wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 12:40 AM GMT

PDB ID	:	2B63
Title	:	Complete RNA Polymerase II-RNA inhibitor complex
Authors	:	Kettenberger, H.; Eisenfuehr, A.; Brueckner, F.; Theis, M.; Famulok, M.; Cramer, P.
Deposited on	:	2005-09-30
Resolution	:	3.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

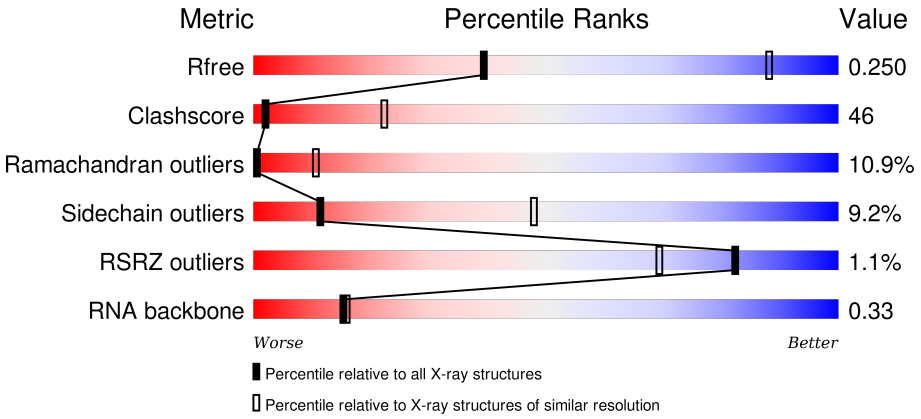
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 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}	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)
RNA backbone	2183	1070 (4.76-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	31	13% 42% 32% 13%
2	A	1733	% 29% 42% 9% • 18%
3	B	1224	% 30% 47% 11% • 9%
4	C	318	27% 45% 12% • 16%

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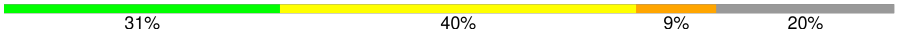
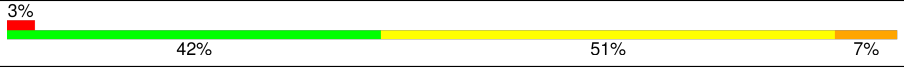
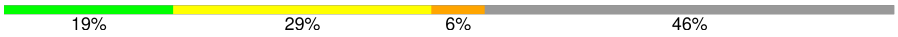
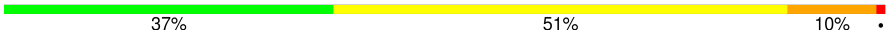
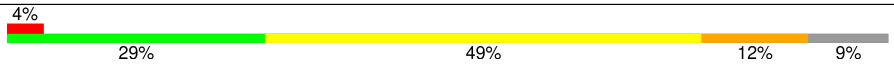
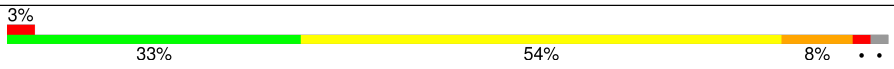
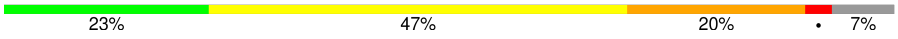
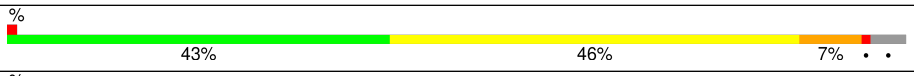
Mol	Chain	Length	Quality of chain
5	D	221	
6	E	215	
7	F	155	
8	G	171	
9	H	146	
10	I	122	
11	J	70	
12	K	120	
13	L	70	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 31731 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 31-MER.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	Br	C	N	O	P			
1	R	31	666	4	296	119	217	30	88	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	1416	11140	7021	1946	2111	62	0	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	B	1112	8836	5594	1548	1639	55	0	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

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

- Molecule 5 is a protein called DNA-directed RNA polymerase II 32 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	D	177	1356	840	241	273	2	0	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

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

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 8 is a protein called DNA-directed RNA polymerase II 19 kDa polypeptide.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	115	Total	C	N	O	S	0	0	0
			924	593	157	172	2			

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

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

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

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

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

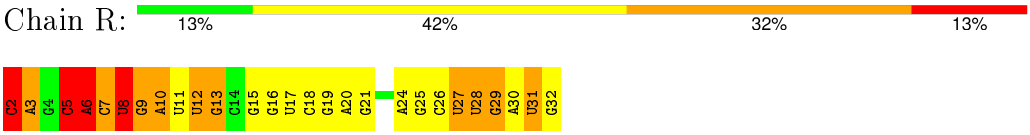
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Mg	0	0
			1	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

