



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 11:24 PM GMT

PDB ID : 4XLQ
Title : Crystal structure of T.aquaticus transcription initiation complex containing upstream fork (-11 base-paired) promoter
Authors : Bae, B.; Darst, S.A.
Deposited on : 2015-01-13
Resolution : 4.60 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 : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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) : rb-20026982

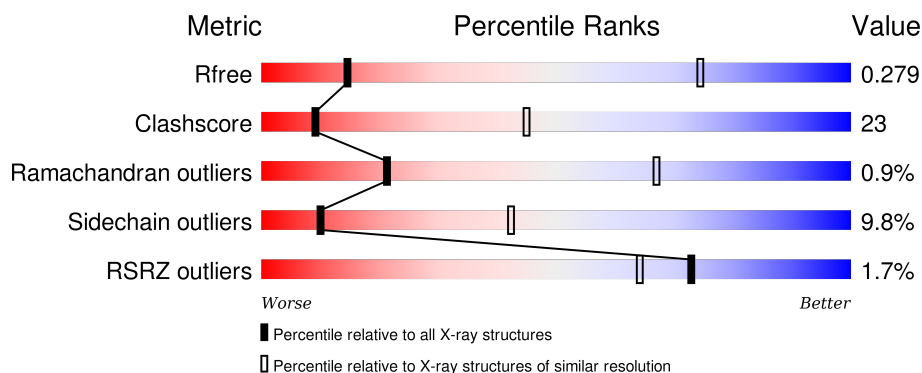
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.60 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	1089 (5.52-3.60)
Clashscore	102246	1004 (5.52-3.64)
Ramachandran outliers	100387	1131 (5.52-3.60)
Sidechain outliers	100360	1112 (5.50-3.60)
RSRZ outliers	91569	1092 (5.52-3.60)

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. 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	314	<div> <div>40%</div> <div>28%</div> <div>•</div> <div>28%</div> </div>
1	B	314	<div> <div>33%</div> <div>34%</div> <div>5%</div> <div>28%</div> </div>
1	G	314	<div> <div>5%</div> <div>36%</div> <div>31%</div> <div>5%</div> <div>28%</div> </div>
1	H	314	<div> <div>35%</div> <div>32%</div> <div>5%</div> <div>28%</div> </div>
2	C	1119	<div> <div>2%</div> <div>45%</div> <div>48%</div> <div>6%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
2	I	1119	<div><div><div></div><div></div><div></div></div><div>2%46%47%6%•</div></div>
3	D	1524	<div><div><div></div><div></div><div></div></div><div>%49%43%6%•</div></div>
3	J	1524	<div><div><div></div><div></div><div></div></div><div>%46%39%5%10%</div></div>
4	E	99	<div><div><div></div><div></div><div></div></div><div>2%59%34%• 6%</div></div>
4	K	99	<div><div><div></div><div></div><div></div></div><div>3%65%28%• 6%</div></div>
5	F	347	<div><div><div></div><div></div><div></div></div><div>56%42%••</div></div>
5	L	347	<div><div><div></div><div></div><div></div></div><div>2%54%43%••</div></div>
6	O	30	<div><div><div></div><div></div><div></div></div><div>13%17%83%</div></div>
6	R	30	<div><div><div></div><div></div><div></div></div><div>13%87%</div></div>
7	P	26	<div><div><div></div><div></div><div></div></div><div>19%8%88%•</div></div>
7	S	26	<div><div><div></div><div></div><div></div></div><div>12%88%</div></div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 56477 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	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	B	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	G	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	H	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1112	Total	C	N	O	S	0	0	0
			8739	5531	1553	1632	23			
2	I	1112	Total	C	N	O	S	0	0	0
			8739	5531	1553	1632	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1490	Total	C	N	O	S	0	0	0
			11761	7439	2088	2196	38			
3	J	1367	Total	C	N	O	S	0	0	0
			10779	6810	1923	2010	36			

- 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
			768	490	136	138	4			
4	K	93	Total	C	N	O	S	0	0	0
			768	490	136	138	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	345	Total	C	N	O	S	0	0	0
			2787	1758	502	523	4			
5	L	345	Total	C	N	O	S	0	0	0
			2787	1758	502	523	4			

- Molecule 6 is a DNA chain called DNA (30-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	O	30	Total	C	N	O	P	0	0	0
			613	296	109	179	29			
6	R	30	Total	C	N	O	P	0	0	0
			613	296	109	179	29			

- Molecule 7 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	P	25	Total	C	N	O	P	0	0	0
			510	245	91	149	25			
7	S	26	Total	C	N	O	P	0	0	0
			527	255	93	154	25			

