



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 07:53 AM UTC

PDB ID : 4YM7 / pdb_00004ym7
Title : RNA polymerase I structure with an alternative dimer hinge
Authors : Kostrewa, D.; Kuhn, C.-D.; Engel, C.; Cramer, P.
Deposited on : 2015-03-06
Resolution : 5.50 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

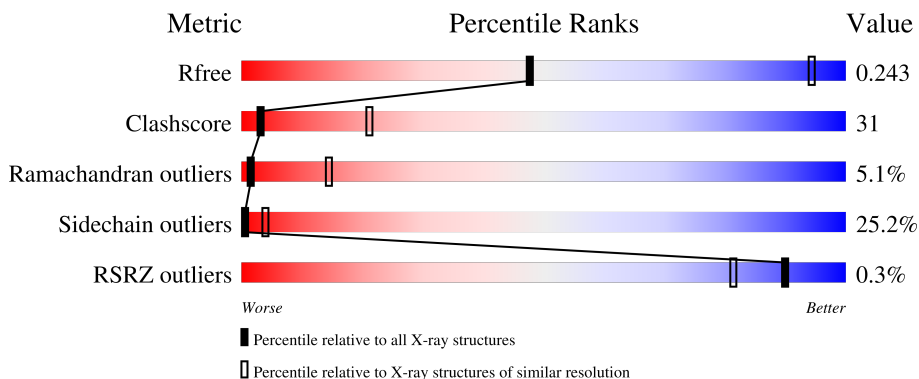
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1088 (7.00-4.00)
Clashscore	190562	1147 (7.00-4.00)
Ramachandran outliers	187476	1012 (7.02-3.98)
Sidechain outliers	187428	1023 (7.04-3.96)
RSRZ outliers	180081	1081 (7.00-4.00)

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 $\leq 5\%$. 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	AA	1664	
1	BA	1664	
1	CA	1664	
1	DA	1664	
1	EA	1664	




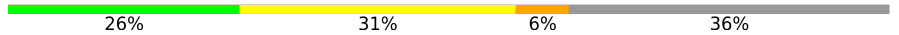
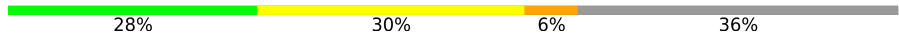
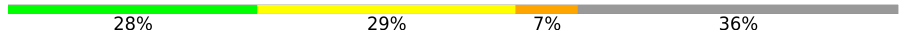














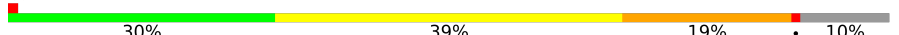
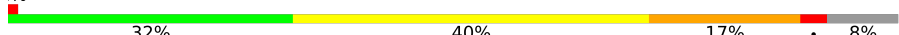
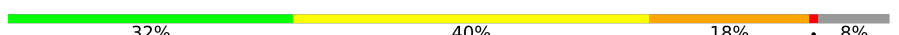
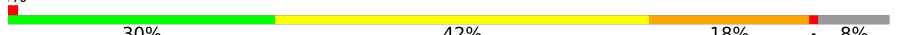

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Mol	Chain	Length	Quality of chain
1	FA	1664	32% 42% 15% 11%
2	AB	1203	36% 43% 15% . .
2	BB	1203	36% 44% 15% . .
2	CB	1203	35% 43% 17% . .
2	DB	1203	33% 46% 16% . .
2	EB	1203	34% 45% 16% . .
2	FB	1203	34% 44% 17% . .
3	AC	335	36% 40% 13% . 9%
3	BC	335	39% 38% 13% . 9%
3	CC	335	32% 44% 14% . 9%
3	DC	335	% 31% 44% 15% . 9%
3	EC	335	% 34% 41% 14% . 9%
3	FC	335	33% 42% 14% . 9%
4	AD	137	23% 15% 5% 58%
4	BD	137	% 21% 17% . 58%
4	CD	137	22% 16% . 58%
4	DD	137	21% 17% . 58%
4	ED	137	19% 19% . 58%
4	FD	137	20% 18% . 58%
5	AE	215	% 40% 49% 10%
5	BE	215	% 44% 44% 12%
5	CE	215	40% 48% 11% .
5	DE	215	37% 51% 11% .
5	EE	215	41% 47% 11%
5	FE	215	37% 52% 11%

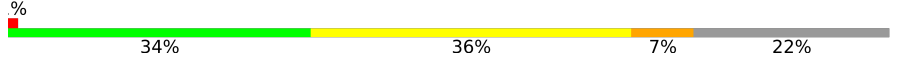


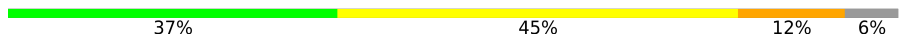
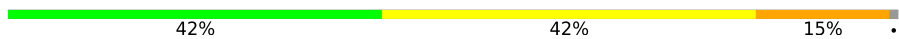
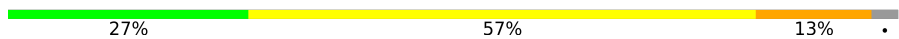
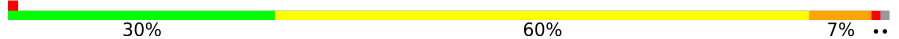
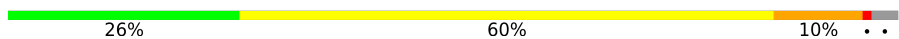
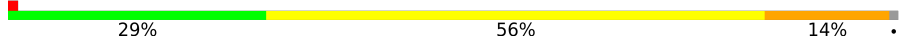
















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Mol	Chain	Length	Quality of chain
6	AF	155	
6	BF	155	 %
6	CF	155	
6	DF	155	
6	EF	155	
6	FF	155	
7	AG	326	 .
7	AO	326	 . 7% 6% 84%
7	BG	326	 .
7	BO	326	 . 8% 5% 84%
7	CG	326	 %
7	CO	326	 6% 5% 5% . 85%
7	DG	326	 .
7	DO	326	 . 6% 6% 84%
7	EG	326	 %
7	EO	326	 . 7% 5% 84%
7	FG	326	 %
7	FO	326	 5% 7% . . 84%
8	AH	146	
8	BH	146	 . 10%
8	CH	146	 %
8	DH	146	 . 8%
8	EH	146	 . 8%
8	FH	146	 %
9	AI	125	 %











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Mol	Chain	Length	Quality of chain
9	BI	125	
9	CI	125	
9	DI	125	
9	EI	125	
9	FI	125	
10	AJ	70	
10	BJ	70	
10	CJ	70	
10	DJ	70	
10	EJ	70	
10	FJ	70	
11	AK	142	
11	BK	142	
11	CK	142	
11	DK	142	
11	EK	142	
11	FK	142	
12	AL	70	
12	BL	70	
12	CL	70	
12	DL	70	
12	EL	70	
12	FL	70	
13	AM	415	
13	BM	415	

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Mol	Chain	Length	Quality of chain
13	CM	415	 10% 12% . . 74%
13	DM	415	 10% 12% . . 74%
13	EM	415	 9% 13% . . 73%
13	FM	415	 9% 11% 5% . 73%
14	AN	233	 22% 27% 9% . 39%
14	BN	233	 24% 27% 8% . 39%
14	CN	233	 23% 25% 11% . 39%
14	DN	233	 23% 27% 10% . 38%
14	EN	233	 22% 28% 8% . 38%
14	FN	233	 21% 27% 11% . 38%

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 204233 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 I subunit RPA190.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AA	1484	11703	7385	2036	2220	62	0	0	0
1	BA	1462	11540	7291	2003	2184	62	0	0	0
1	CA	1483	11695	7381	2035	2217	62	0	0	0
1	DA	1483	11697	7381	2034	2220	62	0	0	0
1	EA	1484	11706	7390	2036	2218	62	0	0	0
1	FA	1484	11709	7392	2036	2219	62	0	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA135.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	AB	1154	9187	5822	1606	1708	51	0	0	0
2	BB	1153	9175	5812	1603	1709	51	0	0	0
2	CB	1170	9304	5892	1629	1732	51	0	0	0
2	DB	1165	9269	5871	1622	1725	51	0	0	0
2	EB	1164	9265	5871	1619	1724	51	0	0	0
2	FB	1165	9270	5872	1622	1725	51	0	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	304	Total	C	N	O	S	0	0	0
			2413	1534	414	457	8			
3	BC	304	Total	C	N	O	S	0	0	0
			2413	1534	414	457	8			
3	CC	304	Total	C	N	O	S	0	0	0
			2413	1534	414	457	8			
3	DC	304	Total	C	N	O	S	0	0	0
			2413	1534	414	457	8			
3	EC	304	Total	C	N	O	S	0	0	0
			2413	1534	414	457	8			
3	FC	304	Total	C	N	O	S	0	0	0
			2413	1534	414	457	8			

- Molecule 4 is a protein called DNA-directed RNA polymerase I subunit RPA14.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	AD	58	Total	C	N	O	0	0	0
			459	289	78	92			
4	BD	58	Total	C	N	O	0	0	0
			459	289	78	92			
4	CD	58	Total	C	N	O	0	0	0
			459	289	78	92			
4	DD	58	Total	C	N	O	0	0	0
			459	289	78	92			
4	ED	58	Total	C	N	O	0	0	0
			459	289	78	92			
4	FD	58	Total	C	N	O	0	0	0
			459	289	78	92			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	215	Total	C	N	O	S	0	0	0
			1760	1116	310	322	12			
5	BE	215	Total	C	N	O	S	0	0	0
			1760	1116	310	322	12			
5	CE	215	Total	C	N	O	S	0	0	0
			1760	1116	310	322	12			
5	DE	215	Total	C	N	O	S	0	0	0
			1760	1116	310	322	12			
5	EE	215	Total	C	N	O	S	0	0	0
			1760	1116	310	322	12			
5	FE	215	Total	C	N	O	S	0	0	0
			1760	1116	310	322	12			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	98	Total	C	N	O	S	0	0	0
			807	512	142	150	3			
6	BF	98	Total	C	N	O	S	0	0	0
			807	512	142	150	3			
6	CF	99	Total	C	N	O	S	0	0	0
			816	517	143	153	3			
6	DF	99	Total	C	N	O	S	0	0	0
			816	517	143	153	3			
6	EF	99	Total	C	N	O	S	0	0	0
			816	517	143	153	3			
6	FF	99	Total	C	N	O	S	0	0	0
			816	517	143	153	3			

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	202	Total	C	N	O	S	0	0	0
			1599	1025	276	293	5			
7	AO	52	Total	C	N	O		0	0	0
			413	253	64	96				
7	BG	195	Total	C	N	O	S	0	0	0
			1539	992	264	278	5			
7	BO	51	Total	C	N	O		0	0	0
			404	248	63	93				
7	CG	202	Total	C	N	O	S	0	0	0
			1599	1025	276	293	5			
7	CO	50	Total	C	N	O		0	0	0
			398	245	62	91				
7	DG	202	Total	C	N	O	S	0	0	0
			1599	1025	276	293	5			
7	DO	52	Total	C	N	O		0	0	0
			413	253	64	96				
7	EG	202	Total	C	N	O	S	0	0	0
			1599	1025	276	293	5			
7	EO	52	Total	C	N	O		0	0	0
			413	253	64	96				
7	FG	202	Total	C	N	O	S	0	0	0
			1599	1025	276	293	5			
7	FO	52	Total	C	N	O		0	0	0
			413	253	64	96				

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	132	Total	C	N	O	S	0	0	0
			1063	670	180	209	4			
8	BH	131	Total	C	N	O	S	0	0	0
			1052	664	176	208	4			
8	CH	131	Total	C	N	O	S	0	0	0
			1052	664	176	208	4			
8	DH	134	Total	C	N	O	S	0	0	0
			1075	677	182	212	4			
8	EH	134	Total	C	N	O	S	0	0	0
			1075	677	182	212	4			
8	FH	134	Total	C	N	O	S	0	0	0
			1075	677	182	212	4			

- Molecule 9 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	124	Total	C	N	O	S	0	0	0
			943	584	160	190	9			
9	BI	97	Total	C	N	O	S	0	0	0
			716	439	120	148	9			
9	CI	124	Total	C	N	O	S	0	0	0
			943	584	160	190	9			
9	DI	124	Total	C	N	O	S	0	0	0
			943	584	160	190	9			
9	EI	117	Total	C	N	O	S	0	0	0
			898	556	152	181	9			
9	FI	124	Total	C	N	O	S	0	0	0
			943	584	160	190	9			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	68	Total	C	N	O	S	0	0	0
			558	356	97	99	6			
10	BJ	69	Total	C	N	O	S	0	0	0
			569	362	101	100	6			
10	CJ	68	Total	C	N	O	S	0	0	0
			558	356	97	99	6			
10	DJ	69	Total	C	N	O	S	0	0	0
			569	362	101	100	6			
10	EJ	68	Total	C	N	O	S	0	0	0
			558	356	97	99	6			
10	FJ	68	Total	C	N	O	S	0	0	0
			558	356	97	99	6			

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	101	Total	C	N	O	S	0	0	0
			793	496	130	162	5			
11	BK	100	Total	C	N	O	S	0	0	0
			786	491	129	161	5			
11	CK	101	Total	C	N	O	S	0	0	0
			793	496	130	162	5			
11	DK	101	Total	C	N	O	S	0	0	0
			793	496	130	162	5			
11	EK	100	Total	C	N	O	S	0	0	0
			786	491	129	161	5			
11	FK	100	Total	C	N	O	S	0	0	0
			786	491	129	161	5			

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	44	Total	C	N	O	S	0	0	0
			352	217	70	61	4			
12	BL	44	Total	C	N	O	S	0	0	0
			352	217	70	61	4			
12	CL	44	Total	C	N	O	S	0	0	0
			352	217	70	61	4			
12	DL	44	Total	C	N	O	S	0	0	0
			352	217	70	61	4			
12	EL	44	Total	C	N	O	S	0	0	0
			352	217	70	61	4			
12	FL	44	Total	C	N	O	S	0	0	0
			352	217	70	61	4			

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	AM	109	Total	C	N	O	0	0	0
			863	548	143	172			
13	BM	109	Total	C	N	O	0	0	0
			863	548	143	172			
13	CM	109	Total	C	N	O	0	0	0
			863	548	143	172			
13	DM	109	Total	C	N	O	0	0	0
			863	548	143	172			
13	EM	110	Total	C	N	O	0	0	0
			869	551	144	174			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	FM	110	Total	C	N	O	0	0	0
			869	551	144	174			

- Molecule 14 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	142	Total	C	N	O	S	0	0	0
			1127	719	183	221	4			
14	BN	143	Total	C	N	O	S	0	0	0
			1130	719	184	223	4			
14	CN	143	Total	C	N	O	S	0	0	0
			1137	728	184	221	4			
14	DN	145	Total	C	N	O	S	0	0	0
			1146	729	186	227	4			
14	EN	144	Total	C	N	O	S	0	0	0
			1140	726	186	224	4			
14	FN	145	Total	C	N	O	S	0	0	0
			1146	729	187	226	4			

- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	AA	2	Total	Zn	0	0
			2	2		
15	AB	1	Total	Zn	0	0
			1	1		
15	AI	2	Total	Zn	0	0
			2	2		
15	AJ	1	Total	Zn	0	0
			1	1		
15	AL	1	Total	Zn	0	0
			1	1		
15	BA	2	Total	Zn	0	0
			2	2		
15	BB	1	Total	Zn	0	0
			1	1		
15	BI	2	Total	Zn	0	0
			2	2		
15	BJ	1	Total	Zn	0	0
			1	1		
15	BL	1	Total	Zn	0	0
			1	1		

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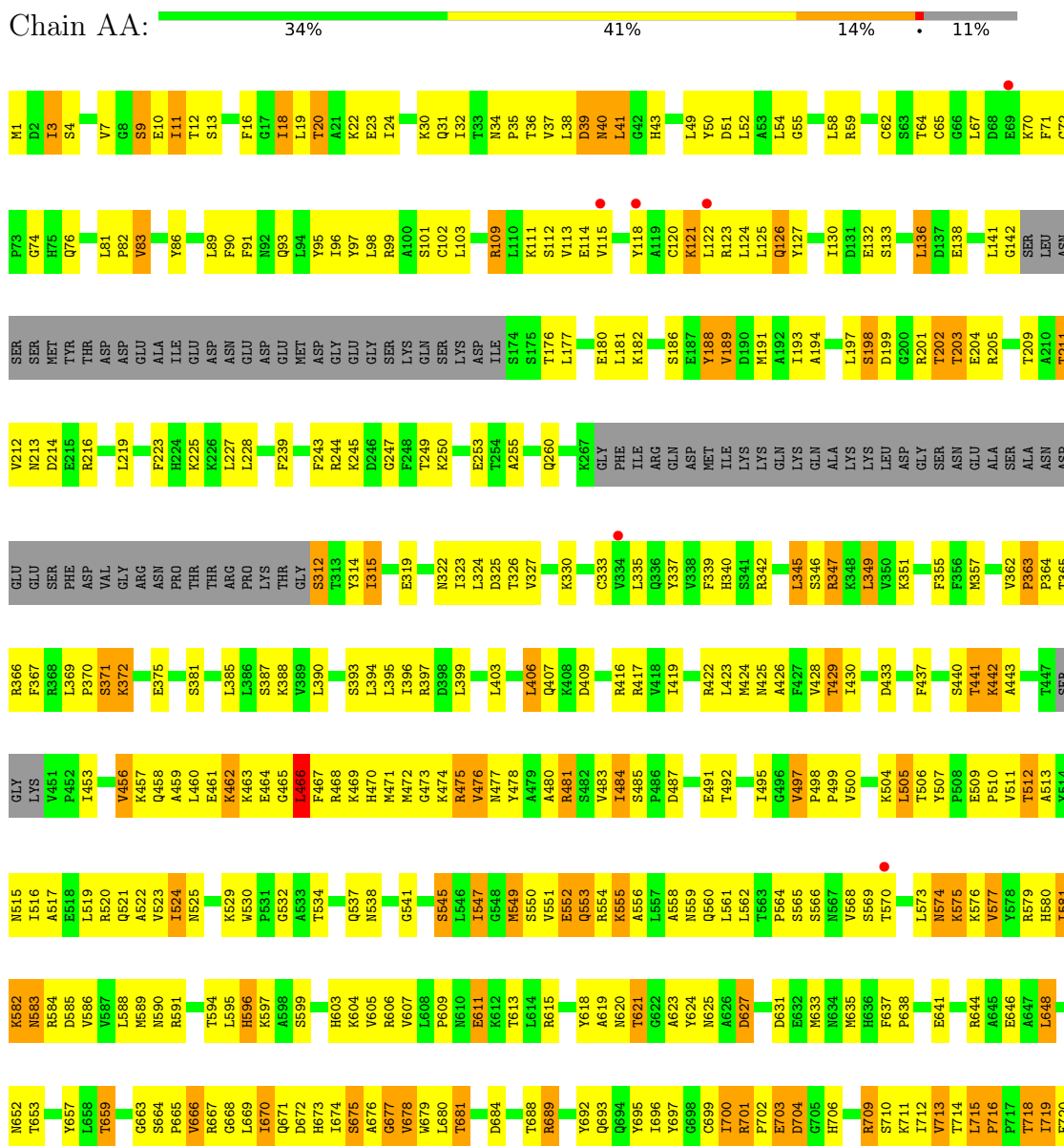
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	CA	2	Total 2	Zn 2	0	0
15	CB	1	Total 1	Zn 1	0	0
15	CI	2	Total 2	Zn 2	0	0
15	CJ	1	Total 1	Zn 1	0	0
15	CL	1	Total 1	Zn 1	0	0
15	DA	2	Total 2	Zn 2	0	0
15	DB	1	Total 1	Zn 1	0	0
15	DI	2	Total 2	Zn 2	0	0
15	DJ	1	Total 1	Zn 1	0	0
15	DL	1	Total 1	Zn 1	0	0
15	EA	2	Total 2	Zn 2	0	0
15	EB	1	Total 1	Zn 1	0	0
15	EI	2	Total 2	Zn 2	0	0
15	EJ	1	Total 1	Zn 1	0	0
15	EL	1	Total 1	Zn 1	0	0
15	FA	2	Total 2	Zn 2	0	0
15	FB	1	Total 1	Zn 1	0	0
15	FI	2	Total 2	Zn 2	0	0
15	FJ	1	Total 1	Zn 1	0	0
15	FL	1	Total 1	Zn 1	0	0

