



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:17 PM GMT

PDB ID : 3WOD
Title : RNA polymerase-gp39 complex
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Deposited on : 2013-12-26
Resolution : 3.60 Å(reported)

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

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

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

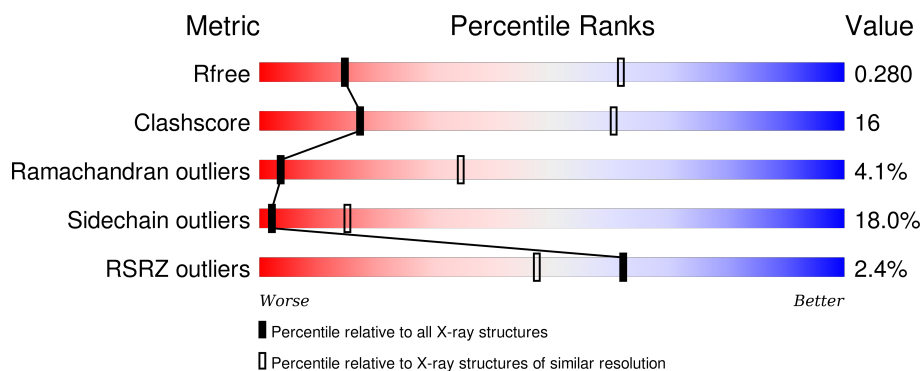
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	315	
1	B	315	
2	C	1119	
3	D	1524	
4	E	99	

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Mol	Chain	Length	Quality of chain
5	F	423	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>3%38%21%6%34%</div></div>
6	G	141	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%65%23%10%</div></div>
6	H	141	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>2%44%16%5%35%</div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 28954 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	225	Total	C	N	O	S	0	0	0
			1772	1132	308	330	2			
1	B	232	Total	C	N	O	S	0	0	0
			1814	1158	316	338	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1118	Total	C	N	O	S	0	0	0
			8817	5575	1573	1645	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1488	Total	C	N	O	S	0	0	0
			11752	7450	2069	2197	36			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	95	Total	C	N	O	S	0	0	0
			769	488	133	144	4			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	61	GLU	VAL	SEE REMARK 999	UNP Q8RQE7
E	92	ILE	LEU	SEE REMARK 999	UNP Q8RQE7
E	95	GLY	VAL	SEE REMARK 999	UNP Q8RQE7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	278	Total	C	N	O	S	0	0	0
			2242	1421	399	420	2			

- Molecule 6 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	127	Total	C	N	O	S	0	0	0
			1035	673	175	184	3			
6	H	91	Total	C	N	O	S	0	0	0
			752	495	125	131	1			

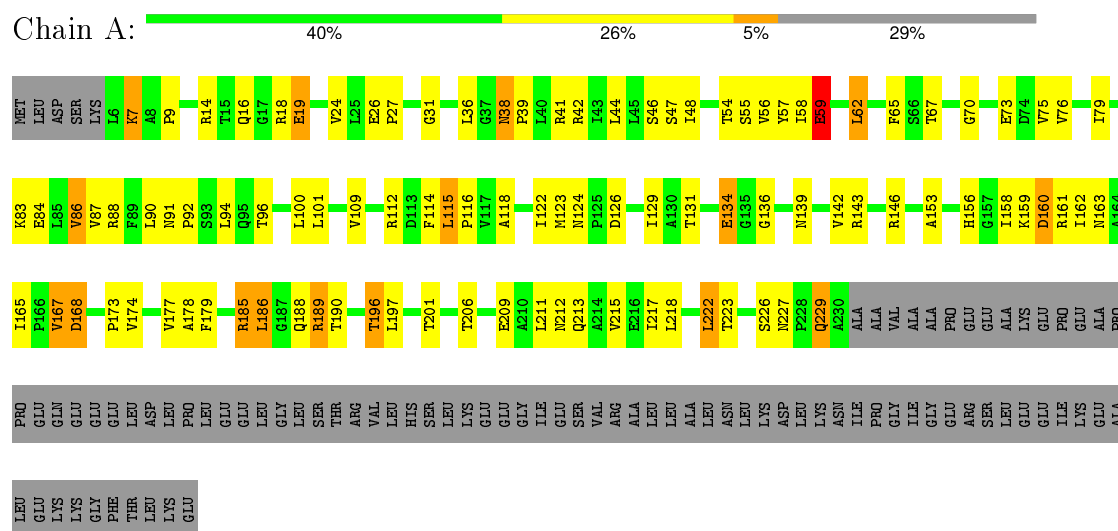
- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	Zn	0	0
			1	1		