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

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

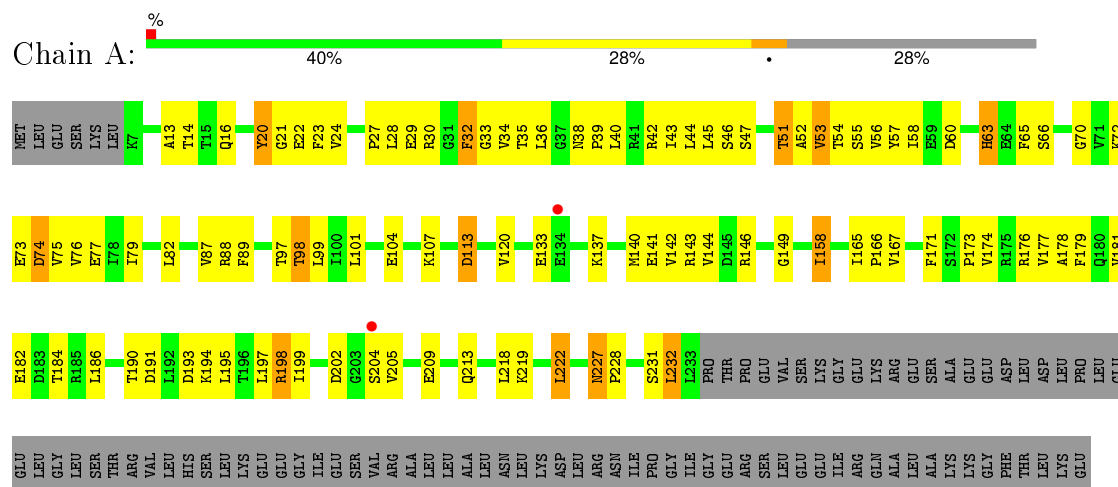
- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

