



wwPDB X-ray Structure Validation Summary Report ⓘ

May 30, 2020 – 02:22 pm BST

PDB ID : 1IW7
Title : Crystal structure of the RNA polymerase holoenzyme from *Thermus thermophilus* at 2.6Å resolution
Authors : RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2002-04-22
Resolution : 2.60 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

<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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

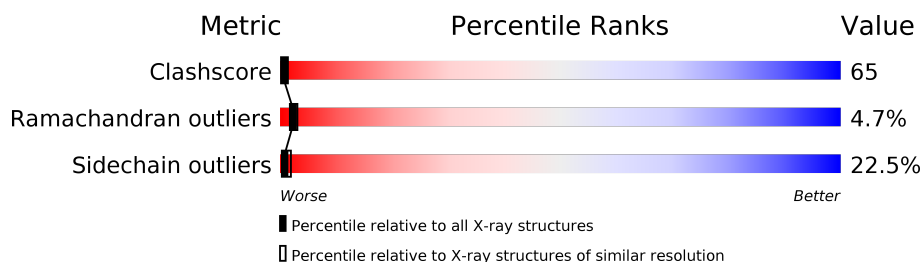
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	315	
1	B	315	
1	K	315	
1	L	315	
2	C	1119	
2	M	1119	
3	D	1524	
3	N	1524	

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Mol	Chain	Length	Quality of chain
4	E	99	<div><div></div><div>24%56%14%</div><div></div><div></div><div></div></div>
4	O	99	<div><div></div><div>24%60%11%</div><div></div><div></div><div></div></div>
5	F	423	<div><div></div><div>20%47%12%</div><div></div><div></div><div></div></div>
5	P	423	<div><div></div><div>21%44%14%</div><div></div><div></div><div></div></div>

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 59529 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 RNA polymerase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	B	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	K	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	L	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1119	Total	C	N	O	S	0	0	0
			8829	5581	1577	1647	24			
2	M	1119	Total	C	N	O	S	0	0	0
			8829	5581	1577	1647	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1392	Total	C	N	O	S	0	0	0
			10801	6823	1925	2020	33			
3	N	1392	Total	C	N	O	S	0	0	0
			10801	6823	1925	2020	33			

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

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

- Molecule 5 is a protein called RNA polymerase sigma-70 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	345	Total	C	N	O	S	0	0	0
			2771	1744	504	519	4			
5	P	345	Total	C	N	O	S	0	0	0
			2771	1744	504	519	4			

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	22	Total	Mg	0	0
			22	22		
6	D	118	Total	Mg	0	0
			118	118		
6	K	20	Total	Mg	0	0
			20	20		
6	E	6	Total	Mg	0	0
			6	6		
6	B	24	Total	Mg	0	0
			24	24		
6	C	63	Total	Mg	0	0
			63	63		
6	A	18	Total	Mg	0	0
			18	18		
6	N	92	Total	Mg	0	0
			92	92		
6	O	8	Total	Mg	0	0
			8	8		
6	L	19	Total	Mg	0	0
			19	19		
6	F	31	Total	Mg	0	0
			31	31		
6	M	64	Total	Mg	0	0
			64	64		

- Molecule 7 is LEAD (II) ION (three-letter code: PB) (formula: Pb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	2	Total	Pb	0	0
			2	2		
7	N	2	Total	Pb	0	0
			2	2		

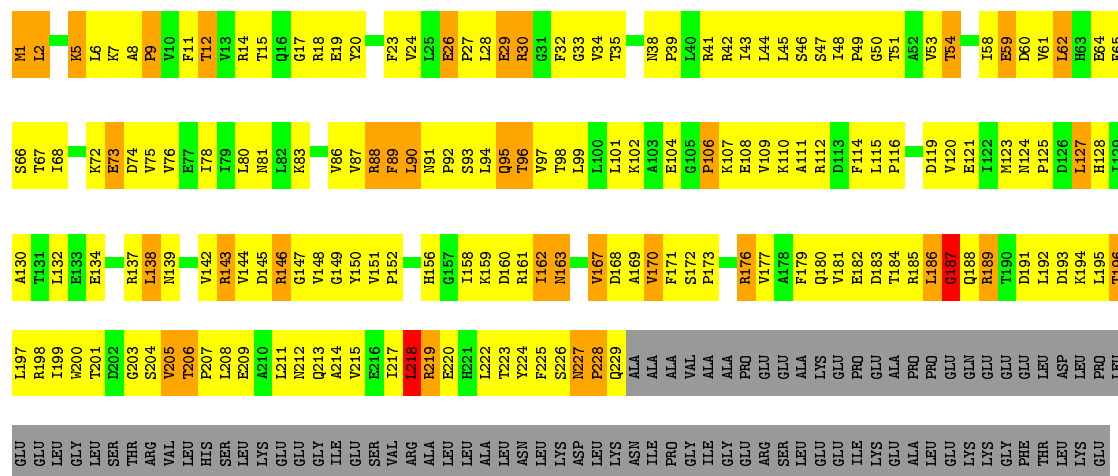
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	194	Total 194	O 194	0	0
8	B	193	Total 193	O 193	0	0
8	C	869	Total 869	O 869	0	0
8	D	1163	Total 1163	O 1163	0	0
8	E	114	Total 114	O 114	0	0
8	F	381	Total 381	O 381	0	0
8	K	161	Total 161	O 161	0	0
8	L	157	Total 157	O 157	0	0
8	M	822	Total 822	O 822	0	0
8	N	983	Total 983	O 983	0	0
8	O	114	Total 114	O 114	0	0
8	P	325	Total 325	O 325	0	0

