wwPDB X-ray Structure Validation Summary Report (i)

Feb 22, 2024 – 11:01 AM EST

PDB ID	:	4XLN
Title	:	Crystal structure of T. aquaticus transcription initiation complex containing bubble promoter and RNA
Authors	:	Bae, B.; Darst, S.A.
Deposited on	:	2015-01-13
Resolution	:	4.00 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 (i) 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 (1)) were used in the production of this report:

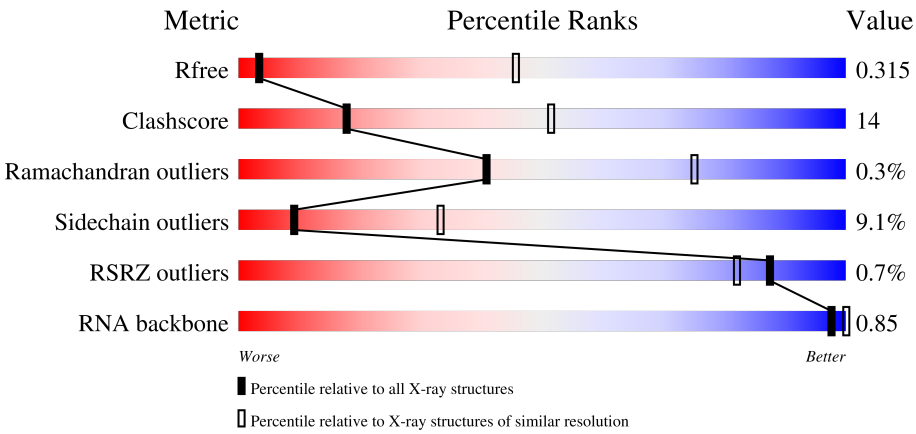
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)
RNA backbone	3102	1048 (5.00-3.00)

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 <=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	47% 23% • 28%
1	B	314	46% 22% • 28%
1	G	314	.% 47% 23% • 28%
1	H	314	46% 22% • 28%

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Mol	Chain	Length	Quality of chain
2	C	1119	%; 59%; 36%
2	I	1119	%; 61%; 35%
3	D	1524	63%; 31%
3	J	1524	59%; 28%; 10%
4	E	99	63%; 27%; 6%
4	K	99	61%; 29%; 6%
5	F	347	2%; 62%; 34%
5	L	347	%; 63%; 33%
6	O	48	8%; 69%; 27%
6	R	48	2%; 65%; 35%
7	P	48	8%; 65%; 29%; 6%
7	S	48	2%; 60%; 29%; 10%
8	Q	4	75%; 25%
8	T	4	50%; 50%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 58255 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
			Total	C	N	O	S			
1	A	227	1770	1130	303	334	3	0	0	0
1	B	227	1770	1130	303	334	3	0	0	0
1	G	227	1770	1130	303	334	3	0	0	0
1	H	227	1770	1130	303	334	3	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	93	768	490	136	138	4	0	0	0
4	K	93	768	490	136	138	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	347	2801	1767	505	525	4	0	0	0
5	L	347	2801	1767	505	525	4	0	0	0

- Molecule 6 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
6	O	48	988	472	182	287	47	0	0	0
6	R	48	988	472	182	287	47	0	0	0

- Molecule 7 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
7	P	48	985	471	183	284	47	0	0	0
7	S	43	882	421	164	255	42	0	0	0

- Molecule 8 is a RNA chain called RNA (5'-D(P*UP*CP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
8	Q	4	85	38	15	28	4	0	0	0
8	T	4	85	38	15	28	4	0	0	0