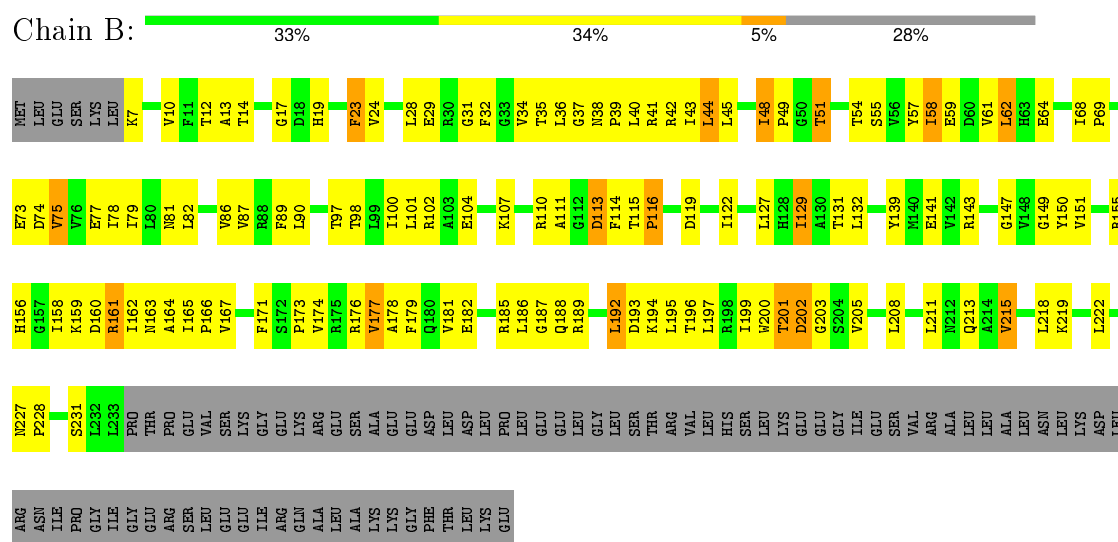
3 Residue-property plots

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

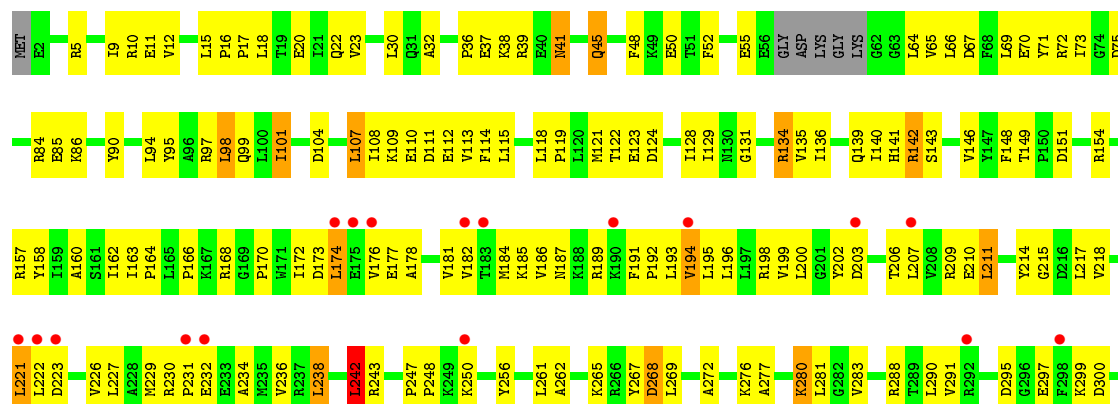


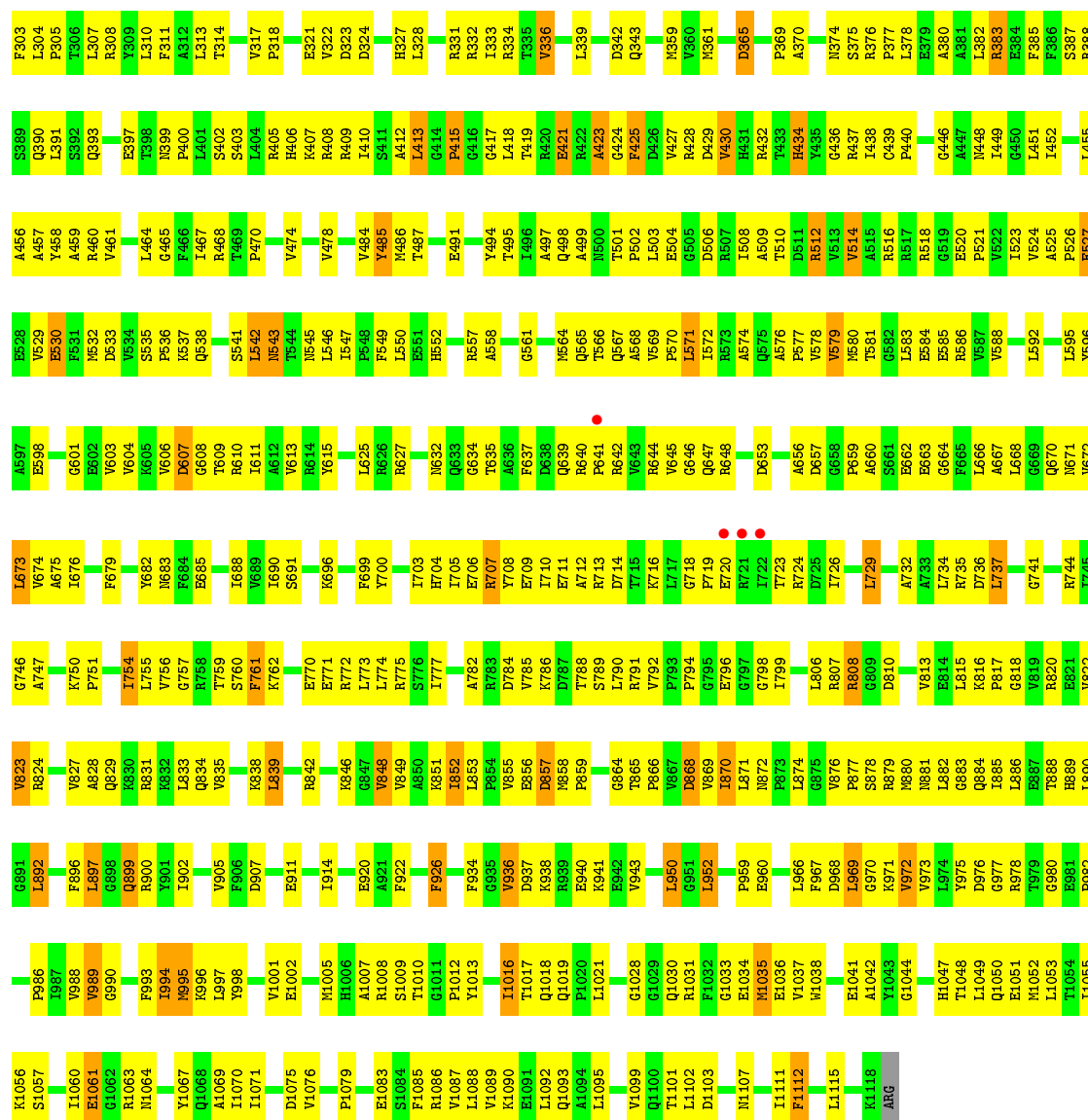
- Molecule 1: DNA-directed RNA polymerase subunit alpha