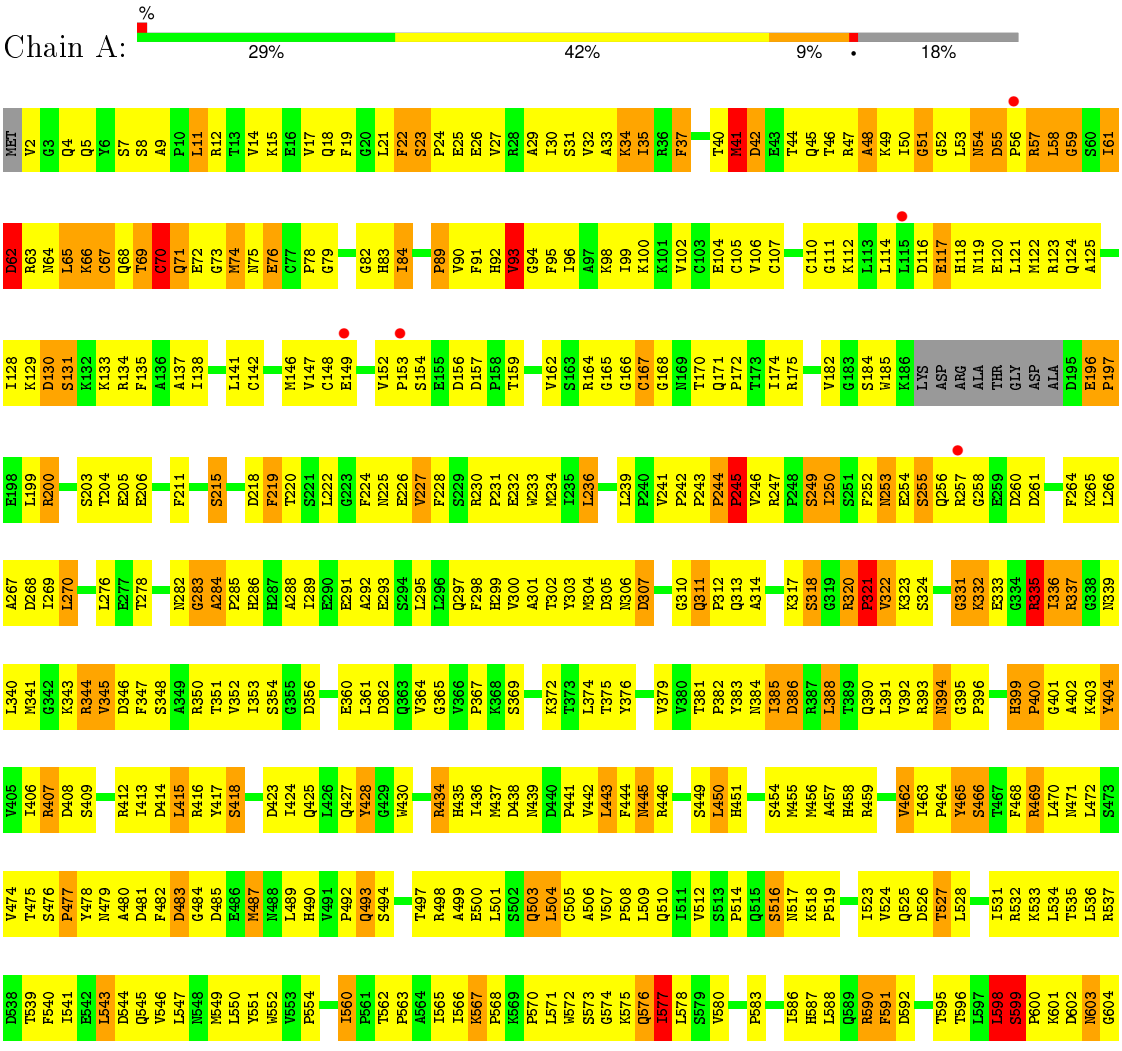
- Molecule 1: 31-MER

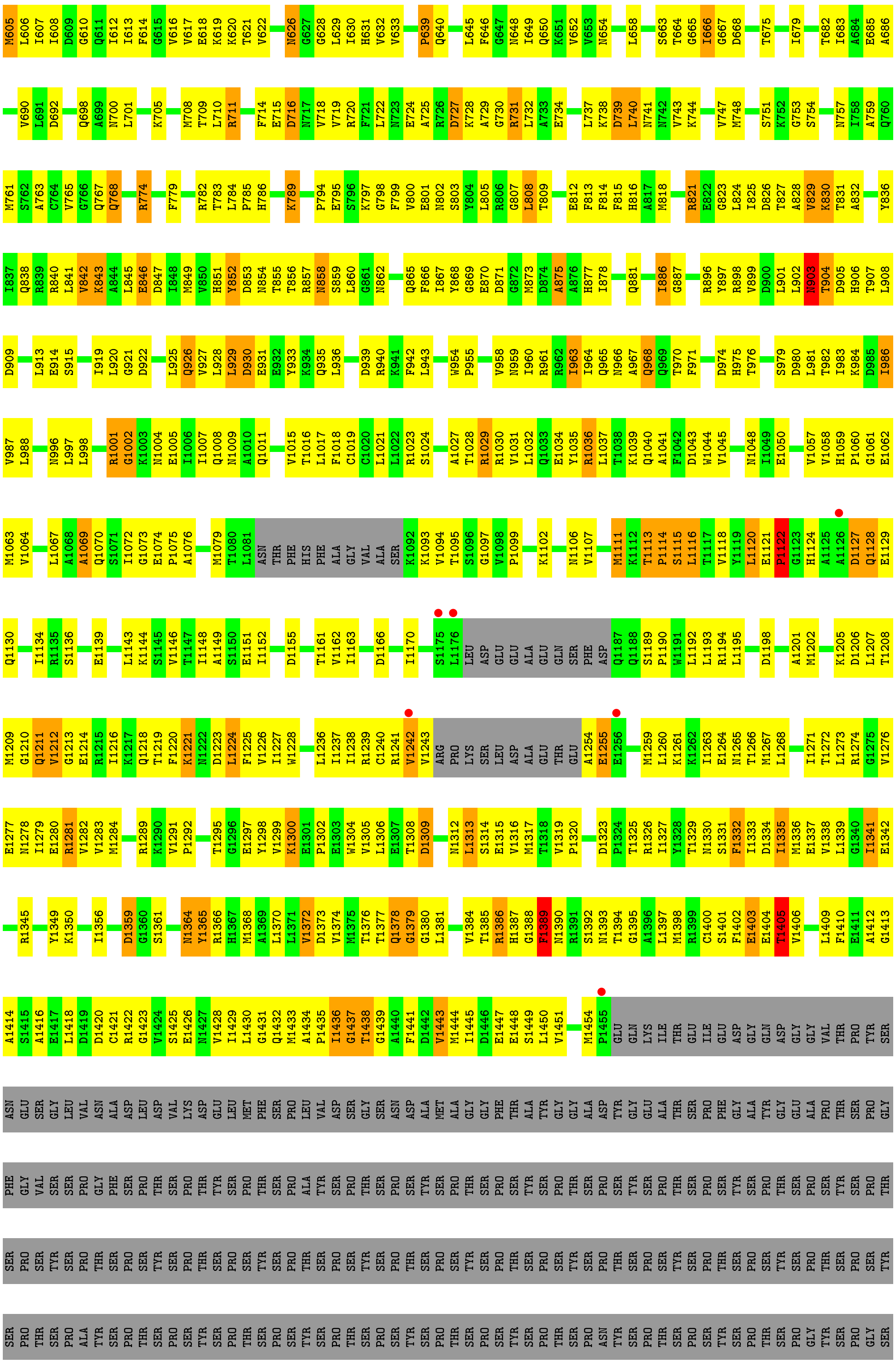
Chain R:



- Molecule 2: DNA-directed RNA polymerase II largest subunit

Chain A:

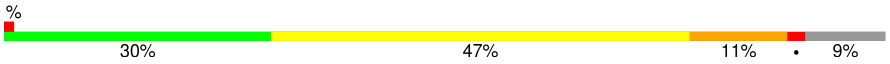


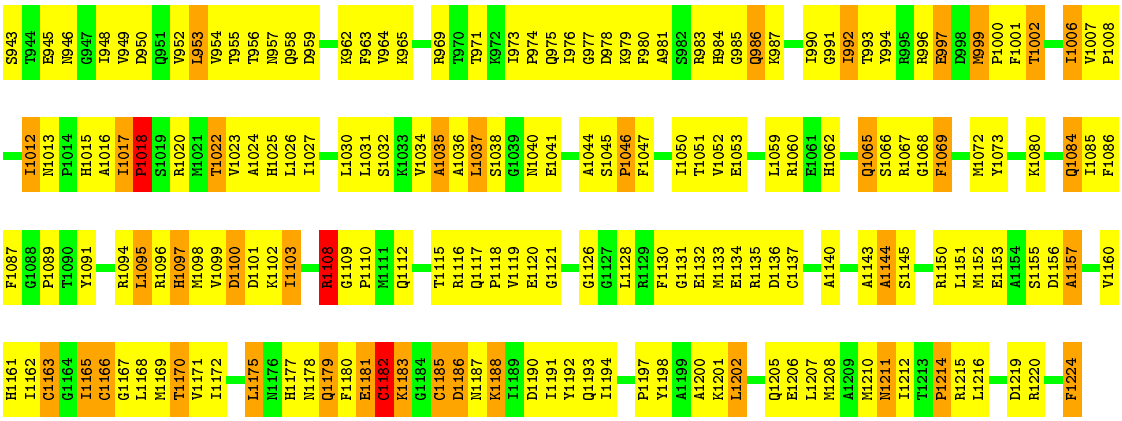

M605 L606 I607 I608 D609 G610 Q611 I612 I613 F614 G615 V616 V617 E618 K619 K620 T621 V622 N626 G627 G628 L629 I630 H631 V632 V633 P639 Q640 L645 F646 G647 N648 I649 Q650 K651 V652 V653 N654 L658 S663 T664 G665 I666 G667 D668 T675 I679 T682 I683 A684 E685 A686
V690 L691 D692 Q698 A699 N700 L701 K705 M708 T709 L710 R711 F714 E715 D716 N717 V718 V719 R720 F721 L722 N723 E724 A725 R726 D727 K728 A729 G730 R731 L732 A733 E734 L737 K738 D739 L740 N741 N742 V743 K744 V747 M748 S751 K752 G753 S754 N757 I758 A759 Q760
M761 S762 A763 C764 V765 G766 Q767 Q768 R774 F779 R782 T783 L784 P785 H786 K789 P794 E795 S796 K797 G798 F799 V800 E801 N802 S803 Y804 L805 R806 G807 L808 T809 E812 F813 F814 F815 H816 A817 M818 R821 E822 G823 L824 I825 D826 T827 A828 V829 K830 T831 A832 Y836
I837 Q838 R839 R840 L841 V842 K843 A844 L845 E846 D847 I848 M849 V850 H851 Y852 D853 N854 T855 T856 R857 N858 S859 L860 G861 N862 Q865 F866 I867 Y868 G869 E870 D871 G872 M873 D874 A875 A876 H877 I878 Q881 I886 G887 R896 Y897 R898 V899 D900 L901 L902 N903 T904 D905 H906 T907 L908
D909 L913 E914 S915 I919 L920 G921 D922 L925 Q926 V927 L928 L929 D930 E931 E932 Y933 K934 Q935 L936 D939 R940 K941 F942 L943 W954 P955 V958 N959 I960 R961 R962 I963 I964 Q965 N966 A967 Q968 Q969 T970 F971 D974 H975 T976 S979 D980 L981 T982 I983 K984 D985 I986
V987 L988 N996 L997 L998 R1001 G1002 K1003 N1004 E1005 I1006 I1007 Q1008 N1009 A1010 Q1011 V1015 T1016 L1017 F1018 C1019 C1020 L1021 L1022 R1023 S1024 A1027 T1028 R1029 R1030 V1031 L1032 Q1033 E1034 Y1035 R1036 L1037 T1038 K1039 Q1040 A1041 F1042 D1043 W1044 V1045 N1048 I1049 E1050 V1057 V1058 H1059 P1060 G1061 E1062
M1063 V1064 L1067 A1068 A1069 Q1070 S1071 I1072 G1073 E1074 P1075 A1076 M1079 T1080 L1081 ASN THR PHE HIS PHE ALA GLY VAL ALA SER K1092 K1093 V1094 T1095 S1096 G1097 V1098 P1099 K1102 N1106 V1107 M1111 K1112 T1113 P1114 S1115 L1116 T1117 V1118 Y1119 L1120 E1121 P1122 G1123 H1124 A1125 A1126 D1127 Q1128 E1129
