Full wwPDB X-ray Structure Validation Report (i)

Oct 19, 2023 – 01:18 AM EDT

PDB ID	:	2NVZ
Title	:	RNA Polymerase II elongation complex with UTP, updated 11/2006
Authors	:	Wang, D.; Bushnell, D.A.; Westover, K.D.; Kaplan, C.D.; Kornberg, R.D.
Deposited on	:	2006-11-14
Resolution	:	4.30 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:

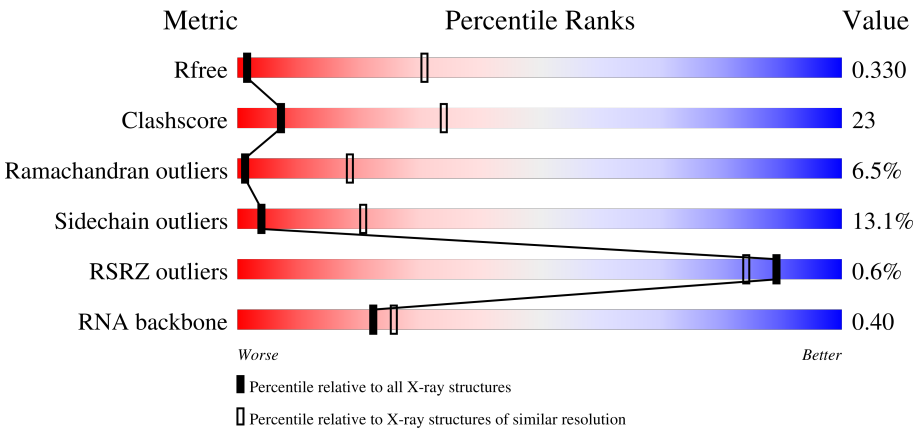
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 4.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1014 (4.80-3.80)
Clashscore	141614	1077 (4.80-3.80)
Ramachandran outliers	138981	1029 (4.80-3.80)
Sidechain outliers	138945	1012 (4.80-3.80)
RSRZ outliers	127900	1075 (4.90-3.70)
RNA backbone	3102	1058 (5.60-3.00)

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% 50%
2	T	28	29% 39% 39% 21%
3	N	14	50% 79% 21%
4	A	1733	42% 31% 6% • 19%

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Mol	Chain	Length	Quality of chain
5	B	1224	44% 38% 7% • 10%
6	C	318	45% 33% 6% 16%
7	E	215	47% 38% 5% 10%
8	F	155	35% 16% •• 46%
9	H	146	51% 29% 9% • 9%
10	I	122	50% 34% 10% • •
11	J	70	47% 37% 7% • 7%
12	K	120	58% 33% • 5%
13	L	70	34% 24% 7% 34%

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 29002 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	1398	10984	6930	1924	2069	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	1096	8701	5508	1518	1620	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
			Total	C	N	O	S			
6	C	266	2095	1317	348	417	13	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	E	193	1594	1016	283	287	8	0	0	0

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

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

- 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
			Total	C	N	O	S			
9	H	133	1068	673	180	211	4	0	0	0

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

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

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

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

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

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

- 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
			Total	C	N	O	S			
13	L	46	363	224	72	63	4	0	0	0

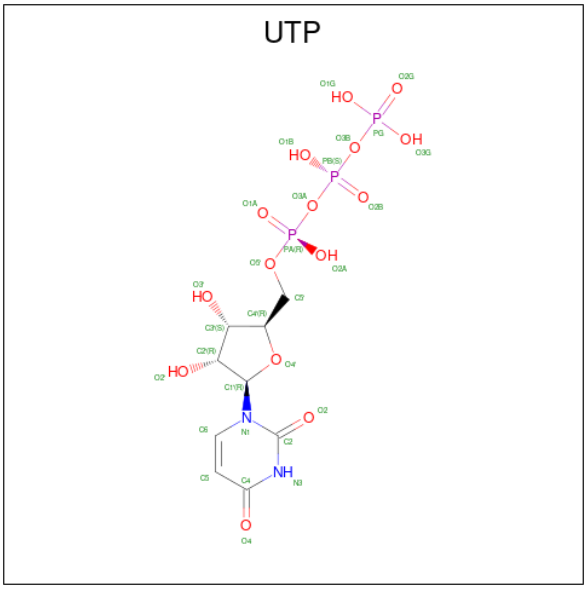
- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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



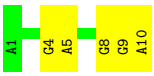
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
16	B	1	29	9	2	15	3	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

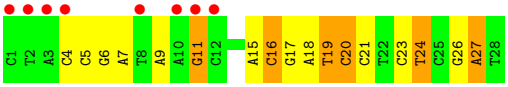
• Molecule 1: 5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*A)-3'

Chain R:



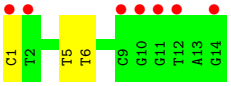
• Molecule 2: 28-MER DNA template strand

Chain T:



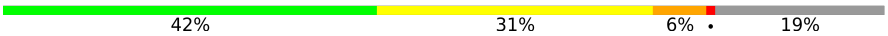
• Molecule 3: 5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*AP*G)-3'

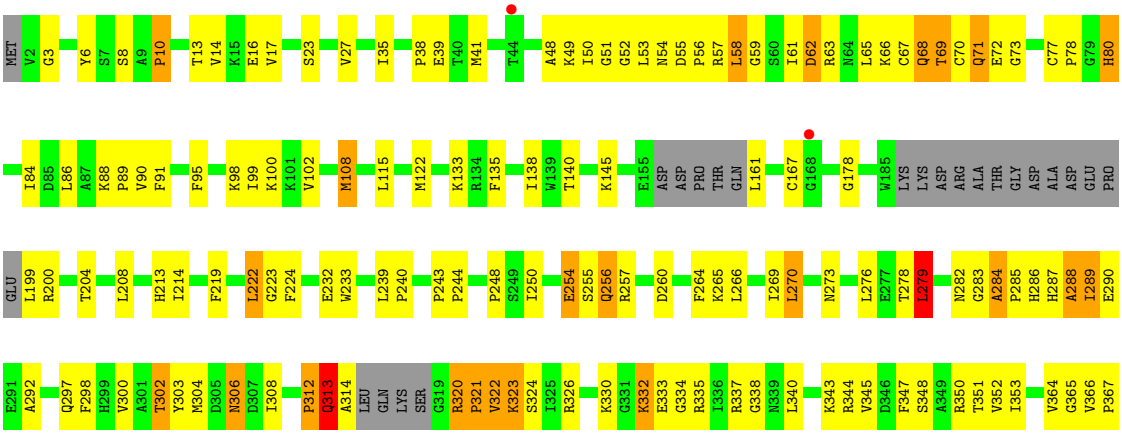
Chain N:

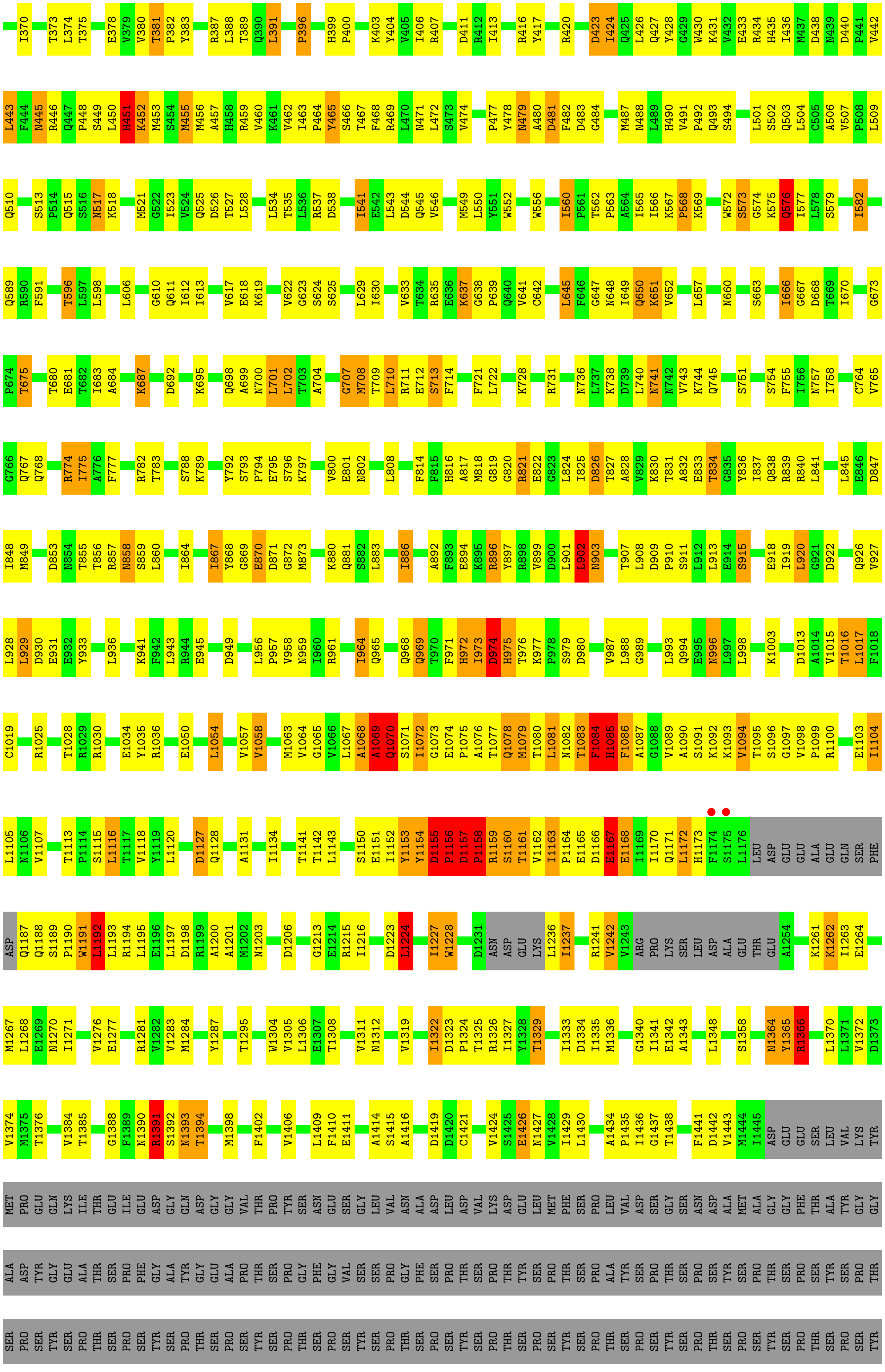


• Molecule 4: DNA-directed RNA polymerase II largest subunit

Chain A:



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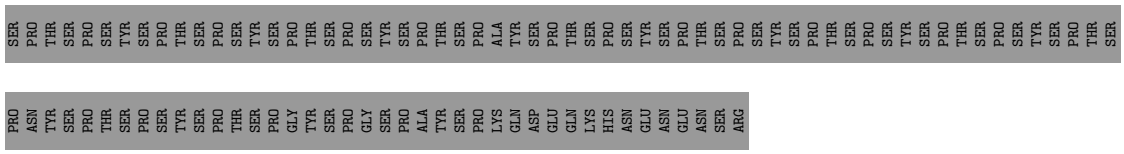
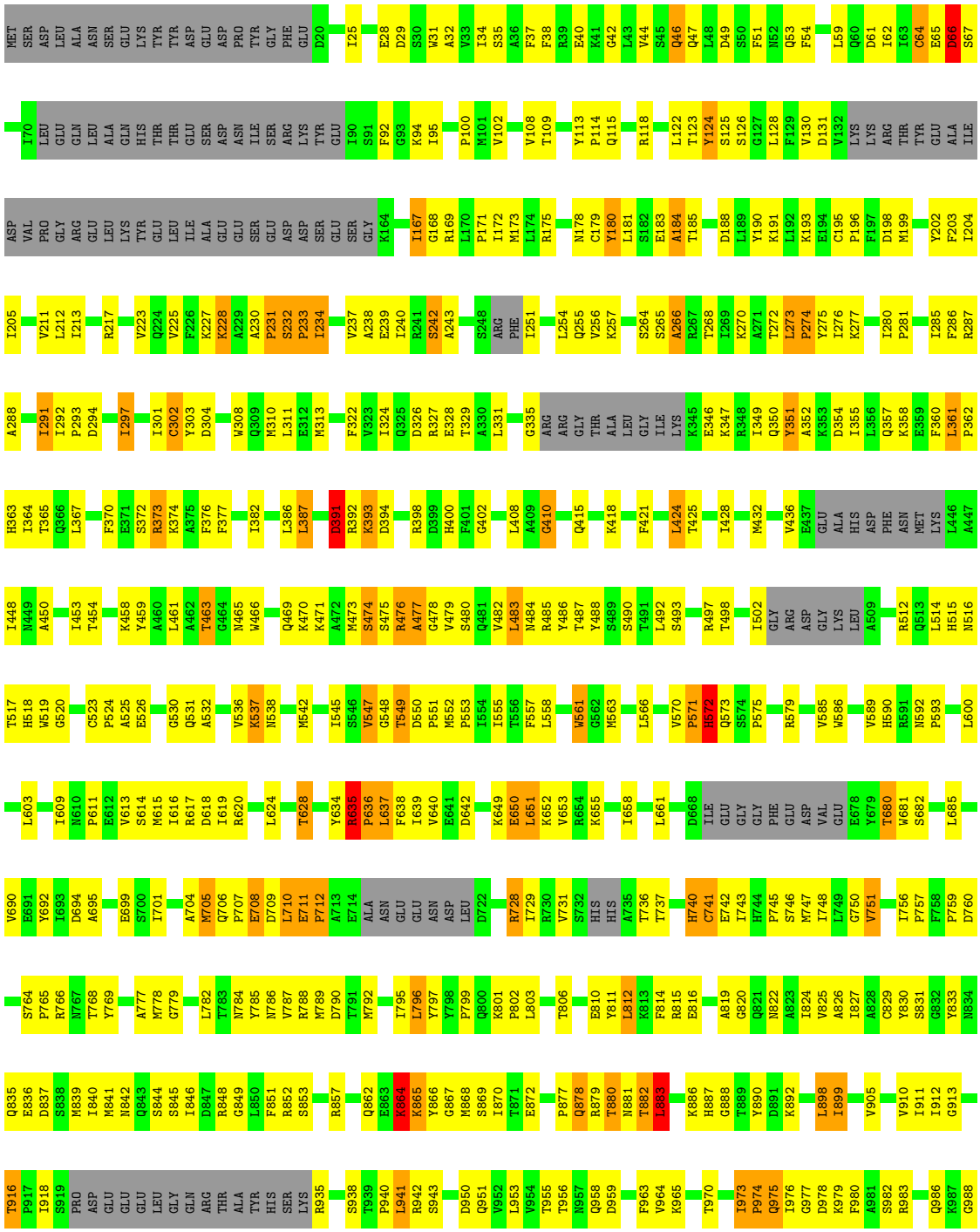
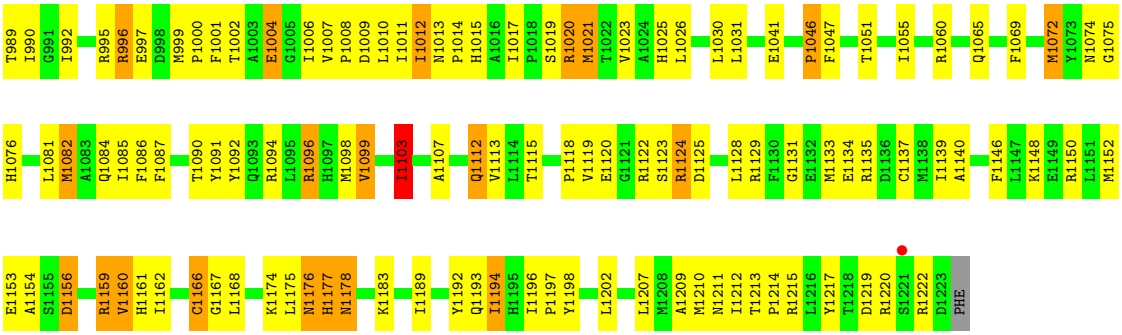
L443 F444 N445 R446 Q447 P448 S449 L450 H451 K452 M453 S454 M455 M456 A457 H458 R459 V460 K461 V462 I463 P464 Y465 S466 T467 F468 R469 L470 N471 L472 S473 V474 P477 Y478 N479 A480 D481 F482 D483 G484 M487 N488 L489 H490 V491 P492 Q493 S494 L501 S502 Q503 L504 C505 A506 V507 P508 L509
Q510 S513 P514 Q515 S516 N517 K518 M521 G522 I523 V524 Q525 D526 T527 L528 L534 T535 L536 R537 D538 I541 E542 L543 D544 Q545 V546 M549 L550 Y551 W552 W556 I560 P561 T562 P563 A564 I565 I566 K567 P568 K569 W572 S573 G574 K575 Q576 I577 L578 S579 I582
Q589 R590 F591 T596 L597 L598 L606 G610 Q611 I612 I613 V617 E618 K619 V622 G623 S624 S625 L629 I630 V633 T634 R635 E636 K637 G638 P639 Q640 V641 C642 L645 F646 G647 N648 I649 Q650 K651 V652 L657 N660 S663 I666 G667 D668 T669 I670 G673
P674 T675 T680 E681 T682 I683 A684 K687 D692 K695 Q698 A699 N700 L701 L702 T703 A704 G707 M708 T709 L710 R711 E712 S713 F714 F721 L722 K728 R731 N736 L737 K738 D739 L740 N741 N742 V743 K744 Q745 S751 S754 F755 I756 N757 I758 C764 V765
G766 Q767 Q768 R774 I775 A776 F777 R782 T783 S788 K789 Y792 S793 P794 E795 S796 K797 V800 E801 N802 L808 F814 F815 H816 A817 M818 G819 G820 R821 E822 G823 L824 I825 D826 T827 A828 V829 K830 T831 A832 E833 T834 G835 Y836 I837 Q838 R839 R840 L841 L845 E846 D847
I848 M849 D853 N854 T855 T856 R857 N858 S859 L860 I864 I867 Y868 G869 E870 D871 G872 M873 K880 Q881 S882 L883 I886 A892 F893 E894 K895 R896 Y897 R898 V899 D900 L901 L902 N903 T907 L908 D909 P910 S911 L912 L913 E914 S915 E918 I919 L920 G921 D922 Q926 V927
L928 L929 D930 E931 E932 Y933 L936 K941 F942 L943 R944 E945 D949 L956 P957 V958 N959 I960 R961 I964 Q965 Q968 Q969 T970 F971 H972 I973 D974 H975 T976 K977 P978 S979 D980 V987 L988 G989 L993 Q994 E995 N996 L997 L998 K1003 D1013 A1014 V1015 T1016 L1017 F1018
C1019 R1025 T1028 R1029 R1030 E1034 Y1035 R1036 E1050 L1054 V1057 V1058 M1063 V1064 G1065 V1066 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 E1103 I1104
L1105 N1106 V1107 T1113 P1114 S1115 L1116 T1117 V1118 Y1119 L1120 D1127 Q1128 A1131 I1134 T1141 T1142 L1143 S1150 E1151 I1152 Y1153 Y1154 D1155 P1156 D1157 P1158 R1159 S1160 T1161 V1162 I1163 P1164 E1165 D1166 E1167 E1168 I1169 I1170 Q1171 L1172 H1173 F1174 S1175 L1176 LEU ASP GLU GLU ALA GLU GLN SER PHE
ASP Q1187 Q1188 S1189 P1190 W1191 L1192 L1193 R1194 L1195 E1196 L1197 D1198 R1199 A1200 A1201 M1202 N1203 D1206 G1213 E1214 R1215 I1216 D1223 L1224 I1227 W1228 D1231 ASN ASP GLU LYS L1236 I1237 R1241 V1242 V1243 ARG PRO LYS SER LEU ASP ALA GLU THR GLU A1254 K1261 K1262 I1263 E1264
M1267 L1268 E1269 N1270 I1271 V1276 E1277 R1281 V1282 V1283 M1284 Y1287 T1295 W1304 V1305 L1306 E1307 T1308 V1311 N1312 V1319 I1322 D1323 P1324 T1325 R1326 I1327 Y1328 T1329 I1333 D1334 I1335 M1336 G1340 I1341 E1342 A1343 L1348 S1358 N1364 Y1365 R1366 L1370 L1371 V1372 D1373
V1374 M1375 T1376 V1384 T1385 G1388 F1389 N1390 R1391 S1392 N1393 T1394 M1398 F1402 V1406 L1409 F1410 E1411 A1414 S1415 A1416 D1419 D1420 C1421 V1424 S1425 E1426 N1427 V1428 I1429 L1430 A1434 P1435 I1436 G1437 T1438 F1441 D1442 V1443 M1444 I1445 ASP GLU GLU SER LEU VAL LYS TYR
MET PRO GLU GLN LYS ILE THR GLU ILE GLU ASP GLY GLN ASP GLY GLY VAL THR PRO TYR SER ASN GLU SER GLY LEU VAL ASN ALA ASP LEU ASP VAL LYS ASP GLU LEU MET PHE SER PRO LEU VAL ASP SER GLY SER ASN ASP ALA MET ALA GLY GLY PHE THR ALA TYR GLY GLY
ALA ASP TYR GLY GLU ALA THR SER PRO PHE GLY ALA TYR GLY GLU ALA PRO THR SER PRO GLY PHE GLY VAL SER SER PRO GLY PHE SER PRO THR SER PRO THR TYR SER PRO THR SER PRO ALA TYR SER PRO THR SER PRO SER TYR SER PRO THR
SER PRO SER TYR SER PRO THR SER PRO SER TYR SER PRO THR SER PRO SER TYR SER PRO THR SER PRO SER TYR SER PRO THR SER PRO SER TYR SER PRO THR SER PRO SER TYR SER PRO THR SER PRO SER TYR SER PRO THR SER PRO SER TYR



