K:11:LEU:HD11	1.84	0.58
4:A:404:TYR:CD2	4:A:412:ARG:HD3	2.37	0.57
4:A:534:LEU:O	4:A:534:LEU:HG	2.03	0.57
5:B:416:LEU:HD23	5:B:420:LEU:HD12	1.85	0.57
5:B:836:GLU:O	5:B:837:ASP:C	2.47	0.57
9:H:137:GLN:O	9:H:139:ASN:N	2.35	0.57
5:B:25:ILE:HG22	5:B:26:THR:O	2.03	0.57
11:J:12:LYS:O	11:J:13:VAL:C	2.47	0.57
6:C:57:VAL:CG1	11:J:60:PHE:HB2	2.32	0.57
4:A:512:VAL:HA	4:A:519:PRO:HA	1.86	0.57
4:A:1119:TYR:HD1	4:A:1326:ARG:HB2	1.69	0.57
5:B:1084:GLN:HE21	6:C:189:THR:HG22	1.68	0.57
4:A:1004:ASN:CG	7:E:167:ARG:HD2	2.30	0.57
4:A:1162:VAL:HG11	10:I:41:PRO:HG2	1.85	0.57
5:B:753:ALA:C	5:B:755:ILE:H	2.11	0.57
11:J:1:MET:H1	11:J:57:ILE:H	1.52	0.57
1:R:7:A:C2	1:R:8:G:C5	2.92	0.57
4:A:57:ARG:C	4:A:68:GLN:HG2	2.28	0.57
4:A:567:LYS:O	4:A:568:PRO:C	2.46	0.57
4:A:1155:ASP:OD1	4:A:1162:VAL:HG23	2.05	0.57
5:B:35:SER:HG	5:B:811:TYR:HE2	1.52	0.57
5:B:764:SER:N	5:B:765:PRO:HD2	2.17	0.57
5:B:778:MET:HE1	5:B:1094:ARG:HH11	1.68	0.57
4:A:11:LEU:HA	5:B:1193:GLN:O	2.05	0.57
4:A:298:PHE:HD2	4:A:302:THR:HB	1.69	0.57
4:A:423:ASP:O	4:A:424:ILE:HB	2.04	0.57
4:A:1446:ASP:O	4:A:1447:GLU:CG	2.45	0.57
11:J:44:TYR:O	11:J:48:ARG:N	2.37	0.57
2:T:21:DC:H2'	2:T:22:DT:H6	1.69	0.57
4:A:47:ARG:CZ	4:A:47:ARG:HA	2.35	0.57
4:A:218:ASP:H	4:A:219:PHE:CB	2.17	0.57
4:A:366:VAL:HG22	4:A:468:PHE:HE2	1.70	0.57
4:A:668:ASP:OD2	4:A:742:ASN:ND2	2.31	0.57
5:B:254:LEU:HD22	5:B:361:LEU:HD11	1.86	0.57
5:B:1180:PHE:O	5:B:1181:GLU:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:56:THR:HG22	6:C:57:VAL:H	1.68	0.57
12:K:39:ASP:OD1	12:K:39:ASP:N	2.38	0.57
13:L:55:ILE:O	13:L:56:LEU:HB2	2.04	0.57
4:A:875:ALA:HB2	4:A:1366:ARG:HD3	1.87	0.57
4:A:1384:VAL:HG23	4:A:1384:VAL:O	2.03	0.57
5:B:428:ILE:O	5:B:432:MET:HB2	2.04	0.57
5:B:1096:ARG:HG3	5:B:1097:HIS:CD2	2.39	0.57
6:C:11:ARG:HD3	6:C:209:TYR:OH	2.05	0.57
6:C:58:LEU:HD12	6:C:145:CYS:SG	2.45	0.57
1:R:8:G:H2'	1:R:9:G:H8	1.69	0.57
1:R:6:G:N3	1:R:7:A:N7	2.53	0.56
4:A:447:GLN:HG2	5:B:1134:GLU:OE2	2.05	0.56
4:A:1353:TYR:C	4:A:1355:VAL:H	2.12	0.56
11:J:43:ARG:C	11:J:47:ARG:HG3	2.29	0.56
4:A:265:LYS:C	4:A:267:ALA:H	2.13	0.56
4:A:452:LYS:N	4:A:1070:GLN:OE1	2.37	0.56
5:B:345:LYS:CA	5:B:346:GLU:HB3	2.29	0.56
5:B:773:MET:CE	5:B:981:ALA:HB2	2.35	0.56
6:C:166:GLU:HG3	12:K:10:PHE:HZ	1.69	0.56
1:R:4:G:H2'	1:R:5:A:C8	2.40	0.56
4:A:587:HIS:HE1	4:A:969:GLN:HG3	1.68	0.56
4:A:1006:ILE:HD11	7:E:167:ARG:HB2	1.87	0.56
4:A:1116:LEU:HD13	4:A:1329:THR:OG1	2.05	0.56
4:A:1389:PHE:O	4:A:1392:SER:HB3	2.05	0.56
5:B:337:ARG:HB2	5:B:340:ALA:CB	2.35	0.56
5:B:647:GLY:CA	5:B:648:HIS:HB2	2.14	0.56
5:B:757:PRO:HG3	5:B:983:ARG:CZ	2.35	0.56
5:B:778:MET:HE1	5:B:1094:ARG:NH1	2.20	0.56
5:B:1013:ASN:O	5:B:1014:PRO:C	2.48	0.56
6:C:196:ASP:O	6:C:200:GLU:HB2	2.05	0.56
4:A:807:GLY:HA3	5:B:728:ARG:NH2	2.20	0.56
5:B:208:SER:OG	5:B:210:LYS:NZ	2.38	0.56
5:B:1033:LYS:CD	11:J:44:TYR:HE1	2.19	0.56
9:H:84:ALA:HA	9:H:87:ARG:HB2	1.86	0.56
12:K:52:ASN:N	12:K:52:ASN:HD22	2.02	0.56
4:A:23:SER:O	4:A:27:VAL:HG23	2.06	0.56
5:B:63:ILE:O	5:B:67:SER:HB3	2.05	0.56
5:B:769:TYR:H	5:B:769:TYR:HD2	1.53	0.56
5:B:1159:ARG:HG3	5:B:1193:GLN:OE1	2.06	0.56
6:C:37:MET:C	6:C:41:ILE:HD11	2.30	0.56
11:J:41:LEU:CB	11:J:47:ARG:HG2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:8:G:N1	2:T:22:DT:N3	2.49	0.56
1:R:10:A:H2	2:T:19:DT:O2	1.88	0.56
4:A:218:ASP:H	4:A:219:PHE:HB3	1.70	0.56
4:A:341:MET:CE	5:B:1135:ARG:CZ	2.83	0.56
5:B:197:PHE:CD1	5:B:817:LEU:HD11	2.41	0.56
5:B:411:PRO:HA	5:B:414:ALA:HB3	1.88	0.56
5:B:711:GLU:HG3	5:B:711:GLU:O	2.06	0.56
4:A:256:GLN:HG3	4:A:257:ARG:H	1.69	0.56
4:A:409:SER:O	4:A:411:ASP:N	2.31	0.56
4:A:1197:LEU:CD1	4:A:1209:MET:HE1	2.31	0.56
5:B:743:ILE:O	5:B:744:HIS:CB	2.54	0.56
6:C:37:MET:O	6:C:41:ILE:CD1	2.52	0.56
4:A:1444:MET:CG	4:A:1445:ILE:N	2.52	0.56
4:A:345:VAL:HG22	5:B:1128:LEU:O	2.06	0.56
5:B:344:LYS:C	5:B:346:GLU:HB3	2.30	0.56
5:B:797:TYR:HD2	5:B:852:ARG:HB2	1.70	0.56
4:A:117:GLU:H	4:A:118:HIS:HB2	1.71	0.56
4:A:754:SER:H	4:A:757:ASN:HD22	1.53	0.56
4:A:849:MET:HB3	4:A:1063:MET:SD	2.46	0.56
5:B:400:HIS:CE1	5:B:517:THR:HG21	2.42	0.56
5:B:807:ARG:HB2	5:B:1045:SER:OG	2.06	0.56
6:C:43:THR:HG22	6:C:44:LEU:H	1.71	0.56
5:B:770:GLN:NE2	5:B:1093:GLN:HE22	2.04	0.55
5:B:778:MET:HE3	5:B:1094:ARG:CD	2.31	0.55
1:R:10:A:H2	2:T:19:DT:C2	2.23	0.55
4:A:131:SER:HB3	4:A:223:GLY:HA2	1.88	0.55
5:B:458:LYS:O	5:B:462:ALA:HB2	2.05	0.55
5:B:797:TYR:CD2	5:B:852:ARG:HB3	2.42	0.55
9:H:2:SER:HB2	9:H:3:ASN:HB3	1.76	0.55
4:A:15:LYS:HE2	5:B:1220:ARG:HG2	1.88	0.55
4:A:246:VAL:O	4:A:246:VAL:HG12	2.06	0.55
4:A:341:MET:HE3	5:B:1135:ARG:CZ	2.37	0.55
4:A:456:MET:HB2	4:A:478:TYR:OH	2.07	0.55
4:A:896:ARG:NH2	4:A:1030:ARG:HH21	2.04	0.55
4:A:1063:MET:HG2	4:A:1436:ILE:HG23	1.85	0.55
4:A:350:ARG:HG3	4:A:350:ARG:NH1	2.21	0.55
5:B:102:VAL:HG12	5:B:110:HIS:HB3	1.89	0.55
12:K:45:LEU:HG	12:K:94:ILE:HD13	1.88	0.55
1:R:2:U:H2'	1:R:3:C:H6	1.68	0.55
2:T:20:DC:H4'	4:A:447:GLN:NE2	2.22	0.55
4:A:265:LYS:HG2	4:A:303:TYR:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:590:ARG:NH2	4:A:620:LYS:O	2.38	0.55
6:C:239:PRO:O	6:C:241:ASP:N	2.40	0.55
6:C:241:ASP:O	6:C:245:VAL:HG23	2.07	0.55
8:F:93:ILE:CD1	8:F:134:ILE:HD11	2.33	0.55
4:A:474:VAL:HG23	4:A:521:MET:HE2	1.88	0.55
5:B:63:ILE:HG22	5:B:64:CYS:N	2.21	0.55
5:B:1212:ILE:O	5:B:1214:PRO:HD3	2.06	0.55
5:B:334:ILE:HG22	5:B:348:ARG:HG3	1.89	0.55
6:C:37:MET:CA	6:C:41:ILE:HD11	2.37	0.55
6:C:73:GLN:NE2	6:C:237:SER:O	2.40	0.55
1:R:8:G:N2	2:T:22:DT:C4	2.74	0.55
4:A:691:LEU:HD13	4:A:695:LYS:HD3	1.89	0.55
5:B:913:GLY:HA2	5:B:938:SER:OG	2.07	0.55
5:B:1007:VAL:CG2	5:B:1008:PRO:HD2	2.37	0.55
1:R:5:A:N1	1:R:6:G:C6	2.74	0.55
5:B:341:LEU:CB	5:B:342:GLY:CA	2.83	0.55
5:B:343:ILE:O	5:B:345:LYS:HG3	2.07	0.55
5:B:773:MET:C	5:B:775:LYS:N	2.64	0.55
5:B:848:ARG:CD	11:J:8:PHE:HA	2.36	0.55
5:B:1087:PHE:HD2	5:B:1088:GLY:N	2.05	0.55
4:A:360:GLU:CD	4:A:360:GLU:N	2.63	0.54
4:A:445:ASN:HA	4:A:454:SER:O	2.07	0.54
6:C:148:ARG:H	6:C:151:GLN:HG3	1.72	0.54
12:K:92:ASN:O	12:K:95:ILE:HB	2.06	0.54
1:R:9:G:P	5:B:776:GLN:NE2	2.80	0.54
4:A:42:ASP:OD2	4:A:45:GLN:HA	2.06	0.54
4:A:1006:ILE:HG13	4:A:1007:ILE:HD12	1.90	0.54
5:B:341:LEU:HD12	5:B:343:ILE:HB	1.86	0.54
4:A:351:THR:O	4:A:486:GLU:HB2	2.08	0.54
5:B:777:ALA:HA	5:B:1095:LEU:HA	1.89	0.54
5:B:1106:ARG:CZ	5:B:1109:GLY:N	2.66	0.54
6:C:164:ALA:HB2	6:C:171:GLY:N	2.23	0.54
2:T:5:DC:H2"	2:T:6:DG:C8	2.43	0.54
4:A:353:ILE:HG21	4:A:487:MET:SD	2.48	0.54
4:A:608:ILE:O	4:A:608:ILE:HG22	2.07	0.54
5:B:261:ARG:N	5:B:264:SER:HB3	2.22	0.54
5:B:336:ARG:O	5:B:337:ARG:O	2.25	0.54
8:F:147:SER:C	8:F:149:GLU:N	2.66	0.54
10:I:106:CYS:SG	10:I:108:HIS:HB3	2.47	0.54
4:A:527:THR:HG21	4:A:650:GLN:HG2	1.89	0.54
5:B:235:SER:HG	5:B:236:HIS:HD1	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1050:ILE:HG23	5:B:1055:ILE:CD1	2.37	0.54
10:I:63:GLY:HA3	10:I:104:LEU:HD11	1.89	0.54
4:A:49:LYS:HZ1	4:A:61:ILE:H	1.56	0.54
4:A:120:GLU:O	4:A:121:LEU:HB2	2.07	0.54
5:B:343:ILE:HG13	5:B:344:LYS:N	2.18	0.54
5:B:639:ILE:HD11	5:B:691:GLU:HB2	1.90	0.54
5:B:764:SER:N	5:B:765:PRO:CD	2.71	0.54
5:B:1072:MET:HE3	5:B:1085:ILE:HB	1.89	0.54
6:C:235:VAL:CG1	11:J:13:VAL:HG22	2.38	0.54
4:A:629:LEU:HD22	4:A:633:VAL:HG23	1.90	0.54
5:B:54:PHE:HE1	5:B:414:ALA:HA	1.72	0.54
5:B:123:THR:HG23	5:B:205:ILE:HA	1.88	0.54
4:A:215:SER:HB3	4:A:218:ASP:OD2	2.08	0.54
4:A:366:VAL:HG22	4:A:468:PHE:CE2	2.43	0.54
4:A:608:ILE:O	4:A:609:ASP:HB3	2.07	0.54
4:A:704:ALA:N	4:A:705:LYS:HA	2.19	0.54
4:A:966:ASN:HB3	4:A:1044:TRP:HH2	1.73	0.54
5:B:44:VAL:HG11	5:B:495:LEU:HD22	1.89	0.54
5:B:341:LEU:HB2	5:B:343:ILE:N	2.23	0.54
5:B:774:GLY:HA2	5:B:777:ALA:HB3	1.90	0.54
6:C:209:TYR:CD1	6:C:209:TYR:N	2.76	0.54
7:E:28:TYR:HA	7:E:64:PRO:HA	1.90	0.54
7:E:77:SER:HB3	7:E:105:PHE:HA	1.89	0.54
9:H:2:SER:N	9:H:3:ASN:C	2.66	0.54
4:A:907:THR:HG21	4:A:920:LEU:HD23	1.90	0.54
5:B:259:TYR:HB2	5:B:268:THR:HG23	1.89	0.54
5:B:708:GLU:C	5:B:710:LEU:N	2.66	0.54
12:K:24:ASP:HB3	12:K:30:ALA:HB3	1.90	0.54
2:T:21:DC:H2'	2:T:22:DT:C6	2.43	0.54
4:A:740:LEU:O	6:C:192:TRP:CD1	2.61	0.54
5:B:103:ASN:ND2	5:B:169:ARG:HH22	2.02	0.54
2:T:18:DA:H2'	2:T:19:DT:C6	2.43	0.53
4:A:54:ASN:N	4:A:54:ASN:ND2	2.52	0.53
4:A:182:VAL:HG12	4:A:183:GLY:H	1.73	0.53
4:A:768:GLN:HB3	4:A:775:ILE:HD11	1.90	0.53
4:A:853:ASP:CG	4:A:855:THR:HG22	2.33	0.53
5:B:982:SER:N	5:B:1092:TYR:CE2	2.76	0.53
6:C:62:PHE:O	6:C:63:ILE:C	2.50	0.53
4:A:879:GLU:OE2	4:A:962:ARG:NH2	2.31	0.53
5:B:140:ILE:CB	5:B:141:ASP:CA	2.70	0.53
5:B:1051:THR:O	5:B:1055:ILE:HD13	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:134:ILE:HD12	6:C:141:GLY:H	1.72	0.53
6:C:166:GLU:O	12:K:6:ARG:CZ	2.56	0.53
10:I:106:CYS:SG	10:I:108:HIS:CB	2.96	0.53
4:A:341:MET:SD	4:A:1428:VAL:HG11	2.49	0.53
4:A:346:ASP:H	5:B:1154:ALA:HB1	1.73	0.53
4:A:662:PHE:HE1	4:A:742:ASN:HB3	1.73	0.53
4:A:901:LEU:HA	4:A:907:THR:HG22	1.88	0.53
4:A:1025:ARG:HG2	4:A:1025:ARG:NH1	2.21	0.53
6:C:98:VAL:H	6:C:122:SER:HB2	1.73	0.53
4:A:944:ARG:HE	4:A:1298:TYR:HE1	1.56	0.53
5:B:764:SER:OG	5:B:765:PRO:HD3	2.07	0.53
11:J:46:CYS:O	11:J:49:MET:HB2	2.09	0.53
4:A:50:ILE:O	4:A:56:PRO:HD3	2.09	0.53
5:B:1031:LEU:HD12	5:B:1031:LEU:C	2.30	0.53
6:C:106:GLU:HA	6:C:106:GLU:OE2	2.08	0.53
4:A:809:THR:HG23	5:B:730:ARG:HH21	1.73	0.53
5:B:833:TYR:OH	12:K:66:PRO:CG	2.57	0.53
9:H:135:LEU:O	9:H:137:GLN:N	2.41	0.53
11:J:53:HIS:CE1	11:J:55:ASP:OD1	2.59	0.53
12:K:6:ARG:C	12:K:8:GLU:H	2.17	0.53
1:R:7:A:N1	1:R:8:G:C5	2.77	0.53
4:A:95:PHE:HE2	4:A:1414:ALA:HB2	1.73	0.53
4:A:719:VAL:HG12	4:A:723:ASN:HD21	1.73	0.53
4:A:1444:MET:O	8:F:133:VAL:N	2.41	0.53
5:B:647:GLY:HA3	5:B:648:HIS:HB3	1.82	0.53
7:E:199:ILE:O	7:E:199:ILE:HG22	2.09	0.53
5:B:558:LEU:C	5:B:560:GLU:H	2.17	0.53
5:B:753:ALA:O	5:B:755:ILE:N	2.39	0.53
4:A:370:ILE:C	4:A:372:LYS:N	2.67	0.53
4:A:589:GLN:HB3	4:A:961:ARG:NH2	2.23	0.53
4:A:845:LEU:O	4:A:847:ASP:N	2.42	0.53
5:B:333:PHE:HB3	5:B:334:ILE:HA	1.91	0.53
5:B:370:PHE:O	5:B:372:SER:N	2.42	0.53
5:B:416:LEU:HD22	5:B:457:LEU:HD23	1.90	0.53
5:B:754:SER:C	5:B:755:ILE:HG12	2.33	0.53
7:E:14:ARG:HB3	7:E:141:VAL:O	2.09	0.53
4:A:567:LYS:HB3	9:H:96:VAL:N	2.17	0.53
5:B:1081:LEU:O	5:B:1083:ALA:N	2.42	0.53
4:A:836:TYR:CE2	4:A:840:ARG:HD2	2.44	0.52
4:A:1209:MET:HE2	4:A:1209:MET:HA	1.91	0.52
5:B:329:THR:HA	5:B:332:ASP:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1085:ILE:O	5:B:1086:PHE:C	2.52	0.52
5:B:1086:PHE:HD2	5:B:1087:PHE:N	2.07	0.52
6:C:177:GLU:HG3	6:C:231:ASN:HD22	1.74	0.52
7:E:37:LEU:HD22	7:E:42:PHE:HB2	1.90	0.52
11:J:1:MET:H1	11:J:57:ILE:N	2.07	0.52
11:J:56:LEU:C	11:J:58:GLU:N	2.62	0.52
4:A:650:GLN:O	4:A:654:ASN:HB2	2.08	0.52
5:B:463:THR:CB	5:B:465:ASN:HD22	2.22	0.52
6:C:124:LEU:C	6:C:126:GLY:N	2.62	0.52
6:C:252:GLN:HE21	12:K:95:ILE:HG23	1.74	0.52
1:R:7:A:N1	1:R:8:G:C6	2.77	0.52
4:A:751:SER:OG	5:B:1015:HIS:CE1	2.63	0.52
4:A:1058:VAL:O	4:A:1060:PRO:HD3	2.09	0.52
7:E:64:PRO:HG3	7:E:76:GLY:HA2	1.90	0.52
2:T:22:DT:H2'	2:T:23:DC:C6	2.44	0.52
4:A:328:ARG:HD3	5:B:1206:GLU:OE1	2.09	0.52
4:A:856:THR:O	4:A:864:ILE:HG12	2.10	0.52
4:A:959:ASN:HD22	4:A:962:ARG:NH2	2.08	0.52
5:B:746:SER:HB2	5:B:1046:PRO:HG2	1.92	0.52
4:A:737:LEU:HD22	4:A:741:ASN:ND2	2.24	0.52
6:C:180:TYR:OH	6:C:188:HIS:HD2	1.93	0.52
4:A:68:GLN:O	4:A:68:GLN:CD	2.53	0.52
4:A:827:THR:CG2	4:A:828:ALA:N	2.72	0.52
4:A:1394:THR:HB	4:A:1399:ARG:HD3	1.92	0.52
10:I:45:ARG:HE	10:I:47:GLU:HG2	1.74	0.52
5:B:757:PRO:CG	5:B:1028:GLU:OE2	2.46	0.52
5:B:1055:ILE:O	5:B:1056:SER:C	2.52	0.52
6:C:57:VAL:CG1	11:J:60:PHE:HD2	2.23	0.52
4:A:423:ASP:CG	4:A:424:ILE:N	2.64	0.52
4:A:1042:PHE:O	4:A:1045:VAL:N	2.43	0.52
4:A:1153:TYR:HB2	4:A:1192:LEU:HD23	1.90	0.52
5:B:1174:LYS:O	5:B:1177:HIS:O	2.28	0.52
5:B:1206:GLU:O	5:B:1210:MET:HB2	2.10	0.52
11:J:41:LEU:HB3	11:J:47:ARG:HG2	1.92	0.52
4:A:116:ASP:HA	4:A:117:GLU:HB2	1.85	0.52
5:B:402:GLY:HA3	5:B:695:ALA:HB3	1.92	0.52
5:B:778:MET:CE	5:B:1094:ARG:HH11	2.22	0.52
4:A:503:GLN:OE1	4:A:503:GLN:HA	2.10	0.52
5:B:104:GLU:OE1	13:L:54:ARG:NH1	2.43	0.52
5:B:826:ALA:O	5:B:828:ALA:N	2.38	0.52
4:A:862:ASN:OD1	7:E:174:GLN:HA	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:343:ILE:H	5:B:345:LYS:NZ	2.08	0.51
4:A:133:LYS:HE3	4:A:1391:ARG:NH1	2.19	0.51
5:B:248:SER:H	5:B:418:LYS:HE3	1.75	0.51
5:B:834:ASN:HD21	5:B:1013:ASN:ND2	2.05	0.51
5:B:1060:ARG:HB2	5:B:1066:SER:HB3	1.91	0.51
6:C:124:LEU:O	6:C:126:GLY:N	2.43	0.51
2:T:26:DG:H4'	5:B:462:ALA:HB1	1.91	0.51
4:A:64:ASN:C	4:A:66:LYS:H	2.18	0.51
5:B:336:ARG:O	5:B:340:ALA:HB3	2.10	0.51
5:B:825:VAL:HA	5:B:1010:LEU:HB3	1.91	0.51
5:B:906:SER:O	5:B:909:ASP:OD2	2.27	0.51
1:R:6:G:C2	1:R:7:A:C5	2.98	0.51
4:A:116:ASP:CA	4:A:117:GLU:CB	2.71	0.51
5:B:1156:ASP:HB3	5:B:1197:PRO:HA	1.92	0.51
7:E:61:GLN:HB2	7:E:79:TRP:HE3	1.75	0.51
10:I:32:CYS:O	10:I:33:SER:HB2	2.10	0.51
11:J:3:VAL:HG23	11:J:53:HIS:CE1	2.46	0.51
4:A:35:ILE:CG2	4:A:84:ILE:HD12	2.40	0.51
4:A:312:PRO:C	4:A:313:GLN:HE21	2.17	0.51
4:A:381:THR:HG21	4:A:383:TYR:CD1	2.45	0.51
4:A:672:ASP:HB2	4:A:736:ASN:HD21	1.76	0.51
5:B:386:LEU:C	5:B:388:CYS:H	2.18	0.51
5:B:1043:ASP:O	5:B:1050:ILE:HD13	2.10	0.51
4:A:596:THR:C	4:A:598:LEU:H	2.19	0.51
4:A:669:THR:HG21	4:A:761:MET:HG3	1.92	0.51
4:A:1040:GLN:N	4:A:1041:ALA:CA	2.74	0.51
4:A:1072:ILE:HD11	4:A:1368:MET:HA	1.92	0.51
12:K:38:GLU:O	12:K:71:PHE:HD2	1.94	0.51
4:A:91:PHE:HA	4:A:235:ILE:HG22	1.92	0.51
4:A:1171:GLN:H	4:A:1172:LEU:C	2.19	0.51
5:B:46:GLN:OE1	5:B:47:GLN:N	2.43	0.51
5:B:364:ILE:O	5:B:365:THR:HB	2.10	0.51
5:B:769:TYR:N	5:B:769:TYR:CD2	2.79	0.51
11:J:5:VAL:CG1	11:J:6:ARG:H	2.07	0.51
4:A:55:ASP:O	4:A:57:ARG:N	2.44	0.51
4:A:323:LYS:HG2	4:A:324:SER:H	1.76	0.51
4:A:1410:PHE:CD2	5:B:1212:ILE:HD11	2.40	0.51
4:A:1448:GLU:CG	4:A:1449:SER:N	2.73	0.51
5:B:37:PHE:O	5:B:38:PHE:HB2	2.11	0.51
5:B:757:PRO:HG3	5:B:983:ARG:NH2	2.26	0.51
5:B:1069:PHE:HA	5:B:1086:PHE:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:116:TYR:HE2	9:H:140:ALA:CB	2.24	0.51
11:J:23:ASN:HB3	11:J:24:LEU:HD12	1.92	0.51
4:A:116:ASP:HA	4:A:117:GLU:CB	2.41	0.51
4:A:218:ASP:HB2	4:A:219:PHE:HB2	1.93	0.51
5:B:637:LEU:HA	5:B:743:ILE:HD11	1.93	0.51
5:B:1015:HIS:C	5:B:1017:ILE:N	2.69	0.51
5:B:1121:GLY:O	5:B:1122:ARG:C	2.53	0.51
6:C:52:GLU:HA	13:L:64:LEU:HD22	1.93	0.51
9:H:62:SER:OG	9:H:63:LEU:N	2.43	0.51
9:H:123:MET:HE2	9:H:142:LEU:HD13	1.91	0.51
1:R:8:G:N2	2:T:22:DT:C6	2.79	0.51
4:A:482:PHE:C	4:A:484:GLY:H	2.19	0.51
4:A:650:GLN:HB3	4:A:654:ASN:ND2	2.26	0.51
4:A:896:ARG:HD2	4:A:897:TYR:CE1	2.45	0.51
5:B:475:SER:C	5:B:477:ALA:N	2.69	0.51
5:B:783:THR:HB	11:J:63:TYR:OH	2.11	0.51
4:A:349:ALA:HB1	4:A:370:ILE:HD13	1.92	0.50
4:A:662:PHE:CG	4:A:663:SER:N	2.79	0.50
4:A:709:THR:HG21	10:I:93:LYS:O	2.11	0.50
4:A:53:LEU:O	4:A:54:ASN:C	2.54	0.50
5:B:797:TYR:CD2	5:B:852:ARG:CB	2.95	0.50
2:T:20:DC:H2'	2:T:21:DC:O4'	2.11	0.50
5:B:408:LEU:C	5:B:410:GLY:N	2.67	0.50
5:B:542:MET:HE1	5:B:743:ILE:HB	1.91	0.50
5:B:1196:ILE:HD12	5:B:1200:ALA:HB3	1.92	0.50
7:E:65:THR:C	7:E:67:GLU:H	2.19	0.50
4:A:92:HIS:HE1	5:B:1211:ASN:HB3	1.76	0.50
4:A:848:ILE:HG22	4:A:856:THR:HG22	1.94	0.50
5:B:885:MET:HE2	5:B:885:MET:N	2.26	0.50
5:B:969:ARG:NH1	6:C:61:GLU:OE1	2.45	0.50
7:E:23:VAL:HG12	7:E:30:ILE:HD11	1.93	0.50
1:R:10:A:H2	2:T:19:DT:N3	2.09	0.50
4:A:346:ASP:HB2	5:B:1154:ALA:CB	2.40	0.50
4:A:578:LEU:C	4:A:580:VAL:H	2.19	0.50
4:A:776:ALA:O	4:A:778:GLY:N	2.44	0.50
4:A:1447:GLU:HA	4:A:1448:GLU:HB3	1.61	0.50
5:B:398:ARG:HB3	5:B:398:ARG:HH11	1.76	0.50
5:B:545:ILE:HG23	5:B:631:GLY:HA2	1.94	0.50
7:E:127:ILE:O	7:E:127:ILE:HG12	2.12	0.50
5:B:257:LYS:HG3	5:B:259:TYR:HE1	1.77	0.50
5:B:637:LEU:HD12	5:B:740:HIS:HB3	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:837:ASP:O	5:B:988:GLY:HA2	2.11	0.50
7:E:65:THR:C	7:E:67:GLU:N	2.69	0.50
7:E:180:ARG:HB2	7:E:215:MET:OXT	2.12	0.50
4:A:663:SER:O	4:A:742:ASN:HB3	2.12	0.50
4:A:1037:LEU:HD22	4:A:1042:PHE:H	1.76	0.50
4:A:1341:ILE:HG21	7:E:178:ILE:HG13	1.92	0.50
4:A:1425:SER:O	4:A:1429:ILE:HG13	2.11	0.50
5:B:235:SER:OG	5:B:236:HIS:ND1	2.44	0.50
5:B:848:ARG:HD2	11:J:8:PHE:O	2.11	0.50
5:B:999:MET:HG3	5:B:1000:PRO:CD	2.34	0.50
5:B:1133:MET:O	5:B:1136:ASP:HB2	2.12	0.50
11:J:41:LEU:O	11:J:47:ARG:NE	2.44	0.50
4:A:630:ILE:HD12	4:A:630:ILE:N	2.02	0.50
5:B:331:LEU:C	5:B:334:ILE:HG13	2.37	0.50
6:C:166:GLU:HG3	12:K:10:PHE:CZ	2.45	0.50
4:A:457:ALA:HB3	4:A:506:ALA:HA	1.94	0.50
4:A:902:LEU:HG	4:A:926:GLN:HG3	1.93	0.50
5:B:293:PRO:HG2	5:B:296:GLU:HB2	1.94	0.50
5:B:1178:ASN:O	5:B:1179:GLN:C	2.55	0.50
6:C:178:PHE:CE1	6:C:230:MET:HE2	2.47	0.50
11:J:8:PHE:H	11:J:49:MET:HE1	1.72	0.50
2:T:24:DT:H2"	2:T:25:DC:C6	2.47	0.49
4:A:390:GLN:O	4:A:393:ARG:O	2.31	0.49
4:A:660:ASN:C	4:A:660:ASN:ND2	2.70	0.49
4:A:920:LEU:HD22	4:A:920:LEU:C	2.36	0.49
4:A:1410:PHE:C	4:A:1412:ALA:H	2.20	0.49
4:A:1444:MET:HB2	4:A:1445:ILE:CB	2.42	0.49
5:B:544:CYS:HB3	5:B:634:TYR:CZ	2.47	0.49
5:B:624:LEU:C	5:B:624:LEU:HD12	2.37	0.49
7:E:88:VAL:HB	7:E:116:ILE:HD13	1.93	0.49
8:F:138:LEU:HB3	8:F:139:PRO:HD2	1.93	0.49
4:A:33:ALA:HB2	4:A:82:GLY:HA2	1.93	0.49
5:B:333:PHE:HB3	5:B:334:ILE:CB	2.42	0.49