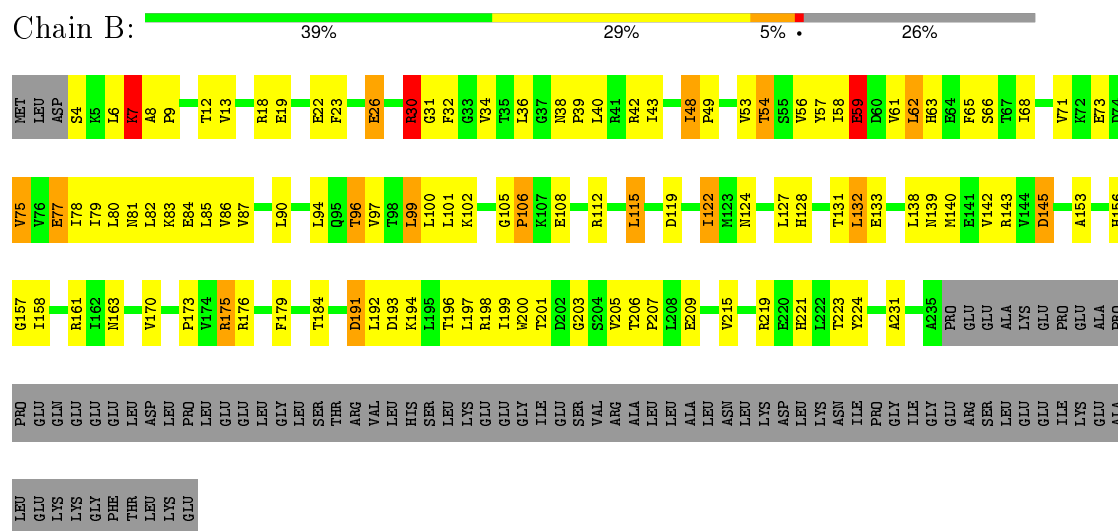
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

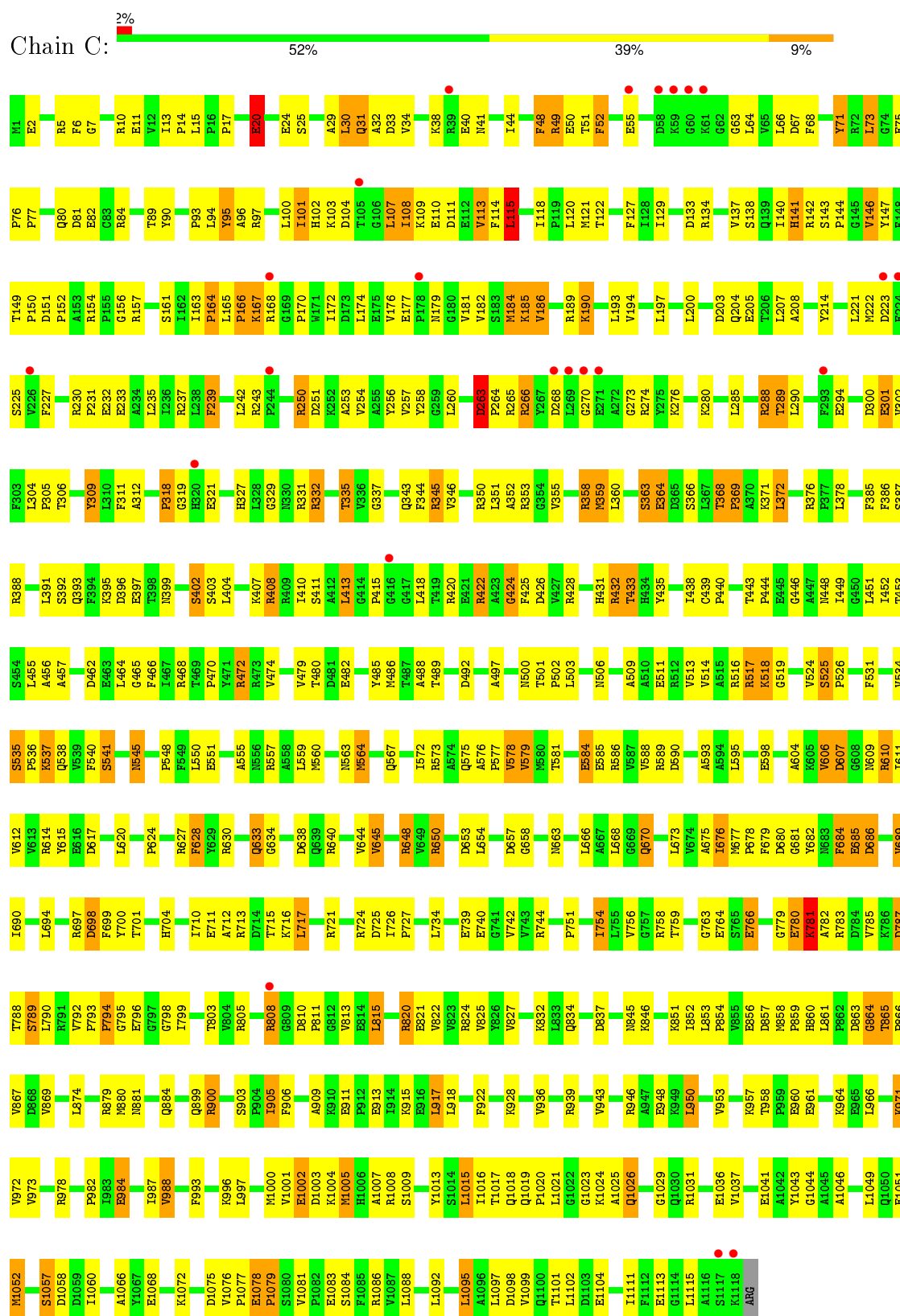
• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 1: DNA-directed RNA polymerase subunit alpha



