



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 08:52 am BST

PDB ID : 5W1S
Title : X-ray crystal structure of Escherichia coli RNA polymerase and TraR complex
Authors : Murakami, K.S.; Molodtsov, V.
Deposited on : 2017-06-04
Resolution : 3.81 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

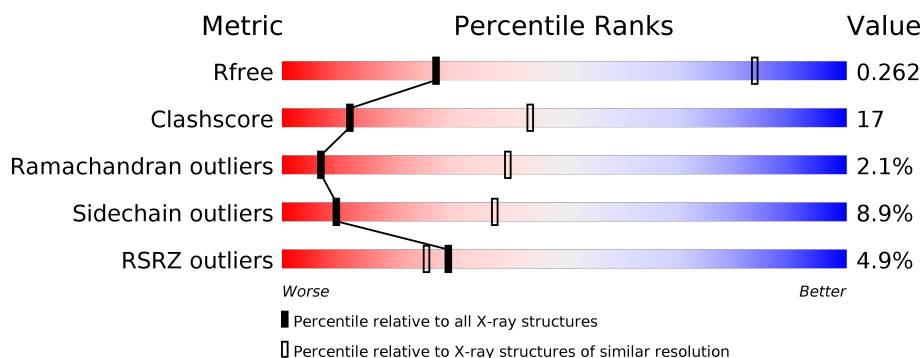
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.81 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	A	329	<div> <div>2%</div> <div> <div>45%</div> <div>41%</div> <div>10%</div> <div>••</div> </div> </div>
1	B	329	<div> <div>3%</div> <div> <div>40%</div> <div>24%</div> <div>•</div> <div>34%</div> </div> </div>
1	G	329	<div> <div>2%</div> <div> <div>37%</div> <div>27%</div> <div>•</div> <div>31%</div> </div> </div>
1	H	329	<div> <div>6%</div> <div> <div>42%</div> <div>22%</div> <div>•</div> <div>34%</div> </div> </div>
2	C	1342	<div> <div>6%</div> <div> <div>57%</div> <div>38%</div> <div>•</div> </div> </div>
2	I	1342	<div> <div>8%</div> <div> <div>62%</div> <div>34%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	D	1407	<div><div><div></div><div></div><div></div><div></div></div><div>%</div><div>48%</div><div>31%</div><div>•</div><div>17%</div></div>
3	J	1407	<div><div><div></div><div></div><div></div><div></div></div><div>2%</div><div>47%</div><div>30%</div><div>•</div><div>18%</div></div>
4	E	91	<div><div><div></div><div></div><div></div><div></div></div><div>%</div><div>63%</div><div>25%</div><div></div><div>10%</div><div>•</div></div>
4	K	91	<div><div><div></div><div></div><div></div><div></div></div><div>18%</div><div>48%</div><div>30%</div><div>•</div><div>21%</div></div>
5	F	613	<div><div><div></div><div></div><div></div><div></div></div><div>4%</div><div>48%</div><div>26%</div><div>•</div><div>24%</div></div>
5	L	613	<div><div><div></div><div></div><div></div><div></div></div><div>3%</div><div>49%</div><div>25%</div><div>•</div><div>23%</div></div>
6	M	79	<div><div><div></div><div></div><div></div><div></div></div><div>4%</div><div>49%</div><div>33%</div><div>5%</div><div>•</div><div>11%</div></div>
6	N	79	<div><div><div></div><div></div><div></div><div></div></div><div>14%</div><div>42%</div><div>39%</div><div>6%</div><div>13%</div></div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 56825 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 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2490	1557	439	486	8			
1	B	217	Total	C	N	O	S	0	0	0
			1677	1047	295	329	6			
1	G	227	Total	C	N	O	S	0	0	0
			1755	1093	311	345	6			
1	H	216	Total	C	N	O	S	0	0	0
			1662	1038	292	326	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0	0
			10564	6628	1838	2055	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10566	6629	1840	2054	43			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1173	Total	C	N	O	S	0	0	0
			9095	5718	1628	1703	46			
3	J	1155	Total	C	N	O	S	0	0	0
			9001	5659	1612	1684	46			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	89	Total	C	N	O	S	0	0	0
			691	421	129	140	1			
4	K	72	Total	C	N	O	S	0	0	0
			573	350	110	112	1			

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	468	Total	C	N	O	S	0	0	0
			3813	2389	678	723	23			
5	L	469	Total	C	N	O	S	0	0	0
			3821	2393	679	726	23			

- Molecule 6 is a protein called Protein TraR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	M	70	Total	C	N	O	S	0	0	0
			557	346	103	103	5			
6	N	69	Total	C	N	O	S	0	0	0
			552	343	102	102	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	74	HIS	-	expression tag	UNP P41065
M	75	HIS	-	expression tag	UNP P41065
M	76	HIS	-	expression tag	UNP P41065
M	77	HIS	-	expression tag	UNP P41065
M	78	HIS	-	expression tag	UNP P41065
M	79	HIS	-	expression tag	UNP P41065
N	74	HIS	-	expression tag	UNP P41065
N	75	HIS	-	expression tag	UNP P41065
N	76	HIS	-	expression tag	UNP P41065
N	77	HIS	-	expression tag	UNP P41065
N	78	HIS	-	expression tag	UNP P41065
N	79	HIS	-	expression tag	UNP P41065

