



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 01:58 AM UTC

PDB ID : 3AOH / pdb_00003aoh
Title : RNA polymerase-Gfh1 complex (Crystal type 1)
Authors : Tagami, S.; Sekine, S.; Kumarevel, T.; Yamamoto, M.; Yokoyama, S.; RIKEN
Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2010-09-28
Resolution : 4.10 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
Xtriage (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

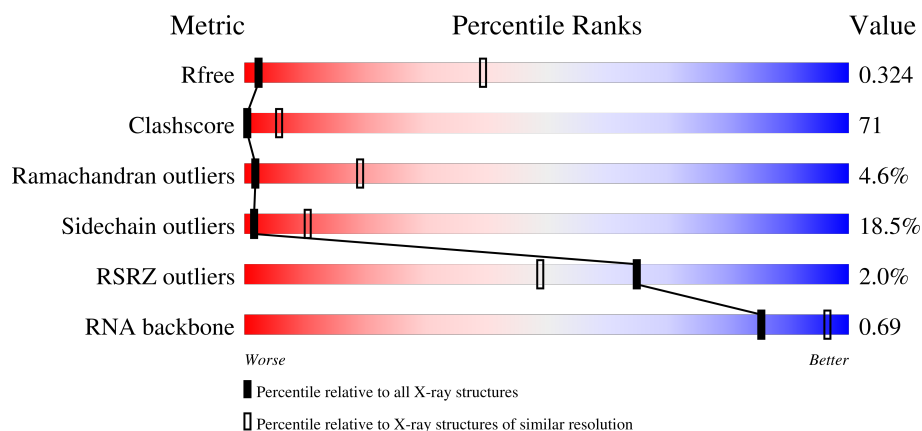
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 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.



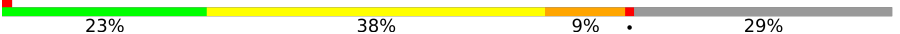
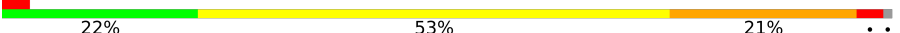
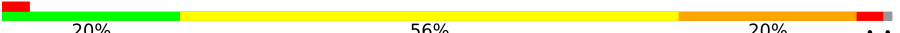
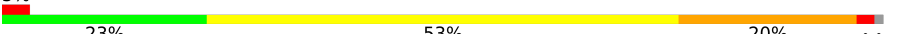
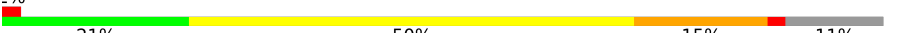
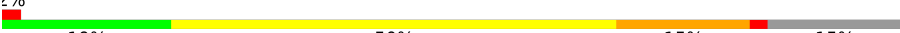
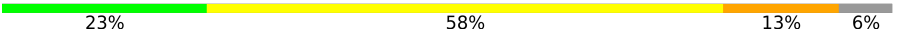
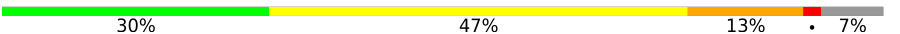
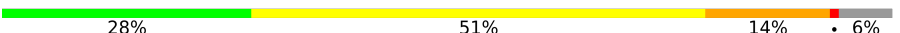
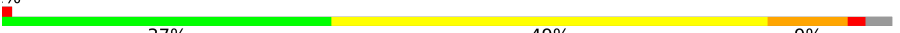
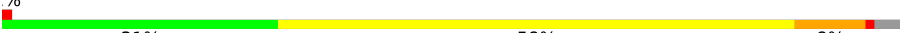
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1243 (4.40-3.80)
Clashscore	190562	1293 (4.40-3.80)
Ramachandran outliers	187476	1206 (4.40-3.80)
Sidechain outliers	187428	1193 (4.40-3.80)
RSRZ outliers	180081	1240 (4.40-3.80)
RNA backbone	3983	1026 (5.04-3.10)

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	A	315	16% 46% 8% 29%
1	B	315	19% 42% 10% 29%
1	F	315	17% 43% 10% 30%
1	G	315	20% 38% 12% 29%

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Mol	Chain	Length	Quality of chain
1	K	315	
1	L	315	
2	C	1119	
2	H	1119	
2	M	1119	
3	D	1524	
3	I	1524	
3	N	1524	
4	E	99	
4	J	99	
4	O	99	
5	P	27	
6	Q	33	
7	X	156	
7	Y	156	
7	Z	156	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 74250 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	223	Total	C	N	O	S	0	0	0
			1759	1123	306	328	2			
1	B	223	Total	C	N	O	S	0	0	0
			1759	1123	306	328	2			
1	F	222	Total	C	N	O	S	0	0	0
			1750	1117	304	327	2			
1	G	223	Total	C	N	O	S	0	0	0
			1759	1123	306	328	2			
1	K	222	Total	C	N	O	S	0	0	0
			1750	1117	304	327	2			
1	L	223	Total	C	N	O	S	0	0	0
			1759	1123	306	328	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1106	Total	C	N	O	S	0	0	0
			8733	5525	1558	1626	24			
2	H	1103	Total	C	N	O	S	0	0	0
			8710	5508	1555	1623	24			
2	M	1105	Total	C	N	O	S	0	0	0
			8729	5523	1557	1625	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1349	Total	C	N	O	S	0	0	0
			10651	6740	1888	1991	32			
3	I	1289	Total	C	N	O	S	0	0	0
			10182	6444	1804	1903	31			
3	N	1351	Total	C	N	O	S	0	0	0
			10667	6749	1891	1995	32			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	93	Total	C	N	O	S	0	0	0
			754	481	131	138	4			
4	J	92	Total	C	N	O	S	0	0	0
			749	478	130	137	4			
4	O	93	Total	C	N	O	S	0	0	0
			754	481	131	138	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	P	6	Total	C	N	O	P	0	0	0
			120	56	22	36	6			

- Molecule 6 is a RNA chain called RNA (5'-R(*CP*CP*CP*CP*GP*GP*AP*AP*GP*AP*UP*CP*AP*UP*CP*UP*UP*CP*CP*GP*GP*GP*GP*GP*AP*U*GP*CP*GP*GP*CP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	Q	7	Total	C	N	O	P	0	0	0
			152	68	31	47	6			

- Molecule 7 is a protein called Anti-cleavage anti-GreA transcription factor Gfh1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	X	152	Total	C	N	O	S	0	0	0
			1169	719	207	239	4			
7	Y	152	Total	C	N	O	S	0	0	0
			1169	719	207	239	4			
7	Z	152	Total	C	N	O	S	0	0	0
			1169	719	207	239	4			

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	1	Total	Zn	0	0
			1	1		
8	I	1	Total	Zn	0	0
			1	1		
8	N	1	Total	Zn	0	0
			1	1		