3 Residue-property plots

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 I subunit RPA190



K721	T862	V838	R1008	K1078	F1155	L1217	T1278	ARG	ASP	E1471	D1539	M1613
P722	K863	N939	T1009	M081	S1158	G1218	S1279	LEU	LYS	F1472	G1540	S1614
Y723	L864	V940	A1010	P1082	T1159	I1219	THR	THR	GLU	K1473	I1541	I1615
P724	D865	V794	V1011	G1082	P1220	P1220	ALA	THR	SER	L1474	T1542	I1616
L725	K866	H941	K1012	S1083	R1221	R1221	GLY	VAL	ASP	E1475	S1543	I1617
W726	D867	H942	T1013	A1084	L1222	L1222	GLY	VAL	SER	L1476	N1544	T1618
T727	T868	M944	S1014	L1085	R1223	R1223	ASN	ALA	ASP	A1477	D1545	K1619
G728	E874	C945	R1015	L1086	E1224	E1224	ASN	ASN	SER	A1478	V1546	Q1620
K729	L946	L946	S1016	E1087	I1225	I1225	ALA	SER	GLU	D1479	V1546	F1621
L730	V800	L947	L1019	E1092	M1226	M1226	ALA	SER	ASP	T1480	G1553	L1622
I731	L875	L947	Q1020	S1093	M1227	M1227	ALA	SER	GLU	E1481	G1554	T1623
I732	L876	L947	S1093	A1094	R1167	R1167	ASN	ASN	ASP	K1482	I1555	K1624
T733	R877	L952	R1021	A1094	A1168	A1168	SER	SER	VAL	L1483	E1556	A1625
I734	L879	R955	C1022	L1095	L1169	L1169	LYS	LYS	ASP	L1484	A1557	V1626
V735	A806	R956	L1023	K1096	A1231	A1231	ARG	ARG	MET	M1485	I1558	L1627
L736	A807	R957	T1024	Y1097	Q1171	Q1171	LEU	LEU	GLU	V1486	V1559	D1628
W737	L736	P958	K1025	Y1097	L1172	L1172	GLU	GLU	GLN	N1487	N1560	M1629
W738	V809	P958	Q1026	S1098	K1173	K1173	GLU	GLU	ASN	I1488	T1561	E1630
P742	V810	M960	L1027	T1101	Y1174	Y1174	ASP	ASP	ASN	V1489	I1562	R1631
D743	S811	V961	E1028	L1102	M1175	M1175	ASP	ASP	LYS	E1490	V1563	E1632
M744	R888	R962	G1029	K1103	R1176	R1176	GLU	GLU	ASP	E1491	I1564	Q1633
P745	S889	V961	V1030	Y1104	S1177	S1177	GLU	GLU	SER	I1492	I1565	L1634
	K814	K964	H1031	R1105	L1178	L1178	GLU	GLU	ILE	C1493	I1566	D1635
	C814	K964	V1032	R1105	I1179	I1179	GLN	GLN	VAL	R1494	N1567	S1636
	R815	T965	S1033	H1108	G1182	G1182	VAL	VAL	GLU	K1495	K1495	P1637
	L816	L965			E1183	E1183	HIS	HIS	GLU	S1496	V1569	S1638
	F817	P967	I1038	E1111	L1184	L1184	LYS	LYS	ASP	I1497	F1570	I1641
	L749	R968	R1039	S1117	V1185	V1185	THR	THR	LYS	I1498	R1571	I1642
	I750	F969	R1039	Y1118	G1186	G1186	LYS	LYS	THR	R1499	R1572	K1645
	R818	K970	L1045	K1119	I1188	I1188	ALA	ALA	GLN	Q1500	I1573	L1646
	N819	P971	V1046	K1119	I1188	I1188	ALA	ALA	GLN	I1501	F1579	M1647
	N752	T821	Q1047	V1123	S1190	S1190	VAL	VAL	VAL	P1502	H1503	M1648
	M753	R822	F1048	L1124	D1262	D1262	TYR	TYR	SER	R1506	R1506	V1649
	I755	V900	M1049	M1128	S1192	S1192	ASP	ASP	ASP	C1507	C1507	G1650
	K756	A825	Y1050	P1129	V1193	V1193	GLU	GLU	GLU	W1508	W1508	T1651
	W757	G829	G1051	P1129	G1194	G1194	PRO	PRO	PRO	H1509	H1509	I1652
	E758	G829	G1052	K1131	E1195	E1195	ASP	ASP	ASP	P1510	P1510	S1653
	V759	D831	D1053	R1131	P1196	P1196	ASP	ASP	THR	E1511	E1511	D1654
	G761	D832	A1054	Y1132	P1196	P1196	THR	THR	THR	F1512	F1512	V1655
	K762	L833	A1054	Y1132	P1196	P1196	THR	THR	THR	E1513	E1513	V1656
	G763	H834	T1055	Y1132	P1196	P1196	THR	THR	THR	M1514	M1514	L1657
	N767	L835	D1056	L1133	S1197	S1197	THR	THR	THR	H1515	H1515	K1658
	E768	T836	D1057	G1134	T1198	T1198	THR	THR	THR	R1516	R1516	V1660
	V769	A837	T1058	S1135	Q1199	Q1199	THR	THR	THR	F1517	F1517	P1661
			K1059	V1136	M1200	M1200	THR	THR	THR	T1518	T1518	F1662
			F920	V1137	T1201	T1201	THR	THR	THR	L1519	L1519	A1663
			P921	E1060	L1202	L1202	MET	MET	MET	V1520	V1520	A1664
			C922	S1061	L1202	L1202	ARG	ARG	ARG	V1524	V1524	
			N923	H1062	M1203	M1203	ARG	ARG	ARG	F1525	F1525	
			M924	M1063	T1204	T1204	GLU	GLU	GLU	Q1527	Q1527	
			S924	Q993	PHE	PHE	ALA	ALA	ALA	A1528	A1528	
			M925	Y996	HIS	HIS	GLU	GLU	GLU	M1529	M1529	
			Q926	F1066	PHE	PHE	GLU	GLU	GLU	V1524	V1524	
			D852	E1067	PHE	PHE	LYS	LYS	LYS	M1525	M1525	
			T853	E1067	ALA	ALA	SER	SER	SER	F1526	F1526	
			M928	C1069	ALA	ALA	SER	SER	SER	Q1527	Q1527	
			G854	C1069	GLY	GLY	ASP	ASP	ASP	D1463	D1463	
			R855	M1000	GLY	GLY	ASP	ASP	ASP	D1464	D1464	
			D782	A1001	GLY	GLY	ASP	ASP	ASP	E1465	E1465	
			E856	G1002	GLY	GLY	GLU	GLU	GLU	S1466	S1466	
			K783	R1003	ALA	ALA	GLU	GLU	GLU	G1467	G1467	
			S784	A933	ALA	ALA	GLY	GLY	GLY	I1468	I1468	
			Q785	K934	ALA	ALA	GLY	GLY	GLY	D1537	D1537	
			A858	E1004	ALA	ALA	ILE	ILE	ILE	V1538	V1538	
			A859	G1005	M1214	M1214	ASP	ASP	ASP			
			E860	L1006	V1215	V1215	ASP	ASP	ASP			
			G787	S936	T1276	T1276	ASP	ASP	ASP			
			A788	N937	G1277	G1277	SER	SER	SER			

• Molecule 1: DNA-directed RNA polymerase I subunit RPA190

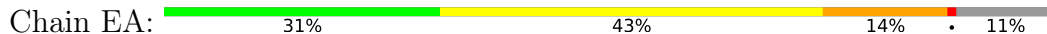


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M928	G932	A933	R934	G935	S936	N937	V940	K943	Q944	C945	L946	L947	L948	Q949	L952	R955	R956	Y957	P958	Q959	K961	L966	R967	S968	F969	K970	P971	Y972	E973	T974	D975	A976	G977	A978	G979	G980	G981	Y982	K983	S984	R985	F986	R987	S988	Q989	M992	S994	M995	F997	H998															
E856	A857	A858	A859	E860	V861	T862	D865	K866	D867	D872	F873	E874	L875	L876	K877	R878	L879	I882	D885	K888	S889	L892	D895	R896	D897	V898	T899	L903	S905	Q906	V907	V908	P913	D914	G915	T916	M917	K918	R919	R920	P921	C922	N923	S924	M925	Q926	Q927	Q928	Q929	Q930															
L781	D782	K783	L784	K785	Y786	G787	A788	S789	K790	Y791	G792	L793	V794	H795	H798	E804	A806	A807	K808	V809	L810	S811	V812	L813	G814	R815	L816	F817	T818	N819	Y820	I821	K822	L823	L824	A825	M830	D831	D832	L833	R834	L835	T836	A837	E838	G839	W842	R843	S850	R851	D852	T853	K854	R855											
V713	T714	L715	P716	T717	Y718	I719	F720	T721	P722	Y723	P724	W725	W726	G727	T728	K729	G730	I731	V732	T733	Y734	L735	L736	L737	N738	V739	G741	P742	R743	M744	T745	G746	L747	N748	I750	S751	K752	N753	K754	I755	K756	N757	E758	Y759	W760	W767	E768	V769	K772	D773	G774	C778	G779	I780											
A845	E846	A847	L848	N849	L850	A851	M852	T853	D854	S855	Q856	V857	L858	T859	G863	S864	G865	P866	R867	G868	L869	O870	O871	D872	H873	L874	S875	A876	G877	V878	W879	L880	T881	S882	K883	D884	T888	R889	Y892	I896	Y897	G898	C899	I700	R701	P702	E703	D704	G705	H706	R709	S710	K711	I712											
R579	H580	I581	K582	N583	R584	D585	V586	W587	L588	N589	N590	R591	T594	L595	H596	P597	A598	S599	M600	M601	G602	H603	K604	V605	R606	L607	L608	P609	N610	E611	R612	T613	L614	R615	Y618	A619	N620	T621	G622	A623	Y624	N625	D631	H632	M633	M634	G635	H636	F637	P638	E641	R644													
V514	N515	L516	L519	R520	R521	A522	V523	L524	N525	G526	G527	D528	K529	W530	P531	G532	K533	K534	Q535	L536	Q537	N538	G541	S545	L546	I547	G548	M549	S550	V551	L552	Q553	R481	S482	V483	I484	S485	E491	T492	V497	P498	N425	V500	F492	V428	T429	L430	Q431	F355	S357	M357	V362	P363	S440	T441										
R366	L369	P370	S371	K372	L373	S374	E375	E379	N380	T381	R382	N383	Q384	L385	L386	L387	S388	V389	L390	S393	L394	L395	L396	R397	D398	L399	L403	L406	Q407	K408	D409	R416	R417	V418	I419	L423	M424	N425	A426	F427	V428	T429	L430	Q431	F355	S357	M357	V362	P363	S440	T441														
K442	A443	Q444	ARG	THR	SER	GLY	K450	L453	V456	K457	A458	Q459	A460	L461	E462	K463	G464	G465	L466	F467	R468	M471	N472	G473	K474	R475	V476	N477	A480	R481	S482	V483	I484	S485	E491	T492	V497	P498	N425	V500	F492	V428	T429	L430	Q431	F355	S357	M357	V362	P363	S440	T441													
H294	K225	K226	L227	L228	K232	C233	D234	F243	R244	K245	E246	G247	F248	A100	S101	C102	L103	F108	R109	L110	K111	S112	M113	N114	P115	D116	M117	L118	L119	L120	K121	L122	R123	L124	L125	M126	A127	I130	D131	E132	S133	L136	D137	E138	E204	R205	L141	GLY	SER	LEU	ASN	ASN	C72	P73	SER	SER	MET	TYR	THR	ASP					
ASP	GLU	ALA	ILE	PHE	ASP	ASN	GLU	ASP	MET	GLU	ASP	GLY	GLU	PRO	THR	THR	ARG	PRO	LYS	THR	GLY	S312	T313	Y314	I315	E319	I323	L324	D325	T326	THR	ASN	ASN	ARG	VAL	L406	E187	Y188	V189	D190	M191	A192	I193	A194	L197	S198	R201	T202	L203	E204	R205	L211	GLY	SER	LEU	ASN	ASN	C72	P73	SER	SER	MET	TYR	THR	ASP
H294	K225	K226	L227	L228	K232	C233	D234	F243	R244	K245	E246	G247	F248	A100	S101	C102	L103	F108	R109	L110	K111	S112	M113	N114	P115	D116	M117	L118	L119	L120	K121	L122	R123	L124	L125	M126	A127	I130	D131	E132	S133	L136	D137	E138	E204	R205	L141	GLY	SER	LEU	ASN	ASN	C72	P73	SER	SER	MET	TYR	THR	ASP					