5:B:755:ILE:HD12	5:B:814:PHE:CE1	2.48	0.49
5:B:769:TYR:HD2	5:B:769:TYR:N	2.08	0.49
5:B:886:LYS:CB	5:B:887:HIS:CA	2.58	0.49
5:B:1184:GLY:C	5:B:1186:ASP:N	2.70	0.49
6:C:57:VAL:CG1	11:J:60:PHE:CB	2.90	0.49
11:J:36:LEU:HD11	11:J:51:LEU:CD1	2.42	0.49
4:A:481:ASP:OD1	4:A:483:ASP:CG	2.56	0.49
4:A:908:LEU:HB3	4:A:912:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:148:VAL:HG12	8:F:148:VAL:O	2.13	0.49
5:B:132:VAL:CG2	5:B:165:VAL:HG21	2.42	0.49
5:B:770:GLN:HE22	5:B:1093:GLN:HE22	1.58	0.49
5:B:833:TYR:OH	12:K:66:PRO:HG3	2.13	0.49
8:F:137:TYR:CD2	8:F:143:PHE:HB3	2.48	0.49
4:A:827:THR:HG22	4:A:828:ALA:H	1.78	0.49
5:B:1119:VAL:O	5:B:1126:GLY:CA	2.61	0.49
11:J:1:MET:H3	11:J:56:LEU:H	1.60	0.49
11:J:64:ASN:N	11:J:65:PRO:HD2	2.26	0.49
2:T:20:DC:O5'	2:T:20:DC:H6	1.96	0.49
4:A:260:ASP:CG	4:A:261:ASP:N	2.71	0.49
5:B:179:CYS:SG	5:B:180:TYR:N	2.86	0.49
6:C:131:HIS:O	6:C:132:PRO:C	2.55	0.49
4:A:271:LYS:O	4:A:275:SER:HB2	2.12	0.49
4:A:399:HIS:CB	4:A:400:PRO:HD3	2.42	0.49
5:B:711:GLU:H	5:B:712:PRO:HD3	1.70	0.49
5:B:848:ARG:HD2	11:J:8:PHE:CA	2.41	0.49
13:L:69:ALA:O	13:L:70:ARG:HG2	2.12	0.49
1:R:8:G:O2'	1:R:9:G:O5'	2.29	0.49
4:A:33:ALA:CB	4:A:82:GLY:HA2	2.43	0.49
4:A:381:THR:CG2	4:A:382:PRO:HD2	2.42	0.49
4:A:540:PHE:HB3	4:A:571:LEU:HD12	1.95	0.49
4:A:590:ARG:O	4:A:591:PHE:HB2	2.13	0.49
5:B:213:ILE:CD1	5:B:481:GLN:OE1	2.61	0.49
5:B:470:LYS:C	5:B:472:ALA:H	2.21	0.49
5:B:880:THR:O	5:B:933:SER:HB2	2.13	0.49
6:C:31:ASN:ND2	6:C:35:ARG:HD2	2.28	0.49
11:J:28:ASP:O	11:J:30:LEU:N	2.46	0.49
4:A:351:THR:HG22	4:A:352:VAL:N	2.13	0.49
4:A:1118:VAL:HG12	4:A:1327:ILE:HD11	1.95	0.49
5:B:391:ASP:HB3	10:I:92:ARG:HB2	1.94	0.49
5:B:829:CYS:SG	5:B:1014:PRO:CG	2.86	0.49
6:C:44:LEU:HD22	6:C:129:ILE:CG2	2.43	0.49
6:C:164:ALA:HB2	6:C:171:GLY:HA2	1.93	0.49
8:F:116:ASP:HB3	8:F:119:ARG:HG3	1.94	0.49
4:A:315:LEU:HD23	4:A:320:ARG:HH21	1.78	0.49
4:A:1400:CYS:C	4:A:1402:PHE:H	2.20	0.49
5:B:493:SER:C	5:B:495:LEU:H	2.21	0.49
5:B:910:VAL:HG13	5:B:938:SER:HB3	1.95	0.49
5:B:980:PHE:HE1	5:B:990:ILE:HD11	1.77	0.49
6:C:99:LEU:HB2	6:C:157:CYS:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:35:ILE:HG21	4:A:84:ILE:HD12	1.94	0.48
4:A:334:GLY:O	4:A:336:ILE:N	2.46	0.48
4:A:873:MET:HG2	4:A:957:PRO:HG3	1.95	0.48
5:B:515:HIS:CD2	5:B:517:THR:H	2.30	0.48
5:B:906:SER:HA	5:B:946:ASN:HA	1.95	0.48
11:J:1:MET:HB2	11:J:56:LEU:HD12	1.95	0.48
4:A:297:GLN:O	4:A:299:HIS:O	2.31	0.48
4:A:444:PHE:HE2	4:A:470:LEU:HD22	1.77	0.48
4:A:453:MET:C	4:A:455:MET:H	2.20	0.48
5:B:332:ASP:CG	5:B:332:ASP:O	2.55	0.48
5:B:708:GLU:HG3	5:B:709:ASP:H	1.78	0.48
5:B:711:GLU:H	5:B:712:PRO:HD2	1.78	0.48
1:R:5:A:H2'	1:R:6:G:H8	1.77	0.48
2:T:18:DA:H2"	2:T:19:DT:C5'	2.44	0.48
4:A:30:ILE:HG23	5:B:1170:THR:HG23	1.94	0.48
4:A:472:LEU:HD11	5:B:835:GLN:NE2	2.28	0.48
4:A:663:SER:CB	5:B:1085:ILE:HA	2.43	0.48
4:A:760:GLN:NE2	4:A:765:VAL:HA	2.29	0.48
4:A:821:ARG:HH12	5:B:514:LEU:HD13	1.78	0.48
5:B:38:PHE:O	5:B:39:ARG:C	2.56	0.48
5:B:801:LYS:O	5:B:801:LYS:HG3	2.12	0.48
5:B:841:MET:HG3	5:B:1009:ASP:O	2.14	0.48
5:B:1174:LYS:HB2	5:B:1179:GLN:O	2.13	0.48
9:H:135:LEU:C	9:H:137:GLN:H	2.21	0.48
12:K:10:PHE:N	12:K:10:PHE:CD2	2.81	0.48
4:A:709:THR:HB	4:A:712:GLU:HB2	1.94	0.48
4:A:850:VAL:HG21	4:A:1058:VAL:HG11	1.94	0.48
4:A:867:ILE:O	4:A:868:TYR:C	2.55	0.48
4:A:1116:LEU:HB2	4:A:1308:THR:HB	1.96	0.48
11:J:1:MET:O	11:J:2:ILE:O	2.32	0.48
5:B:840:ILE:HG21	5:B:994:TYR:CD1	2.47	0.48
4:A:55:ASP:O	4:A:56:PRO:C	2.56	0.48
5:B:658:ILE:HA	5:B:661:LEU:HD12	1.95	0.48
7:E:59:SER:OG	7:E:81:GLU:HG3	2.13	0.48
2:T:19:DT:H2'	2:T:20:DC:O5'	2.14	0.48
4:A:851:HIS:ND1	4:A:857:ARG:HD2	2.29	0.48
4:A:1319:VAL:HG12	4:A:1320:PRO:O	2.14	0.48
5:B:635:ARG:HB2	5:B:636:PRO:HD2	1.94	0.48
5:B:653:VAL:CG1	5:B:689:LEU:HD13	2.41	0.48
5:B:755:ILE:HG23	5:B:809:MET:HE2	1.95	0.48
5:B:762:ASN:HB2	5:B:767:ASN:HD21	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:843:GLN:N	5:B:994:TYR:O	2.44	0.48
5:B:882:THR:HG23	5:B:883:LEU:N	2.28	0.48
7:E:112:TYR:HE2	7:E:134:THR:HB	1.77	0.48
5:B:744:HIS:HA	5:B:745:PRO:HD3	1.63	0.48
5:B:794:ASN:C	5:B:795:ILE:HD12	2.38	0.48
5:B:882:THR:HG23	5:B:883:LEU:H	1.77	0.48
5:B:1177:HIS:O	5:B:1178:ASN:C	2.57	0.48
6:C:258:ILE:CD1	12:K:42:LEU:HD21	2.44	0.48
9:H:2:SER:N	9:H:3:ASN:CA	2.77	0.48
4:A:442:VAL:O	4:A:457:ALA:HA	2.13	0.48
4:A:453:MET:HG3	4:A:456:MET:HE1	1.95	0.48
4:A:541:ILE:HG22	4:A:545:GLN:NE2	2.28	0.48
5:B:824:ILE:HD11	11:J:48:ARG:HH21	1.76	0.48
6:C:209:TYR:N	6:C:209:TYR:HD1	2.11	0.48
9:H:2:SER:CA	9:H:3:ASN:CB	2.65	0.48
4:A:667:GLY:CA	4:A:670:ILE:HG12	2.33	0.48
4:A:778:GLY:HA3	5:B:516:ASN:HB2	1.96	0.48
5:B:493:SER:O	5:B:495:LEU:N	2.47	0.48
5:B:743:ILE:O	5:B:744:HIS:HB2	2.13	0.48
7:E:135:PHE:HB3	7:E:140:LEU:HD11	1.95	0.48
1:R:8:G:O3'	5:B:776:GLN:NE2	2.47	0.47
5:B:980:PHE:O	5:B:987:LYS:O	2.32	0.47
5:B:1166:CYS:O	5:B:1215:ARG:NH1	2.47	0.47
10:I:40:SER:C	10:I:42:LEU:N	2.71	0.47
4:A:300:VAL:O	4:A:301:ALA:C	2.58	0.47
4:A:368:LYS:O	4:A:370:ILE:N	2.47	0.47
4:A:506:ALA:C	4:A:508:PRO:HD2	2.39	0.47
4:A:658:LEU:HD21	5:B:1076:HIS:HD2	1.80	0.47
4:A:1161:THR:HG22	4:A:1163:ILE:H	1.79	0.47
5:B:653:VAL:HG12	5:B:689:LEU:CD1	2.42	0.47
5:B:827:ILE:HG22	5:B:827:ILE:O	2.13	0.47
10:I:118:ARG:NH1	10:I:118:ARG:CG	2.64	0.47
4:A:920:LEU:HD13	4:A:920:LEU:O	2.14	0.47
4:A:947:PHE:CE2	4:A:954:TRP:CE2	3.02	0.47
4:A:1059:HIS:CE1	8:F:155:LEU:HD21	2.42	0.47
5:B:824:ILE:CD1	11:J:48:ARG:NH2	2.76	0.47
4:A:330:LYS:O	4:A:334:GLY:HA3	2.14	0.47
4:A:675:THR:HA	4:A:678:GLU:HB2	1.95	0.47
4:A:843:LYS:HZ1	5:B:1135:ARG:NH2	2.11	0.47
4:A:1314:SER:HA	4:A:1317:MET:HE2	1.97	0.47
5:B:241:ARG:HA	5:B:253:THR:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:842:ASN:HB2	5:B:1009:ASP:HA	1.96	0.47
6:C:173:ALA:O	6:C:174:ALA:HB3	2.15	0.47
11:J:36:LEU:CD1	11:J:51:LEU:HD13	2.44	0.47
4:A:1064:VAL:O	4:A:1064:VAL:CG1	2.62	0.47
5:B:1007:VAL:HG23	5:B:1008:PRO:HD2	1.97	0.47
5:B:1121:GLY:O	5:B:1124:ARG:N	2.47	0.47
12:K:82:ASP:HA	12:K:83:PRO:HD2	1.71	0.47
4:A:760:GLN:HE21	4:A:765:VAL:HA	1.78	0.47
4:A:1447:GLU:CA	4:A:1448:GLU:CG	2.67	0.47
5:B:471:LYS:HD2	5:B:471:LYS:O	2.14	0.47
11:J:43:ARG:O	11:J:47:ARG:HG3	2.14	0.47
4:A:242:PRO:HD2	4:A:266:LEU:HD11	1.96	0.47
4:A:264:PHE:O	4:A:268:ASP:HB2	2.15	0.47
4:A:525:GLN:CB	5:B:835:GLN:HG2	2.45	0.47
4:A:807:GLY:HA3	5:B:728:ARG:HH21	1.78	0.47
4:A:944:ARG:HD3	4:A:1298:TYR:OH	2.15	0.47
4:A:1403:GLU:O	4:A:1404:GLU:C	2.57	0.47
5:B:758:PHE:HD2	5:B:761:HIS:CD2	2.33	0.47
5:B:995:ARG:HD2	5:B:997:GLU:OE2	2.15	0.47
5:B:1084:GLN:NE2	6:C:189:THR:HG22	2.29	0.47
6:C:144:ILE:HG22	6:C:145:CYS:CB	2.42	0.47
1:R:3:C:H2'	1:R:4:G:C8	2.50	0.47
5:B:824:ILE:CD1	11:J:48:ARG:HH21	2.27	0.47
5:B:835:GLN:O	5:B:836:GLU:O	2.33	0.47
5:B:941:LEU:HD21	5:B:946:ASN:N	2.30	0.47
5:B:942:ARG:HB2	5:B:945:GLU:HB2	1.96	0.47
7:E:121:MET:HA	7:E:124:VAL:HG23	1.96	0.47
11:J:45:CYS:O	11:J:48:ARG:HG3	2.14	0.47
4:A:250:ILE:HD11	5:B:1113:VAL:HG21	1.96	0.47
4:A:483:ASP:HB2	5:B:987:LYS:CE	2.43	0.47
4:A:789:LYS:HD3	5:B:620:ARG:HH12	1.79	0.47
4:A:1410:PHE:O	4:A:1412:ALA:N	2.48	0.47
5:B:31:TRP:CD1	5:B:807:ARG:HH12	2.33	0.47
5:B:70:ILE:HD13	5:B:70:ILE:HA	1.84	0.47
5:B:199:MET:HE2	5:B:495:LEU:CD1	2.45	0.47
5:B:210:LYS:NZ	5:B:482:VAL:HG13	2.30	0.47
5:B:213:ILE:HD11	5:B:481:GLN:OE1	2.15	0.47
5:B:1015:HIS:O	5:B:1017:ILE:N	2.48	0.47
6:C:180:TYR:CE1	6:C:188:HIS:HD2	2.32	0.47
9:H:2:SER:N	9:H:3:ASN:CB	2.78	0.47
11:J:5:VAL:HG12	11:J:6:ARG:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:5:A:C2	1:R:6:G:C6	3.02	0.47
4:A:574:GLY:O	4:A:575:LYS:C	2.56	0.47
4:A:618:GLU:C	4:A:618:GLU:CD	2.83	0.47
4:A:784:LEU:HB3	4:A:785:PRO:CD	2.44	0.47
4:A:908:LEU:HD22	4:A:1032:LEU:HD12	1.97	0.47
4:A:1098:VAL:N	4:A:1099:PRO:HD2	2.30	0.47
5:B:800:GLN:OE1	5:B:822:ASN:N	2.37	0.47
6:C:194:GLU:H	6:C:194:GLU:HG3	1.46	0.47
6:C:241:ASP:CG	6:C:242:GLN:N	2.73	0.47
6:C:264:GLN:C	6:C:266:ASP:H	2.22	0.47
4:A:1171:GLN:N	4:A:1172:LEU:O	2.48	0.46
4:A:1322:ILE:HG12	4:A:1323:ASP:N	2.30	0.46
5:B:1050:ILE:HG23	5:B:1055:ILE:HD11	1.97	0.46
9:H:118:PHE:HE1	9:H:123:MET:HB2	1.80	0.46
12:K:6:ARG:C	12:K:8:GLU:N	2.73	0.46
13:L:55:ILE:O	13:L:56:LEU:CB	2.62	0.46
4:A:761:MET:HA	4:A:804:TYR:H	1.80	0.46
4:A:870:GLU:HB2	7:E:204:THR:CG2	2.44	0.46
5:B:542:MET:HE1	5:B:743:ILE:HG13	1.98	0.46
5:B:967:ARG:HG2	5:B:967:ARG:HH11	1.80	0.46
11:J:48:ARG:HH11	11:J:49:MET:CE	2.24	0.46
4:A:1075:PRO:O	4:A:1076:ALA:C	2.59	0.46
5:B:1139:ILE:O	5:B:1140:ALA:C	2.58	0.46
5:B:1198:TYR:C	5:B:1198:TYR:CD2	2.94	0.46
4:A:871:ASP:HA	4:A:1014:ALA:HB1	1.97	0.46
4:A:1098:VAL:O	4:A:1099:PRO:C	2.58	0.46
5:B:345:LYS:N	5:B:346:GLU:HB2	2.31	0.46
5:B:1111:MET:HG2	5:B:1117:GLN:C	2.40	0.46
1:R:8:G:H2'	1:R:9:G:O5'	2.15	0.46
1:R:10:A:H4'	4:A:485:ASP:OD1	2.15	0.46
1:R:10:A:OP1	5:B:979:LYS:HE3	2.15	0.46
4:A:737:LEU:CB	4:A:738:LYS:HB2	2.44	0.46
4:A:875:ALA:HB2	4:A:1366:ARG:CD	2.46	0.46
4:A:1391:ARG:HD3	4:A:1391:ARG:C	2.40	0.46
4:A:1410:PHE:C	4:A:1412:ALA:N	2.72	0.46
5:B:492:LEU:HD23	5:B:492:LEU:HA	1.70	0.46
5:B:845:SER:O	5:B:846:ILE:C	2.58	0.46
5:B:941:LEU:HG	5:B:942:ARG:N	2.30	0.46
11:J:7:CYS:N	11:J:14:VAL:HG22	2.29	0.46
4:A:665:GLY:O	4:A:668:ASP:HB2	2.16	0.46
4:A:901:LEU:H	4:A:926:GLN:HE21	1.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:254:LEU:HG	5:B:255:GLN:N	2.30	0.46
5:B:778:MET:O	5:B:796:LEU:HD11	2.14	0.46
6:C:90:ASP:O	6:C:91:HIS:HB3	2.16	0.46
4:A:115:LEU:HD21	4:A:145:LYS:HD2	1.97	0.46
4:A:393:ARG:O	4:A:394:ASN:CB	2.51	0.46
5:B:386:LEU:C	5:B:388:CYS:N	2.73	0.46
5:B:592:ASN:HD21	5:B:595:ARG:HD2	1.80	0.46
5:B:918:ILE:HD13	5:B:918:ILE:HA	1.80	0.46
6:C:11:ARG:HD3	6:C:209:TYR:CE2	2.51	0.46
8:F:107:VAL:HG12	8:F:109:VAL:H	1.80	0.46
1:R:6:G:C2	1:R:7:A:N7	2.84	0.46
4:A:18:GLN:NE2	4:A:1418:LEU:HD12	2.30	0.46
4:A:450:LEU:H	4:A:450:LEU:HD12	1.80	0.46
4:A:534:LEU:O	4:A:574:GLY:HA3	2.15	0.46
4:A:1336:MET:HE3	4:A:1336:MET:HB3	1.86	0.46
4:A:1343:ALA:O	4:A:1344:GLY:C	2.58	0.46
5:B:275:TYR:O	5:B:336:ARG:NH2	2.47	0.46
5:B:344:LYS:C	5:B:346:GLU:CB	2.88	0.46
9:H:96:VAL:HG23	9:H:143:LEU:HG	1.98	0.46
2:T:15:DA:C2'	2:T:16:DC:O5'	2.62	0.46
4:A:18:GLN:HB3	5:B:1215:ARG:HB2	1.98	0.46
4:A:70:CYS:HB2	5:B:1172:ILE:CG2	2.46	0.46
4:A:375:THR:HA	4:A:434:ARG:O	2.16	0.46
4:A:481:ASP:OD2	16:A:2003[B]:UTP:O2A	2.34	0.46
4:A:1313:LEU:C	4:A:1315:GLU:H	2.24	0.46
4:A:1446:ASP:O	4:A:1448:GLU:HG2	2.16	0.46
5:B:210:LYS:HD3	5:B:210:LYS:HA	1.73	0.46
5:B:258:LEU:HB2	5:B:385:LEU:HD21	1.98	0.46
5:B:557:PHE:C	5:B:557:PHE:CD2	2.94	0.46
11:J:48:ARG:O	11:J:52:THR:OG1	2.34	0.46
4:A:117:GLU:N	4:A:118:HIS:C	2.74	0.46
4:A:477:PRO:HG2	4:A:521:MET:HE3	1.97	0.46
4:A:1144:LYS:HG3	4:A:1268:LEU:HB3	1.96	0.46
5:B:709:ASP:C	5:B:710:LEU:HD22	2.40	0.46
7:E:169:ARG:HD3	8:F:138:LEU:HD22	1.96	0.46
11:J:44:TYR:HA	11:J:47:ARG:CG	2.45	0.46
4:A:862:ASN:HA	7:E:174:GLN:HB3	1.97	0.45
5:B:25:ILE:CG2	5:B:29:ASP:HB2	2.44	0.45
5:B:579:ARG:HD2	5:B:586:TRP:CZ2	2.51	0.45
5:B:680:THR:O	5:B:681:TRP:C	2.58	0.45
5:B:997:GLU:H	5:B:997:GLU:HG3	1.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:171:GLN:HG3	4:A:172:PRO:HD2	1.98	0.45
4:A:218:ASP:O	4:A:221:SER:HB2	2.16	0.45
4:A:1105:LEU:HD22	4:A:1384:VAL:HG21	1.99	0.45
5:B:402:GLY:CA	5:B:695:ALA:HB3	2.46	0.45
5:B:841:MET:HG3	5:B:842:ASN:H	1.81	0.45
6:C:82:TYR:HB3	6:C:84:ARG:HG2	1.98	0.45
7:E:157:SER:O	7:E:158:SER:C	2.60	0.45
2:T:19:DT:C2'	2:T:20:DC:O5'	2.64	0.45
4:A:1155:ASP:OD2	4:A:1161:THR:HA	2.17	0.45
4:A:1341:ILE:CG2	7:E:178:ILE:HG13	2.45	0.45
4:A:1365:TYR:O	4:A:1366:ARG:C	2.59	0.45
5:B:287:ARG:HD3	5:B:292:ILE:HA	1.97	0.45
5:B:516:ASN:HD22	5:B:516:ASN:N	2.04	0.45
5:B:1089:PRO:C	5:B:1090:THR:OG1	2.59	0.45
6:C:57:VAL:CG1	11:J:60:PHE:CD2	2.99	0.45
9:H:137:GLN:C	9:H:139:ASN:N	2.60	0.45
11:J:16:ASP:OD1	11:J:16:ASP:N	2.50	0.45
4:A:312:PRO:O	4:A:313:GLN:NE2	2.39	0.45
4:A:323:LYS:O	4:A:324:SER:CB	2.64	0.45
4:A:563:PRO:HG3	4:A:572:TRP:CZ2	2.52	0.45
4:A:679:ILE:HG23	4:A:729:ALA:HB1	1.98	0.45
4:A:960:ILE:O	4:A:961:ARG:C	2.59	0.45
5:B:333:PHE:CB	5:B:334:ILE:CB	2.94	0.45
5:B:621:GLU:O	5:B:622:LYS:C	2.60	0.45
5:B:795:ILE:O	5:B:854:LEU:N	2.40	0.45
4:A:672:ASP:HB2	4:A:736:ASN:ND2	2.32	0.45
4:A:1341:ILE:HG22	7:E:182:ASP:OD2	2.17	0.45
4:A:1364:ASN:HD22	4:A:1365:TYR:N	2.14	0.45
5:B:412:LEU:HA	5:B:412:LEU:HD23	1.67	0.45
5:B:793:ALA:HB3	5:B:856:PHE:CB	2.43	0.45
5:B:893:LEU:HD13	5:B:897:GLY:O	2.17	0.45
5:B:996:ARG:NH1	11:J:10:CYS:O	2.46	0.45
7:E:105:PHE:HB3	7:E:106:GLN:H	1.62	0.45
11:J:12:LYS:O	11:J:14:VAL:HG13	2.15	0.45
11:J:25:LEU:HB3	11:J:30:LEU:O	2.17	0.45
4:A:737:LEU:HA	4:A:738:LYS:CG	2.45	0.45
4:A:1072:ILE:O	4:A:1072:ILE:HG22	2.16	0.45
5:B:273:LEU:HD11	5:B:285:ILE:HD12	1.98	0.45
5:B:696:GLU:O	5:B:699:GLU:HB2	2.17	0.45
5:B:724:ASP:HA	5:B:725:PRO:HD3	1.80	0.45
12:K:37:LYS:HA	12:K:69:ALA:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:396:PRO:HG3	4:A:416:ARG:HB3	1.98	0.45
4:A:453:MET:HG3	4:A:456:MET:HE3	1.98	0.45
4:A:464:PRO:HB2	12:K:4:PRO:HD3	1.99	0.45
4:A:860:LEU:HD21	4:A:1393:ASN:O	2.16	0.45
4:A:1111:MET:HE1	4:A:1331:SER:HA	1.98	0.45
4:A:1128:GLN:HG2	4:A:1304:TRP:NE1	2.32	0.45
5:B:202:TYR:HB3	5:B:211:VAL:HG22	1.97	0.45
5:B:624:LEU:C	5:B:624:LEU:HD13	2.40	0.45
5:B:828:ALA:HB2	5:B:1085:ILE:HG23	1.94	0.45
5:B:1050:ILE:HG23	5:B:1055:ILE:HD13	1.99	0.45
6:C:76:ASP:N	6:C:76:ASP:OD1	2.49	0.45
12:K:101:LEU:O	12:K:101:LEU:HD22	2.16	0.45
1:R:1:A:C2	1:R:2:U:C4	3.05	0.45
4:A:403:LYS:O	4:A:415:LEU:CD1	2.65	0.45
4:A:737:LEU:HD13	4:A:744:LYS:HB2	1.98	0.45
4:A:1074:GLU:O	4:A:1075:PRO:C	2.60	0.45
4:A:1376:THR:HG22	7:E:212:ARG:NH2	2.29	0.45
5:B:581:PHE:HB2	5:B:625:LYS:HA	1.98	0.45
5:B:873:THR:O	5:B:914:LYS:HA	2.17	0.45
6:C:166:GLU:O	12:K:6:ARG:NH1	2.50	0.45
6:C:178:PHE:CD1	6:C:230:MET:HE2	2.52	0.45
7:E:197:LYS:HE3	7:E:199:ILE:HD11	1.98	0.45
4:A:21:LEU:HD23	4:A:22:PHE:H	1.81	0.45
4:A:1344:GLY:O	4:A:1345:ARG:C	2.60	0.45
5:B:762:ASN:OD1	5:B:984:HIS:HD2	1.99	0.45
6:C:120:ILE:H	6:C:120:ILE:HD12	1.81	0.45
11:J:48:ARG:C	11:J:48:ARG:CD	2.89	0.45
4:A:222:LEU:HD12	4:A:222:LEU:O	2.17	0.45
4:A:814:PHE:CE1	5:B:514:LEU:HD21	2.52	0.45
4:A:1345:ARG:HG2	4:A:1372:VAL:CG1	2.47	0.45
5:B:1065:GLN:HG3	5:B:1065:GLN:O	2.16	0.45
11:J:56:LEU:O	11:J:57:ILE:C	2.60	0.45
4:A:1017:LEU:O	4:A:1018:PHE:C	2.61	0.44
4:A:1340:GLY:HA2	7:E:183:PRO:HD2	1.99	0.44
5:B:254:LEU:CD2	5:B:361:LEU:HD11	2.46	0.44
5:B:1027:ILE:O	5:B:1029:CYS:N	2.50	0.44
9:H:93:TYR:HB3	9:H:144:ILE:O	2.17	0.44
4:A:403:LYS:CB	4:A:404:TYR:HD1	2.31	0.44
4:A:406:ILE:O	4:A:430:TRP:HB3	2.17	0.44
4:A:842:VAL:C	4:A:844:ALA:H	2.25	0.44
4:A:1025:ARG:HH11	4:A:1025:ARG:HG3	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1027:ALA:O	4:A:1031:VAL:HG23	2.17	0.44
4:A:1110:ASN:H	4:A:1110:ASN:ND2	2.14	0.44
5:B:702:LEU:HD21	5:B:735:ALA:HB1	1.98	0.44
5:B:848:ARG:HG3	11:J:8:PHE:HA	1.99	0.44
5:B:1198:TYR:CD2	5:B:1198:TYR:O	2.70	0.44
8:F:82:THR:HG22	8:F:84:TYR:HB2	1.99	0.44
8:F:130:ILE:HA	8:F:131:PRO:HD3	1.75	0.44
4:A:567:LYS:HD3	9:H:95:TYR:CG	2.52	0.44
4:A:645:LEU:HD11	4:A:649:ILE:HD11	1.98	0.44
4:A:665:GLY:CA	5:B:1086:PHE:CD1	2.79	0.44
4:A:1198:ASP:HB3	4:A:1201:ALA:HB3	1.99	0.44
5:B:195:CYS:C	5:B:197:PHE:H	2.25	0.44
5:B:261:ARG:H	5:B:264:SER:HB3	1.83	0.44
5:B:1080:LYS:HB2	6:C:188:HIS:HB3	1.99	0.44
6:C:167:HIS:CD2	6:C:169:LYS:H	2.35	0.44
4:A:70:CYS:HB2	5:B:1172:ILE:HG22	1.99	0.44
4:A:262:LEU:HB2	4:A:323:LYS:HE3	1.99	0.44
4:A:652:VAL:O	4:A:653:VAL:C	2.59	0.44
4:A:704:ALA:HB3	4:A:705:LYS:C	2.43	0.44
4:A:1089:VAL:HG11	4:A:1092:LYS:HD3	1.99	0.44
5:B:212:LEU:HD12	5:B:409:ALA:CB	2.47	0.44
5:B:341:LEU:HD12	5:B:343:ILE:CG2	2.48	0.44
5:B:979:LYS:HE2	5:B:987:LYS:HD2	1.99	0.44
6:C:138:GLU:OE1	6:C:138:GLU:N	2.50	0.44
10:I:65:ASP:HA	10:I:66:PRO:HD3	1.84	0.44
11:J:7:CYS:HA	11:J:49:MET:CE	2.38	0.44
4:A:50:ILE:HG22	4:A:51:GLY:H	1.82	0.44
4:A:265:LYS:CG	4:A:303:TYR:HB2	2.47	0.44
4:A:350:ARG:NH1	4:A:488:ASN:OD1	2.50	0.44
4:A:446:ARG:HD2	4:A:478:TYR:O	2.18	0.44
4:A:549:MET:HE1	4:A:656:TRP:HD1	1.82	0.44
4:A:909:ASP:HA	4:A:910:PRO:HD2	1.83	0.44
4:A:1025:ARG:CG	4:A:1025:ARG:NH1	2.62	0.44
4:A:1393:ASN:HD22	4:A:1393:ASN:N	2.16	0.44
5:B:745:PRO:HB2	5:B:1047:PHE:CD1	2.52	0.44
5:B:981:ALA:C	5:B:982:SER:O	2.60	0.44
9:H:93:TYR:HD1	9:H:143:LEU:HB3	1.82	0.44
9:H:94:ASP:OD1	9:H:94:ASP:N	2.50	0.44
11:J:7:CYS:HB2	11:J:49:MET:HG2	1.99	0.44
11:J:56:LEU:O	11:J:59:LYS:N	2.43	0.44
4:A:332:LYS:O	4:A:333:GLU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:719:VAL:O	4:A:723:ASN:ND2	2.51	0.44
4:A:1223:ASP:HA	4:A:1243:VAL:HB	2.00	0.44
5:B:212:LEU:CD1	5:B:409:ALA:HA	2.43	0.44
8:F:128:LYS:NZ	8:F:151:LEU:O	2.35	0.44
4:A:416:ARG:CG	4:A:416:ARG:NH1	2.57	0.44
4:A:845:LEU:O	4:A:846:GLU:C	2.59	0.44
4:A:979:SER:OG	4:A:981:LEU:HD12	2.17	0.44
5:B:493:SER:C	5:B:495:LEU:N	2.74	0.44
5:B:1215:ARG:HB3	5:B:1217:TYR:HE1	1.82	0.44
4:A:438:ASP:HA	4:A:460:VAL:O	2.17	0.44
4:A:1112:LYS:O	4:A:1114:PRO:HD3	2.18	0.44
5:B:38:PHE:C	5:B:40:GLU:N	2.75	0.44
5:B:195:CYS:SG	5:B:197:PHE:N	2.90	0.44
5:B:385:LEU:HD23	5:B:386:LEU:HD23	2.00	0.44
5:B:1072:MET:HE3	5:B:1085:ILE:CD1	2.42	0.44