VAL LEU HIS SER LYS LEU GLU GLY ILE GLU VAL ARG ALA LEU LEU ASN LEU LEU LYS ASP LYS LEU LYS ASN ILE PRO GLY ILE GLY GLU ANG SER LEU GLU TLE TLE

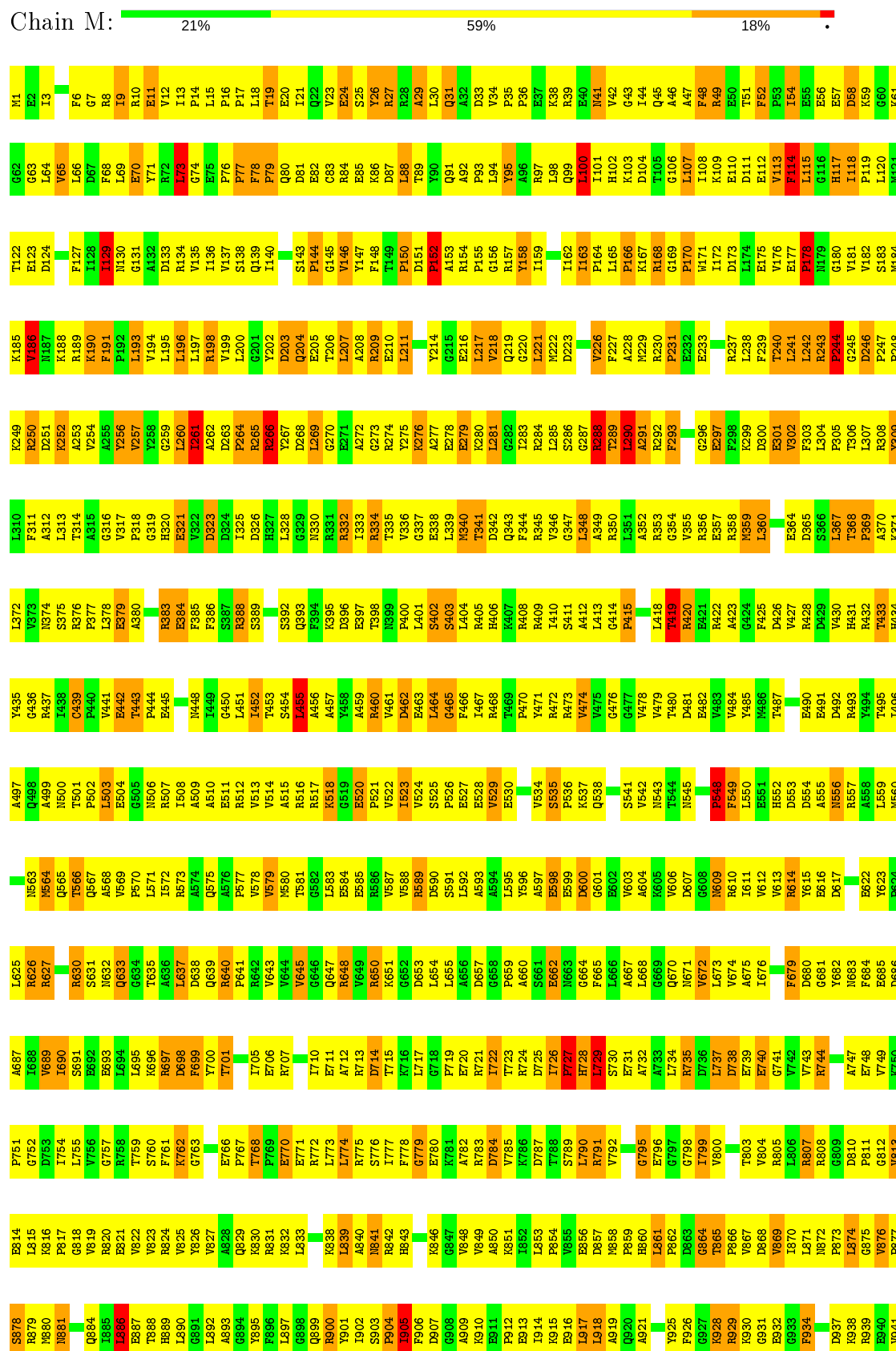
• Molecule 1: RNA polymerase alpha subunit