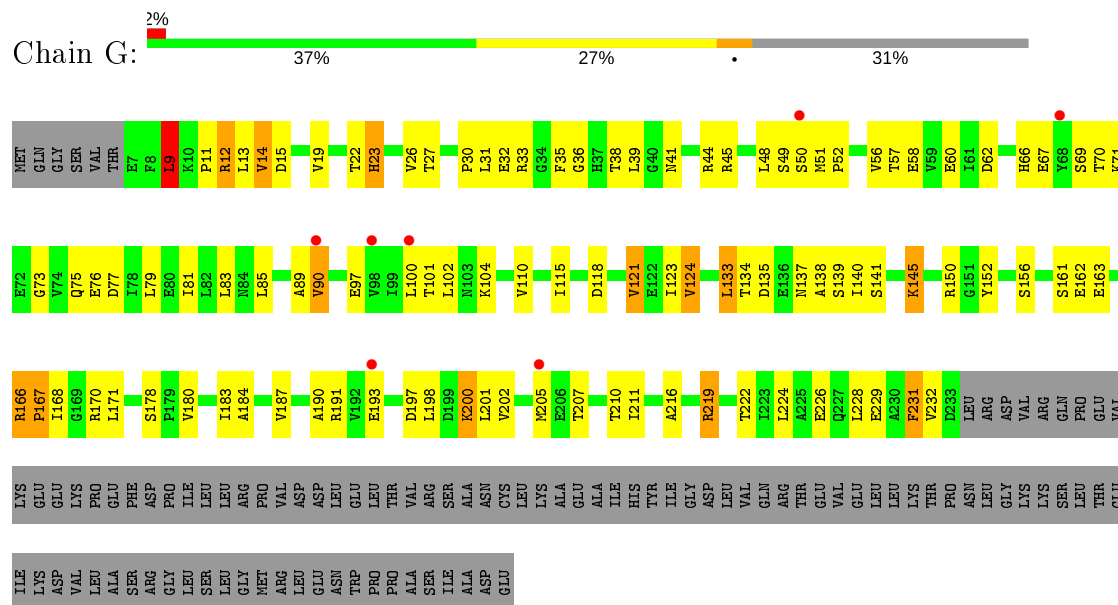
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	J	1	Total	Mg	0	0
			1	1		
7	D	1	Total	Mg	0	0
			1	1		

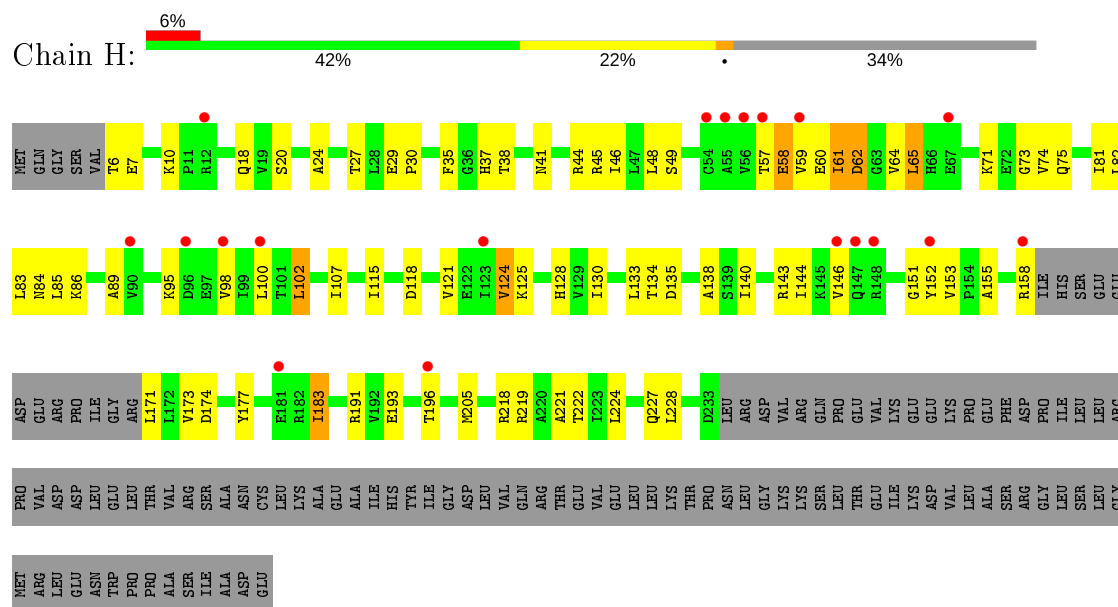
- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	J	2	Total 2	Zn 2	0	0
8	D	2	Total 2	Zn 2	0	0
8	N	1	Total 1	Zn 1	0	0
8	M	1	Total 1	Zn 1	0	0

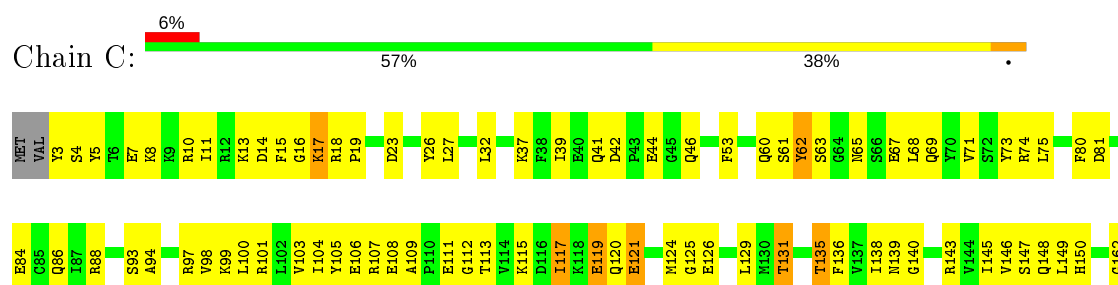
- Molecule 1: DNA-directed RNA polymerase subunit alpha