Q1130 I1134 R1135 S1136 E1139 L1143 K1144 S1145 V1146 T1147 I1148 A1149 S1150 E1151 I1152 D1155 T1161 V1162 I1163 D1166 I1170 S1175 L1176 LEU ASP GLU GLU ALA GLU GLN SER PHE ASP Q1187 Q1188 S1189 P1190 W1191 L1192 L1193 R1194 L1195 D1198 A1201 M1202 K1205 D1206 L1207 T1208
M1209 G1210 Q1211 V1212 G1213 E1214 R1215 I1216 K1217 Q1218 T1219 F1220 K1221 N1222 D1223 L1224 F1225 V1226 I1227 W1228 L1236 I1237 I1238 R1239 C1240 R1241 V1242 V1243 ARG PRO LYS SER LEU ASP ALA GLU THR GLU A1254 E1255 E1256 M1259 L1260 K1261 K1262 I1263 E1264 N1265 T1266 M1267 L1268 I1271 T1272 L1273 R1274 G1275 V1276
E1277 N1278 I1279 E1280 R1281 V1282 V1283 M1284 R1289 K1290 V1291 P1292 T1295 G1296 E1297 Y1298 V1299 K1300 E1301 P1302 E1303 W1304 V1305 L1306 E1307 T1308 D1309 N1312 L1313 S1314 E1315 V1316 M1317 T1318 V1319 P1320 D1323 P1324 T1325 R1326 I1327 Y1328 T1329 N1330 S1331 F1332 I1333 D1334 I1335 M1336 E1337 V1338 L1339 G1340 I1341 E1342
R1345 Y1349 K1350 I1356 D1359 G1360 S1361 N1364 Y1365 R1366 H1367 M1368 A1369 L1370 L1371 V1372 D1373 V1374 M1375 T1376 T1377 Q1378 G1379 G1380 L1381 V1384 T1385 R1386 H1387 G1388 F1389 N1390 R1391 S1392 N1393 T1394 G1395 A1396 L1397 M1398 R1399 C1400 S1401 F1402 E1403 E1404 T1405 V1406 L1409 F1410 E1411 A1412 G1413
A1414 S1415 A1416 E1417 L1418 D1419 D1420 C1421 R1422 G1423 V1424 S1425 E1426 N1427 V1428 I1429 L1430 G1431 Q1432 M1433 A1434 P1435 I1436 G1437 T1438 G1439 A1440 F1441 D1442 V1443 M1444 I1445 D1446 E1447 E1448 S1449 L1450 V1451 M1454 P1455 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 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 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 ASN TYR SER PRO THR SER PRO SER TYR SER PRO THR SER PRO SER TYR SER PRO GLY TYR SER PRO GLY SER

PRO ALA TYR SER PRO LYS GLN ASP GLU GLN LYS HIS ASN GLU ASN GLU ASN SER ARG

- Molecule 3: DNA-directed RNA polymerase II 140 kDa polypeptide

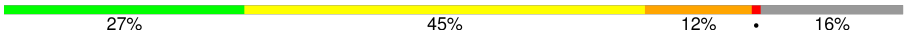
Chain B:

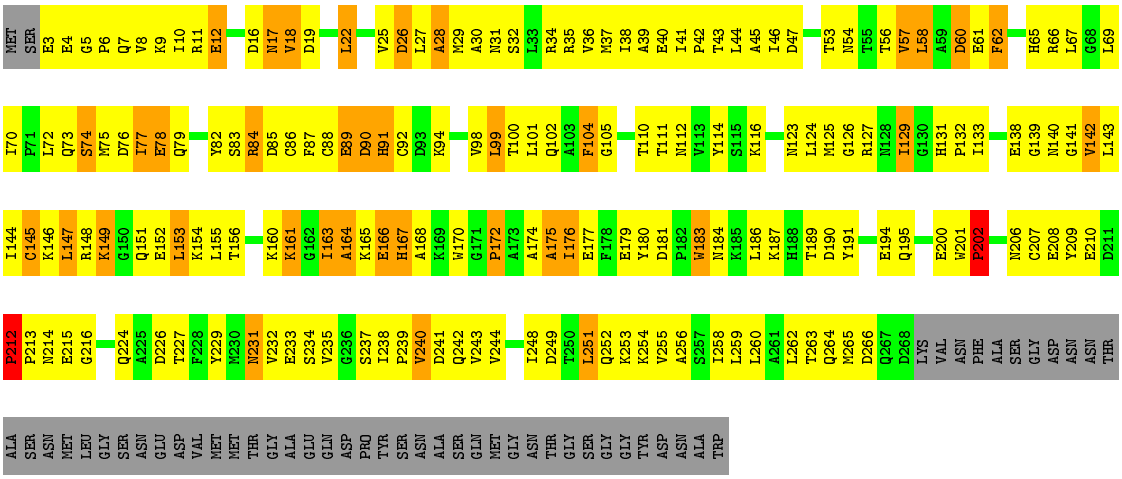




• Molecule 4: DNA-directed RNA polymerase II 45 kDa polypeptide

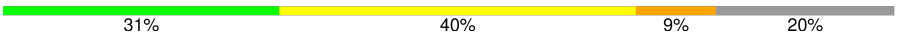
Chain C:

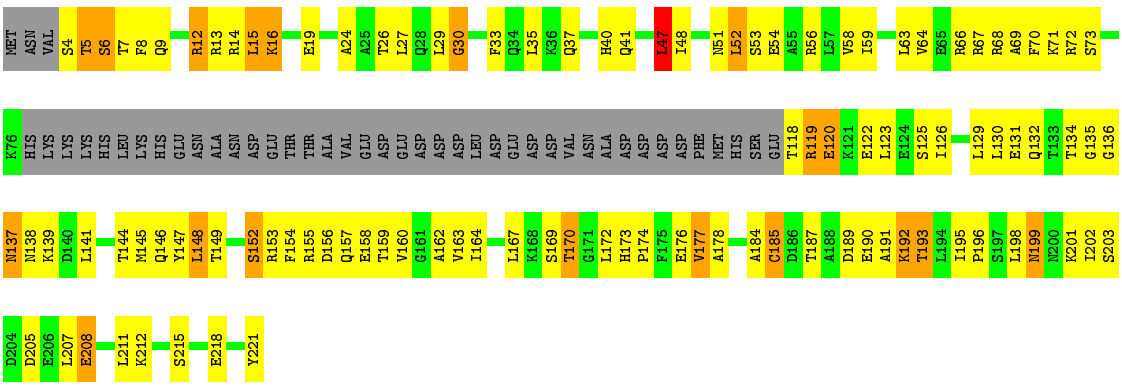




• Molecule 5: DNA-directed RNA polymerase II 32 kDa polypeptide

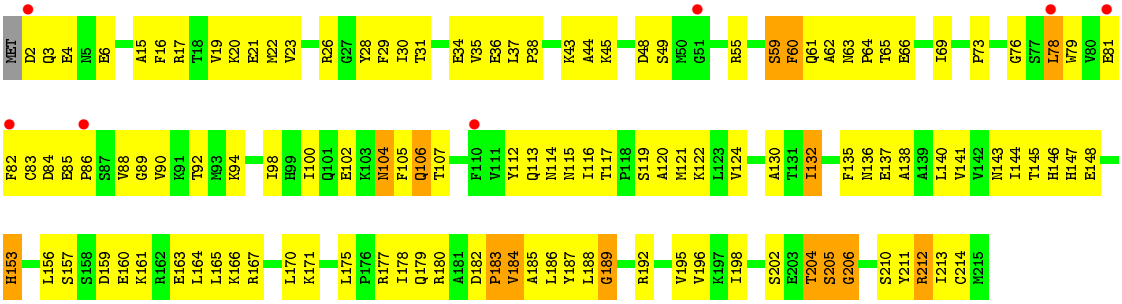
Chain D:



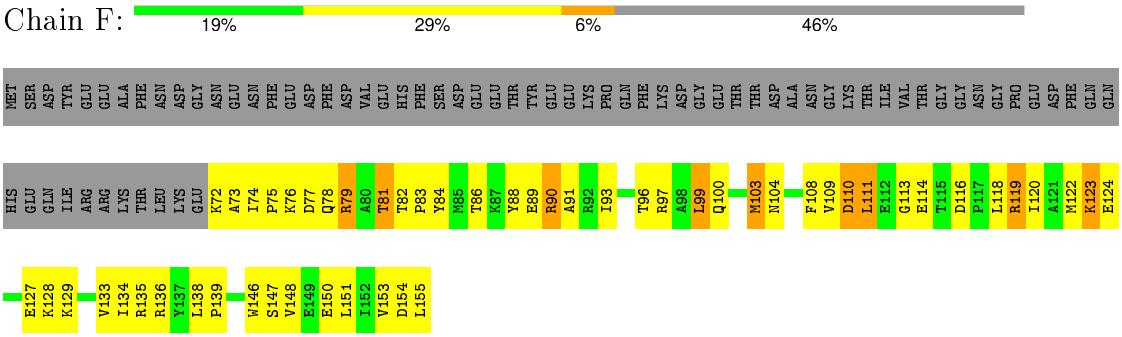


• Molecule 6: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

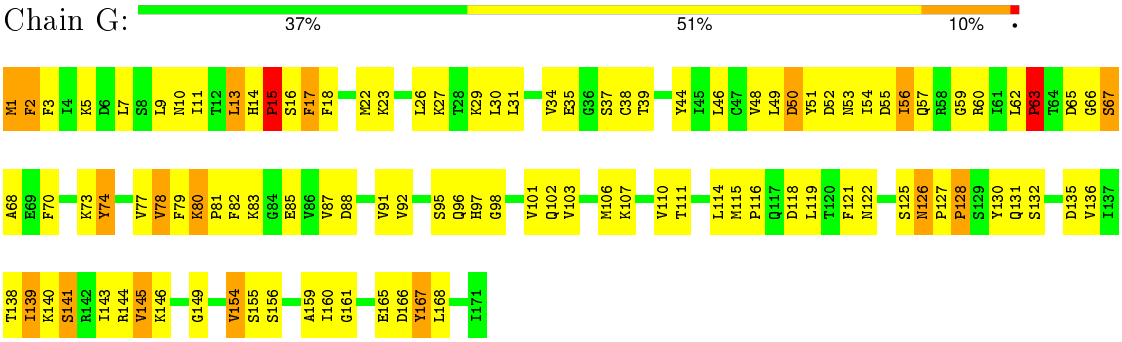
Chain E:



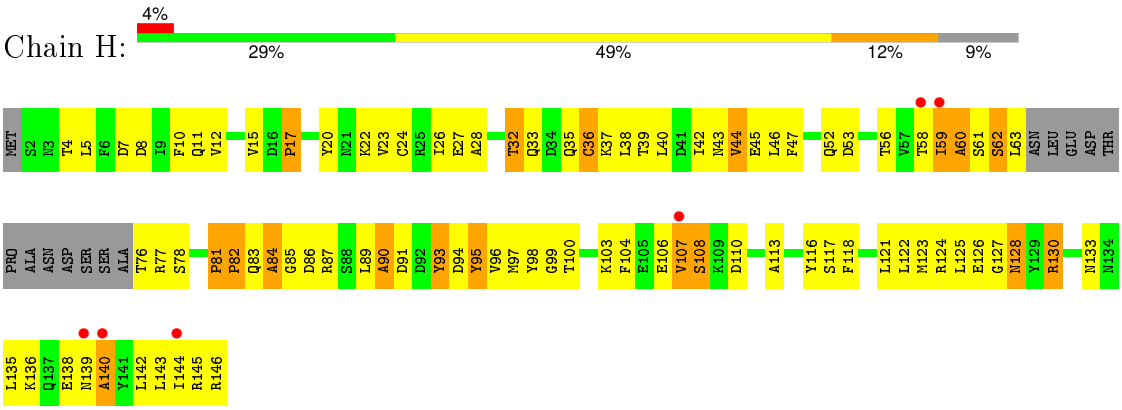
• Molecule 7: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide



• Molecule 8: DNA-directed RNA polymerase II 19 kDa polypeptide

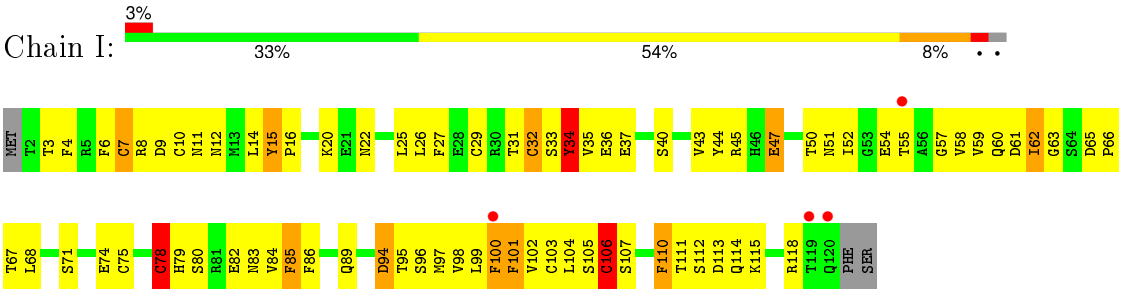


• Molecule 9: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide



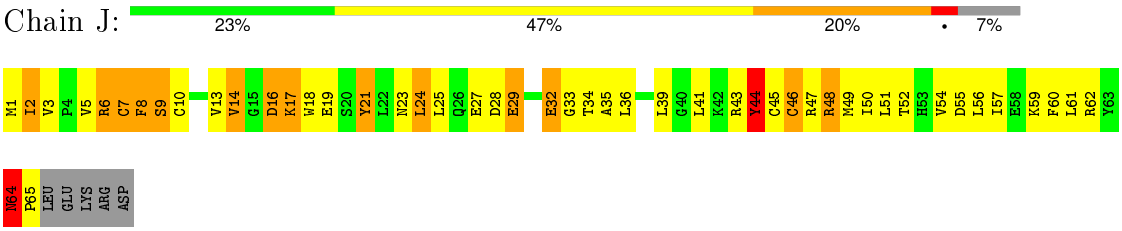
• Molecule 10: DNA-directed RNA polymerase II subunit 9

Chain I:



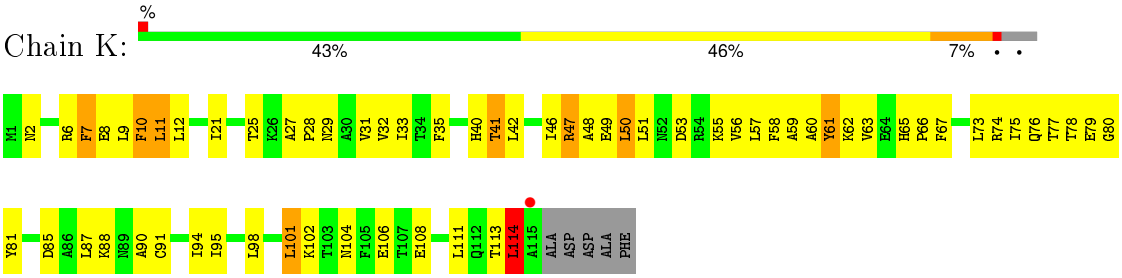
• Molecule 11: DNA-directed RNA polymerases I/II/III subunit 10

Chain J:



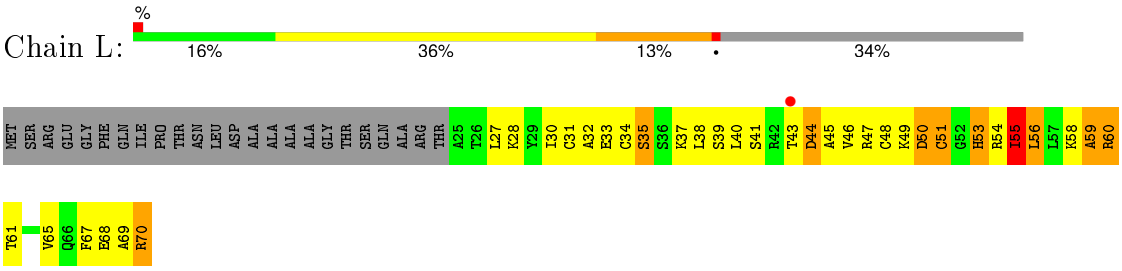
• Molecule 12: DNA-directed RNA polymerase II 13.6 kDa polypeptide

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 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	224.59Å 399.81Å 286.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 49.15 – 3.77	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-3.80) 99.1 (49.15-3.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 3.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.252 , 0.273 0.226 , 0.250	Depositor DCC
R_{free} test set	2527 reflections (2.04%)	DCC
Wilson B-factor (Å^2)	121.4	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 64.6	EDS
Estimated twinning fraction	0.015 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.018 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 248494 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	31731	wwPDB-VP
Average B, all atoms (Å^2)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5BU, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	R	0.93	1/652 (0.2%)	1.19	4/1017 (0.4%)
2	A	0.48	0/11339	0.74	5/15334 (0.0%)
3	B	0.47	0/9008	0.78	19/12146 (0.2%)
4	C	0.47	0/2133	0.75	1/2891 (0.0%)
5	D	0.45	0/1365	0.68	0/1837
6	E	0.44	0/1788	0.67	0/2406
7	F	0.56	0/691	0.76	0/933
8	G	0.51	0/1368	0.75	0/1844
9	H	0.39	0/1086	0.64	0/1470
10	I	0.39	0/989	0.70	0/1331
11	J	0.51	0/541	0.82	0/727
12	K	0.46	0/942	0.68	0/1272
13	L	0.53	0/365	0.75	0/485
All	All	0.48	1/32267 (0.0%)	0.76	29/43693 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	R	0	2
11	J	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	2	C	C3'-C2'	5.33	1.58	1.52

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	503	GLY	N-CA-C	-10.94	85.76	113.10
3	B	273	LEU	C-N-CD	-9.80	99.03	120.60
1	R	2	C	O4'-C1'-N1	9.55	115.84	108.20
3	B	508	LEU	N-CA-C	-8.97	86.78	111.00
1	R	5	C	C2'-C3'-O3'	7.04	124.98	109.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	J	44	TYR	Sidechain
1	R	2	C	Sidechain
1	R	5	C	Sidechain

5.2 Too-close contacts

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	666	0	331	42	0
2	A	11140	0	11217	1087	0
3	B	8836	0	8871	910	0
4	C	2095	0	2051	242	0
5	D	1356	0	1319	118	0
6	E	1752	0	1776	129	0
7	F	679	0	701	56	0
8	G	1340	0	1357	132	0
9	H	1068	0	1040	123	0
10	I	971	0	928	83	0
11	J	532	0	542	84	0
12	K	924	0	934	78	0
13	L	363	0	386	41	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	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	31731	0	31453	2875	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 46.

The worst 5 of 2875 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)
5:D:40:HIS:HB3	8:G:73:LYS:NZ	1.60	1.16
2:A:1329:THR:HG22	2:A:1331:SER:H	1.01	1.12
3:B:827:ILE:HG12	3:B:1012:ILE:HD11	1.18	1.11
3:B:463:THR:HB	3:B:465:ASN:HB2	1.32	1.10
1:R:3:A:OP2	3:B:531:GLN:HB3	1.50	1.10

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
2	A	1406/1733 (81%)	973 (69%)	278 (20%)	155 (11%)	0 10
3	B	1096/1224 (90%)	754 (69%)	214 (20%)	128 (12%)	0 9
4	C	264/318 (83%)	172 (65%)	62 (24%)	30 (11%)	0 9
5	D	173/221 (78%)	116 (67%)	36 (21%)	21 (12%)	0 8
6	E	212/215 (99%)	155 (73%)	42 (20%)	15 (7%)	1 23
7	F	82/155 (53%)	72 (88%)	9 (11%)	1 (1%)	16 63
8	G	169/171 (99%)	133 (79%)	19 (11%)	17 (10%)	1 13
9	H	129/146 (88%)	89 (69%)	23 (18%)	17 (13%)	0 6
10	I	117/122 (96%)	83 (71%)	23 (20%)	11 (9%)	1 15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
11	J	63/70 (90%)	35 (56%)	14 (22%)	14 (22%)	0 1
12	K	113/120 (94%)	83 (74%)	25 (22%)	5 (4%)	3 35
13	L	44/70 (63%)	19 (43%)	16 (36%)	9 (20%)	0 2
All	All	3868/4565 (85%)	2684 (69%)	761 (20%)	423 (11%)	0 11

5 of 423 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	31	SER
2	A	48	ALA
2	A	55	ASP
2	A	57	ARG
2	A	58	LEU