6:C:46:ILE:HD13	6:C:159:ALA:HB2	2.00	0.44
6:C:84:ARG:CD	12:K:11:LEU:HD11	2.47	0.44
8:F:125:LEU:O	8:F:125:LEU:HG	2.17	0.44
4:A:469:ARG:HB3	4:A:469:ARG:CZ	2.48	0.43
4:A:886:ILE:HG21	4:A:950:GLY:O	2.18	0.43
4:A:1356:ILE:HG21	4:A:1363:VAL:HG23	1.99	0.43
4:A:1364:ASN:O	4:A:1365:TYR:C	2.60	0.43
5:B:337:ARG:CG	5:B:339:THR:HG23	2.45	0.43
5:B:337:ARG:CB	5:B:340:ALA:H	2.28	0.43
5:B:753:ALA:C	5:B:755:ILE:N	2.74	0.43
5:B:996:ARG:HE	6:C:38:ILE:HD12	1.83	0.43
5:B:1073:TYR:CE2	5:B:1080:LYS:HG2	2.52	0.43
2:T:6:DG:C6	2:T:7:DA:C6	3.06	0.43
4:A:253:ASN:N	4:A:253:ASN:ND2	2.65	0.43
4:A:397:ASN:HD22	4:A:397:ASN:HA	1.58	0.43
4:A:525:GLN:HB3	5:B:835:GLN:HG2	2.00	0.43
4:A:628:GLY:O	4:A:632:VAL:HG23	2.17	0.43
4:A:658:LEU:HD21	5:B:1076:HIS:CD2	2.53	0.43
4:A:780:VAL:N	5:B:699:GLU:OE1	2.38	0.43
4:A:789:LYS:O	4:A:790:ASP:HB2	2.18	0.43
4:A:795:GLU:CD	4:A:795:GLU:H	2.26	0.43
4:A:1127:ASP:O	4:A:1129:GLU:N	2.51	0.43
4:A:1128:GLN:HG2	4:A:1304:TRP:CE2	2.54	0.43
5:B:112:LEU:CD1	5:B:116:GLU:HB3	2.48	0.43
5:B:519:TRP:CH2	5:B:748:ILE:HD13	2.53	0.43
5:B:542:MET:HE1	5:B:743:ILE:CB	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1044:ALA:O	5:B:1045:SER:C	2.61	0.43
5:B:1104:HIS:HD2	5:B:1128:LEU:HD21	1.83	0.43
6:C:34:ARG:HG3	6:C:176:ILE:HG21	1.99	0.43
8:F:103:MET:O	8:F:105:ALA:N	2.51	0.43
9:H:50:ALA:O	9:H:53:ASP:CB	2.63	0.43
11:J:44:TYR:CA	11:J:47:ARG:HB2	2.30	0.43
4:A:367:PRO:HA	4:A:463:ILE:HD12	1.99	0.43
4:A:374:LEU:HB3	4:A:436:ILE:CD1	2.44	0.43
4:A:545:GLN:C	4:A:547:LEU:N	2.76	0.43
4:A:583:PRO:C	4:A:586:ILE:HD13	2.44	0.43
4:A:665:GLY:O	4:A:666:ILE:C	2.60	0.43
5:B:337:ARG:CD	5:B:339:THR:CG2	2.76	0.43
5:B:473:MET:HE3	5:B:473:MET:HB2	1.73	0.43
5:B:1023:VAL:O	5:B:1024:ALA:C	2.61	0.43
6:C:25:VAL:HG12	6:C:26:ASP:N	2.32	0.43
10:I:55:THR:HG22	10:I:58:VAL:HG21	2.00	0.43
11:J:3:VAL:HG21	11:J:18:TRP:CE3	2.53	0.43
4:A:298:PHE:O	4:A:298:PHE:CD1	2.72	0.43
4:A:578:LEU:C	4:A:580:VAL:N	2.76	0.43
4:A:1126:ALA:O	4:A:1127:ASP:C	2.61	0.43
5:B:332:ASP:O	5:B:332:ASP:OD1	2.36	0.43
7:E:176:PRO:O	7:E:212:ARG:HA	2.18	0.43
4:A:285:PRO:HB2	4:A:288:ALA:HB3	2.00	0.43
4:A:335:ARG:CD	5:B:1202:LEU:HD12	2.48	0.43
4:A:432:VAL:O	4:A:434:ARG:N	2.52	0.43
4:A:1195:LEU:HD11	4:A:1267:MET:HE1	2.01	0.43
5:B:116:GLU:HG2	5:B:120:ARG:CD	2.48	0.43
5:B:363:HIS:O	5:B:364:ILE:HB	2.18	0.43
5:B:697:GLU:C	5:B:699:GLU:N	2.75	0.43
5:B:764:SER:H	5:B:765:PRO:HD2	1.81	0.43
5:B:841:MET:HA	5:B:1009:ASP:O	2.19	0.43
5:B:1099:VAL:O	5:B:1101:ASP:N	2.50	0.43
6:C:31:ASN:HD21	6:C:35:ARG:HD2	1.84	0.43
7:E:72:PHE:HA	7:E:73:PRO:HD3	1.85	0.43
1:R:6:G:H8	1:R:6:G:O5'	2.02	0.43
4:A:242:PRO:HA	4:A:243:PRO:HD3	1.82	0.43
4:A:343:LYS:NZ	5:B:1197:PRO:HG3	2.32	0.43
4:A:501:LEU:HD13	4:A:501:LEU:HA	1.75	0.43
4:A:513:SER:HA	4:A:514:PRO:HD3	1.73	0.43
4:A:1243:VAL:HG22	4:A:1244:ARG:HA	2.00	0.43
5:B:345:LYS:N	5:B:346:GLU:CB	2.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:601:ARG:O	5:B:605:ARG:HD2	2.18	0.43
7:E:153:HIS:CG	7:E:184:VAL:HG11	2.54	0.43
4:A:589:GLN:HB3	4:A:961:ARG:HH22	1.82	0.43
4:A:873:MET:HG3	4:A:1056:SER:O	2.18	0.43
4:A:1131:ALA:HA	4:A:1134:ILE:HD12	1.99	0.43
5:B:138:GLU:O	5:B:139:ALA:O	2.36	0.43
5:B:409:ALA:O	5:B:413:LEU:HB2	2.18	0.43
5:B:567:GLU:H	5:B:567:GLU:CD	2.27	0.43
5:B:637:LEU:HD11	5:B:740:HIS:HB3	1.92	0.43
5:B:850:LEU:HD13	11:J:8:PHE:HD1	1.84	0.43
5:B:1099:VAL:C	5:B:1103:ILE:HD12	2.43	0.43
11:J:21:TYR:HE1	11:J:36:LEU:HG	1.83	0.43
4:A:50:ILE:HG22	4:A:51:GLY:N	2.34	0.43
4:A:247:ARG:O	4:A:248:PRO:O	2.36	0.43
4:A:299:HIS:O	4:A:300:VAL:C	2.61	0.43
4:A:775:ILE:H	4:A:775:ILE:HG12	1.50	0.43
4:A:809:THR:O	4:A:810:PRO:C	2.61	0.43
4:A:820:GLY:O	4:A:821:ARG:C	2.62	0.43
4:A:868:TYR:CD2	4:A:1058:VAL:HG21	2.54	0.43
4:A:947:PHE:CD2	4:A:954:TRP:NE1	2.86	0.43
5:B:115:GLN:O	5:B:116:GLU:C	2.61	0.43
5:B:174:LEU:HD13	5:B:202:TYR:CD1	2.54	0.43
5:B:834:ASN:ND2	5:B:1012:ILE:O	2.49	0.43
7:E:105:PHE:O	7:E:106:GLN:HB2	2.18	0.43
10:I:43:VAL:O	10:I:43:VAL:HG12	2.19	0.43
4:A:265:LYS:O	4:A:268:ASP:N	2.48	0.43
4:A:573:SER:O	4:A:574:GLY:C	2.61	0.43
4:A:909:ASP:C	4:A:911:SER:N	2.76	0.43
4:A:1004:ASN:CB	4:A:1007:ILE:HD13	2.17	0.43
5:B:99:LYS:HD3	5:B:178:ASN:O	2.18	0.43
5:B:166:PHE:C	5:B:167:ILE:HG12	2.43	0.43
5:B:307:ASP:O	5:B:311:LEU:HG	2.18	0.43
5:B:758:PHE:HB2	5:B:1024:ALA:HB1	2.01	0.43
6:C:128:ASN:O	6:C:129:ILE:HG13	2.18	0.43
7:E:84:ASP:O	7:E:113:GLN:NE2	2.51	0.43
8:F:109:VAL:HG22	8:F:110:ASP:N	2.33	0.43
9:H:2:SER:HB2	9:H:3:ASN:CG	2.33	0.43
11:J:63:TYR:C	11:J:65:PRO:HD2	2.44	0.43
4:A:117:GLU:N	4:A:118:HIS:CB	2.79	0.43
4:A:363:GLN:HG2	4:A:459:ARG:HB2	2.01	0.43
4:A:381:THR:HG23	8:F:104:ASN:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:709:THR:CB	4:A:712:GLU:HB2	2.48	0.43
4:A:775:ILE:O	4:A:797:LYS:HE2	2.19	0.43
4:A:825:ILE:HD12	5:B:512:ARG:HB3	1.99	0.43
5:B:474:SER:O	5:B:475:SER:C	2.62	0.43
5:B:710:LEU:HD13	5:B:733:HIS:HA	2.00	0.43
5:B:756:ILE:HG21	5:B:767:ASN:OD1	2.18	0.43
5:B:758:PHE:CE1	5:B:1044:ALA:HA	2.54	0.43
5:B:780:VAL:O	5:B:782:LEU:N	2.52	0.43
5:B:1030:LEU:C	5:B:1032:SER:H	2.26	0.43
2:T:19:DT:O4	2:T:20:DC:N4	2.52	0.42
4:A:222:LEU:O	4:A:222:LEU:CD1	2.67	0.42
4:A:372:LYS:O	4:A:435:HIS:CD2	2.72	0.42
4:A:471:ASN:CG	4:A:472:LEU:N	2.77	0.42
4:A:542:GLU:O	4:A:546:VAL:HG23	2.19	0.42
4:A:738:LYS:HB3	4:A:741:ASN:HB2	2.01	0.42
4:A:764:CYS:HB2	4:A:801:GLU:O	2.19	0.42
4:A:884:ASP:O	4:A:885:THR:C	2.61	0.42
4:A:1042:PHE:O	4:A:1043:ASP:C	2.62	0.42
5:B:1027:ILE:O	5:B:1028:GLU:C	2.62	0.42
5:B:1086:PHE:C	5:B:1086:PHE:HD2	2.27	0.42
6:C:204:SER:C	6:C:206:ASN:N	2.77	0.42
7:E:150:VAL:HA	7:E:151:PRO:HD3	1.85	0.42
4:A:67:CYS:C	4:A:68:GLN:HG3	2.44	0.42
4:A:171:GLN:HE21	4:A:171:GLN:HB2	1.66	0.42
4:A:920:LEU:C	4:A:920:LEU:CD1	2.83	0.42
5:B:215:GLN:HE22	5:B:499:ASN:HD22	1.66	0.42
5:B:605:ARG:CZ	5:B:639:ILE:HD13	2.49	0.42
5:B:753:ALA:HA	5:B:756:ILE:CD1	2.49	0.42
5:B:763:GLN:HG2	5:B:765:PRO:HD2	2.01	0.42
5:B:848:ARG:HD2	11:J:8:PHE:C	2.44	0.42
5:B:872:GLU:OE2	5:B:916:THR:HB	2.19	0.42
5:B:1006:ILE:HG22	5:B:1007:VAL:N	2.33	0.42
4:A:877:HIS:C	4:A:878:ILE:HD12	2.44	0.42
4:A:974:ASP:C	4:A:976:THR:H	2.27	0.42
4:A:1355:VAL:HG12	4:A:1356:ILE:HD13	2.00	0.42
5:B:121:ASN:OD1	5:B:963:PHE:CE1	2.72	0.42
5:B:185:THR:O	5:B:186:GLU:C	2.62	0.42
11:J:24:LEU:N	11:J:24:LEU:CD1	2.83	0.42
4:A:273:ASN:HA	4:A:296:LEU:HD11	2.00	0.42
4:A:735:VAL:C	4:A:737:LEU:H	2.28	0.42
4:A:845:LEU:HD12	4:A:1069:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1412:ALA:HA	4:A:1417:GLU:HG2	2.02	0.42
5:B:35:SER:OG	5:B:811:TYR:HE2	2.02	0.42
5:B:879:ARG:HB3	5:B:880:THR:H	1.65	0.42
12:K:35:PHE:O	12:K:70:ARG:HA	2.19	0.42
4:A:37:PHE:HA	4:A:38:PRO:HD3	1.94	0.42
4:A:88:LYS:HA	4:A:89:PRO:HD3	1.75	0.42
4:A:116:ASP:CB	4:A:117:GLU:CB	2.57	0.42
4:A:1079:MET:HE1	4:A:1355:VAL:HG13	2.00	0.42
5:B:582:VAL:HG23	5:B:626:ILE:HB	2.01	0.42
5:B:597:MET:SD	5:B:624:LEU:HD21	2.60	0.42
5:B:619:ILE:HG13	10:I:65:ASP:HB2	2.01	0.42
5:B:889:THR:HG22	5:B:891:ASP:HB2	2.01	0.42
5:B:941:LEU:HG	5:B:942:ARG:H	1.84	0.42
5:B:1086:PHE:C	5:B:1086:PHE:CD2	2.96	0.42
6:C:208:GLU:HB3	6:C:209:TYR:CE1	2.55	0.42
2:T:18:DA:H2	16:A:2003[B]:UTP:O2	2.02	0.42
4:A:404:TYR:HD2	4:A:412:ARG:CD	2.26	0.42
4:A:650:GLN:HB3	4:A:654:ASN:HD21	1.84	0.42
4:A:770:VAL:O	4:A:773:LYS:O	2.37	0.42
4:A:1021:LEU:O	4:A:1024:SER:N	2.52	0.42
5:B:66:ASP:OD2	5:B:422:LYS:HE3	2.20	0.42
5:B:695:ALA:O	5:B:696:GLU:C	2.62	0.42
5:B:856:PHE:CD2	5:B:967:ARG:HD2	2.55	0.42
6:C:39:ALA:O	6:C:164:ALA:HB3	2.20	0.42
4:A:38:PRO:HA	4:A:270:LEU:HD13	2.02	0.42
4:A:53:LEU:CG	4:A:54:ASN:N	2.71	0.42
4:A:306:ASN:O	4:A:307:ASP:CB	2.67	0.42
4:A:541:ILE:HD13	4:A:546:VAL:HG22	2.02	0.42
4:A:778:GLY:HA3	5:B:516:ASN:CG	2.45	0.42
4:A:780:VAL:H	5:B:699:GLU:CD	2.25	0.42
4:A:896:ARG:HB3	4:A:897:TYR:CD1	2.55	0.42
4:A:1140:HIS:CE1	4:A:1272:THR:HG22	2.55	0.42
5:B:95:ILE:HG23	5:B:95:ILE:O	2.19	0.42
5:B:797:TYR:CD2	5:B:852:ARG:HD2	2.54	0.42
5:B:797:TYR:HB2	5:B:852:ARG:O	2.20	0.42
5:B:855:PHE:HD1	5:B:856:PHE:H	1.66	0.42
10:I:85:PHE:HB3	10:I:101:PHE:CD2	2.55	0.42
11:J:36:LEU:HD11	11:J:51:LEU:HD12	2.02	0.42
4:A:284:ALA:HB1	4:A:289:ILE:HD11	2.00	0.42
4:A:374:LEU:HD13	4:A:491:VAL:HG21	2.02	0.42
4:A:533:LYS:HE2	4:A:745:GLN:HE22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:784:LEU:HD12	4:A:815:PHE:CZ	2.55	0.42
4:A:1069:ALA:O	4:A:1070:GLN:C	2.63	0.42
5:B:169:ARG:N	5:B:454:THR:OG1	2.52	0.42
5:B:470:LYS:O	5:B:471:LYS:HG3	2.20	0.42
5:B:516:ASN:O	5:B:518:HIS:N	2.53	0.42
5:B:823:ALA:CB	5:B:1010:LEU:HD22	2.49	0.42
6:C:80:LEU:HD12	6:C:127:ARG:NH2	2.35	0.42
7:E:37:LEU:HD23	7:E:38:PRO:O	2.20	0.42
4:A:129:LYS:O	4:A:130:ASP:HB2	2.19	0.42
4:A:297:GLN:O	4:A:300:VAL:HB	2.20	0.42
4:A:535:THR:CG2	4:A:617:VAL:H	2.30	0.42
4:A:996:ASN:HB3	4:A:1050:GLU:OE2	2.20	0.42
5:B:836:GLU:C	5:B:838:SER:N	2.77	0.42
5:B:1099:VAL:C	5:B:1101:ASP:N	2.68	0.42
7:E:124:VAL:HB	7:E:125:PRO:HD3	2.02	0.42
7:E:173:SER:OG	7:E:174:GLN:N	2.52	0.42
10:I:45:ARG:HE	10:I:47:GLU:CG	2.32	0.42
1:R:5:A:N3	1:R:6:G:C8	2.88	0.42
4:A:323:LYS:NZ	4:A:324:SER:H	2.17	0.42
4:A:368:LYS:O	4:A:372:LYS:N	2.52	0.42
4:A:403:LYS:O	4:A:415:LEU:HG	2.19	0.42
5:B:274:PRO:C	5:B:276:ILE:H	2.28	0.42
5:B:363:HIS:O	5:B:364:ILE:CB	2.67	0.42
5:B:1187:ASN:HD21	5:B:1190:ASP:HB3	1.84	0.42
6:C:180:TYR:HB3	6:C:228:PHE:CD2	2.55	0.42
10:I:116:ASN:OD1	10:I:116:ASN:N	2.53	0.42
12:K:58:PHE:HE2	12:K:74:ARG:HE	1.68	0.42
12:K:65:HIS:C	12:K:67:PHE:H	2.28	0.42
5:B:697:GLU:C	5:B:699:GLU:H	2.28	0.41
5:B:777:ALA:HB2	5:B:1095:LEU:HD23	2.03	0.41
5:B:1213:THR:HG21	5:B:1215:ARG:HH21	1.85	0.41
6:C:22:LEU:O	6:C:227:THR:HA	2.20	0.41
6:C:43:THR:HG22	6:C:44:LEU:N	2.34	0.41
6:C:175:ALA:HB3	11:J:43:ARG:CZ	2.50	0.41
8:F:112:GLU:C	8:F:114:GLU:H	2.27	0.41
11:J:24:LEU:O	11:J:25:LEU:HG	2.20	0.41
4:A:242:PRO:HD2	4:A:266:LEU:CD1	2.50	0.41
4:A:313:GLN:HG2	4:A:322:VAL:HG22	2.02	0.41
4:A:457:ALA:HB2	4:A:501:LEU:HD12	2.01	0.41
4:A:543:LEU:O	4:A:544:ASP:C	2.63	0.41
4:A:1356:ILE:HG22	4:A:1361:SER:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:685:LEU:HD21	5:B:692:TYR:CE1	2.55	0.41
5:B:1006:ILE:HG22	5:B:1007:VAL:H	1.85	0.41
7:E:137:GLU:O	7:E:141:VAL:HG23	2.20	0.41
12:K:73:LEU:HD21	12:K:75:ILE:HD11	2.00	0.41
3:N:3:DG:H2"	3:N:4:DC:O5'	2.20	0.41
4:A:357:PRO:HG3	5:B:832:GLY:HA3	2.02	0.41
4:A:780:VAL:HG13	4:A:789:LYS:HE2	2.01	0.41
4:A:863:VAL:C	4:A:864:ILE:HD13	2.46	0.41
4:A:886:ILE:HD11	4:A:943:LEU:HB3	2.01	0.41
5:B:683:SER:O	5:B:687:GLU:HB2	2.20	0.41
5:B:805:THR:CG2	5:B:815:ARG:HH21	2.24	0.41
5:B:841:MET:CG	5:B:842:ASN:N	2.83	0.41
5:B:1091:TYR:HD1	5:B:1091:TYR:HA	1.70	0.41
6:C:148:ARG:N	6:C:151:GLN:HG3	2.34	0.41
6:C:177:GLU:HB2	6:C:231:ASN:HB3	2.02	0.41
11:J:12:LYS:HB2	11:J:46:CYS:SG	2.60	0.41
4:A:709:THR:HB	4:A:712:GLU:CB	2.51	0.41
5:B:273:LEU:O	5:B:276:ILE:HG22	2.20	0.41
5:B:334:ILE:HA	5:B:334:ILE:HD13	1.94	0.41
5:B:490:SER:CB	5:B:775:LYS:HG2	2.47	0.41
5:B:768:THR:O	5:B:771:SER:OG	2.29	0.41
5:B:1023:VAL:O	5:B:1026:LEU:N	2.54	0.41
8:F:85:MET:SD	8:F:90:ARG:HB3	2.60	0.41
11:J:10:CYS:SG	11:J:43:ARG:HD2	2.60	0.41
13:L:26:THR:HA	13:L:62:LYS:NZ	2.35	0.41
2:T:13:DA:N6	3:N:2:DT:C6	2.88	0.41
4:A:499:ALA:HA	8:F:118:LEU:HD11	2.02	0.41
4:A:596:THR:C	4:A:598:LEU:N	2.78	0.41
4:A:811:GLN:HE22	5:B:731:VAL:HG21	1.86	0.41
4:A:827:THR:C	4:A:829:VAL:N	2.66	0.41
4:A:915:SER:HB3	4:A:919:ILE:HD13	2.03	0.41
5:B:31:TRP:CH2	5:B:807:ARG:HB3	2.55	0.41
5:B:176:SER:O	5:B:178:ASN:N	2.52	0.41
7:E:156:LEU:HD23	7:E:197:LYS:HB2	2.03	0.41
9:H:131:ASN:HB3	9:H:132:LEU:H	1.56	0.41
4:A:548:ASN:OD1	12:K:60:ALA:HB1	2.21	0.41
4:A:650:GLN:O	4:A:651:LYS:C	2.62	0.41
4:A:660:ASN:ND2	4:A:661:GLY:O	2.53	0.41
4:A:991:LYS:O	4:A:994:GLN:HB3	2.20	0.41
5:B:398:ARG:HB3	5:B:398:ARG:NH1	2.35	0.41
5:B:733:HIS:HB2	5:B:734:HIS:H	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:864:LYS:HD3	5:B:865:LYS:N	2.36	0.41
5:B:1048:THR:HB	5:B:1049:ASP:H	1.69	0.41
5:B:1084:GLN:HE21	6:C:189:THR:HG21	1.81	0.41
5:B:1133:MET:O	5:B:1134:GLU:C	2.64	0.41
6:C:259:LEU:HD13	12:K:91:CYS:HB3	2.03	0.41
11:J:8:PHE:N	11:J:49:MET:CE	2.70	0.41
12:K:100:ALA:C	12:K:102:LYS:N	2.77	0.41
4:A:117:GLU:N	4:A:118:HIS:CA	2.82	0.41
4:A:303:TYR:CD2	4:A:304:MET:HG3	2.55	0.41
4:A:363:GLN:HE21	4:A:459:ARG:NH1	2.19	0.41
4:A:455:MET:HE1	5:B:1134:GLU:HG3	2.03	0.41
4:A:662:PHE:HD1	4:A:663:SER:H	1.50	0.41
5:B:120:ARG:HH21	5:B:956:THR:HG22	1.85	0.41
5:B:463:THR:HB	5:B:465:ASN:ND2	2.31	0.41
5:B:788:ARG:NH1	5:B:790:ASP:OD1	2.54	0.41
12:K:57:LEU:HD21	12:K:78:THR:HG23	2.03	0.41
12:K:82:ASP:OD2	12:K:84:LYS:HB2	2.21	0.41
4:A:42:ASP:OD1	4:A:45:GLN:N	2.54	0.41
4:A:657:LEU:HD21	5:B:829:CYS:HB2	2.03	0.41
5:B:393:LYS:HD2	5:B:393:LYS:HA	1.90	0.41
5:B:490:SER:HB3	5:B:775:LYS:CG	2.47	0.41
5:B:644:GLU:HB3	5:B:645:SER:H	1.70	0.41
5:B:708:GLU:O	5:B:712:PRO:CG	2.68	0.41
5:B:846:ILE:HG22	5:B:847:ASP:OD1	2.20	0.41
12:K:65:HIS:CD2	12:K:67:PHE:HB2	2.56	0.41
2:T:17:DG:OP1	4:A:337:ARG:NH2	2.52	0.41
4:A:173:THR:HB	4:A:184:SER:HB3	2.02	0.41
4:A:219:PHE:CZ	4:A:230:ARG:HG2	2.55	0.41
4:A:332:LYS:HA	4:A:332:LYS:HD2	1.71	0.41
4:A:672:ASP:HB2	4:A:736:ASN:OD1	2.20	0.41
4:A:1040:GLN:C	4:A:1041:ALA:O	2.63	0.41
4:A:1140:HIS:HE1	4:A:1272:THR:HG22	1.86	0.41
5:B:60:GLN:HE22	5:B:94:LYS:HA	1.85	0.41
5:B:168:GLY:H	5:B:450:ALA:HB1	1.86	0.41
5:B:176:SER:C	5:B:178:ASN:N	2.78	0.41
5:B:256:VAL:HG11	5:B:382:ILE:HD13	2.03	0.41
5:B:418:LYS:C	5:B:420:LEU:H	2.28	0.41
5:B:453:ILE:O	5:B:454:THR:C	2.62	0.41
5:B:590:HIS:CD2	5:B:596:LEU:HD22	2.56	0.41
5:B:778:MET:HE3	5:B:1094:ARG:CG	2.51	0.41
5:B:797:TYR:CD1	6:C:62:PHE:CE2	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:906:SER:OG	5:B:946:ASN:HB2	2.20	0.41
5:B:1131:GLY:O	5:B:1134:GLU:N	2.54	0.41
6:C:169:LYS:HD2	6:C:170:TRP:CD2	2.56	0.41
7:E:173:SER:O	7:E:175:LEU:N	2.53	0.41
9:H:95:TYR:HB3	9:H:144:ILE:HB	2.03	0.41
12:K:12:LEU:HA	12:K:37:LYS:HG3	2.02	0.41
4:A:265:LYS:C	4:A:267:ALA:N	2.79	0.41
4:A:751:SER:OG	5:B:1015:HIS:HE1	2.02	0.41
5:B:140:ILE:CG2	5:B:141:ASP:HB3	2.34	0.41
5:B:1028:GLU:OE1	5:B:1090:THR:HG22	2.21	0.41
6:C:32:SER:O	6:C:36:VAL:CG1	2.64	0.41
6:C:35:ARG:NH1	12:K:41:THR:OG1	2.54	0.41
4:A:1091:SER:C	4:A:1093:LYS:N	2.76	0.40
5:B:28:GLU:O	5:B:28:GLU:HG3	2.21	0.40
5:B:781:PHE:HE1	5:B:788:ARG:NH1	2.19	0.40
6:C:31:ASN:O	6:C:35:ARG:HG3	2.21	0.40
6:C:248:ILE:HD13	12:K:101:LEU:HD13	2.04	0.40
7:E:144:ILE:HG13	7:E:145:THR:N	2.36	0.40
4:A:74:MET:O	4:A:75:ASN:HB3	2.20	0.40
4:A:298:PHE:CD2	4:A:302:THR:HB	2.53	0.40
4:A:497:THR:HG23	5:B:1146:PHE:HB2	2.04	0.40
4:A:575:LYS:HB3	4:A:612:ILE:HD11	2.03	0.40
4:A:1192:LEU:HG	4:A:1193:LEU:N	2.35	0.40
4:A:1424:VAL:O	4:A:1426:GLU:N	2.54	0.40
5:B:354:ASP:O	5:B:358:LYS:N	2.53	0.40
5:B:549:THR:HG22	5:B:550:ASP:H	1.86	0.40
5:B:731:VAL:O	5:B:732:SER:CB	2.69	0.40
5:B:778:MET:HG3	5:B:1094:ARG:O	2.20	0.40
9:H:81:PRO:HA	9:H:82:PRO:HD3	1.97	0.40
2:T:20:DC:H2'	2:T:21:DC:C6	2.55	0.40
4:A:537:ARG:NH2	4:A:599:SER:O	2.49	0.40
4:A:540:PHE:HZ	9:H:121:LEU:HD11	1.86	0.40
4:A:780:VAL:HG12	5:B:699:GLU:CD	2.46	0.40
4:A:1436:ILE:O	4:A:1437:GLY:C	2.64	0.40
5:B:31:TRP:CD1	5:B:807:ARG:NH1	2.90	0.40
5:B:731:VAL:O	5:B:732:SER:HB2	2.21	0.40
6:C:56:THR:HG21	6:C:145:CYS:SG	2.61	0.40
6:C:146:LYS:O	6:C:147:LEU:HD23	2.21	0.40
11:J:56:LEU:C	11:J:58:GLU:H	2.28	0.40
4:A:117:GLU:O	4:A:123:ARG:HG2	2.21	0.40
4:A:334:GLY:C	4:A:336:ILE:N	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:443:LEU:HD21	4:A:455:MET:HG3	2.03	0.40
4:A:482:PHE:C	4:A:484:GLY:N	2.79	0.40
4:A:569:LYS:HA	4:A:570:PRO:HD3	1.95	0.40
4:A:1308:THR:HG22	4:A:1309:ASP:N	2.36	0.40
4:A:1393:ASN:HD22	4:A:1393:ASN:H	1.70	0.40
5:B:95:ILE:HD12	5:B:130:VAL:CG1	2.51	0.40
5:B:333:PHE:H	5:B:334:ILE:HG12	1.84	0.40
5:B:333:PHE:H	5:B:334:ILE:HG13	1.85	0.40
5:B:708:GLU:H	5:B:708:GLU:HG2	1.71	0.40
5:B:784:ASN:OD1	5:B:784:ASN:N	2.50	0.40
5:B:980:PHE:CE2	5:B:1094:ARG:CG	2.76	0.40
5:B:1027:ILE:C	5:B:1029:CYS:N	2.79	0.40
6:C:73:GLN:HE21	6:C:74:SER:N	2.19	0.40
6:C:167:HIS:HD2	6:C:169:LYS:H	1.69	0.40
12:K:47:ARG:HD2	12:K:60:ALA:HA	2.03	0.40
4:A:356:ASP:HA	4:A:357:PRO:HD2	1.79	0.40
4:A:362:ASP:HB3	4:A:508:PRO:HD3	2.02	0.40
4:A:1444:MET:HB2	4:A:1445:ILE:HG12	1.95	0.40
5:B:229:ALA:O	5:B:261:ARG:NH2	2.54	0.40
5:B:643:ASP:O	5:B:644:GLU:CB	2.69	0.40
6:C:35:ARG:O	6:C:38:ILE:N	2.53	0.40
6:C:239:PRO:O	6:C:240:VAL:C	2.64	0.40
7:E:101:GLN:OE1	7:E:127:ILE:HG13	2.21	0.40
12:K:38:GLU:OE1	12:K:38:GLU:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	A	1401/1733 (81%)	1052 (75%)	250 (18%)	99 (7%)	1 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	B	1105/1224 (90%)	836 (76%)	177 (16%)	92 (8%)	0 4
6	C	264/318 (83%)	197 (75%)	54 (20%)	13 (5%)	1 11
7	E	212/215 (99%)	184 (87%)	22 (10%)	6 (3%)	4 19
8	F	83/155 (54%)	70 (84%)	7 (8%)	6 (7%)	1 5
9	H	129/146 (88%)	99 (77%)	22 (17%)	8 (6%)	1 7
10	I	117/122 (96%)	88 (75%)	22 (19%)	7 (6%)	1 7
11	J	63/70 (90%)	49 (78%)	7 (11%)	7 (11%)	0 2
12	K	112/120 (93%)	96 (86%)	14 (12%)	2 (2%)	6 26
13	L	44/70 (63%)	26 (59%)	14 (32%)	4 (9%)	0 3
All	All	3530/4173 (85%)	2697 (76%)	589 (17%)	244 (7%)	1 6