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

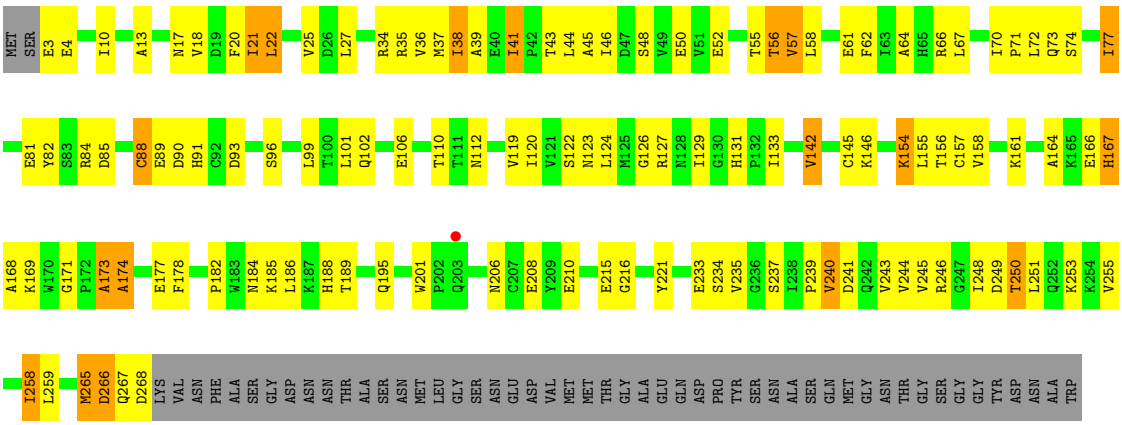
Chain B: 44% 38% 7% • 10%





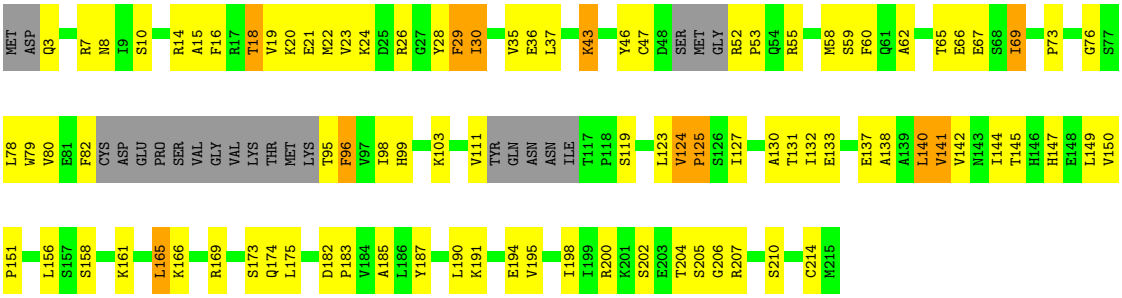
- Molecule 6: DNA-directed RNA polymerase II 45 kDa polypeptide

Chain C: 45% 33% 6% 16%



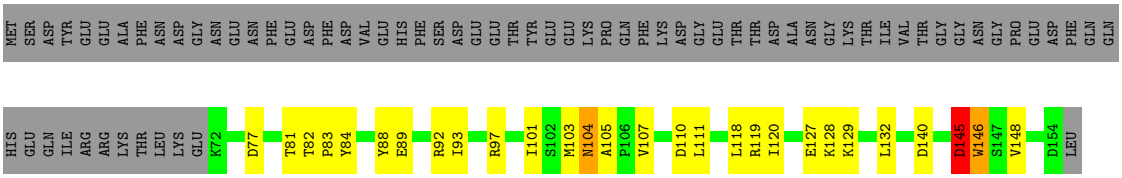
- Molecule 7: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

Chain E: 47% 38% 5% 10%



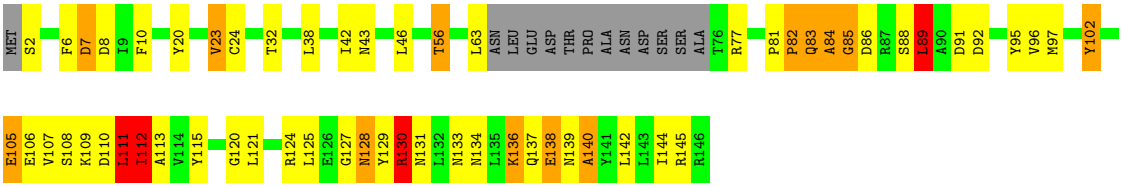
- Molecule 8: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide

Chain F: 35% 16% •• 46%



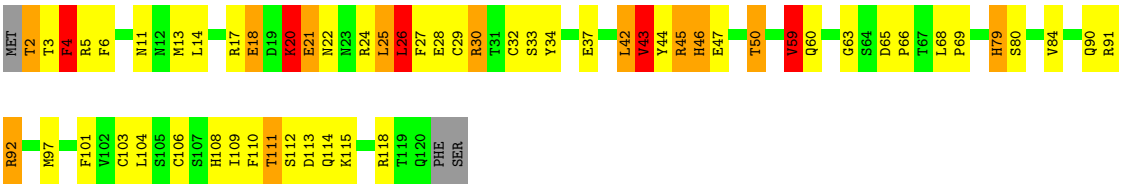
• Molecule 9: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide

Chain H:



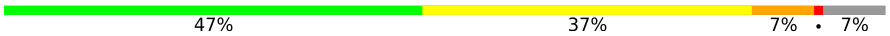
• Molecule 10: DNA-directed RNA polymerase II subunit 9

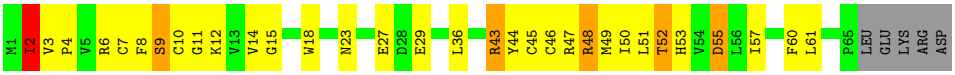
Chain I:



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

Chain J:



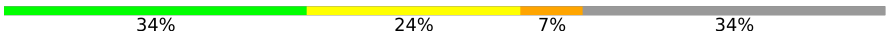


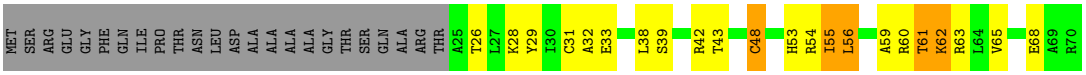
• Molecule 12: DNA-directed RNA polymerase II 13.6 kDa polypeptide

Chain K:

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

Chain L:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	169.65Å 222.34Å 194.32Å 90.00° 101.67° 90.00°	Depositor
Resolution (Å)	40.00 – 4.30 39.94 – 4.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-4.30) 86.4 (39.94-4.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	3.67 (at 4.28Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.270 , 0.332 0.277 , 0.330	Depositor DCC
R_{free} test set	4179 reflections (10.09%)	wwPDB-VP
Wilson B-factor (Å^2)	97.0	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 60.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	29002	wwPDB-VP
Average B, all atoms (Å^2)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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 (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	R	0.81	0/243	1.33	0/378
2	T	0.87	0/634	1.63	17/975 (1.7%)
3	N	0.77	0/317	1.35	1/488 (0.2%)
4	A	0.45	1/11180 (0.0%)	0.67	3/15117 (0.0%)
5	B	0.45	0/8866	0.65	1/11956 (0.0%)
6	C	0.43	0/2133	0.60	0/2891
7	E	0.44	0/1625	0.61	0/2182
8	F	0.43	0/682	0.61	1/922 (0.1%)
9	H	0.47	0/1086	0.77	2/1470 (0.1%)
10	I	0.48	0/989	0.74	0/1331
11	J	0.47	0/541	0.62	0/727
12	K	0.46	0/937	0.60	0/1265
13	L	0.53	0/365	0.79	0/485
All	All	0.47	1/29598 (0.0%)	0.72	25/40187 (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	9
5	B	0	1
9	H	0	2
All	All	0	12

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1158	PRO	CG-CD	5.94	1.70	1.50

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	23	DC	O4'-C4'-C3'	-9.30	100.42	106.00
2	T	16	DC	O4'-C1'-N1	9.29	114.50	108.00
2	T	11	DG	O4'-C1'-N9	8.90	114.23	108.00
2	T	23	DC	O4'-C1'-N1	8.24	113.77	108.00
2	T	20	DC	O4'-C4'-C3'	-8.15	101.11	106.00
2	T	19	DT	C4-C5-C7	8.11	123.86	119.00
2	T	15	DA	P-O3'-C3'	7.71	128.96	119.70
2	T	19	DT	C6-C5-C7	-7.40	118.46	122.90
2	T	27	DA	O4'-C4'-C3'	-7.23	101.61	104.50
2	T	20	DC	C4'-C3'-C2'	-6.19	97.53	103.10
5	B	883	LEU	CA-CB-CG	6.16	129.46	115.30
2	T	23	DC	C4'-C3'-C2'	-6.04	97.66	103.10
2	T	16	DC	O4'-C4'-C3'	-6.00	102.10	104.50
3	N	1	DC	O4'-C1'-N1	5.97	112.18	108.00
4	A	1070	GLN	N-CA-C	-5.95	94.95	111.00
2	T	4	DC	O4'-C1'-N1	5.54	111.88	108.00
2	T	5	DC	C1'-O4'-C4'	-5.42	104.69	110.10
4	A	1069	ALA	N-CA-C	-5.38	96.46	111.00
2	T	24	DT	N3-C4-O4	5.37	123.12	119.90
9	H	89	LEU	CA-CB-CG	5.32	127.54	115.30
2	T	5	DC	O4'-C1'-N1	5.20	111.64	108.00
4	A	701	LEU	CA-CB-CG	5.09	127.02	115.30
8	F	118	LEU	CA-CB-CG	5.07	126.97	115.30
9	H	111	LEU	CA-CB-CG	5.04	126.89	115.30
2	T	4	DC	C1'-O4'-C4'	-5.03	105.07	110.10

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	1068	ALA	Peptide
4	A	1069	ALA	Peptide
4	A	1070	GLN	Peptide
4	A	1079	MET	Peptide
4	A	1084	PHE	Peptide
4	A	1155	ASP	Peptide
4	A	1157	ASP	Peptide
4	A	451	HIS	Peptide
4	A	974	ASP	Peptide
5	B	1176	ASN	Peptide
9	H	128	ASN	Peptide