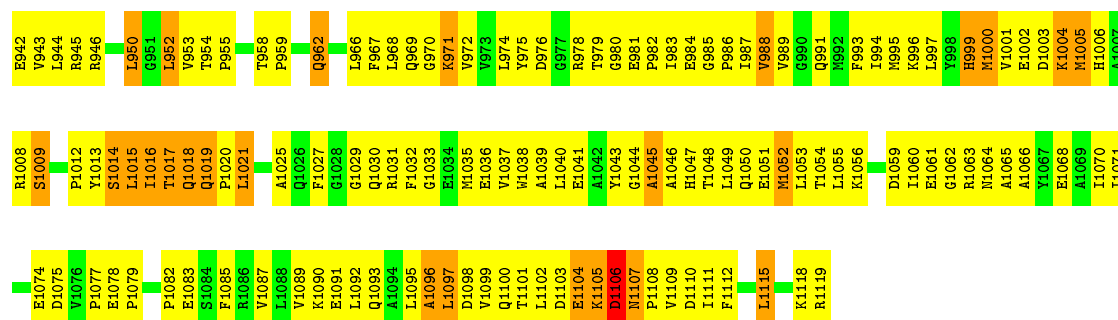
Chain K: 17% 43% 11% 27%



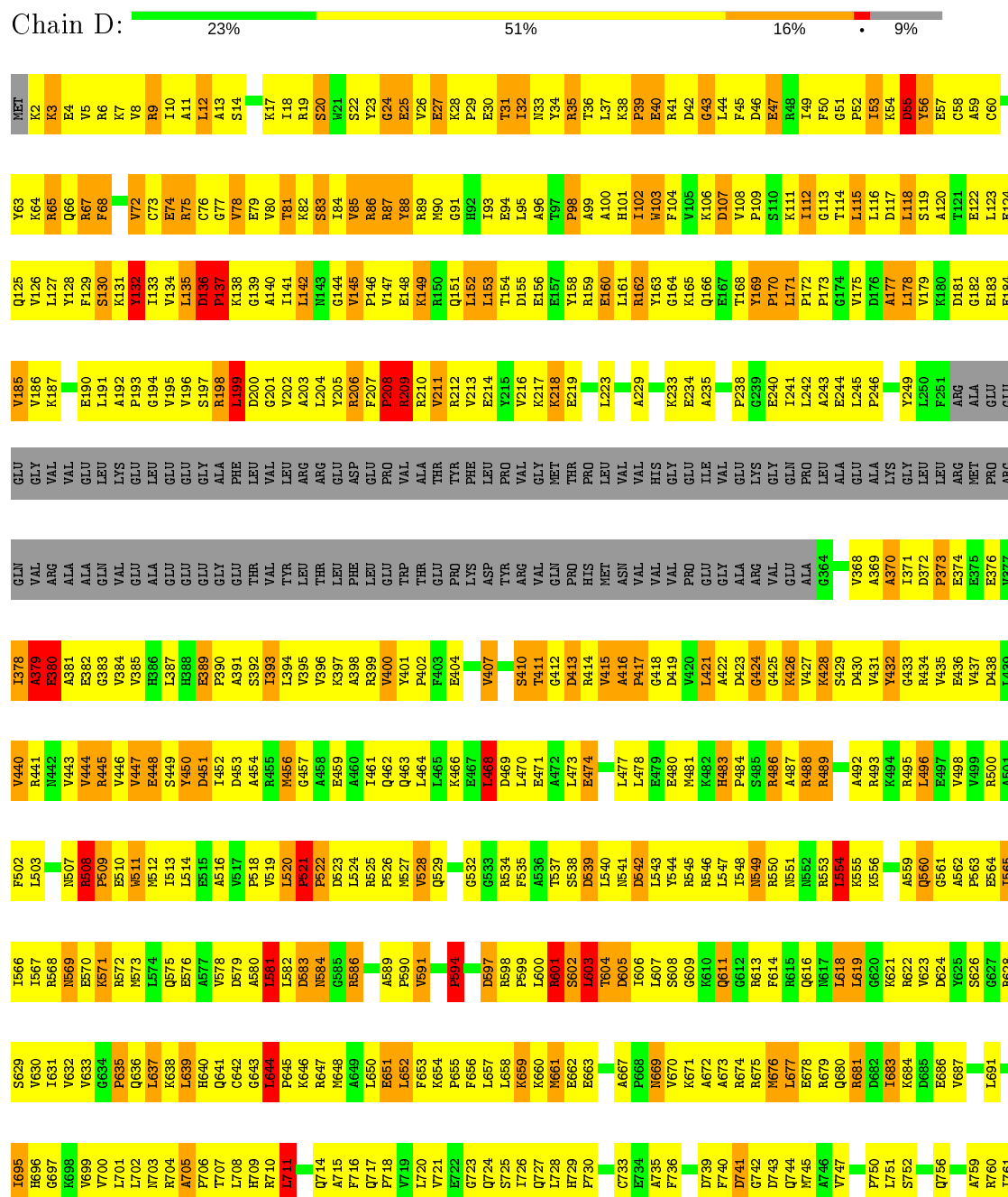
Q1093	A1094	L1095	A1096	L1097	D1098	V1099	Q1100	T1101	L1102	D1103	E1104	K1105	D1106	M1107	P1108	V1109	I1110	F1111	F1112	L1115	A1116	S1117	K1118	R1119
L966	F967	L968	Q969	G970	K971	Y975	D976	G977	R978	Q979	G980	E981	P982	R983	E984	G985	P986	L987	V988	G989	Q990	Q991	L992	F993
L1031	F1032	G1033	E1034	L1035	E1036	V1037	A1038	A1039	L1040	E1041	A1042	L1043	L1044	E1045	A1046	H1047	T1048	L1049	Q1050	E1051	M1052	L1053	T1054	L1055
L1063	A1064	A1065	A1066	Y1067	I1070	L1071	K1072	G1073	E1074	D1075	L1076	P1077	E1078	P1079	S1080	L1081	P1082	E1083	S1084	F1085	L1086	V1087	L1088	V1089
Q1093	A1094	L1095	A1096	L1097	D1098	V1099	Q1100	T1101	L1102	D1103	E1104	K1105	D1106	M1107	P1108	V1109	I1110	F1111	F1112	L1115	A1116	S1117	K1118	R1119
L966	F967	L968	Q969	G970	K971	Y975	D976	G977	R978	Q979	G980	E981	P982	R983	E984	G985	P986	L987	V988	G989	Q990	Q991	L992	F993
L1031	F1032	G1033	E1034	L1035	E1036	V1037	A1038	A1039	L1040	E1041	A1042	L1043	L1044	E1045	A1046	H1047	T1048	L1049	Q1050	E1051	M1052	L1053	T1054	L1055
L1063	A1064	A1065	A1066	Y1067	I1070	L1071	K1072	G1073	E1074	D1075	L1076	P1077	E1078	P1079	S1080	L1081	P1082	E1083	S1084	F1085	L1086	V1087	L1088	V1089
K188	R189	K190	F191	L192	P193	V194	L195	L196	I197	L198	V199	L200	E201	Y202	D203	Q204	E205	T206	L207	A208	R209	E210	T211	L212
A253	V254	A255	L256	V257	Y258	G259	L260	L261	A262	D263	P264	R265	E266	R331	R332	I333	E334	T335	V336	G337	E338	L339	M340	T341
A315	G316	G319	R320	E321	V322	D323	D324	I325	D326	H327	L328	R331	S402	I333	E334	L404	R405	H406	R407	R408	R409	L410	S411	A412
K488	R489	K490	F491	L492	P493	V494	L495	L496	I497	L498	V499	L500	E501	Y502	D503	Q504	E505	T506	L507	A508	R509	E510	T511	L512
A523	V524	A525	L526	V527	Y528	G529	L530	L531	A532	D533	P534	R535	E536	R537	E538	E539	E540	E541	E542	E543	E544	E545	E546	E547
A583	V584	A585	L586	V587	Y588	G589	L590	L591	A592	D593	P594	R595	E596	R657	E658	L659	P660	T661	E662	R663	E664	F665	L666	G667
K688	R689	K690	F691	L692	P693	V694	L695	L696	I697	L698	V699	L700	E701	Y702	D703	Q704	E705	T706	L707	A708	R709	E710	T711	L712