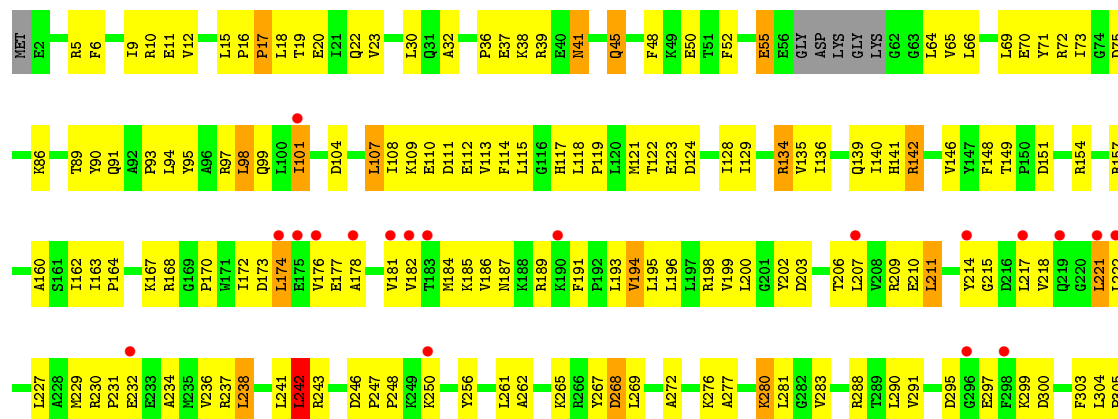
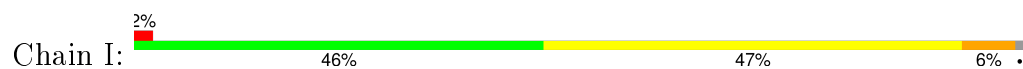
- Molecule 1: DNA-directed RNA polymerase subunit alpha