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Mol	Chain	Res	Type	Group
9	H	130	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	216	0	109	6	0
2	T	566	0	316	18	0
3	N	284	0	161	2	0
4	A	10984	0	11069	568	0
5	B	8701	0	8728	479	0
6	C	2095	0	2051	92	0
7	E	1594	0	1622	52	0
8	F	670	0	690	15	0
9	H	1068	0	1040	52	0
10	I	971	0	928	63	0
11	J	532	0	542	38	0
12	K	919	0	929	32	0
13	L	363	0	387	13	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	B	29	0	11	2	0
All	All	29002	0	28583	1299	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (1299) 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)
4:A:701:LEU:HA	4:A:702:LEU:CB	1.68	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:975:HIS:HB3	4:A:976:THR:OG1	1.41	1.19
4:A:335:ARG:HD2	5:B:1202:LEU:HD12	1.27	1.16
4:A:1167:GLU:CB	4:A:1168:GLU:HA	1.75	1.15
5:B:1019:SER:HB2	5:B:1020:ARG:HB2	1.24	1.15
4:A:707:GLY:HA2	4:A:709:THR:H	0.99	1.14
4:A:712:GLU:H	4:A:713:SER:HB2	0.98	1.14
4:A:709:THR:HA	4:A:710:LEU:HB3	1.19	1.13
5:B:227:LYS:HA	5:B:228:LYS:HB2	1.29	1.12
10:I:3:THR:HA	10:I:4:PHE:CG	1.85	1.11
6:C:39:ALA:HA	6:C:164:ALA:HB3	1.33	1.11
4:A:1167:GLU:HB2	4:A:1168:GLU:CA	1.81	1.09
5:B:705:MET:HB3	5:B:706:GLN:HB2	1.08	1.08
4:A:1080:THR:O	4:A:1082:ASN:N	1.86	1.08
5:B:877:PRO:HA	5:B:878:GLN:CB	1.84	1.07
9:H:85:GLY:HA2	9:H:86:ASP:HB2	1.14	1.06
5:B:868:MET:H	5:B:869:SER:HB3	0.92	1.06
10:I:20:LYS:HA	10:I:21:GLU:O	1.57	1.05
4:A:707:GLY:HA2	4:A:709:THR:N	1.72	1.04
5:B:327:ARG:HB3	5:B:328:GLU:HB2	1.09	1.04
5:B:293:PRO:HA	5:B:294:ASP:HB2	1.40	1.03
4:A:701:LEU:CA	4:A:702:LEU:HB2	1.88	1.03
5:B:635:ARG:HB2	5:B:636:PRO:HD2	1.04	1.03
13:L:42:ARG:HB2	13:L:43:THR:HB	1.35	1.03
10:I:25:LEU:HA	10:I:26:LEU:CB	1.89	1.02
5:B:256:VAL:HG11	5:B:382:ILE:HD11	1.40	1.02
4:A:712:GLU:N	4:A:713:SER:HB2	1.73	1.02
10:I:45:ARG:HA	10:I:46:HIS:HB2	1.05	1.02
5:B:868:MET:N	5:B:869:SER:HB3	1.74	1.02
5:B:636:PRO:HB2	5:B:637:LEU:HB3	1.43	1.00
5:B:1019:SER:CB	5:B:1020:ARG:HB2	1.91	1.00
5:B:868:MET:H	5:B:869:SER:CB	1.75	1.00
9:H:111:LEU:HB3	9:H:128:ASN:HB2	1.41	0.99
9:H:85:GLY:CA	9:H:86:ASP:HB2	1.91	0.99
4:A:709:THR:HA	4:A:710:LEU:CB	1.92	0.99
5:B:1002:THR:HG22	5:B:1006:ILE:H	1.26	0.99
5:B:877:PRO:HA	5:B:878:GLN:HB2	1.44	0.98
10:I:45:ARG:HA	10:I:46:HIS:CB	1.93	0.98
4:A:1091:SER:HB2	4:A:1092:LYS:C	1.84	0.98
5:B:635:ARG:CB	5:B:636:PRO:HD2	1.92	0.98
4:A:712:GLU:H	4:A:713:SER:CB	1.76	0.98
10:I:25:LEU:HA	10:I:26:LEU:HB2	1.44	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:635:ARG:HB2	5:B:636:PRO:CD	1.94	0.97
4:A:802:ASN:HD21	5:B:729:ILE:H	0.98	0.97
4:A:67:CYS:CB	4:A:70:CYS:HB2	1.93	0.97
9:H:85:GLY:HA2	9:H:86:ASP:CB	1.94	0.97
4:A:1071:SER:H	4:A:1072:ILE:HB	1.26	0.96
10:I:63:GLY:HA3	10:I:104:LEU:HD21	1.45	0.96
10:I:45:ARG:CA	10:I:46:HIS:HB2	1.95	0.96
4:A:868:TYR:HE1	4:A:1064:VAL:HG11	1.30	0.95
4:A:1236:LEU:HA	4:A:1237:ILE:HB	1.46	0.95
4:A:782:ARG:HB3	4:A:789:LYS:HA	1.46	0.95
5:B:766:ARG:HH21	5:B:1020:ARG:HA	1.26	0.95
4:A:284:ALA:H	4:A:285:PRO:HD3	1.29	0.94
5:B:350:GLN:HB3	5:B:351:TYR:HB2	1.48	0.94
4:A:284:ALA:H	4:A:285:PRO:CD	1.80	0.94
4:A:701:LEU:HA	4:A:702:LEU:HB2	0.95	0.94
6:C:58:LEU:HD11	11:J:2:ILE:HD12	1.50	0.93
5:B:882:THR:HB	5:B:883:LEU:HA	1.49	0.92
4:A:709:THR:CA	4:A:710:LEU:HB3	2.00	0.91
6:C:67:LEU:O	6:C:70:ILE:HG22	1.69	0.91
5:B:327:ARG:CB	5:B:328:GLU:HB2	2.01	0.90
1:R:10:A:H61	2:T:19:DT:H3	1.16	0.90
4:A:282:ASN:HB3	4:A:283:GLY:CA	2.02	0.90
9:H:84:ALA:HA	9:H:85:GLY:C	1.92	0.90
4:A:108:MET:HE3	4:A:167:CYS:HB2	1.52	0.90
5:B:122:LEU:HD22	5:B:958:GLN:HG3	1.51	0.89
1:R:4:G:H2'	1:R:5:A:H8	1.38	0.89
5:B:124:TYR:HH	5:B:179:CYS:HG	1.17	0.89
6:C:74:SER:O	6:C:77:ILE:HB	1.74	0.87
5:B:642:ASP:HB3	5:B:649:LYS:HG3	1.55	0.87
5:B:636:PRO:HB2	5:B:637:LEU:CB	2.05	0.86
5:B:995:ARG:HB3	5:B:997:GLU:OE2	1.76	0.86
1:R:4:G:H2'	1:R:5:A:C8	2.10	0.85
4:A:567:LYS:HB2	4:A:568:PRO:HD2	1.56	0.85
4:A:1085:HIS:H	4:A:1085:HIS:CD2	1.88	0.85
4:A:1152:ILE:HA	4:A:1153:TYR:HB2	1.57	0.84
5:B:705:MET:HB3	5:B:706:GLN:CB	2.01	0.84
4:A:630:ILE:HD12	4:A:630:ILE:H	1.43	0.84
5:B:705:MET:CB	5:B:706:GLN:HB2	2.03	0.84
1:R:9:G:N2	2:T:21:DC:H1'	1.92	0.83
4:A:67:CYS:HB2	4:A:70:CYS:HB2	1.59	0.83
4:A:1082:ASN:N	4:A:1083:THR:HA	1.90	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1191:TRP:HA	4:A:1192:LEU:HB2	1.58	0.83
5:B:782:LEU:HD13	5:B:784:ASN:HD21	1.43	0.83
4:A:483:ASP:HA	5:B:988:GLY:HA2	1.61	0.83
5:B:557:PHE:O	5:B:561:TRP:HB3	1.79	0.83
4:A:1083:THR:OG1	4:A:1084:PHE:HB3	1.79	0.83
4:A:1097:GLY:H	4:A:1100:ARG:HB2	1.41	0.83
5:B:899:ILE:HD11	5:B:911:ILE:HG12	1.60	0.83
4:A:868:TYR:CE1	4:A:1064:VAL:HG11	2.12	0.82
5:B:827:ILE:HG12	5:B:1012:ILE:HD11	1.59	0.82
7:E:165:LEU:HD21	7:E:175:LEU:HD21	1.61	0.82
10:I:25:LEU:CA	10:I:26:LEU:HB2	2.08	0.82
4:A:335:ARG:HD2	5:B:1202:LEU:CD1	2.06	0.82
6:C:184:ASN:ND2	6:C:189:THR:O	2.13	0.82
5:B:877:PRO:HA	5:B:878:GLN:HB3	1.62	0.81
5:B:973:ILE:HG22	5:B:974:PRO:HD2	1.63	0.81
4:A:1191:TRP:HA	4:A:1192:LEU:CB	2.10	0.81
5:B:571:PRO:HB2	5:B:572:HIS:HA	1.60	0.81
5:B:498:THR:HB	5:B:537:LYS:O	1.81	0.81
10:I:20:LYS:HA	10:I:21:GLU:C	2.01	0.81
4:A:326:ARG:HG2	4:A:1406:VAL:HG21	1.60	0.81
6:C:248:ILE:HG23	12:K:98:LEU:HD22	1.61	0.81
5:B:327:ARG:HB3	5:B:328:GLU:CB	2.04	0.81
10:I:43:VAL:HB	10:I:44:TYR:HA	1.61	0.81
11:J:3:VAL:HG21	11:J:18:TRP:CG	2.16	0.80
5:B:349:ILE:HA	5:B:352:ALA:HB2	1.63	0.80
1:R:9:G:H22	2:T:21:DC:H1'	1.46	0.80
4:A:902:LEU:O	4:A:903:ASN:HB2	1.81	0.80
16:B:3000:UTP:O2A	16:B:3000:UTP:H4'	1.79	0.80
4:A:423:ASP:CG	4:A:424:ILE:H	1.85	0.79
4:A:1159:ARG:HB2	4:A:1161:THR:N	1.97	0.79
5:B:824:ILE:HG12	11:J:48:ARG:HH12	1.45	0.79
5:B:955:THR:HG22	5:B:956:THR:H	1.46	0.79
4:A:1083:THR:N	4:A:1084:PHE:O	2.16	0.79
4:A:1089:VAL:N	4:A:1090:ALA:HA	1.98	0.78
5:B:1008:PRO:HB3	5:B:1087:PHE:HE1	1.45	0.78
4:A:707:GLY:CA	4:A:709:THR:H	1.91	0.78
5:B:996:ARG:HG3	5:B:1007:VAL:HG21	1.64	0.78
5:B:493:SER:OG	5:B:751:VAL:HB	1.83	0.78
5:B:600:LEU:HB3	5:B:615:MET:SD	2.24	0.78
5:B:839:MET:HE3	5:B:1010:LEU:HD11	1.66	0.77
4:A:86:LEU:HA	4:A:273:ASN:HD21	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:351:THR:HG22	4:A:352:VAL:N	1.99	0.77
5:B:256:VAL:HG11	5:B:382:ILE:CD1	2.14	0.77
6:C:58:LEU:HD11	11:J:2:ILE:CD1	2.13	0.77
10:I:17:ARG:O	10:I:26:LEU:HB3	1.85	0.77
5:B:572:HIS:H	5:B:573:GLN:C	1.88	0.77
4:A:834:THR:HG21	4:A:1080:THR:HG21	1.66	0.77
5:B:801:LYS:O	11:J:52:THR:HG22	1.83	0.77
4:A:681:GLU:HA	4:A:684:ALA:HB3	1.66	0.77
5:B:796:LEU:HB3	5:B:799:PRO:HG3	1.67	0.77
4:A:278:THR:O	4:A:279:LEU:HB2	1.86	0.76
5:B:705:MET:H	5:B:710:LEU:HD13	1.51	0.76
5:B:277:LYS:HD2	5:B:335:GLY:H	1.50	0.76
13:L:32:ALA:H	13:L:55:ILE:HD13	1.50	0.76
13:L:42:ARG:CB	13:L:43:THR:HB	2.16	0.76
4:A:1228:TRP:HD1	4:A:1228:TRP:O	1.68	0.76
5:B:877:PRO:CA	5:B:878:GLN:CB	2.63	0.75
6:C:93:ASP:OD1	6:C:122:SER:HB2	1.87	0.75
4:A:675:THR:HG21	4:A:736:ASN:HD21	1.49	0.75
5:B:911:ILE:HG22	5:B:912:ILE:HG13	1.68	0.75
4:A:67:CYS:HB3	4:A:70:CYS:HB2	1.66	0.75
4:A:1072:ILE:HG22	4:A:1073:GLY:N	2.02	0.75
5:B:572:HIS:H	5:B:573:GLN:CA	1.99	0.75
4:A:701:LEU:CA	4:A:702:LEU:CB	2.58	0.75
4:A:1167:GLU:HB2	4:A:1168:GLU:HA	0.86	0.75
4:A:1155:ASP:CG	4:A:1190:PRO:HA	2.07	0.75
4:A:1159:ARG:HB2	4:A:1160:SER:C	2.07	0.75
4:A:579:SER:HA	4:A:582:ILE:CG1	2.17	0.74
4:A:1427:ASN:HB2	4:A:1434:ALA:HB2	1.69	0.74
4:A:1069:ALA:HB1	4:A:1070:GLN:HA	1.69	0.74
4:A:630:ILE:HD12	4:A:630:ILE:N	2.02	0.74
6:C:244:VAL:HG21	12:K:105:PHE:CZ	2.23	0.74
4:A:446:ARG:HH12	4:A:448:PRO:HD2	1.52	0.74
6:C:34:ARG:O	6:C:38:ILE:HG12	1.87	0.74
5:B:227:LYS:HA	5:B:228:LYS:CB	2.15	0.74
10:I:3:THR:HA	10:I:4:PHE:CB	2.17	0.74
9:H:111:LEU:HA	9:H:112:ILE:HB	1.70	0.73
4:A:1071:SER:N	4:A:1072:ILE:HB	2.02	0.73
5:B:1002:THR:HG23	5:B:1004:GLU:H	1.51	0.73
6:C:58:LEU:HD12	6:C:145:CYS:SG	2.28	0.73
4:A:565:ILE:HG23	4:A:567:LYS:HE3	1.70	0.73
4:A:1092:LYS:HB3	4:A:1093:LYS:HA	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1093:LYS:HB3	4:A:1094:VAL:HB	1.71	0.73
2:T:6:DG:H2"	2:T:7:DA:C8	2.23	0.73
4:A:751:SER:HB2	5:B:1015:HIS:HE1	1.53	0.73
6:C:186:LEU:HB3	6:C:188:HIS:HD2	1.53	0.73
5:B:864:LYS:H	5:B:872:GLU:HB2	1.54	0.73
4:A:282:ASN:HB3	4:A:283:GLY:HA3	1.70	0.73
10:I:20:LYS:HG2	10:I:24:ARG:H	1.54	0.73
5:B:611:PRO:HB3	5:B:685:LEU:HD11	1.70	0.72
10:I:43:VAL:CB	10:I:44:TYR:HA	2.17	0.72
13:L:42:ARG:HB2	13:L:43:THR:CB	2.16	0.72
4:A:638:GLY:H	4:A:641:VAL:HB	1.54	0.72
4:A:915:SER:HB2	4:A:919:ILE:HG12	1.72	0.72
5:B:636:PRO:CB	5:B:637:LEU:HA	2.18	0.72
4:A:51:GLY:HA2	4:A:56:PRO:HG3	1.70	0.72
5:B:1001:PHE:HE1	6:C:178:PHE:HB3	1.53	0.72
4:A:1091:SER:HB2	4:A:1092:LYS:O	1.88	0.72
10:I:101:PHE:HE1	10:I:112:SER:HB3	1.52	0.72
11:J:43:ARG:HG3	11:J:46:CYS:SG	2.29	0.72
4:A:975:HIS:HB3	4:A:976:THR:HG1	1.51	0.72
5:B:882:THR:HG21	5:B:935:ARG:HA	1.70	0.72
4:A:579:SER:HA	4:A:582:ILE:HG13	1.71	0.72
4:A:828:ALA:HB2	5:B:530:GLY:HA2	1.72	0.72
5:B:705:MET:O	5:B:742:GLU:HB3	1.90	0.72
4:A:751:SER:HB2	5:B:1015:HIS:CE1	2.25	0.71
5:B:636:PRO:CB	5:B:637:LEU:CA	2.69	0.71
5:B:126:SER:OG	5:B:172:ILE:HD11	1.90	0.71
5:B:526:GLU:HG2	5:B:538:ASN:HD22	1.54	0.71
5:B:642:ASP:HA	5:B:649:LYS:HA	1.72	0.71
4:A:1017:LEU:HB2	7:E:205:SER:HA	1.72	0.71
5:B:357:GLN:HA	5:B:374:LYS:NZ	2.05	0.71
4:A:288:ALA:HA	4:A:290:GLU:N	2.06	0.70
4:A:961:ARG:HH11	4:A:961:ARG:HG3	1.56	0.70
4:A:899:VAL:HB	4:A:929:LEU:HD11	1.74	0.70
4:A:1072:ILE:HG22	4:A:1073:GLY:H	1.56	0.70
10:I:4:PHE:C	10:I:4:PHE:HD1	1.94	0.70
5:B:842:ASN:HB3	5:B:845:SER:OG	1.91	0.70
4:A:1075:PRO:O	4:A:1079:MET:N	2.24	0.70
5:B:1156:ASP:HB2	5:B:1198:TYR:H	1.55	0.70
4:A:886:ILE:HD11	4:A:943:LEU:HB3	1.73	0.70
5:B:1019:SER:CA	5:B:1020:ARG:HB2	2.22	0.70
11:J:44:TYR:HA	11:J:47:ARG:HB2	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:802:ASN:HD21	5:B:729:ILE:N	1.83	0.69
5:B:636:PRO:HB2	5:B:637:LEU:CA	2.23	0.69
4:A:288:ALA:HA	4:A:290:GLU:H	1.57	0.69
5:B:1177:HIS:HA	5:B:1178:ASN:HB2	1.74	0.69
6:C:142:VAL:HG13	11:J:15:GLY:HA3	1.73	0.69
5:B:986:GLN:HE21	5:B:1025:HIS:CD2	2.10	0.69
9:H:105:GLU:HG3	9:H:106:GLU:H	1.58	0.69
5:B:168:GLY:H	5:B:450:ALA:HB1	1.57	0.69
5:B:997:GLU:OE1	6:C:39:ALA:HB2	1.92	0.69
4:A:657:LEU:HD21	5:B:829:CYS:HB3	1.75	0.69
10:I:25:LEU:HA	10:I:26:LEU:HB3	1.72	0.69
4:A:1064:VAL:O	4:A:1068:ALA:N	2.26	0.69
10:I:25:LEU:CA	10:I:26:LEU:CB	2.70	0.68
10:I:33:SER:HA	10:I:34:TYR:HB3	1.75	0.68
5:B:280:ILE:HB	5:B:285:ILE:HD11	1.76	0.68
5:B:363:HIS:O	5:B:364:ILE:HB	1.93	0.68
6:C:18:VAL:HG12	6:C:20:PHE:HD2	1.59	0.68
4:A:446:ARG:NH1	4:A:448:PRO:HD2	2.09	0.68
4:A:1083:THR:N	4:A:1084:PHE:C	2.47	0.68
4:A:668:ASP:HB3	4:A:743:VAL:HG23	1.74	0.67
4:A:1200:ALA:HB2	4:A:1203:ASN:HB2	1.77	0.67
5:B:65:GLU:O	5:B:66:ASP:HB3	1.95	0.67
5:B:827:ILE:HG12	5:B:1012:ILE:CD1	2.25	0.67
4:A:711:ARG:HA	4:A:713:SER:HB2	1.77	0.67
4:A:834:THR:HG21	4:A:1080:THR:CG2	2.25	0.67
4:A:1084:PHE:CD1	4:A:1085:HIS:HA	2.30	0.67
6:C:21:ILE:HG22	6:C:22:LEU:H	1.59	0.67
5:B:308:TRP:HA	5:B:311:LEU:HD12	1.77	0.67
5:B:852:ARG:HG2	5:B:973:ILE:HG23	1.76	0.67
10:I:17:ARG:HB2	10:I:26:LEU:HD12	1.77	0.66
4:A:1085:HIS:H	4:A:1085:HIS:HD2	1.41	0.66
4:A:1085:HIS:CD2	4:A:1085:HIS:N	2.63	0.66
5:B:287:ARG:NH1	5:B:324:ILE:O	2.28	0.66
6:C:101:LEU:HD23	6:C:155:LEU:HD12	1.78	0.66
4:A:1069:ALA:HA	4:A:1072:ILE:HG21	1.77	0.66
4:A:1143:LEU:HB3	4:A:1268:LEU:HA	1.76	0.66
4:A:1228:TRP:O	4:A:1228:TRP:CD1	2.48	0.66
5:B:542:MET:HB3	5:B:636:PRO:HD3	1.78	0.66
5:B:1112:GLN:HG3	5:B:1119:VAL:HG12	1.76	0.65
4:A:630:ILE:H	4:A:630:ILE:CD1	2.09	0.65
5:B:230:ALA:N	5:B:231:PRO:HD3	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1137:CYS:O	5:B:1140:ALA:HB3	1.95	0.65
4:A:1104:ILE:HG22	4:A:1105:LEU:HD12	1.79	0.65
4:A:1159:ARG:HD2	4:A:1161:THR:HG23	1.77	0.65
4:A:994:GLN:HG3	4:A:1019:CYS:SG	2.36	0.65
9:H:88:SER:O	9:H:89:LEU:HB3	1.95	0.65
4:A:69:THR:HG21	5:B:1174:LYS:HE3	1.78	0.65
4:A:782:ARG:NH2	5:B:699:GLU:O	2.29	0.65
4:A:1348:LEU:HG	4:A:1372:VAL:HG22	1.79	0.65
5:B:313:MET:HE2	5:B:386:LEU:HD22	1.78	0.65
5:B:709:ASP:HB3	5:B:710:LEU:HD12	1.79	0.65
5:B:25:ILE:HD11	5:B:653:VAL:HB	1.78	0.65
5:B:835:GLN:HA	5:B:1013:ASN:HD22	1.62	0.65
5:B:636:PRO:HB3	5:B:637:LEU:HA	1.78	0.64
5:B:639:ILE:HA	5:B:740:HIS:HB3	1.78	0.64
4:A:381:THR:HG22	4:A:382:PRO:HD2	1.79	0.64
4:A:406:ILE:HB	4:A:431:LYS:HB2	1.79	0.64
4:A:407:ARG:HD2	4:A:413:ILE:HD13	1.79	0.64
6:C:112:ASN:HD21	6:C:146:LYS:HE2	1.62	0.64
8:F:145:ASP:O	8:F:146:TRP:HB2	1.97	0.64
4:A:545:GLN:O	4:A:549:MET:HG3	1.97	0.64
5:B:421:PHE:O	5:B:424:LEU:HD23	1.96	0.64
5:B:572:HIS:N	5:B:573:GLN:HB3	2.12	0.64
5:B:711:GLU:H	5:B:712:PRO:CD	2.09	0.64
5:B:728:ARG:NH1	5:B:760:ASP:OD2	2.28	0.64
4:A:1092:LYS:HB3	4:A:1093:LYS:CA	2.26	0.64
4:A:1197:LEU:HA	4:A:1198:ASP:HB3	1.78	0.64
5:B:778:MET:HE1	5:B:853:SER:HB3	1.78	0.64
5:B:848:ARG:NH1	11:J:8:PHE:O	2.30	0.64
4:A:802:ASN:ND2	5:B:729:ILE:H	1.82	0.64
5:B:474:SER:HB2	5:B:476:ARG:HG3	1.79	0.64
5:B:886:LYS:HG2	5:B:940:PRO:HG3	1.78	0.64
6:C:84:ARG:HD2	12:K:11:LEU:HD11	1.79	0.64
5:B:572:HIS:H	5:B:573:GLN:HB3	1.61	0.64
5:B:579:ARG:HA	5:B:589:VAL:HA	1.80	0.64
4:A:849:MET:HB3	4:A:1063:MET:SD	2.38	0.64
5:B:113:TYR:HB3	5:B:114:PRO:HD2	1.79	0.64
4:A:845:LEU:HB2	4:A:1065:GLY:O	1.98	0.63
4:A:282:ASN:CB	4:A:283:GLY:HA3	2.28	0.63
5:B:286:PHE:HB3	5:B:297:ILE:HD11	1.81	0.63
4:A:10:PRO:HG2	5:B:1192:TYR:HA	1.81	0.63
5:B:882:THR:CG2	5:B:935:ARG:HA	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:472:LEU:HD13	5:B:835:GLN:NE2	2.13	0.63
4:A:868:TYR:HE2	4:A:1366:ARG:HE	1.45	0.63
4:A:975:HIS:CB	4:A:976:THR:OG1	2.34	0.63
4:A:1421:CYS:HA	4:A:1426:GLU:HG2	1.81	0.62
5:B:67:SER:HB2	5:B:92:PHE:H	1.63	0.62
5:B:572:HIS:H	5:B:573:GLN:CB	2.12	0.62
4:A:265:LYS:HZ1	4:A:323:LYS:HE2	1.64	0.62
4:A:282:ASN:HB3	4:A:283:GLY:HA2	1.79	0.62
5:B:115:GLN:HG2	5:B:193:LYS:HB2	1.80	0.62
5:B:913:GLY:HA2	5:B:938:SER:HB3	1.81	0.62
10:I:4:PHE:C	10:I:4:PHE:CD1	2.69	0.62
4:A:269:ILE:HD11	4:A:300:VAL:HG23	1.81	0.62
5:B:785:TYR:HE2	11:J:60:PHE:CE1	2.17	0.62
4:A:731:ARG:HG3	4:A:755:PHE:CE1	2.34	0.62
5:B:400:HIS:CE1	5:B:517:THR:HG21	2.35	0.62
5:B:524:PRO:HG3	5:B:748:ILE:HD12	1.79	0.62
5:B:785:TYR:CE2	11:J:60:PHE:CE1	2.87	0.62
4:A:901:LEU:HG	4:A:926:GLN:HE21	1.64	0.62
5:B:782:LEU:HD13	5:B:784:ASN:ND2	2.13	0.62
4:A:466:SER:O	5:B:1103:ILE:HD11	1.99	0.62
4:A:845:LEU:O	4:A:848:ILE:HG12	2.00	0.62
4:A:1084:PHE:HA	4:A:1085:HIS:C	2.19	0.62
5:B:1008:PRO:HB3	5:B:1087:PHE:CE1	2.32	0.62
5:B:1082:MET:HG2	6:C:188:HIS:O	1.99	0.62
6:C:20:PHE:HD1	6:C:21:ILE:O	1.82	0.62
7:E:16:PHE:CE2	7:E:20:LYS:HE2	2.34	0.62
5:B:877:PRO:CA	5:B:878:GLN:HB3	2.29	0.62
4:A:1083:THR:HG23	4:A:1084:PHE:HD2	1.64	0.62
5:B:634:TYR:CE1	5:B:692:TYR:CD1	2.88	0.62
5:B:827:ILE:HD12	5:B:1086:PHE:HD2	1.63	0.62
4:A:1093:LYS:H	4:A:1095:THR:H	1.49	0.61
4:A:1324:PRO:HB2	7:E:142:VAL:HG11	1.80	0.61
6:C:186:LEU:HB3	6:C:188:HIS:CD2	2.34	0.61
5:B:778:MET:CE	5:B:853:SER:HB3	2.29	0.61
6:C:57:VAL:HG21	11:J:60:PHE:HB3	1.82	0.61
4:A:567:LYS:CB	4:A:568:PRO:HD2	2.30	0.61
5:B:955:THR:HG22	5:B:956:THR:N	2.13	0.61
9:H:82:PRO:O	9:H:83:GLN:HB3	2.00	0.61
12:K:47:ARG:HH11	12:K:47:ARG:HB3	1.64	0.61
5:B:745:PRO:HB2	5:B:1047:PHE:CD1	2.35	0.61
6:C:166:GLU:O	6:C:167:HIS:HB2	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:62:ALA:HB3	7:E:78:LEU:HB3	1.83	0.61
12:K:20:LYS:HB3	12:K:34:THR:HB	1.81	0.61
4:A:68:GLN:O	4:A:68:GLN:HG2	2.01	0.61
5:B:227:LYS:CA	5:B:228:LYS:HB2	2.18	0.61
9:H:111:LEU:HD12	9:H:127:GLY:HA2	1.82	0.61
4:A:320:ARG:HB2	4:A:321:PRO:HA	1.83	0.61
4:A:840:ARG:HG2	4:A:1402:PHE:HZ	1.65	0.61
4:A:1162:VAL:HA	4:A:1163:ILE:O	2.00	0.61
5:B:364:ILE:HD13	5:B:585:VAL:HG13	1.82	0.61
6:C:171:GLY:C	6:C:173:ALA:H	2.03	0.61
5:B:351:TYR:H	5:B:354:ASP:HB2	1.66	0.61
12:K:47:ARG:HD2	12:K:60:ALA:HA	1.82	0.61
4:A:523:ILE:HD13	4:A:622:VAL:HG22	1.83	0.60
5:B:803:LEU:N	5:B:822:ASN:HD21	1.99	0.60
6:C:99:LEU:HB2	6:C:157:CYS:HB2	1.81	0.60
9:H:109:LYS:CG	9:H:110:ASP:HB2	2.31	0.60
5:B:785:TYR:CE2	11:J:60:PHE:HE1	2.18	0.60
4:A:961:ARG:NH1	4:A:965:GLN:HE22	2.00	0.60
5:B:123:THR:HG23	5:B:205:ILE:HA	1.81	0.60
6:C:56:THR:HG21	6:C:145:CYS:SG	2.40	0.60
4:A:1070:GLN:O	4:A:1074:GLU:HB2	2.01	0.60
4:A:1410:PHE:HD2	5:B:1212:ILE:HD11	1.66	0.60
5:B:549:THR:HB	5:B:628:THR:CG2	2.31	0.60
5:B:779:GLY:O	5:B:795:ILE:HA	2.01	0.60
4:A:834:THR:OG1	4:A:1077:THR:HA	2.02	0.60
4:A:901:LEU:H	4:A:926:GLN:NE2	1.99	0.60
6:C:45:ALA:HA	6:C:72:LEU:HD13	1.83	0.60
11:J:43:ARG:HH11	11:J:43:ARG:HB3	1.66	0.60
2:T:6:DG:H2"	2:T:7:DA:H8	1.65	0.60
4:A:68:GLN:HE22	4:A:80:HIS:CE1	2.20	0.60
1:R:10:A:N6	2:T:19:DT:H3	1.92	0.60
4:A:440:ASP:O	4:A:460:VAL:HG23	2.02	0.60
4:A:675:THR:CG2	4:A:736:ASN:HD21	2.14	0.60
9:H:83:GLN:HG3	9:H:83:GLN:O	2.01	0.60
4:A:472:LEU:HD13	5:B:835:GLN:HE22	1.67	0.59
5:B:1176:ASN:O	5:B:1177:HIS:CG	2.55	0.59
4:A:855:THR:HG23	4:A:857:ARG:HE	1.65	0.59
4:A:1390:ASN:HD21	4:A:1402:PHE:HB3	1.68	0.59
5:B:977:GLY:HA3	5:B:1099:VAL:CG1	2.32	0.59
5:B:1156:ASP:OD2	5:B:1156:ASP:N	2.34	0.59
5:B:391:ASP:CA	5:B:392:ARG:HB2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:21:ILE:HG12	12:K:33:ILE:HG12	1.84	0.59
4:A:899:VAL:HB	4:A:929:LEU:CD1	2.31	0.59
5:B:706:GLN:HB3	5:B:709:ASP:HB2	1.85	0.59
5:B:806:THR:HG22	5:B:1046:PRO:HD3	1.83	0.59
4:A:370:ILE:HG22	4:A:374:LEU:HD12	1.84	0.59
4:A:451:HIS:HB3	4:A:453:MET:N	2.16	0.59
5:B:801:LYS:O	11:J:52:THR:CG2	2.50	0.59
9:H:84:ALA:HA	9:H:86:ASP:N	2.16	0.59
4:A:901:LEU:HD22	4:A:919:ILE:HG22	1.85	0.59
4:A:567:LYS:O	4:A:569:LYS:N	2.34	0.59
5:B:424:LEU:O	5:B:428:ILE:HG12	2.02	0.59
5:B:882:THR:CB	5:B:883:LEU:HA	2.23	0.59
8:F:81:THR:HG22	8:F:82:THR:H	1.67	0.59
4:A:1223:ASP:O	4:A:1224:LEU:HB2	2.02	0.59
5:B:25:ILE:HD12	5:B:651:LEU:HD13	1.84	0.59
5:B:213:ILE:HD13	5:B:497:ARG:HB3	1.85	0.59
4:A:90:VAL:HG13	4:A:297:GLN:OE1	2.03	0.59
4:A:579:SER:OG	4:A:612:ILE:HG22	2.02	0.59
4:A:699:ALA:N	4:A:700:ASN:HA	2.17	0.59
5:B:849:GLY:HA2	5:B:852:ARG:HD2	1.84	0.59
5:B:1031:LEU:HD13	5:B:1055:ILE:HD12	1.85	0.59
4:A:1093:LYS:HB3	4:A:1094:VAL:CB	2.33	0.59
5:B:287:ARG:HH21	5:B:294:ASP:CG	2.06	0.59
7:E:111:VAL:HG12	7:E:137:GLU:HG2	1.84	0.59
5:B:558:LEU:HB3	5:B:563:MET:SD	2.42	0.58
5:B:1212:ILE:O	5:B:1214:PRO:HD3	2.03	0.58
4:A:449:SER:HB2	5:B:1137:CYS:SG	2.43	0.58
4:A:399:HIS:CE1	4:A:462:VAL:HG11	2.38	0.58
4:A:579:SER:HA	4:A:582:ILE:HG12	1.85	0.58
5:B:292:ILE:HD12	5:B:326:ASP:HA	1.84	0.58
5:B:709:ASP:HB3	5:B:710:LEU:HB2	1.85	0.58
5:B:831:SER:HB2	5:B:833:TYR:HD1	1.66	0.58
7:E:65:THR:C	7:E:67:GLU:H	2.06	0.58
4:A:364:VAL:HG12	4:A:459:ARG:O	2.02	0.58
5:B:239:GLU:HG3	5:B:255:GLN:HG2	1.84	0.58
5:B:351:TYR:CD2	5:B:355:ILE:HD11	2.38	0.58
5:B:365:THR:HG21	5:B:370:PHE:CD1	2.38	0.58
4:A:526:ASP:HB2	5:B:835:GLN:NE2	2.18	0.58
5:B:1162:ILE:HG12	5:B:1194:ILE:HD12	1.85	0.58
5:B:862:GLN:HG2	5:B:963:PHE:HD1	1.69	0.58
4:A:1084:PHE:HD1	4:A:1086:PHE:HA	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:35:SER:HA	5:B:811:TYR:HE2	1.69	0.58
7:E:124:VAL:HB	7:E:125:PRO:HD3	1.85	0.58
8:F:127:GLU:O	8:F:129:LYS:N	2.36	0.58
4:A:800:VAL:HG11	4:A:808:LEU:HG	1.86	0.58
4:A:928:LEU:HA	4:A:931:GLU:HB2	1.86	0.58
2:T:27:DA:H2'	2:T:27:DA:N3	2.19	0.58
7:E:198:ILE:HB	7:E:210:SER:HB3	1.86	0.58
4:A:793:SER:HB2	4:A:794:PRO:HD2	1.86	0.57
4:A:1154:TYR:O	4:A:1192:LEU:HG	2.04	0.57
5:B:975:GLN:O	5:B:990:ILE:HD12	2.03	0.57
5:B:1168:LEU:HD21	5:B:1214:PRO:HD2	1.86	0.57
6:C:251:LEU:O	6:C:255:VAL:HG23	2.05	0.57
9:H:56:THR:O	9:H:144:ILE:HA	2.05	0.57
13:L:38:LEU:HD21	13:L:48:CYS:HA	1.85	0.57