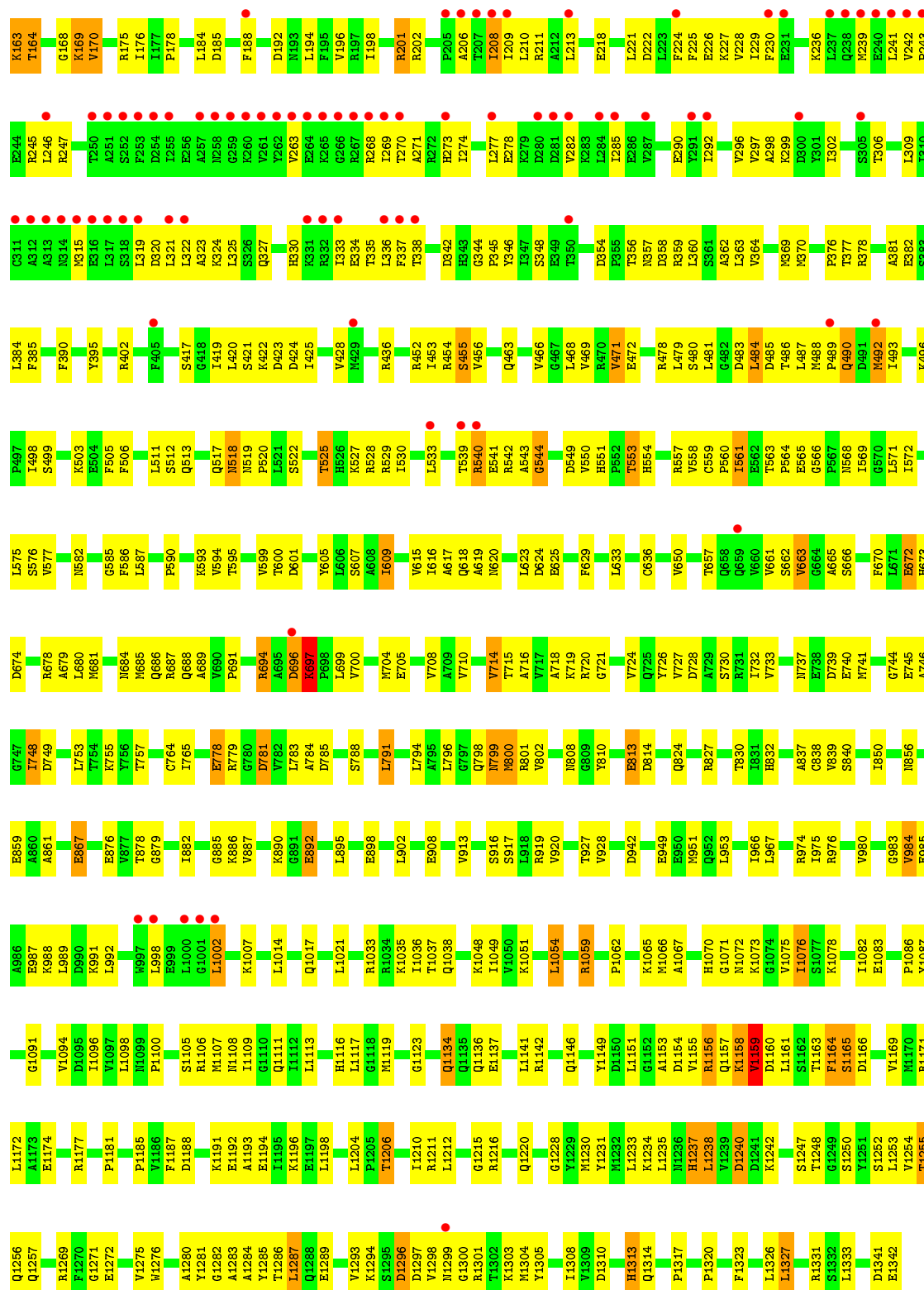


- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 2: DNA-directed RNA polymerase subunit beta





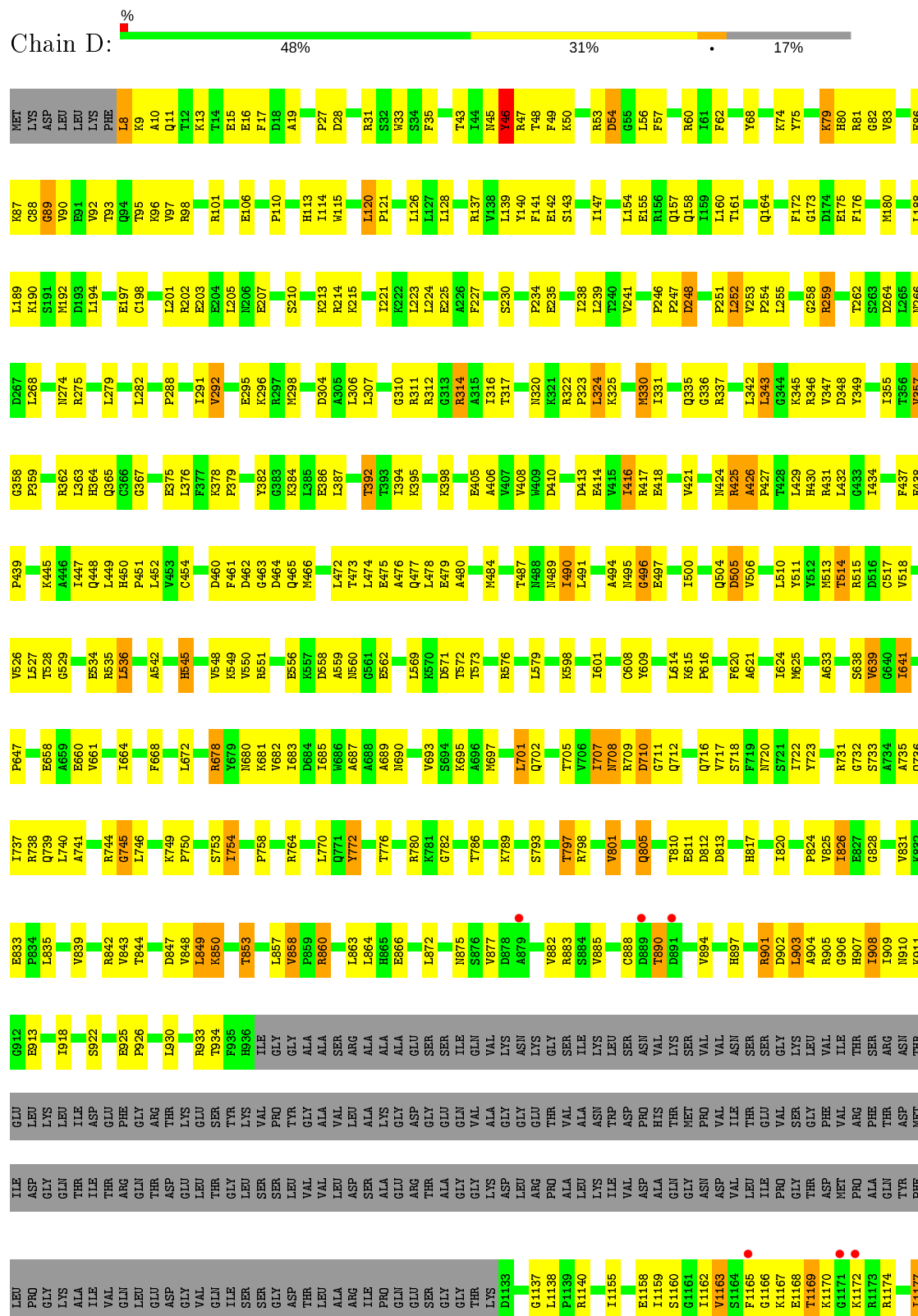
• Molecule 2: DNA-directed RNA polymerase subunit beta