P1342	K372	L1272	L1145	E1145	F1068	M1000	E856	Q785	L719	L648	R520	L195	K372
D1343	L373	I1273	S1146	S1146	C1069	A1001	A857	Y786	F720	M652	Q521	V461	L373
I1344	G374	E1274	F1147	F1147	G1092	R1003	A858	G787	K721	T653	A522	P452	G374
A1347	E375	T1275	L1148	L1148	M1072	E1004	V861	S789	P724	Q656	I524	I453	E375
V1349	E379	L1276	M1151	M1151	Y1074	L1007	R862	K790	L725	Y657	N525	V456	E379
ARG	R880	THR	L1154	L1154	A1075	D1008	R863	Y791	L726	L688	G526	K457	R880
LEU	S381	ASN	S1158	S1158	L1076	T1009	L864	G792	R726	Y659	P527	Q458	S381
GLN	Q382	THR	I1159	I1159	Y1078	Y1090	D865	I793	G728	K529	D528	Q459	Q382
THR	L385	ALA	D1160	D1160	X1079	V1011	R866	H794	K729	W530	W530	E461	L385
ASP	L386	ASP	G1160	G1160	K1079	V1010	D867	H795	Q730	P665	P531	K462	L386
GLY	L387	GLY	V1161	V1161	Y1080	T1012	D872	H798	I731	G666	G532	K463	L387
ASN	K388	ASN	N1162	N1162	H1081	G1013	F873	S799	I732	R687	A535	E464	K388
ALA	V389	ALA	S1083	S1083	F1082	S1014	E874	Y800	T733	G688	T594	G465	V389
ASN	L390	ASN	L1084	L1084	A1084	R1015	E875	V800	T734	L669	Q535	L466	L390
SER	T391	SER	K1165	K1165	L1085	S1016	L875	P803	G735	G670	I536	F467	T391
SER	S393	SER	F1166	F1166	Y1018	G1017	L876	R804	L736	O671	Q537	R468	S393
ASN	L394	ASN	R1167	R1167	L1086	L1019	R878	V805	L737	D672	N538	K469	L394
LYS	L403	LYS	A1168	A1168	E1087	Q1020	L879	A806	W739	H673	E539	H470	L403
ARG	L406	ARG	L1169	L1169	E1092	R1021	T882	R807	V739	I674	K604	M471	L406
LEU	Q407	LEU	M1170	M1170	R956	C1022	I882	K808	L749	G814	L546	N477	Q407
GLN	K408	GLN	Q1171	Q1171	A1094	L1023	S889	R809	T750	R612	I547	A479	K408
GLU	D409	GLU	L1172	L1172	L1095	L1024	D885	V809	D743	K612	G548	A480	D409
ASP	R410	ASP	K1173	K1173	K1096	H1031	R886	L810	M744	L614	L543	R481	R410
ASP	L419	ASP	Y1174	Y1174	K1096	Q1026	N887	S811	P745	V678	W544	S482	L419
ASN	L419	ASN	M1175	M1175	H1101	L1027	R888	V812	M748	L680	S545	R475	L419
ASN	L419	ASN	R1176	R1176	L1102	E1028	R889	L813	N748	L680	S545	R476	L419
GLU	L419	GLU	L1177	L1177	L1102	E1028	S890	G814	L749	L680	S545	R477	L419
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GLN	L419	GLN	L1179	L1179	Y1104	G1029	R892	R815	T750	T681	I547	A479	L419
SER	L419	SER	I1179	I1179	Y1104	G1029	R892	R815	T750	T681	I547	A479	L419
SER	L419	SER	L1182	L1182	H1108	S1033	T896	M819	K752	W551	V551	S482	L419
LYS	L419	LYS	E1183	E1183	E1111	I1038	S897	Y820	L755	Y692	E552	I484	L419
THR	L419	THR	G1186	G1186	S1117	R1039	S897	Y820	L755	Y692	E552	I484	L419
THR	L419	THR	I1187	I1187	V1118	D1040	S897	Y820	L755	Y692	E552	I484	L419
VAL	L419	VAL	I1188	I1188	K1119	A1041	V900	T822	Y759	Y695	N620	T492	L419
SER	L419	SER	I1189	I1189	E1111	I1038	T904	A825	W760	I696	N620	T492	L419
TYR	L419	TYR	S1190	S1190	P1122	V1046	S905	M830	G763	Y697	N559	V497	L419
ASP	L419	ASP	L1192	L1192	V1123	Q1047	Q906	D831	Y624	G698	Q560	P498	L419
GLU	L419	GLU	V1193	V1193	F1228	M1048	V907	D832	N625	C699	L561	P499	L419
PRO	L419	PRO	G1194	G1194	M128	F1048	V912	L834	N767	R701	L562	V500	L419
ASP	L419	ASP	E1195	E1195	P1129	Y1060	F913	L855	E768	F702	P564	F501	L419
ASP	L419	ASP	P1196	P1196	A1130	T1058	F913	L855	E768	F702	P564	F501	L419
GLU	L419	GLU	S1197	S1197	K1131	D1063	D914	T836	L770	E703	S565	K504	L419
GLU	L419	GLU	T1198	T1198	A1054	A1054	G915	A837	F771	D704	S566	L505	L419
ILE	L419	ILE	Q1199	Q1199	I1055	I1055	M917	E838	K772	G705	N567	T506	L419
GLU	L419	GLU	M1200	M1200	D1066	D1066	K918	G339	D773	H706	V568	Y507	L419
THR	L419	THR	L1262	L1262	S1135	I1057	K919	M840	G774	R709	S569	F508	L419
THR	L419	THR	L1263	L1263	V1136	T1057	K919	M840	G774	R709	S569	F508	L419
MET	L419	MET	S1264	S1264	V1136	T1057	K919	M840	G774	R709	S569	F508	L419
ARG	L419	ARG	N1203	N1203	E1137	K1059	F920	W842	L776	S710	L573	P510	L419
GLU	L419	GLU	L1204	L1204	E1138	E1060	P921	R843	L777	K711	N574	V511	L419
ALA	L419	ALA	V1266	V1266	M1139	S1061	G922	R843	C778	I712	K575	T512	L419
GLU	L419	GLU	L1268	L1268	F1140	H1062	N923	S850	G779	V713	K576	A513	L419
LYS	L419	LYS	D1268	D1268	Q1141	M1083	N925	H851	T714	L714	W577	Y514	L419
SER	L419	SER	K1337	K1337	D1442	H998	Q926	D852	L781	L715	Y578	M515	L419
SER	L419	SER	L1271	L1271	K1143	A1066	A927	T853	D782	P716	H579	I516	L419
SER	L419	SER	I1271	I1271	L1144	E1067	M928	G854	K783	T718	H580	SER	L419
SER	L419	SER	L1271	L1271	L1144	E1067	M928	G854	K783	T718	H580	SER	L419

M1648
V1649
G1650
T1651
G1652
D1655
V1656
L1657
A1658
V1659
P1660
P1661
M1662
A1663
A1664

● Molecule 1: DNA-directed RNA polymerase I subunit RPA190



M1	D2	I3	V7	G8	S9	E10	I11	T12	S13	V14	D15	F16	G17	I18	L19	T20	K22	A21	S28	K30	Q31	I32	T36	L38	D39	M40	L41	G42	H43	G47	G48	L49	Y50	D51	L52	A53	L54	G55	L58	L61	C62	L67	K70	F71	C72	P73	G74
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H75	Q76	G77	H78	L81	P82	V83	Y86	N87	P88	L89	F90	F91	N92	I93	Q93	L94	Y95	I96	Y97	L98	R99	A100	S101	C102	L103	R109	L110	E114	V115	H116	L117	R117	Y118	A119	C120	K121	L122	R123	L124	L125	Y126	Y127	L130	S133	L136	T203	E138	L141	G142	S143	LEU
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ASN	SER	SER	MET	THR	THR	ASP	ASP	GLU	ALA	ILE	GLY	GLY	GLY	GLY	GLY	SER	LYS	GLN	GLY	GLY	GLY	GLY	GLY	GLY	ASP	ILE	ILE	SER	S175	T176	L177	L178	M179	E180	H181	L181	K182	S186	E187	Y188	Y189	D190	M191	A192	Y127	I193	A194	L197	S198	D199	L202	T203	E204	R205	T209	A210
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T211	V212	N213	D214	E215	R216	L219	F223	H224	GLY	K225	K226	L227	L228	F239	F243	K244	K245	D246	G247	F248	T249	K250	E253	T254	A255	L256	N257	Q260	L261	K267	K268	F269	ILE	ARG	GLN	GLN	ASP	MET	ILE	LYS	LYS	LYS	GLN	LYS	LYS	LYS	GLN	ALA	LYS	LYS	LEU	ASP	GLY	SER	ASN	GLU	ALA
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SER	ALA	ASN	ASP	GLU	GLU	SER	PHE	ASP	VAL	GLY	ARG	ASN	PRO	THR	THR	THR	THR	ARG	PRO	LYS	THR	GLY	S312	I315	E319	I323	L324	D325	T326	V327	K330	C333	V334	L335	Q336	Y337	F338	F339	H340	S341	R342	L345	S346	R347	K348	L349	Q350	K351	F355	K357	P363	P364
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A443	Q444	T447	SER	GLY	LYS	V451	P452	I453	V456	Q458	A459	L460	E461	K462	K463	E464	G465	L466	F467	R468	K469	H470	M471	M472	G473	K474	R475	V476	N477	Y478	A479	A480	R481	S482	V483	L484	S485	P488	E491	T492	I495	G496	V497	P498	P499	V500	F501	K504	L505	T506	Y507	P508
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N574	K575	K576	V577	V578	R579	H580	L581	K582	N583	R584	D585	V586	M589	N590	R591	T594	L595	H596	K597	A598	S599	M600	H601	G602	L603	K604	H605	R606	G607	L608	P609	N610	E611	K612	T613	L614	R615	Y618	E619	N620	T621	G622	A623	Y624	N625	A626	D627	D631	E632	M633	M635	H636	F637	P638
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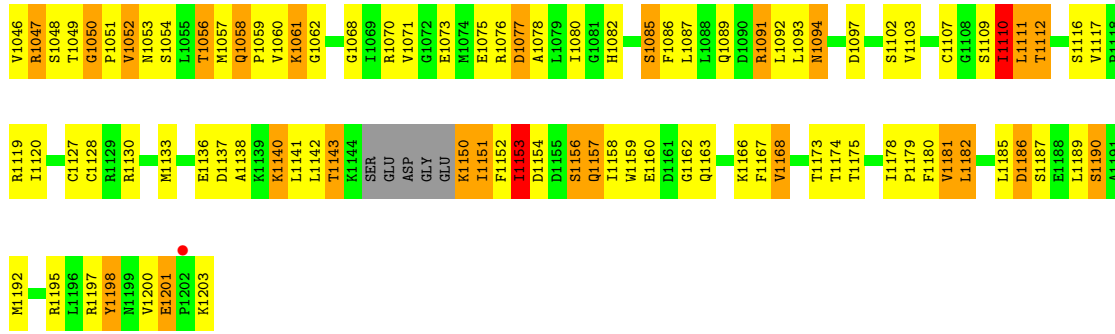
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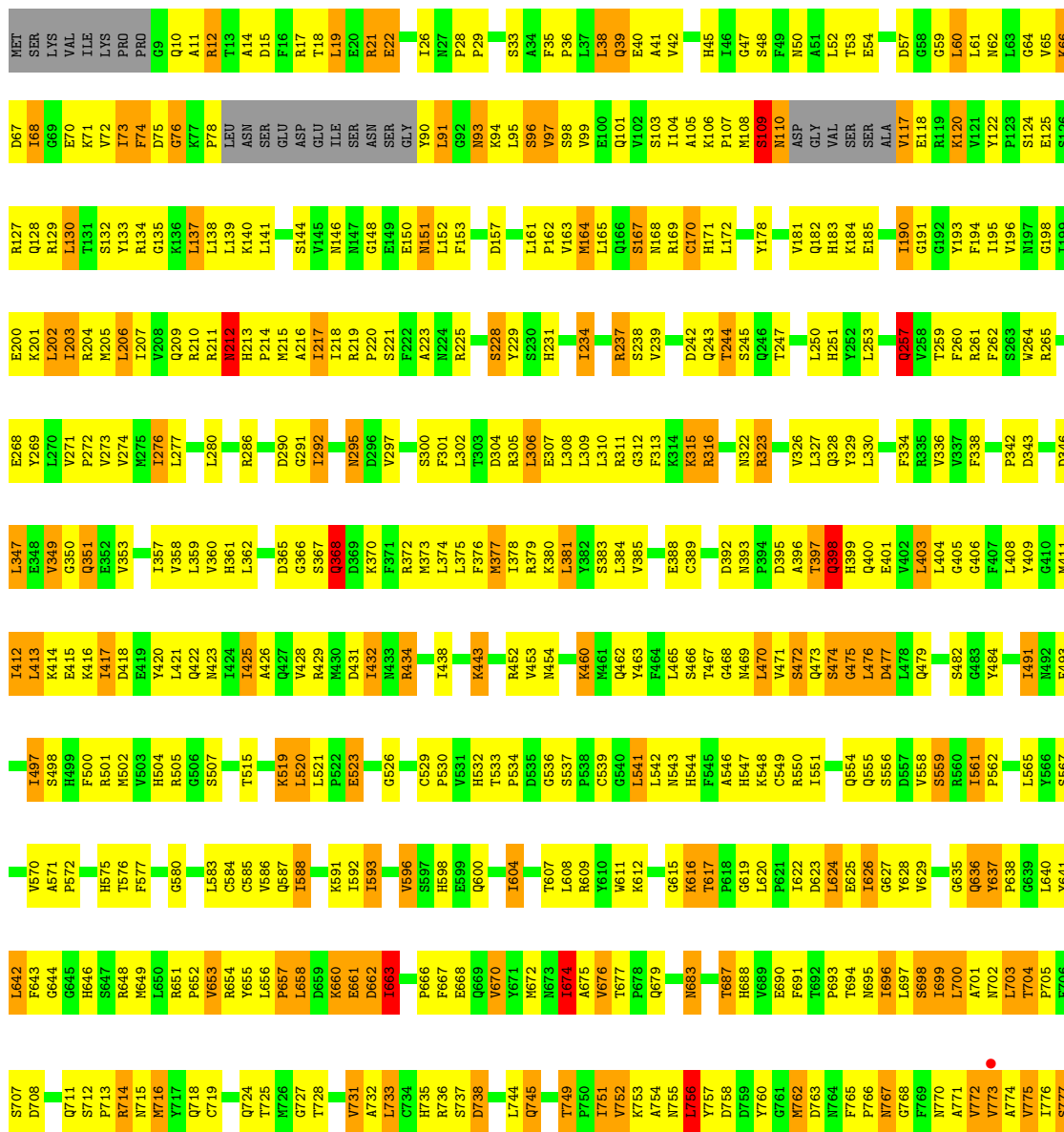
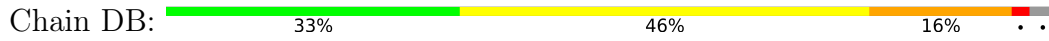
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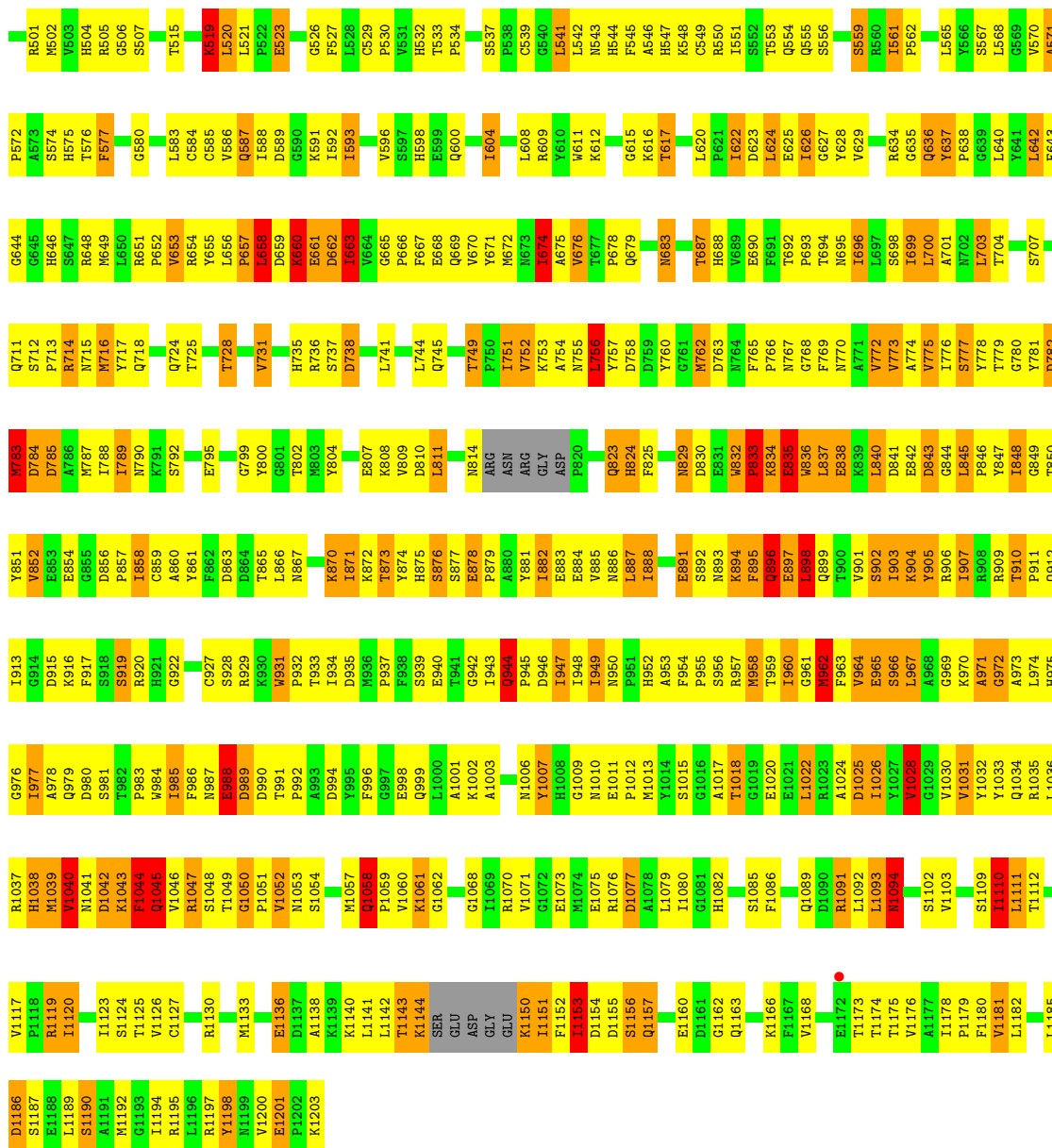
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L1202	S1135	T1058	Y987	P921	R843	L777	V713	E646	V577	A513	GLY	K372	GLY	ASP
M1203	S1136	K1059	S988	C922	T714	C778	T714	A647	Y578	Y514	LYS	G374	ARG	GLU
PHE	S1137	E1060	N923	N923	S850	G779	L715	L648	H579	N515	ALA	G374	ASN	ALA
PHE	E1138	H1061	P952	S924	V851	I780	P716	H649	H580	W516	PRO	E375	PRO	ILE
ALA	M1139	S1062	Q953	N925	D852	L781	P717	L650	I581	A517	THR	K225	THR	THR
ALA	F1140	M1063	Q926	Q926	T863	D782	T718	A651	K582	E518	THR	K226	THR	ASP
GLY	Q1141	F1066	Y986	A927	G854	K783	I719	N652	N583	L519	THR	E379	THR	ASN
HIS	K1142	E1067	H988	N928	R855	S784	F720	T653	R584	S381	PRO	K380	PRO	GLU
GLY	K1143	F1068	H988	N928	E856	Q785	K721	D654	D585	Q521	PRO	S381	PRO	GLU
ALA	L1144	F1068	H988	N928	A857	Y786	P722	S655	V586	A522	THR	N383	THR	ASP
ALA	E1145	C1069	A1001	G932	A858	G787	Y723	O656	Y523	Q384	THR	Q384	THR	MET
M1214	F1147	M1072	G1002	A933	V861	A788	P724	V657	N590	I594	GLY	S312	GLY	ASP
V1215	L1148	Y1073	R1003	K934	T862	S789	L725	L658	R591	N525	GLY	F313	GLY	GLU
L1216	M1151	Y1074	G1004	G935	N863	K790	W726	T659	T594	G526	GLY	G247	GLY	GLU
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L1219	M1151	Y1074	G1004	G935	N863	K790	W726	T659	T594	G526	GLY	G247	GLY	GLU
P1220	L1154	L1076	L1007	N938	D865	I793	G728	G663	H596	K529	LYS	L390	LYS	SER
R1221	L1154	L1076	L1007	N938	D865	I793	G728	G663	H596	K529	LYS	L390	LYS	SER
R1222	L1154	L1076	L1007	N938	D865	I793	G728	G663	H596	K529	LYS	L390	LYS	SER
R1223	L1154	L1076	L1007	N938	D865	I793	G728	G663	H596	K529	LYS	L390	LYS	SER
E1224	L1154	L1076	L1007	N938	D865	I793	G728	G663	H596	K529	LYS	L390	LYS	SER
I1225	L1154	L1076	L1007	N938	D865	I793	G728	G663	H596	K529	LYS	L390	LYS	SER
V1226	L1154	L1076	L1007	N938	D865	I793	G728	G663	H596	K529	LYS	L390	LYS	SER
M1227	L1154	L1076	L1007	N938	D865	I793	G728	G663	H596	K529	LYS	L390	LYS	SER
T1228	K1165	E1087	S1016	L947	R878	R789	T740	H673	R606	M588	GLN	L403	GLN	S175
A1229	F1166	E1087	S1016	L947	R878	R789	T740	H673	R606	M588	GLN	L403	GLN	T176
S1230	R1167	E1087	S1016	L947	R878	R789	T740	H673	R606	M588	GLN	L403	GLN	T177
L1231	A1168	E1087	S1016	L947	R878	R789	T740	H673	R606	M588	GLN	L403	GLN	L178
A1232	M1169	E1087	S1016	L947	R878	R789	T740	H673	R606	M588	GLN	L403	GLN	N179
L1233	L1170	E1087	S1016	L947	R878	R789	T740	H673	R606	M588	GLN	L403	GLN	E180
K1234	Q1171	E1087	S1016	L947	R878	R789	T740	H673	R606	M588	GLN	L403	GLN	L181
L1235	L1172	E1087	S1016	L947	R878	R789	T740	H673	R606	M588	GLN	L403	GLN	K182
P1236	K1173	E1087	S1016	L947	R878	R789	T740	H673	R606	M588	GLN	L403	GLN	S186
Q1237	Y1174	E1087	S1016	L947	R878	R789	T740	H673	R606	M588	GLN	L403	GLN	E187
M1238	M1175	E1087	S1016	L947	R878	R789	T740	H673	R606	M588	GLN	L403	GLN	Y188
T1239	R1176	E1087	S1016	L947	R878	R789	T740	H673	R606	M588	GLN	L403	GLN	V189
L1240	S1177	E1087	S1016	L947	R878	R789	T740	H673	R606	M588	GLN	L403	GLN	D190
P1241	L1178	E1087	S1016	L947	R878	R789	T740	H673	R606	M588	GLN	L403	GLN	M191
I1242	G1182	E1087	S1016	L947	R878	R789	T740	H673	R606	M588	GLN	L403	GLN	A192
M1243	E1183	E1087	S1016	L947	R878	R789	T740	H673	R606	M588	GLN	L403	GLN	I193
N1244	A1184	E1087	S1016	L947	R878	R789	T740	H673	R606	M588	GLN	L403	GLN	A194
D1245	V1185	E1087	S1016	L947	R878	R789	T740	H673	R606	M588	GLN	L403	GLN	L197
V1246	G1186	E1087	S1016	L947	R878	R789	T740	H673	R606	M588	GLN	L403	GLN	S198
S1247	L1187	E1087	S1016	L947	R878	R789	T740	H673	R606	M588	GLN	L403	GLN	D199
D1248	I1188	E1087	S1016	L947	R878	R789	T740	H673	R606	M588	GLN	L403	GLN	T202
E1249	A1189	E1087	S1016	L947	R878	R789	T740	H673	R606	M588	GLN	L403	GLN	T203
Q1250	S1190	E1087	S1016	L947	R878	R789	T740	H673	R606	M588	GLN	L403	GLN	E204
A1251	Q1191	E1087	S1016	L947	R878	R789	T740	H673	R606	M588	GLN	L403	GLN	R205
D1252	S1192	E1087	S1016	L947	R878	R789	T740	H673	R606	M588	GLN	L403	GLN	T209
T1253	V1193	E1087	S1016	L947	R878	R789	T740	H673	R606	M588	GLN	L403	GLN	A210
F1254	L1194	E1087	S1016	L947	R878	R789	T740	H673	R606	M588	GLN	L403	GLN	T211
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K1256	P1196	E1087	S1016	L947	R878	R789	T740	H673	R606	M588	GLN	L403	GLN	N213
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S1259	Q1199	E1087	S1016	L947	R878	R789	T740	H673	R606	M588	GLN	L403	GLN	R216
K1260	M1200	E1087	S1016	L947	R878	R789	T740	H673	R606	M588	GLN	L403	GLN	ASP