7:E:144:ILE:HG13	7:E:145:THR:H	1.69	0.57
4:A:115:LEU:HD11	4:A:145:LYS:HD2	1.87	0.57
5:B:1177:HIS:CA	5:B:1178:ASN:HB2	2.34	0.57
11:J:57:ILE:O	11:J:61:LEU:HG	2.05	0.57
5:B:391:ASP:N	5:B:392:ARG:HB2	2.20	0.57
5:B:941:LEU:HD23	5:B:942:ARG:H	1.70	0.57
5:B:977:GLY:HA3	5:B:1099:VAL:HG13	1.87	0.57
4:A:17:VAL:HB	4:A:1419:ASP:HB3	1.86	0.57
5:B:270:LYS:HA	5:B:281:PRO:HA	1.86	0.57
4:A:534:LEU:O	4:A:574:GLY:HA3	2.05	0.57
4:A:901:LEU:HA	4:A:907:THR:HG23	1.87	0.57
5:B:525:ALA:O	5:B:768:THR:HG23	2.03	0.57
4:A:1077:THR:O	4:A:1081:LEU:HB3	2.05	0.56
4:A:313:GLN:HE21	4:A:322:VAL:HG11	1.70	0.56
4:A:1092:LYS:CB	4:A:1093:LYS:HB2	2.35	0.56
5:B:1019:SER:CA	5:B:1020:ARG:CB	2.82	0.56
10:I:20:LYS:HG2	10:I:24:ARG:N	2.20	0.56
4:A:648:ASN:O	4:A:652:VAL:HG23	2.05	0.56
4:A:698:GLN:HA	10:I:97:MET:O	2.06	0.56
5:B:361:LEU:HD21	5:B:377:PHE:CD2	2.40	0.56
5:B:373:ARG:HA	5:B:566:LEU:HD23	1.88	0.56
4:A:95:PHE:O	4:A:99:ILE:HG13	2.05	0.56
4:A:596:THR:C	4:A:598:LEU:H	2.09	0.56
10:I:14:LEU:HD23	10:I:27:PHE:HB3	1.87	0.56
10:I:92:ARG:HA	10:I:92:ARG:NE	2.20	0.56
4:A:663:SER:CB	5:B:827:ILE:O	2.54	0.56
5:B:354:ASP:O	5:B:358:LYS:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:969:GLN:HA	4:A:972:HIS:HB3	1.88	0.56
4:A:351:THR:HG22	4:A:352:VAL:H	1.70	0.56
4:A:477:PRO:HG3	4:A:521:MET:HE2	1.88	0.56
10:I:3:THR:HA	10:I:4:PHE:CD2	2.37	0.56
4:A:731:ARG:CG	4:A:755:PHE:HE1	2.19	0.56
5:B:764:SER:N	5:B:765:PRO:HD2	2.21	0.56
5:B:974:PRO:HA	5:B:1094:ARG:HH21	1.70	0.56
4:A:855:THR:CG2	4:A:857:ARG:HE	2.18	0.56
4:A:1096:SER:N	4:A:1097:GLY:HA3	2.21	0.56
5:B:180:TYR:HD1	5:B:180:TYR:H	1.54	0.56
7:E:15:ALA:HA	7:E:141:VAL:H	1.70	0.56
11:J:53:HIS:HE1	11:J:55:ASP:OD1	1.89	0.56
4:A:464:PRO:HG2	12:K:67:PHE:CD1	2.41	0.55
4:A:596:THR:HB	4:A:598:LEU:HB2	1.88	0.55
4:A:731:ARG:HG3	4:A:755:PHE:CZ	2.40	0.55
4:A:1092:LYS:HB3	4:A:1093:LYS:CB	2.36	0.55
5:B:1019:SER:N	5:B:1020:ARG:HB3	2.20	0.55
5:B:1160:VAL:HG12	5:B:1161:HIS:H	1.71	0.55
4:A:1319:VAL:HB	4:A:1322:ILE:HD12	1.88	0.55
5:B:469:GLN:HE21	5:B:470:LYS:HE3	1.71	0.55
5:B:1120:GLU:HB3	5:B:1124:ARG:HH12	1.71	0.55
9:H:109:LYS:H	9:H:110:ASP:C	2.10	0.55
4:A:1105:LEU:HB3	4:A:1384:VAL:HB	1.89	0.55
5:B:485:ARG:NH2	5:B:782:LEU:HD11	2.21	0.55
4:A:284:ALA:N	4:A:285:PRO:CD	2.56	0.55
4:A:442:VAL:HG12	4:A:491:VAL:HG22	1.88	0.55
4:A:868:TYR:CE1	4:A:1064:VAL:HG21	2.41	0.55
5:B:708:GLU:HA	5:B:711:GLU:HG2	1.88	0.55
5:B:879:ARG:O	5:B:880:THR:HG22	2.06	0.55
6:C:18:VAL:HG12	6:C:20:PHE:CD2	2.41	0.55
6:C:82:TYR:HB2	6:C:85:ASP:HB2	1.88	0.55
11:J:3:VAL:HG22	11:J:53:HIS:CE1	2.42	0.55
4:A:456:MET:HB2	4:A:478:TYR:OH	2.06	0.55
4:A:1151:GLU:HA	10:I:45:ARG:HB3	1.89	0.55
4:A:389:THR:OG1	4:A:426:LEU:HD12	2.07	0.55
4:A:667:GLY:HA2	4:A:670:ILE:HG13	1.89	0.55
5:B:810:GLU:HB2	5:B:815:ARG:HH22	1.71	0.55
4:A:351:THR:CG2	4:A:352:VAL:N	2.68	0.55
4:A:617:VAL:HG12	4:A:622:VAL:HB	1.89	0.55
4:A:683:ILE:HG22	4:A:687:LYS:HG3	1.88	0.55
5:B:518:HIS:CE1	5:B:537:LYS:HE2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:614:SER:HB3	5:B:694:ASP:OD1	2.07	0.55
5:B:878:GLN:HG3	5:B:881:ASN:HB2	1.87	0.55
6:C:3:GLU:HB3	12:K:104:ASN:HD21	1.72	0.55
4:A:219:PHE:O	4:A:222:LEU:O	2.24	0.55
5:B:303:TYR:HH	5:B:586:TRP:HH2	1.55	0.55
5:B:512:ARG:NH2	5:B:532:ALA:HA	2.21	0.55
10:I:42:LEU:CD2	10:I:43:VAL:H	2.20	0.55
4:A:666:ILE:HD11	5:B:1030:LEU:HD13	1.88	0.55
7:E:29:PHE:O	7:E:30:ILE:HB	2.07	0.55
10:I:101:PHE:HB2	10:I:110:PHE:CZ	2.41	0.55
4:A:1075:PRO:O	4:A:1079:MET:HG3	2.07	0.54
5:B:350:GLN:HB3	5:B:351:TYR:CB	2.31	0.54
4:A:438:ASP:HA	4:A:460:VAL:O	2.07	0.54
4:A:1092:LYS:HB2	4:A:1093:LYS:HB2	1.90	0.54
4:A:1093:LYS:CB	4:A:1094:VAL:HB	2.36	0.54
5:B:391:ASP:HA	5:B:392:ARG:HB2	1.88	0.54
5:B:707:PRO:HA	5:B:741:CYS:SG	2.47	0.54
5:B:851:PHE:CD2	5:B:1094:ARG:HB2	2.42	0.54
7:E:26:ARG:NH2	7:E:133:GLU:OE1	2.31	0.54
9:H:115:TYR:CE2	9:H:124:ARG:HG3	2.42	0.54
4:A:683:ILE:HG21	4:A:801:GLU:HG3	1.88	0.54
4:A:629:LEU:O	4:A:633:VAL:HG23	2.08	0.54
4:A:1287:TYR:HD2	4:A:1305:VAL:HB	1.72	0.54
7:E:35:VAL:C	7:E:37:LEU:H	2.11	0.54
11:J:6:ARG:HA	11:J:12:LYS:O	2.07	0.54
4:A:1227:ILE:HA	4:A:1228:TRP:CG	2.42	0.54
5:B:1004:GLU:O	6:C:177:GLU:HG2	2.07	0.54
5:B:1159:ARG:HD3	5:B:1193:GLN:CG	2.37	0.54
4:A:827:THR:OG1	4:A:1083:THR:HG21	2.07	0.54
4:A:909:ASP:C	4:A:911:SER:H	2.11	0.54
6:C:173:ALA:O	6:C:233:GLU:O	2.24	0.54
4:A:1073:GLY:O	4:A:1077:THR:OG1	2.15	0.54
4:A:232:GLU:HG3	4:A:233:TRP:CD1	2.43	0.54
4:A:350:ARG:HD3	4:A:488:ASN:OD1	2.07	0.54
4:A:375:THR:HA	4:A:434:ARG:O	2.08	0.54
6:C:66:ARG:NH2	11:J:4:PRO:HA	2.23	0.54
4:A:8:SER:O	4:A:10:PRO:HD3	2.08	0.53
5:B:515:HIS:H	5:B:518:HIS:CD2	2.25	0.53
10:I:17:ARG:HA	10:I:18:GLU:HB3	1.90	0.53
5:B:237:VAL:HG22	5:B:257:LYS:HG2	1.90	0.53
5:B:573:GLN:O	5:B:575:PRO:HD3	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1194:ARG:O	4:A:1195:LEU:HB2	2.08	0.53
5:B:840:ILE:HB	5:B:1011:ILE:HD13	1.90	0.53
5:B:973:ILE:CG2	5:B:974:PRO:HD2	2.37	0.53
9:H:96:VAL:HA	9:H:142:LEU:O	2.09	0.53
4:A:278:THR:O	4:A:279:LEU:CB	2.57	0.53
4:A:930:ASP:HA	4:A:933:TYR:HB3	1.91	0.53
4:A:973:ILE:HG23	4:A:974:ASP:HA	1.90	0.53
4:A:1264:GLU:HA	4:A:1267:MET:HB2	1.91	0.53
5:B:115:GLN:CD	5:B:118:ARG:HH21	2.12	0.53
5:B:827:ILE:HD12	5:B:1086:PHE:CD2	2.42	0.53
9:H:81:PRO:HB2	9:H:82:PRO:CD	2.39	0.53
5:B:515:HIS:H	5:B:518:HIS:HD2	1.57	0.53
6:C:182:PRO:HG3	6:C:206:ASN:O	2.09	0.53
10:I:43:VAL:CG1	10:I:44:TYR:HA	2.38	0.53
4:A:343:LYS:HZ1	5:B:1197:PRO:HB3	1.72	0.53
4:A:573:SER:O	4:A:576:GLN:HB2	2.08	0.53
6:C:64:ALA:HA	6:C:67:LEU:HD12	1.90	0.53
7:E:7:ARG:HA	7:E:10:SER:HB3	1.91	0.53
4:A:847:ASP:HB3	4:A:1424:VAL:HG23	1.90	0.53
4:A:1115:SER:HA	4:A:1308:THR:O	2.08	0.53
6:C:13:ALA:HA	6:C:17:ASN:O	2.09	0.53
13:L:60:ARG:HG3	13:L:61:THR:H	1.73	0.53
4:A:1236:LEU:CA	4:A:1237:ILE:HB	2.30	0.53
5:B:223:VAL:HG22	5:B:240:ILE:HD12	1.91	0.53
7:E:35:VAL:O	7:E:37:LEU:N	2.38	0.53
11:J:9:SER:HB2	11:J:45:CYS:HB2	1.91	0.53
4:A:482:PHE:C	4:A:484:GLY:H	2.12	0.53
5:B:637:LEU:HA	5:B:743:ILE:HD11	1.91	0.53
5:B:1159:ARG:HE	5:B:1193:GLN:NE2	2.08	0.53
7:E:28:TYR:CE1	7:E:78:LEU:HD13	2.44	0.53
4:A:380:VAL:HG22	4:A:430:TRP:H	1.74	0.52
4:A:794:PRO:C	4:A:796:SER:H	2.12	0.52
4:A:818:MET:HG2	5:B:514:LEU:HD23	1.91	0.52
4:A:902:LEU:HG	4:A:926:GLN:HG3	1.92	0.52
4:A:1067:LEU:O	4:A:1069:ALA:O	2.28	0.52
5:B:122:LEU:CD2	5:B:958:GLN:HG3	2.32	0.52
5:B:293:PRO:HA	5:B:294:ASP:CB	2.25	0.52
5:B:785:TYR:HE2	11:J:60:PHE:CZ	2.25	0.52
7:E:194:GLU:O	7:E:214:CYS:HB2	2.08	0.52
5:B:408:LEU:HD23	5:B:545:ILE:HG21	1.92	0.52
5:B:589:VAL:HG12	5:B:590:HIS:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:17:ARG:HB3	10:I:18:GLU:O	2.09	0.52
4:A:276:LEU:HD11	4:A:292:ALA:HB1	1.90	0.52
4:A:565:ILE:CG2	4:A:567:LYS:HE3	2.37	0.52
5:B:649:LYS:HE2	5:B:737:THR:HA	1.92	0.52
9:H:109:LYS:HG2	9:H:110:ASP:HB2	1.90	0.52
4:A:266:LEU:O	4:A:269:ILE:HG22	2.09	0.52
4:A:579:SER:HB3	4:A:611:GLN:HA	1.91	0.52
4:A:623:GLY:C	4:A:625:SER:H	2.13	0.52
5:B:557:PHE:O	5:B:561:TRP:CB	2.53	0.52
5:B:1159:ARG:HD3	5:B:1193:GLN:HG3	1.91	0.52
12:K:82:ASP:OD1	12:K:83:PRO:HD2	2.10	0.52
4:A:98:LYS:O	4:A:102:VAL:HG23	2.09	0.52
4:A:446:ARG:HD2	4:A:480:ALA:HB2	1.92	0.52
5:B:571:PRO:N	5:B:572:HIS:HB2	2.25	0.52
6:C:62:PHE:O	6:C:66:ARG:HG3	2.08	0.52
4:A:848:ILE:HD12	4:A:864:ILE:HG13	1.90	0.52
5:B:708:GLU:O	5:B:712:PRO:HD3	2.09	0.52
10:I:21:GLU:O	10:I:22:ASN:HB3	2.10	0.52
4:A:681:GLU:HA	4:A:684:ALA:CB	2.39	0.52
4:A:1156:PRO:O	4:A:1157:ASP:HB2	2.09	0.52
6:C:3:GLU:HG3	6:C:4:GLU:H	1.75	0.52
9:H:95:TYR:HB3	9:H:144:ILE:HB	1.91	0.52
4:A:1200:ALA:HA	4:A:1201:ALA:C	2.29	0.52
2:T:26:DG:C2	2:T:27:DA:H1'	2.44	0.52
4:A:1100:ARG:O	4:A:1103:GLU:HB2	2.10	0.52
5:B:498:THR:O	5:B:536:VAL:HA	2.10	0.52
4:A:642:CYS:O	4:A:645:LEU:HB3	2.10	0.52
4:A:751:SER:CB	5:B:1015:HIS:CE1	2.93	0.52
4:A:768:GLN:NE2	4:A:1087:ALA:HB1	2.25	0.52
4:A:869:GLY:O	7:E:204:THR:HG21	2.10	0.52
4:A:1093:LYS:HB3	4:A:1094:VAL:CG2	2.39	0.52
4:A:1424:VAL:HG11	5:B:1139:ILE:HD13	1.91	0.52
5:B:471:LYS:O	5:B:474:SER:HB3	2.10	0.52
12:K:92:ASN:HA	12:K:95:ILE:HD12	1.92	0.52
5:B:40:GLU:OE1	5:B:682:SER:HB2	2.10	0.51
6:C:37:MET:HA	6:C:41:ILE:HD11	1.92	0.51
9:H:129:TYR:O	9:H:130:ARG:HG2	2.09	0.51
4:A:387:ARG:O	4:A:391:LEU:HD23	2.11	0.51
4:A:423:ASP:CG	4:A:424:ILE:N	2.59	0.51
4:A:663:SER:HA	5:B:1014:PRO:HG3	1.91	0.51
11:J:6:ARG:HB3	11:J:11:GLY:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:58:LEU:HD21	4:A:243:PRO:HB3	1.92	0.51
4:A:407:ARG:HD3	4:A:411:ASP:HB2	1.93	0.51
5:B:603:LEU:HB3	5:B:609:ILE:HG12	1.93	0.51
5:B:1177:HIS:HA	5:B:1178:ASN:CB	2.38	0.51
6:C:48:SER:HB3	6:C:158:VAL:HB	1.92	0.51
4:A:399:HIS:HB3	4:A:400:PRO:HD3	1.93	0.51
5:B:638:PHE:O	5:B:740:HIS:HB2	2.10	0.51
5:B:1075:GLY:O	6:C:35:ARG:HD2	2.11	0.51
6:C:35:ARG:NH1	12:K:41:THR:OG1	2.43	0.51
10:I:101:PHE:CE1	10:I:112:SER:HB3	2.39	0.51
13:L:55:ILE:HD12	13:L:56:LEU:H	1.76	0.51
2:T:16:DC:C6	2:T:17:DG:C8	2.98	0.51
4:A:546:VAL:HG21	4:A:572:TRP:CE3	2.46	0.51
4:A:550:LEU:HD12	4:A:556:TRP:NE1	2.25	0.51
4:A:1156:PRO:HG2	4:A:1163:ILE:HG12	1.93	0.51
4:A:1394:THR:HG22	4:A:1398:MET:HE1	1.92	0.51
5:B:613:VAL:HG22	5:B:628:THR:HG23	1.93	0.51
6:C:66:ARG:NH2	11:J:3:VAL:O	2.43	0.51
4:A:710:LEU:HA	4:A:713:SER:HB2	1.92	0.51
4:A:1120:LEU:HD13	4:A:1304:TRP:O	2.11	0.51
5:B:288:ALA:HB1	5:B:331:LEU:HG	1.93	0.51
5:B:518:HIS:HE1	5:B:537:LYS:HE2	1.75	0.51
5:B:815:ARG:HD3	5:B:1041:GLU:OE2	2.11	0.51
5:B:1019:SER:N	5:B:1020:ARG:CB	2.74	0.51
4:A:1391:ARG:O	4:A:1393:ASN:N	2.43	0.51
4:A:1411:GLU:HA	4:A:1414:ALA:HB3	1.92	0.51
4:A:1434:ALA:O	4:A:1436:ILE:N	2.44	0.51
5:B:1156:ASP:CB	5:B:1198:TYR:H	2.21	0.51
4:A:403:LYS:O	4:A:433:GLU:O	2.29	0.51
4:A:731:ARG:HG2	4:A:755:PHE:HE1	1.76	0.51
4:A:834:THR:O	4:A:837:ILE:HB	2.11	0.51
5:B:637:LEU:O	5:B:690:VAL:HG13	2.10	0.51
5:B:745:PRO:O	5:B:747:MET:N	2.44	0.51
5:B:983:ARG:HH11	5:B:1091:TYR:HB3	1.76	0.51
10:I:29:CYS:H	10:I:33:SER:HB2	1.76	0.51
10:I:43:VAL:HB	10:I:44:TYR:CA	2.38	0.51
11:J:43:ARG:HB3	11:J:43:ARG:NH1	2.26	0.51
4:A:443:LEU:HD12	5:B:1146:PHE:CZ	2.46	0.50
4:A:814:PHE:HB2	5:B:519:TRP:HZ3	1.76	0.50
4:A:1071:SER:H	4:A:1072:ILE:CB	2.11	0.50
5:B:552:MET:HB2	5:B:553:PRO:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:66:ARG:HH21	11:J:4:PRO:HA	1.75	0.50
9:H:115:TYR:HE2	9:H:124:ARG:HG3	1.76	0.50
12:K:65:HIS:O	12:K:67:PHE:N	2.44	0.50
4:A:330:LYS:O	4:A:334:GLY:HA3	2.10	0.50
4:A:663:SER:HB2	5:B:827:ILE:O	2.11	0.50
4:A:1091:SER:HB2	4:A:1093:LYS:N	2.26	0.50
6:C:57:VAL:HG11	11:J:60:PHE:CD1	2.46	0.50
6:C:133:ILE:HD11	6:C:237:SER:HA	1.92	0.50
4:A:59:GLY:HA2	4:A:67:CYS:SG	2.52	0.50
4:A:1171:GLN:C	4:A:1173:HIS:N	2.64	0.50
5:B:364:ILE:O	5:B:365:THR:HB	2.11	0.50
6:C:36:VAL:HG21	6:C:251:LEU:HD13	1.93	0.50
9:H:6:PHE:O	9:H:7:ASP:HB3	2.11	0.50
9:H:105:GLU:CG	9:H:106:GLU:H	2.23	0.50
13:L:29:TYR:HB3	13:L:56:LEU:HD22	1.93	0.50
4:A:374:LEU:O	4:A:436:ILE:HG13	2.11	0.50
4:A:407:ARG:HD2	4:A:413:ILE:CD1	2.42	0.50
4:A:1063:MET:HG3	4:A:1436:ILE:HG23	1.93	0.50
4:A:1069:ALA:C	4:A:1071:SER:N	2.65	0.50
5:B:168:GLY:HA2	5:B:454:THR:OG1	2.11	0.50
6:C:77:ILE:HD12	6:C:161:LYS:HE3	1.93	0.50
8:F:103:MET:O	8:F:105:ALA:N	2.45	0.50
4:A:961:ARG:HH11	4:A:961:ARG:CG	2.24	0.50
4:A:1390:ASN:ND2	4:A:1402:PHE:HB3	2.26	0.50
6:C:18:VAL:CG2	6:C:240:VAL:HB	2.42	0.50
11:J:14:VAL:HB	11:J:50:ILE:HD11	1.93	0.50
4:A:667:GLY:HA2	4:A:670:ILE:CG1	2.42	0.50
4:A:1157:ASP:C	4:A:1159:ARG:N	2.65	0.50
4:A:1167:GLU:CB	4:A:1168:GLU:CA	2.62	0.50
5:B:635:ARG:O	5:B:636:PRO:O	2.30	0.50
5:B:1002:THR:HG22	5:B:1006:ILE:N	2.10	0.50
10:I:33:SER:HA	10:I:34:TYR:CB	2.39	0.50
4:A:407:ARG:CD	4:A:413:ILE:HD13	2.41	0.50
4:A:712:GLU:H	4:A:713:SER:CA	2.24	0.50
4:A:822:GLU:O	4:A:825:ILE:HB	2.11	0.50
4:A:452:LYS:HB3	5:B:1140:ALA:HB1	1.93	0.50
5:B:54:PHE:HB2	5:B:410:GLY:HA2	1.93	0.50
5:B:124:TYR:OH	5:B:179:CYS:SG	2.49	0.50
5:B:190:TYR:CZ	5:B:196:PRO:HG3	2.47	0.50
10:I:111:THR:HG22	10:I:112:SER:H	1.76	0.50
4:A:350:ARG:O	4:A:351:THR:OG1	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:382:PRO:HD3	4:A:428:TYR:CE2	2.46	0.49
4:A:528:LEU:HD23	4:A:751:SER:HA	1.94	0.49
13:L:28:LYS:HB2	13:L:39:SER:HA	1.94	0.49
4:A:868:TYR:HE1	4:A:1064:VAL:CG1	2.15	0.49
5:B:108:VAL:HG12	5:B:109:THR:H	1.77	0.49
5:B:179:CYS:SG	5:B:181:LEU:HG	2.52	0.49
5:B:549:THR:HG22	5:B:550:ASP:H	1.76	0.49
9:H:102:TYR:CD2	9:H:102:TYR:N	2.80	0.49
10:I:3:THR:HG22	10:I:4:PHE:CE2	2.47	0.49
10:I:42:LEU:HD22	10:I:43:VAL:H	1.76	0.49
4:A:455:MET:CE	5:B:1134:GLU:HG3	2.42	0.49
4:A:1082:ASN:C	4:A:1084:PHE:O	2.51	0.49
4:A:1086:PHE:N	4:A:1086:PHE:CD1	2.79	0.49
5:B:357:GLN:HA	5:B:374:LYS:HZ1	1.76	0.49
5:B:579:ARG:HB3	5:B:589:VAL:HG22	1.94	0.49
5:B:708:GLU:O	5:B:708:GLU:HG2	2.12	0.49
5:B:848:ARG:HD2	11:J:8:PHE:HA	1.93	0.49
5:B:1177:HIS:CB	5:B:1178:ASN:HB2	2.42	0.49
10:I:5:ARG:HG2	10:I:6:PHE:H	1.77	0.49
4:A:575:LYS:HD2	9:H:120:GLY:HA3	1.94	0.49
4:A:754:SER:N	4:A:757:ASN:HD22	2.11	0.49
4:A:826:ASP:HA	4:A:830:LYS:H	1.76	0.49
4:A:961:ARG:O	4:A:965:GLN:NE2	2.45	0.49
6:C:52:GLU:HB3	6:C:154:LYS:HB3	1.94	0.49
4:A:903:ASN:O	4:A:907:THR:OG1	2.30	0.49
4:A:976:THR:H	4:A:1036:ARG:NH1	2.11	0.49
4:A:1436:ILE:HG22	4:A:1437:GLY:N	2.27	0.49
5:B:59:LEU:HA	5:B:62:ILE:HD12	1.93	0.49
5:B:549:THR:HB	5:B:628:THR:HG21	1.95	0.49
5:B:955:THR:CG2	5:B:956:THR:H	2.23	0.49
5:B:1084:GLN:HG2	6:C:201:TRP:CZ2	2.48	0.49
4:A:445:ASN:HB2	4:A:455:MET:HG2	1.95	0.49
4:A:853:ASP:OD2	4:A:855:THR:HG22	2.12	0.49
5:B:976:ILE:HD11	5:B:992:ILE:HA	1.94	0.49
4:A:731:ARG:CG	4:A:755:PHE:CE1	2.95	0.49
5:B:291:ILE:HD12	5:B:291:ILE:H	1.78	0.49
4:A:1152:ILE:CA	4:A:1153:TYR:HB2	2.36	0.49
5:B:880:THR:H	5:B:883:LEU:HD12	1.77	0.49
4:A:788:SER:HB3	10:I:69:PRO:HD3	1.93	0.49
4:A:1070:GLN:O	4:A:1074:GLU:N	2.46	0.49
4:A:1161:THR:O	4:A:1163:ILE:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:811:TYR:N	5:B:811:TYR:CD1	2.80	0.49
8:F:81:THR:HG22	8:F:82:THR:N	2.27	0.49
13:L:62:LYS:H	13:L:62:LYS:HD2	1.78	0.49
4:A:1311:VAL:HG22	4:A:1329:THR:HG21	1.95	0.49
4:A:1341:ILE:HB	7:E:182:ASP:OD1	2.13	0.49
5:B:302:CYS:HB2	5:B:310:MET:HG2	1.95	0.49
11:J:23:ASN:O	11:J:27:GLU:HB3	2.11	0.49
4:A:886:ILE:HD11	4:A:943:LEU:CB	2.43	0.48
4:A:1411:GLU:O	4:A:1415:SER:N	2.38	0.48
5:B:978:ASP:HB2	5:B:980:PHE:HE1	1.78	0.48
6:C:239:PRO:O	6:C:243:VAL:HG23	2.13	0.48
4:A:987:VAL:C	4:A:989:GLY:H	2.16	0.48
5:B:593:PRO:HG2	5:B:617:ARG:CZ	2.43	0.48
4:A:320:ARG:CB	4:A:321:PRO:HA	2.43	0.48
4:A:707:GLY:CA	4:A:709:THR:N	2.62	0.48
4:A:1409:LEU:HD13	5:B:1207:LEU:HD21	1.95	0.48
5:B:198:ASP:OD2	5:B:202:TYR:OH	2.31	0.48
5:B:230:ALA:C	5:B:232:SER:HB3	2.33	0.48
5:B:487:THR:HG22	5:B:488:TYR:N	2.27	0.48
5:B:825:VAL:HG21	5:B:1090:THR:HB	1.95	0.48
5:B:872:GLU:HG2	5:B:916:THR:HB	1.94	0.48
4:A:517:ASN:ND2	4:A:1364:ASN:OD1	2.44	0.48
4:A:663:SER:HB3	5:B:827:ILE:O	2.14	0.48
4:A:1340:GLY:HA2	7:E:183:PRO:HD2	1.95	0.48
5:B:640:VAL:HG13	5:B:650:GLU:O	2.14	0.48
4:A:442:VAL:CG1	4:A:491:VAL:HG22	2.43	0.48
4:A:491:VAL:H	5:B:1150:ARG:NH2	2.11	0.48
4:A:775:ILE:HB	4:A:797:LYS:O	2.13	0.48
4:A:821:ARG:O	4:A:825:ILE:HG12	2.13	0.48
4:A:1118:VAL:O	4:A:1305:VAL:HG13	2.13	0.48
7:E:43:LYS:O	7:E:47:CYS:HB3	2.12	0.48
4:A:332:LYS:C	4:A:334:GLY:H	2.17	0.48
4:A:492:PRO:O	4:A:493:GLN:NE2	2.46	0.48
4:A:754:SER:H	4:A:757:ASN:HD22	1.60	0.48
4:A:768:GLN:HE22	4:A:1087:ALA:HB1	1.79	0.48
6:C:173:ALA:O	6:C:174:ALA:HB3	2.13	0.48
12:K:38:GLU:HG3	12:K:42:LEU:HD22	1.96	0.48
4:A:350:ARG:HH11	4:A:488:ASN:HD21	1.60	0.48
4:A:515:GLN:HG3	4:A:1071:SER:HB3	1.96	0.48
4:A:1082:ASN:HB3	4:A:1084:PHE:O	2.12	0.48
5:B:619:ILE:HG13	10:I:65:ASP:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:636:PRO:CB	5:B:637:LEU:HB3	2.29	0.48
2:T:24:DT:OP1	5:B:857:ARG:NH2	2.46	0.48
5:B:1175:LEU:HB2	5:B:1176:ASN:HA	1.94	0.48
6:C:3:GLU:HG2	12:K:104:ASN:OD1	2.13	0.48
7:E:185:ALA:HA	7:E:190:LEU:HD23	1.94	0.48
4:A:702:LEU:HG	4:A:704:ALA:HB2	1.96	0.48
4:A:1030:ARG:HD3	4:A:1034:GLU:HG3	1.94	0.48
5:B:520:GLY:HA2	5:B:748:ILE:HA	1.94	0.48
2:T:17:DG:H5"	2:T:18:DA:OP1	2.13	0.48
4:A:332:LYS:H	4:A:337:ARG:HB2	1.79	0.48
4:A:897:TYR:CD2	4:A:936:LEU:HD21	2.48	0.48
5:B:571:PRO:HB2	5:B:572:HIS:CA	2.36	0.48
10:I:103:CYS:SG	10:I:106:CYS:CB	3.00	0.48
4:A:56:PRO:HA	4:A:57:ARG:HA	1.62	0.47
4:A:1364:ASN:C	4:A:1364:ASN:HD22	2.18	0.47
4:A:1370:LEU:O	4:A:1374:VAL:HG23	2.14	0.47
5:B:95:ILE:HD12	5:B:130:VAL:HG22	1.96	0.47
5:B:839:MET:O	5:B:990:ILE:HA	2.14	0.47
4:A:338:GLY:HA2	5:B:1129:ARG:HH22	1.79	0.47
4:A:623:GLY:O	4:A:625:SER:N	2.44	0.47
4:A:818:MET:CG	5:B:514:LEU:HD23	2.43	0.47
5:B:996:ARG:HH12	6:C:173:ALA:CB	2.27	0.47
6:C:35:ARG:HH12	12:K:41:THR:N	2.13	0.47
7:E:55:ARG:HB3	7:E:82:PHE:HB3	1.96	0.47
5:B:486:TYR:OH	5:B:1096:ARG:HB3	2.14	0.47
7:E:18:THR:HG21	7:E:140:LEU:HB2	1.96	0.47
4:A:707:GLY:O	4:A:1283:VAL:HG21	2.14	0.47
4:A:836:TYR:CZ	4:A:840:ARG:HD2	2.49	0.47
4:A:1081:LEU:O	4:A:1083:THR:HG22	2.13	0.47
4:A:1343:ALA:HB2	7:E:150:VAL:HG22	1.97	0.47
5:B:294:ASP:H	5:B:297:ILE:HB	1.78	0.47
5:B:978:ASP:OD2	5:B:1094:ARG:NH2	2.47	0.47
2:T:26:DG:C6	2:T:27:DA:C8	3.02	0.47
4:A:340:LEU:HD13	4:A:1429:ILE:HG23	1.95	0.47
4:A:490:HIS:ND1	5:B:1150:ARG:NH1	2.63	0.47
5:B:638:PHE:O	5:B:740:HIS:CB	2.63	0.47
5:B:841:MET:HA	5:B:1009:ASP:O	2.13	0.47
6:C:173:ALA:O	6:C:174:ALA:CB	2.63	0.47
7:E:144:ILE:HG13	7:E:145:THR:N	2.30	0.47
10:I:30:ARG:HB2	10:I:30:ARG:NH1	2.29	0.47
4:A:380:VAL:HG21	4:A:427:GLN:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:420:ARG:O	4:A:424:ILE:HG13	2.14	0.47
4:A:833:GLU:O	4:A:837:ILE:HG12	2.14	0.47
4:A:901:LEU:HD12	4:A:926:GLN:HG2	1.95	0.47
4:A:1069:ALA:CB	4:A:1070:GLN:HA	2.41	0.47
5:B:95:ILE:HD12	5:B:130:VAL:CG2	2.45	0.47
7:E:131:THR:HG21	7:E:191:LYS:HD3	1.96	0.47
7:E:140:LEU:HA	7:E:141:VAL:HB	1.96	0.47
4:A:350:ARG:NH1	4:A:488:ASN:HD21	2.11	0.47
4:A:867:ILE:HG22	4:A:872:GLY:CA	2.45	0.47
4:A:1076:ALA:O	4:A:1080:THR:HG22	2.15	0.47
4:A:1084:PHE:CD1	4:A:1086:PHE:HA	2.49	0.47
4:A:1261:LYS:C	4:A:1263:ILE:H	2.17	0.47
5:B:38:PHE:O	5:B:42:GLY:N	2.47	0.47
5:B:256:VAL:CG1	5:B:382:ILE:HD11	2.29	0.47
5:B:487:THR:O	5:B:490:SER:OG	2.14	0.47
6:C:124:LEU:C	6:C:126:GLY:H	2.17	0.47
9:H:63:LEU:C	9:H:89:LEU:HB2	2.35	0.47
4:A:399:HIS:O	4:A:435:HIS:HD2	1.97	0.47
4:A:503:GLN:O	4:A:504:LEU:HD12	2.14	0.47
4:A:526:ASP:HB2	5:B:835:GLN:HE21	1.80	0.47
5:B:51:PHE:CD2	5:B:173:MET:HB3	2.50	0.47
5:B:570:VAL:C	5:B:572:HIS:HB2	2.35	0.47
7:E:10:SER:O	7:E:14:ARG:HG3	2.15	0.47
4:A:975:HIS:HB3	4:A:976:THR:CB	2.39	0.47
5:B:243:ALA:HB2	5:B:251:ILE:HD13	1.96	0.47
10:I:43:VAL:HG12	10:I:44:TYR:HA	1.97	0.47
11:J:9:SER:CB	11:J:45:CYS:HB2	2.45	0.47
4:A:61:ILE:HG13	4:A:62:ASP:N	2.30	0.47
4:A:91:PHE:HB2	4:A:297:GLN:HE22	1.80	0.47
5:B:32:ALA:O	5:B:35:SER:HB2	2.15	0.47
5:B:979:LYS:HA	5:B:989:THR:HG22	1.96	0.47
4:A:792:TYR:OH	10:I:91:ARG:NH2	2.48	0.46
5:B:777:ALA:HB1	5:B:819:ALA:HB1	1.97	0.46
7:E:205:SER:O	7:E:207:ARG:N	2.47	0.46
10:I:101:PHE:HB2	10:I:110:PHE:CE1	2.50	0.46
4:A:457:ALA:O	4:A:507:VAL:HG23	2.16	0.46
4:A:1342:GLU:HG3	7:E:198:ILE:HG21	1.98	0.46
5:B:1120:GLU:HB3	5:B:1124:ARG:NH1	2.30	0.46
5:B:1209:ALA:C	5:B:1211:ASN:H	2.19	0.46
4:A:58:LEU:HD22	4:A:244:PRO:HD2	1.97	0.46
4:A:298:PHE:O	4:A:302:THR:OG1	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:416:ARG:HG3	4:A:417:TYR:CD1	2.49	0.46
4:A:793:SER:CB	4:A:794:PRO:HD2	2.45	0.46
4:A:1191:TRP:CA	4:A:1192:LEU:CB	2.90	0.46
5:B:62:ILE:HG23	5:B:418:LYS:HG2	1.97	0.46
5:B:265:SER:O	5:B:266:ALA:HB3	2.14	0.46
5:B:785:TYR:HA	5:B:788:ARG:HB2	1.96	0.46