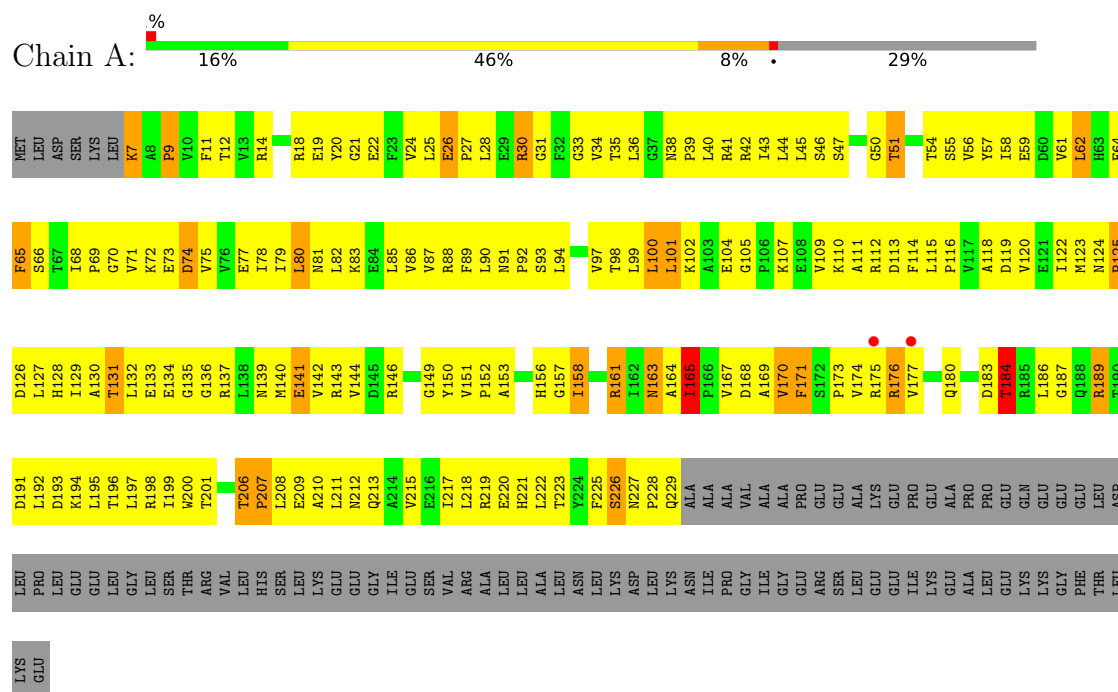
- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	1	Total 1	Mg 1	0	0
9	I	1	Total 1	Mg 1	0	0
9	N	1	Total 1	Mg 1	0	0

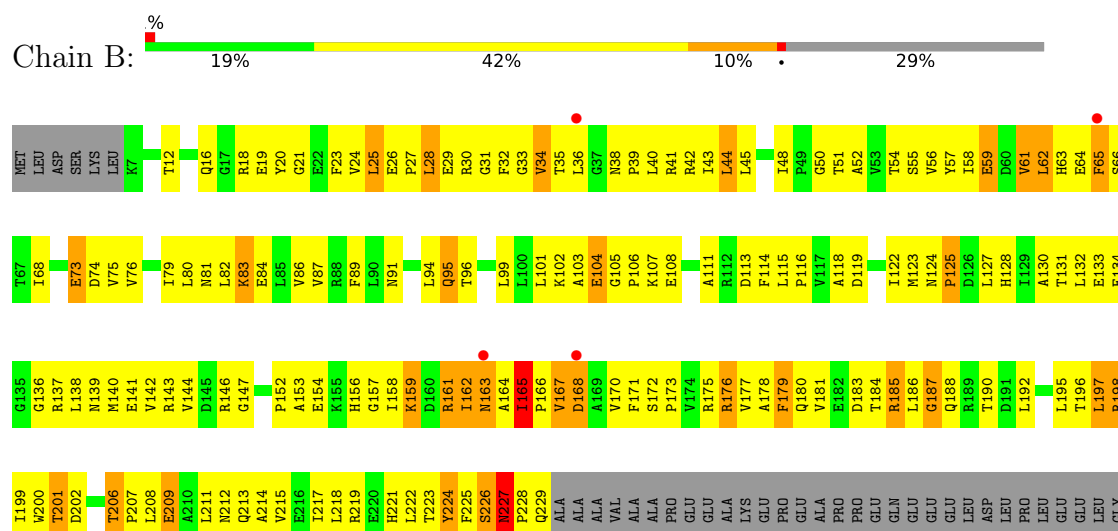
3 Residue-property plots

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 subunit alpha



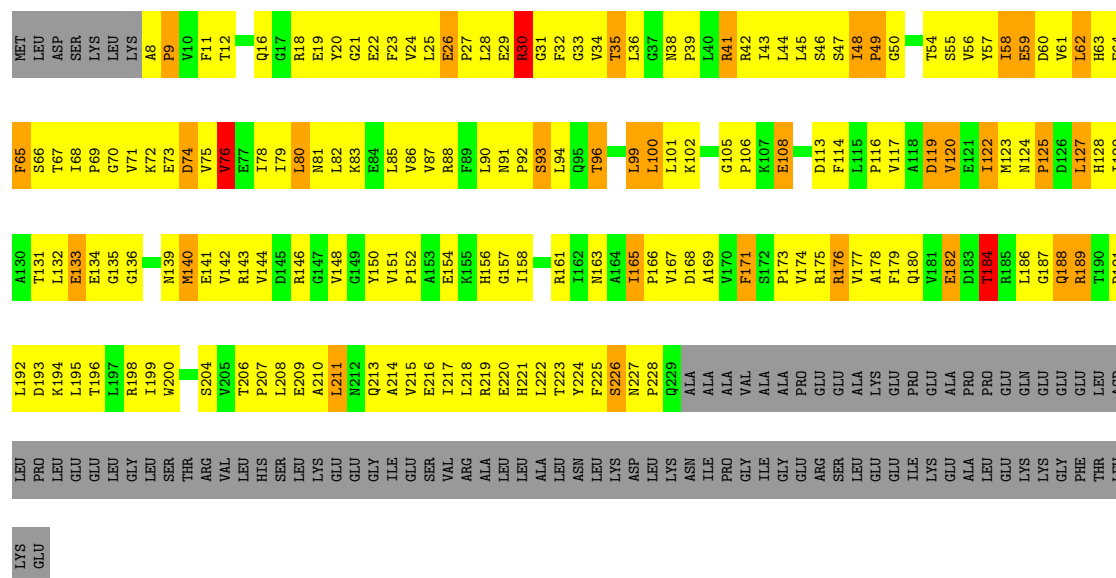
• Molecule 1: DNA-directed RNA polymerase subunit alpha



LEU SER THR ARG VAL HIS SER LEU GLU GLY ILE GLU SER VAL ARG ALA LEU LEU ALA LEU LEU LEU LEU ASN PRO GLY ILE GLU ARG SER LEU LEU GLU ILE ILE LYS LYS ALA GLU

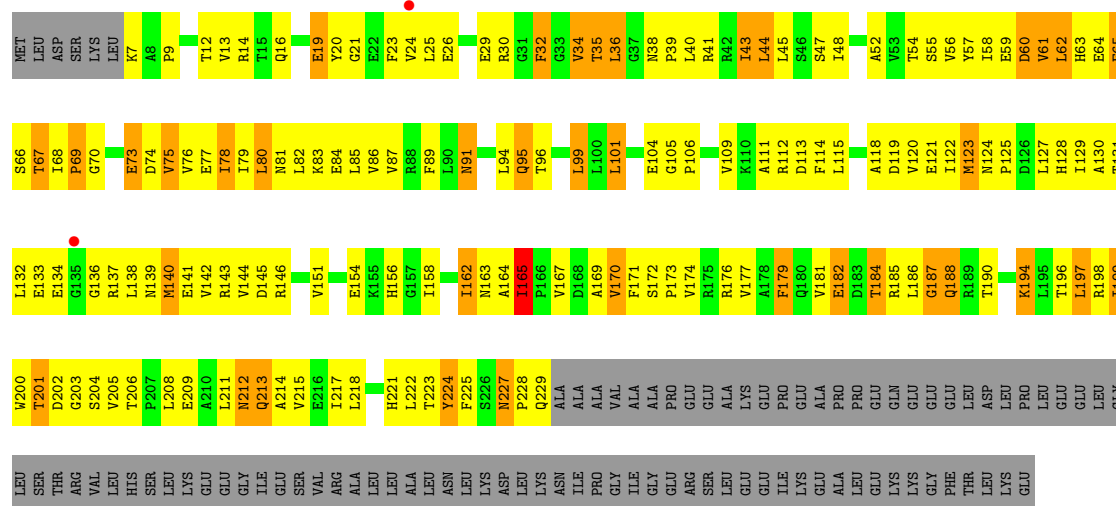
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain F: 17% 43% 10% 30%