All (244) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	55	ASP
4	A	68	GLN
4	A	93	VAL
4	A	117	GLU
4	A	118	HIS
4	A	119	ASN
4	A	121	LEU
4	A	248	PRO
4	A	250	ILE
4	A	254	GLU
4	A	300	VAL
4	A	394	ASN
4	A	399	HIS
4	A	610	GLY
4	A	777	PHE
4	A	828	ALA
4	A	846	GLU
4	A	885	THR
4	A	1004	ASN
4	A	1041	ALA
4	A	1042	PHE
4	A	1127	ASP
4	A	1128	GLN
4	A	1365	TYR
4	A	1424	VAL

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Mol	Chain	Res	Type
4	A	1448	GLU
5	B	229	ALA
5	B	333	PHE
5	B	334	ILE
5	B	341	LEU
5	B	409	ALA
5	B	468	GLU
5	B	476	ARG
5	B	644	GLU
5	B	648	HIS
5	B	711	GLU
5	B	732	SER
5	B	744	HIS
5	B	773	MET
5	B	827	ILE
5	B	837	ASP
5	B	846	ILE
5	B	946	ASN
5	B	976	ILE
5	B	982	SER
5	B	1014	PRO
5	B	1045	SER
5	B	1082	MET
5	B	1096	ARG
5	B	1100	ASP
5	B	1122	ARG
5	B	1223	ASP
6	C	60	ASP
6	C	240	VAL
8	F	73	ALA
8	F	104	ASN
9	H	3	ASN
9	H	108	SER
9	H	131	ASN
9	H	136	LYS
9	H	138	GLU
10	I	33	SER
11	J	6	ARG
11	J	13	VAL
11	J	29	GLU
11	J	32	GLU
13	L	55	ILE