4:A:254:GLU:HA	4:A:255:SER:HA	1.70	0.46
4:A:617:VAL:CG1	4:A:622:VAL:HB	2.45	0.46
9:H:23:VAL:HA	9:H:43:ASN:HA	1.95	0.46
9:H:139:ASN:O	9:H:140:ALA:HB2	2.15	0.46
4:A:370:ILE:HG22	4:A:374:LEU:CD1	2.45	0.46
4:A:396:PRO:HB3	4:A:403:LYS:HG2	1.96	0.46
4:A:445:ASN:CB	4:A:455:MET:HG2	2.46	0.46
4:A:666:ILE:HD12	4:A:666:ILE:H	1.79	0.46
5:B:286:PHE:HB3	5:B:297:ILE:CD1	2.45	0.46
4:A:239:LEU:HD12	4:A:240:PRO:HD2	1.96	0.46
4:A:367:PRO:HD2	4:A:370:ILE:HD12	1.98	0.46
4:A:490:HIS:HB3	5:B:1150:ARG:CZ	2.45	0.46
4:A:1170:ILE:HA	4:A:1171:GLN:O	2.16	0.46
5:B:169:ARG:HB2	5:B:454:THR:HG23	1.97	0.46
5:B:328:GLU:HA	5:B:329:THR:HA	1.63	0.46
5:B:950:ASP:O	5:B:951:GLN:HG3	2.16	0.46
10:I:114:GLN:HA	10:I:115:LYS:HA	1.69	0.46
4:A:312:PRO:O	4:A:313:GLN:HB2	2.15	0.46
4:A:767:GLN:NE2	4:A:774:ARG:HB2	2.31	0.46
5:B:471:LYS:O	5:B:471:LYS:HG2	2.16	0.46
5:B:704:ALA:HB1	5:B:710:LEU:HB3	1.98	0.46
5:B:892:LYS:O	5:B:899:ILE:HG23	2.16	0.46
6:C:50:GLU:HB2	6:C:156:THR:OG1	2.15	0.46
9:H:6:PHE:HZ	9:H:134:ASN:HB2	1.81	0.46
9:H:106:GLU:HA	9:H:112:ILE:H	1.81	0.46
4:A:838:GLN:O	4:A:840:ARG:N	2.49	0.46
5:B:213:ILE:CD1	5:B:497:ARG:HB3	2.45	0.46
5:B:361:LEU:HD21	5:B:377:PHE:HD2	1.79	0.46
9:H:81:PRO:HB2	9:H:82:PRO:HD2	1.98	0.46
4:A:345:VAL:HA	5:B:1154:ALA:O	2.16	0.46
4:A:892:ALA:O	4:A:896:ARG:HB2	2.16	0.46
4:A:1050:GLU:O	4:A:1054:LEU:HD13	2.16	0.46
4:A:1116:LEU:HB3	4:A:1308:THR:HB	1.98	0.46
5:B:230:ALA:O	5:B:232:SER:O	2.34	0.46
2:T:9:DA:H61	3:N:6:DT:H3	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:637:LYS:HA	4:A:638:GLY:HA2	1.65	0.46
5:B:125:SER:HB2	5:B:169:ARG:HB3	1.97	0.46
5:B:707:PRO:HB3	5:B:741:CYS:SG	2.55	0.46
5:B:955:THR:HG23	13:L:54:ARG:O	2.16	0.46
6:C:41:ILE:CG2	6:C:246:ARG:HB3	2.46	0.46
4:A:282:ASN:CB	4:A:283:GLY:CA	2.78	0.45
4:A:467:THR:HG23	5:B:976:ILE:HG23	1.97	0.45
4:A:513:SER:HB3	4:A:518:LYS:O	2.16	0.45
4:A:722:LEU:HD11	4:A:794:PRO:HB3	1.98	0.45
4:A:824:LEU:HD21	5:B:769:TYR:HE1	1.81	0.45
4:A:901:LEU:H	4:A:926:GLN:HE21	1.62	0.45
4:A:1015:VAL:O	4:A:1017:LEU:N	2.49	0.45
5:B:709:ASP:CB	5:B:710:LEU:HB2	2.46	0.45
5:B:845:SER:HB2	11:J:8:PHE:HB3	1.96	0.45
2:T:11:DG:N2	3:N:5:DT:O2	2.49	0.45
4:A:10:PRO:HD2	5:B:1193:GLN:HB2	1.96	0.45
4:A:452:LYS:HD2	4:A:510:GLN:HE22	1.81	0.45
5:B:372:SER:O	5:B:376:PHE:HD1	1.99	0.45
5:B:492:LEU:HD13	5:B:812:LEU:HD12	1.98	0.45
5:B:996:ARG:CG	5:B:1007:VAL:HG21	2.41	0.45
10:I:79:HIS:HA	10:I:80:SER:O	2.16	0.45
4:A:563:PRO:HD3	4:A:572:TRP:CZ2	2.52	0.45
4:A:712:GLU:N	4:A:713:SER:CB	2.53	0.45
4:A:741:ASN:HD22	4:A:744:LYS:H	1.62	0.45
4:A:907:THR:HG22	4:A:908:LEU:N	2.31	0.45
5:B:61:ASP:HA	5:B:64:CYS:HB2	1.98	0.45
5:B:212:LEU:HA	5:B:479:VAL:O	2.15	0.45
5:B:331:LEU:HB3	5:B:352:ALA:HB1	1.97	0.45
5:B:680:THR:HB	5:B:681:TRP:H	1.56	0.45
5:B:830:TYR:CZ	5:B:1000:PRO:HD3	2.51	0.45
6:C:88:CYS:SG	6:C:89:GLU:N	2.89	0.45
4:A:1098:VAL:N	4:A:1099:PRO:HD2	2.32	0.45
5:B:1076:HIS:ND1	12:K:40:HIS:NE2	2.64	0.45
8:F:101:ILE:HD13	8:F:120:ILE:HG22	1.99	0.45
9:H:38:LEU:HD13	9:H:125:LEU:HD13	1.99	0.45
12:K:37:LYS:O	12:K:38:GLU:HG2	2.16	0.45
4:A:663:SER:OG	5:B:1085:ILE:HA	2.16	0.45
4:A:1068:ALA:C	4:A:1069:ALA:O	2.53	0.45
5:B:831:SER:HB2	5:B:833:TYR:CD1	2.49	0.45
5:B:996:ARG:HH12	6:C:173:ALA:HB1	1.81	0.45
6:C:215:GLU:HG3	6:C:216:GLY:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:199:LEU:HB3	4:A:200:ARG:H	1.56	0.45
4:A:901:LEU:HB2	4:A:926:GLN:HG2	1.98	0.45
4:A:959:ASN:OD1	4:A:961:ARG:HB3	2.17	0.45
4:A:1191:TRP:HA	4:A:1192:LEU:HB3	1.96	0.45
8:F:93:ILE:HG12	8:F:148:VAL:HG21	1.98	0.45
10:I:59:VAL:HG12	10:I:60:GLN:H	1.81	0.45
4:A:868:TYR:CD2	4:A:868:TYR:C	2.90	0.45
4:A:1080:THR:HG23	4:A:1081:LEU:H	1.81	0.45
5:B:572:HIS:N	5:B:573:GLN:C	2.64	0.45
5:B:1177:HIS:HB2	5:B:1178:ASN:HB2	1.98	0.45
7:E:69:ILE:HD13	7:E:73:PRO:HA	1.99	0.45
9:H:108:SER:HB3	9:H:111:LEU:H	1.81	0.45
4:A:975:HIS:NE2	9:H:136:LYS:CB	2.80	0.45
5:B:1166:CYS:O	5:B:1168:LEU:N	2.48	0.45
5:B:1175:LEU:HA	5:B:1177:HIS:O	2.16	0.45
12:K:7:PHE:C	12:K:9:LEU:H	2.19	0.45
12:K:97:LYS:O	12:K:100:ALA:HB3	2.16	0.45
13:L:32:ALA:H	13:L:55:ILE:CD1	2.26	0.45
4:A:630:ILE:N	4:A:630:ILE:CD1	2.72	0.45
4:A:1074:GLU:HB3	4:A:1075:PRO:HD3	1.98	0.45
5:B:579:ARG:HA	5:B:589:VAL:HG13	1.97	0.45
5:B:814:PHE:C	5:B:816:GLU:H	2.20	0.45
6:C:127:ARG:HG3	6:C:129:ILE:HG22	1.99	0.45
4:A:783:THR:O	5:B:516:ASN:OD1	2.35	0.45
5:B:600:LEU:HD22	5:B:615:MET:SD	2.57	0.45
4:A:68:GLN:O	4:A:68:GLN:CG	2.65	0.44
4:A:1069:ALA:CB	4:A:1070:GLN:CA	2.95	0.44
4:A:1072:ILE:CG2	4:A:1073:GLY:N	2.72	0.44
5:B:476:ARG:O	5:B:477:ALA:C	2.55	0.44
6:C:70:ILE:HA	6:C:71:PRO:HD2	1.64	0.44
6:C:265:MET:C	6:C:267:GLN:H	2.20	0.44
10:I:50:THR:HB	10:I:90:GLN:HE22	1.81	0.44
4:A:324:SER:O	4:A:326:ARG:N	2.45	0.44
4:A:1069:ALA:HA	4:A:1072:ILE:CG2	2.45	0.44
4:A:1083:THR:H	4:A:1084:PHE:C	2.17	0.44
4:A:1323:ASP:OD1	4:A:1325:THR:HG22	2.17	0.44
5:B:459:TYR:O	5:B:463:THR:OG1	2.35	0.44
5:B:1000:PRO:HB2	5:B:1072:MET:HE3	2.00	0.44
5:B:1148:LYS:O	5:B:1152:MET:HB2	2.17	0.44
9:H:88:SER:O	9:H:89:LEU:CB	2.63	0.44
4:A:1197:LEU:HA	4:A:1198:ASP:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1074:ASN:C	5:B:1074:ASN:OD1	2.54	0.44
6:C:124:LEU:O	6:C:127:ARG:HG2	2.17	0.44
4:A:222:LEU:O	4:A:224:PHE:N	2.50	0.44
4:A:265:LYS:NZ	4:A:323:LYS:HE2	2.32	0.44
4:A:915:SER:HB2	4:A:919:ILE:CG1	2.45	0.44
4:A:1118:VAL:CG2	4:A:1306:LEU:HB2	2.48	0.44
5:B:115:GLN:HG2	5:B:193:LYS:CB	2.46	0.44
5:B:1176:ASN:O	5:B:1177:HIS:ND1	2.51	0.44
7:E:46:TYR:CD2	7:E:58:MET:HG3	2.53	0.44
7:E:173:SER:O	7:E:175:LEU:N	2.51	0.44
4:A:351:THR:HB	4:A:468:PHE:CD1	2.52	0.44
4:A:692:ASP:O	4:A:695:LYS:HG2	2.17	0.44
4:A:1327:ILE:O	7:E:147:HIS:HE1	2.01	0.44
5:B:638:PHE:HB3	5:B:651:LEU:HD21	1.99	0.44
6:C:46:ILE:O	6:C:169:LYS:HE3	2.18	0.44
10:I:21:GLU:O	10:I:22:ASN:CB	2.65	0.44
4:A:1171:GLN:C	4:A:1173:HIS:H	2.21	0.44
5:B:487:THR:CG2	5:B:488:TYR:N	2.80	0.44
5:B:999:MET:CE	5:B:1000:PRO:HD2	2.47	0.44
5:B:1124:ARG:O	5:B:1125:ASP:C	2.55	0.44
6:C:101:LEU:HB3	6:C:155:LEU:HB2	2.00	0.44
4:A:451:HIS:HB3	4:A:453:MET:H	1.81	0.44
4:A:541:ILE:CD1	4:A:577:ILE:HD11	2.48	0.44
4:A:855:THR:HG23	4:A:855:THR:O	2.18	0.44
5:B:756:ILE:O	5:B:759:PRO:HD3	2.17	0.44
8:F:145:ASP:O	8:F:146:TRP:CB	2.65	0.44
9:H:129:TYR:O	9:H:130:ARG:CG	2.65	0.44
10:I:63:GLY:CA	10:I:104:LEU:HD21	2.32	0.44
4:A:304:MET:SD	5:B:1210:MET:HG3	2.58	0.44
4:A:344:ARG:HB3	5:B:1118:PRO:HD2	1.99	0.44
4:A:1150:SER:HB3	10:I:46:HIS:CD2	2.53	0.44
4:A:1325:THR:HG23	4:A:1326:ARG:HG3	2.00	0.44
16:B:3000:UTP:H5'1	16:B:3000:UTP:H6	1.83	0.44
12:K:58:PHE:HB3	12:K:76:GLN:HB3	2.00	0.44
4:A:366:VAL:O	4:A:463:ILE:HG13	2.18	0.44
4:A:1327:ILE:O	7:E:147:HIS:CE1	2.71	0.44
5:B:287:ARG:HG2	5:B:292:ILE:HA	1.99	0.44
5:B:387:LEU:HD13	5:B:392:ARG:HD2	1.99	0.44
5:B:459:TYR:C	5:B:459:TYR:CD2	2.91	0.44
5:B:547:VAL:CG1	5:B:548:GLY:N	2.81	0.44
5:B:865:LYS:HB2	5:B:865:LYS:HE3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:365:GLY:HA3	4:A:469:ARG:HB2	2.00	0.43
4:A:479:ASN:ND2	4:A:1078:GLN:OE1	2.50	0.43
4:A:873:MET:C	4:A:1058:VAL:HG13	2.38	0.43
4:A:1070:GLN:O	4:A:1074:GLU:CB	2.64	0.43
4:A:1083:THR:C	4:A:1084:PHE:O	2.57	0.43
5:B:242:SER:HB2	5:B:362:PRO:HD2	2.00	0.43
6:C:43:THR:HG22	6:C:44:LEU:H	1.83	0.43
6:C:71:PRO:HB2	6:C:133:ILE:HB	1.98	0.43
7:E:19:VAL:O	7:E:23:VAL:HG23	2.17	0.43
11:J:43:ARG:HD2	11:J:46:CYS:SG	2.58	0.43
4:A:413:ILE:HG22	4:A:413:ILE:O	2.18	0.43
4:A:451:HIS:O	4:A:1070:GLN:NE2	2.52	0.43
4:A:871:ASP:OD1	4:A:1366:ARG:NH2	2.50	0.43
4:A:956:LEU:HA	4:A:957:PRO:HD3	1.68	0.43
5:B:273:LEU:HD21	5:B:360:PHE:HB2	1.99	0.43
5:B:572:HIS:N	5:B:573:GLN:CB	2.77	0.43
5:B:986:GLN:HE21	5:B:1025:HIS:HD2	1.64	0.43
6:C:45:ALA:HA	6:C:72:LEU:CD1	2.46	0.43
7:E:52:ARG:HA	7:E:53:PRO:HD3	1.74	0.43
4:A:668:ASP:HB3	4:A:743:VAL:CG2	2.46	0.43
4:A:870:GLU:OE2	7:E:200:ARG:NH1	2.51	0.43
5:B:46:GLN:OE1	5:B:47:GLN:HG2	2.18	0.43
5:B:563:MET:HA	5:B:590:HIS:ND1	2.33	0.43
5:B:1194:ILE:HD13	5:B:1194:ILE:H	1.84	0.43
9:H:95:TYR:HE2	9:H:97:MET:HG3	1.83	0.43
9:H:105:GLU:HB3	9:H:113:ALA:HB3	1.99	0.43
5:B:898:LEU:HD22	5:B:964:VAL:HG11	2.00	0.43
4:A:350:ARG:HB2	5:B:1128:LEU:HD11	1.99	0.43
4:A:383:TYR:OH	8:F:107:VAL:HG21	2.19	0.43
4:A:751:SER:CB	5:B:1015:HIS:HE1	2.26	0.43
4:A:816:HIS:CD2	5:B:764:SER:H	2.36	0.43
4:A:1089:VAL:H	4:A:1090:ALA:HA	1.77	0.43
5:B:31:TRP:O	5:B:34:ILE:HB	2.17	0.43
5:B:53:GLN:O	5:B:53:GLN:HG3	2.16	0.43
5:B:1209:ALA:C	5:B:1211:ASN:N	2.71	0.43
12:K:58:PHE:HE2	12:K:74:ARG:HB3	1.84	0.43
4:A:378:GLU:OE1	4:A:434:ARG:NH1	2.48	0.43
4:A:443:LEU:HD12	5:B:1146:PHE:CE2	2.54	0.43
4:A:1091:SER:CB	4:A:1092:LYS:C	2.72	0.43
5:B:463:THR:HB	5:B:465:ASN:H	1.84	0.43
5:B:790:ASP:N	5:B:790:ASP:OD1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:2:THR:OG1	10:I:43:VAL:HG13	2.18	0.43
11:J:2:ILE:HG13	11:J:57:ILE:HG21	1.99	0.43
11:J:48:ARG:HH21	11:J:49:MET:HE1	1.84	0.43
4:A:135:PHE:HA	4:A:138:ILE:HD12	2.00	0.43
4:A:304:MET:SD	5:B:1210:MET:HA	2.59	0.43
4:A:313:GLN:HB3	4:A:314:ALA:H	1.66	0.43
4:A:374:LEU:CB	4:A:436:ILE:HD11	2.49	0.43
4:A:567:LYS:HD2	9:H:46:LEU:HD13	2.01	0.43
4:A:1159:ARG:CB	4:A:1160:SER:C	2.83	0.43
4:A:1277:GLU:H	4:A:1277:GLU:HG2	1.70	0.43
5:B:124:TYR:HB2	5:B:204:ILE:HB	2.01	0.43
5:B:172:ILE:HG22	5:B:173:MET:O	2.19	0.43
5:B:230:ALA:N	5:B:231:PRO:CD	2.81	0.43
12:K:40:HIS:CE1	12:K:63:VAL:HG11	2.53	0.43
2:T:19:DT:H2'	2:T:20:DC:C6	2.54	0.43
4:A:88:LYS:HA	4:A:89:PRO:HD3	1.91	0.43
4:A:353:ILE:HA	4:A:468:PHE:O	2.19	0.43
4:A:1092:LYS:CB	4:A:1093:LYS:CB	2.97	0.43
5:B:555:ILE:HA	5:B:558:LEU:HD12	2.00	0.43
5:B:1010:LEU:HD12	5:B:1010:LEU:HA	1.75	0.43
5:B:1213:THR:HB	5:B:1215:ARG:NH1	2.34	0.43
6:C:91:HIS:HB2	6:C:96:SER:OG	2.19	0.43
7:E:138:ALA:HA	7:E:140:LEU:N	2.33	0.43
8:F:93:ILE:HD11	8:F:132:LEU:HB2	2.00	0.43
9:H:43:ASN:ND2	9:H:46:LEU:HD12	2.34	0.43
12:K:65:HIS:C	12:K:67:PHE:H	2.22	0.43
4:A:77:CYS:SG	4:A:80:HIS:NE2	2.91	0.43
4:A:826:ASP:HB2	4:A:830:LYS:HB3	2.01	0.43
4:A:1171:GLN:O	4:A:1173:HIS:N	2.52	0.43
4:A:1441:PHE:CZ	8:F:89:GLU:HA	2.54	0.43
5:B:890:TYR:CE2	5:B:910:VAL:HG11	2.54	0.43
5:B:1069:PHE:HA	5:B:1085:ILE:O	2.19	0.43
5:B:1098:MET:O	5:B:1099:VAL:C	2.57	0.43
4:A:38:PRO:CB	4:A:39:GLU:HA	2.47	0.43
4:A:819:GLY:O	4:A:820:GLY:C	2.57	0.43
4:A:961:ARG:HH11	4:A:965:GLN:HE22	1.65	0.43
5:B:1074:ASN:HB2	5:B:1081:LEU:HD21	2.01	0.43
4:A:848:ILE:HG21	4:A:1370:LEU:HD11	2.01	0.42
4:A:867:ILE:HG22	4:A:872:GLY:HA3	2.01	0.42
4:A:979:SER:OG	4:A:980:ASP:N	2.53	0.42
5:B:802:PRO:HA	5:B:1091:TYR:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:824:ILE:HG12	11:J:48:ARG:NH1	2.24	0.42
5:B:846:ILE:HG23	5:B:974:PRO:HG2	2.01	0.42
6:C:34:ARG:HG3	6:C:35:ARG:N	2.34	0.42
7:E:59:SER:HB3	7:E:80:VAL:O	2.18	0.42
10:I:3:THR:CA	10:I:4:PHE:CB	2.93	0.42
4:A:471:ASN:O	4:A:474:VAL:HG12	2.19	0.42
4:A:502:SER:HA	4:A:506:ALA:HB2	2.01	0.42
5:B:37:PHE:O	5:B:38:PHE:HB2	2.19	0.42
5:B:402:GLY:CA	5:B:695:ALA:HB3	2.49	0.42
5:B:820:GLY:N	5:B:1091:TYR:OH	2.49	0.42
5:B:999:MET:HE2	5:B:1000:PRO:HD2	2.01	0.42
10:I:4:PHE:HD1	10:I:5:ARG:N	2.17	0.42
12:K:40:HIS:HB3	12:K:61:TYR:HE1	1.84	0.42
12:K:82:ASP:OD2	12:K:84:LYS:HB2	2.20	0.42
4:A:562:THR:HA	4:A:563:PRO:HD2	1.81	0.42
4:A:647:GLY:O	4:A:651:LYS:HG3	2.19	0.42
4:A:711:ARG:CA	4:A:713:SER:HB2	2.48	0.42
5:B:31:TRP:HA	5:B:34:ILE:HG13	2.01	0.42
8:F:82:THR:HA	8:F:83:PRO:HD3	1.87	0.42
12:K:32:VAL:HG22	12:K:74:ARG:HG3	2.00	0.42
2:T:18:DA:H2'	2:T:19:DT:C6	2.55	0.42
4:A:465:TYR:HB3	5:B:976:ILE:HG21	2.01	0.42
4:A:1364:ASN:HD22	4:A:1366:ARG:HG2	1.84	0.42
7:E:141:VAL:HG12	7:E:142:VAL:HG23	2.00	0.42
13:L:60:ARG:HG3	13:L:61:THR:N	2.34	0.42
4:A:1155:ASP:OD1	4:A:1190:PRO:HA	2.18	0.42
5:B:254:LEU:HD12	5:B:272:THR:O	2.20	0.42
5:B:658:ILE:HA	5:B:661:LEU:HD12	2.02	0.42
5:B:886:LYS:O	5:B:888:GLY:N	2.42	0.42
6:C:43:THR:HG22	6:C:44:LEU:N	2.34	0.42
4:A:351:THR:CG2	4:A:352:VAL:H	2.32	0.42
4:A:589:GLN:HB3	4:A:961:ARG:HH22	1.84	0.42
4:A:1078:GLN:O	4:A:1082:ASN:HB2	2.20	0.42
5:B:67:SER:HB2	5:B:92:PHE:HD1	1.85	0.42
5:B:483:LEU:HD22	5:B:484:ASN:H	1.85	0.42
5:B:745:PRO:HB2	5:B:1047:PHE:HD1	1.84	0.42
5:B:973:ILE:H	5:B:973:ILE:HG13	1.47	0.42
6:C:21:ILE:O	6:C:22:LEU:HB2	2.18	0.42
5:B:620:ARG:HH21	10:I:68:LEU:HD21	1.84	0.42
5:B:867:GLY:HA2	5:B:868:MET:HA	1.65	0.42
5:B:1011:ILE:HD12	5:B:1011:ILE:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1139:ILE:H	5:B:1139:ILE:HG13	1.66	0.42
4:A:14:VAL:HG21	4:A:1430:LEU:HD22	2.01	0.42
4:A:538:ASP:HB2	9:H:20:TYR:CD2	2.54	0.42
4:A:606:LEU:HD23	4:A:613:ILE:HG21	2.01	0.42
4:A:841:LEU:HD22	4:A:1072:ILE:HG21	2.01	0.42
5:B:232:SER:HA	5:B:233:PRO:HD3	2.00	0.42
5:B:911:ILE:HG22	5:B:912:ILE:CG1	2.43	0.42
7:E:22:MET:HG3	7:E:187:TYR:CD1	2.54	0.42
9:H:111:LEU:HB2	9:H:112:ILE:HG22	2.01	0.42
10:I:42:LEU:HD22	10:I:43:VAL:N	2.34	0.42
4:A:964:ILE:O	4:A:968:GLN:HG2	2.20	0.42
4:A:1197:LEU:HB3	4:A:1198:ASP:O	2.19	0.42
5:B:265:SER:O	5:B:266:ALA:CB	2.68	0.42
6:C:61:GLU:HA	6:C:64:ALA:HB3	2.01	0.42
11:J:3:VAL:HG21	11:J:18:TRP:CB	2.49	0.42
4:A:582:ILE:HG22	4:A:610:GLY:HA2	2.02	0.42
4:A:745:GLN:H	4:A:745:GLN:HG2	1.62	0.42
4:A:1057:VAL:HG12	4:A:1058:VAL:O	2.19	0.42
5:B:211:VAL:O	5:B:480:SER:HA	2.20	0.42
5:B:796:LEU:HD22	5:B:799:PRO:HA	2.02	0.42
5:B:802:PRO:HA	5:B:822:ASN:ND2	2.35	0.42
5:B:826:ALA:O	5:B:1011:ILE:HA	2.20	0.42
7:E:79:TRP:HE1	7:E:96:PHE:HE1	1.66	0.42
4:A:482:PHE:C	4:A:484:GLY:N	2.73	0.41
4:A:704:ALA:HB1	4:A:710:LEU:HD22	2.01	0.41
4:A:858:ASN:ND2	4:A:860:LEU:H	2.18	0.41
4:A:1414:ALA:C	4:A:1416:ALA:H	2.23	0.41
5:B:67:SER:HB2	5:B:92:PHE:CD1	2.55	0.41
5:B:123:THR:O	5:B:125:SER:N	2.43	0.41
6:C:18:VAL:HG23	6:C:240:VAL:HB	2.02	0.41
7:E:161:LYS:HG3	7:E:195:VAL:HG21	2.02	0.41
7:E:202:SER:OG	7:E:204:THR:HG22	2.20	0.41
4:A:831:THR:O	4:A:834:THR:HG23	2.20	0.41
4:A:1096:SER:O	4:A:1100:ARG:HG3	2.21	0.41
4:A:1364:ASN:O	4:A:1365:TYR:C	2.57	0.41
4:A:1410:PHE:CD2	5:B:1212:ILE:HD11	2.52	0.41
5:B:831:SER:CB	5:B:833:TYR:HD1	2.32	0.41
5:B:977:GLY:HA3	5:B:1099:VAL:HG11	2.02	0.41
12:K:43:GLY:HA2	12:K:71:PHE:CE1	2.55	0.41
5:B:125:SER:HA	5:B:171:PRO:HA	2.01	0.41
5:B:789:MET:HE2	5:B:965:LYS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:537:ARG:HG2	4:A:575:LYS:HE3	2.00	0.41
4:A:575:LYS:O	4:A:576:GLN:C	2.59	0.41
4:A:754:SER:H	4:A:757:ASN:ND2	2.18	0.41
4:A:777:PHE:CE2	4:A:782:ARG:HA	2.55	0.41
5:B:363:HIS:O	5:B:364:ILE:CB	2.66	0.41
5:B:1150:ARG:HA	5:B:1150:ARG:HD3	1.90	0.41
6:C:234:SER:HB3	6:C:240:VAL:HG13	2.02	0.41
6:C:245:VAL:HA	6:C:248:ILE:HD12	2.03	0.41
6:C:250:THR:HA	6:C:253:LYS:HB2	2.02	0.41
7:E:149:LEU:O	7:E:151:PRO:HD3	2.20	0.41
4:A:77:CYS:HA	4:A:78:PRO:HD3	1.83	0.41
4:A:323:LYS:N	4:A:323:LYS:HD3	2.35	0.41
4:A:365:GLY:N	4:A:469:ARG:O	2.50	0.41
4:A:847:ASP:HA	4:A:1063:MET:HE1	2.03	0.41
4:A:1441:PHE:HZ	8:F:88:TYR:C	2.24	0.41
5:B:195:CYS:HB3	5:B:198:ASP:HB2	2.02	0.41
5:B:391:ASP:HA	5:B:393:LYS:N	2.36	0.41
5:B:757:PRO:HD3	5:B:983:ARG:HE	1.85	0.41
6:C:241:ASP:HB3	12:K:109:TRP:CE2	2.55	0.41
2:T:20:DC:OP1	5:B:1131:GLY:HA3	2.19	0.41
4:A:23:SER:O	4:A:27:VAL:HG23	2.21	0.41
5:B:128:LEU:HB2	5:B:167:ILE:O	2.21	0.41
5:B:183:GLU:CA	5:B:184:ALA:HB3	2.51	0.41
5:B:636:PRO:HB3	5:B:743:ILE:CG1	2.51	0.41
9:H:23:VAL:HG11	9:H:121:LEU:HD22	2.02	0.41
9:H:84:ALA:CA	9:H:85:GLY:C	2.76	0.41
12:K:42:LEU:O	12:K:46:ILE:HB	2.21	0.41
4:A:552:TRP:CE3	4:A:651:LYS:HB3	2.55	0.41
4:A:909:ASP:C	4:A:911:SER:N	2.74	0.41
4:A:1083:THR:CA	4:A:1084:PHE:O	2.68	0.41
5:B:273:LEU:HD23	5:B:274:PRO:HD2	2.01	0.41
5:B:549:THR:HB	5:B:628:THR:HG22	2.02	0.41
5:B:1103:ILE:O	5:B:1103:ILE:HG22	2.21	0.41
5:B:1177:HIS:CA	5:B:1178:ASN:CB	2.98	0.41
6:C:22:LEU:CD2	6:C:25:VAL:HG21	2.51	0.41
6:C:73:GLN:HB3	6:C:131:HIS:H	1.86	0.41
6:C:102:GLN:OE1	6:C:154:LYS:HD2	2.20	0.41
9:H:92:ASP:O	9:H:145:ARG:HD3	2.20	0.41
10:I:103:CYS:SG	10:I:106:CYS:HB2	2.60	0.41
4:A:16:GLU:HB2	5:B:1217:TYR:HB2	2.03	0.41
4:A:645:LEU:HD11	4:A:649:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:710:LEU:HA	4:A:712:GLU:N	2.36	0.41
4:A:1131:ALA:HA	4:A:1134:ILE:HD12	2.03	0.41
4:A:1193:LEU:HD21	4:A:1264:GLU:HB3	2.03	0.41
5:B:51:PHE:CE1	5:B:203:PHE:HE2	2.39	0.41
5:B:523:CYS:SG	5:B:750:GLY:N	2.94	0.41
5:B:1023:VAL:O	5:B:1026:LEU:HB2	2.21	0.41
9:H:105:GLU:HG3	9:H:106:GLU:N	2.30	0.41
11:J:3:VAL:HA	11:J:4:PRO:HD3	1.88	0.41
4:A:399:HIS:CE1	4:A:462:VAL:HG21	2.56	0.41
4:A:619:LYS:O	4:A:623:GLY:HA3	2.21	0.41
4:A:857:ARG:HA	4:A:864:ILE:HG12	2.03	0.41
4:A:858:ASN:C	4:A:858:ASN:HD22	2.24	0.41
4:A:1438:THR:CG2	8:F:92:ARG:HB2	2.51	0.41
5:B:29:ASP:HB3	5:B:658:ILE:HD13	2.03	0.41
5:B:997:GLU:C	5:B:999:MET:H	2.24	0.41
7:E:140:LEU:HA	7:E:142:VAL:H	1.84	0.41
12:K:40:HIS:HB3	12:K:61:TYR:CE1	2.56	0.41
4:A:61:ILE:HG13	4:A:62:ASP:H	1.86	0.41
4:A:452:LYS:HB3	5:B:1140:ALA:CB	2.50	0.41
4:A:675:THR:HG21	4:A:736:ASN:ND2	2.26	0.41
4:A:1072:ILE:HD13	4:A:1072:ILE:HA	1.86	0.41
4:A:1200:ALA:CB	4:A:1203:ASN:HB2	2.50	0.41
5:B:634:TYR:HE1	5:B:692:TYR:CD1	2.36	0.41
6:C:36:VAL:HG23	12:K:41:THR:HG21	2.02	0.41
6:C:258:ILE:H	6:C:258:ILE:HG13	1.60	0.41
4:A:86:LEU:HD23	4:A:273:ASN:HD22	1.86	0.40
4:A:256:GLN:HE21	4:A:256:GLN:HB3	1.62	0.40
4:A:347:PHE:H	5:B:1107:ALA:HA	1.86	0.40
4:A:481:ASP:HA	5:B:836:GLU:HG2	2.03	0.40
4:A:527:THR:HG23	4:A:650:GLN:HA	2.04	0.40
4:A:814:PHE:O	4:A:817:ALA:HB3	2.22	0.40
5:B:183:GLU:N	5:B:184:ALA:HB3	2.36	0.40
5:B:212:LEU:HD21	5:B:461:LEU:CD1	2.50	0.40
5:B:238:ALA:HB3	5:B:256:VAL:HB	2.03	0.40
5:B:293:PRO:CA	5:B:294:ASP:HB2	2.29	0.40
5:B:550:ASP:HA	5:B:551:PRO:HD3	1.97	0.40
4:A:764:CYS:HA	4:A:802:ASN:O	2.21	0.40
4:A:794:PRO:C	4:A:796:SER:N	2.73	0.40
4:A:1192:LEU:HD13	4:A:1193:LEU:N	2.35	0.40
4:A:1366:ARG:HG2	4:A:1366:ARG:H	1.77	0.40
6:C:124:LEU:C	6:C:126:GLY:N	2.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:59:SER:O	7:E:60:PHE:HB3	2.21	0.40
9:H:8:ASP:HB3	9:H:10:PHE:CE1	2.56	0.40
2:T:18:DA:H8	4:A:832:ALA:HA	1.87	0.40
4:A:977:LYS:HD3	4:A:977:LYS:HA	1.69	0.40
4:A:993:LEU:HA	4:A:996:ASN:HD21	1.86	0.40
5:B:421:PHE:HA	5:B:453:ILE:HD11	2.03	0.40
7:E:21:GLU:O	7:E:24:LYS:HG2	2.21	0.40
7:E:79:TRP:CZ2	7:E:99:HIS:NE2	2.90	0.40
9:H:137:GLN:HG2	9:H:138:GLU:H	1.85	0.40
10:I:65:ASP:HA	10:I:66:PRO:HD3	1.90	0.40
4:A:560:ILE:H	4:A:560:ILE:HG12	1.58	0.40
4:A:1189:SER:HB2	4:A:1242:VAL:O	2.22	0.40
4:A:1271:ILE:HD13	4:A:1271:ILE:HA	1.99	0.40
5:B:327:ARG:O	5:B:331:LEU:HD12	2.21	0.40
6:C:166:GLU:O	6:C:167:HIS:CB	2.69	0.40
4:A:38:PRO:HG3	4:A:270:LEU:HB3	2.04	0.40
4:A:71:GLN:O	4:A:73:GLY:N	2.53	0.40
4:A:380:VAL:HG12	4:A:388:LEU:HD13	2.03	0.40
4:A:818:MET:HA	5:B:514:LEU:HB3	2.03	0.40
4:A:841:LEU:O	4:A:845:LEU:HG	2.22	0.40
4:A:894:GLU:C	4:A:896:ARG:H	2.25	0.40
4:A:975:HIS:NE2	9:H:136:LYS:HB2	2.36	0.40
4:A:1213:GLY:HA2	4:A:1216:ILE:HD12	2.03	0.40
5:B:108:VAL:HG12	5:B:109:THR:N	2.37	0.40
8:F:82:THR:HG22	8:F:84:TYR:HB2	2.04	0.40
9:H:42:ILE:HG23	9:H:95:TYR:CE1	2.56	0.40
9:H:111:LEU:HD12	9:H:127:GLY:CA	2.50	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	1384/1733 (80%)	1055 (76%)	224 (16%)	105 (8%)	1 15
5	B	1074/1224 (88%)	855 (80%)	161 (15%)	58 (5%)	2 22
6	C	264/318 (83%)	217 (82%)	35 (13%)	12 (4%)	2 24
7	E	185/215 (86%)	146 (79%)	26 (14%)	13 (7%)	1 17
8	F	81/155 (52%)	62 (76%)	15 (18%)	4 (5%)	2 23
9	H	129/146 (88%)	87 (67%)	30 (23%)	12 (9%)	0 12
10	I	117/122 (96%)	73 (62%)	32 (27%)	12 (10%)	0 9
11	J	63/70 (90%)	56 (89%)	4 (6%)	3 (5%)	2 23
12	K	112/120 (93%)	98 (88%)	13 (12%)	1 (1%)	17 56
13	L	44/70 (63%)	29 (66%)	11 (25%)	4 (9%)	1 12
All	All	3453/4173 (83%)	2678 (78%)	551 (16%)	224 (6%)	1 18