• Molecule 1: DNA-directed RNA polymerase subunit alpha

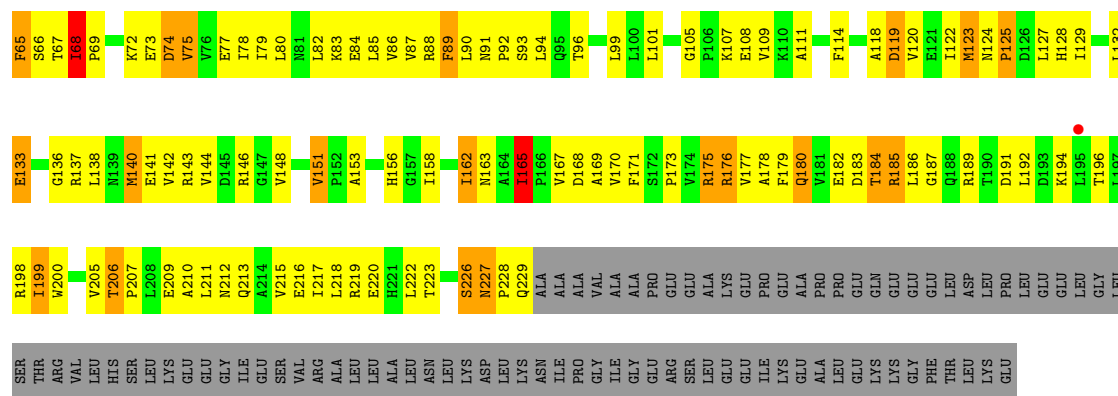
Chain G: 20% 38% 12% 29%



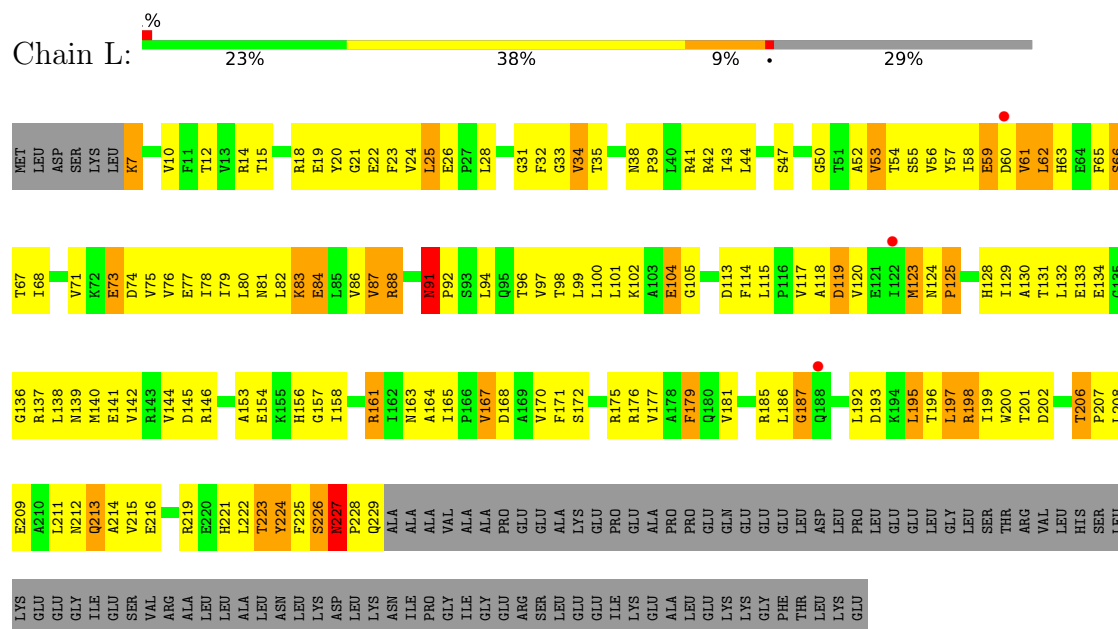
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain K: 22% 39% 9% 30%

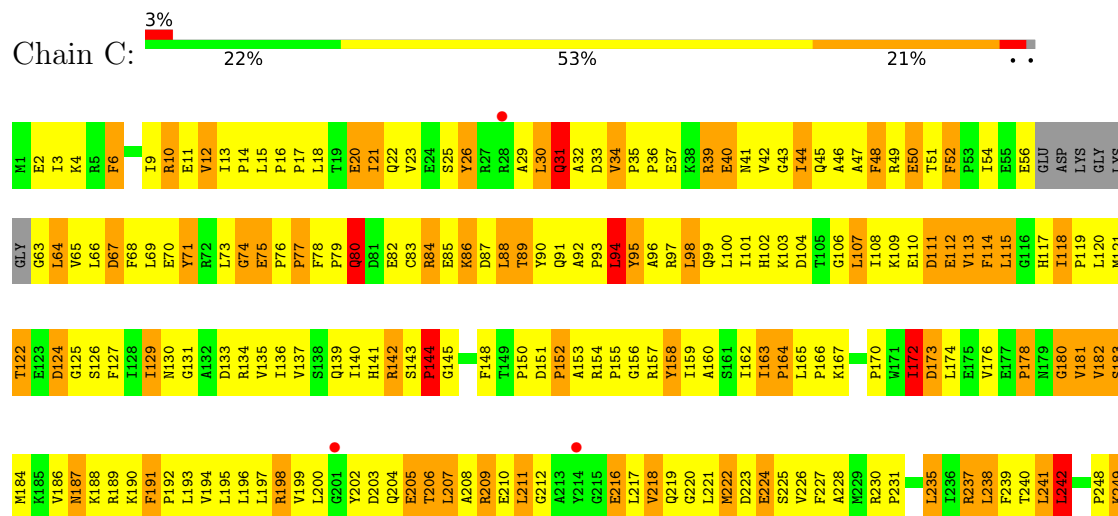




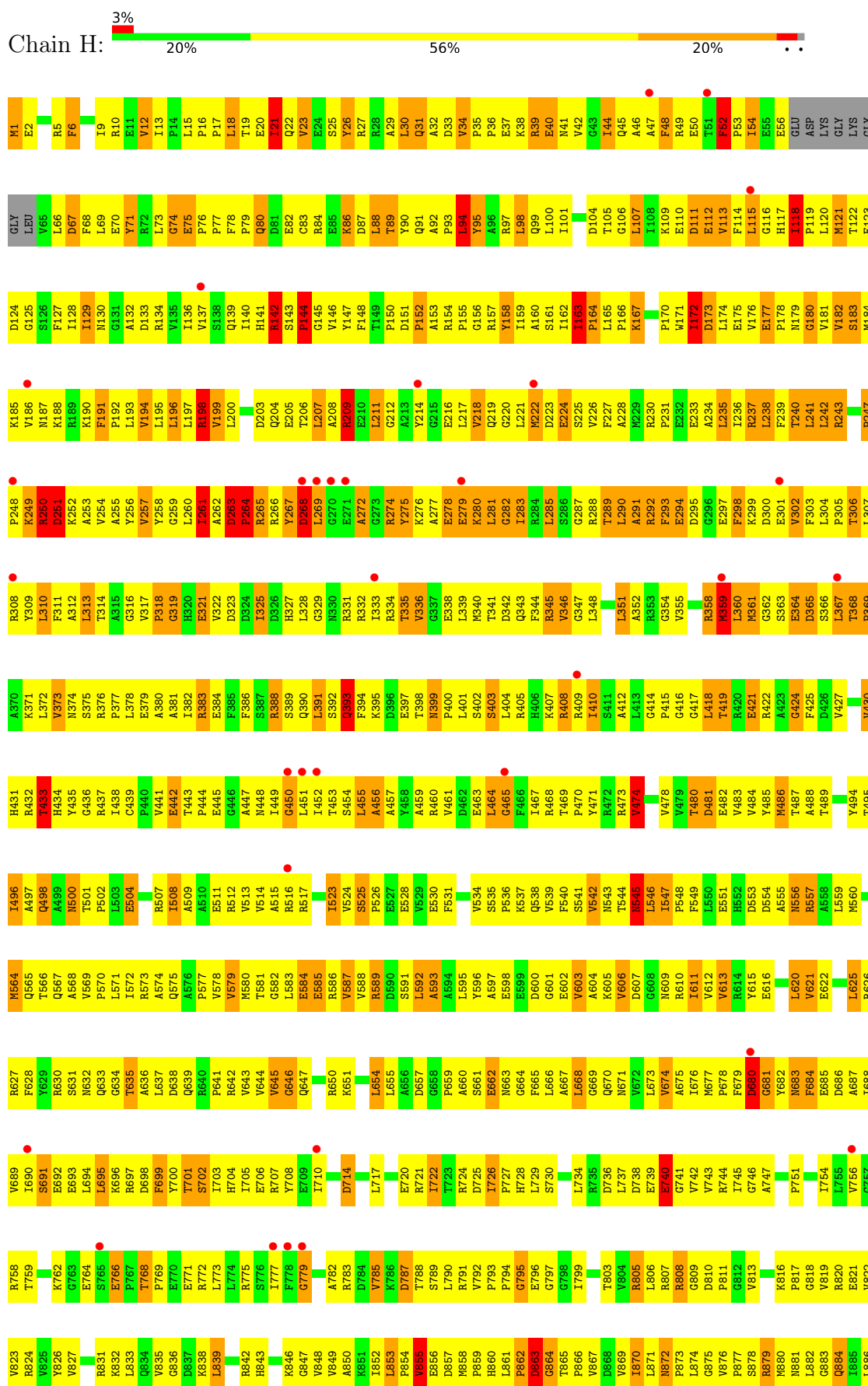
• Molecule 1: DNA-directed RNA polymerase subunit alpha

