wwPDB X-ray Structure Validation Summary Report (i)

Dec 4, 2023 – 05:00 pm GMT

PDB ID	:	2VUM
Title	:	Alpha-amanitin inhibited complete RNA polymerase II elongation complex
Authors	:	Brueckner, F.; Cramer, P.
Deposited on	:	2008-05-27
Resolution	:	3.40 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
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:

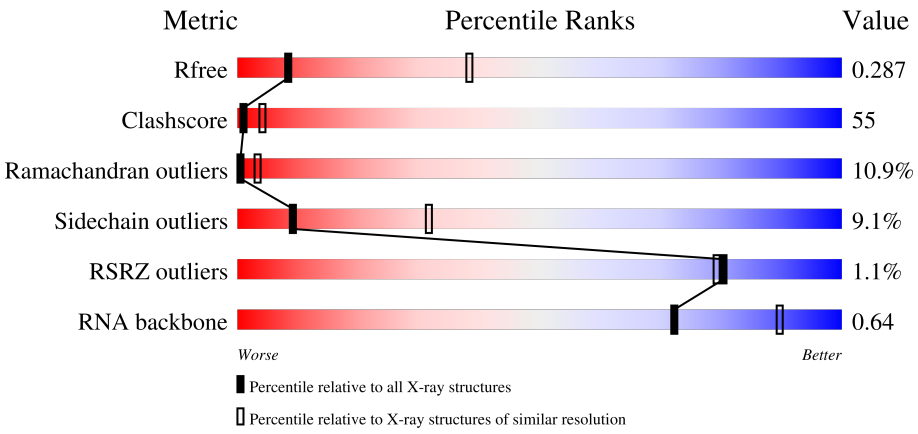
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)
RNA backbone	3102	1006 (3.84-2.96)

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	A	1733	24% 47% 10% • 18%
2	B	1224	% 24% 53% 12% • 10%
3	C	318	28% 43% 12% • 16%
4	D	221	29% 42% 9% • 20%

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Mol	Chain	Length	Quality of chain
5	E	215	3% 32% 58% 10%
6	F	155	12% 35% 7% 46%
7	G	171	33% 57% 9%
8	H	146	3% 24% 51% 14% 9%
9	I	122	6% 29% 56% 10%
10	J	70	17% 56% 19% 7%
11	K	120	32% 52% 10% 5%
12	L	70	7% 14% 30% 20% 34%
13	M	8	25% 50% 25%
14	N	14	7% 14% 79% 7%
15	P	11	9% 82% 9%
16	T	26	12% 15% 77%

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 32083 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 protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1418	11158	7032	1949	2115	62	0	0	0

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1106	8792	5568	1538	1631	55	0	0	0

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3.

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

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4.

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

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC1.

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

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC2.

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

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7.

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

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC3.

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

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

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

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC5.

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

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11.

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

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4.

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

- Molecule 13 is a protein called AMATOXIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	M	8	64	39	10	14	1	0	0	0

- Molecule 14 is a DNA chain called 5'-D(*AP*AP*AP*CP*TP*AP*CP*TP*TP*GP *AP*GP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
14	N	13	262	127	47	76	12	0	0	0

- Molecule 15 is a RNA chain called 5'-R(*AP*AP*AP*GP*AP*CP*CP*AP*GP*GP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
15	P	10	214	97	44	64	9	0	0	0

- Molecule 16 is a DNA chain called 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP *GP* TP*TP*AP*CP*GP*CP*CP*BRUP*GP*GP*TP*CP*AP*TP*T)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	Br	C	N	O	P			
16	T	25	509	1	243	92	149	24	0	0	0