All (224) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	63	ARG
4	A	223	GLY
4	A	284	ALA
4	A	313	GLN
4	A	404	TYR
4	A	517	ASN
4	A	525	GLN
4	A	568	PRO
4	A	702	LEU
4	A	710	LEU
4	A	903	ASN
4	A	998	LEU
4	A	1016	THR
4	A	1081	LEU
4	A	1084	PHE
4	A	1085	HIS
4	A	1156	PRO
4	A	1158	PRO
4	A	1163	ILE
4	A	1165	GLU
4	A	1172	LEU
4	A	1191	TRP
4	A	1365	TYR
4	A	1392	SER

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Mol	Chain	Res	Type
4	A	1393	ASN
5	B	66	ASP
5	B	184	ALA
5	B	231	PRO
5	B	274	PRO
5	B	636	PRO
5	B	711	GLU
5	B	878	GLN
5	B	882	THR
5	B	1178	ASN
6	C	110	THR
6	C	167	HIS
6	C	173	ALA
6	C	174	ALA
7	E	130	ALA
8	F	104	ASN
8	F	128	LYS
9	H	77	ARG
9	H	84	ALA
10	I	21	GLU
10	I	26	LEU
10	I	46	HIS
10	I	47	GLU
13	L	26	THR
4	A	55	ASP
4	A	71	GLN
4	A	250	ILE
4	A	279	LEU
4	A	288	ALA
4	A	312	PRO
4	A	423	ASP
4	A	424	ILE
4	A	479	ASN
4	A	543	LEU
4	A	576	GLN
4	A	624	SER
4	A	637	LYS
4	A	713	SER
4	A	1069	ALA
4	A	1072	ILE
4	A	1094	VAL
4	A	1127	ASP