1986	F986	N987	E988	D989	D990	T991	F992	A993	D994	Y995	F996	E997	E998	Q999	L1000	A1001	K1002	A1003	M1006	Y1007	H1008	G1009	M1010	E1011	F1012	M1013	Y1014	G1015	G1016	A1017	T1018	G1019	E1020	E1021	L1022	G1023	A1024	D1025	I1026	Y1027	Y1028	V1029	V1030	V1031	Y1032	Q1033	Q1034	R1035	L1036	R1037	H1038	M1039	Y1040	N1041	D1042	K1043	F1044	Q1045																																																																																																																																																																																																																																																																																																																																																																									
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G922	Q923	K924	C927	S928	D929	R930	W931	R931	R932	T933	I934	D935	H936	P937	F938	S939	E940	I943	Q944	P945	D946	I947	I948	I949	N950	A953	F954	Y955	G956	R957	N958	T959	I960	R961	H962	F963	V964	E965	S966	L967	A968	G969	R970	A971	A972	A973	Q1034	L1036	R1037	H1038	M1039	Y1040	N1041	D1042	K1043	F1044	Q1045																																																																																																																																																																																																																																																																																																																																																																										
R796	G799	Y800	G801	D802	T803	L804	R805	Y806	K807	E808	K809	R810	L811	A812	L813	S814	A815	ARG	ASN	ARG	ARG	GLY	ASP	P820	I821	T822	Q823	H824	F825	G828	G829	E830	E831	R832	N833	K834	F835	G836	L837	R838	R839	V901	S902	I903	K904	Y905	R906	I907	A908	R909	T910	R911	Q912	I913	K916	S919	R920	H921																																																																																																																																																																																																																																																																																																																																																																									
V731	A732	L733	C734	H735	R736	S737	D738	L741	M742	M743	L744	Q745	T749	P750	V751	V752	K753	A754	M755	L756	H757	D758	D759	Y760	G761	Q762	H763	D764	F765	P766	M767	G768	F769	N770	A771	V772	V773	A774	V775	I776	S777	Y778	T779	G780	Y781	D782	M783	D784	D785	A786	M787	I788	N789	K791	S792	T795	E796																																																																																																																																																																																																																																																																																																																																																																										
I663	V664	G665	P666	F667	G668	Q669	Y670	Y671	M672	M673	I674	A675	V676	Q679	M680	N681	N682	H686	T687	H688	V689	E690	F691	T692	P693	G694	M695	D696	F697	S698	L699	L700	A701	N702	L703	T704	P705	F706	S707	D708	F709	N710	Q711	S712	P713	R714	R715	N716	Y717	Q718	C719	Q724	T725	M726	G727	T728	G729	E796																																																																																																																																																																																																																																																																																																																																																																									
K591	L592	L593	E594	G595	P596	S597	H598	L604	M605	H606	L607	M608	H609	H610	M611	K612	G613	K614	T617	L620	P621	F622	D623	L624	E625	M626	G627	L628	L629	Q654	Q655	V656	S657	L658	L659	H664	S662	L663	L664	L665	L666	M667	N668	M669	H670	P672	A673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000	L1001	L1002	L1003	L1004	L1005	L1006	L1007	L1008	L1009	L1010	L1011	L1012	L1013	L1014	L1015	L1016	L1017	L1018	L1019	L1020	L1021	L1022	L1023	L1024	L1025	L1026	L1027	L1028	L1029	L1030	L1031	L1032	L1033	L1034	L1035	L1036	L1037	L1038	L1039	L1040	L1041	L1042	L1043	L1044	L1045
1432	H433	R434	I438	F443	L450	M451	R452	V453	M454	S459	M460	M461	Y463	S466	T467	G468	M469	V471	S472	Q388	R389	Q390	L391	L392	L393	F313	K314	R315	R316	N322	R323	V326	L327	Q328	F334	R335	V336	D343	D346	L347	E348	V349	G350	O351	E352	V353	L357	V358	L359	V360	H361	L362	D431																																																																																																																																																																																																																																																																																																																																																																														
G366	S367	D368	K370	F371	R372	K373	L374	L375	F376	M377	L378	R379	K380	L381	Y382	S383	L384	V385	C389	D392	A396	T397	R399	H399	Q400	Q401	N402	L403	L404	G405	L408	Y409	G410	M411	L412	L413	K414	E415	K416	L417	D418	E419	F420	L421	Q422	H423	L424	R425	A426	Q427	V428	R429	T430	H431	R432	H433	R434	I438	F443	L450	M451	R452	V453	M454	S459	M460	M461	Y463	S466	T467	G468	M469	V471	S472	Q388	R389	Q390	L391	L392	L393	F313	K314	R315	R316	N322	R323	V326	L327	Q328	F334	R335	V336	D343	D346	L347	E348	V349	G350	O351	E352	V353	L357	V358	L359	V360	H361	L362	D431																																																																																																																																																																																																																																																																																																																							
173	F74	D75	G76	K77	L139	L140	L141	S144	V145	ASP	GLU	ILE	PRO	PRO	G9	Q10	A11	R12	T13	A14	R17	T18	L19	E20	R21	E22	I26	S33	A34	F35	L95	S96	V97	S98	V99	E100	H101	S103	I104	A105	K106	M108	S109	N110	ASP	GLY	VAL	SER	SER	SER	ALA	V117	E118	R119	G120	G125	G126	R127	Q128	L129	L130	T131	S132	Y133	L134																																																																																																																																																																																																																																																																																																																																																																		
L277	L280	R286	R212	R214	R215	A216	I217	G294	G295	M296	P220	V297	K298	F301	L302	T303	D304	R305	E307	L234	R237	S238	V239	D242	Q243	T244	S245	Q246	T247	L250	H251	Y252	L253	Q257	T259	F260	R261	F262	S263	F264	R265	K266	N267	E268	Y269	V271	L272	L359	V360	H361	L362	D431																																																																																																																																																																																																																																																																																																																																																																															

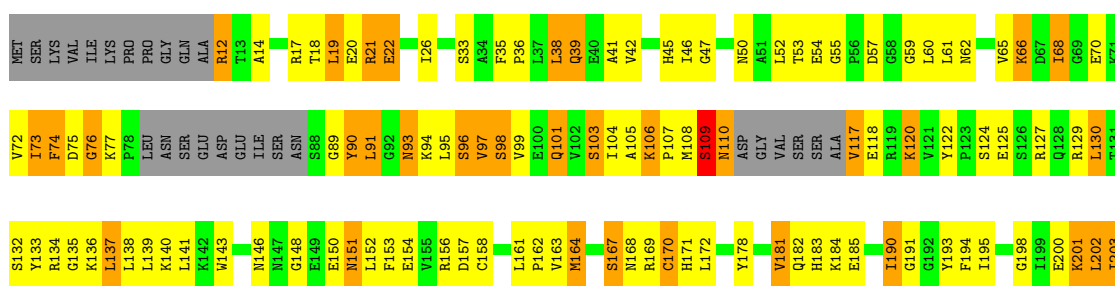


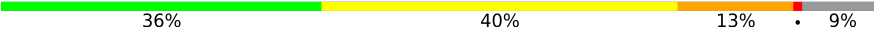
● Molecule 2: DNA-directed RNA polymerase I subunit RPA135

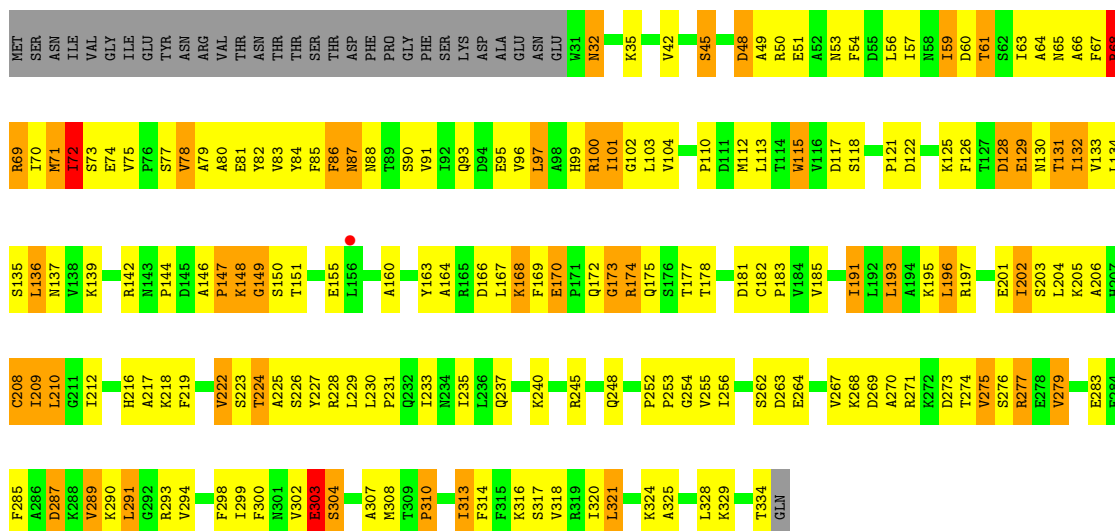




● Molecule 2: DNA-directed RNA polymerase I subunit RPA135

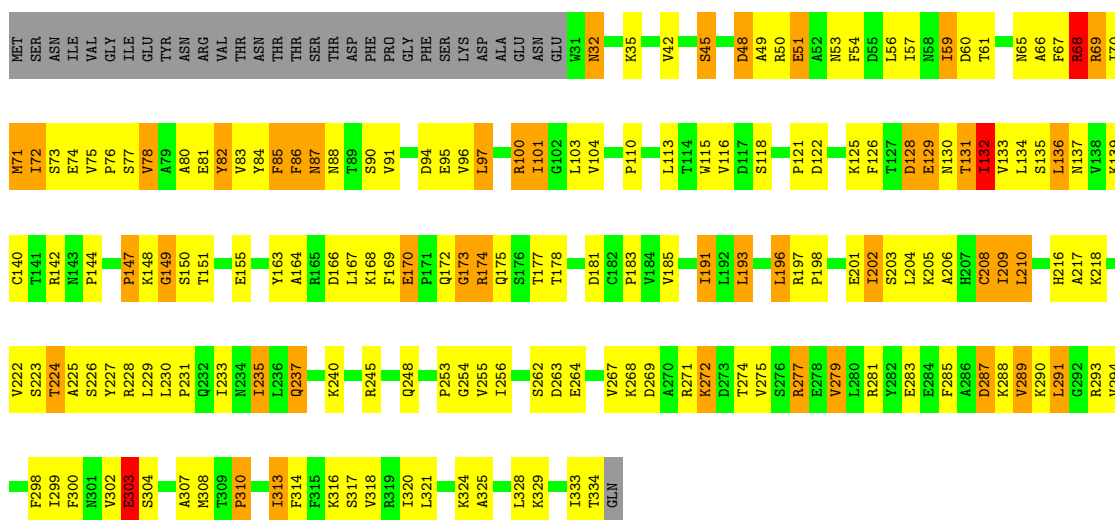


Chain AC:  36% 40% 13% 9%



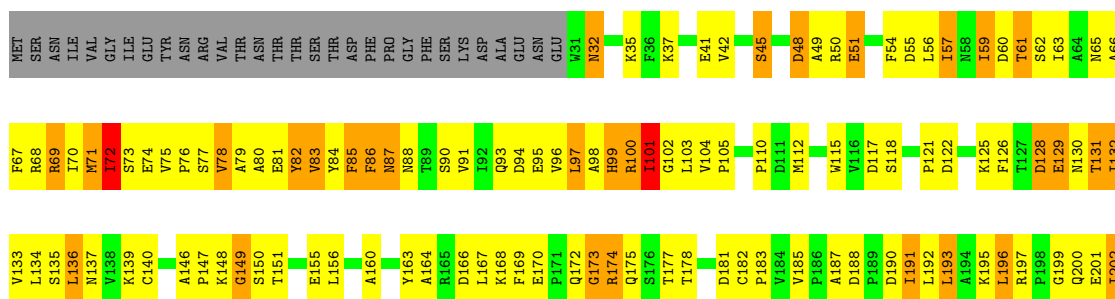
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

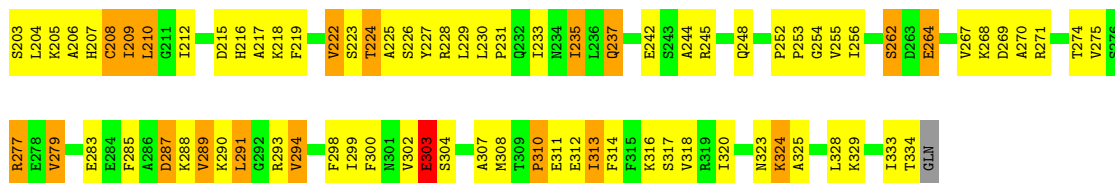
Chain BC:  39% 38% 13% 9%



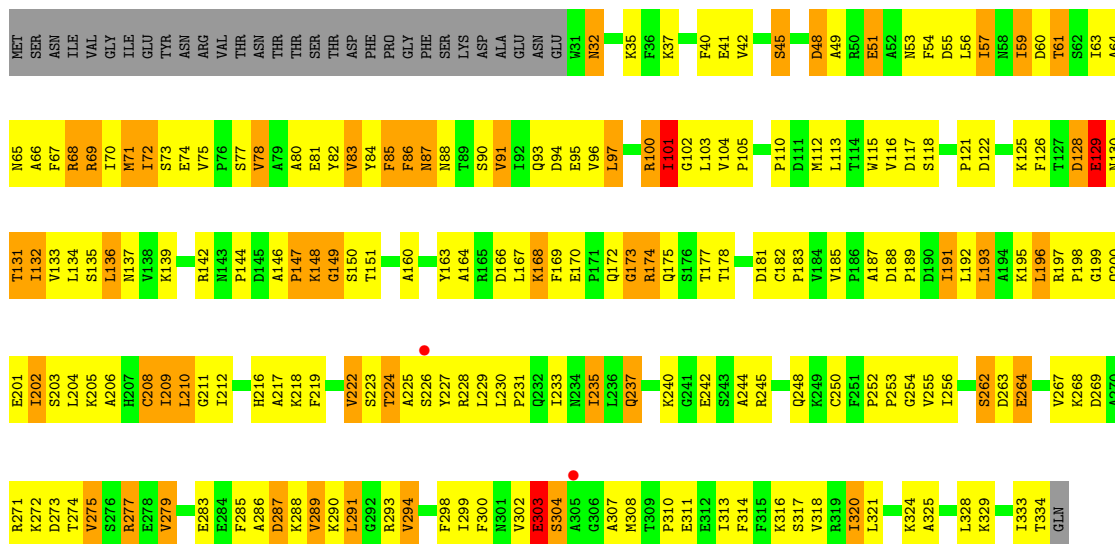
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