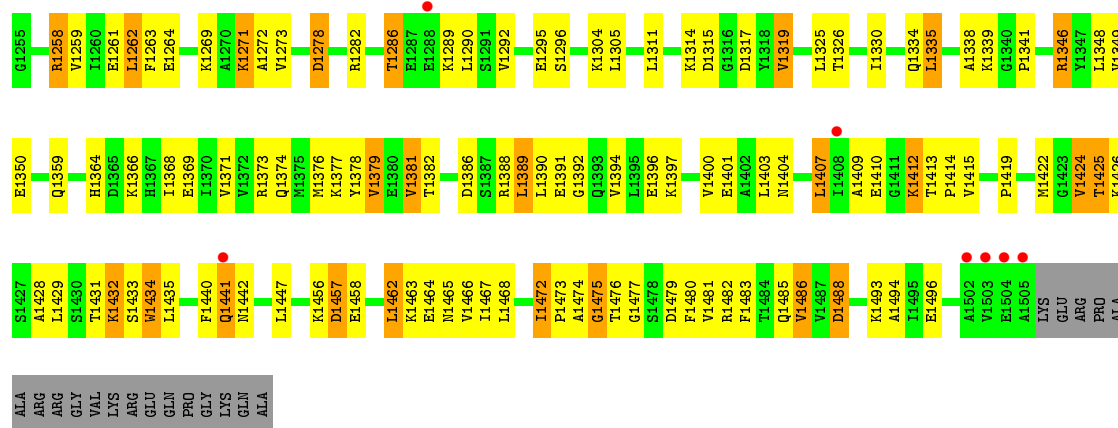
• Molecule 2: DNA-directed RNA polymerase subunit beta



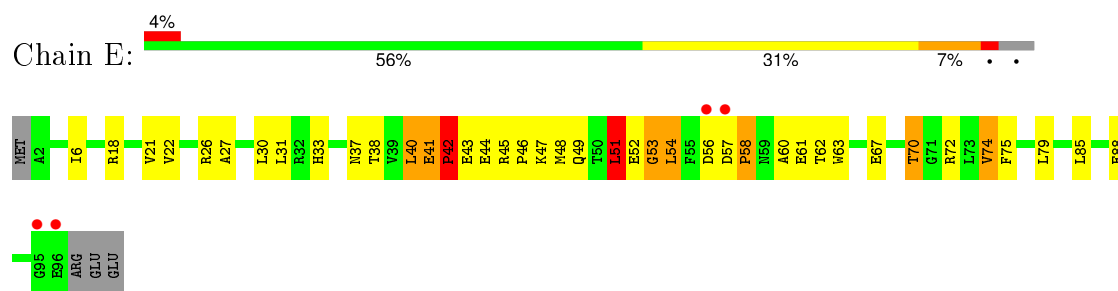
• Molecule 3: DNA-directed RNA polymerase subunit beta'