A723	V724	A725	L726	V727	Y728	G729	L730	L731	A732	D733	P734	R735	E736	R737	E738	E739	E740	E741	E742	E743	E744	E745	E746	E747
A783	V784	A785	L786	V787	Y788	G789	L790	L791	A792	D793	P794	R795	E796	R857	E858	L859	P860	T861	E862	R863	E864	F865	L866	G867
K888	R889	K890	F891	L892	P893	V894	L895	L896	I897	L898	V899	L900	E901	Y902	D903	Q904	E905	T906	L907	A908	R909	E910	T911	L912
A923	V924	A925	L926	V927	Y928	G929	L930	L931	A932	D933	P934	R935	E936	R997	E998	L999	P1000	T1001	E1002	R1003	E1004	F1005	L1006	G1007
K1088	R1089	K1090	F1091	L1092	P1093	V1094	L1095	L1096	I1097	L1098	V1099	L1100	E1101	Y1102	D1103	Q1104	E1105	T1106	L1107	A1108	R1109	E1110	T1111	L1112
A1123	V1124	A1125	L1126	V1127	Y1128	G1129	L1130	L1131	A1132	D1133	P1134	R1135	E1136	R1197	E1198	L1199	P1200	T1201	E1202	R1203	E1204	F1205	L1206	G1207
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A1323	V1324	A1325	L1326	V1327	Y1328	G1329	L1330	L1331	A1332	D1333	P1334	R1335	E1336	R1397	E1398	L1399	P1400	T1401	E1402	R1403	E1404	F1405	L1406	G1407
K1488	R1489	K1490	F1491	L1492	P1493	V1494	L1495	L1496	I1497	L1498	V1499	L1500	E1501	Y1502	D1503	Q1504	E1505	T1506	L1507	A1508	R1509	E1510	T1511	L1512
A1523	V1524	A1525	L1526	V1527	Y1528	G1529	L1530	L1531	A1532	D1533	P1534	R1535	E1536	R1537	E1538	E1539	E1540	E1541	E1542	E1543	E1544	E1545	E1546	E1547
A1583	V1584	A1585	L1586	V1587	Y1588	G1589	L1590	L1591	A1592	D1593	P1594	R1595	E1596	R1657	E1658	L1659	P1660	T1661	E1662	R1663	E1664	F1665	L1666	G1667
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A1723	V1724	A1725	L1726	V1727	Y1728	G1729	L1730	L1731	A1732	D1733	P1734	R1735	E1736	R1737	E1738	E1739	E1740	E1741	E1742	E1743	E1744	E1745	E1746	E1747
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A3783	V3784	A3785	L3786	V3787	Y3788	G3789	L3790	L3791	A3792	D3793	P3794	R3795	E3796	R3857	E3858	L3859	P3860	T3861	E3862	R3863	E3864	F3865	L3866	G3867
K3888	R3889	K3890	F3891	L3892	P3893	V3894	L3895	L3896	I3897	L3898	V3899	L3900	E3901	Y3902	D3903	Q3904	E3905	T3906	L3907	A3908	R3909	E3910	T3911	L3912
A3923	V3924	A3925	L3926	V3927	Y3928	G3929	L3930	L3931	A3932	D3933	P3934	R3935	E3936	R3997	E3998	L3999	P4000	T4001	E4002	R4003	E4004	F4005	L4006	G4007
K4088	R4089																							