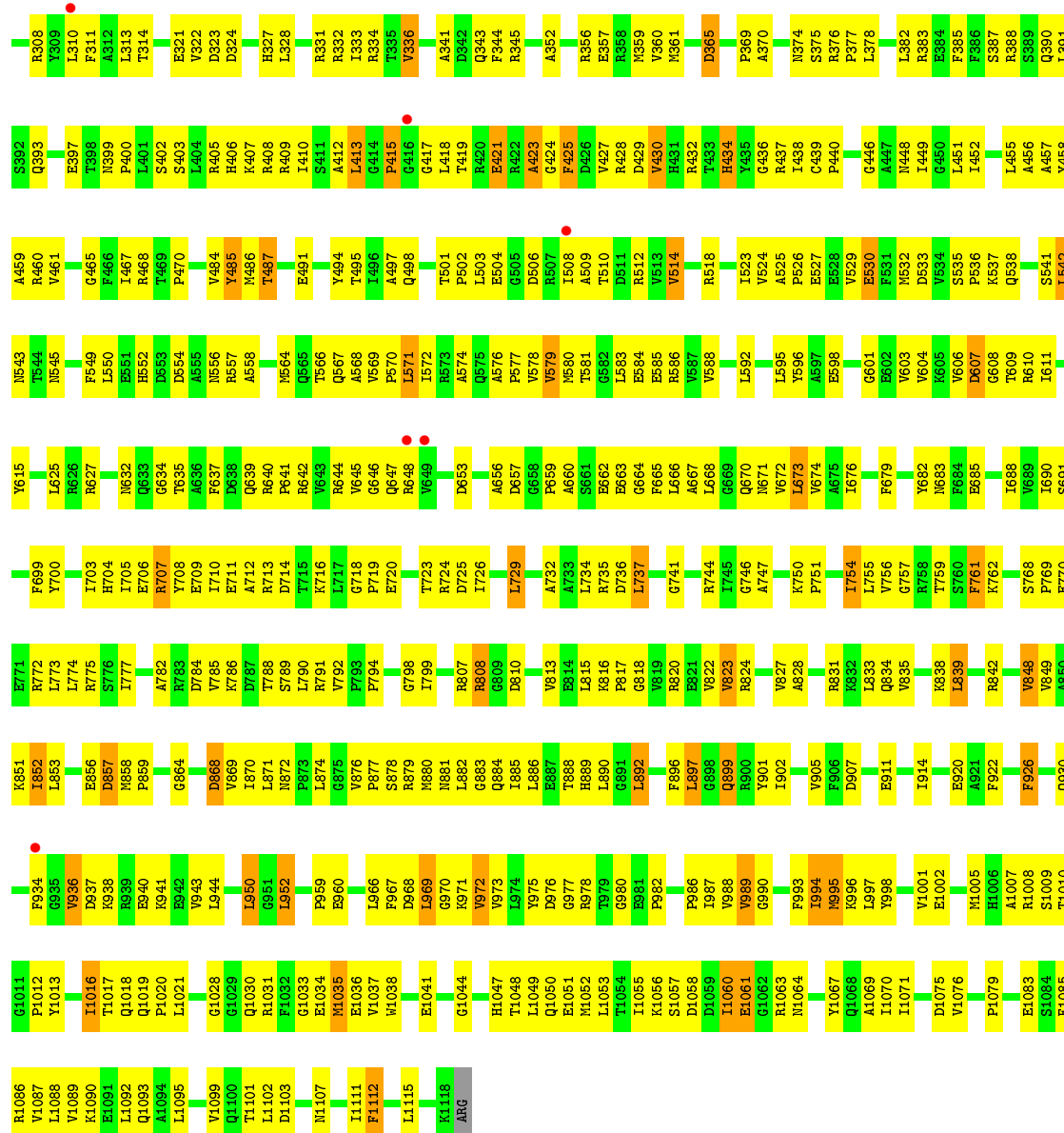






• Molecule 2: DNA-directed RNA polymerase subunit beta

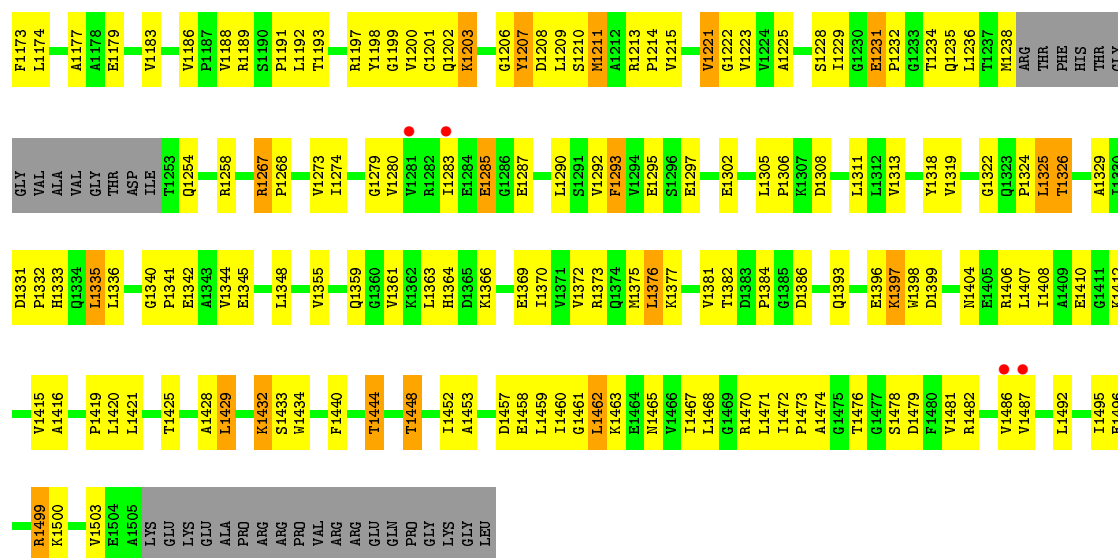




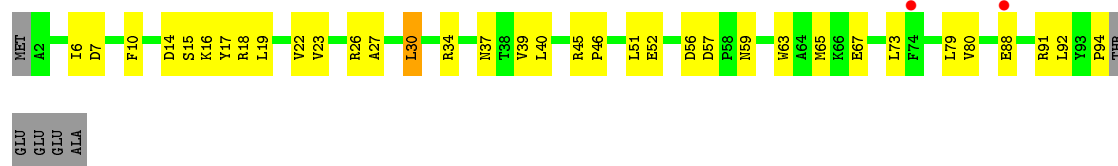
E1464	I1370	D1278	R1213	D1139	V1057	L964	L981	G801	V719	K646	R572	R493	V384	V300
M1465	V1371	G1279	P1214	I1140	R1058	D968	R884	A802	L720	R647	R573	K494	R388	G301
V1466	V1372	V1280	V1215	S1059	S1059	R969	I885	G803	I726	A648	L574	R495	E389	L304
L1468	R1373	E1285	S1142	S1142	S1060	K970	V886	F806	L728	E575	E575	F502	P390	A305
G1469	K1377	E1285	L1144	L1144	R1062	L971	G887	E810	R729	E651	A577	E502	A391	E306
R1470	Y1378	D1288	V1221	E1063	E1063	R972	V890	E811	H729	L652	V578	R508	S392	G309
L1471	V1379	R1289	G1222	G1064	L1064	Q973	G891	A812	V732	F653	D579	P509	I393	L310
L1472	E1380	L1290	V1223	L1065	L1065	I974	D892	L813	V732	P655	A580	E510	L394	R312
P1473	V1381	F1293	V1224	A1150	V1066	E975	E893	L814	A735	P656	V581	W511	V395	L311
L1474	D1382	F1293	A1225	V1153	V1067	Q976	E894	A815	A735	P656	V582	M512	V396	R312
G1475	D1383	V1294	A1225	V1153	L1068	A977	V895	A815	D739	L657	D583	I513	K397	L313
L1476	P1384	E1295	S1228	L1156	E1069	Y978	V896	R818	F740	L658	R584	L514	P314	P314
G1477	G1385	S1296	I1229	L1156	E1069	Y978	V896	R818	F740	L658	G585	E515	R315	R315
S1478	D1386	E1297	G1230	E1231	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315
L1479	E1302	E1297	E1231	R1159	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315
F1480	E1302	E1297	E1231	R1159	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315
V1481	E1303	E1297	E1231	R1159	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315
R1482	G1304	E1297	E1231	R1159	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315
F1483	L1305	E1297	E1231	R1159	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315
D1399	P1306	E1297	E1231	R1159	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315
V1486	K1307	E1297	E1231	R1159	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315
V1487	R1310	E1297	E1231	R1159	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315
T1491	L1311	E1297	E1231	R1159	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315
L1492	P1312	E1297	E1231	R1159	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315
R1499	V1313	E1297	E1231	R1159	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315
K1500	Y1318	E1297	E1231	R1159	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315
V1503	P1324	E1297	E1231	R1159	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315
E1504	L1325	E1297	E1231	R1159	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315
A1505	T1326	E1297	E1231	R1159	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315
LYS	R1327	E1297	E1231	R1159	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315
GLU	T1330	E1297	E1231	R1159	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315
LYS	D1331	E1297	E1231	R1159	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315
ALA	P1332	E1297	E1231	R1159	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315
PRO	H1333	E1297	E1231	R1159	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315
ARG	L1336	E1297	E1231	R1159	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315
ARG	E1342	E1297	E1231	R1159	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315
VAL	A1343	E1297	E1231	R1159	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315
ARG	R1346	E1297	E1231	R1159	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315
GLN	Q1353	E1297	E1231	R1159	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315
PRO	R1357	E1297	E1231	R1159	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315
LYS	V1361	E1297	E1231	R1159	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315
LEU	K1362	E1297	E1231	R1159	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315
	L1363	E1297	E1231	R1159	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315
	H1364	E1297	E1231	R1159	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315
	D1365	E1297	E1231	R1159	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315
	L1459	E1297	E1231	R1159	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315
	I1460	E1297	E1231	R1159	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315
	G1461	E1297	E1231	R1159	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315
	L1462	E1297	E1231	R1159	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315
	K1463	E1297	E1231	R1159	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315
	E1369	E1297	E1231	R1159	H1075	I983	Q897	R818	F740	L658	R586	E515	R315	R315