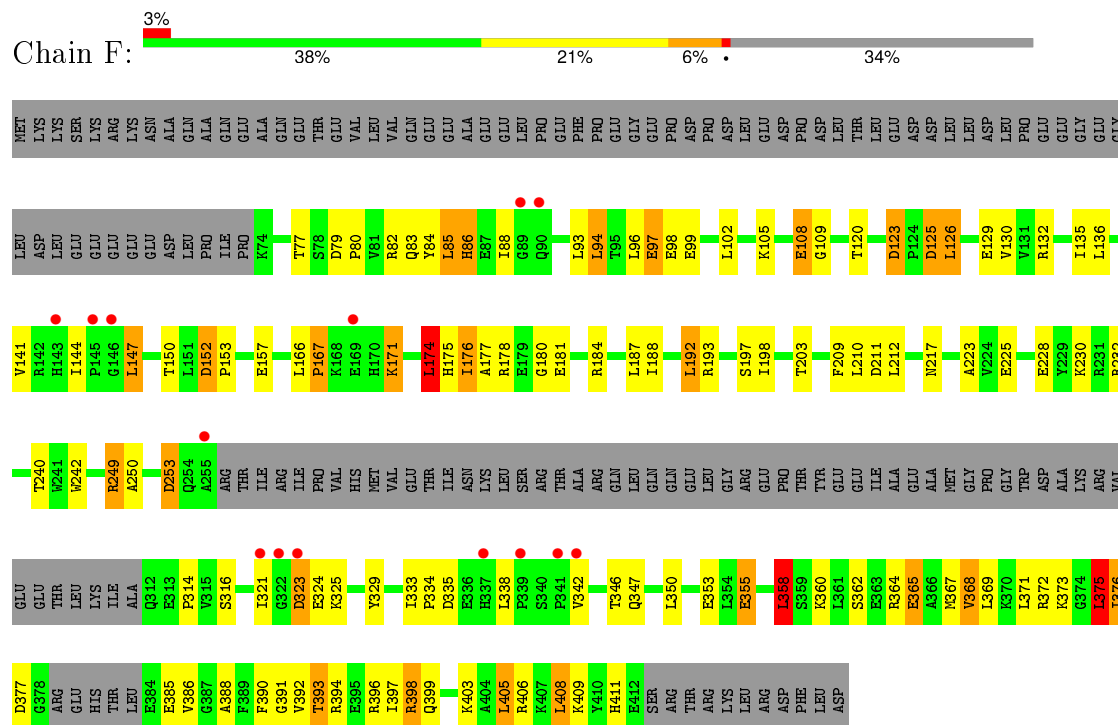
L1174	R1096	T984	R394	I827	R760	R881	G532	A454	E375	E294	G222	V145	G77	MET
I1175	R1097	E987	R895	R828	I761	D682	G533	R495	E376	G295	L223	P146	V78	K2
I1183	L1098	R896	R896	R829	Q762	E686	F535	M456	E377	E296	R224	E148	E79	V5
L1184	L1109	R897	R897	A830	R763	E687	R534	I461	I378	I297	L225	R149	R80	R6
E1185	L1101	R898	R898	G831	L764	R765	R535	L461	I379	E298	P226	R150	R82	K7
V1186	T1102	R899	R899	R832	S765	R766	D539	L465	E380	E299	L227	Q151	S83	V8
P1187	H1103	R900	R900	S835	R767	A690	L540	L465	E381	E300	A228	Q152	R84	R9
E1188	E1104	R901	R901	R836	L770	V694	N541	L465	E382	G301	A229	L153	R85	I10
L1189	L1105	R902	R902	R837	S771	I695	L543	L468	E383	Q302	E230	T154	R86	A11
T1190	Q1106	R903	R903	R838	S772	H696	L544	D469	G383	P303	E231	T155	R87	L12
L1191	R1002	R904	R904	R839	S773	G697	R546	E471	L387	A305	K233	E156	R88	A13
E1192	K1003	R905	R905	R840	S774	R697	L547	A472	H388	E306	E234	E157	R89	S22
Q1193	Q1004	R906	R906	R841	P777	R703	R550	K473	E389	A307	A235	L161	R90	Y23
Q1194	A1006	R907	R907	R842	L778	R704	R553	K474	P390	L311	Y236	R162	R91	E30
Q1195	V1007	R908	R908	R843	L779	R705	R554	K475	A391	R312	Y237	R163	R92	T31
Q1196	I1008	R909	R909	R844	S780	R706	L554	L478	L394	R313	P238	Q165	A96	I32
Q1197	E1109	R910	R910	R845	S781	R707	R555	E479	K397	P314	L242	Q166	H101	N33
L1198	L1110	R911	R911	R846	R782	R708	R556	E480	V400	V317	L245	Q167	I102	R35
Q1199	Q1111	R912	R912	R847	R783	R709	L557	M481	K397	V317	P246	E167	F104	T36
Q1200	L1112	R913	R913	R848	R784	R710	R558	E482	V400	A324	L250	G174	Y103	L37
Q1201	T1113	R914	R914	R849	R785	R711	R559	E483	D405	E325	F251	P173	P109	K38
Q1202	Y1114	R915	R915	R850	R786	R712	R560	E484	E406	E326	R252	V175	P39	P39
Q1203	Y1115	R916	R916	R851	R787	R713	R561	E485	V407	E327	A253	D176	R41	E40
Q1204	Y1116	R917	R917	R852	R788	R714	R562	E486	E408	G328	E254	A177	K11	R41
Q1205	Y1117	R918	R918	R853	R789	R715	R563	E487	E409	E329	T330	L178	I112	D42
Q1206	Y1118	R919	R919	R854	R790	R716	R564	E488	E410	E330	E255	G43	G13	G43
Q1207	Y1119	R920	R920	R855	R791	R717	R565	E489	E411	E331	E256	D181	T114	L44
Q1208	Y1120	R921	R921	R856	R792	R718	R566	E490	E412	E332	V259	G182	F45	F45
Q1209	Y1121	R922	R922	R857	R793	R719	R567	E491	E413	E333	E260	E183	D46	D46
Q1210	Y1122	R923	R923	R858	R794	R720	R568	E492	E414	E334	E261	E184	E47	E47
Q1211	Y1123	R924	R924	R859	R795	R721	R569	E493	E415	E335	E262	E185	R48	R48