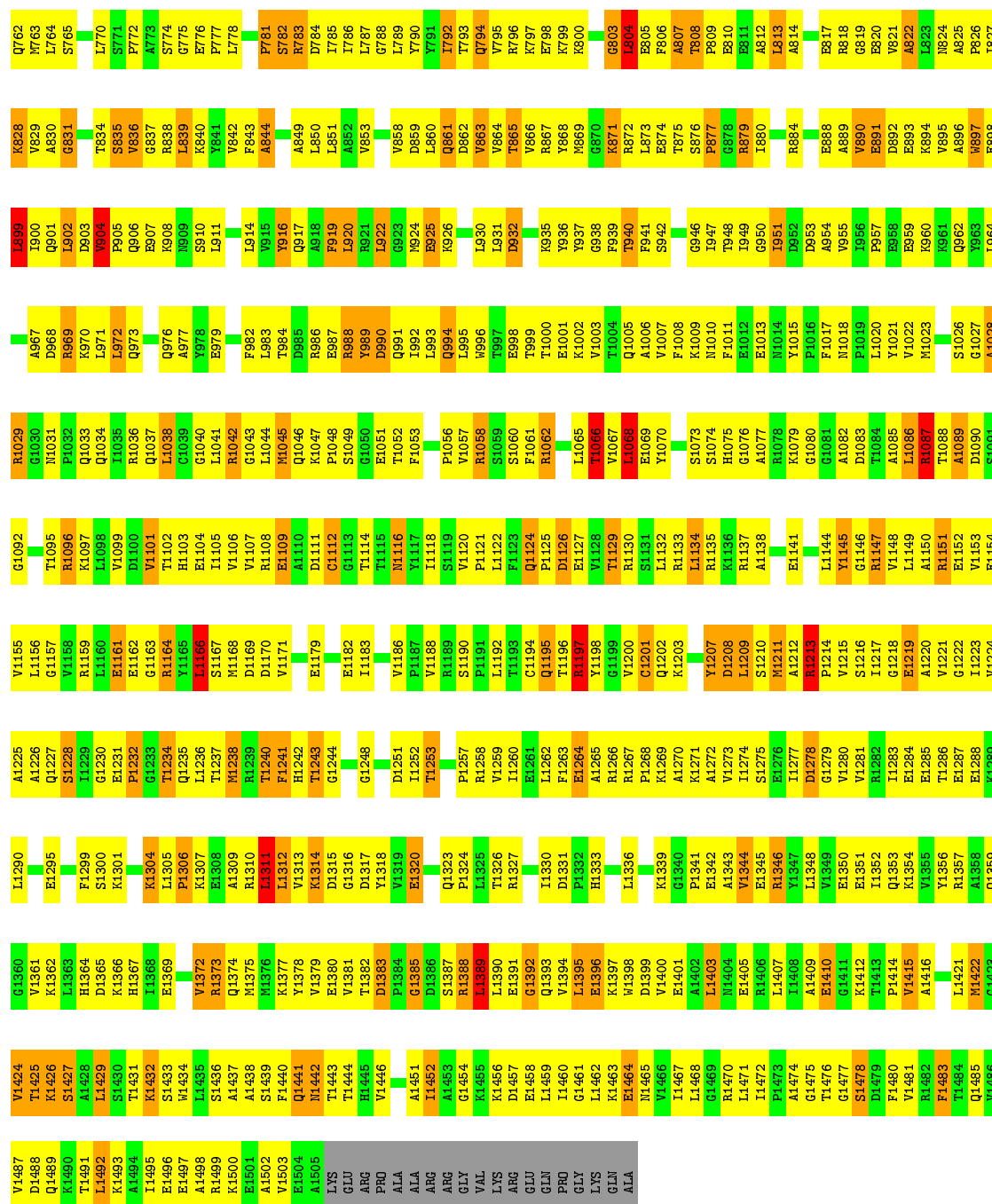
● Molecule 2: RNA polymerase beta subunit





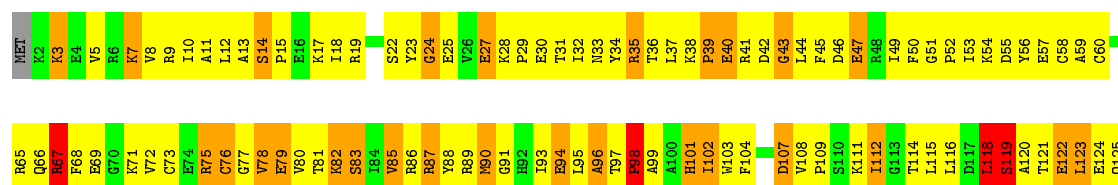
• Molecule 3: RNA polymerase beta subunit