Chain CC:  32% 44% 14% 9%

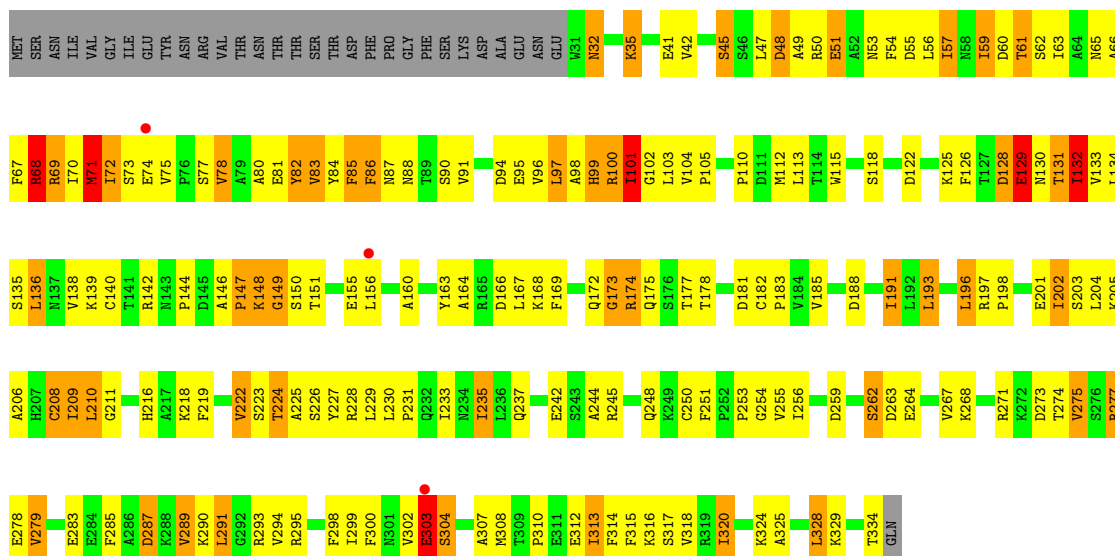




• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1



• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

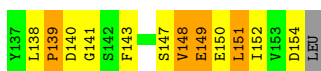
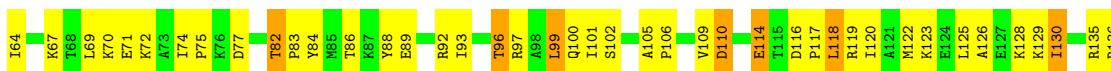
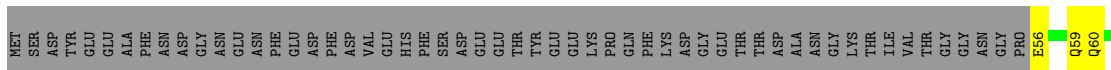


• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1



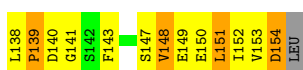
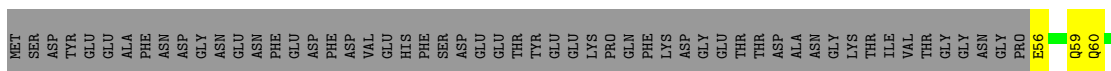
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain CF: 27% 30% 7% 36%



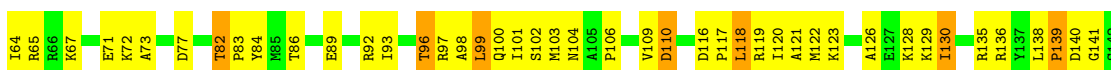
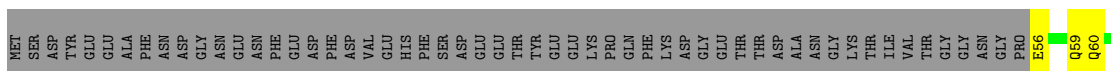
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain DF: 26% 31% 6% 36%



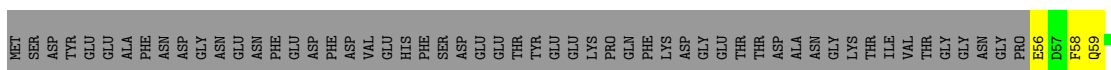
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

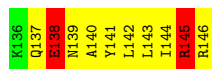
Chain EF: 28% 30% 6% 36%



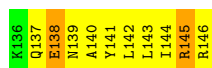
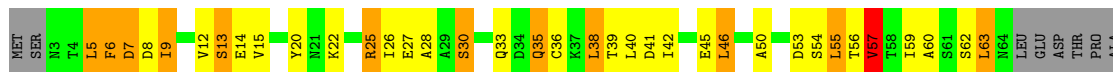
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain FF: 28% 29% 7% 36%

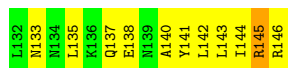
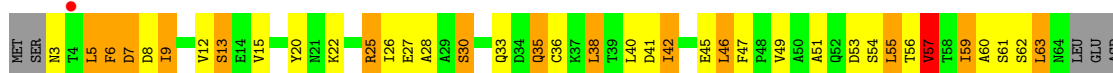




• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



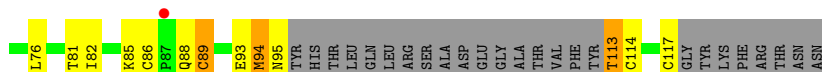
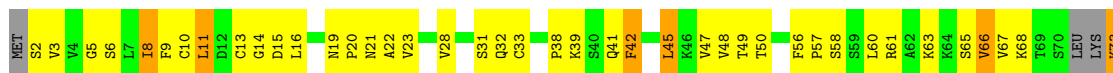
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



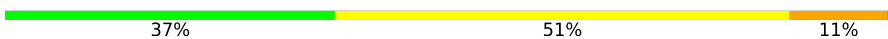
• Molecule 9: DNA-directed RNA polymerase I subunit RPA12

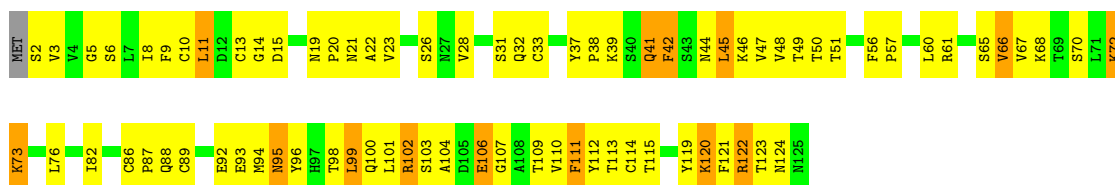


• Molecule 9: DNA-directed RNA polymerase I subunit RPA12



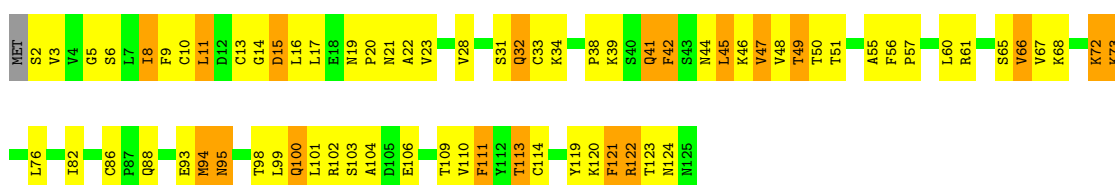
- Molecule 9: DNA-directed RNA polymerase I subunit RPA12

Chain CI:  37% 51% 11% .



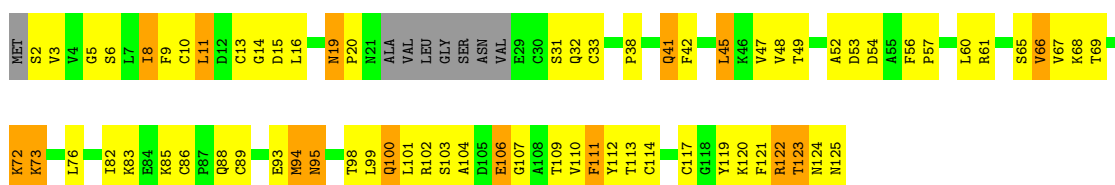
- Molecule 9: DNA-directed RNA polymerase I subunit RPA12

Chain DI:  42% 42% 15% .



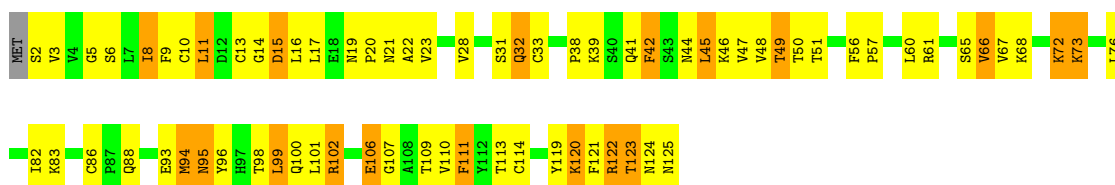
- Molecule 9: DNA-directed RNA polymerase I subunit RPA12

Chain EI:  37% 45% 12% 6%



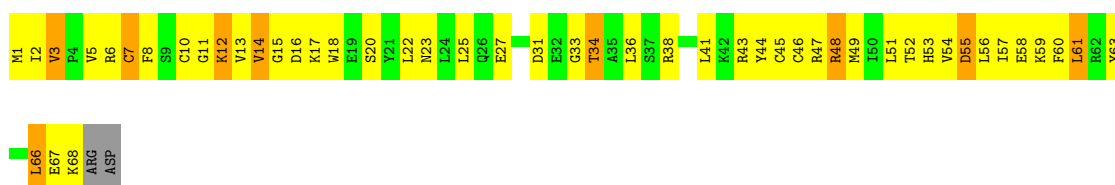
- Molecule 9: DNA-directed RNA polymerase I subunit RPA12

Chain FI:  42% 42% 15% .




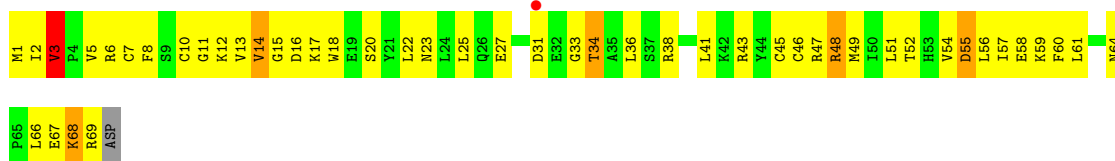
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain AJ:  27% 57% 13% .



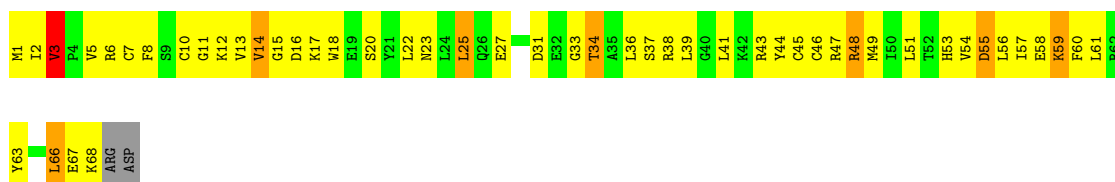
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain BJ: 



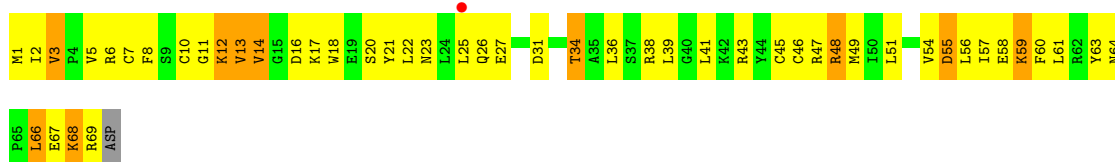
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain CJ: 



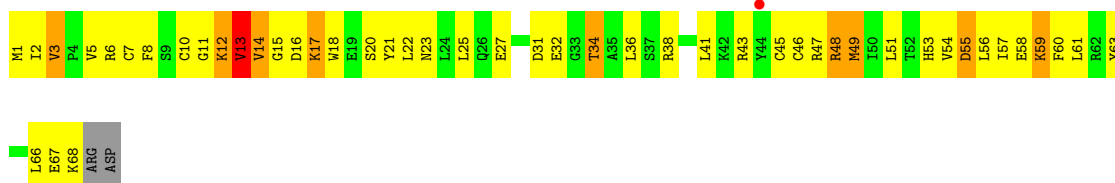
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain DJ: 

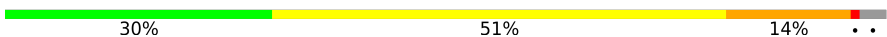


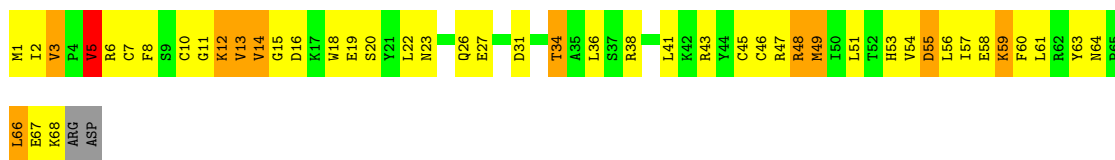
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain EJ: 

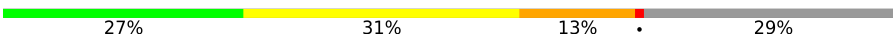


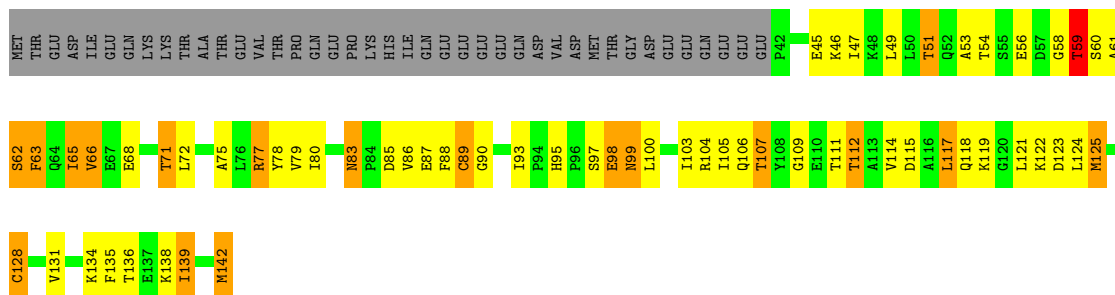
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain FJ: 




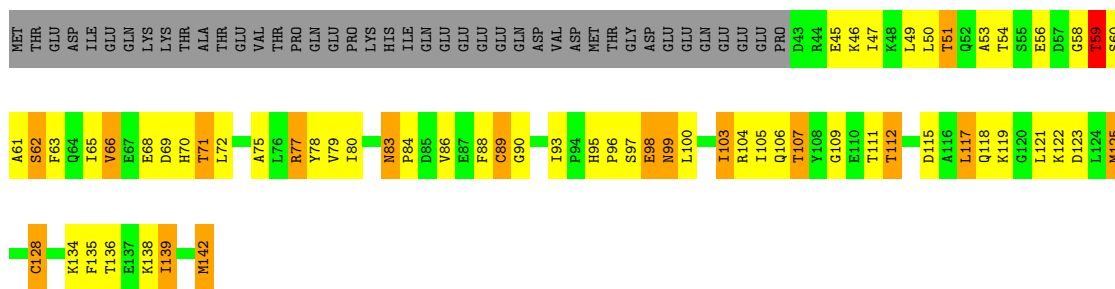
- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

Chain AK: 




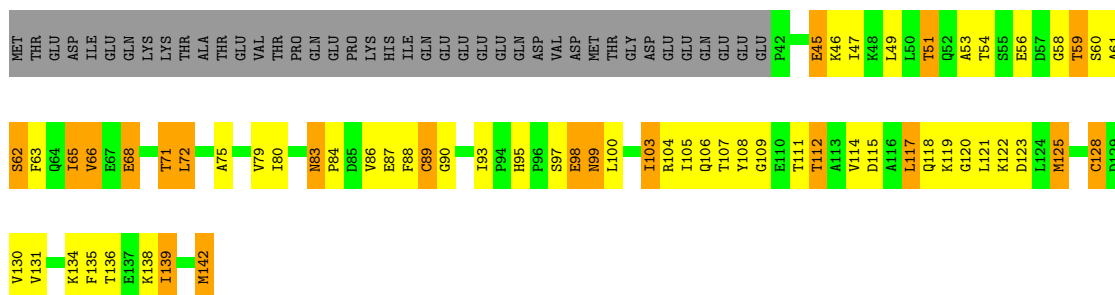
- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

Chain BK: 

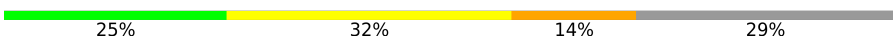


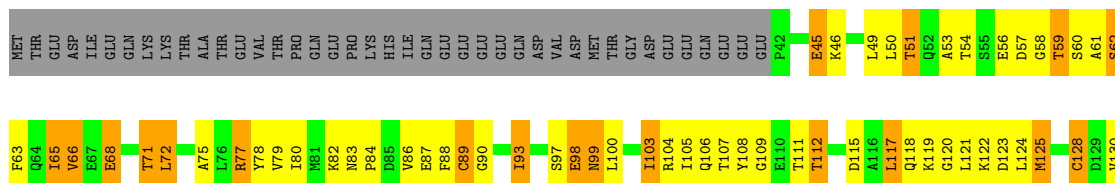
- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

Chain CK: 