Q1212	Y1124	R925	R925	R860	R796	R722	R570	E494	E416	E336	E263	E186	I49	I49
Q1213	Y1125	R926	R926	R861	R797	R723	R571	E495	E417	E337	E264	K187	A120	A120
Q1214	Y1126	R927	R927	R862	R798	R724	R572	E496	E418	E338	E265	G188	T121	P82
Q1215	Y1127	R928	R928	R863	R799	R725	R573	E497	E419	E339	E266	Q189	E122	I83
Q1216	Y1128	R929	R929	R864	R800	R726	R574	E498	E420	E340	F269	E190	L123	F54
Q1217	Y1129	R930	R930	R865	R801	R727	R575	E499	E421	E341	V271	L191	E124	D55
Q1218	Y1130	R931	R931	R866	R802	R728	R576	E500	E422	E342	E274	A192	Y56	Y56
Q1219	Y1131	R932	R932	R867	R803	R729	R577	E501	E423	E343	E275	P193	E57	E57
Q1220	Y1132	R933	R933	R868	R804	R730	R578	E502	E424	E344	E276	L199	C58	C58
Q1221	Y1133	R934	R934	R869	R805	R731	R579	E503	E425	E345	E277	L129	A59	A59
Q1222	Y1134	R935	R935	R870	R806	R732	R580	E504	E426	E346	E278	G61	C60	C60
Q1223	Y1135	R936	R936	R871	R807	R733	R581	E505	E427	E347	E279	A203	G62	G62
Q1224	Y1136	R937	R937	R872	R808	R734	R582	E506	E428	E348	E280	L204	Y63	Y63
Q1225	Y1137	R938	R938	R873	R809	R735	R583	E507	E429	E349	E281	Y205	K64	K64
Q1226	Y1138	R939	R939	R874	R810	R736	R584	E508	E430	E350	E282	R206	R65	R65
Q1227	Y1139	R940	R940	R875	R811	R737	R585	E509	E431	E351	E283	F207	Q66	Q66
Q1228	Y1140	R941	R941	R876	R812	R738	R586	E510	E432	E352	E284	E214	R67	R67
Q1229	Y1141	R942	R942	R877	R813	R739	R587	E511	E433	E353	E285	E215	F68	F68
Q1230	Y1142	R943	R943	R878	R814	R740	R588	E512	E434	E354	E286	Y216	A140	A140
Q1231	Y1143	R944	R944	R879	R815	R741	R589	E513	E435	E355	E287	V217	C73	C73
Q1232	Y1144	R945	R945	R880	R816	R742	R590	E514	E436	E356	E288	E219	E74	E74
Q1233	Y1145	R946	R946	R881	R817	R743	R591	E515	E437	E357	E289	E219	R75	R75
Q1234	Y1146	R947	R947	R882	R818	R744	R592	E516	E438	E358	E290	E219	N143	N143
Q1235	Y1147	R948	R948	R883	R819	R745	R593	E517	E439	E359	E291	E219	G144	G144
Q1236	Y1148	R949	R949	R884	R820	R746	R594	E518	E440	E360	E292	E219	C76	C76
Q1237	Y1149	R950	R950	R885	R821	R747	R595	E519	E441	E361	E293	E219		
Q1238	Y1150	R951	R951	R886	R822	R748	R596	E520	E442	E362	E294	E219		
Q1239	Y1151	R952	R952	R887	R823	R749	R597	E521	E443	E363	E295	E219		
Q1240	Y1152	R953	R953	R888	R824	R750	R598	E522	E444	E364	E296	E219		
Q1241	Y1153	R954	R954	R889	R825	R751	R599	E523	E445	E365	E297	E219		
Q1242	Y1154	R955	R955	R890	R826	R752	R600	E524	E446	E366	E298	E219		
Q1243	Y1155	R956	R956	R891	R827	R753	R601	E525	E447	E367	E299	E219		