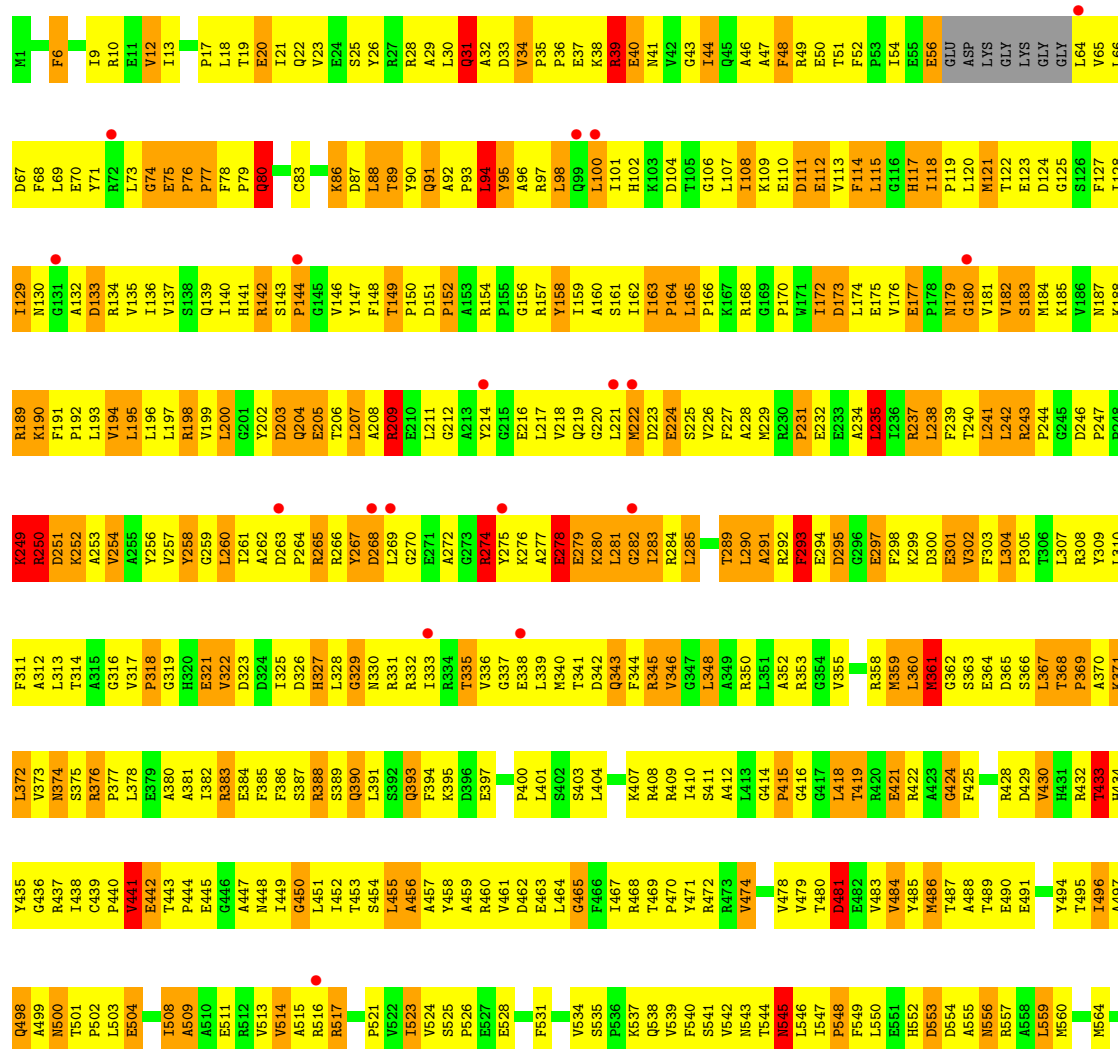


• Molecule 2: DNA-directed RNA polymerase subunit beta

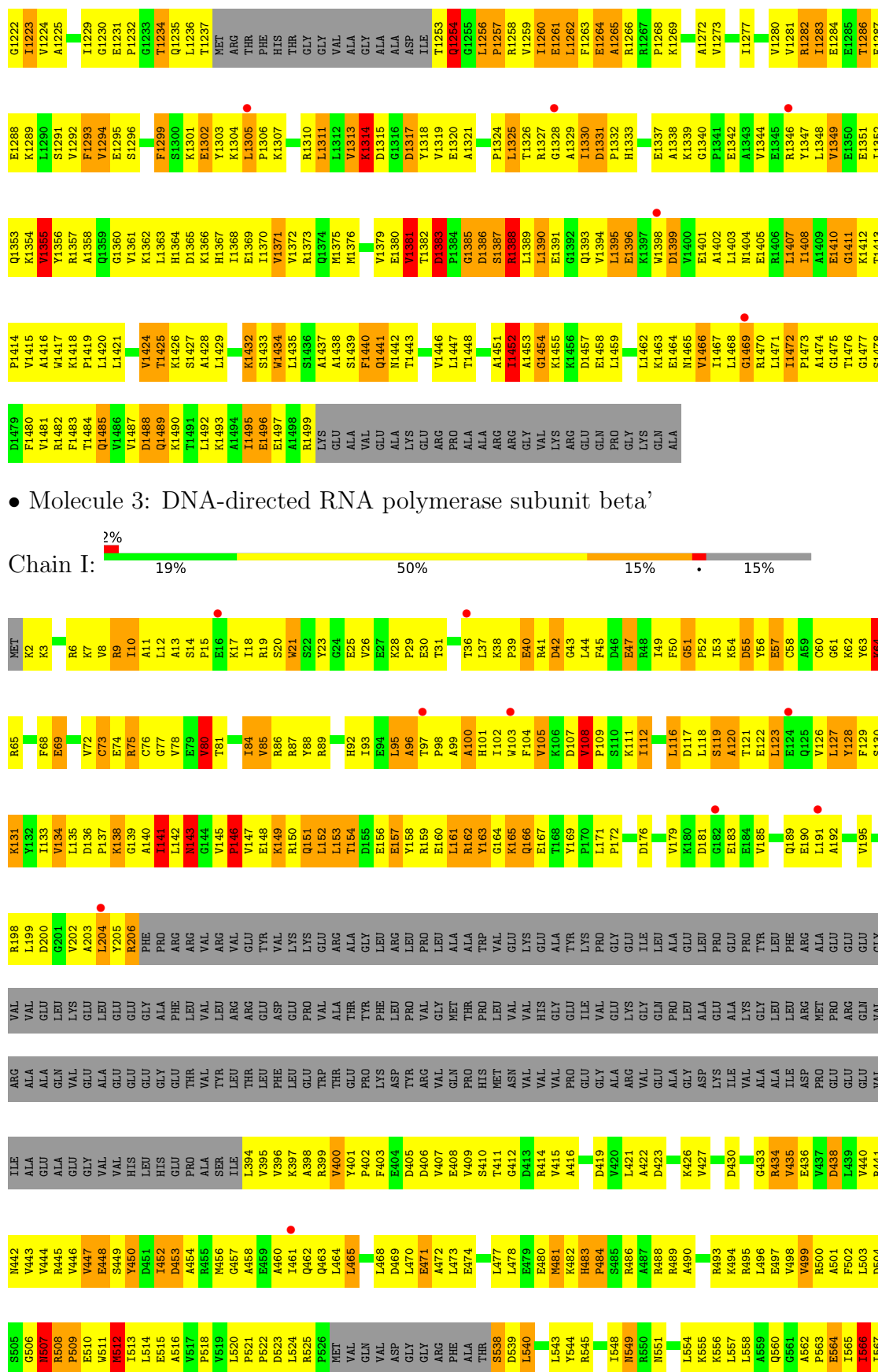






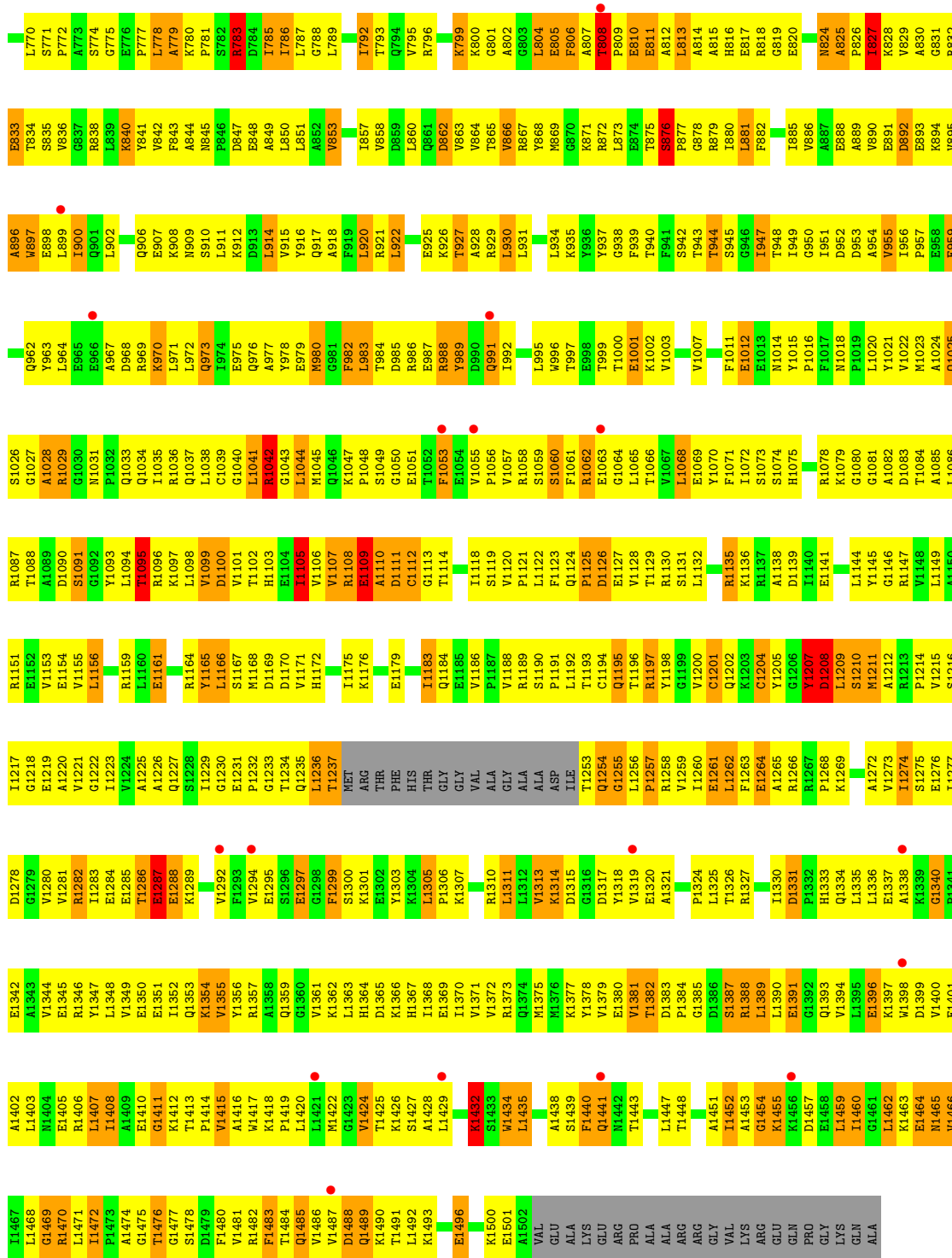


V1155	A1089	G1027	E958	K994	A830	H767	L702	Q641	W578	MS12	E448	V384	GLY
L1160	D1090	A1028	E959	V995	G831	H770	N703	C642	D579	IS13	S449	V385	VAL
E1161	S1091	R1029	G963	W897	A896	L771	R704	G643	A580	LS14	I452	L387	VAL
	G1092	G1030	L964	E898	E833	S771	A705	G644	E581	E515	I453	H388	GLU
	Y1093	N1031		E899	S772	P772	T706	P645	L582	A516	A454	H389	LYS
	L1094	P1032		S835	S773	A773	T707	K646	D583	V517	A455	P390	VAL
	T1095	Q1033		V936	S774	S774	L708	K647	N584	P518	R455	A391	GLU
	R1096	Q1034		G837	G775	G775	H709	K648	G585	V519	M456	A392	LEU
	R1097	Q1035		G838	E776	E776	R710	K649	R586	L520	G457	S992	GLU
	L1098	R1036		L839	R777	P777	L711	E650		P521	A458	L393	GLU
	V1099	Q1037		D903	L840		G712	E651	A589	P522	E459	L394	GLY
	D1100	L1038		Q901	R841	A779	I713	L652	P590	D523	A460	V395	ALA
	V1101	G1039		Q906	Y841	R780	Q714	E653	V591	L524	I461	V396	PHE
	T1102	G1040		K908	V842	P781	A715	K654	E592	R525	Q462	K397	LEU
	H1173	L1041		K908	F843	S782		P655	N593	P525	Q463	A398	VAL
	L1174	R1042		N909	F844	R783	F716	P656	E594	VAL	L465	R399	LEU
	L1175	G1043		S910	N845	D784	Q717	L657	G595	GLN	K466	Y401	ARG
	K1176	L1044		K912	P846	I785	P718	L658	S596	VAL	D469	Y402	ARG
		M1045		D913	D847	I786	V719	K659		VAL	L470	F403	ASP
		Q1046		L914	E848	I786	L720	K660	L600	ASP	E471	F404	GLY
				V915	A849	L787	V721	M661	R601	GLY	A472	D405	GLY
				A918	L850	L788		E662	S602	ARG	A473	D406	PRO
					L851	L789	Q724	E663	L603	ARG	E474	D407	VAL
					A852	Y790	S725	K664	T604	PHE	E475	V407	THR
					V853	Y791	I726	G665	D605	ALA	E476	E408	THR