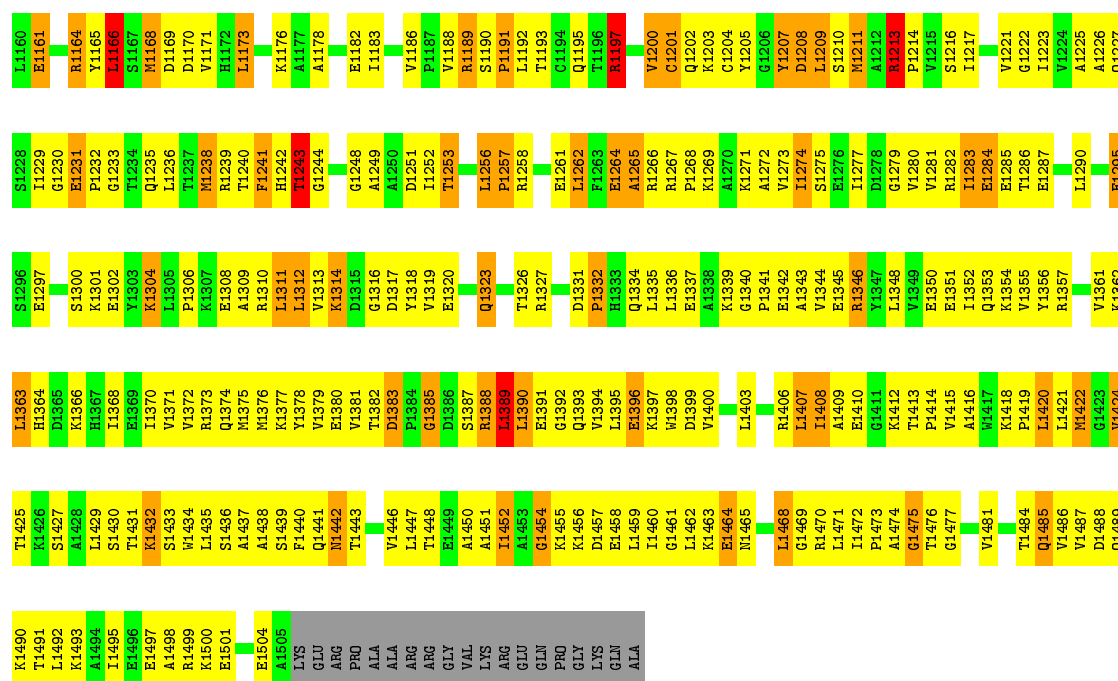


• Molecule 3: RNA polymerase beta subunit

Chain N: 23% 51% 16% 9%

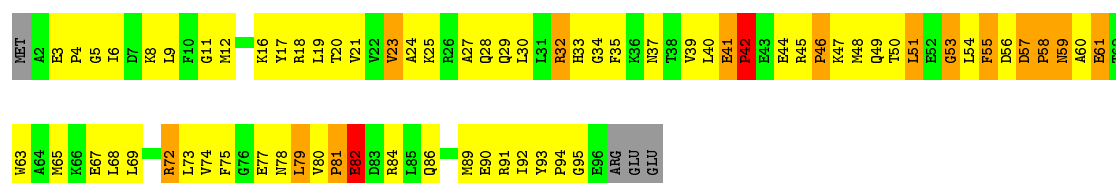


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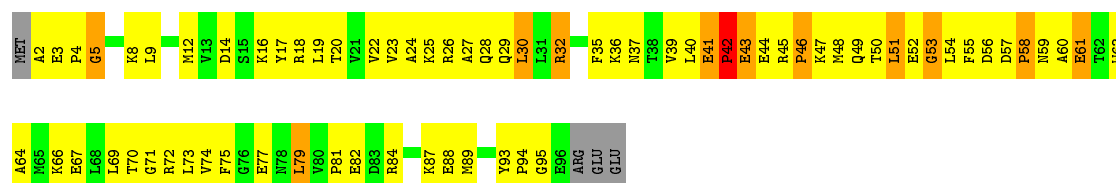
• Molecule 4: RNA polymerase omega subunit

Chain E: 24% 56% 14%



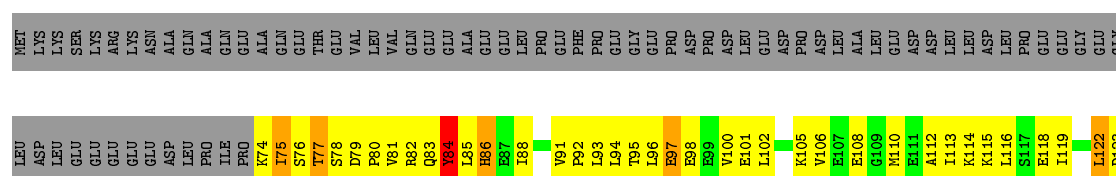
• Molecule 4: RNA polymerase omega subunit