Q1244	Y1156	R957	R957	R892	R828	R754	R602	E526	E448	E368	E300	E219		
Q1245	Y1157	R958	R958	R893	R829	R755	R603	E527	E449	E369	E301	E219		
Q1246	Y1158	R959	R959	R894	R830	R756	R604	E528	E450	E370	E302	E219		
Q1247	Y1159	R960	R960	R895	R831	R757	R605	E529	E451	E371	E303	E219		
Q1248	Y1160	R961	R961	R896	R832	R758	R606	E530	E452	E372	E304	E219		
Q1249	Y1161	R962	R962	R897	R833	R759	R607	E531	E453	E373	E305	E219		
Q1250	Y1162	R963	R963	R898	R834	R760	R608	E532	E454	E374	E306	E219		
Q1251	Y1163	R964	R964	R899	R835	R761	R609	E533	E455	E375	E307	E219		
Q1252	Y1164	R965	R965	R900	R836	R762	R610	E534	E456	E376	E308	E219		
Q1253	Y1165	R966	R966	R901	R837	R763	R611	E535	E457	E377	E309	E219		
Q1254	Y1166	R967	R967	R902	R838	R764	R612	E536	E458	E378	E310	E219		
Q1255	Y1167	R968	R968	R903	R839	R765	R613	E537	E459	E379	E311	E219		
Q1256	Y1168	R969	R969	R904	R840	R766	R614	E538	E460	E380	E312	E219		
Q1257	Y1169	R970	R970	R905	R841	R767	R615	E539	E461	E381	E313	E219		
Q1258	Y1170	R971	R971	R906	R842	R768	R616	E540	E462	E382	E314	E219		
Q1259	Y1171	R972	R972	R907	R843	R769	R617	E541	E463	E383	E315	E219		
Q1260	Y1172	R973	R973	R908	R844	R770	R618	E542	E464	E384	E316	E219		
Q1261	Y1173	R974	R974	R909	R845	R771	R619	E543	E465	E385	E317	E219		
Q1262	Y1174	R975	R975	R910	R846	R772	R620	E544	E466	E386	E318	E219		
Q1263	Y1175	R976	R976	R911	R847	R773	R621	E545	E467	E387	E319	E219		
Q1264	Y1176	R977	R977	R912	R848	R774	R622	E546	E468	E388	E320	E219		
Q1265	Y1177	R978	R978	R913	R849	R775	R623	E547	E469	E389	E321	E219		
Q1266	Y1178	R979	R979	R914	R850	R776	R624	E548	E470	E390	E322	E219		
Q1267	Y1179	R980	R980	R915	R851	R777	R625	E549	E471	E391	E323	E219		
Q1268	Y1180	R981	R981	R916	R852	R778	R626	E550	E472	E392	E324	E219		
Q1269	Y1181	R982	R982	R917	R853	R779	R627	E551	E473	E393	E325	E219		
Q1270	Y1182	R983	R983	R918	R854	R780	R628	E552	E474	E394	E326	E219		
Q1271	Y1183	R984	R984	R919	R855	R781	R629	E553	E475	E395	E327	E219		
Q1272	Y1184	R985	R985	R920	R856	R782	R630	E554	E476	E396	E328	E219		
Q1273	Y1185	R986	R986	R921	R857	R783	R631	E555	E477	E397	E329	E219		
Q1274	Y1186	R987	R987	R922	R858	R784	R632	E556	E478	E398	E330	E219		
Q1275	Y1187	R988	R988	R923	R859	R785	R633	E557	E479	E399	E331	E219		
Q1276	Y1188	R989	R989	R924	R860	R786	R634	E558	E480	E400	E332	E219		
Q1277	Y1189	R990	R990	R925	R861	R787	R635	E559	E481	E401	E333	E219		
Q1278	Y1190	R991	R991	R926	R862	R788	R636	E560	E48					