					A854	I792	Q727	I666	L606	THR	K475	V409	TYR
					H855	T793	L728	A667	L607	SS38	E476	S410	PHE
					G856	Q794	H729	P668	S608	GLY	L477	T411	LEU
					V858	V795	P730	N669	G609	THR	L478	G412	PRO
					D859	V796	L731	K670	K610	ALA	E479	D413	VAL
					R860	E798	V732	K671	G611	ALA	E480	R414	VAL
					L860	K300	C733	A672	G612	LYS	M481	V415	GLY
					Q861	G801	E734	A673	R613	THR	K482	A416	THR
					D862	A735	A735	R674	F614	THR	H483	P417	PRO
					V863	F736	N737	R675	R615	THR	P484	G418	LEU
					L864	R803	R803	M676	G616	THR	S485	D419	VAL
					T865	L804	A738	L677	N617	THR	R486	V420	VAL
					V866	E805	D739	E678	L618	THR	R489	L421	HIS
					R867	F806	F740	R679	L619	THR	A492	D422	GLY
					Y868	A807	D743	Q680	G620	THR	R493	D423	GLY
					M869	T808	Q744	R681	K621	THR	K494	G424	ILE
						P809	M745	D682	R622	THR	R495	V427	VAL
					R872	E811	A746	L683	V623	THR	K496	V361	LYS
					T875	A812	V747	K684	D624	THR	L496	E362	GLY
					S876	L813	H748	D685	Y625	THR	E497	V431	GLN
					P877	A814	V749	E686	S626	THR	V498	Y432	PRO
					G878	A815	P750	V687	G627	THR	V499	G433	LEU
					R879	H816	F754	W688	R628	THR	R500	K366	ALA
					L881	R818	A755	A690	S629	THR	V435	I367	ALA
					F882	G819	Q756	L691	V630	THR	A501	V368	GLU
					I885	E820	A757	E692	V631	THR	F502	E436	ALA
					E888	V821	E758	V694	G634	THR	L503	D438	LYS
					A889		A759	V694	E634	THR	D504		GLY
					V890		Q762	L695	K571	THR	S505	E376	LEU
					E891		M763	P635	R572	THR	G506	V377	LEU
					E892		L764	Q636	M573	THR	N607	I378	ARG
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					E894		L765	K638	Q575	THR	P509	R445	PRO
					E895		A766	L639	E576	THR	E510	V446	ARG
					E896			V700	E576	THR	A577		GLN
					E897			L701	H640	THR	W511	V447	