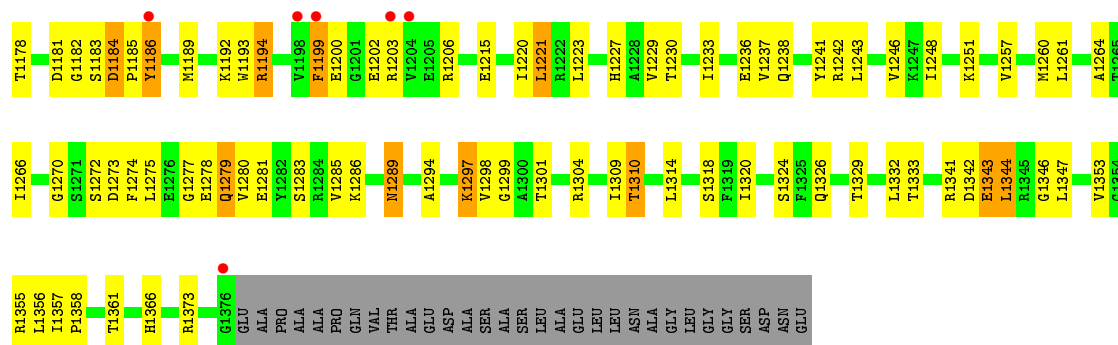


R1216	R1142	R1058	F972	I870	V661	F564	L484	R368	K236	H150	F80	MET
Q1146	Q1149	R1059	S973	V871	S662	E565	D485	M369	L237	R151	B84	VAL
E1222	R976	R974	R975	Y872	V663	G566	M488	M370	M239	P153	B85	Y3
V1225	D1150	P1062	R976	A875	F670	P567	Q493	A381	R245	F156	Q86	Y5
G1152	L1151	G1063	L979	L833	E672	L575	D491	L384	R267	F157	R88	E7
Y1229	G1152	K1065	V980	V884	H673	S576	M492	L389	L284	D158	T91	K8
M1230	D1154	A1067	A981	V884	D674	S582	I493	F388	I285	D160	S92	R9
L1233	G1155	G983	G982	G885	R678	N582	Q497	L389	R267	D160	A94	R10
K1234	R1156	H1070	G984	G886	A679	Y584	I498	Y395	V289	T164	R95	R12
H1237	K1158	N1071	E985	V887	K684	G585	S499	D396	H165	H165	L96	K13
L1238	V1159	N1072	A986	K890	Q686	F586	V502	L397	G168	G168	R97	D14
D1239	K988	K1073	K987	L892	Q686	E588	K503	L397	K169	K169	R98	F15
V1240	L1161	L989	L989	P787	R687	T589	F506	V400	V170	V170	K99	G16
M1243	S1162	L1076	L895	D790	Q688	P590	F506	L409	R175	R175	L100	R18
H1244	T1163	K1078	T896	L791	A689	V594	Q513	L420	H176	H176	R101	P19
S1247	F1164	L1079	P897	L791	A689	T595	F514	D423	D185	D185	Y105	Y26
G1249	S1165	N1080	E998	L794	R694	D596	M515	D423	F186	F186	R106	S29
S1250	D1166	E1083	R903	A795	A695	G597	Q517	D424	R107	R107	I30	I30
L1253	L1172	L1082	R903	L796	D696	V598	Q518	I425	C311	C311	O31	O31
T1254	E1174	L1082	E308	G797	K697	V599	M518	I425	R197	R197	L32	L32
Q1256	E1175	P1086	K909	Q798	T600	T600	N519	V428	N314	N314	P110	P110
L1273	M1176	Y1087	A910	Q799	D601	H604	T524	M429	D320	D320	G112	G112
T1285	R1177	G1091	V913	M800	H604	S607	H526	V442	D321	D321	K115	K115
Q1280	M1180	L1096	S917	L712	S712	A608	K527	D443	K324	K324	D116	D116
E1281	P1181	V1097	L918	G713	V713	L608	R528	N450	L325	L325	D116	D116
E1282	I1182	L1098	R919	V714	G714	E610	R529	S326	R201	R201	I117	I117
Y1285	A1183	N1099	V920	G909	N810	E610	S530	R451	K118	K118	E119	E119
T1286	L1184	P1100	P921	N811	R720	L616	S531	R452	R202	R202	G120	G120
L1287	P1185	L1004	N922	N811	R720	L616	A532	R454	K203	K203	Q120	Q120
Q1288	D1188	S1105	G923	F812	V724	A617	A532	R454	H330	H330	L204	L204
E1289	G1189	R1106	V924	E813	Q725	Q618	P535	R454	K331	K331	V122	V122
D1296	A1190	N1108	V928	D814	A729	A619	G536	S465	R332	R332	Y123	Y123
D1297	K1191	L1109	V933	E820	A729	N620	L538	S465	T207	T207	M124	M124
G1300	A1193	Q1111	V933	Q824	I732	N622	T539	E461	K208	K208	G125	G125
R1301	I1195	E1114	D842	R827	I734	F629	R540	Q463	L210	L210	I127	I127
L1210	Y1285	T1115	K943	F828	K735	L633	R541	R465	R211	R211	M130	M130
L1212	T1286	L1117	R944	T736	V736	V634	R542	V466	K212	K212	T131	T131
T1308	L1198	L1117	E949	T737	N737	T635	G544	V469	Y215	Y215	D132	D132
N1312	L1199	L1124	R950	E738	E738	C636	V547	R470	Q219	Q219	T135	T135
	G1202	I1124	M951	E740	E740	V650	R548	V471	I220	I220	L138	L138
	D1203	T1128	I960	N741	N741	M653	V550	V475	L221	L221	M139	M139
	T1206	M1129	P743	Y742	Y742	P653	K476	K476	F224	F224	G140	G140
	I1210	A1130	E963	G744	G744	D654	E477	E477	R230	R230	R143	R143
	R1301	M1131	I1049	E745	E745	V655	R478	R478	E231	E231	Y146	Y146
	T1308	E1137	I966	A746	A746	S656	L479	L479	T232	T232	L147	L147
		K1140	L867	G747	G747	T657	S480	S480	R233	R233	Q148	Q148
		L1141	E968	I748	I748	Q658	G482	G482	D234	D234	L149	L149
			P855	D749	D749	P659	I561	I561	N235	N235		
			N856	I750	I750	V660						