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

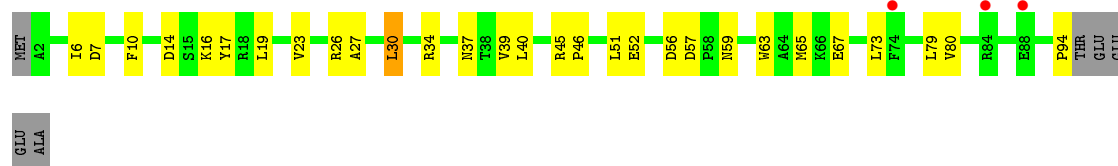




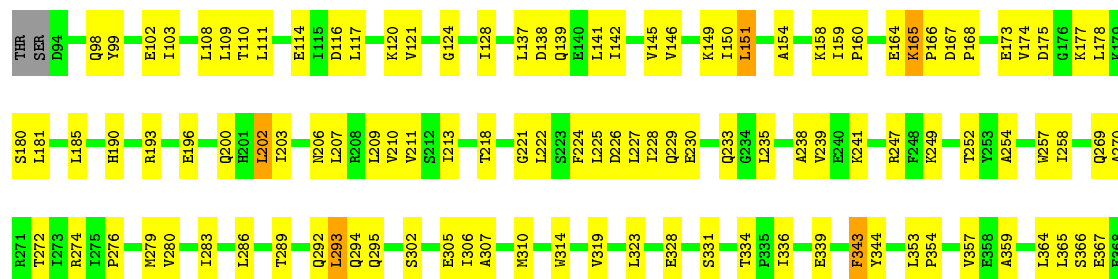
• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 4: DNA-directed RNA polymerase subunit omega