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Mol	Chain	Res	Type
4	A	1153	TYR
4	A	1154	TYR
4	A	1160	SER
4	A	1167	GLU
4	A	1192	LEU
4	A	1224	LEU
4	A	1391	ARG
5	B	228	LYS
5	B	266	ALA
5	B	276	ILE
5	B	301	ILE
5	B	391	ASP
5	B	410	GLY
5	B	474	SER
5	B	478	GLY
5	B	705	MET
5	B	708	GLU
5	B	864	LYS
5	B	996	ARG
5	B	1020	ARG
5	B	1021	MET
5	B	1167	GLY
5	B	1177	HIS
6	C	22	LEU
6	C	142	VAL
6	C	266	ASP
7	E	30	ILE
7	E	36	GLU
7	E	141	VAL
7	E	174	GLN
7	E	206	GLY
8	F	145	ASP
9	H	82	PRO
9	H	85	GLY
9	H	89	LEU
9	H	107	VAL
9	H	112	ILE
9	H	140	ALA
4	A	48	ALA
4	A	72	GLU
4	A	214	ILE
4	A	257	ARG

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Mol	Chain	Res	Type
4	A	289	ILE
4	A	465	TYR
4	A	741	ASN
4	A	972	HIS
4	A	1206	ASP
5	B	477	ALA
5	B	482	VAL
5	B	531	GLN
5	B	792	MET
6	C	88	CYS
6	C	90	ASP
9	H	91	ASP
9	H	131	ASN
10	I	4	PHE
13	L	56	LEU
4	A	54	ASN
4	A	287	HIS
4	A	321	PRO
4	A	591	PHE
4	A	651	LYS
4	A	708	MET
4	A	775	ILE
4	A	975	HIS
4	A	1003	LYS
4	A	1262	LYS
4	A	1270	ASN
4	A	1435	PRO
5	B	100	PRO
5	B	124	TYR
5	B	458	LYS
5	B	572	HIS
5	B	635	ARG
5	B	710	LEU
5	B	865	LYS
5	B	887	HIS
5	B	1017	ILE
5	B	1046	PRO
5	B	1103	ILE
5	B	1112	GLN
7	E	125	PRO
8	F	146	TRP
10	I	20	LYS

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Mol	Chain	Res	Type
10	I	113	ASP
11	J	10	CYS
11	J	29	GLU
12	K	66	PRO
4	A	10	PRO
4	A	58	LEU
4	A	178	GLY
4	A	213	HIS
4	A	254	GLU
4	A	306	ASN
4	A	332	LYS
4	A	333	GLU
4	A	639	PRO
4	A	650	GLN
4	A	673	GLY
4	A	870	GLU
4	A	902	LEU
4	A	910	PRO
4	A	920	LEU
4	A	922	ASP
4	A	958	VAL
4	A	969	GLN
4	A	1013	ASP
4	A	1155	ASP
4	A	1164	PRO
4	A	1366	ARG
5	B	64	CYS
5	B	232	SER
5	B	476	ARG
5	B	652	LYS
5	B	786	ASN
5	B	870	ILE
5	B	974	PRO
6	C	21	ILE
6	C	38	ILE
7	E	29	PHE
7	E	66	GLU
7	E	96	PHE
7	E	166	LYS
9	H	7	ASP
9	H	23	VAL
10	I	11	ASN

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Mol	Chain	Res	Type
10	I	18	GLU
11	J	2	ILE
13	L	59	ALA
4	A	248	PRO
4	A	707	GLY
4	A	883	LEU
4	A	886	ILE
4	A	1388	GLY
5	B	233	PRO
5	B	275	TYR
5	B	436	VAL
5	B	571	PRO
5	B	712	PRO
5	B	731	VAL
5	B	746	SER
6	C	168	ALA
7	E	76	GLY
10	I	118	ARG
4	A	1107	VAL
4	A	1237	ILE
13	L	55	ILE
4	A	35	ILE
4	A	1157	ASP
4	A	52	GLY
5	B	592	ASN
10	I	59	VAL
4	A	3	GLY
7	E	124	VAL
10	I	43	VAL
4	A	396	PRO
5	B	234	ILE
5	B	751	VAL

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	1218/1520 (80%)	1055 (87%)	163 (13%)	4 20
5	B	951/1061 (90%)	827 (87%)	124 (13%)	4 21
6	C	234/274 (85%)	207 (88%)	27 (12%)	5 24
7	E	177/197 (90%)	160 (90%)	17 (10%)	8 30
8	F	73/137 (53%)	65 (89%)	8 (11%)	6 25
9	H	117/128 (91%)	103 (88%)	14 (12%)	5 23
10	I	113/116 (97%)	92 (81%)	21 (19%)	1 10
11	J	60/65 (92%)	51 (85%)	9 (15%)	3 17
12	K	99/102 (97%)	88 (89%)	11 (11%)	6 25
13	L	40/57 (70%)	31 (78%)	9 (22%)	1 6
All	All	3082/3657 (84%)	2679 (87%)	403 (13%)	4 21