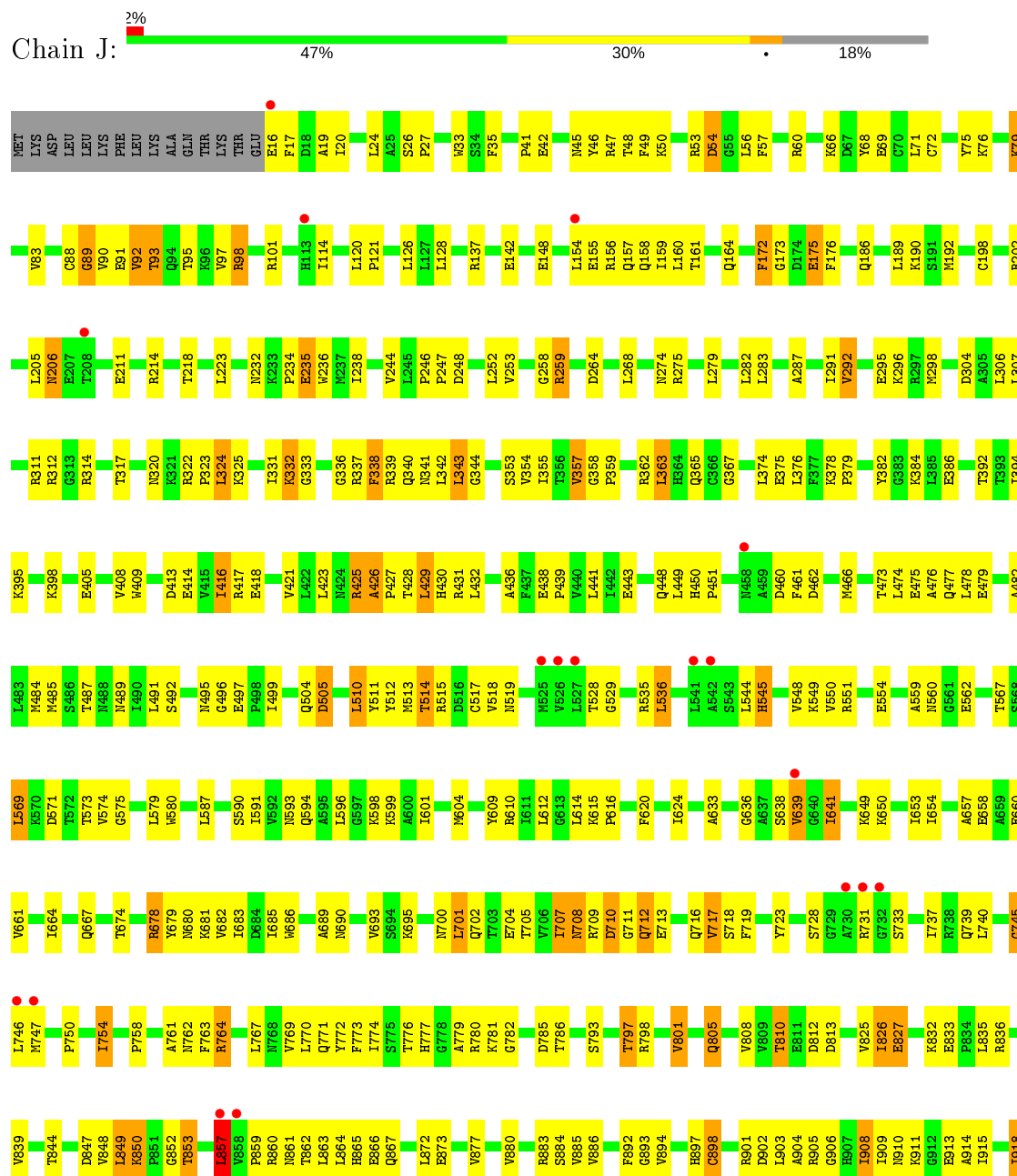


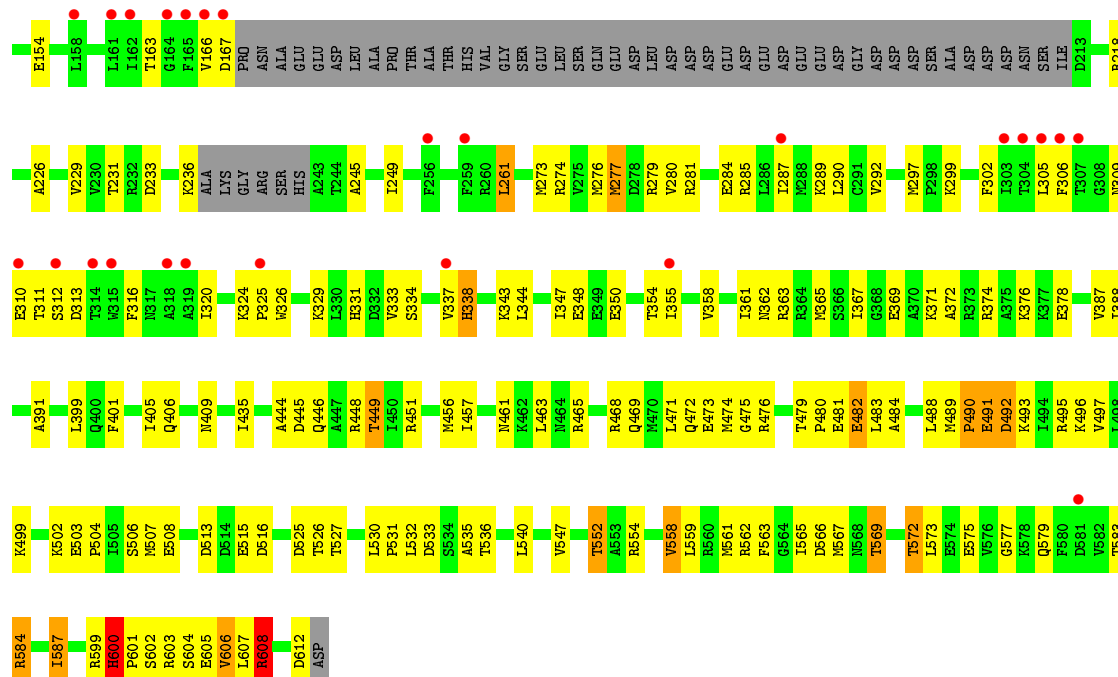
• Molecule 3: DNA-directed RNA polymerase subunit beta'