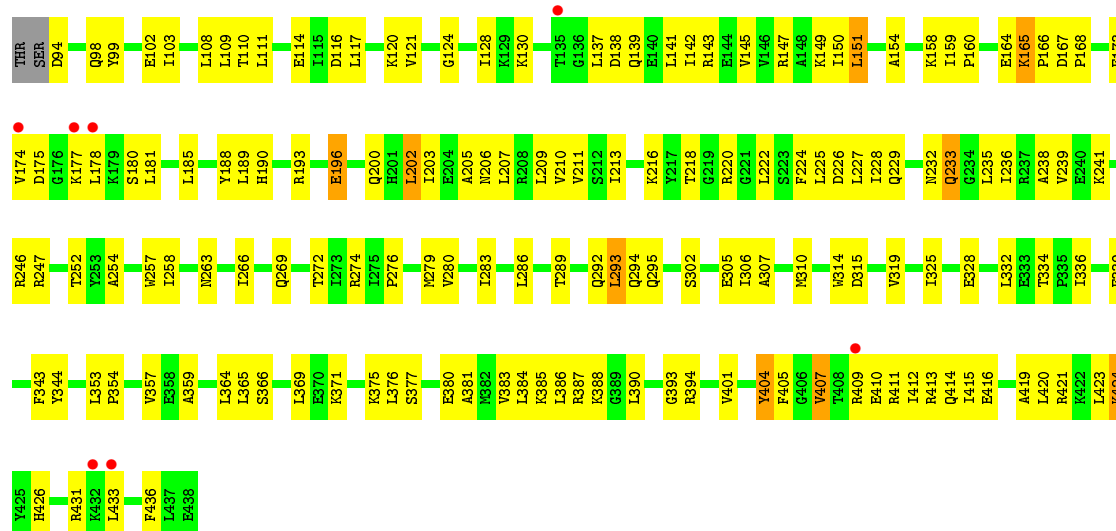


• Molecule 5: RNA polymerase sigma factor SigA





• Molecule 5: RNA polymerase sigma factor SigA



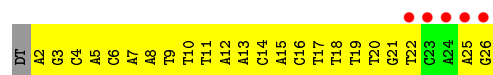
• Molecule 6: DNA (30-MER)



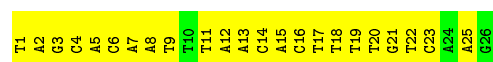
• Molecule 6: DNA (30-MER)



• Molecule 7: DNA (26-MER)



• Molecule 7: DNA (26-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	288.23Å 288.23Å 535.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.81 – 4.60 49.81 – 4.60	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.81-4.60) 98.6 (49.81-4.60)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 4.64Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1839)	Depositor
R, R_{free}	0.245 , 0.281 0.240 , 0.279	Depositor DCC
R_{free} test set	6217 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	154.6	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 174.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.17$	Xtriage
Outliers	0 of 123373 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	56477	wwPDB-VP
Average B, all atoms (Å ²)	175.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% 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 [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	0.31	0/1804	0.64	1/2455 (0.0%)
1	B	0.30	0/1804	0.61	0/2455
1	G	0.31	0/1804	0.64	1/2455 (0.0%)
1	H	0.30	0/1804	0.61	0/2455
2	C	0.27	0/8905	0.55	2/12040 (0.0%)
2	I	0.27	0/8905	0.55	2/12040 (0.0%)
3	D	0.28	0/11963	0.55	3/16165 (0.0%)
3	J	0.28	0/10959	0.57	1/14802 (0.0%)
4	E	0.25	0/783	0.54	0/1054
4	K	0.25	0/783	0.53	0/1054
5	F	0.27	0/2829	0.55	1/3804 (0.0%)
5	L	0.27	0/2829	0.55	1/3804 (0.0%)
6	O	0.50	0/687	0.92	0/1059
6	R	0.50	0/687	0.91	0/1059
7	P	0.54	0/571	0.93	0/878
7	S	0.54	0/590	0.93	0/908
All	All	0.29	0/57707	0.59	12/78487 (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
2	I	0	3
3	D	0	1
3	J	0	1
All	All	0	8

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	311	LEU	CA-CB-CG	7.45	132.43	115.30
3	D	1134	LEU	CA-CB-CG	6.98	131.36	115.30
2	I	417	GLY	N-CA-C	6.42	129.14	113.10
2	C	417	GLY	N-CA-C	6.40	129.09	113.10
3	J	1134	LEU	CA-CB-CG	5.63	128.26	115.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	415	PRO	Peptide
2	C	423	ALA	Peptide
2	C	737	LEU	Peptide
3	D	1208	ASP	Peptide
2	I	415	PRO	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	1770	0	1799	89	0
1	B	1770	0	1799	101	0
1	G	1770	0	1799	103	0
1	H	1770	0	1799	95	0
2	C	8739	0	8841	499	0
2	I	8739	0	8841	485	0
3	D	11761	0	11976	585	0
3	J	10779	0	10993	503	0
4	E	768	0	784	37	0
4	K	768	0	784	29	0
5	F	2787	0	2866	120	0
5	L	2787	0	2866	133	0
6	O	613	0	343	28	0
6	R	613	0	343	26	0
7	P	510	0	284	27	0
7	S	527	0	297	25	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
9	D	1	0	0	0	0
9	J	1	0	0	0	0
All	All	56477	0	56414	2598	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 23.

The worst 5 of 2598 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:C:707:ARG:HE	2:C:824:ARG:HE	1.17	0.90
6:R:24:DC:H42	7:S:3:DG:H1	1.18	0.90
4:E:30:LEU:HD12	4:E:37:ASN:HD21	1.39	0.88
3:D:105:VAL:HA	3:D:112:ILE:HD11	1.55	0.88
4:K:30:LEU:HD12	4:K:37:ASN:HD21	1.39	0.87