• Molecule 4: DNA-directed RNA polymerase subunit omega

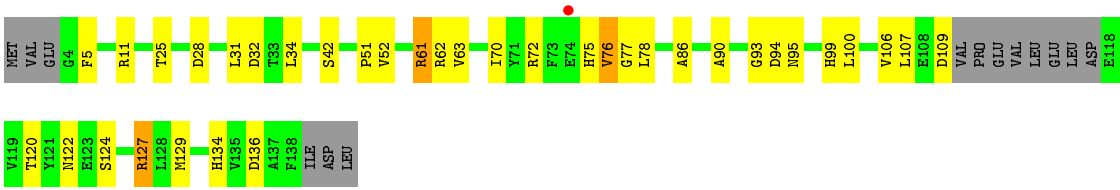


• Molecule 5: RNA polymerase sigma factor

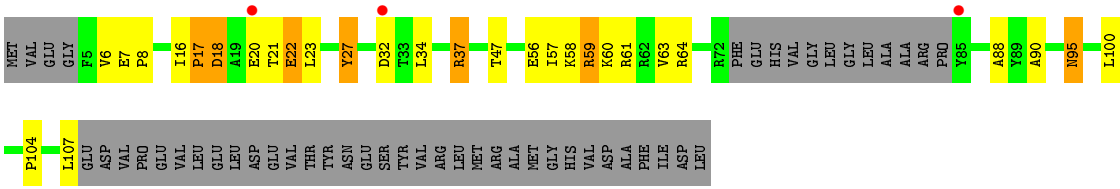


• Molecule 6: Putative uncharacterized protein





● Molecule 6: Putative uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	294.44Å 294.44Å 223.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.88 – 3.60 19.88 – 3.58	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.88-3.60) 99.3 (19.88-3.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.22	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 3.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.250 , 0.279 0.249 , 0.280	Depositor DCC
R_{free} test set	6371 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	64.5	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 20.7	EDS
Estimated twinning fraction	0.166 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.16$	Xtriage
Outliers	0 of 129363 reflections	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	28954	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
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	A	0.35	0/1804	0.63	1/2454 (0.0%)
1	B	0.32	0/1846	0.59	0/2511
2	C	0.33	0/8985	0.61	2/12150 (0.0%)
3	D	0.32	0/11958	0.60	4/16166 (0.0%)
4	E	0.31	0/783	0.66	0/1054
5	F	0.33	0/2276	0.59	3/3058 (0.1%)
6	G	0.27	0/1065	0.53	0/1449
6	H	0.27	0/775	0.48	0/1057
All	All	0.32	0/29492	0.60	10/39899 (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	3
3	D	0	3
4	E	0	3
5	F	0	1
All	All	0	10

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	795	GLY	N-CA-C	-6.48	96.90	113.10
1	A	115	LEU	CA-CB-CG	6.18	129.51	115.30
3	D	581	LEU	CA-CB-CG	5.89	128.84	115.30
5	F	174	LEU	CA-CB-CG	5.88	128.81	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	804	LEU	CA-CB-CG	5.79	128.61	115.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	260	LEU	Peptide
2	C	685	GLU	Peptide
2	C	794	PRO	Peptide
3	D	1196	THR	Peptide
3	D	561	GLY	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	1772	0	1821	63	0
1	B	1814	0	1868	73	0
2	C	8817	0	8920	305	0
3	D	11752	0	11990	447	0
4	E	769	0	775	29	0
5	F	2242	0	2305	62	0
6	G	1035	0	1013	19	0
6	H	752	0	748	20	0
7	D	1	0	0	0	0
All	All	28954	0	29440	943	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 16.