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

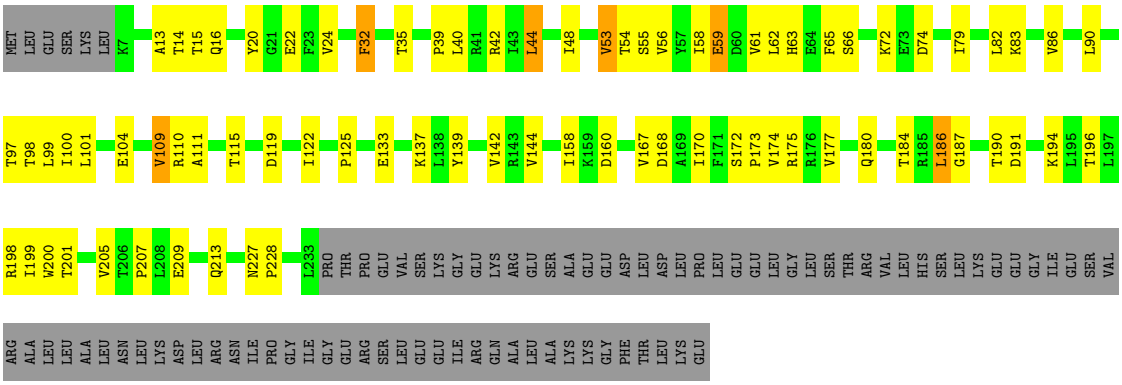
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
10	D	1	1	1	0	0
			Total	Mg		
10	J	1	1	1	0	0

3 Residue-property plots (i)

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.

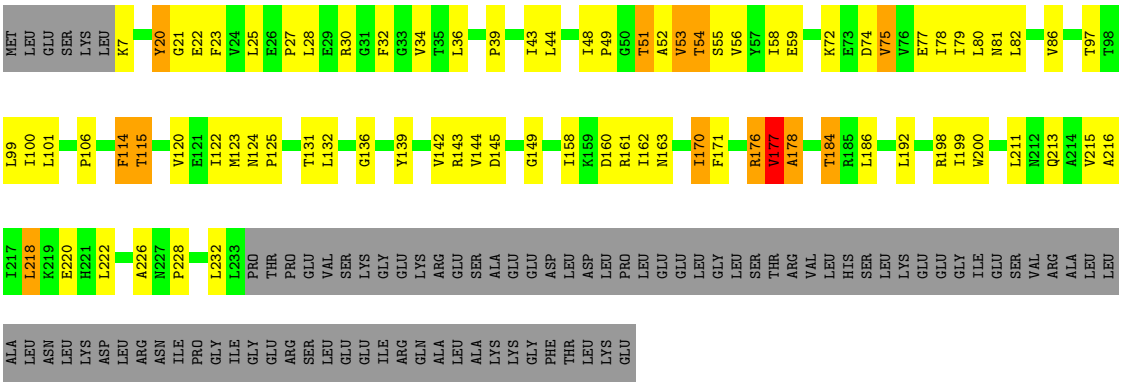
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A: 47% 23% • 28%



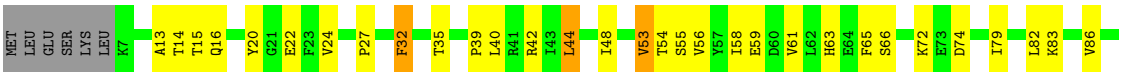
• Molecule 1: DNA-directed RNA polymerase subunit alpha