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	225/314 (72%)	200 (89%)	23 (10%)	2 (1%)	21	67
1	B	225/314 (72%)	200 (89%)	20 (9%)	5 (2%)	8	51
1	G	225/314 (72%)	200 (89%)	23 (10%)	2 (1%)	21	67
1	H	225/314 (72%)	201 (89%)	18 (8%)	6 (3%)	6	47
2	C	1108/1119 (99%)	958 (86%)	139 (12%)	11 (1%)	19	65
2	I	1108/1119 (99%)	956 (86%)	140 (13%)	12 (1%)	17	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	1486/1524 (98%)	1315 (88%)	162 (11%)	9 (1%)	30	74
3	J	1361/1524 (89%)	1201 (88%)	150 (11%)	10 (1%)	26	71
4	E	91/99 (92%)	75 (82%)	16 (18%)	0	100	100
4	K	91/99 (92%)	75 (82%)	16 (18%)	0	100	100
5	F	343/347 (99%)	299 (87%)	42 (12%)	2 (1%)	30	74
5	L	343/347 (99%)	302 (88%)	40 (12%)	1 (0%)	46	83
All	All	6831/7434 (92%)	5982 (88%)	789 (12%)	60 (1%)	21	67

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	VAL
3	D	1128	VAL
3	D	1209	LEU
1	G	53	VAL
3	J	1128	VAL

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	194/270 (72%)	179 (92%)	15 (8%)	16	55
1	B	194/270 (72%)	172 (89%)	22 (11%)	7	36
1	G	194/270 (72%)	178 (92%)	16 (8%)	14	51
1	H	194/270 (72%)	171 (88%)	23 (12%)	6	34
2	C	931/936 (100%)	840 (90%)	91 (10%)	10	42
2	I	931/936 (100%)	840 (90%)	91 (10%)	10	42
3	D	1252/1281 (98%)	1114 (89%)	138 (11%)	8	37
3	J	1150/1281 (90%)	1028 (89%)	122 (11%)	8	39
4	E	83/88 (94%)	79 (95%)	4 (5%)	31	69
4	K	83/88 (94%)	79 (95%)	4 (5%)	31	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	F	296/299 (99%)	276 (93%)	20 (7%)	20	59
5	L	296/299 (99%)	276 (93%)	20 (7%)	20	59
All	All	5798/6288 (92%)	5232 (90%)	566 (10%)	10	42

5 of 566 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	1382	THR
1	H	113	ASP
3	J	1293	PHE
3	D	1459	LEU
5	F	409	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	1235	GLN
1	G	63	HIS
4	K	37	ASN
3	D	1359	GLN
5	F	294	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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 [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 ⓘ

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	227/314 (72%)	0.08	2 (0%) 85 80	107, 189, 236, 264	0
1	B	227/314 (72%)	-0.23	0 100 100	94, 161, 214, 264	0
1	G	227/314 (72%)	0.39	16 (7%) 19 15	116, 199, 240, 276	0
1	H	227/314 (72%)	-0.13	2 (0%) 85 80	116, 173, 216, 267	0
2	C	1112/1119 (99%)	-0.03	21 (1%) 70 61	90, 179, 243, 314	0
2	I	1112/1119 (99%)	0.01	25 (2%) 65 56	94, 185, 244, 315	0
3	D	1490/1524 (97%)	-0.13	13 (0%) 85 80	64, 149, 204, 259	0
3	J	1367/1524 (89%)	-0.08	18 (1%) 79 71	79, 159, 217, 264	0
4	E	93/99 (93%)	0.05	2 (2%) 65 56	100, 159, 205, 238	0
4	K	93/99 (93%)	0.03	3 (3%) 51 41	112, 168, 216, 253	0
5	F	345/347 (99%)	-0.10	1 (0%) 94 92	115, 185, 255, 300	0
5	L	345/347 (99%)	-0.11	7 (2%) 68 59	121, 188, 252, 300	0
6	O	30/30 (100%)	0.70	4 (13%) 4 6	154, 221, 293, 311	0
6	R	30/30 (100%)	0.22	0 100 100	164, 221, 257, 267	0
7	P	25/26 (96%)	0.81	5 (20%) 1 3	172, 235, 306, 326	0
7	S	26/26 (100%)	0.07	0 100 100	184, 224, 263, 283	0
All	All	6976/7546 (92%)	-0.05	119 (1%) 73 64	64, 171, 235, 326	0

The worst 5 of 119 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	176	VAL	5.1
2	I	175	GLU	4.6
2	C	221	LEU	4.4
1	G	13	ALA	4.1
2	C	175	GLU	3.7

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
8	ZN	D	2001	1/1	0.99	0.13	-0.59	107,107,107,107	0
8	ZN	J	2001	1/1	0.97	0.12	-1.01	166,166,166,166	0
8	ZN	D	2002	1/1	0.96	0.16	-1.20	182,182,182,182	0
8	ZN	J	2002	1/1	0.93	0.07	-1.44	147,147,147,147	0
9	MG	D	2003	1/1	0.82	0.45	-	286,286,286,286	0
9	MG	J	2003	1/1	0.84	0.41	-	331,331,331,331	0

6.5 Other polymers [i](#)

There are no such residues in this entry.