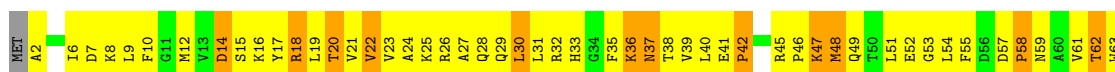
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L1395	Q1334	L1209	G1080	N1018	Y146	G1080	N1018	E821	A757	H696	R569
L1396	L1335	S1210	T1084	P1019	R147	T1084	P1019	E822	E758	H697	E570
K1397	L1336	M1211	T1084	L1020	R147	T1084	P1019	E823	A759	E698	K571
V1398	E1337	A1212	L1086	Y1021	L148	A1086	Y1021	E824	V699	K698	R572
D1399	L1338	R1213	L1086	Y1022	L149	A1086	Y1022	E825	Q762	V700	M573
V1400	L1339	P1214	E1087	M1023	A1150	P1214	M1023	E826	W763	L701	L574
E1401	G1340	S1215	T1088	A1024	A1151	T1088	A1024	E827	L764	L702	Q575
A1402	P1341	S1216	S1091	Q1025	E1152	S1091	Q1025	E828	S765	N703	E576
L1403	G1342	T1217	G1092	S1026	E1153	G1092	S1026	E829	A766	R704	A577
N1404	E1345	G1218	G1092	G1027	E1154	E1092	G1027	E830	G643	A705	V578
E1405	R1346	E1219	Y1093	A1028	E1155	Y1093	A1028	E831	L644	P706	D579
R1406	E1347	A1220	L1094	R1028	L1156	L1094	R1028	E832	K645	T707	A580
L1407	Y1347	V1221	T1095	G1030	L1156	T1095	G1030	E833	K646	L707	L581
E1410	L1348	G1222	R1096	M1031	E1161	R1096	M1031	E834	R647	R710	L582
V1411	V1349	I1223	K1097	P1032	E1162	K1097	P1032	E835	A648	L711	D583
G1412	E1350	V1224	L1098	Q1033	G1163	L1098	Q1033	E836	L650	G712	N584
L1413	L1351	A1225	L1098	Q1034	R1164	L1098	Q1034	E837	E651	G713	G585
P1414	I1352	A1226	D1100	I1035	V1165	D1100	I1035	E838	L652	W714	R586
V1415	Q1353	L1290	V1101	R1036	L1166	V1101	R1036	E839	F653	A715	P590
K1354	K1354	S1291	T1102	Q1037	S1167	T1102	Q1037	E840	A779	F716	V591
A1416	V1355	F1292	H1103	L1038	M1168	H1103	L1038	E841	K780	K717	T592
W1417	L1356	F1293	E1104	C1039	D1169	E1104	C1039	E842	P781	Q718	N593
K1418	R1357	V1294	T1105	G1040	D1170	T1105	G1040	E843	S782	F718	P594
P1419	A1358	E1295	V1106	L1041	V1171	V1106	L1041	E844	R783	W719	
L1420	Q1359	S1296	V1107	R1042	H1172	V1107	R1042	E845	D784	L720	
G1360	V1360	E1297	R1108	G1043	L1173	R1108	G1043	E846	L785	W721	
L1421	L1361	G1298	E1109	L1044	L1174	E1109	L1044	E847	R786	E722	R598
M1422	K1362	F1299	A1110	M1045	K1175	A1110	M1045	E848	L787	G723	P599
G1423	L1363	S1300	D1111	Q1046	K1176	D1111	Q1046	E849	G788	Q724	L600
H1424	H1364	K1301	C1112	Q1047	A1177	C1112	Q1047	E850	L789	S725	R601
K1425	K1365	E1302	G1113	P1048	E1178	G1113	P1048	E851	Y790	W726	S602
S1427	K1366	L1303	T1114	S1049	E1179	T1114	S1049	E852	Y791	Q727	L603
A1428	H1367	K1304	T1115	G1050	E1182	T1115	G1050	E853	L792	L726	T604
L1429	L1368	L1305	N1116	E1051	I1183	N1116	E1051	E854	W793	H729	D605
E1369	E1369	P1306	Y1117	T1052	I1184	Y1117	T1052	E855	A697	P730	L606
T1430	S1370	K1307	L1118	F1053	Q1184	L1118	F1053	E856	N669	W731	L607
K1432	V1371	L1307	S1119	E1054	E1185	S1119	E1054	E857	V670	V732	S608
L1433	V1372	L1307	V1120	V1055	V1186	V1120	V1055	E858	K671	C733	
W1434	Q1374	L1312	P1121	P1056	P1187	P1121	P1056	E859	A672	E734	G612
L1435	M1375	V1313	L1122	V1057	V1188	L1122	V1057	E860	A673	A735	R613
A1438	K1376	D1251	F1123	R1058	R1189	F1123	R1058	E861	M676	F736	F614
S1439	F1440	L1252	Q1124	S1059	S1190	Q1124	S1059	E862	L677	N737	R615
N1441	Q1441	T1253	P1125	T1060	P1191	P1125	T1060	E863	E678	A738	Q616
T1443	G1377	L1315	D1126	F1061	L1192	D1126	F1061	E864	L679	D739	N617
G1444	V1378	G1316	E1127	R1062	T1193	E1127	R1062	E865	R679	F740	L618
L1447	E1380	D1317	V1128	E1063	C1194	V1128	E1063	E866	Q680	D741	L619
T1448	V1381	L1319	T1129	G1064	Q1195	T1129	G1064	E867	R681	G742	G620
A1451	L1382	E1320	R1130	L1065	T1196	R1130	L1065	E868	D682	Q743	K621
I1452	D1383	A1321	S1131	T1066	R1197	S1131	T1066	E869	L683	W745	R622
A1453	P1384	Q1322	L1132	V1067	Y1198	L1132	V1067	E870	K684	A746	V623
G1454	G1385	P1324	R1135	L1068	G1199	R1135	L1068	E871	D685	V747	D624
L1455	S1387	L1325	K1136	E1069	V1200	K1136	E1069	E872	E686	W747	Y625
K1456	L1388	T1326	Q1202	V1070	C1201	Q1202	V1070	E873	V687	H748	S626
K1457	G1454	R1327	A1264	F1071	Q1202	A1264	F1071	E874	W688	V749	G627
K1458	L1389	R1327	L1137	I1072	K1203	L1137	I1072	E875	R689	R750	R628
K1459	L1390	R1266	D1139	S1073	C1204	D1139	S1073	E876	A814	A814	S629
K1459	E1391	R1267	T1140	S1074	Y1205	T1140	S1074	E877	L691	S752	V630
K1459	G1392	D1267	E1141	R1078	Y1207	E1141	R1078	E878	E692	S753	I631
E1458	Q1393	K1269	A1142			A1142		E879	V694	F754	V632
								E880			V633