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

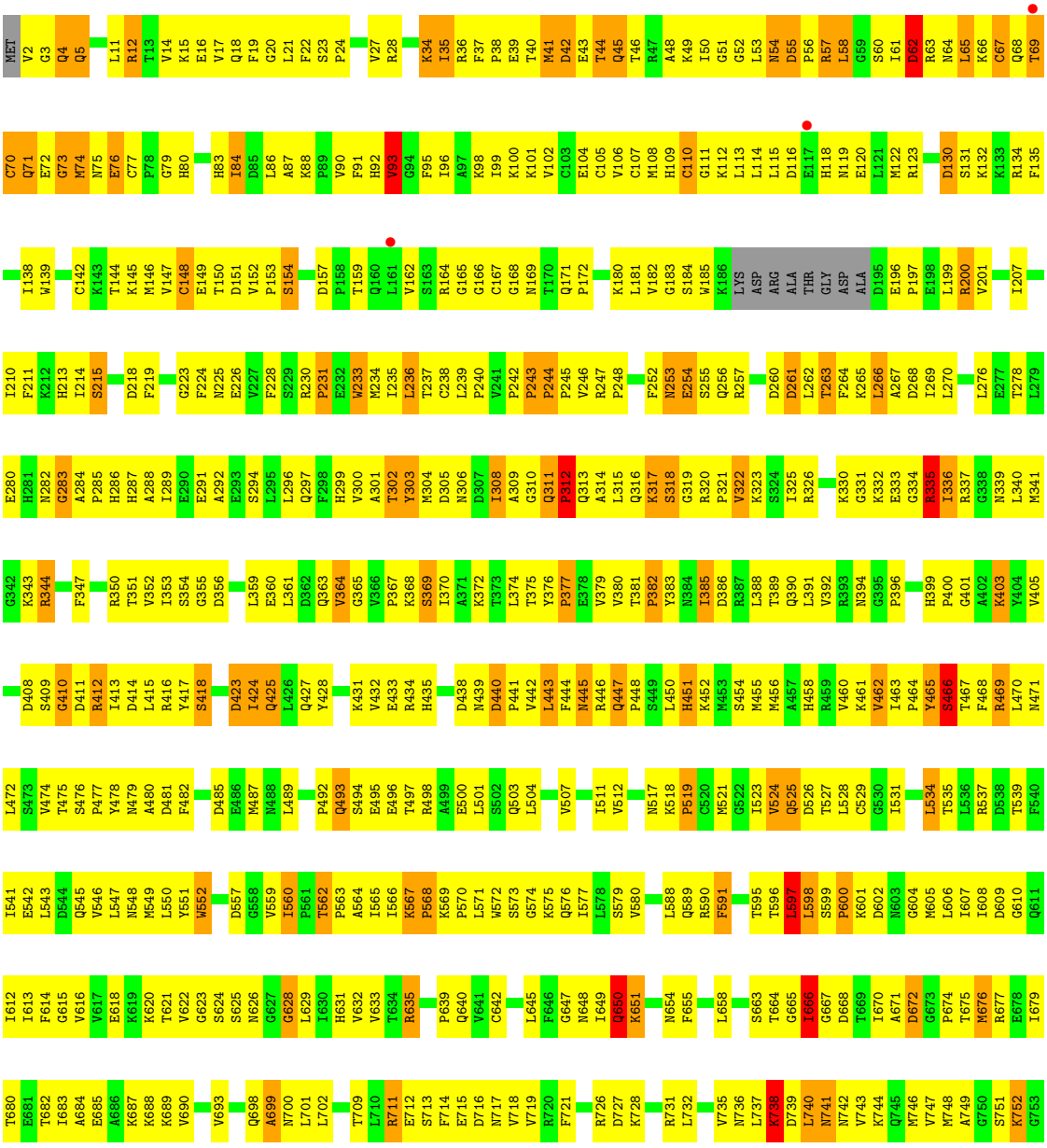
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
18	A	1	1	1	0	0

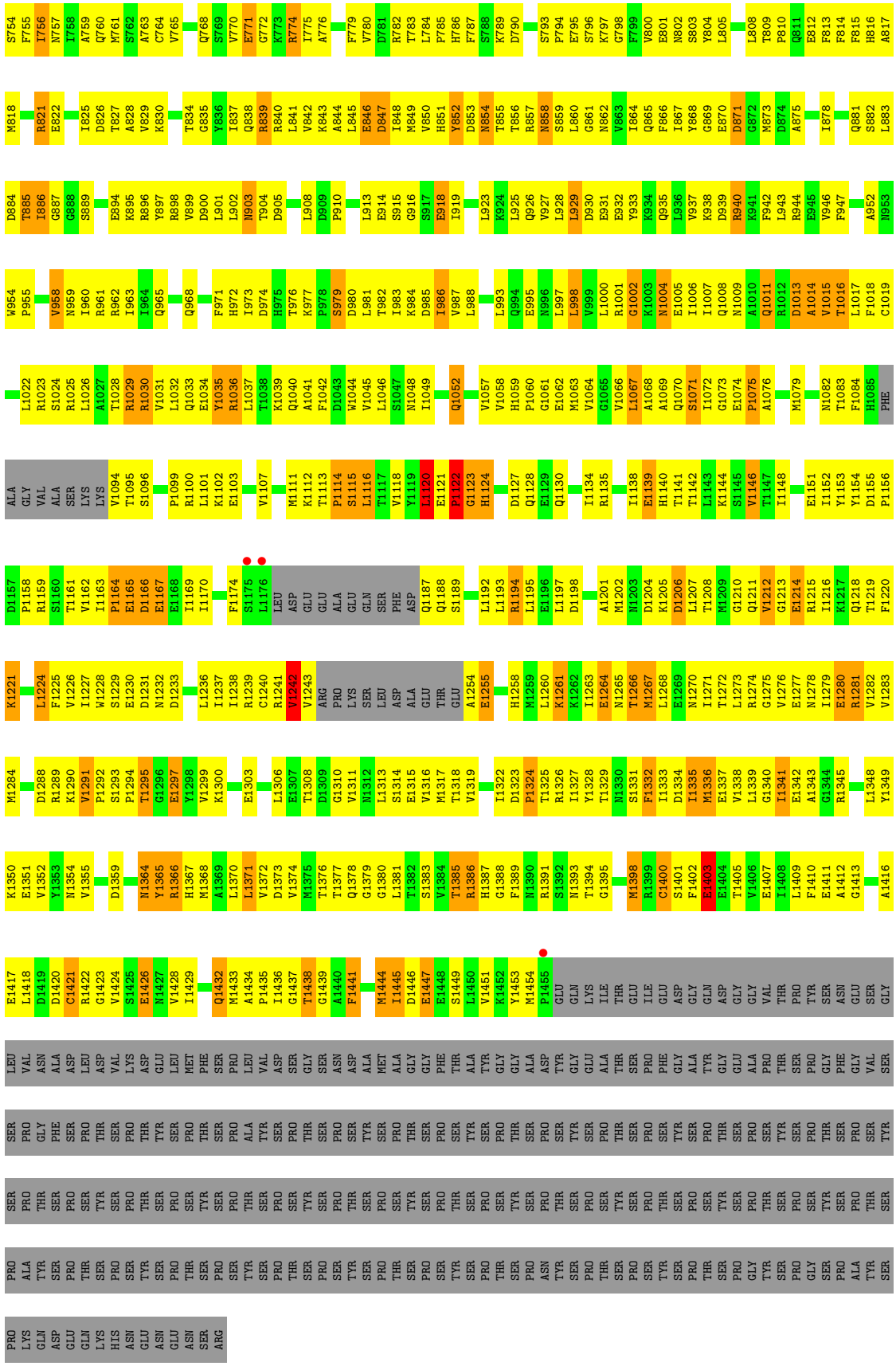
3 Residue-property plots (i)