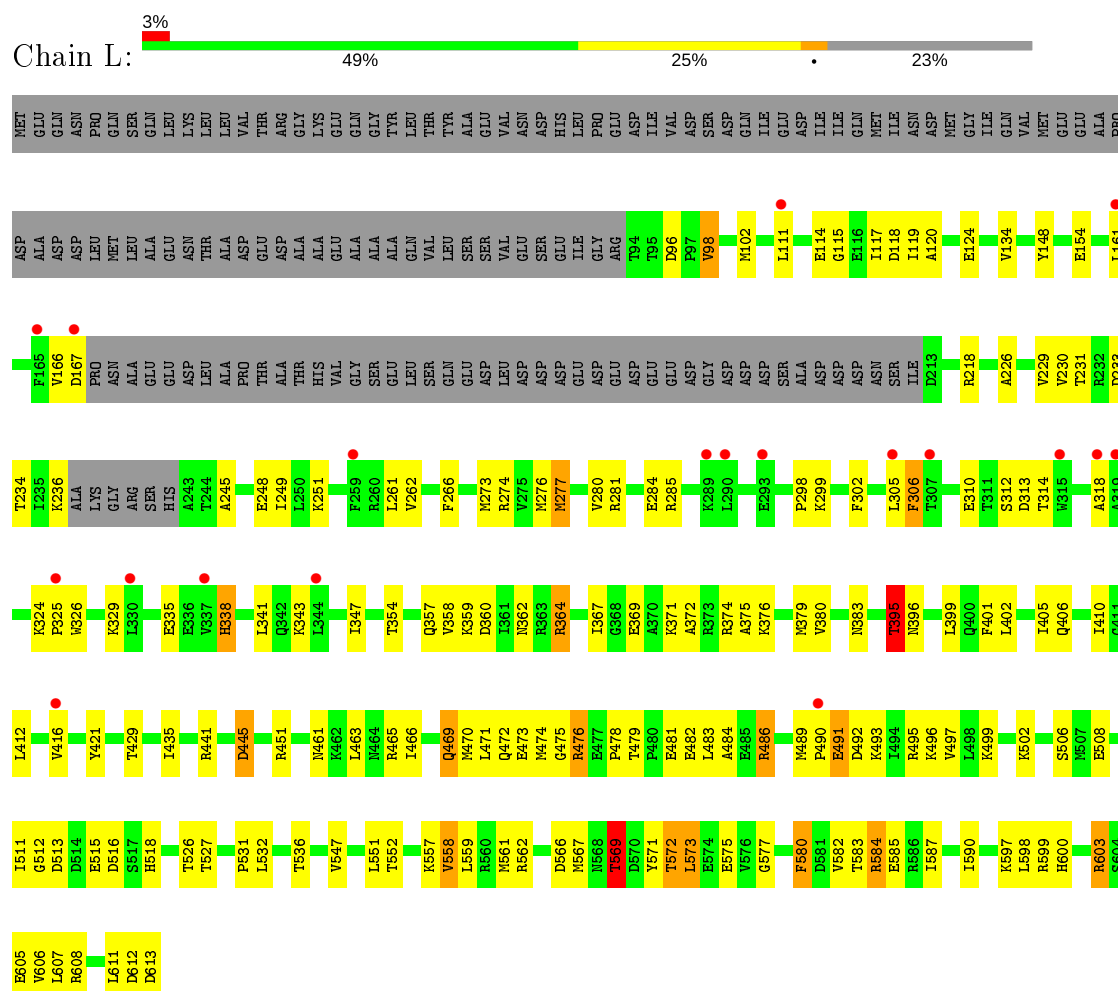


• Molecule 3: DNA-directed RNA polymerase subunit beta'

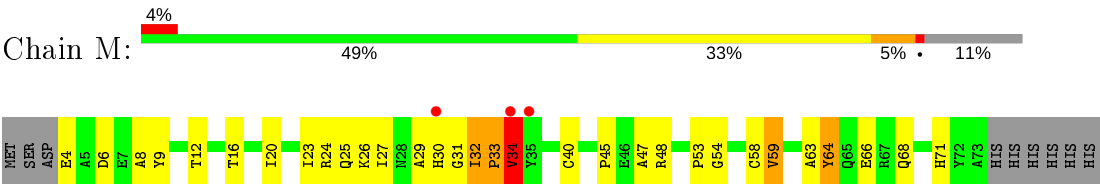




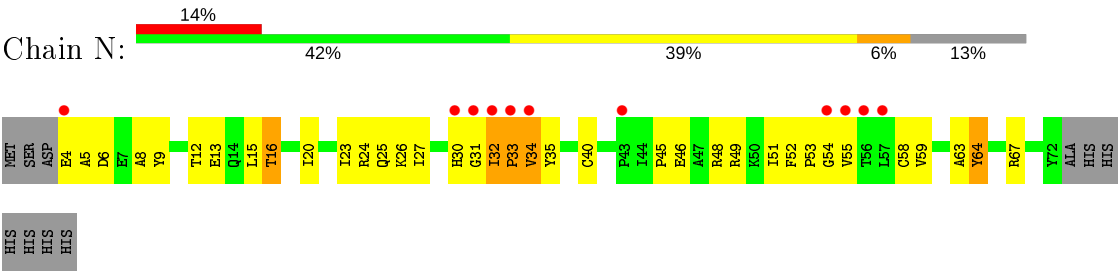
• Molecule 5: RNA polymerase sigma factor RpoD



● Molecule 6: Protein TraR



● Molecule 6: Protein TraR



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	186.48Å 206.04Å 310.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.84 – 3.81 49.84 – 3.81	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.84-3.81) 86.5 (49.84-3.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.60 (at 3.77Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.208 , 0.262 0.208 , 0.262	Depositor DCC
R_{free} test set	2000 reflections (1.70%)	wwPDB-VP
Wilson B-factor (Å ²)	156.4	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 180.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	56825	wwPDB-VP
Average B, all atoms (Å ²)	239.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% 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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.29	0/2524	0.63	1/3421 (0.0%)
1	B	0.30	0/1697	0.60	0/2300
1	G	0.28	0/1777	0.59	0/2408
1	H	0.29	0/1681	0.63	2/2278 (0.1%)
2	C	0.30	0/10733	0.58	1/14482 (0.0%)
2	I	0.29	0/10735	0.56	0/14484
3	D	0.31	0/9235	0.59	0/12472