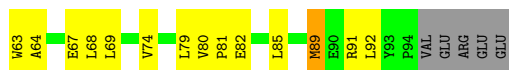
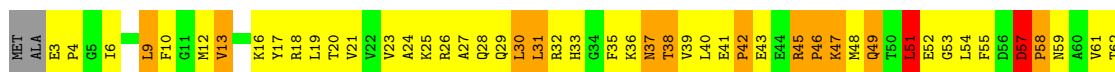
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 23% 58% 13% 6%



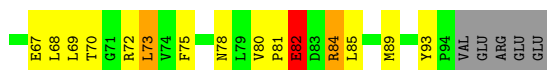
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain J: 30% 47% 13% • 7%

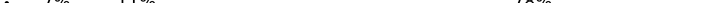


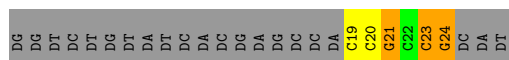
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain 0: 28% 51% 14% 6%

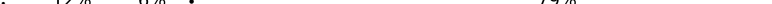


- Molecule 5: DNA (5'-D(*GP*GP*TP*CP*TP*GP*TP*AP*TP*CP*AP*CP*GP*AP*GP*CP*CP*AP*CP*CP*GP*CP*CP*GP*CP*AP*T)-3')

Chain P:  7% 11% 82%

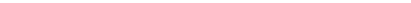


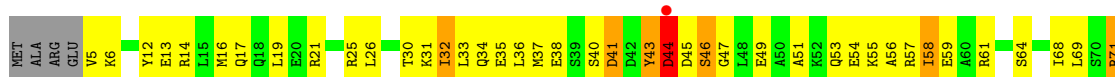
- Molecule 6: RNA (5'-R(*CP*CP*CP*CP*GP*GP*AP*AP*GP*AP*UP*CP*AP*UP*CP*UP*UP*CP*CP*GP*GP*GP*GP*GP*AP*U*GP*CP*GP*GP*CP*GP*G)-3')

Chain Q:  12% 6% . 79%



- Molecule 7: Anti-cleavage anti-GreA transcription factor Gfh1

Chain X:  37% 49% 9% . .



R147
E148
F149

V152
A153
I154
H155
G156

• Molecule 7: Anti-cleavage anti-GreA transcription factor Gfh1



MET ALA ARG GLU V5 K6 A10 G11 Y12 E13 R14 Q17 Q18 L19 E20 R21 E22 R23 L26 Q27 E28 A29 T30 K31 I32 L33 Q34 E35 L36 K37 S40 D41 D42 Y43 D44 S46 G47 L48 E49 A50 A51 K52 Q53 E54 K55 A56 R57 I58 E59 A60 R61 I62 I68

R71 A72 V73 I74 L75 E76 E77 G84 L85 V89 E90 L91 E92 S96 G97 E98 R99 V102 Q103 V104 V105 S106 P107 A108 E109 A110 N111 V112 L113 D114 T115 P116 M117 K118 T119 S120 D121 S123 A122 L123 P124 M125 G126 K127 A128 L129 L130 R133 V134 G135 D136 V137 L138 S139 D141

T142 P143 K144 G145 R146 R147 E148 F149 R150 V151 V152 A153 I154 H155 G156

• Molecule 7: Anti-cleavage anti-GreA transcription factor Gfh1



MET ALA ARG GLU K6 L7 A10 G11 Y12 E13 R14 L15 R16 Q17 E20 R21 E22 R25 E28 A29 T30 K31 I32 L33 Q34 E35 L36 K37 S38 E39 S40 D41 D42 Y43 D44 S46 G47 L48 E49 K52 Q53 E54 K55 A56 R57 I58 E59 A60 R61 I62 D63 S64 L65

E66 D67 I68 L69 S70 R71 A72 V73 I74 L75 E76 E77 G78 S79 G80 E81 V82 I83 G84 L85 V88 V89 E90 L91 E92 E98 R99 V102 Q103 V104 P107 A108 E109 A110 N111 V112 L113 D114 T115 P116 M117 K118 T119 S120 D121 S123 A122 L123 P124 M125 G126 K127 A128 L129 L130 H132

R133 V134 G135 D136 V137 L138 S139 D141 R146 R147 E148 F149 V152 A153 I154 H155 G156

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	192.76Å 260.70Å 198.56Å 90.00° 117.58° 90.00°	Depositor
Resolution (Å)	49.87 – 4.10 49.87 – 4.10	Depositor EDS
% Data completeness (in resolution range)	96.9 (49.87-4.10) 96.9 (49.87-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 4.14Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.262 , 0.318 0.271 , 0.324	Depositor DCC
R_{free} test set	3932 reflections (2.98%)	wwPDB-VP
Wilson B-factor (Å ²)	136.4	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 118.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	74250	wwPDB-VP
Average B, all atoms (Å ²)	171.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.77% 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, 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	0.56	0/1791	1.10	10/2436 (0.4%)
1	B	0.57	0/1791	1.10	10/2436 (0.4%)
1	F	0.57	1/1782 (0.1%)	1.13	10/2425 (0.4%)
1	G	0.60	0/1791	1.09	10/2436 (0.4%)
1	K	0.56	1/1782 (0.1%)	1.09	14/2425 (0.6%)
1	L	0.54	0/1791	1.10	13/2436 (0.5%)
2	C	0.62	0/8900	1.24	86/12038 (0.7%)
2	H	0.65	1/8876 (0.0%)	1.25	97/12006 (0.8%)
2	M	0.59	0/8896	1.20	86/12033 (0.7%)
3	D	0.61	1/10832 (0.0%)	1.21	118/14638 (0.8%)
3	I	0.62	2/10351 (0.0%)	1.21	89/13979 (0.6%)
3	N	0.61	0/10848	1.20	109/14658 (0.7%)
4	E	0.55	0/768	1.08	2/1035 (0.2%)
4	J	0.57	0/763	1.13	4/1028 (0.4%)
4	O	0.74	1/768 (0.1%)	1.26	5/1035 (0.5%)
5	P	0.56	0/133	1.21	2/202 (1.0%)
6	Q	0.80	0/170	0.93	1/265 (0.4%)
7	X	0.53	0/1178	1.02	4/1582 (0.3%)
7	Y	0.53	0/1178	1.08	8/1582 (0.5%)
7	Z	0.51	0/1178	1.08	7/1582 (0.4%)
All	All	0.61	7/75567 (0.0%)	1.19	685/102257 (0.7%)

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	H	0	1
2	M	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	I	0	1
3	N	0	1
5	P	0	1
6	Q	0	1
7	Z	0	1
All	All	0	9

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	51	LEU	C-O	-6.79	1.16	1.23
1	K	12	THR	CA-CB	6.02	1.63	1.53
2	H	972	VAL	CA-CB	-5.49	1.47	1.54
3	I	800	LYS	CA-C	-5.44	1.45	1.52
1	F	76	VAL	CA-CB	-5.36	1.47	1.54

The worst 5 of 685 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	143	ASN	N-CA-C	-15.09	95.74	114.75
3	I	143	ASN	N-CA-C	-14.81	96.09	114.75
3	D	1209	LEU	N-CA-C	-14.11	89.14	109.18
3	N	1209	LEU	N-CA-C	-14.07	89.20	109.18
3	I	1209	LEU	N-CA-C	-13.70	89.72	109.18

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	258	TYR	Sidechain
2	C	71	TYR	Sidechain
2	H	71	TYR	Sidechain
3	I	1070	TYR	Sidechain
2	M	258	TYR	Sidechain

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	1759	0	1805	218	0
1	B	1759	0	1805	230	0
1	F	1750	0	1792	264	0
1	G	1759	0	1805	237	0
1	K	1750	0	1792	202	0
1	L	1759	0	1805	200	0
2	C	8733	0	8834	1435	1
2	H	8710	0	8811	1470	2
2	M	8729	0	8831	1433	0
3	D	10651	0	10880	1804	2
3	I	10182	0	10418	1590	0
3	N	10667	0	10894	1687	1
4	E	754	0	769	100	0
4	J	749	0	764	110	0
4	O	754	0	769	110	0
5	P	120	0	67	10	0
6	Q	152	0	78	7	0
7	X	1169	0	1186	116	0
7	Y	1169	0	1186	132	0
7	Z	1169	0	1186	152	0
8	D	1	0	0	0	0
8	I	1	0	0	0	0
8	N	1	0	0	0	0
9	D	1	0	0	0	0
9	I	1	0	0	0	0
9	N	1	0	0	0	0
All	All	74250	0	75477	10688	3

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 71.