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: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1

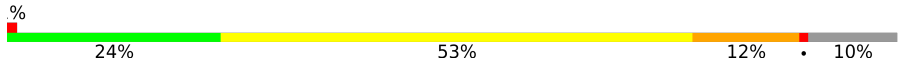
Chain A: 24% 47% 10% • 18%

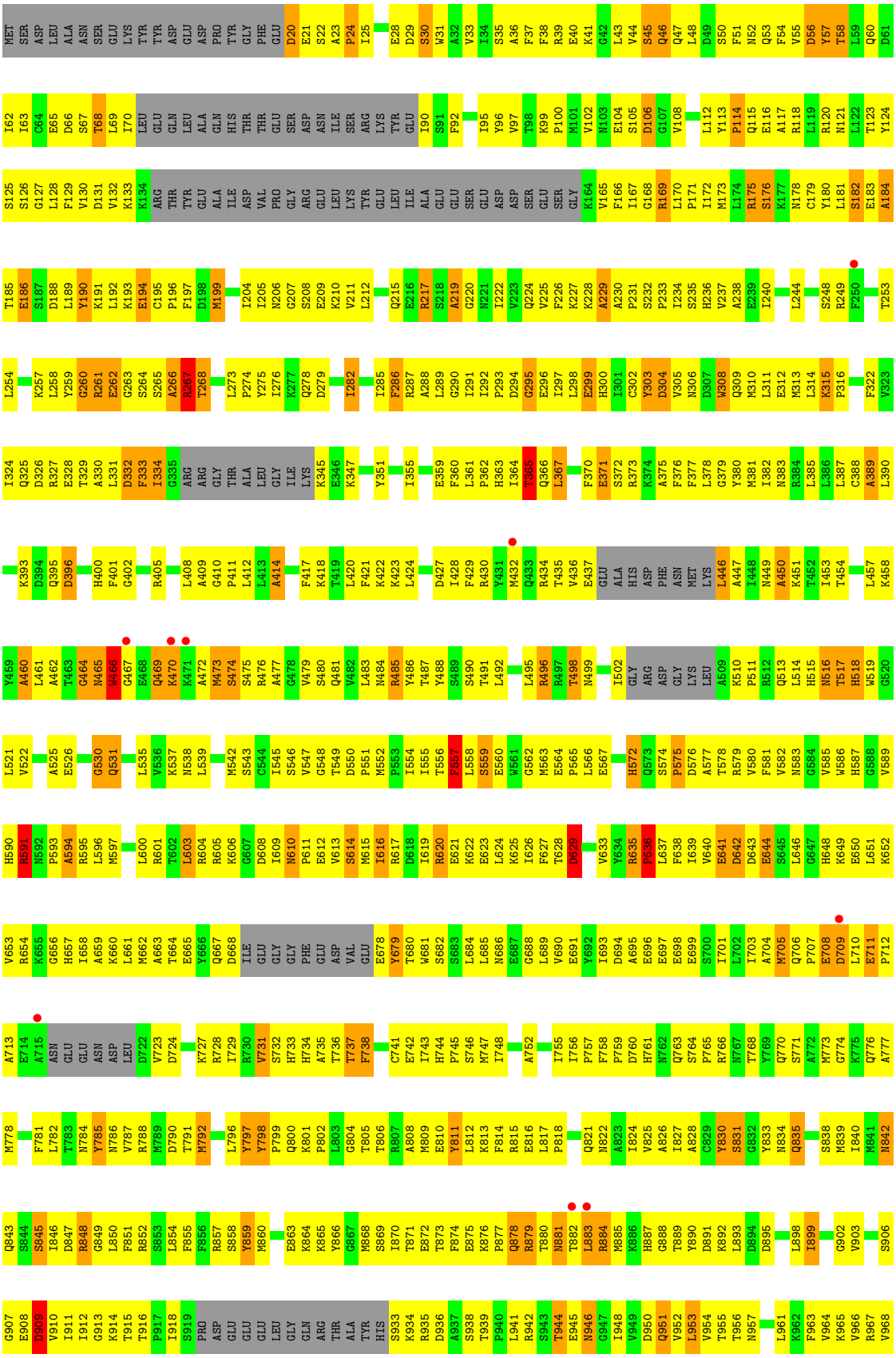




- Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2

Chain B:





R969 T970 T971 K972 I973 P974 Q975 I976 G977 F980 A981 S982 R983 H984 G985 Q986 K987 G988 T989 I990 G991 I992 T993 Y994 R995 R996 E997 D998 M999 P1000 F1001 T1002 A1003 E1004 G1005 I1006 V1007 P1008 D1009 L1010 I1011 I1012 N1013 P1014 H1015 A1016 I1017 P1018 S1019 R1020 M1021 T1022 V1023 A1024 H1025 L1026 I1027 E1028 C1029