3	J	0.29	0/9140	0.56	2/12341 (0.0%)
4	E	0.27	0/693	0.52	0/935
4	K	0.26	0/575	0.43	0/774
5	F	0.28	0/3864	0.54	1/5194 (0.0%)
5	L	0.27	0/3872	0.53	0/5205
6	M	0.34	0/567	0.64	1/766 (0.1%)
6	N	0.37	0/562	0.64	1/759 (0.1%)
All	All	0.29	0/57655	0.57	9/77819 (0.0%)

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
2	C	0	2
2	I	0	2
3	D	0	2
3	J	0	2
5	F	0	1
All	All	0	9

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	LEU	CA-CB-CG	6.11	129.35	115.30
6	M	32	ILE	C-N-CD	-6.10	107.18	120.60
1	H	29	GLU	C-N-CD	-5.98	107.44	120.60
3	J	1221	LEU	CA-CB-CG	5.83	128.71	115.30
6	N	32	ILE	C-N-CD	-5.66	108.16	120.60

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	109	ALA	Peptide
2	C	236	LYS	Peptide
3	D	1184	ASP	Peptide
3	D	901	ARG	Peptide
5	F	600	HIS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2490	0	2542	120	0
1	B	1677	0	1703	61	0
1	G	1755	0	1773	78	0
1	H	1662	0	1687	59	0
2	C	10564	0	10571	426	0
2	I	10566	0	10576	351	0
3	D	9095	0	9222	385	0
3	J	9001	0	9167	375	0
4	E	691	0	695	26	0
4	K	573	0	587	20	0
5	F	3813	0	3880	119	0
5	L	3821	0	3884	109	0
6	M	557	0	547	31	0
6	N	552	0	542	44	0
7	D	1	0	0	0	0
7	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	2	0	0	0	0
8	J	2	0	0	0	0
8	M	1	0	0	0	0
8	N	1	0	0	0	0
All	All	56825	0	57376	1966	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 17.