The worst 5 of 10688 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)
2:H:282:GLY:O	2:H:283:ILE:HG13	1.34	1.25
3:D:1093:TYR:OH	3:D:1097:LYS:HE3	1.07	1.25
3:D:1093:TYR:OH	3:D:1097:LYS:CE	1.85	1.23
2:C:987:ILE:HG23	3:D:948:THR:HG21	1.20	1.20
3:I:108:VAL:HB	3:I:109:PRO:HD3	1.20	1.19

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:223:ASP:O	3:N:562:ALA:O[2_647]	1.66	0.54
3:D:562:ALA:O	2:H:223:ASP:O[2_646]	2.02	0.18
3:D:159:ARG:O	2:H:209:ARG:NH1[2_646]	2.15	0.05

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	221/315 (70%)	181 (82%)	33 (15%)	7 (3%)	3	24
1	B	221/315 (70%)	188 (85%)	28 (13%)	5 (2%)	5	31
1	F	220/315 (70%)	182 (83%)	32 (14%)	6 (3%)	4	28
1	G	221/315 (70%)	190 (86%)	27 (12%)	4 (2%)	6	35
1	K	220/315 (70%)	183 (83%)	29 (13%)	8 (4%)	2	22
1	L	221/315 (70%)	189 (86%)	26 (12%)	6 (3%)	4	28
2	C	1102/1119 (98%)	873 (79%)	169 (15%)	60 (5%)	1	17
2	H	1099/1119 (98%)	882 (80%)	157 (14%)	60 (6%)	1	17
2	M	1101/1119 (98%)	892 (81%)	150 (14%)	59 (5%)	1	17
3	D	1341/1524 (88%)	1055 (79%)	221 (16%)	65 (5%)	2	18
3	I	1281/1524 (84%)	1006 (78%)	216 (17%)	59 (5%)	2	19
3	N	1343/1524 (88%)	1068 (80%)	211 (16%)	64 (5%)	2	18
4	E	91/99 (92%)	71 (78%)	15 (16%)	5 (6%)	1	17
4	J	90/99 (91%)	71 (79%)	14 (16%)	5 (6%)	1	17
4	O	91/99 (92%)	70 (77%)	16 (18%)	5 (6%)	1	17
7	X	150/156 (96%)	119 (79%)	26 (17%)	5 (3%)	3	24
7	Y	150/156 (96%)	121 (81%)	26 (17%)	3 (2%)	6	33
7	Z	150/156 (96%)	123 (82%)	21 (14%)	6 (4%)	2	21
All	All	9313/10584 (88%)	7464 (80%)	1417 (15%)	432 (5%)	2	19

5 of 432 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	GLU
1	A	226	SER
2	C	44	ILE
2	C	80	GLN
2	C	152	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	196/273 (72%)	171 (87%)	25 (13%)	4	19
1	B	196/273 (72%)	168 (86%)	28 (14%)	3	16
1	F	195/273 (71%)	158 (81%)	37 (19%)	1	10
1	G	196/273 (72%)	156 (80%)	40 (20%)	1	8
1	K	195/273 (71%)	168 (86%)	27 (14%)	3	17
1	L	196/273 (72%)	167 (85%)	29 (15%)	3	15
2	C	932/941 (99%)	716 (77%)	216 (23%)	1	5
2	H	930/941 (99%)	729 (78%)	201 (22%)	1	6
2	M	932/941 (99%)	741 (80%)	191 (20%)	1	8
3	D	1142/1279 (89%)	936 (82%)	206 (18%)	2	11
3	I	1092/1279 (85%)	902 (83%)	190 (17%)	2	12
3	N	1143/1279 (89%)	955 (84%)	188 (16%)	2	13
4	E	82/88 (93%)	69 (84%)	13 (16%)	2	14
4	J	82/88 (93%)	68 (83%)	14 (17%)	2	12
4	O	82/88 (93%)	69 (84%)	13 (16%)	2	14
7	X	128/131 (98%)	110 (86%)	18 (14%)	3	17
7	Y	128/131 (98%)	107 (84%)	21 (16%)	2	13
7	Z	128/131 (98%)	109 (85%)	19 (15%)	3	15
All	All	7975/8955 (89%)	6499 (82%)	1476 (18%)	1	10

5 of 1476 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	I	1305	LEU
2	M	635	THR
3	I	1492	LEU
3	I	1304	LYS
2	M	91	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 268 such sidechains are listed below:

Mol	Chain	Res	Type
3	N	616	GLN
3	N	762	GLN
7	X	27	GLN
1	G	38	ASN
1	F	213	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	Q	6/33 (18%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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 6 ligands modelled in this entry, 6 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	223/315 (70%)	0.22	2 (0%) 81 65	81, 153, 225, 265	0
1	B	223/315 (70%)	0.18	4 (1%) 67 51	97, 154, 223, 265	0
1	F	222/315 (70%)	-0.03	0 100 100	84, 150, 216, 265	0
1	G	223/315 (70%)	0.12	2 (0%) 81 65	85, 150, 216, 248	0
1	K	222/315 (70%)	0.06	1 (0%) 87 74	110, 167, 229, 262	0
1	L	223/315 (70%)	0.10	3 (1%) 75 58	103, 164, 222, 265	0
2	C	1106/1119 (98%)	0.22	32 (2%) 53 40	70, 158, 243, 265	0
2	H	1103/1119 (98%)	0.30	35 (3%) 50 38	73, 155, 251, 267	0
2	M	1105/1119 (98%)	0.26	32 (2%) 53 40	79, 166, 255, 265	0
3	D	1349/1524 (88%)	0.21	24 (1%) 67 51	74, 171, 259, 267	0
3	I	1289/1524 (84%)	0.21	26 (2%) 65 49	70, 173, 259, 267	0
3	N	1351/1524 (88%)	0.23	29 (2%) 63 48	76, 167, 254, 267	0
4	E	93/99 (93%)	0.15	0 100 100	114, 183, 262, 265	0
4	J	92/99 (92%)	0.08	0 100 100	92, 176, 254, 265	0
4	O	93/99 (93%)	0.07	0 100 100	99, 173, 246, 265	0
5	P	6/27 (22%)	1.19	0 100 100	198, 198, 198, 198	0
6	Q	7/33 (21%)	0.86	0 100 100	188, 198, 198, 198	0
7	X	152/156 (97%)	0.06	1 (0%) 84 69	105, 187, 241, 267	0
7	Y	152/156 (97%)	0.14	1 (0%) 84 69	99, 186, 246, 267	0
7	Z	152/156 (97%)	0.09	0 100 100	109, 171, 248, 267	0
All	All	9386/10644 (88%)	0.21	192 (2%) 65 49	70, 166, 252, 267	0

The worst 5 of 192 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	271	GLU	5.7
2	H	1091	GLU	4.6
2	M	1084	SER	4.5
2	C	271	GLU	4.4
2	C	269	LEU	4.3

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($\text{\AA}^2$)	Q<0.9
9	MG	N	2006	1/1	0.56	0.23	94,94,94,94	0
9	MG	I	2005	1/1	0.75	0.18	94,94,94,94	0
8	ZN	D	2001	1/1	0.98	0.04	94,94,94,94	0
9	MG	D	2004	1/1	0.99	0.06	94,94,94,94	0
8	ZN	I	2002	1/1	0.99	0.02	94,94,94,94	0
8	ZN	N	2003	1/1	0.99	0.05	94,94,94,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.