The worst 5 of 943 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)
3:D:820:GLU:HG3	3:D:836:VAL:HG21	1.51	0.92
2:C:164:PRO:HA	2:C:266:ARG:HH22	1.36	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:54:LEU:HA	4:E:58:PRO:HD2	1.57	0.85
2:C:63:GLY:HA3	2:C:103:LYS:HG2	1.58	0.83
3:D:133:ILE:HG21	3:D:454:ALA:HB1	1.60	0.83

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	223/315 (71%)	198 (89%)	22 (10%)	3 (1%)	15	60
1	B	230/315 (73%)	207 (90%)	14 (6%)	9 (4%)	4	36
2	C	1116/1119 (100%)	947 (85%)	128 (12%)	41 (4%)	4	38
3	D	1484/1524 (97%)	1209 (82%)	200 (14%)	75 (5%)	2	28
4	E	93/99 (94%)	75 (81%)	12 (13%)	6 (6%)	1	22
5	F	272/423 (64%)	225 (83%)	36 (13%)	11 (4%)	4	35
6	G	123/141 (87%)	116 (94%)	5 (4%)	2 (2%)	12	56
6	H	87/141 (62%)	81 (93%)	4 (5%)	2 (2%)	8	50
All	All	3628/4077 (89%)	3058 (84%)	421 (12%)	149 (4%)	3	34

5 of 149 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	GLU
1	B	7	LYS
1	B	59	GLU
1	B	75	VAL
2	C	31	GLN

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	197/273 (72%)	164 (83%)	33 (17%)	2	18
1	B	200/273 (73%)	172 (86%)	28 (14%)	4	28
2	C	940/941 (100%)	756 (80%)	184 (20%)	1	12
3	D	1254/1279 (98%)	1018 (81%)	236 (19%)	2	13
4	E	83/87 (95%)	70 (84%)	13 (16%)	3	22
5	F	241/371 (65%)	200 (83%)	41 (17%)	2	18
6	G	107/121 (88%)	92 (86%)	15 (14%)	4	28
6	H	79/121 (65%)	71 (90%)	8 (10%)	9	43
All	All	3101/3466 (90%)	2543 (82%)	558 (18%)	2	15

5 of 558 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	55	ASP
3	D	456	MET
5	F	253	ASP
3	D	85	VAL
3	D	227	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	327	HIS
5	F	218	GLN
3	D	909	ASN
2	C	31	GLN
3	D	569	ASN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	225/315 (71%)	-0.75	0	100 100	11, 37, 83, 144	0
1	B	232/315 (73%)	-0.64	0	100 100	14, 47, 104, 158	0
2	C	1118/1119 (99%)	-0.49	23 (2%)	67 52	8, 59, 151, 222	0
3	D	1488/1524 (97%)	-0.28	44 (2%)	54 38	8, 85, 179, 244	0
4	E	95/99 (95%)	-0.27	4 (4%)	40 28	40, 74, 183, 242	0
5	F	278/423 (65%)	-0.03	14 (5%)	32 22	44, 119, 192, 255	0
6	G	127/141 (90%)	-0.38	1 (0%)	87 78	27, 73, 137, 179	0
6	H	91/141 (64%)	-0.06	3 (3%)	50 36	73, 113, 161, 175	0
All	All	3654/4077 (89%)	-0.37	89 (2%)	62 47	8, 74, 170, 255	0

The worst 5 of 89 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	294	HIS	7.5
2	C	60	GLY	6.5
3	D	1408	ILE	6.2
3	D	230	TRP	6.1
2	C	270	GLY	6.1

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(\AA^2)	Q<0.9
7	ZN	D	1601	1/1	0.97	0.10	-1.37	110,110,110,110	0

6.5 Other polymers [i](#)

There are no such residues in this entry.