L1030 L1031 G1039 G1042 D1043 A1044 S1045 P1046 F1047 I1055 R1060 Q1065 S1066 R1067 G1068 F1069 E1070 V1071 M1072 Y1073 N1074 G1075 K1079 K1080 L1081 Q1084 I1085 F1086 F1087 G1088 P1089 T1090 Y1091 Y1092 Q1093 R1094 L1095 R1096 H1097 M1098 V1099 D1100 D1101 K1102 I1103 H1104 A1105 R1106 A1107 R1108 G1109 P1110

T1115 R1116 V1119 E1120 G1121 R1122 D1125 G1126 G1127 L1128 R1129 F1130 G1131 E1132 M1133 E1134 R1135 D1136 I1139 A1140 V1071 H1141 G1142 F1146 L1147 K1148 E1149 R1150 L1151 M1152 E1153 A1154 S1155 D1156 A1157 F1158 R1159 V1160 H1161 I1162 C1163 G1164 I1165 C1166 G1167 L1168 M1169 T1170 V1171 I1172 A1173 K1174 L1175 N1176 H1177 N1178 Q1179

F1180 E1181 C1182 K1183 G1184 C1185 D1186 N1187 K1188 I1189 D1190 I1191 Y1192 Q1193 I1194 H1195 I1196 P1197 Y1198 A1199 A1200 K1201 L1202 L1203 F1204 Q1205 E1206 L1207 M1208 A1209 M1210 N1211 I1212 R1215 L1216 Y1217 T1218 D1219 R1220 S1221 R1222 D1223 F1224

- Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

Chain C: 28% 43% 12% • 16%

MET SER E3 E4 G5 P6 Q7 V8 K9 I10 R11 E12 D16 N17 V18 D19 F20 V25 D26 L27 A28 M29 A30 N31 S32 L33 R34 R35 V36 M37 I38 A39 T43 L44 A45 I46 D47 V51 E52 T55 T56 V57 L58 A59 D60 E61 F62 I63 A64 H65 R66 L67 G68 L69 I70

F71 L72 Q73 S74 M75 D76 I77 L80 E81 Y82 S83 R84 C88 E89 D90 H91 C92 D93 K94 C95 S96 V97 V98 L99 T100 L101 Q102 A103 F104 S107 E108 S109 T110 T111 N112 V113 Y114 S115 K116 D117 L118 V119 I120 V121 S122 N123 L124 M125 G126 R127 N128 I129 G130 H131 P132 I133 I134

Q135 D136 K137 E138 G139 N140 G141 V142 L143 I144 G145 K146 L147 R148 K149 L153 K154 L155 T156 C157 V158 K161 G162 I163 A164 K165 E166 H167 A168 K169 W170 G171 P172 A173 A174 A175 I176 E177 F178 E179 Y180 D181 P182 W183 N184 K185 L186 T189 D190 Y191 W192 Y193 E194 W201 P202

K205 N206 C207 E208 Y209 P212 P213 N214 F219 D220 Y221 K222 D226 T227 M230 N231 Y232 E233 S234 V235 G236 S237 I238 P239 V240 D241 Q242 V243 V244 V245 R246 G247 I248 L251 Q252 K253 K254 V255 A256 S257 I258 L259 L260 A261 L262 T263 Q264 D268 LYS VAL ASN PHE ALA SER

GLY ASP ASN ASN THR ALA SER ASN MET LEU LEU GLY SER ASN GLU ASP VAL MET MET THR GLY ALA GLU GLN ASP PRO TYR SER ASN ALA SER GLN MET GLY ASN THR GLY SER GLY GLY TYR ASP ASN ALA TRP

- Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4

Chain D: 29% 42% 9% • 20%

MET ASN VAL S4 T5 S6 T7 R13 R14 L15 K16 K17 V18 E21 E22 N23 A24 A25 T26 L27 Q28 L29 G30 F33 Q34 L35 K36 Q37 H40 Q41 E46 L47 I48 A49 L50 N51 L52 S53 E54 A55 R56 L57 V58 I59 V64 E65 R66 R67 R68 A69 F70 Q74 K75