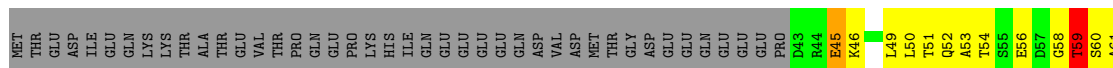
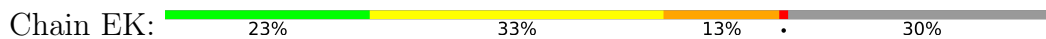
- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

Chain DK: 

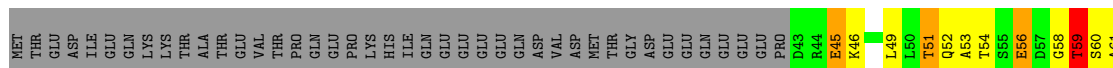
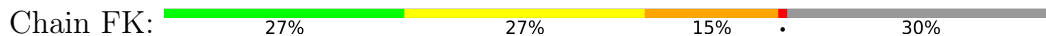




- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2



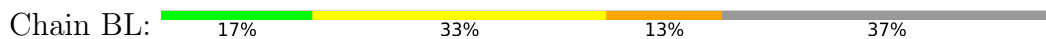
- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2



- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

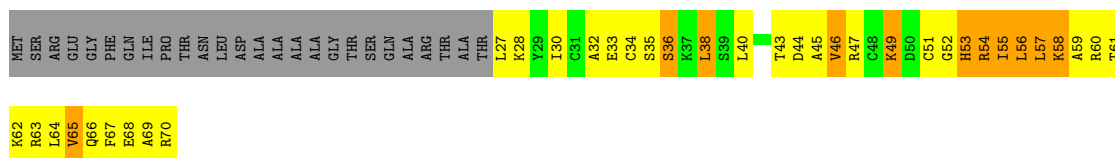


- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



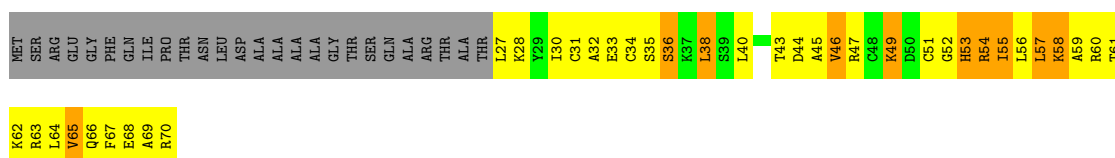
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain CL:



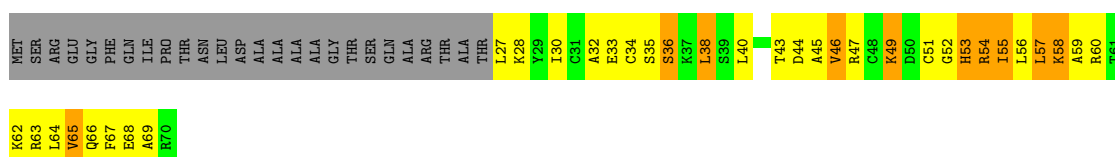
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain DL:



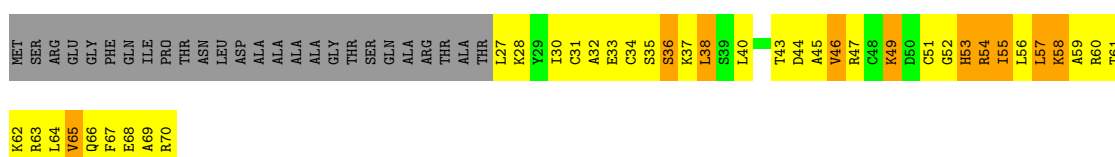
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain EL:



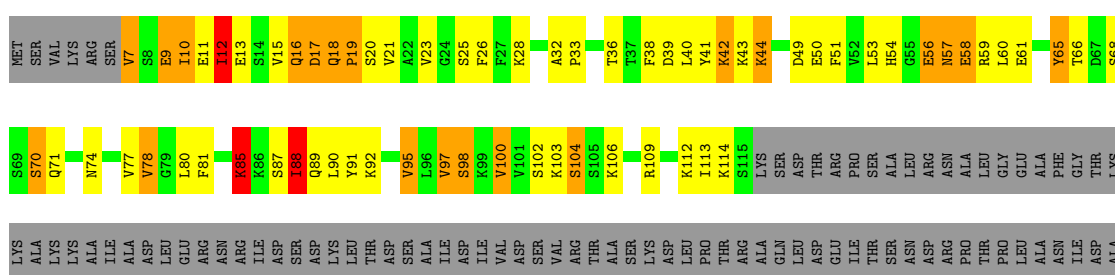
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain FL:



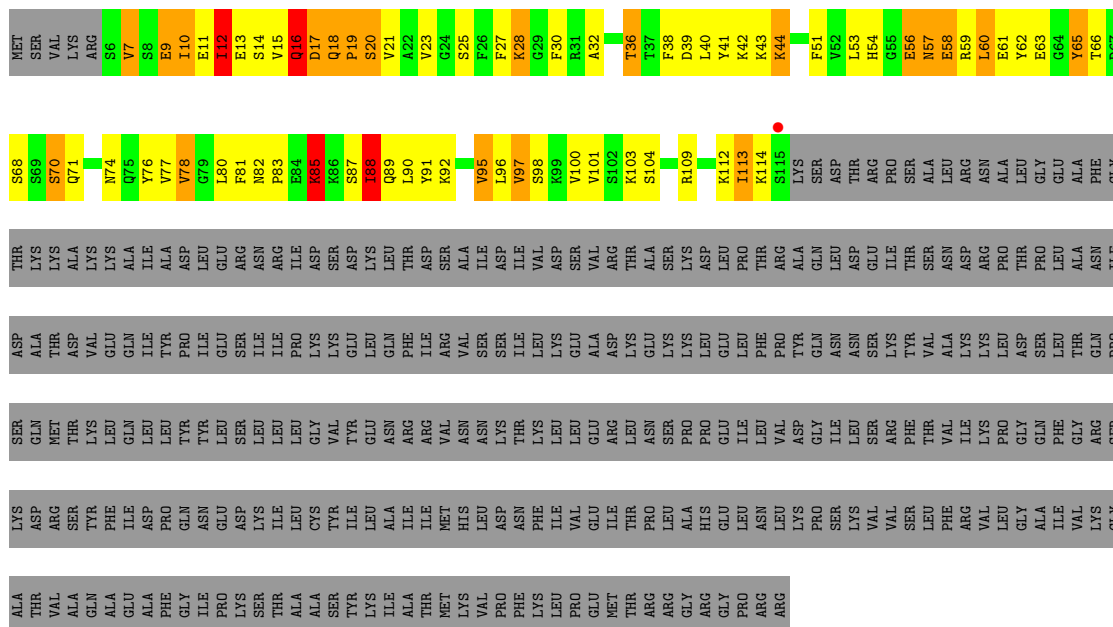
• Molecule 13: DNA-directed RNA polymerase I subunit RPA49

Chain AM:




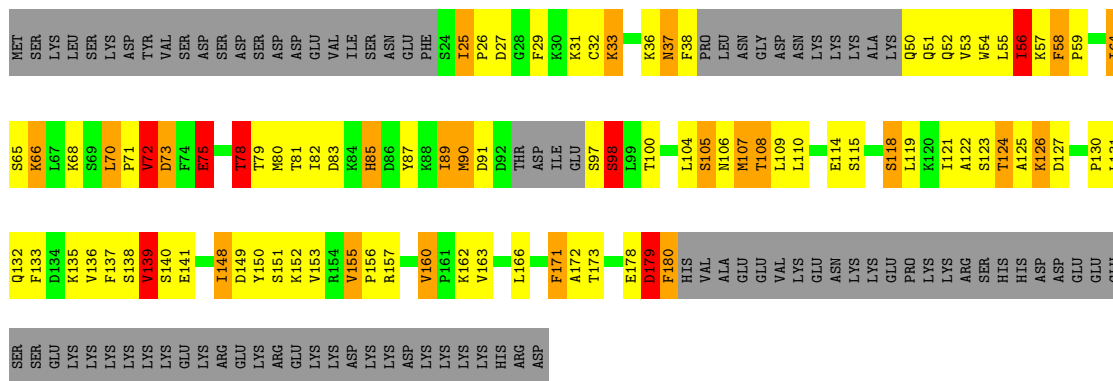
- Molecule 13: DNA-directed RNA polymerase I subunit RPA49

Chain FM:  9% 11% 5% 73%




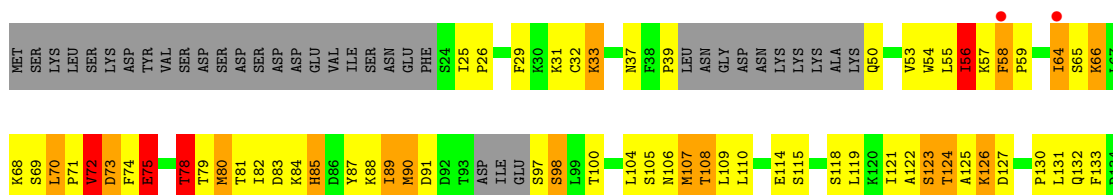
- Molecule 14: DNA-directed RNA polymerase I subunit RPA34

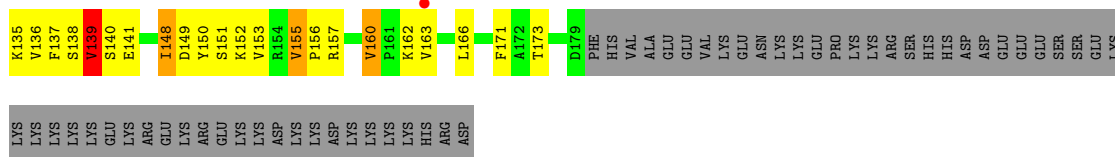
Chain AN:  22% 27% 9% 39%



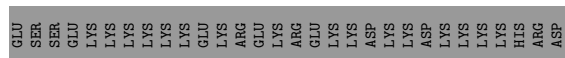
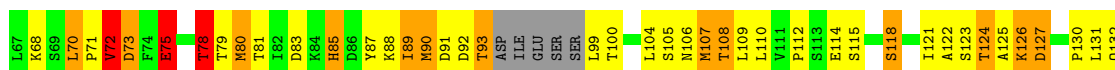
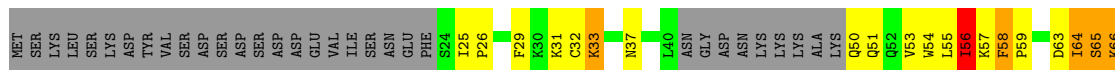
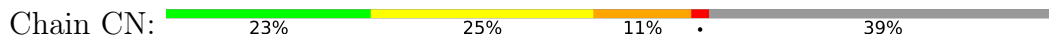
- Molecule 14: DNA-directed RNA polymerase I subunit RPA34

Chain BN:  24% 27% 8% 39%

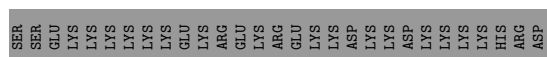
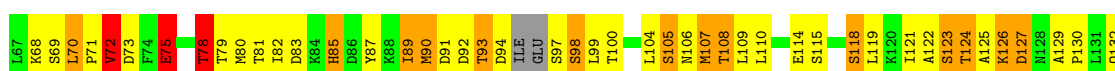
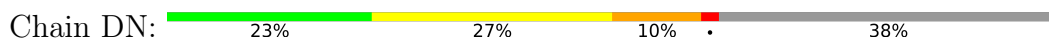




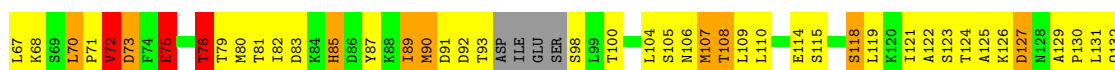
• Molecule 14: DNA-directed RNA polymerase I subunit RPA34



• Molecule 14: DNA-directed RNA polymerase I subunit RPA34



• Molecule 14: DNA-directed RNA polymerase I subunit RPA34



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	619.48Å 306.62Å 251.78Å 90.00° 97.50° 90.00°	Depositor
Resolution (Å)	49.69 – 5.50 49.69 – 5.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.69-5.50) 98.9 (49.69-5.50)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 5.39Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.196 , 0.235 0.204 , 0.243	Depositor DCC
R_{free} test set	1987 reflections (1.31%)	wwPDB-VP
Wilson B-factor (Å ²)	117.0	Xtrriage
Anisotropy	0.698	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 235.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	204233	wwPDB-VP
Average B, all atoms (Å ²)	195.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	AA	0.78	3/11916 (0.0%)	1.03	28/16097 (0.2%)
1	BA	0.70	3/11752 (0.0%)	1.00	23/15875 (0.1%)
1	CA	0.85	5/11908 (0.0%)	1.05	30/16086 (0.2%)
1	DA	0.85	3/11910 (0.0%)	1.06	26/16090 (0.2%)
1	EA	0.88	9/11919 (0.1%)	1.07	35/16099 (0.2%)
1	FA	0.88	7/11923 (0.1%)	1.05	28/16106 (0.2%)
2	AB	0.74	2/9389 (0.0%)	1.03	38/12685 (0.3%)
2	BB	0.72	2/9377 (0.0%)	1.02	32/12671 (0.3%)
2	CB	0.88	7/9509 (0.1%)	1.08	45/12847 (0.4%)
2	DB	0.87	4/9474 (0.0%)	1.08	39/12802 (0.3%)
2	EB	0.87	5/9470 (0.1%)	1.08	40/12796 (0.3%)
2	FB	0.87	5/9475 (0.1%)	1.09	44/12802 (0.3%)
3	AC	0.78	0/2465	1.03	7/3342 (0.2%)
3	BC	0.69	0/2465	1.00	6/3342 (0.2%)
3	CC	0.87	2/2465 (0.1%)	1.07	6/3342 (0.2%)
3	DC	0.84	2/2465 (0.1%)	1.05	5/3342 (0.1%)
3	EC	0.93	3/2465 (0.1%)	1.07	8/3342 (0.2%)
3	FC	0.89	2/2465 (0.1%)	1.08	6/3342 (0.2%)
4	AD	0.76	0/465	1.09	2/630 (0.3%)
4	BD	0.65	0/465	1.06	2/630 (0.3%)
4	CD	0.87	0/465	1.10	2/630 (0.3%)
4	DD	0.82	0/465	1.11	2/630 (0.3%)
4	ED	0.86	0/465	1.07	2/630 (0.3%)
4	FD	0.85	0/465	1.11	2/630 (0.3%)
5	AE	0.66	0/1796	0.97	2/2416 (0.1%)
5	BE	0.61	0/1796	0.96	2/2416 (0.1%)
5	CE	0.74	0/1796	1.02	3/2416 (0.1%)
5	DE	0.78	0/1796	1.03	2/2416 (0.1%)
5	EE	0.74	0/1796	0.98	0/2416
5	FE	0.81	0/1796	1.01	3/2416 (0.1%)
6	AF	0.73	0/821	1.01	0/1106
6	BF	0.60	0/821	0.97	2/1106 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	CF	0.79	0/830	1.06	1/1118 (0.1%)
6	DF	0.81	1/830 (0.1%)	1.09	2/1118 (0.2%)
6	EF	0.79	1/830 (0.1%)	1.07	2/1118 (0.2%)
6	FF	0.83	0/830	1.07	0/1118
7	AG	0.81	0/1637	1.08	7/2226 (0.3%)
7	AO	1.05	0/417	1.08	1/562 (0.2%)
7	BG	0.70	0/1577	1.04	8/2145 (0.4%)
7	BO	1.08	0/408	1.05	1/550 (0.2%)
7	CG	0.91	0/1637	1.09	8/2226 (0.4%)
7	CO	1.18	1/402 (0.2%)	1.37	3/542 (0.6%)
7	DG	0.89	0/1637	1.10	5/2226 (0.2%)
7	DO	1.14	0/417	1.34	5/562 (0.9%)
7	EG	0.87	1/1637 (0.1%)	1.07	8/2226 (0.4%)
7	EO	1.06	0/417	1.19	1/562 (0.2%)
7	FG	0.94	2/1637 (0.1%)	1.12	10/2226 (0.4%)
7	FO	1.07	1/417 (0.2%)	1.26	6/562 (1.1%)
8	AH	0.83	0/1081	1.01	2/1463 (0.1%)
8	BH	0.64	1/1070 (0.1%)	0.90	2/1449 (0.1%)
8	CH	0.86	0/1070	1.03	7/1449 (0.5%)
8	DH	0.88	2/1093 (0.2%)	1.00	2/1480 (0.1%)
8	EH	0.90	4/1093 (0.4%)	1.06	5/1480 (0.3%)
8	FH	1.06	3/1093 (0.3%)	1.12	8/1480 (0.5%)
9	AI	0.91	1/956 (0.1%)	1.01	3/1288 (0.2%)
9	BI	0.74	0/721	0.93	2/969 (0.2%)
9	CI	0.92	1/956 (0.1%)	1.01	3/1288 (0.2%)
9	DI	0.92	0/956	1.01	3/1288 (0.2%)
9	EI	1.01	1/910 (0.1%)	1.08	3/1223 (0.2%)
9	FI	1.02	3/956 (0.3%)	1.03	2/1288 (0.2%)
10	AJ	0.70	0/567	0.99	0/761
10	BJ	0.67	0/578	1.00	2/775 (0.3%)
10	CJ	0.85	0/567	1.03	3/761 (0.4%)
10	DJ	0.76	0/578	0.98	1/775 (0.1%)
10	EJ	0.89	1/567 (0.2%)	1.01	0/761
10	FJ	0.83	0/567	1.01	0/761
11	AK	0.80	0/804	1.08	4/1083 (0.4%)
11	BK	0.65	0/796	1.02	2/1072 (0.2%)
11	CK	0.88	0/804	1.07	4/1083 (0.4%)
11	DK	0.82	0/804	1.06	2/1083 (0.2%)
11	EK	0.82	0/796	1.07	4/1072 (0.4%)
11	FK	0.80	0/796	1.05	4/1072 (0.4%)
12	AL	0.81	0/354	0.97	1/468 (0.2%)
12	BL	0.75	0/354	0.94	0/468
12	CL	0.86	0/354	1.03	2/468 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
12	DL	0.82	0/354	1.00	1/468 (0.2%)
12	EL	0.89	0/354	1.06	1/468 (0.2%)
12	FL	0.82	0/354	0.98	1/468 (0.2%)
13	AM	0.82	0/879	1.01	0/1180
13	BM	0.81	0/879	1.01	1/1180 (0.1%)
13	CM	0.91	0/879	1.04	2/1180 (0.2%)
13	DM	0.88	0/879	1.03	1/1180 (0.1%)
13	EM	0.87	0/885	1.07	1/1188 (0.1%)
13	FM	0.89	0/885	1.04	2/1188 (0.2%)
14	AN	0.90	2/1148 (0.2%)	1.06	1/1546 (0.1%)
14	BN	0.88	2/1151 (0.2%)	1.06	2/1552 (0.1%)
14	CN	0.96	2/1159 (0.2%)	1.12	2/1563 (0.1%)
14	DN	0.95	1/1167 (0.1%)	1.19	7/1574 (0.4%)
14	EN	0.99	2/1161 (0.2%)	1.17	9/1566 (0.6%)
14	FN	0.99	2/1167 (0.2%)	1.20	6/1574 (0.4%)
All	All	0.83	99/208122 (0.0%)	1.05	648/281066 (0.2%)