All (403) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	6	TYR
4	A	13	THR
4	A	41	MET
4	A	49	LYS
4	A	50	ILE
4	A	53	LEU
4	A	62	ASP
4	A	65	LEU
4	A	66	LYS
4	A	68	GLN
4	A	69	THR
4	A	80	HIS
4	A	84	ILE
4	A	100	LYS
4	A	108	MET
4	A	122	MET
4	A	133	LYS
4	A	140	THR
4	A	161	LEU
4	A	204	THR
4	A	208	LEU
4	A	222	LEU
4	A	256	GLN
4	A	260	ASP

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Mol	Chain	Res	Type
4	A	264	PHE
4	A	270	LEU
4	A	279	LEU
4	A	286	HIS
4	A	289	ILE
4	A	302	THR
4	A	303	TYR
4	A	306	ASN
4	A	308	ILE
4	A	313	GLN
4	A	320	ARG
4	A	322	VAL
4	A	323	LYS
4	A	348	SER
4	A	373	THR
4	A	381	THR
4	A	391	LEU
4	A	443	LEU
4	A	445	ASN
4	A	450	LEU
4	A	451	HIS
4	A	452	LYS
4	A	455	MET
4	A	481	ASP
4	A	487	MET
4	A	494	SER
4	A	501	LEU
4	A	509	LEU
4	A	535	THR
4	A	541	ILE
4	A	544	ASP
4	A	560	ILE
4	A	566	ILE
4	A	573	SER
4	A	576	GLN
4	A	582	ILE
4	A	596	THR
4	A	618	GLU
4	A	635	ARG
4	A	645	LEU
4	A	660	ASN
4	A	666	ILE

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Mol	Chain	Res	Type
4	A	675	THR
4	A	680	THR
4	A	687	LYS
4	A	708	MET
4	A	714	PHE
4	A	721	PHE
4	A	728	LYS
4	A	738	LYS
4	A	740	LEU
4	A	758	ILE
4	A	765	VAL
4	A	774	ARG
4	A	795	GLU
4	A	821	ARG
4	A	826	ASP
4	A	834	THR
4	A	839	ARG
4	A	856	THR
4	A	858	ASN
4	A	859	SER
4	A	867	ILE
4	A	880	LYS
4	A	881	GLN
4	A	896	ARG
4	A	902	LEU
4	A	913	LEU
4	A	915	SER
4	A	918	GLU
4	A	920	LEU
4	A	927	VAL
4	A	929	LEU
4	A	941	LYS
4	A	945	GLU
4	A	949	ASP
4	A	964	ILE
4	A	971	PHE
4	A	973	ILE
4	A	974	ASP
4	A	988	LEU
4	A	996	ASN
4	A	1016	THR
4	A	1017	LEU

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Mol	Chain	Res	Type
4	A	1025	ARG
4	A	1028	THR
4	A	1035	TYR
4	A	1054	LEU
4	A	1058	VAL
4	A	1078	GLN
4	A	1083	THR
4	A	1085	HIS
4	A	1086	PHE
4	A	1104	ILE
4	A	1113	THR
4	A	1116	LEU
4	A	1127	ASP
4	A	1128	GLN
4	A	1141	THR
4	A	1142	THR
4	A	1156	PRO
4	A	1158	PRO
4	A	1159	ARG
4	A	1161	THR
4	A	1166	ASP
4	A	1167	GLU
4	A	1168	GLU
4	A	1172	LEU
4	A	1187	GLN
4	A	1188	GLN
4	A	1192	LEU
4	A	1215	ARG
4	A	1224	LEU
4	A	1227	ILE
4	A	1228	TRP
4	A	1241	ARG
4	A	1242	VAL
4	A	1262	LYS
4	A	1276	VAL
4	A	1281	ARG
4	A	1284	MET
4	A	1295	THR
4	A	1312	ASN
4	A	1322	ILE
4	A	1329	THR
4	A	1333	ILE

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Mol	Chain	Res	Type
4	A	1334	ASP
4	A	1335	ILE
4	A	1336	MET
4	A	1358	SER
4	A	1364	ASN
4	A	1366	ARG
4	A	1376	THR
4	A	1385	THR
4	A	1391	ARG
4	A	1394	THR
4	A	1426	GLU
4	A	1442	ASP
4	A	1443	VAL
5	B	28	GLU
5	B	44	VAL
5	B	46	GLN
5	B	49	ASP
5	B	66	ASP
5	B	94	LYS
5	B	102	VAL
5	B	131	ASP
5	B	167	ILE
5	B	175	ARG
5	B	178	ASN
5	B	180	TYR
5	B	185	THR
5	B	188	ASP
5	B	191	LYS
5	B	199	MET
5	B	217	ARG
5	B	225	VAL
5	B	234	ILE
5	B	242	SER
5	B	264	SER
5	B	268	THR
5	B	273	LEU
5	B	291	ILE
5	B	297	ILE
5	B	302	CYS
5	B	304	ASP
5	B	322	PHE
5	B	346	GLU

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Mol	Chain	Res	Type
5	B	347	LYS
5	B	351	TYR
5	B	361	LEU
5	B	367	LEU
5	B	373	ARG
5	B	387	LEU
5	B	391	ASP
5	B	393	LYS
5	B	394	ASP
5	B	398	ARG
5	B	415	GLN
5	B	424	LEU
5	B	425	THR
5	B	432	MET
5	B	448	ILE
5	B	463	THR
5	B	466	TRP
5	B	473	MET
5	B	475	SER
5	B	483	LEU
5	B	502	ILE
5	B	537	LYS
5	B	547	VAL
5	B	549	THR
5	B	561	TRP
5	B	572	HIS
5	B	616	ILE
5	B	618	ASP
5	B	624	LEU
5	B	628	THR
5	B	635	ARG
5	B	637	LEU
5	B	650	GLU
5	B	651	LEU
5	B	655	LYS
5	B	680	THR
5	B	701	ILE
5	B	728	ARG
5	B	736	THR
5	B	740	HIS
5	B	741	CYS
5	B	787	VAL

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Mol	Chain	Res	Type
5	B	796	LEU
5	B	797	TYR
5	B	812	LEU
5	B	837	ASP
5	B	844	SER
5	B	864	LYS
5	B	866	TYR
5	B	880	THR
5	B	883	LEU
5	B	898	LEU
5	B	899	ILE
5	B	905	VAL
5	B	916	THR
5	B	918	ILE
5	B	941	LEU
5	B	943	SER
5	B	953	LEU
5	B	959	ASP
5	B	970	THR
5	B	973	ILE
5	B	975	GLN
5	B	982	SER
5	B	1004	GLU
5	B	1012	ILE
5	B	1021	MET
5	B	1051	THR
5	B	1060	ARG
5	B	1065	GLN
5	B	1072	MET
5	B	1082	MET
5	B	1092	TYR
5	B	1096	ARG
5	B	1099	VAL
5	B	1103	ILE
5	B	1113	VAL
5	B	1115	THR
5	B	1122	ARG
5	B	1123	SER
5	B	1124	ARG
5	B	1133	MET
5	B	1135	ARG
5	B	1153	GLU

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Mol	Chain	Res	Type
5	B	1156	ASP
5	B	1159	ARG
5	B	1160	VAL
5	B	1166	CYS
5	B	1183	LYS
5	B	1189	ILE
5	B	1194	ILE
5	B	1196	ILE
5	B	1219	ASP
5	B	1220	ARG
5	B	1222	ARG
6	C	10	ILE
6	C	27	LEU
6	C	41	ILE
6	C	55	THR
6	C	56	THR
6	C	57	VAL
6	C	77	ILE
6	C	81	GLU
6	C	106	GLU
6	C	119	VAL
6	C	120	ILE
6	C	123	ASN
6	C	154	LYS
6	C	185	LYS
6	C	195	GLN
6	C	208	GLU
6	C	210	GLU
6	C	221	TYR
6	C	235	VAL
6	C	240	VAL
6	C	249	ASP
6	C	250	THR
6	C	258	ILE
6	C	259	LEU
6	C	265	MET
6	C	266	ASP
6	C	268	ASP
7	E	3	GLN
7	E	8	ASN
7	E	18	THR
7	E	43	LYS

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Mol	Chain	Res	Type
7	E	69	ILE
7	E	95	THR
7	E	98	ILE
7	E	103	LYS
7	E	119	SER
7	E	123	LEU
7	E	127	ILE
7	E	132	ILE
7	E	140	LEU
7	E	156	LEU
7	E	158	SER
7	E	165	LEU
7	E	169	ARG
8	F	77	ASP
8	F	97	ARG
8	F	104	ASN
8	F	110	ASP
8	F	111	LEU
8	F	119	ARG
8	F	140	ASP
8	F	145	ASP
9	H	2	SER
9	H	24	CYS
9	H	32	THR
9	H	56	THR
9	H	83	GLN
9	H	89	LEU
9	H	102	TYR
9	H	105	GLU
9	H	111	LEU
9	H	112	ILE
9	H	130	ARG
9	H	133	ASN
9	H	136	LYS
9	H	138	GLU
10	I	2	THR
10	I	4	PHE
10	I	13	MET
10	I	20	LYS
10	I	25	LEU
10	I	26	LEU
10	I	28	GLU

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Mol	Chain	Res	Type
10	I	30	ARG
10	I	32	CYS
10	I	37	GLU
10	I	42	LEU
10	I	43	VAL
10	I	45	ARG
10	I	50	THR
10	I	59	VAL
10	I	79	HIS
10	I	84	VAL
10	I	92	ARG
10	I	108	HIS
10	I	109	ILE
10	I	111	THR
11	J	2	ILE
11	J	7	CYS
11	J	9	SER
11	J	36	LEU
11	J	43	ARG
11	J	48	ARG
11	J	51	LEU
11	J	52	THR
11	J	55	ASP
12	K	11	LEU
12	K	12	LEU
12	K	22	ASP
12	K	40	HIS
12	K	41	THR
12	K	52	ASN
12	K	53	ASP
12	K	63	VAL
12	K	85	ASP
12	K	91	CYS
12	K	101	LEU
13	L	31	CYS
13	L	33	GLU
13	L	48	CYS
13	L	53	HIS
13	L	61	THR
13	L	62	LYS
13	L	63	ARG
13	L	65	VAL

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Mol	Chain	Res	Type
13	L	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	68	GLN
4	A	83	HIS
4	A	109	HIS
4	A	225	ASN
4	A	256	GLN
4	A	273	ASN
4	A	313	GLN
4	A	390	GLN
4	A	397	ASN
4	A	399	HIS
4	A	435	HIS
4	A	510	GLN
4	A	517	ASN
4	A	576	GLN
4	A	654	ASN
4	A	660	ASN
4	A	700	ASN
4	A	736	ASN
4	A	741	ASN
4	A	757	ASN
4	A	802	ASN
4	A	838	GLN
4	A	858	ASN
4	A	926	GLN
4	A	965	GLN
4	A	966	ASN
4	A	968	GLN
4	A	972	HIS
4	A	996	ASN
4	A	1085	HIS
4	A	1110	ASN
4	A	1128	GLN
4	A	1222	ASN
4	A	1312	ASN
4	A	1364	ASN
4	A	1390	ASN
5	B	121	ASN

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Mol	Chain	Res	Type
5	B	325	GLN
5	B	363	HIS
5	B	366	GLN
5	B	469	GLN
5	B	481	GLN
5	B	513	GLN
5	B	515	HIS
5	B	516	ASN
5	B	518	HIS
5	B	531	GLN
5	B	744	HIS
5	B	763	GLN
5	B	776	GLN
5	B	794	ASN
5	B	822	ASN
5	B	835	GLN
5	B	975	GLN
5	B	984	HIS
5	B	1013	ASN
5	B	1015	HIS
5	B	1025	HIS
5	B	1084	GLN
5	B	1177	HIS
6	C	7	GLN
6	C	73	GLN
6	C	112	ASN
6	C	188	HIS
6	C	203	GLN
6	C	224	GLN
6	C	242	GLN
6	C	252	GLN
7	E	8	ASN
7	E	101	GLN
7	E	147	HIS
8	F	78	GLN
9	H	33	GLN
9	H	128	ASN
10	I	90	GLN
10	I	116	ASN
11	J	53	HIS
12	K	65	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	8/10 (80%)	1 (12%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	8	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
16	UTP	B	3000	15	22,30,30	2.08	4 (18%)	27,47,47	1.39	4 (14%)

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	B	3000	15	-	6/20/38/38	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	3000	UTP	C6-N1	5.25	1.42	1.35
16	B	3000	UTP	C4-N3	5.06	1.41	1.33
16	B	3000	UTP	O4'-C1'	3.87	1.46	1.41
16	B	3000	UTP	PG-O2G	3.32	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	B	3000	UTP	PB-O3B-PG	-3.37	121.26	132.83
16	B	3000	UTP	O1G-PG-O3B	2.57	113.25	104.64
16	B	3000	UTP	PB-O3A-PA	-2.46	124.38	132.83
16	B	3000	UTP	C5'-C4'-C3'	-2.01	107.63	115.18

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	B	3000	UTP	C5'-O5'-PA-O1A
16	B	3000	UTP	C4'-C5'-O5'-PA
16	B	3000	UTP	O4'-C4'-C5'-O5'
16	B	3000	UTP	C3'-C4'-C5'-O5'
16	B	3000	UTP	PB-O3A-PA-O5'
16	B	3000	UTP	PB-O3B-PG-O2G

There are no ring outliers.

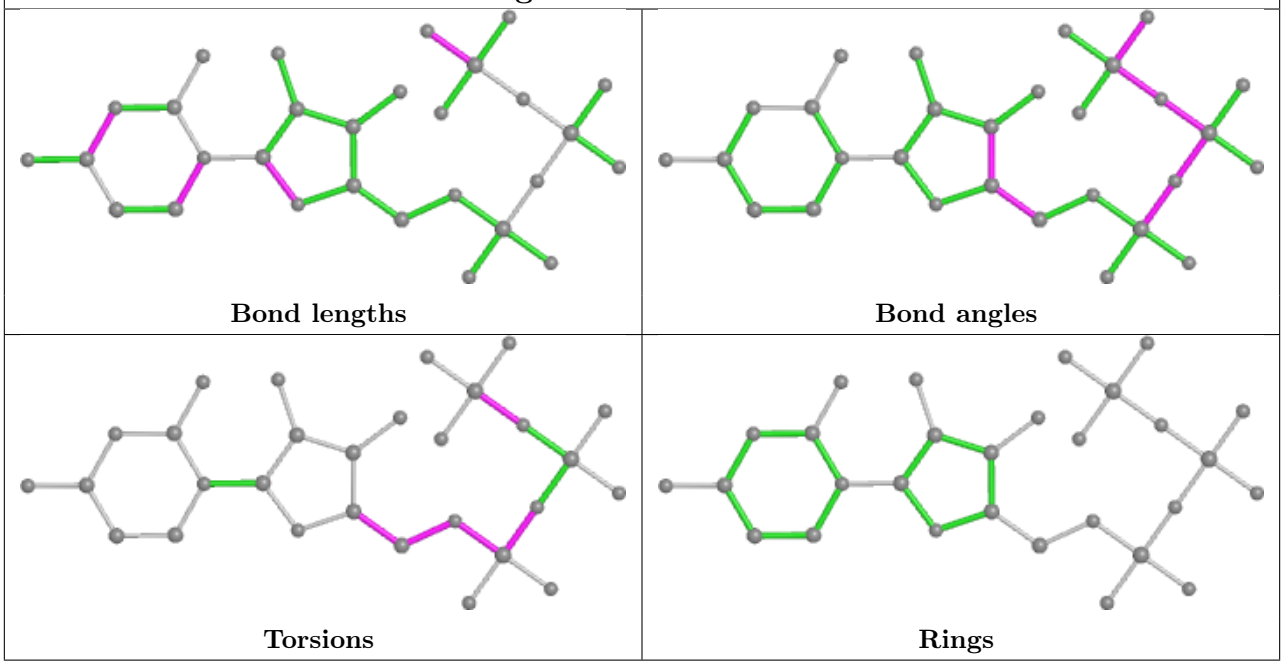
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	3000	UTP	2	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.

Ligand UTP B 3000



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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%)	-0.36	0	100	100	89, 111, 136, 141	0
2	T	28/28 (100%)	0.73	8 (28%)	0	0	81, 200, 285, 291	0
3	N	14/14 (100%)	1.65	7 (50%)	0	0	265, 273, 290, 292	0
4	A	1398/1733 (80%)	-0.38	4 (0%)	94	90	84, 118, 171, 184	0
5	B	1096/1224 (89%)	-0.38	1 (0%)	95	95	86, 114, 151, 165	0
6	C	266/318 (83%)	-0.42	1 (0%)	92	87	99, 118, 146, 150	0
7	E	193/215 (89%)	-0.32	0	100	100	98, 130, 163, 167	0
8	F	83/155 (53%)	-0.36	0	100	100	111, 127, 138, 144	0
9	H	133/146 (91%)	-0.26	0	100	100	120, 141, 176, 181	0
10	I	119/122 (97%)	-0.22	0	100	100	118, 149, 168, 173	0
11	J	65/70 (92%)	-0.56	0	100	100	103, 119, 134, 136	0
12	K	114/120 (95%)	-0.34	0	100	100	99, 118, 134, 136	0
13	L	46/70 (65%)	-0.06	0	100	100	137, 178, 191, 193	0
All	All	3565/4225 (84%)	-0.35	21 (0%)	89	84	81, 120, 168, 292	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	T	2	DT	4.9
2	T	3	DA	3.7
2	T	10	DA	3.2
3	N	11	DG	3.2
2	T	1	DC	3.1
4	A	168	GLY	2.8
3	N	1	DC	2.8
3	N	12	DT	2.7
3	N	10	DG	2.6

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Mol	Chain	Res	Type	RSRZ
4	A	1175	SER	2.4
2	T	12	DC	2.4
3	N	2	DT	2.2
3	N	9	DC	2.1
5	B	1221	SER	2.1
2	T	11	DG	2.1
4	A	44	THR	2.1
2	T	4	DC	2.1
6	C	203	GLN	2.1
4	A	1174	PHE	2.0
3	N	14	DG	2.0
2	T	8	DT	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)

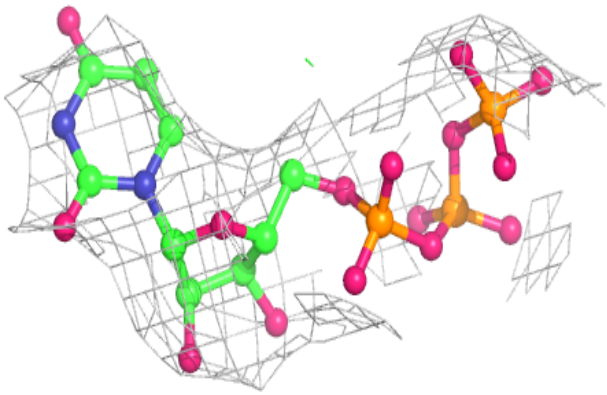
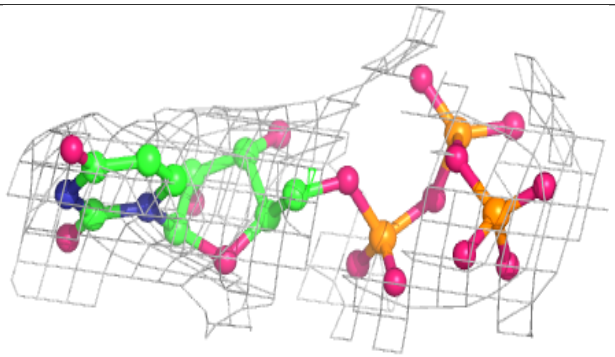
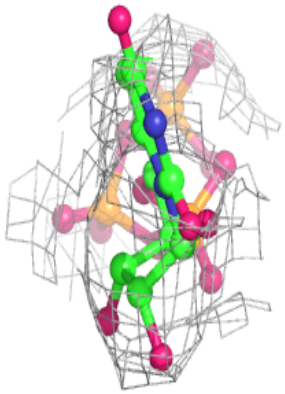
There are no monosaccharides in this entry.

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, 95th 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
15	MG	A	2001	1/1	0.84	0.14	97,97,97,97	0
15	MG	A	2002	1/1	0.88	0.19	102,102,102,102	0
14	ZN	A	1734	1/1	0.92	0.07	177,177,177,177	0
14	ZN	I	204	1/1	0.95	0.04	157,157,157,157	0
14	ZN	L	105	1/1	0.95	0.11	181,181,181,181	0
14	ZN	A	1735	1/1	0.95	0.05	165,165,165,165	0
14	ZN	I	203	1/1	0.95	0.09	121,121,121,121	0
16	UTP	B	3000	29/29	0.96	0.16	110,112,113,113	0
14	ZN	B	1307	1/1	0.97	0.05	147,147,147,147	0
14	ZN	J	101	1/1	0.97	0.12	112,112,112,112	0
14	ZN	C	319	1/1	0.98	0.03	117,117,117,117	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 B 3000: $2mF_o$-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 (i)

There are no such residues in this entry.