The worst 5 of 1966 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:HG2	1:B:38:THR:HB	1.42	1.02
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.42	1.01
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.38	1.00
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.44	0.99
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.46	0.96

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	317/329 (96%)	247 (78%)	52 (16%)	18 (6%)	1	21
1	B	213/329 (65%)	194 (91%)	15 (7%)	4 (2%)	8	42
1	G	225/329 (68%)	199 (88%)	20 (9%)	6 (3%)	5	35
1	H	212/329 (64%)	196 (92%)	12 (6%)	4 (2%)	8	42
2	C	1338/1342 (100%)	1201 (90%)	118 (9%)	19 (1%)	11	46
2	I	1338/1342 (100%)	1197 (90%)	120 (9%)	21 (2%)	9	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	1169/1407 (83%)	1038 (89%)	104 (9%)	27 (2%)	6	38
3	J	1151/1407 (82%)	1026 (89%)	99 (9%)	26 (2%)	6	38
4	E	87/91 (96%)	80 (92%)	5 (6%)	2 (2%)	6	38
4	K	70/91 (77%)	61 (87%)	8 (11%)	1 (1%)	11	46
5	F	462/613 (75%)	426 (92%)	28 (6%)	8 (2%)	9	43
5	L	463/613 (76%)	425 (92%)	30 (6%)	8 (2%)	9	43
6	M	68/79 (86%)	56 (82%)	7 (10%)	5 (7%)	1	16
6	N	67/79 (85%)	56 (84%)	6 (9%)	5 (8%)	1	15
All	All	7180/8380 (86%)	6402 (89%)	624 (9%)	154 (2%)	7	40

5 of 154 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	107	ILE
1	A	136	GLU
1	A	162	GLU
1	A	167	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	278/286 (97%)	226 (81%)	52 (19%)	1	11
1	B	186/286 (65%)	171 (92%)	15 (8%)	11	41
1	G	193/286 (68%)	169 (88%)	24 (12%)	4	24
1	H	183/286 (64%)	172 (94%)	11 (6%)	19	50
2	C	1154/1157 (100%)	1052 (91%)	102 (9%)	10	38
2	I	1154/1157 (100%)	1058 (92%)	96 (8%)	11	40
3	D	962/1168 (82%)	882 (92%)	80 (8%)	11	40
3	J	960/1168 (82%)	876 (91%)	84 (9%)	10	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	72/75 (96%)	63 (88%)	9 (12%)	4	24
4	K	62/75 (83%)	59 (95%)	3 (5%)	25	56
5	F	417/540 (77%)	387 (93%)	30 (7%)	14	45
5	L	418/540 (77%)	380 (91%)	38 (9%)	9	36
6	M	59/68 (87%)	55 (93%)	4 (7%)	16	47
6	N	59/68 (87%)	56 (95%)	3 (5%)	24	54
All	All	6157/7160 (86%)	5606 (91%)	551 (9%)	9	38

5 of 551 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	3	ARG
1	G	207	THR
5	L	154	GLU
4	E	58	LEU
5	F	552	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	129	GLN
1	G	66	HIS
5	L	131	GLN
5	F	131	GLN
5	F	446	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	319/329 (96%)	-0.01	8 (2%) 57 49	152, 220, 344, 468	0
1	B	217/329 (65%)	-0.05	9 (4%) 37 31	140, 238, 332, 383	0
1	G	227/329 (68%)	-0.06	7 (3%) 49 40	204, 265, 358, 416	0
1	H	216/329 (65%)	0.41	19 (8%) 10 8	204, 298, 387, 432	0
2	C	1340/1342 (99%)	0.23	83 (6%) 20 16	104, 197, 403, 528	0
2	I	1340/1342 (99%)	0.38	109 (8%) 12 10	127, 264, 377, 485	0
3	D	1173/1407 (83%)	-0.07	12 (1%) 82 76	101, 174, 294, 419	0
3	J	1155/1407 (82%)	0.07	34 (2%) 51 42	125, 213, 329, 431	0
4	E	89/91 (97%)	-0.34	1 (1%) 80 74	160, 216, 269, 393	0
4	K	72/91 (79%)	1.28	16 (22%) 0 0	227, 323, 429, 471	0
5	F	468/613 (76%)	0.08	25 (5%) 26 23	137, 239, 365, 477	0
5	L	469/613 (76%)	-0.06	19 (4%) 37 31	162, 251, 379, 489	0
6	M	70/79 (88%)	0.12	3 (4%) 35 30	226, 315, 399, 479	0
6	N	69/79 (87%)	0.45	11 (15%) 1 2	325, 403, 501, 568	0
All	All	7224/8380 (86%)	0.14	356 (4%) 29 25	101, 230, 372, 568	0

The worst 5 of 356 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	338	THR	14.4
2	C	252	SER	10.7
2	C	241	LEU	9.4
3	J	1198	VAL	9.2
2	C	251	ALA	9.1

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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(\AA^2)	Q<0.9
7	MG	D	2001	1/1	0.42	0.18	251,251,251,251	0
8	ZN	N	101	1/1	0.78	0.06	465,465,465,465	0
8	ZN	M	101	1/1	0.84	0.04	468,468,468,468	0
8	ZN	J	2002	1/1	0.87	0.15	229,229,229,229	0
8	ZN	D	2002	1/1	0.94	0.15	182,182,182,182	0
8	ZN	D	2003	1/1	0.97	0.49	334,334,334,334	0
7	MG	J	2001	1/1	0.98	0.47	170,170,170,170	0
8	ZN	J	2003	1/1	0.99	0.24	126,126,126,126	0

6.5 Other polymers [i](#)

There are no such residues in this entry.