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Mol	Chain	Res	Type
13	L	56	LEU
4	A	56	PRO
4	A	62	ASP
4	A	69	THR
4	A	76	GLU
4	A	126	LEU
4	A	266	LEU
4	A	299	HIS
4	A	324	SER
4	A	369	SER
4	A	410	GLY
4	A	424	ILE
4	A	452	LYS
4	A	593	GLU
4	A	624	SER
4	A	738	LYS
4	A	870	GLU
4	A	916	GLY
4	A	979	SER
4	A	1081	LEU
4	A	1411	GLU
4	A	1437	GLY
4	A	1444	MET
5	B	67	SER
5	B	106	ASP
5	B	139	ALA
5	B	290	GLY
5	B	337	ARG
5	B	346	GLU
5	B	371	GLU
5	B	453	ILE
5	B	471	LYS
5	B	563	MET
5	B	754	SER
5	B	785	TYR
5	B	836	GLU
5	B	879	ARG
5	B	883	LEU
5	B	885	MET
5	B	1012	ILE
5	B	1046	PRO
5	B	1066	SER

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Mol	Chain	Res	Type
5	B	1069	PHE
5	B	1108	ARG
5	B	1126	GLY
5	B	1155	SER
5	B	1157	ALA
6	C	102	GLN
6	C	215	GLU
7	E	106	GLN
7	E	172	GLU
7	E	174	GLN
8	F	78	GLN
9	H	18	GLY
9	H	92	ASP
10	I	3	THR
10	I	34	TYR
10	I	47	GLU
11	J	2	ILE
12	K	7	PHE
4	A	54	ASN
4	A	219	PHE
4	A	257	ARG
4	A	315	LEU
4	A	335	ARG
4	A	377	PRO
4	A	423	ASP
4	A	465	TYR
4	A	517	ASN
4	A	544	ASP
4	A	761	MET
4	A	975	HIS
4	A	1083	THR
4	A	1221	LYS
4	A	1312	ASN
4	A	1394	THR
5	B	37	PHE
5	B	137	TYR
5	B	177	LYS
5	B	410	GLY
5	B	469	GLN
5	B	709	ASP
5	B	712	PRO
5	B	733	HIS