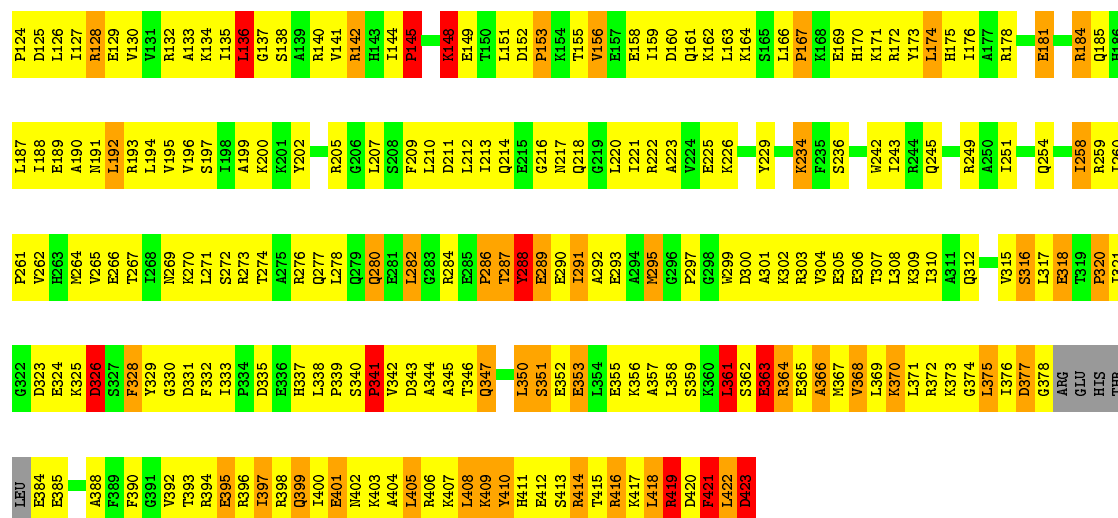
Chain O: 24% 60% 11%



• Molecule 5: RNA polymerase sigma-70 subunit

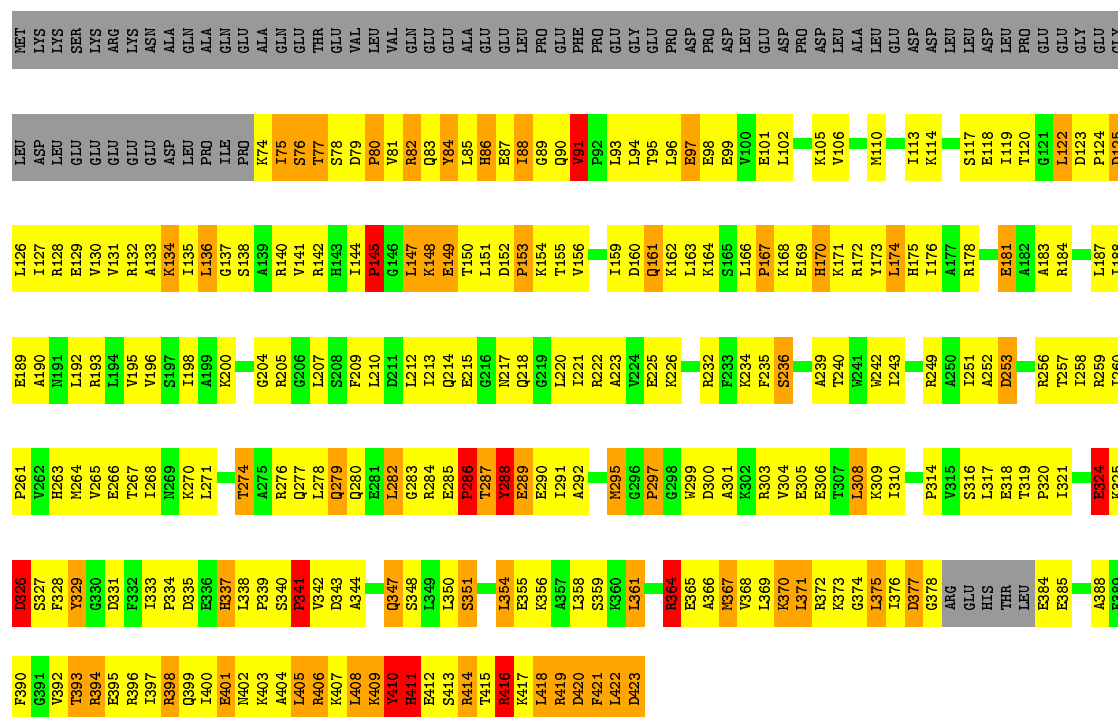
Chain F: 20% 47% 12% 18%





• Molecule 5: RNA polymerase sigma-70 subunit

Chain P: 21% 44% 14% 18%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	236.35Å 236.35Å 249.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.60)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.228 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	59529	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PB, 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	0.68	0/1838	0.87	4/2498 (0.2%)
1	B	0.68	0/1838	0.85	7/2498 (0.3%)
1	K	0.66	1/1838 (0.1%)	0.85	5/2498 (0.2%)
1	L	0.67	0/1838	0.90	4/2498 (0.2%)
2	C	0.72	3/8997 (0.0%)	0.97	30/12164 (0.2%)
2	M	0.73	2/8997 (0.0%)	0.97	26/12164 (0.2%)
3	D	0.71	8/10979 (0.1%)	1.01	52/14844 (0.4%)
3	N	0.73	6/10979 (0.1%)	1.02	38/14844 (0.3%)
4	E	0.72	0/783	1.01	2/1054 (0.2%)
4	O	0.71	0/783	1.02	2/1054 (0.2%)
5	F	0.90	8/2812 (0.3%)	1.08	20/3781 (0.5%)
5	P	0.85	4/2812 (0.1%)	1.12	20/3781 (0.5%)
All	All	0.73	32/54494 (0.1%)	0.99	210/73678 (0.3%)

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
3	D	0	3
3	N	0	3
5	F	0	1
All	All	0	7

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	401	GLU	CG-CD	13.42	1.72	1.51
5	F	401	GLU	CB-CG	13.27	1.77	1.52
5	P	401	GLU	CG-CD	13.01	1.71	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	401	GLU	CB-CG	12.94	1.76	1.52
5	F	423	ASP	C-OXT	11.47	1.45	1.23