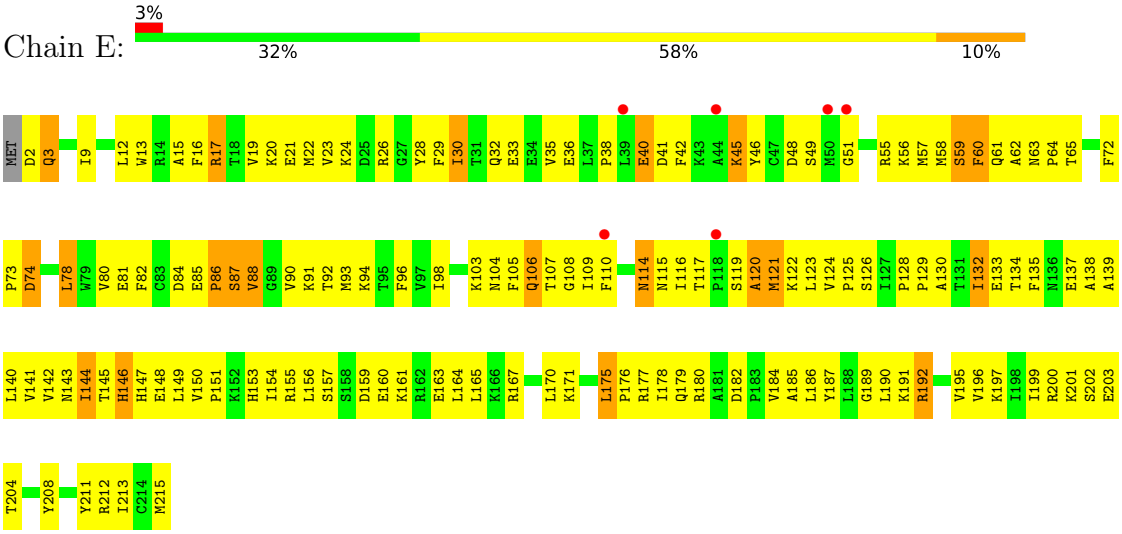
K76 HIS LYS LYS LYS HIS LEU LYS HIS GLU ASN ALA ASN ASP GLU THR THR ALA VAL GLU ASP GLU ASP ASP ASP LEU ASP GLU ASP ASP VAL ASN ALA ASP ASP ASP ASP PHE MET HIS SER GLU T118 R119 E120 K121 E122 L123 E124 S125 I126 D127 V128 L129 L130 E131 Q132 T133 T134 G135

G136 N137 N138 K139 D140 L141 T144 M145 Q146 Y147 L148 T149 S152 R153 F154 R155 D156 T159 V160 G161 A162 V163 I164 Q165 T170 G171 L172 H173 R174 F175 E176 V177 A178 S182 L183 A184 C185 D186 T187 E190 A191 K192 T193 L194 I195 P196 S197 L198 N199 N200 K201 I202 S203 D204

D205 E206 L207 E208 R209 I210 L211 K212 E213 L214 S215 E218 T219 L220 Y221

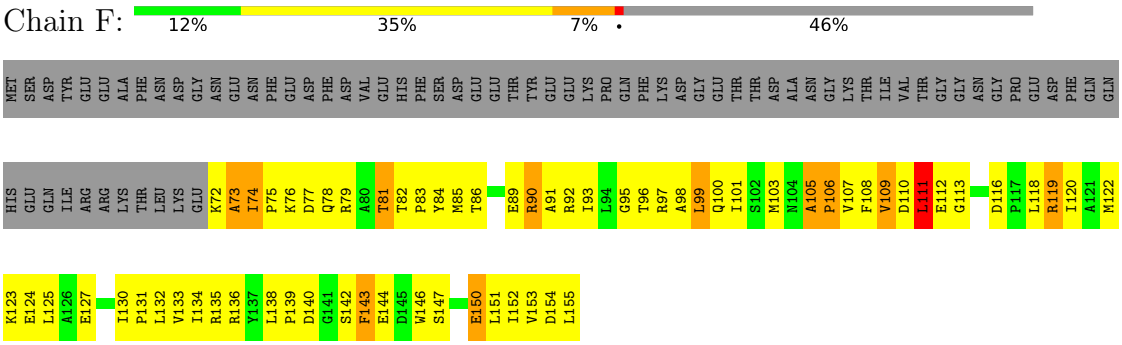
- Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC1

Chain E:



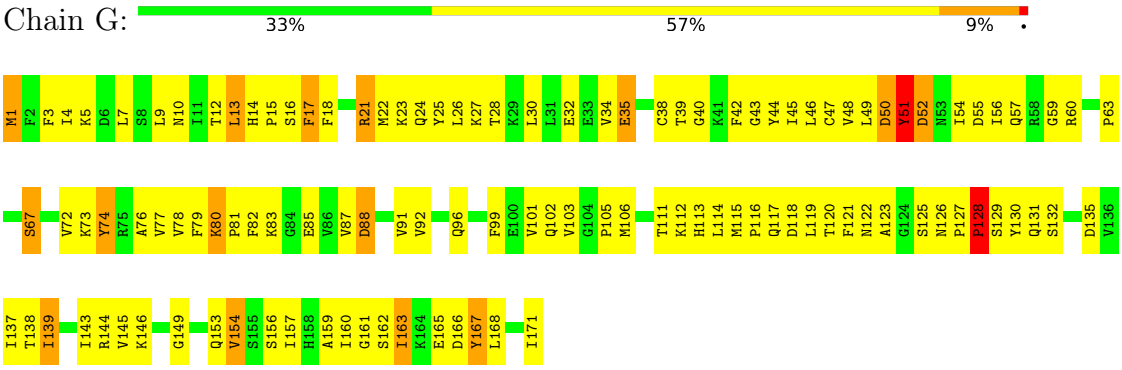
- Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC2

Chain F:



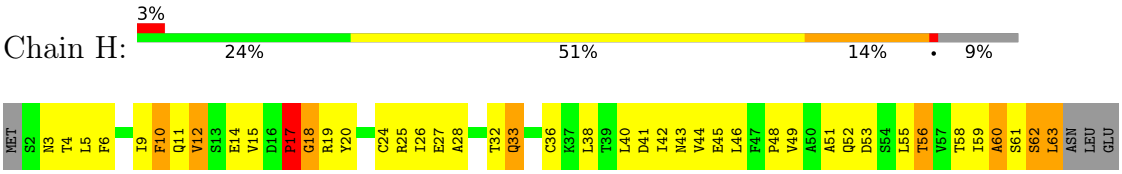
- Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