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Mol	Chain	Res	Type
5	B	772	ALA
5	B	868	MET
5	B	887	HIS
5	B	1016	ALA
5	B	1030	LEU
5	B	1057	LYS
5	B	1181	GLU
6	C	63	ILE
6	C	125	MET
6	C	164	ALA
8	F	106	PRO
10	I	11	ASN
10	I	58	VAL
4	A	149	GLU
4	A	214	ILE
4	A	267	ALA
4	A	307	ASP
4	A	309	ALA
4	A	312	PRO
4	A	371	ALA
4	A	433	GLU
4	A	483	ASP
4	A	569	LYS
4	A	958	VAL
4	A	1084	PHE
4	A	1425	SER
5	B	65	GLU
5	B	419	THR
5	B	477	ALA
5	B	758	PHE
5	B	894	ASP
5	B	997	GLU
5	B	1010	LEU
5	B	1097	HIS
5	B	1098	MET
5	B	1211	ASN
6	C	28	ALA
6	C	174	ALA
7	E	48	ASP
7	E	76	GLY
7	E	105	PHE
9	H	137	GLN

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Mol	Chain	Res	Type
11	J	40	GLY
4	A	65	LEU
4	A	168	GLY
4	A	249	SER
4	A	308	ILE
4	A	736	ASN
4	A	875	ALA
4	A	1107	VAL
4	A	1206	ASP
4	A	1366	ARG
5	B	479	VAL
5	B	482	VAL
5	B	483	LEU
5	B	513	GLN
5	B	792	MET
5	B	864	LYS
5	B	1017	ILE
5	B	1065	GLN
6	C	142	VAL
6	C	181	ASP
8	F	154	ASP
13	L	42	ARG
13	L	53	HIS
4	A	418	SER
4	A	579	SER
4	A	652	VAL
4	A	910	PRO
4	A	1172	LEU
4	A	1314	SER
5	B	681	TRP
5	B	1003	ALA
6	C	213	PRO
12	K	41	THR
5	B	1054	GLY
4	A	886	ILE
5	B	364	ILE
5	B	1214	PRO
10	I	76	PRO
11	J	14	VAL
4	A	567	LYS
4	A	639	PRO
4	A	810	PRO

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Mol	Chain	Res	Type
5	B	63	ILE
5	B	301	ILE
5	B	780	VAL
6	C	132	PRO
4	A	829	VAL
4	A	1099	PRO
5	B	196	PRO
8	F	131	PRO
4	A	775	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	1231/1520 (81%)	981 (80%)	250 (20%)	1	4
5	B	972/1061 (92%)	776 (80%)	196 (20%)	1	4
6	C	234/274 (85%)	198 (85%)	36 (15%)	2	10
7	E	196/197 (100%)	177 (90%)	19 (10%)	8	28
8	F	75/137 (55%)	68 (91%)	7 (9%)	8	29
9	H	117/128 (91%)	99 (85%)	18 (15%)	2	10
10	I	113/116 (97%)	92 (81%)	21 (19%)	1	6
11	J	60/65 (92%)	37 (62%)	23 (38%)	0	0
12	K	99/102 (97%)	79 (80%)	20 (20%)	1	4
13	L	40/57 (70%)	33 (82%)	7 (18%)	2	8
All	All	3137/3657 (86%)	2540 (81%)	597 (19%)	1	6

All (597) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	4	GLN
4	A	11	LEU
4	A	21	LEU
4	A	36	ARG

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Mol	Chain	Res	Type
4	A	40	THR
4	A	43	GLU
4	A	54	ASN
4	A	55	ASP
4	A	57	ARG
4	A	58	LEU
4	A	61	ILE
4	A	62	ASP
4	A	63	ARG
4	A	69	THR
4	A	70	CYS
4	A	86	LEU
4	A	93	VAL
4	A	101	LYS
4	A	118	HIS
4	A	121	LEU
4	A	147	VAL
4	A	161	LEU
4	A	171	GLN
4	A	174	ILE
4	A	182	VAL
4	A	208	LEU
4	A	227	VAL
4	A	235	ILE
4	A	237	THR
4	A	250	ILE
4	A	252	PHE
4	A	253	ASN
4	A	263	THR
4	A	265	LYS
4	A	270	LEU
4	A	271	LYS
4	A	276	LEU
4	A	290	GLU
4	A	291	GLU
4	A	296	LEU
4	A	297	GLN
4	A	298	PHE
4	A	302	THR
4	A	303	TYR
4	A	313	GLN
4	A	315	LEU