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
2	A	1239/1520 (82%)	1146 (92%)	93 (8%)	17 57
3	B	964/1061 (91%)	854 (89%)	110 (11%)	7 37
4	C	234/274 (85%)	211 (90%)	23 (10%)	10 44
5	D	140/200 (70%)	128 (91%)	12 (9%)	13 51
6	E	196/197 (100%)	186 (95%)	10 (5%)	29 69
7	F	74/137 (54%)	63 (85%)	11 (15%)	4 26
8	G	152/152 (100%)	137 (90%)	15 (10%)	10 44
9	H	117/128 (91%)	113 (97%)	4 (3%)	44 79
10	I	113/116 (97%)	97 (86%)	16 (14%)	4 29
11	J	60/65 (92%)	51 (85%)	9 (15%)	3 26
12	K	99/102 (97%)	90 (91%)	9 (9%)	12 48
13	L	40/57 (70%)	37 (92%)	3 (8%)	17 57
All	All	3428/4009 (86%)	3113 (91%)	315 (9%)	11 48

5 of 315 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	531	GLN
3	B	953	LEU
10	I	101	PHE
3	B	603	LEU
3	B	778	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	449	ASN
3	B	686	ASN
10	I	12	ASN
3	B	469	GLN
3	B	518	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	31/31 (100%)	16 (51%)	3 (9%)

5 of 16 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	3	A
1	R	6	A
1	R	7	C
1	R	8	U
1	R	9	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	R	2	C
1	R	5	C
1	R	6	A

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
1	5BU	R	12	1	13,22,23	2.24	4 (30%)	14,32,35	4.74	5 (35%)
1	5BU	R	17	1	13,22,23	1.65	2 (15%)	14,32,35	4.47	3 (21%)
1	5BU	R	27	1	13,22,23	2.09	2 (15%)	14,32,35	4.48	3 (21%)
1	5BU	R	28	1	13,22,23	2.88	4 (30%)	14,32,35	4.74	3 (21%)

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
1	5BU	R	12	1	-	0/3/25/26	0/2/2/2
1	5BU	R	17	1	-	0/3/25/26	0/2/2/2
1	5BU	R	27	1	-	0/3/25/26	0/2/2/2
1	5BU	R	28	1	-	0/3/25/26	0/2/2/2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	12	5BU	C4-N3	2.18	1.37	1.33
1	R	28	5BU	C4-N3	2.71	1.38	1.33
1	R	17	5BU	C4-N3	2.87	1.38	1.33
1	R	12	5BU	C6-N1	2.92	1.39	1.35
1	R	27	5BU	C4-N3	3.42	1.39	1.33

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	R	17	5BU	C5-C4-N3	-8.99	114.40	124.00
1	R	27	5BU	C5-C4-N3	-8.50	114.92	124.00
1	R	12	5BU	C5-C4-N3	-8.23	115.21	124.00
1	R	28	5BU	C5-C4-N3	-7.86	115.61	124.00
1	R	12	5BU	BR-C5-C4	-2.05	118.03	121.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	R	12	5BU	4	0
1	R	17	5BU	3	0
1	R	27	5BU	1	0
1	R	28	5BU	4	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	R	23/31 (74%)	0.22	0 100 100	86, 105, 133, 157	0
2	A	1416/1733 (81%)	-0.35	11 (0%) 87 77	22, 86, 159, 180	0
3	B	1112/1224 (90%)	-0.25	15 (1%) 79 65	26, 95, 168, 180	0
4	C	266/318 (83%)	-0.42	0 100 100	47, 82, 139, 156	0
5	D	177/221 (80%)	-0.33	0 100 100	56, 108, 156, 177	0
6	E	214/215 (99%)	-0.09	7 (3%) 50 34	56, 141, 179, 180	0
7	F	84/155 (54%)	-0.52	0 100 100	28, 59, 98, 122	0
8	G	171/171 (100%)	-0.32	0 100 100	54, 82, 124, 133	0
9	H	133/146 (91%)	0.27	6 (4%) 37 24	105, 144, 178, 180	0
10	I	119/122 (97%)	0.02	4 (3%) 49 34	82, 135, 166, 180	0
11	J	65/70 (92%)	-0.53	0 100 100	48, 78, 125, 133	0
12	K	115/120 (95%)	-0.40	1 (0%) 85 74	45, 83, 113, 143	0
13	L	46/70 (65%)	-0.07	1 (2%) 65 50	73, 139, 174, 179	0
All	All	3941/4596 (85%)	-0.28	45 (1%) 82 69	22, 92, 168, 180	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	1176	LEU	5.0
3	B	882	THR	4.4
2	A	149	GLU	3.8
3	B	883	LEU	3.6
6	E	51	GLY	3.5

6.2 Non-standard residues in protein, DNA, RNA chains (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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	5BU	R	17	21/22	0.90	0.18	-	88,105,129,149	0
1	5BU	R	12	21/22	0.88	0.18	-	96,112,134,153	0
1	5BU	R	28	21/22	0.78	0.25	-	130,138,155,167	0
1	5BU	R	27	21/22	0.76	0.24	-	140,148,161,171	0

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
14	ZN	I	1121	1/1	0.99	0.14	0.21	85,85,85,85	0
14	ZN	A	2456	1/1	0.97	0.11	-0.84	73,73,73,73	0
14	ZN	B	2225	1/1	0.99	0.13	-1.16	66,66,66,66	0
14	ZN	I	1122	1/1	0.99	0.08	-1.27	176,176,176,176	0
14	ZN	L	1071	1/1	0.97	0.05	-1.33	114,114,114,114	0
14	ZN	C	1269	1/1	0.98	0.07	-1.41	48,48,48,48	0
14	ZN	A	2457	1/1	0.99	0.10	-1.59	46,46,46,46	0
14	ZN	J	1066	1/1	0.99	0.13	-2.45	65,65,65,65	0
15	MG	A	2458	1/1	0.98	0.35	-	20,20,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.