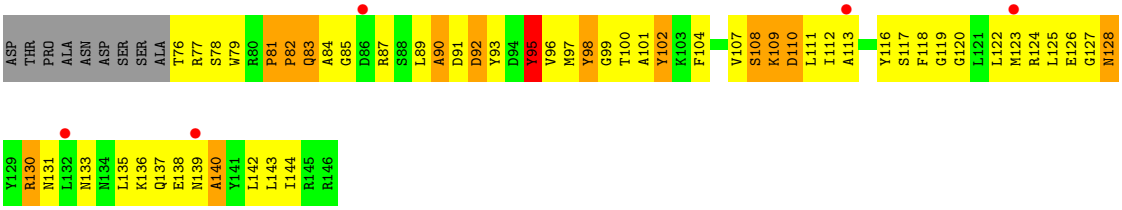
Chain G:



- Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC3

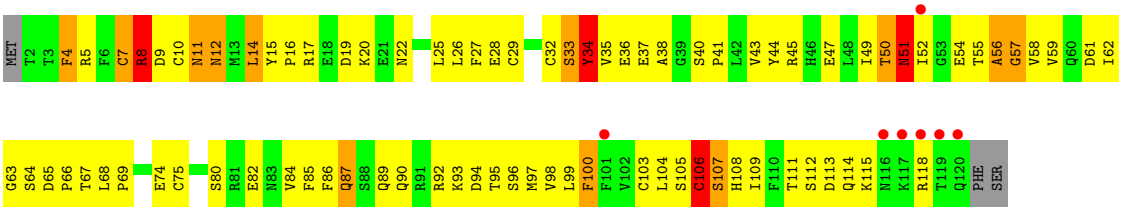
Chain H:





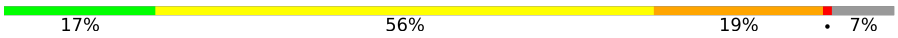
• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9

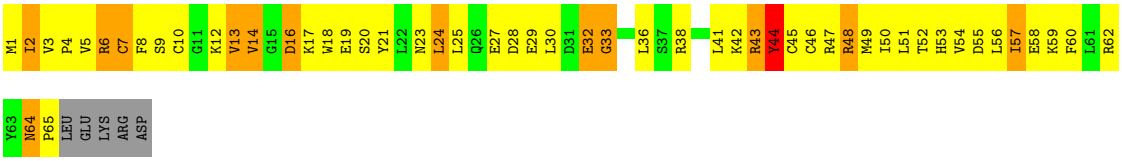
Chain I:



• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC5

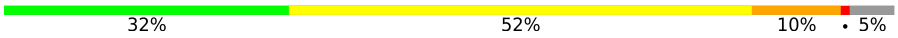
Chain J:

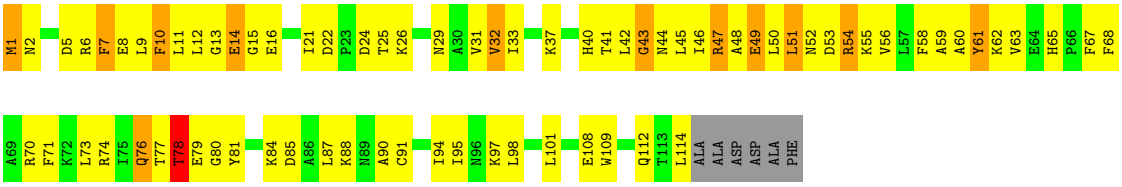




• Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11

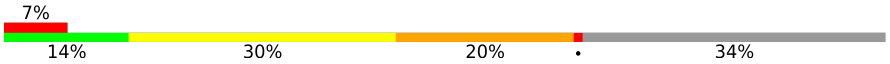
Chain K:

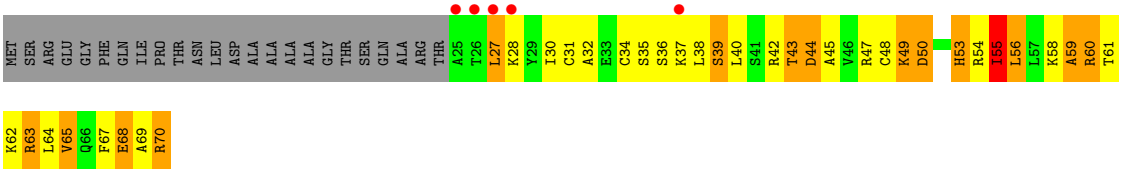




• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4

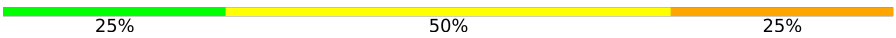
Chain L:





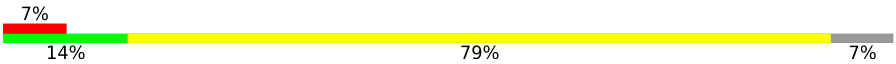
• Molecule 13: AMATOXIN

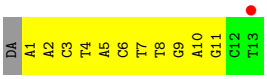
Chain M:



• Molecule 14: 5'-D(*AP*AP*AP*CP*TP*AP*CP*TP*TP*GP *AP*GP*CP*T)-3'

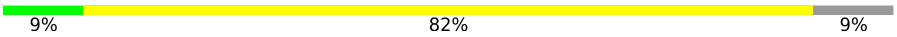
Chain N:

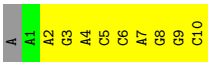




• Molecule 15: 5'-R(*AP*AP*AP*GP*AP*CP*CP*AP*GP*GP*C)-3'

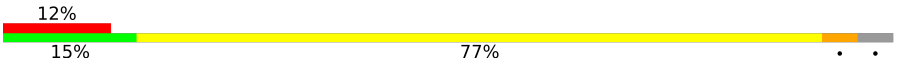
Chain P:

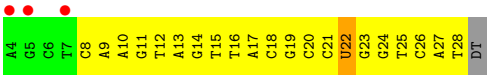




• Molecule 16: 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP *GP*TP*TP*AP*CP*GP*CP*CP*BRUP*GP*GP*TP*CP*AP*TP*T)-3'

Chain T:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	220.62Å 394.23Å 283.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.40 49.75 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-3.40) 99.9 (49.75-3.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 3.19Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.255 , 0.288 0.251 , 0.287	Depositor DCC
R_{free} test set	7809 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å^2)	72.7	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 42.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	0.077 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.085 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	32083	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 1.82% 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: TRX, ILX, ZN, MG, CSX, HYP, BRU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.44	0/11359	0.73	1/15364 (0.0%)
2	B	0.43	0/8963	0.73	0/12086
3	C	0.44	0/2133	0.71	1/2891 (0.0%)
4	D	0.40	0/1365	0.65	0/1837
5	E	0.40	0/1788	0.63	0/2406
6	F	0.49	0/691	0.75	0/933
7	G	0.45	0/1368	0.71	0/1844
8	H	0.41	0/1086	0.66	0/1470
9	I	0.39	0/989	0.67	0/1331
10	J	0.46	0/541	0.76	0/727
11	K	0.48	0/937	0.71	0/1265
12	L	0.44	0/365	0.77	0/485
13	M	1.80	1/22 (4.5%)	1.60	0/26
14	N	0.59	0/293	0.84	0/450
15	P	0.45	0/240	0.77	0/373
16	T	0.55	0/547	0.95	0/840
All	All	0.44	1/32687 (0.0%)	0.72	2/44328 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	7	GLY	N-CA	5.81	1.54	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	39	ALA	N-CA-C	5.43	125.66	111.00
1	A	266	LEU	N-CA-C	-5.29	96.70	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11158	0	11222	1335	0
2	B	8792	0	8823	1107	0
3	C	2095	0	2051	245	0
4	D	1356	0	1319	127	0
5	E	1752	0	1776	162	0
6	F	679	0	701	86	0
7	G	1340	0	1357	170	0
8	H	1068	0	1040	160	0
9	I	971	0	931	108	0
10	J	532	0	543	128	0
11	K	919	0	929	103	0
12	L	363	0	388	54	0
13	M	64	0	50	4	0
14	N	262	0	149	20	0
15	P	214	0	111	7	0
16	T	509	0	281	41	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
18	A	1	0	0	0	0
All	All	32083	0	31671	3527	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 55.

The worst 5 of 3527 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1329:THR:HG22	1:A:1331:SER:H	1.05	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1159:ARG:HB3	2:B:1159:ARG:HH11	1.14	1.10
6:F:109:VAL:HG12	6:F:110:ASP:H	1.15	1.09
1:A:40:THR:HB	1:A:41:MET:HE2	1.15	1.09
3:C:43:THR:HG22	3:C:44:LEU:H	1.08	1.08

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	
1	A	1408/1733 (81%)	984 (70%)	283 (20%)	141 (10%)	0	4
2	B	1088/1224 (89%)	740 (68%)	220 (20%)	128 (12%)	0	3
3	C	264/318 (83%)	187 (71%)	52 (20%)	25 (10%)	0	4
4	D	173/221 (78%)	116 (67%)	37 (21%)	20 (12%)	0	3
5	E	212/215 (99%)	150 (71%)	41 (19%)	21 (10%)	0	4
6	F	82/155 (53%)	58 (71%)	14 (17%)	10 (12%)	0	2
7	G	169/171 (99%)	126 (75%)	30 (18%)	13 (8%)	1	6
8	H	129/146 (88%)	95 (74%)	17 (13%)	17 (13%)	0	1
9	I	117/122 (96%)	74 (63%)	28 (24%)	15 (13%)	0	2
10	J	63/70 (90%)	38 (60%)	14 (22%)	11 (18%)	0	0
11	K	112/120 (93%)	86 (77%)	17 (15%)	9 (8%)	1	6
12	L	44/70 (63%)	19 (43%)	13 (30%)	12 (27%)	0	0
13	M	3/8 (38%)	3 (100%)	0	0	100	100
All	All	3864/4573 (84%)	2676 (69%)	766 (20%)	422 (11%)	0	3

5 of 422 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	A	54	ASN
1	A	57	ARG
1	A	67	CYS
1	A	71	GLN

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	
1	A	1241/1520 (82%)	1134 (91%)	107 (9%)	10	35
2	B	960/1061 (90%)	870 (91%)	90 (9%)	8	30
3	C	234/274 (85%)	207 (88%)	27 (12%)	5	20
4	D	140/200 (70%)	125 (89%)	15 (11%)	6	24
5	E	196/197 (100%)	185 (94%)	11 (6%)	21	51
6	F	74/137 (54%)	65 (88%)	9 (12%)	5	18
7	G	152/152 (100%)	142 (93%)	10 (7%)	16	46
8	H	117/128 (91%)	107 (92%)	10 (8%)	10	35
9	I	113/116 (97%)	103 (91%)	10 (9%)	10	33
10	J	60/65 (92%)	53 (88%)	7 (12%)	5	20
11	K	99/102 (97%)	88 (89%)	11 (11%)	6	22
12	L	40/57 (70%)	34 (85%)	6 (15%)	3	12
13	M	2/2 (100%)	2 (100%)	0	100	100
All	All	3428/4011 (86%)	3115 (91%)	313 (9%)	9	32