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Mol	Chain	Res	Type
4	A	316	GLN
4	A	320	ARG
4	A	323	LYS
4	A	325	ILE
4	A	337	ARG
4	A	350	ARG
4	A	351	THR
4	A	352	VAL
4	A	360	GLU
4	A	375	THR
4	A	379	VAL
4	A	393	ARG
4	A	394	ASN
4	A	404	TYR
4	A	407	ARG
4	A	416	ARG
4	A	424	ILE
4	A	436	ILE
4	A	437	MET
4	A	438	ASP
4	A	440	ASP
4	A	442	VAL
4	A	443	LEU
4	A	447	GLN
4	A	449	SER
4	A	450	LEU
4	A	451	HIS
4	A	452	LYS
4	A	460	VAL
4	A	462	VAL
4	A	463	ILE
4	A	466	SER
4	A	469	ARG
4	A	470	LEU
4	A	471	ASN
4	A	472	LEU
4	A	474	VAL
4	A	475	THR
4	A	489	LEU
4	A	490	HIS
4	A	501	LEU
4	A	509	LEU

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Mol	Chain	Res	Type
4	A	512	VAL
4	A	513	SER
4	A	532	ARG
4	A	533	LYS
4	A	534	LEU
4	A	535	THR
4	A	541	ILE
4	A	549	MET
4	A	557	ASP
4	A	559	VAL
4	A	566	ILE
4	A	567	LYS
4	A	588	LEU
4	A	596	THR
4	A	598	LEU
4	A	599	SER
4	A	612	ILE
4	A	618	GLU
4	A	622	VAL
4	A	629	LEU
4	A	630	ILE
4	A	649	ILE
4	A	657	LEU
4	A	660	ASN
4	A	662	PHE
4	A	664	THR
4	A	672	ASP
4	A	675	THR
4	A	676	MET
4	A	678	GLU
4	A	688	LYS
4	A	691	LEU
4	A	701	LEU
4	A	702	LEU
4	A	708	MET
4	A	709	THR
4	A	710	LEU
4	A	722	LEU
4	A	740	LEU
4	A	744	LYS
4	A	761	MET
4	A	762	SER

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Mol	Chain	Res	Type
4	A	764	CYS
4	A	768	GLN
4	A	770	VAL
4	A	775	ILE
4	A	786	HIS
4	A	801	GLU
4	A	803	SER
4	A	809	THR
4	A	821	ARG
4	A	827	THR
4	A	829	VAL
4	A	845	LEU
4	A	848	ILE
4	A	864	ILE
4	A	867	ILE
4	A	878	ILE
4	A	880	LYS
4	A	883	LEU
4	A	884	ASP
4	A	886	ILE
4	A	896	ARG
4	A	908	LEU
4	A	915	SER
4	A	919	ILE
4	A	920	LEU
4	A	923	LEU
4	A	924	LYS
4	A	925	LEU
4	A	926	GLN
4	A	929	LEU
4	A	931	GLU
4	A	938	LYS
4	A	960	ILE
4	A	965	GLN
4	A	982	THR
4	A	988	LEU
4	A	999	VAL
4	A	1000	LEU
4	A	1005	GLU
4	A	1006	ILE
4	A	1007	ILE
4	A	1012	ARG

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Mol	Chain	Res	Type
4	A	1015	VAL
4	A	1024	SER
4	A	1025	ARG
4	A	1029	ARG
4	A	1038	THR
4	A	1040	GLN
4	A	1045	VAL
4	A	1047	SER
4	A	1048	ASN
4	A	1067	LEU
4	A	1077	THR
4	A	1082	ASN
4	A	1084	PHE
4	A	1085	HIS
4	A	1089	VAL
4	A	1095	THR
4	A	1098	VAL
4	A	1110	ASN
4	A	1115	SER
4	A	1116	LEU
4	A	1120	LEU
4	A	1129	GLU
4	A	1141	THR
4	A	1146	VAL
4	A	1148	ILE
4	A	1171	GLN
4	A	1173	HIS
4	A	1174	PHE
4	A	1187	GLN
4	A	1192	LEU
4	A	1199	ARG
4	A	1205	LYS
4	A	1221	LYS
4	A	1222	ASN
4	A	1223	ASP
4	A	1237	ILE
4	A	1242	VAL
4	A	1243	VAL
4	A	1261	LYS
4	A	1264	GLU
4	A	1270	ASN
4	A	1274	ARG

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Mol	Chain	Res	Type
4	A	1280	GLU
4	A	1288	ASP
4	A	1291	VAL
4	A	1297	GLU
4	A	1301	GLU
4	A	1322	ILE
4	A	1326	ARG
4	A	1329	THR
4	A	1331	SER
4	A	1333	ILE
4	A	1336	MET
4	A	1354	ASN
4	A	1355	VAL
4	A	1356	ILE
4	A	1359	ASP
4	A	1364	ASN
4	A	1366	ARG
4	A	1372	VAL
4	A	1381	LEU
4	A	1382	THR
4	A	1385	THR
4	A	1386	ARG
4	A	1391	ARG
4	A	1393	ASN
4	A	1398	MET
4	A	1403	GLU
4	A	1406	VAL
4	A	1408	ILE
4	A	1418	LEU
4	A	1426	GLU
4	A	1428	VAL
4	A	1436	ILE
4	A	1443	VAL
4	A	1444	MET
4	A	1445	ILE
4	A	1448	GLU
5	B	26	THR
5	B	35	SER
5	B	46	GLN
5	B	63	ILE
5	B	65	GLU
5	B	68	THR

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Mol	Chain	Res	Type
5	B	70	ILE
5	B	89	GLU
5	B	94	LYS
5	B	95	ILE
5	B	108	VAL
5	B	109	THR
5	B	115	GLN
5	B	116	GLU
5	B	123	THR
5	B	128	LEU
5	B	131	ASP
5	B	135	ARG
5	B	140	ILE
5	B	167	ILE
5	B	176	SER
5	B	183	GLU
5	B	187	SER
5	B	199	MET
5	B	204	ILE
5	B	223	VAL
5	B	234	ILE
5	B	240	ILE
5	B	245	GLU
5	B	246	LYS
5	B	257	LYS
5	B	268	THR
5	B	276	ILE
5	B	280	ILE
5	B	298	LEU
5	B	299	GLU
5	B	314	LEU
5	B	323	VAL
5	B	324	ILE
5	B	334	ILE
5	B	346	GLU
5	B	349	ILE
5	B	356	LEU
5	B	361	LEU
5	B	364	ILE
5	B	365	THR
5	B	368	GLU
5	B	371	GLU

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Mol	Chain	Res	Type
5	B	372	SER
5	B	384	ARG
5	B	391	ASP
5	B	396	ASP
5	B	398	ARG
5	B	408	LEU
5	B	413	LEU
5	B	416	LEU
5	B	419	THR
5	B	420	LEU
5	B	429	PHE
5	B	436	VAL
5	B	437	GLU
5	B	448	ILE
5	B	452	THR
5	B	471	LYS
5	B	473	MET
5	B	479	VAL
5	B	481	GLN
5	B	482	VAL
5	B	487	THR
5	B	492	LEU
5	B	493	SER
5	B	495	LEU
5	B	500	THR
5	B	516	ASN
5	B	527	THR
5	B	529	GLU
5	B	536	VAL
5	B	539	LEU
5	B	543	SER
5	B	544	CYS
5	B	545	ILE
5	B	547	VAL
5	B	568	ASP
5	B	582	VAL
5	B	604	ARG
5	B	605	ARG
5	B	613	VAL
5	B	617	ARG
5	B	624	LEU
5	B	628	THR

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Mol	Chain	Res	Type
5	B	635	ARG
5	B	637	LEU
5	B	642	ASP
5	B	644	GLU
5	B	646	LEU
5	B	650	GLU
5	B	651	LEU
5	B	653	VAL
5	B	655	LYS
5	B	662	MET
5	B	664	THR
5	B	666	TYR
5	B	693	ILE
5	B	705	MET
5	B	706	GLN
5	B	732	SER
5	B	739	THR
5	B	743	ILE
5	B	746	SER
5	B	751	VAL
5	B	755	ILE
5	B	760	ASP
5	B	762	ASN
5	B	769	TYR
5	B	778	MET
5	B	780	VAL
5	B	790	ASP
5	B	791	THR
5	B	792	MET
5	B	796	LEU
5	B	797	TYR
5	B	805	THR
5	B	807	ARG
5	B	815	ARG
5	B	824	ILE
5	B	825	VAL
5	B	829	CYS
5	B	835	GLN
5	B	844	SER
5	B	846	ILE
5	B	857	ARG
5	B	864	LYS

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Mol	Chain	Res	Type
5	B	865	LYS
5	B	870	ILE
5	B	878	GLN
5	B	879	ARG
5	B	883	LEU
5	B	885	MET
5	B	886	LYS
5	B	918	ILE
5	B	939	THR
5	B	944	THR
5	B	945	GLU
5	B	946	ASN
5	B	956	THR
5	B	957	ASN
5	B	963	PHE
5	B	964	VAL
5	B	970	THR
5	B	971	THR
5	B	972	LYS
5	B	978	ASP
5	B	983	ARG
5	B	995	ARG
5	B	997	GLU
5	B	999	MET
5	B	1002	THR
5	B	1028	GLU
5	B	1031	LEU
5	B	1032	SER
5	B	1045	SER
5	B	1060	ARG
5	B	1065	GLN
5	B	1069	PHE
5	B	1077	THR
5	B	1082	MET
5	B	1087	PHE
5	B	1090	THR
5	B	1091	TYR
5	B	1094	ARG
5	B	1099	VAL
5	B	1102	LYS
5	B	1113	VAL
5	B	1119	VAL

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Mol	Chain	Res	Type
5	B	1122	ARG
5	B	1124	ARG
5	B	1132	GLU
5	B	1138	MET
5	B	1145	SER
5	B	1147	LEU
5	B	1148	LYS
5	B	1150	ARG
5	B	1151	LEU
5	B	1160	VAL
5	B	1163	CYS
5	B	1175	LEU
5	B	1176	ASN
5	B	1182	CYS
5	B	1183	LYS
5	B	1185	CYS
5	B	1186	ASP
5	B	1188	LYS
5	B	1189	ILE
5	B	1194	ILE
5	B	1221	SER
5	B	1223	ASP
6	C	4	GLU
6	C	14	SER
6	C	36	VAL
6	C	37	MET
6	C	40	GLU
6	C	41	ILE
6	C	51	VAL
6	C	62	PHE
6	C	65	HIS
6	C	67	LEU
6	C	77	ILE
6	C	80	LEU
6	C	97	VAL
6	C	100	THR
6	C	102	GLN
6	C	106	GLU
6	C	137	LYS
6	C	140	ASN
6	C	144	ILE
6	C	148	ARG

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Mol	Chain	Res	Type
6	C	149	LYS
6	C	166	GLU
6	C	169	LYS
6	C	181	ASP
6	C	194	GLU
6	C	200	GLU
6	C	203	GLN
6	C	209	TYR
6	C	215	GLU
6	C	224	GLN
6	C	227	THR
6	C	235	VAL
6	C	240	VAL
6	C	241	ASP
6	C	263	THR
6	C	266	ASP
7	E	31	THR
7	E	52	ARG
7	E	65	THR
7	E	66	GLU
7	E	72	PHE
7	E	88	VAL
7	E	92	THR
7	E	94	LYS
7	E	98	ILE
7	E	127	ILE
7	E	137	GLU
7	E	158	SER
7	E	159	ASP
7	E	162	ARG
7	E	169	ARG
7	E	177	ARG
7	E	190	LEU
7	E	199	ILE
7	E	215	MET
8	F	72	LYS
8	F	86	THR
8	F	93	ILE
8	F	111	LEU
8	F	118	LEU
8	F	125	LEU
8	F	138	LEU

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Mol	Chain	Res	Type
9	H	4	THR
9	H	15	VAL
9	H	24	CYS
9	H	26	ILE
9	H	31	THR
9	H	35	GLN
9	H	39	THR
9	H	44	VAL
9	H	78	SER
9	H	80	ARG
9	H	86	ASP
9	H	94	ASP
9	H	102	TYR
9	H	106	GLU
9	H	123	MET
9	H	130	ARG
9	H	132	LEU
9	H	145	ARG
10	I	17	ARG
10	I	28	GLU
10	I	29	CYS
10	I	31	THR
10	I	32	CYS
10	I	44	TYR
10	I	49	ILE
10	I	55	THR
10	I	70	ARG
10	I	75	CYS
10	I	83	ASN
10	I	91	ARG
10	I	92	ARG
10	I	95	THR
10	I	96	SER
10	I	98	VAL
10	I	102	VAL
10	I	104	LEU
10	I	109	ILE
10	I	116	ASN
10	I	118	ARG
11	J	2	ILE
11	J	3	VAL
11	J	6	ARG

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Mol	Chain	Res	Type
11	J	7	CYS
11	J	9	SER
11	J	12	LYS
11	J	13	VAL
11	J	16	ASP
11	J	22	LEU
11	J	23	ASN
11	J	25	LEU
11	J	29	GLU
11	J	30	LEU
11	J	31	ASP
11	J	38	ARG
11	J	43	ARG
11	J	44	TYR
11	J	48	ARG
11	J	49	MET
11	J	51	LEU
11	J	52	THR
11	J	55	ASP
11	J	56	LEU
12	K	10	PHE
12	K	11	LEU
12	K	12	LEU
12	K	18	LYS
12	K	20	LYS
12	K	21	ILE
12	K	38	GLU
12	K	50	LEU
12	K	52	ASN
12	K	72	LYS
12	K	73	LEU
12	K	74	ARG
12	K	78	THR
12	K	91	CYS
12	K	97	LYS
12	K	101	LEU
12	K	103	THR
12	K	107	THR
12	K	113	THR
12	K	114	LEU
13	L	30	ILE
13	L	31	CYS

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Mol	Chain	Res	Type
13	L	34	CYS
13	L	47	ARG
13	L	48	CYS
13	L	54	ARG
13	L	57	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	54	ASN
4	A	64	ASN
4	A	68	GLN
4	A	83	HIS
4	A	92	HIS
4	A	171	GLN
4	A	225	ASN
4	A	253	ASN
4	A	256	GLN
4	A	273	ASN
4	A	282	ASN
4	A	316	GLN
4	A	397	ASN
4	A	425	GLN
4	A	447	GLN
4	A	479	ASN
4	A	517	ASN
4	A	545	GLN
4	A	587	HIS
4	A	589	GLN
4	A	654	ASN
4	A	660	ASN
4	A	700	ASN
4	A	723	ASN
4	A	741	ASN
4	A	742	ASN
4	A	757	ASN
4	A	760	GLN
4	A	768	GLN
4	A	811	GLN
4	A	877	HIS
4	A	926	GLN
4	A	965	GLN

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Mol	Chain	Res	Type
4	A	1008	GLN
4	A	1033	GLN
4	A	1110	ASN
4	A	1140	HIS
4	A	1211	GLN
4	A	1364	ASN
4	A	1390	ASN
4	A	1393	ASN
5	B	103	ASN
5	B	178	ASN
5	B	278	GLN
5	B	300	HIS
5	B	366	GLN
5	B	383	ASN
5	B	400	HIS
5	B	465	ASN
5	B	499	ASN
5	B	515	HIS
5	B	516	ASN
5	B	518	HIS
5	B	592	ASN
5	B	657	HIS
5	B	706	GLN
5	B	734	HIS
5	B	762	ASN
5	B	767	ASN
5	B	770	GLN
5	B	822	ASN
5	B	834	ASN
5	B	878	GLN
5	B	887	HIS
5	B	957	ASN
5	B	984	HIS
5	B	986	GLN
5	B	1015	HIS
5	B	1104	HIS
5	B	1161	HIS
5	B	1195	HIS
6	C	17	ASN
6	C	73	GLN
6	C	112	ASN
6	C	140	ASN

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Mol	Chain	Res	Type
6	C	167	HIS
6	C	188	HIS
6	C	224	GLN
6	C	231	ASN
6	C	242	GLN
6	C	252	GLN
7	E	54	GLN
7	E	99	HIS
7	E	104	ASN
7	E	147	HIS
7	E	174	GLN
9	H	33	GLN
9	H	133	ASN
9	H	139	ASN
10	I	83	ASN
11	J	53	HIS
12	K	29	ASN
12	K	40	HIS
12	K	52	ASN
12	K	65	HIS
12	K	76	GLN
12	K	96	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	8/10 (80%)	2 (25%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	8	G
1	R	9	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 10 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
16	UTP	A	2003[A]	-	29,30,30	1.30	1 (3%)	43,47,47	1.60	7 (16%)
16	UTP	A	2003[B]	-	29,30,30	1.29	1 (3%)	43,47,47	1.61	7 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	UTP	A	2003[A]	-	-	6/22/38/38	0/2/2/2
16	UTP	A	2003[B]	-	-	1/22/38/38	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	2003[B]	UTP	PG-O2G	3.54	1.61	1.50
16	A	2003[A]	UTP	PG-O2G	3.51	1.61	1.50

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	A	2003[B]	UTP	C4-N3-C2	-5.43	119.87	126.61
16	A	2003[A]	UTP	C4-N3-C2	-5.41	119.89	126.61
16	A	2003[A]	UTP	N3-C2-N1	3.80	119.84	114.89
16	A	2003[B]	UTP	N3-C2-N1	3.80	119.83	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	A	2003[B]	UTP	C5-C4-N3	3.78	120.10	114.80
16	A	2003[A]	UTP	C5-C4-N3	3.76	120.07	114.80
16	A	2003[B]	UTP	O4-C4-C5	-3.04	119.92	125.16
16	A	2003[A]	UTP	O4-C4-C5	-3.01	119.97	125.16
16	A	2003[B]	UTP	O1G-PG-O3B	2.45	112.86	104.64
16	A	2003[A]	UTP	O1G-PG-O3B	2.45	112.86	104.64
16	A	2003[B]	UTP	C4'-O4'-C1'	-2.45	104.06	109.47
16	A	2003[A]	UTP	C4'-O4'-C1'	-2.42	104.12	109.47
16	A	2003[B]	UTP	O2-C2-N1	-2.11	120.05	122.80
16	A	2003[A]	UTP	O2-C2-N1	-2.09	120.07	122.80

There are no chirality outliers.