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	EA	0	1

The worst 5 of 99 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	FH	76	THR	CA-C	12.85	1.60	1.53
1	EA	75	HIS	CD2-NE2	11.71	1.50	1.37
8	FH	76	THR	N-CA	11.10	1.53	1.46
1	FA	1013	THR	CA-CB	10.15	1.65	1.52
1	EA	75	HIS	CG-CD2	9.99	1.46	1.35

The worst 5 of 648 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	FN	38	PHE	CA-C-N	12.24	135.15	119.84
14	FN	38	PHE	C-N-CA	12.24	135.15	119.84
8	FH	76	THR	N-CA-C	10.57	117.45	108.78
2	EB	571	ALA	CA-C-N	10.46	130.56	119.89
2	EB	571	ALA	C-N-CA	10.46	130.56	119.89

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	EA	75	HIS	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	AA	11703	0	11787	788	0
1	BA	11540	0	11624	746	0
1	CA	11695	0	11780	843	0
1	DA	11697	0	11775	853	0
1	EA	11706	0	11788	831	0
1	FA	11709	0	11790	849	0
2	AB	9187	0	9100	624	0
2	BB	9175	0	9074	606	0
2	CB	9304	0	9216	663	0
2	DB	9269	0	9175	684	0
2	EB	9265	0	9179	673	0
2	FB	9270	0	9180	685	0
3	AC	2413	0	2404	172	0
3	BC	2413	0	2404	154	0
3	CC	2413	0	2404	190	0
3	DC	2413	0	2404	184	0
3	EC	2413	0	2404	174	0
3	FC	2413	0	2404	180	0
4	AD	459	0	462	25	0
4	BD	459	0	462	33	0
4	CD	459	0	462	27	0
4	DD	459	0	462	26	0
4	ED	459	0	462	30	0
4	FD	459	0	462	32	0
5	AE	1760	0	1788	89	0
5	BE	1760	0	1788	89	0
5	CE	1760	0	1788	97	0
5	DE	1760	0	1788	104	0
5	EE	1760	0	1788	89	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	FE	1760	0	1788	112	0
6	AF	807	0	827	45	0
6	BF	807	0	827	44	0
6	CF	816	0	833	41	0
6	DF	816	0	833	40	0
6	EF	816	0	833	44	0
6	FF	816	0	833	39	0
7	AG	1599	0	1602	116	0
7	AO	413	0	389	49	0
7	BG	1539	0	1552	112	0
7	BO	404	0	383	46	0
7	CG	1599	0	1602	111	0
7	CO	398	0	378	42	0
7	DG	1599	0	1602	123	0
7	DO	413	0	389	36	0
7	EG	1599	0	1602	121	0
7	EO	413	0	389	49	0
7	FG	1599	0	1602	116	0
7	FO	413	0	389	38	0
8	AH	1063	0	1034	61	0
8	BH	1052	0	1021	62	0
8	CH	1052	0	1021	73	0
8	DH	1075	0	1046	72	0
8	EH	1075	0	1046	67	0
8	FH	1075	0	1046	65	0
9	AI	943	0	929	65	0
9	BI	716	0	709	40	0
9	CI	943	0	929	67	0
9	DI	943	0	929	65	0
9	EI	898	0	880	58	0
9	FI	943	0	929	66	0
10	AJ	558	0	572	43	0
10	BJ	569	0	585	38	0
10	CJ	558	0	572	47	0
10	DJ	569	0	585	40	0
10	EJ	558	0	572	36	0
10	FJ	558	0	572	40	0
11	AK	793	0	790	42	0
11	BK	786	0	782	42	0
11	CK	793	0	790	47	0
11	DK	793	0	790	52	0
11	EK	786	0	782	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	FK	786	0	782	49	0
12	AL	352	0	374	48	0
12	BL	352	0	374	26	0
12	CL	352	0	374	44	0
12	DL	352	0	374	42	0
12	EL	352	0	374	35	0
12	FL	352	0	374	45	0
13	AM	863	0	864	62	0
13	BM	863	0	864	78	0
13	CM	863	0	864	61	0
13	DM	863	0	864	59	0
13	EM	869	0	869	70	0
13	FM	869	0	869	73	0
14	AN	1127	0	1133	88	0
14	BN	1130	0	1138	83	0
14	CN	1137	0	1148	87	0
14	DN	1146	0	1153	79	0
14	EN	1140	0	1150	80	0
14	FN	1146	0	1155	80	0
15	AA	2	0	0	0	0
15	AB	1	0	0	0	0
15	AI	2	0	0	0	0
15	AJ	1	0	0	0	0
15	AL	1	0	0	0	0
15	BA	2	0	0	0	0
15	BB	1	0	0	0	0
15	BI	2	0	0	0	0
15	BJ	1	0	0	0	0
15	BL	1	0	0	0	0
15	CA	2	0	0	0	0
15	CB	1	0	0	0	0
15	CI	2	0	0	0	0
15	CJ	1	0	0	0	0
15	CL	1	0	0	0	0
15	DA	2	0	0	0	0
15	DB	1	0	0	0	0
15	DI	2	0	0	0	0
15	DJ	1	0	0	0	0
15	DL	1	0	0	0	0
15	EA	2	0	0	0	0
15	EB	1	0	0	0	0
15	EI	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	EJ	1	0	0	0	0
15	EL	1	0	0	0	0
15	FA	2	0	0	0	0
15	FB	1	0	0	0	0
15	FI	2	0	0	0	0
15	FJ	1	0	0	0	0
15	FL	1	0	0	0	0
All	All	204233	0	204265	12684	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 31.

The worst 5 of 12684 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)
7:FG:11:ARG:HG2	7:FG:11:ARG:HH11	1.10	1.15
7:DG:11:ARG:HH11	7:DG:11:ARG:HG3	1.13	1.11
7:AG:11:ARG:HH11	7:AG:11:ARG:HG3	1.14	1.10
7:EG:11:ARG:HH11	7:EG:11:ARG:HG2	1.13	1.10
7:CG:11:ARG:HG3	7:CG:11:ARG:HH11	1.11	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	AA	1470/1664 (88%)	1124 (76%)	276 (19%)	70 (5%)	2 16
1	BA	1448/1664 (87%)	1124 (78%)	259 (18%)	65 (4%)	2 16
1	CA	1469/1664 (88%)	1131 (77%)	268 (18%)	70 (5%)	2 16
1	DA	1469/1664 (88%)	1138 (78%)	263 (18%)	68 (5%)	2 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	EA	1468/1664 (88%)	1127 (77%)	272 (18%)	69 (5%)	2	16
1	FA	1470/1664 (88%)	1127 (77%)	274 (19%)	69 (5%)	2	16
2	AB	1142/1203 (95%)	926 (81%)	158 (14%)	58 (5%)	1	14
2	BB	1141/1203 (95%)	923 (81%)	164 (14%)	54 (5%)	2	16
2	CB	1160/1203 (96%)	921 (79%)	171 (15%)	68 (6%)	1	12
2	DB	1155/1203 (96%)	923 (80%)	172 (15%)	60 (5%)	1	14
2	EB	1154/1203 (96%)	928 (80%)	165 (14%)	61 (5%)	1	14
2	FB	1155/1203 (96%)	925 (80%)	165 (14%)	65 (6%)	1	14
3	AC	302/335 (90%)	231 (76%)	53 (18%)	18 (6%)	1	12
3	BC	302/335 (90%)	232 (77%)	53 (18%)	17 (6%)	1	14
3	CC	302/335 (90%)	234 (78%)	52 (17%)	16 (5%)	1	14
3	DC	302/335 (90%)	233 (77%)	51 (17%)	18 (6%)	1	12
3	EC	302/335 (90%)	233 (77%)	52 (17%)	17 (6%)	1	14
3	FC	302/335 (90%)	233 (77%)	51 (17%)	18 (6%)	1	12
4	AD	54/137 (39%)	49 (91%)	5 (9%)	0	100	100
4	BD	54/137 (39%)	50 (93%)	4 (7%)	0	100	100
4	CD	54/137 (39%)	49 (91%)	5 (9%)	0	100	100
4	DD	54/137 (39%)	50 (93%)	4 (7%)	0	100	100
4	ED	54/137 (39%)	50 (93%)	3 (6%)	1 (2%)	6	31
4	FD	54/137 (39%)	49 (91%)	4 (7%)	1 (2%)	6	31
5	AE	213/215 (99%)	176 (83%)	31 (15%)	6 (3%)	4	24
5	BE	213/215 (99%)	174 (82%)	32 (15%)	7 (3%)	3	20
5	CE	213/215 (99%)	174 (82%)	33 (16%)	6 (3%)	4	24
5	DE	213/215 (99%)	176 (83%)	31 (15%)	6 (3%)	4	24
5	EE	213/215 (99%)	175 (82%)	32 (15%)	6 (3%)	4	24
5	FE	213/215 (99%)	174 (82%)	33 (16%)	6 (3%)	4	24
6	AF	96/155 (62%)	85 (88%)	10 (10%)	1 (1%)	12	48
6	BF	96/155 (62%)	87 (91%)	8 (8%)	1 (1%)	12	48
6	CF	97/155 (63%)	87 (90%)	9 (9%)	1 (1%)	12	48
6	DF	97/155 (63%)	85 (88%)	11 (11%)	1 (1%)	12	48
6	EF	97/155 (63%)	88 (91%)	8 (8%)	1 (1%)	12	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	FF	97/155 (63%)	88 (91%)	7 (7%)	2 (2%)	5	29
7	AG	198/326 (61%)	143 (72%)	40 (20%)	15 (8%)	1	9
7	AO	50/326 (15%)	31 (62%)	11 (22%)	8 (16%)	0	2
7	BG	191/326 (59%)	139 (73%)	37 (19%)	15 (8%)	1	9
7	BO	49/326 (15%)	33 (67%)	11 (22%)	5 (10%)	0	6
7	CG	198/326 (61%)	145 (73%)	38 (19%)	15 (8%)	1	9
7	CO	48/326 (15%)	32 (67%)	10 (21%)	6 (12%)	0	4
7	DG	198/326 (61%)	142 (72%)	38 (19%)	18 (9%)	0	8
7	DO	50/326 (15%)	31 (62%)	12 (24%)	7 (14%)	0	3
7	EG	198/326 (61%)	144 (73%)	40 (20%)	14 (7%)	1	10
7	EO	50/326 (15%)	30 (60%)	13 (26%)	7 (14%)	0	3
7	FG	198/326 (61%)	141 (71%)	40 (20%)	17 (9%)	0	8
7	FO	50/326 (15%)	34 (68%)	13 (26%)	3 (6%)	1	12
8	AH	128/146 (88%)	106 (83%)	19 (15%)	3 (2%)	5	27
8	BH	127/146 (87%)	105 (83%)	17 (13%)	5 (4%)	2	18
8	CH	127/146 (87%)	106 (84%)	18 (14%)	3 (2%)	4	26
8	DH	130/146 (89%)	104 (80%)	20 (15%)	6 (5%)	2	16
8	EH	130/146 (89%)	106 (82%)	17 (13%)	7 (5%)	1	14
8	FH	130/146 (89%)	106 (82%)	19 (15%)	5 (4%)	2	19
9	AI	122/125 (98%)	91 (75%)	28 (23%)	3 (2%)	4	25
9	BI	91/125 (73%)	70 (77%)	19 (21%)	2 (2%)	5	28
9	CI	122/125 (98%)	93 (76%)	25 (20%)	4 (3%)	3	20
9	DI	122/125 (98%)	93 (76%)	26 (21%)	3 (2%)	4	25
9	EI	113/125 (90%)	85 (75%)	25 (22%)	3 (3%)	4	25
9	FI	122/125 (98%)	92 (75%)	25 (20%)	5 (4%)	2	17
10	AJ	66/70 (94%)	45 (68%)	16 (24%)	5 (8%)	1	9
10	BJ	67/70 (96%)	45 (67%)	18 (27%)	4 (6%)	1	12
10	CJ	66/70 (94%)	47 (71%)	15 (23%)	4 (6%)	1	12
10	DJ	67/70 (96%)	47 (70%)	16 (24%)	4 (6%)	1	12
10	EJ	66/70 (94%)	47 (71%)	15 (23%)	4 (6%)	1	12
10	FJ	66/70 (94%)	47 (71%)	16 (24%)	3 (4%)	2	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	AK	99/142 (70%)	79 (80%)	17 (17%)	3 (3%)	3	22
11	BK	98/142 (69%)	80 (82%)	15 (15%)	3 (3%)	3	21
11	CK	99/142 (70%)	85 (86%)	11 (11%)	3 (3%)	3	22
11	DK	99/142 (70%)	81 (82%)	14 (14%)	4 (4%)	2	18
11	EK	98/142 (69%)	80 (82%)	14 (14%)	4 (4%)	2	17
11	FK	98/142 (69%)	82 (84%)	13 (13%)	3 (3%)	3	21
12	AL	42/70 (60%)	34 (81%)	5 (12%)	3 (7%)	1	10
12	BL	42/70 (60%)	33 (79%)	6 (14%)	3 (7%)	1	10
12	CL	42/70 (60%)	33 (79%)	6 (14%)	3 (7%)	1	10
12	DL	42/70 (60%)	33 (79%)	6 (14%)	3 (7%)	1	10
12	EL	42/70 (60%)	33 (79%)	6 (14%)	3 (7%)	1	10
12	FL	42/70 (60%)	34 (81%)	5 (12%)	3 (7%)	1	10
13	AM	107/415 (26%)	81 (76%)	17 (16%)	9 (8%)	0	8
13	BM	107/415 (26%)	81 (76%)	17 (16%)	9 (8%)	0	8
13	CM	107/415 (26%)	79 (74%)	19 (18%)	9 (8%)	0	8
13	DM	107/415 (26%)	82 (77%)	15 (14%)	10 (9%)	0	8
13	EM	108/415 (26%)	80 (74%)	18 (17%)	10 (9%)	0	8
13	FM	108/415 (26%)	80 (74%)	18 (17%)	10 (9%)	0	8
14	AN	136/233 (58%)	106 (78%)	17 (12%)	13 (10%)	0	7
14	BN	137/233 (59%)	110 (80%)	16 (12%)	11 (8%)	1	9
14	CN	137/233 (59%)	109 (80%)	17 (12%)	11 (8%)	1	9
14	DN	139/233 (60%)	112 (81%)	16 (12%)	11 (8%)	1	9
14	EN	138/233 (59%)	111 (80%)	15 (11%)	12 (9%)	0	8
14	FN	139/233 (60%)	112 (81%)	15 (11%)	12 (9%)	0	8
All	All	25348/33372 (76%)	19889 (78%)	4164 (16%)	1295 (5%)	1	14