5 of 313 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	148	LEU
9	I	87	GLN
4	D	221	TYR
7	G	13	LEU
11	K	47	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 96 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	975	GLN
4	D	137	ASN
2	B	1065	GLN
3	C	73	GLN
4	D	173	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	9/11 (81%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

5 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	$\#\|Z\| > 2$
13	CSX	M	8	13	3,6,7	1.01	0	1,6,8	1.64	0
13	TRX	M	4	13	14,16,17	1.18	1 (7%)	15,22,24	2.63	4 (26%)
13	ILX	M	3	13	8,9,10	1.35	1 (12%)	9,11,13	2.14	2 (22%)
13	HYP	M	2	13	6,8,9	0.89	0	5,10,12	1.70	2 (40%)
16	BRU	T	22	16,15	18,21,22	0.38	0	26,30,33	0.95	2 (7%)

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
13	CSX	M	8	13	-	0/1/5/7	-
13	TRX	M	4	13	-	0/4/6/8	0/2/2/2
13	ILX	M	3	13	-	0/11/12/14	-
13	HYP	M	2	13	-	0/0/11/13	0/1/1/1
16	BRU	T	22	16,15	-	0/7/21/22	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	4	TRX	CZ3-CH2	3.06	1.44	1.38
13	M	3	ILX	CB-CA	-3.03	1.51	1.54

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	M	4	TRX	CB-CG-CD1	-7.20	119.07	127.97
13	M	3	ILX	CB-CA-C	-5.50	105.52	112.94
13	M	4	TRX	CB-CG-CD2	4.90	133.87	126.25
13	M	4	TRX	CZ2-CE2-CD2	3.01	125.04	121.16
16	T	22	BRU	C6-C5-C4	-2.88	117.74	120.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	4	TRX	1	0
13	M	3	ILX	1	0
16	T	22	BRU	4	0

5.5 Carbohydrates (i)

There are no monosaccharides 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 (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	A	1418/1733 (81%)	-0.26	6 (0%)	92	92	37, 86, 139, 189	0
2	B	1106/1224 (90%)	-0.15	9 (0%)	86	85	37, 96, 148, 181	0
3	C	266/318 (83%)	-0.33	0	100	100	48, 83, 117, 141	0
4	D	177/221 (80%)	-0.24	0	100	100	66, 107, 145, 149	0
5	E	214/215 (99%)	-0.01	6 (2%)	53	51	66, 127, 171, 180	0
6	F	84/155 (54%)	-0.45	0	100	100	42, 70, 99, 108	0
7	G	171/171 (100%)	-0.21	0	100	100	70, 90, 126, 136	0
8	H	133/146 (91%)	0.25	5 (3%)	40	39	91, 125, 152, 168	0
9	I	119/122 (97%)	0.03	7 (5%)	22	23	84, 125, 158, 175	0
10	J	65/70 (92%)	-0.35	0	100	100	44, 76, 113, 128	0
11	K	114/120 (95%)	-0.34	0	100	100	56, 83, 109, 133	0
12	L	46/70 (65%)	0.50	5 (10%)	5	6	76, 152, 166, 169	0
13	M	4/8 (50%)	-0.51	0	100	100	88, 90, 91, 97	0
14	N	13/14 (92%)	0.64	1 (7%)	13	15	151, 178, 218, 221	0
15	P	10/11 (90%)	-0.35	0	100	100	89, 111, 162, 172	0
16	T	24/26 (92%)	0.19	3 (12%)	3	4	80, 159, 224, 233	0
All	All	3964/4624 (85%)	-0.19	42 (1%)	80	79	37, 93, 152, 233	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	L	27	LEU	6.8
1	A	1176	LEU	6.7
2	B	471	LYS	5.9
16	T	4	DA	5.3
2	B	883	LEU	4.9

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. 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
16	BRU	T	22	20/21	0.82	0.18	69,75,79,82	0
13	TRX	M	4	15/16	0.95	0.26	88,91,93,93	0
13	CSX	M	8	7/8	0.97	0.15	92,94,95,97	0
13	HYP	M	2	8/9	0.97	0.12	84,85,86,87	0
13	ILX	M	3	10/11	0.98	0.17	85,86,88,91	0

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
17	ZN	I	1122	1/1	0.94	0.09	144,144,144,144	0
17	ZN	L	1071	1/1	0.95	0.09	107,107,107,107	0
17	ZN	A	2456	1/1	0.97	0.08	78,78,78,78	0
17	ZN	C	1269	1/1	0.99	0.13	67,67,67,67	0
17	ZN	I	1121	1/1	0.99	0.16	96,96,96,96	0
17	ZN	A	2457	1/1	0.99	0.14	53,53,53,53	0
17	ZN	J	1066	1/1	0.99	0.21	72,72,72,72	0
17	ZN	B	2225	1/1	0.99	0.18	65,65,65,65	0
18	MG	A	2458	1/1	0.99	0.16	43,43,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.