All (7) torsion outliers are listed below:

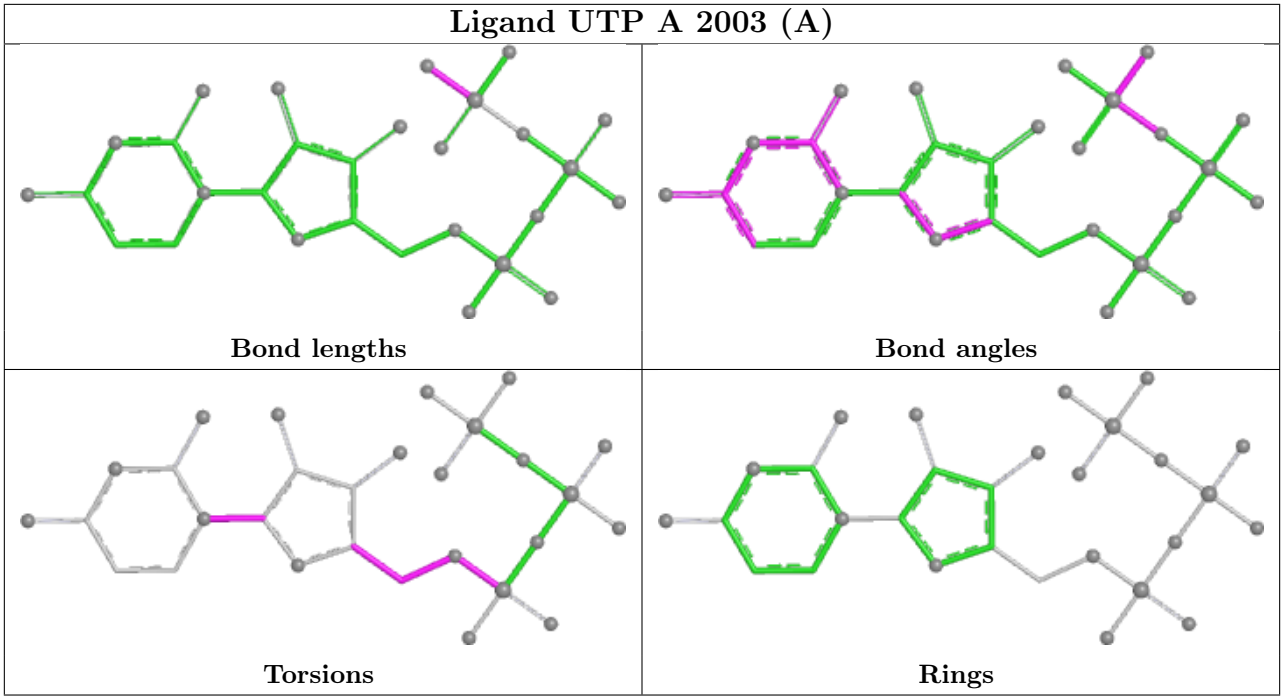
Mol	Chain	Res	Type	Atoms
16	A	2003[A]	UTP	C4'-C5'-O5'-PA
16	A	2003[A]	UTP	C3'-C4'-C5'-O5'
16	A	2003[A]	UTP	O4'-C4'-C5'-O5'
16	A	2003[A]	UTP	C5'-O5'-PA-O1A
16	A	2003[B]	UTP	C4'-C5'-O5'-PA
16	A	2003[A]	UTP	C2'-C1'-N1-C6
16	A	2003[A]	UTP	C2'-C1'-N1-C2

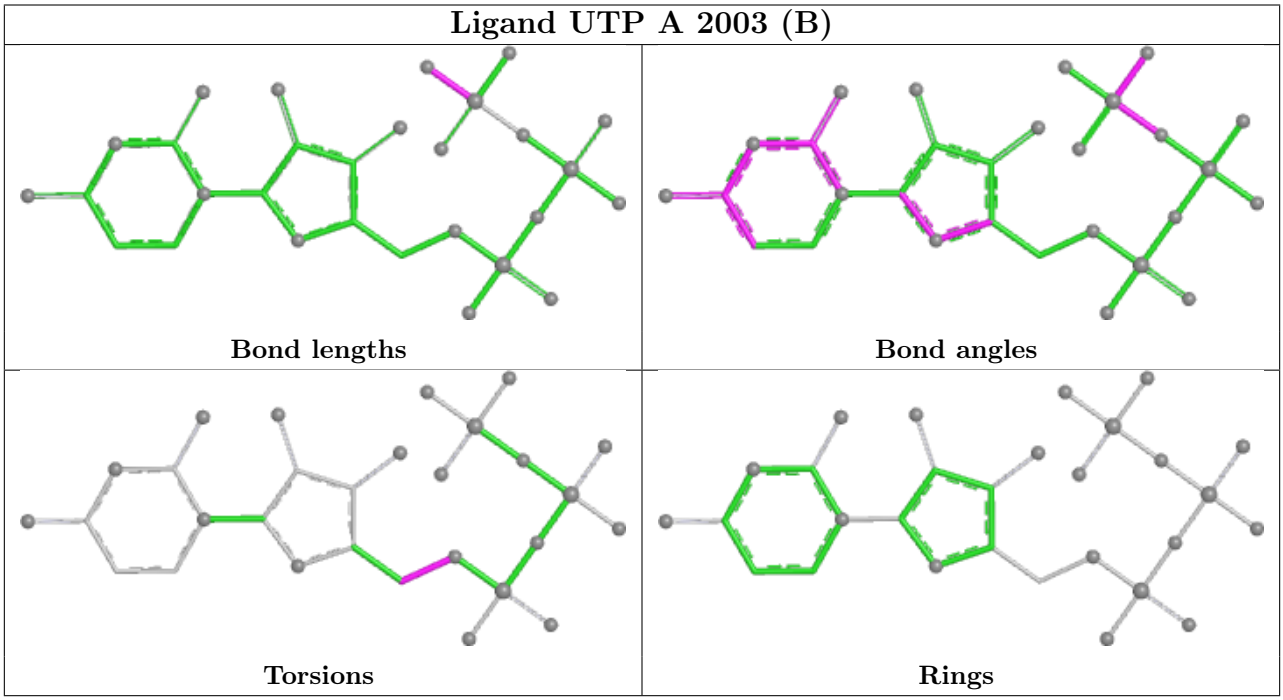
There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	2003[A]	UTP	9	0
16	A	2003[B]	UTP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	R	10/10 (100%)	2.09	5 (50%) 0 0	118, 142, 150, 153	0
2	T	28/28 (100%)	1.42	7 (25%) 2 3	138, 167, 200, 200	0
3	N	14/14 (100%)	0.88	0 100 100	155, 184, 200, 200	0
4	A	1411/1733 (81%)	0.22	45 (3%) 50 37	101, 149, 166, 193	0
5	B	1121/1224 (91%)	0.32	46 (4%) 41 29	84, 141, 159, 176	0
6	C	266/318 (83%)	-0.06	2 (0%) 82 71	109, 139, 155, 178	0
7	E	214/215 (99%)	-0.18	2 (0%) 81 68	147, 163, 172, 177	0
8	F	85/155 (54%)	0.43	2 (2%) 59 45	144, 160, 173, 178	0
9	H	133/146 (91%)	-0.02	2 (1%) 72 57	141, 154, 173, 182	0
10	I	119/122 (97%)	0.22	4 (3%) 48 35	134, 153, 168, 171	0
11	J	65/70 (92%)	0.06	0 100 100	99, 120, 137, 144	0
12	K	114/120 (95%)	-0.06	1 (0%) 81 68	130, 147, 166, 171	0
13	L	46/70 (65%)	0.37	1 (2%) 62 47	148, 174, 178, 178	0
All	All	3626/4225 (85%)	0.21	117 (3%) 50 37	84, 147, 169, 200	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	B	339	THR	5.4
4	A	1087	ALA	5.3
4	A	345	VAL	5.1
4	A	318	SER	4.8
1	R	10	A	4.4
5	B	1120	GLU	4.1
5	B	340	ALA	4.1
5	B	1101	ASP	4.1
4	A	1440	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
4	A	1433	MET	3.6
4	A	1091	SER	3.5
5	B	615	MET	3.4
10	I	13	MET	3.4
5	B	1173	ALA	3.4
5	B	338	GLY	3.3
5	B	356	LEU	3.3
5	B	344	LYS	3.3
4	A	60	SER	3.2
4	A	1090	ALA	3.2
4	A	346	ASP	3.1
5	B	1100	ASP	3.1
4	A	1403	GLU	3.1
4	A	1437	GLY	3.0
5	B	335	GLY	3.0
2	T	21	DC	3.0
13	L	27	LEU	2.9
4	A	904	THR	2.9
1	R	6	G	2.9
2	T	20	DC	2.9
8	F	115	THR	2.8
5	B	70	ILE	2.8
4	A	1083	THR	2.8
4	A	1443	VAL	2.8
5	B	1042	GLY	2.8
2	T	24	DT	2.7
5	B	1130	PHE	2.7
5	B	446	LEU	2.7
4	A	1082	ASN	2.7
5	B	529	GLU	2.7
5	B	883	LEU	2.7
5	B	1221	SER	2.6
5	B	1172	ILE	2.6
2	T	22	DT	2.6
12	K	91	CYS	2.6
5	B	1098	MET	2.6
5	B	343	ILE	2.6
4	A	810	PRO	2.5
4	A	1438	THR	2.5
10	I	2	THR	2.5
4	A	1434	ALA	2.5
4	A	1446	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
2	T	10	DA	2.5
5	B	447	ALA	2.4
5	B	140	ILE	2.4
5	B	167	ILE	2.4
1	R	7	A	2.4
4	A	355	GLY	2.4
4	A	171	GLN	2.4
5	B	1155	SER	2.4
5	B	401	PHE	2.4
4	A	486	GLU	2.4
4	A	608	ILE	2.4
4	A	740	LEU	2.4
4	A	1436	ILE	2.3
4	A	1435	PRO	2.3
5	B	113	TYR	2.3
7	E	93	MET	2.3
4	A	1086	PHE	2.3
5	B	89	GLU	2.3
10	I	41	PRO	2.3
4	A	261	ASP	2.3
5	B	467	GLY	2.2
8	F	137	TYR	2.2
4	A	398	GLU	2.2
4	A	341	MET	2.2
4	A	1176	LEU	2.2
4	A	1441	PHE	2.2
5	B	136	THR	2.2
4	A	513	SER	2.2
4	A	61	ILE	2.2
4	A	471	ASN	2.2
6	C	200	GLU	2.2
9	H	139	ASN	2.2
4	A	329	LEU	2.2
5	B	342	GLY	2.2
1	R	2	U	2.2
4	A	813	PHE	2.2
4	A	1272	THR	2.1
2	T	23	DC	2.1
5	B	112	LEU	2.1
5	B	1099	VAL	2.1
5	B	498	THR	2.1
5	B	448	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
5	B	991	GLY	2.1
5	B	837	ASP	2.1
4	A	808	LEU	2.1
9	H	90	ALA	2.1
5	B	1087	PHE	2.1
2	T	11	DG	2.1
4	A	292	ALA	2.1
4	A	473	SER	2.1
4	A	1000	LEU	2.1
5	B	406	LEU	2.1
5	B	1128	LEU	2.1
10	I	52	ILE	2.1
1	R	9	G	2.1
5	B	1157	ALA	2.1
7	E	66	GLU	2.1
5	B	1009	ASP	2.0
6	C	174	ALA	2.0
4	A	811	GLN	2.0
4	A	72	GLU	2.0
5	B	711	GLU	2.0
5	B	341	LEU	2.0
5	B	869	SER	2.0
5	B	509	ALA	2.0
4	A	168	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

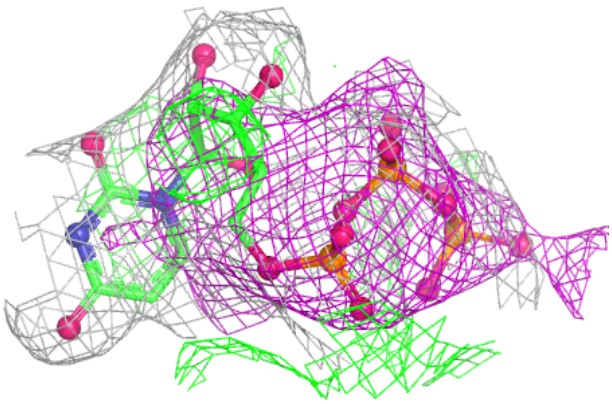
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

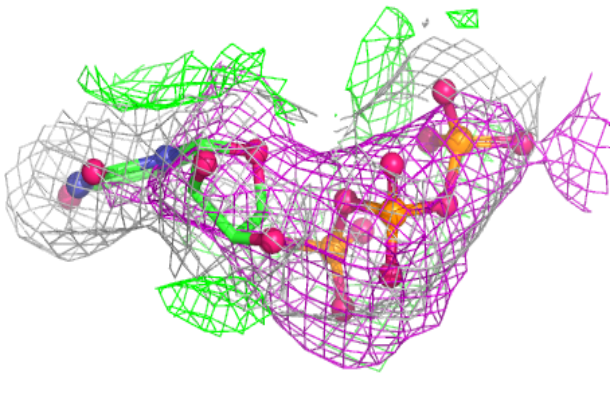
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
16	UTP	A	2003[A]	29/29	0.62	0.18	132,133,138,138	29
16	UTP	A	2003[B]	29/29	0.62	0.18	137,137,137,137	29
15	MG	A	2001	1/1	0.76	0.14	124,124,124,124	0
15	MG	A	2002	1/1	0.94	0.16	59,59,59,59	0
14	ZN	L	105	1/1	0.96	0.12	175,175,175,175	0
14	ZN	A	1734	1/1	0.97	0.20	157,157,157,157	0
14	ZN	B	1307	1/1	0.98	0.15	142,142,142,142	0
14	ZN	I	203	1/1	0.98	0.12	141,141,141,141	0
14	ZN	I	204	1/1	0.98	0.14	154,154,154,154	0
14	ZN	A	1735	1/1	0.98	0.09	149,149,149,149	0
14	ZN	J	101	1/1	0.99	0.09	109,109,109,109	0
14	ZN	C	319	1/1	0.99	0.09	149,149,149,149	0

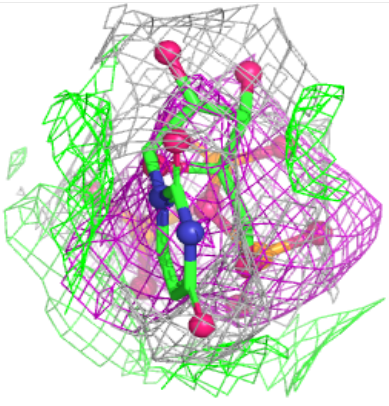
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around UTP A 2003 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

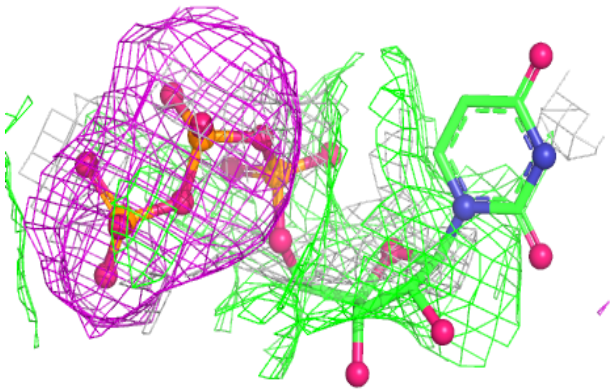


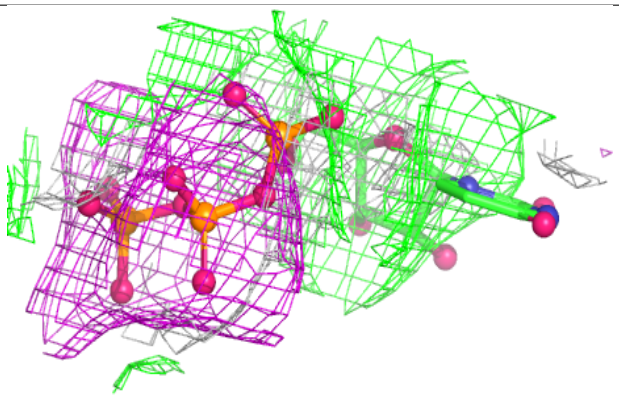


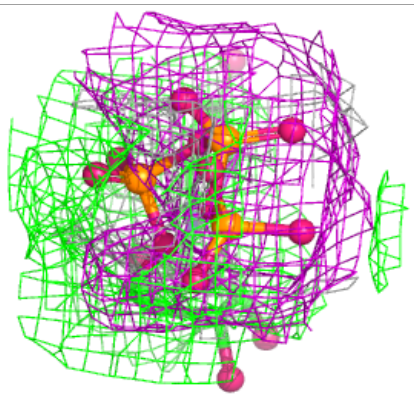


Electron density around UTP A 2003 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers

There are no such residues in this entry.