The worst 5 of 210 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	229	GLN	CA-C-O	17.63	157.12	120.10
5	P	416	ARG	NE-CZ-NH1	13.69	127.14	120.30
2	C	243	ARG	C-N-CD	-12.01	94.19	120.60
2	M	163	ILE	C-N-CD	-11.12	96.14	120.60
3	D	380	GLU	CA-C-O	-11.07	96.85	120.10

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	132	TYR	Sidechain
3	D	379	ALA	Peptide
3	D	380	GLU	Mainchain
5	F	421	PHE	Sidechain
3	N	132	TYR	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	A	1806	0	1861	247	0
1	B	1806	0	1861	213	0
1	K	1806	0	1861	216	0
1	L	1806	0	1861	213	0
2	C	8829	0	8933	1312	0
2	M	8829	0	8933	1273	0
3	D	10801	0	10887	1543	0
3	N	10801	0	10885	1539	0
4	E	769	0	775	94	0
4	O	769	0	775	106	0
5	F	2771	0	2843	392	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	2771	0	2844	429	0
6	A	18	0	0	0	0
6	B	24	0	0	0	0
6	C	63	0	0	0	0
6	D	118	0	0	1	0
6	E	6	0	0	0	0
6	F	31	0	0	0	0
6	K	20	0	0	0	0
6	L	19	0	0	0	0
6	M	64	0	0	0	0
6	N	92	0	0	0	0
6	O	8	0	0	0	0
6	P	22	0	0	0	0
7	D	2	0	0	0	0
7	N	2	0	0	0	0
8	A	194	0	0	44	0
8	B	193	0	0	50	0
8	C	869	0	0	254	0
8	D	1163	0	0	325	0
8	E	114	0	0	30	0
8	F	381	0	0	67	0
8	K	161	0	0	49	0
8	L	157	0	0	52	0
8	M	822	0	0	266	0
8	N	983	0	0	291	0
8	O	114	0	0	30	0
8	P	325	0	0	75	0
All	All	59529	0	54319	7072	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 65.

The worst 5 of 7072 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)
5:F:419:ARG:CB	5:F:419:ARG:CG	1.76	1.60
5:P:401:GLU:CB	5:P:401:GLU:CG	1.76	1.56
5:F:401:GLU:CB	5:F:401:GLU:CG	1.77	1.55
3:N:218:LYS:CB	8:N:9902:HOH:O	1.85	1.18
1:A:94:LEU:HD21	1:A:119:ASP:HB2	1.26	1.16

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	227/315 (72%)	201 (88%)	21 (9%)	5 (2%)	6	12
1	B	227/315 (72%)	200 (88%)	24 (11%)	3 (1%)	12	24
1	K	227/315 (72%)	199 (88%)	24 (11%)	4 (2%)	8	16
1	L	227/315 (72%)	199 (88%)	25 (11%)	3 (1%)	12	24
2	C	1117/1119 (100%)	923 (83%)	139 (12%)	55 (5%)	2	2
2	M	1117/1119 (100%)	928 (83%)	135 (12%)	54 (5%)	2	2
3	D	1388/1524 (91%)	1119 (81%)	196 (14%)	73 (5%)	2	2
3	N	1388/1524 (91%)	1113 (80%)	200 (14%)	75 (5%)	2	2
4	E	93/99 (94%)	72 (77%)	13 (14%)	8 (9%)	1	0
4	O	93/99 (94%)	71 (76%)	15 (16%)	7 (8%)	1	1
5	F	341/423 (81%)	295 (86%)	31 (9%)	15 (4%)	2	3
5	P	341/423 (81%)	288 (84%)	34 (10%)	19 (6%)	2	2
All	All	6786/7590 (89%)	5608 (83%)	857 (13%)	321 (5%)	2	2

5 of 321 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	GLY
2	C	111	ASP
2	C	152	PRO
2	C	231	PRO
2	C	244	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	202/273 (74%)	165 (82%)	37 (18%)	1	2
1	B	202/273 (74%)	164 (81%)	38 (19%)	1	2
1	K	202/273 (74%)	160 (79%)	42 (21%)	1	2
1	L	202/273 (74%)	161 (80%)	41 (20%)	1	2
2	C	941/941 (100%)	730 (78%)	211 (22%)	1	1
2	M	941/941 (100%)	718 (76%)	223 (24%)	1	1
3	D	1123/1279 (88%)	865 (77%)	258 (23%)	1	1
3	N	1123/1279 (88%)	841 (75%)	282 (25%)	0	1
4	E	83/87 (95%)	68 (82%)	15 (18%)	1	2
4	O	83/87 (95%)	68 (82%)	15 (18%)	1	2
5	F	295/370 (80%)	232 (79%)	63 (21%)	1	1
5	P	295/370 (80%)	239 (81%)	56 (19%)	1	2
All	All	5692/6446 (88%)	4411 (78%)	1281 (22%)	1	1

5 of 1281 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	234	LYS
2	M	57	GLU
3	N	1332	PRO
5	F	324	GLU
1	K	170	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 165 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	1489	GLN
1	L	95	GLN
3	N	1374	GLN
4	E	33	HIS

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Mol	Chain	Res	Type
1	K	38	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 489 ligands modelled in this entry, 489 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
3	D	1
3	N	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	380:GLU	C	381:ALA	N	1.17
1	N	380:GLU	C	381:ALA	N	1.17

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.