5 of 1295 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AA	39	ASP
1	AA	547	ILE
1	AA	551	VAL
1	AA	710	SER
1	AA	851	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	
1	AA	1310/1465 (89%)	993 (76%)	317 (24%)	1	5
1	BA	1290/1465 (88%)	978 (76%)	312 (24%)	1	5
1	CA	1308/1465 (89%)	990 (76%)	318 (24%)	1	4
1	DA	1309/1465 (89%)	983 (75%)	326 (25%)	0	4
1	EA	1309/1465 (89%)	986 (75%)	323 (25%)	1	4
1	FA	1309/1465 (89%)	990 (76%)	319 (24%)	1	4
2	AB	1012/1053 (96%)	758 (75%)	254 (25%)	0	4
2	BB	1010/1053 (96%)	758 (75%)	252 (25%)	0	4
2	CB	1024/1053 (97%)	758 (74%)	266 (26%)	0	4
2	DB	1020/1053 (97%)	763 (75%)	257 (25%)	0	4
2	EB	1021/1053 (97%)	766 (75%)	255 (25%)	0	4
2	FB	1021/1053 (97%)	757 (74%)	264 (26%)	0	4
3	AC	268/296 (90%)	212 (79%)	56 (21%)	1	7
3	BC	268/296 (90%)	212 (79%)	56 (21%)	1	7
3	CC	268/296 (90%)	215 (80%)	53 (20%)	1	8
3	DC	268/296 (90%)	213 (80%)	55 (20%)	1	7
3	EC	268/296 (90%)	212 (79%)	56 (21%)	1	7
3	FC	268/296 (90%)	212 (79%)	56 (21%)	1	7
4	AD	55/116 (47%)	45 (82%)	10 (18%)	2	9
4	BD	55/116 (47%)	46 (84%)	9 (16%)	2	11
4	CD	55/116 (47%)	46 (84%)	9 (16%)	2	11
4	DD	55/116 (47%)	45 (82%)	10 (18%)	2	9
4	ED	55/116 (47%)	45 (82%)	10 (18%)	2	9
4	FD	55/116 (47%)	46 (84%)	9 (16%)	2	11
5	AE	197/197 (100%)	154 (78%)	43 (22%)	1	6
5	BE	197/197 (100%)	155 (79%)	42 (21%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	CE	197/197 (100%)	152 (77%)	45 (23%)	1	6
5	DE	197/197 (100%)	152 (77%)	45 (23%)	1	6
5	EE	197/197 (100%)	155 (79%)	42 (21%)	1	6
5	FE	197/197 (100%)	153 (78%)	44 (22%)	1	6
6	AF	88/137 (64%)	73 (83%)	15 (17%)	2	10
6	BF	88/137 (64%)	73 (83%)	15 (17%)	2	10
6	CF	89/137 (65%)	72 (81%)	17 (19%)	1	8
6	DF	89/137 (65%)	73 (82%)	16 (18%)	2	9
6	EF	89/137 (65%)	73 (82%)	16 (18%)	2	9
6	FF	89/137 (65%)	73 (82%)	16 (18%)	2	9
7	AG	180/291 (62%)	126 (70%)	54 (30%)	0	2
7	AO	50/291 (17%)	28 (56%)	22 (44%)	0	0
7	BG	173/291 (60%)	123 (71%)	50 (29%)	0	2
7	BO	49/291 (17%)	32 (65%)	17 (35%)	0	1
7	CG	180/291 (62%)	122 (68%)	58 (32%)	0	2
7	CO	48/291 (16%)	30 (62%)	18 (38%)	0	1
7	DG	180/291 (62%)	123 (68%)	57 (32%)	0	2
7	DO	50/291 (17%)	29 (58%)	21 (42%)	0	0
7	EG	180/291 (62%)	125 (69%)	55 (31%)	0	2
7	EO	50/291 (17%)	33 (66%)	17 (34%)	0	1
7	FG	180/291 (62%)	122 (68%)	58 (32%)	0	2
7	FO	50/291 (17%)	34 (68%)	16 (32%)	0	2
8	AH	116/128 (91%)	83 (72%)	33 (28%)	0	3
8	BH	115/128 (90%)	82 (71%)	33 (29%)	0	3
8	CH	115/128 (90%)	79 (69%)	36 (31%)	0	2
8	DH	117/128 (91%)	81 (69%)	36 (31%)	0	2
8	EH	117/128 (91%)	84 (72%)	33 (28%)	0	3
8	FH	117/128 (91%)	83 (71%)	34 (29%)	0	2
9	AI	109/110 (99%)	84 (77%)	25 (23%)	1	6
9	BI	86/110 (78%)	69 (80%)	17 (20%)	1	8
9	CI	109/110 (99%)	82 (75%)	27 (25%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	DI	109/110 (99%)	82 (75%)	27 (25%)	1	4
9	EI	104/110 (94%)	78 (75%)	26 (25%)	0	4
9	FI	109/110 (99%)	84 (77%)	25 (23%)	1	6
10	AJ	63/65 (97%)	46 (73%)	17 (27%)	0	3
10	BJ	64/65 (98%)	49 (77%)	15 (23%)	1	5
10	CJ	63/65 (97%)	46 (73%)	17 (27%)	0	3
10	DJ	64/65 (98%)	47 (73%)	17 (27%)	0	3
10	EJ	63/65 (97%)	45 (71%)	18 (29%)	0	3
10	FJ	63/65 (97%)	45 (71%)	18 (29%)	0	3
11	AK	91/130 (70%)	64 (70%)	27 (30%)	0	2
11	BK	90/130 (69%)	63 (70%)	27 (30%)	0	2
11	CK	91/130 (70%)	66 (72%)	25 (28%)	0	3
11	DK	91/130 (70%)	64 (70%)	27 (30%)	0	2
11	EK	90/130 (69%)	64 (71%)	26 (29%)	0	2
11	FK	90/130 (69%)	63 (70%)	27 (30%)	0	2
12	AL	39/57 (68%)	26 (67%)	13 (33%)	0	2
12	BL	39/57 (68%)	26 (67%)	13 (33%)	0	2
12	CL	39/57 (68%)	26 (67%)	13 (33%)	0	2
12	DL	39/57 (68%)	26 (67%)	13 (33%)	0	2
12	EL	39/57 (68%)	26 (67%)	13 (33%)	0	2
12	FL	39/57 (68%)	26 (67%)	13 (33%)	0	2
13	AM	99/371 (27%)	71 (72%)	28 (28%)	0	3
13	BM	99/371 (27%)	70 (71%)	29 (29%)	0	2
13	CM	99/371 (27%)	72 (73%)	27 (27%)	0	3
13	DM	99/371 (27%)	74 (75%)	25 (25%)	0	4
13	EM	100/371 (27%)	72 (72%)	28 (28%)	0	3
13	FM	100/371 (27%)	71 (71%)	29 (29%)	0	2
14	AN	132/220 (60%)	89 (67%)	43 (33%)	0	2
14	BN	133/220 (60%)	93 (70%)	40 (30%)	0	2
14	CN	133/220 (60%)	91 (68%)	42 (32%)	0	2
14	DN	135/220 (61%)	92 (68%)	43 (32%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	EN	134/220 (61%)	92 (69%)	42 (31%)	0	2
14	FN	135/220 (61%)	94 (70%)	41 (30%)	0	2
All	All	22843/29562 (77%)	17084 (75%)	5759 (25%)	0	4

5 of 5759 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	DK	62	SER
7	EG	250	ILE
7	DO	276	LYS
11	DK	45	GLU
2	EB	57	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 590 such sidechains are listed below:

Mol	Chain	Res	Type
3	EC	323	ASN
8	FH	52	GLN
7	EG	119	HIS
3	EC	301	ASN
1	FA	1447	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 42 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	EA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	EA	1261:VAL	C	1262:LEU	N	2.28

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	AA	1484/1664 (89%)	-0.32	8 (0%) 87 77	174, 197, 249, 308	0
1	BA	1462/1664 (87%)	-0.19	10 (0%) 84 73	242, 262, 287, 314	0
1	CA	1483/1664 (89%)	-0.36	2 (0%) 92 87	143, 164, 201, 253	0
1	DA	1483/1664 (89%)	-0.30	8 (0%) 87 77	147, 170, 215, 278	0
1	EA	1484/1664 (89%)	-0.34	7 (0%) 87 77	149, 171, 207, 250	0
1	FA	1484/1664 (89%)	-0.36	4 (0%) 90 81	142, 160, 203, 262	0
2	AB	1154/1203 (95%)	-0.30	2 (0%) 91 84	179, 212, 250, 276	0
2	BB	1153/1203 (95%)	-0.26	3 (0%) 90 81	233, 245, 265, 279	0
2	CB	1170/1203 (97%)	-0.35	3 (0%) 90 81	144, 169, 196, 227	0
2	DB	1165/1203 (96%)	-0.34	1 (0%) 92 87	148, 169, 191, 222	0
2	EB	1164/1203 (96%)	-0.35	2 (0%) 91 84	148, 162, 188, 225	0
2	FB	1165/1203 (96%)	-0.34	1 (0%) 92 87	142, 164, 191, 212	0
3	AC	304/335 (90%)	-0.39	1 (0%) 90 81	190, 209, 237, 253	0
3	BC	304/335 (90%)	-0.19	0 100 100	248, 278, 311, 332	0
3	CC	304/335 (90%)	-0.31	0 100 100	162, 175, 191, 207	0
3	DC	304/335 (90%)	-0.31	2 (0%) 84 73	167, 182, 197, 206	0
3	EC	304/335 (90%)	-0.38	3 (0%) 79 67	158, 173, 190, 203	0
3	FC	304/335 (90%)	-0.33	0 100 100	154, 170, 187, 198	0
4	AD	58/137 (42%)	-0.17	0 100 100	207, 243, 266, 270	0
4	BD	58/137 (42%)	-0.19	1 (1%) 69 58	262, 281, 301, 303	0
4	CD	58/137 (42%)	-0.25	0 100 100	171, 184, 195, 200	0
4	DD	58/137 (42%)	-0.34	0 100 100	177, 190, 204, 207	0
4	ED	58/137 (42%)	-0.37	0 100 100	185, 202, 214, 215	0
4	FD	58/137 (42%)	-0.35	0 100 100	162, 186, 211, 212	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
5	AE	215/215 (100%)	-0.35	2 (0%) 81 69	186, 214, 234, 243	0
5	BE	215/215 (100%)	-0.20	2 (0%) 81 69	255, 281, 296, 307	0
5	CE	215/215 (100%)	-0.40	0 100 100	152, 178, 194, 206	0
5	DE	215/215 (100%)	-0.32	0 100 100	156, 187, 209, 222	0
5	EE	215/215 (100%)	-0.34	0 100 100	158, 189, 211, 228	0
5	FE	215/215 (100%)	-0.34	0 100 100	149, 179, 199, 212	0
6	AF	98/155 (63%)	-0.35	0 100 100	181, 190, 240, 243	0
6	BF	98/155 (63%)	-0.10	1 (1%) 79 67	251, 265, 299, 302	0
6	CF	99/155 (63%)	-0.37	0 100 100	148, 157, 185, 188	0
6	DF	99/155 (63%)	-0.32	0 100 100	152, 162, 201, 207	0
6	EF	99/155 (63%)	-0.32	0 100 100	154, 168, 211, 214	0
6	FF	99/155 (63%)	-0.29	0 100 100	144, 152, 209, 213	0
7	AG	202/326 (61%)	-0.23	1 (0%) 87 77	199, 249, 286, 305	0
7	AO	52/326 (15%)	-0.31	0 100 100	209, 235, 287, 294	0
7	BG	195/326 (59%)	-0.27	0 100 100	259, 290, 311, 319	0
7	BO	51/326 (15%)	-0.43	0 100 100	244, 259, 301, 312	0
7	CG	202/326 (61%)	-0.34	2 (0%) 79 67	171, 186, 215, 221	0
7	CO	50/326 (15%)	-0.42	0 100 100	159, 187, 235, 247	0
7	DG	202/326 (61%)	-0.24	0 100 100	165, 205, 241, 251	0
7	DO	52/326 (15%)	-0.31	0 100 100	167, 197, 258, 276	0
7	EG	202/326 (61%)	-0.28	2 (0%) 79 67	181, 209, 227, 234	0
7	EO	52/326 (15%)	-0.31	0 100 100	168, 190, 233, 246	0
7	FG	202/326 (61%)	-0.22	2 (0%) 79 67	158, 197, 226, 232	0
7	FO	52/326 (15%)	-0.43	0 100 100	163, 191, 241, 257	0
8	AH	132/146 (90%)	-0.31	0 100 100	180, 190, 197, 206	0
8	BH	131/146 (89%)	-0.23	0 100 100	282, 313, 328, 335	0
8	CH	131/146 (89%)	-0.37	1 (0%) 82 71	162, 175, 183, 187	0
8	DH	134/146 (91%)	-0.30	1 (0%) 84 73	167, 182, 196, 231	0
8	EH	134/146 (91%)	-0.36	0 100 100	164, 185, 201, 209	0
8	FH	134/146 (91%)	-0.32	1 (0%) 84 73	151, 162, 173, 203	0
9	AI	124/125 (99%)	-0.17	1 (0%) 82 71	189, 209, 254, 260	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
9	BI	97/125 (77%)	-0.14	1 (1%) 79 67	254, 264, 300, 307	0
9	CI	124/125 (99%)	-0.42	0 100 100	162, 179, 201, 206	0
9	DI	124/125 (99%)	-0.27	0 100 100	166, 187, 207, 214	0
9	EI	117/125 (93%)	-0.25	0 100 100	160, 177, 203, 235	0
9	FI	124/125 (99%)	-0.24	0 100 100	159, 181, 203, 211	0
10	AJ	68/70 (97%)	-0.18	0 100 100	194, 209, 227, 240	0
10	BJ	69/70 (98%)	-0.11	1 (1%) 73 61	245, 263, 275, 279	0
10	CJ	68/70 (97%)	-0.41	0 100 100	162, 172, 183, 195	0
10	DJ	69/70 (98%)	-0.28	1 (1%) 73 61	164, 174, 184, 191	0
10	EJ	68/70 (97%)	-0.35	1 (1%) 72 59	155, 165, 177, 180	0
10	FJ	68/70 (97%)	-0.33	0 100 100	155, 165, 179, 186	0
11	AK	101/142 (71%)	-0.43	0 100 100	186, 193, 213, 220	0
11	BK	100/142 (70%)	-0.35	0 100 100	259, 288, 305, 311	0
11	CK	101/142 (71%)	-0.42	0 100 100	157, 168, 182, 190	0
11	DK	101/142 (71%)	-0.37	0 100 100	161, 175, 190, 197	0
11	EK	100/142 (70%)	-0.49	0 100 100	154, 168, 182, 190	0
11	FK	100/142 (70%)	-0.41	0 100 100	150, 159, 174, 180	0
12	AL	44/70 (62%)	-0.44	0 100 100	201, 238, 253, 256	0
12	BL	44/70 (62%)	-0.16	0 100 100	241, 248, 255, 256	0
12	CL	44/70 (62%)	-0.35	0 100 100	163, 184, 192, 193	0
12	DL	44/70 (62%)	-0.38	0 100 100	167, 184, 191, 195	0
12	EL	44/70 (62%)	-0.42	0 100 100	158, 176, 188, 191	0
12	FL	44/70 (62%)	-0.46	0 100 100	159, 183, 193, 196	0
13	AM	109/415 (26%)	-0.32	0 100 100	228, 248, 259, 263	0
13	BM	109/415 (26%)	-0.32	0 100 100	247, 257, 278, 284	0
13	CM	109/415 (26%)	-0.37	0 100 100	181, 196, 202, 205	0
13	DM	109/415 (26%)	-0.29	1 (0%) 81 69	181, 197, 211, 218	0
13	EM	110/415 (26%)	-0.38	0 100 100	173, 189, 198, 203	0
13	FM	110/415 (26%)	-0.44	1 (0%) 81 69	177, 191, 198, 200	0
14	AN	142/233 (60%)	-0.13	0 100 100	194, 234, 266, 270	0
14	BN	143/233 (61%)	-0.12	3 (2%) 63 53	254, 266, 283, 297	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
14	CN	143/233 (61%)	-0.37	0 100 100	166, 187, 208, 219	0
14	DN	145/233 (62%)	-0.24	1 (0%) 84 73	167, 197, 213, 220	0
14	EN	144/233 (61%)	-0.25	1 (0%) 84 73	160, 184, 203, 214	0
14	FN	145/233 (62%)	-0.23	1 (0%) 84 73	157, 184, 204, 214	0
All	All	25720/33372 (77%)	-0.31	86 (0%) 90 81	142, 184, 273, 335	0

The worst 5 of 86 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BA	1489	VAL	4.5
5	AE	30	ILE	4.3
14	BN	64	ILE	3.8
3	EC	74	GLU	3.5
2	BB	1192	MET	3.3

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	ZN	BI	3002	1/1	0.93	0.11	311,311,311,311	0
15	ZN	DI	3002	1/1	0.97	0.04	195,195,195,195	0
15	ZN	BA	3001	1/1	0.98	0.05	248,248,248,248	0
15	ZN	BA	3002	1/1	0.98	0.04	283,283,283,283	0
15	ZN	AA	3001	1/1	0.98	0.05	222,222,222,222	0
15	ZN	AI	3001	1/1	0.98	0.04	247,247,247,247	0
15	ZN	EA	3002	1/1	0.98	0.03	215,215,215,215	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	ZN	EB	3001	1/1	0.98	0.05	169,169,169,169	0
15	ZN	FA	3001	1/1	0.98	0.06	178,178,178,178	0
15	ZN	FL	3001	1/1	0.98	0.04	184,184,184,184	0
15	ZN	AI	3002	1/1	0.99	0.03	213,213,213,213	0
15	ZN	BJ	3001	1/1	0.99	0.03	267,267,267,267	0
15	ZN	BL	3001	1/1	0.99	0.03	245,245,245,245	0
15	ZN	CA	3001	1/1	0.99	0.04	168,168,168,168	0
15	ZN	CA	3002	1/1	0.99	0.03	205,205,205,205	0
15	ZN	CB	3001	1/1	0.99	0.03	167,167,167,167	0
15	ZN	CI	3001	1/1	0.99	0.04	194,194,194,194	0
15	ZN	CI	3002	1/1	0.99	0.05	195,195,195,195	0
15	ZN	CL	3001	1/1	0.99	0.05	185,185,185,185	0
15	ZN	DA	3001	1/1	0.99	0.04	177,177,177,177	0
15	ZN	DA	3002	1/1	0.99	0.02	211,211,211,211	0
15	ZN	AJ	3001	1/1	0.99	0.06	197,197,197,197	0
15	ZN	EA	3001	1/1	0.99	0.08	171,171,171,171	0
15	ZN	AL	3001	1/1	0.99	0.04	241,241,241,241	0
15	ZN	AB	3001	1/1	0.99	0.04	214,214,214,214	0
15	ZN	EI	3001	1/1	0.99	0.05	187,187,187,187	0
15	ZN	EI	3002	1/1	0.99	0.03	198,198,198,198	0
15	ZN	EL	3001	1/1	0.99	0.06	176,176,176,176	0
15	ZN	AA	3002	1/1	0.99	0.03	262,262,262,262	0
15	ZN	FA	3002	1/1	0.99	0.02	202,202,202,202	0
15	ZN	FI	3002	1/1	0.99	0.03	190,190,190,190	0
15	ZN	BI	3001	1/1	0.99	0.06	257,257,257,257	0
15	ZN	DJ	3001	1/1	1.00	0.04	167,167,167,167	0
15	ZN	EJ	3001	1/1	1.00	0.02	159,159,159,159	0
15	ZN	DL	3001	1/1	1.00	0.03	184,184,184,184	0
15	ZN	BB	3001	1/1	1.00	0.04	252,252,252,252	0
15	ZN	DB	3001	1/1	1.00	0.07	172,172,172,172	0
15	ZN	FB	3001	1/1	1.00	0.06	163,163,163,163	0
15	ZN	FI	3001	1/1	1.00	0.05	189,189,189,189	0
15	ZN	DI	3001	1/1	1.00	0.04	195,195,195,195	0
15	ZN	FJ	3001	1/1	1.00	0.02	157,157,157,157	0
15	ZN	CJ	3001	1/1	1.00	0.06	164,164,164,164	0

6.5 Other polymers [i](#)

There are no such residues in this entry.