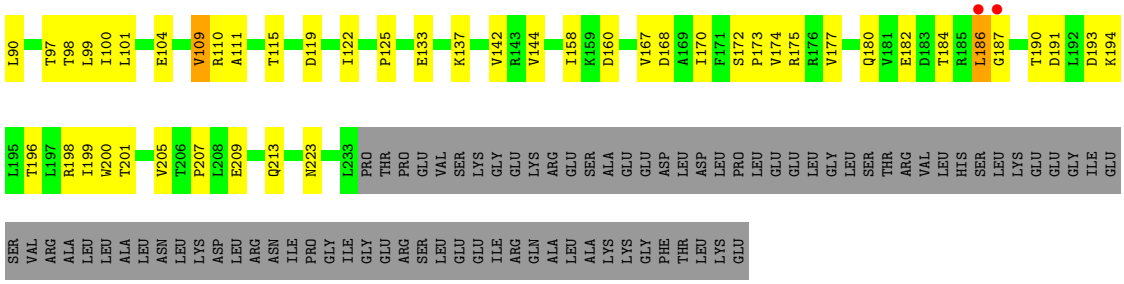
Chain B: 46% 22% • 28%



• Molecule 1: DNA-directed RNA polymerase subunit alpha

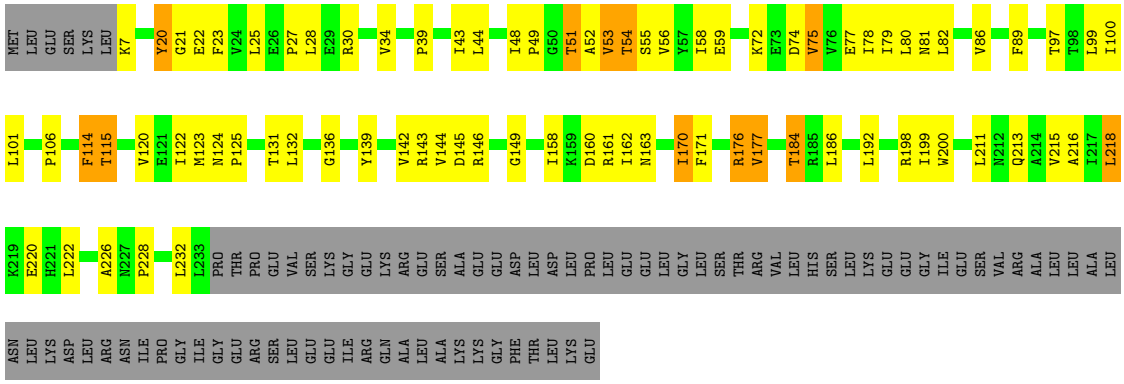
Chain G: % 47% 23% • 28%





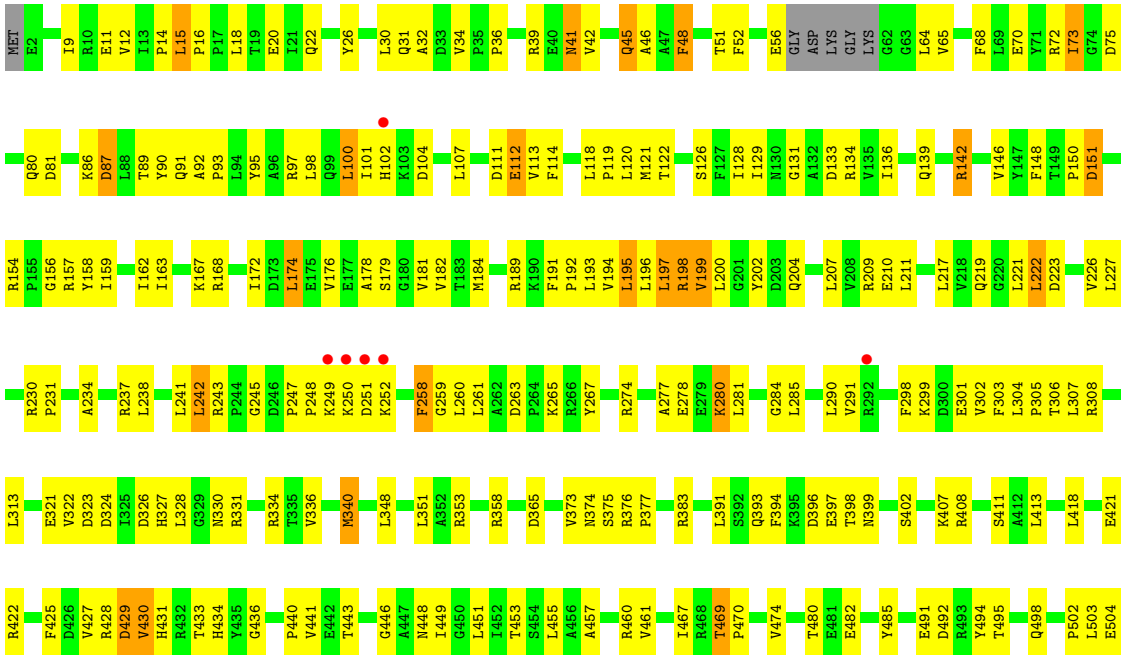
- Molecule 1: DNA-directed RNA polymerase subunit alpha

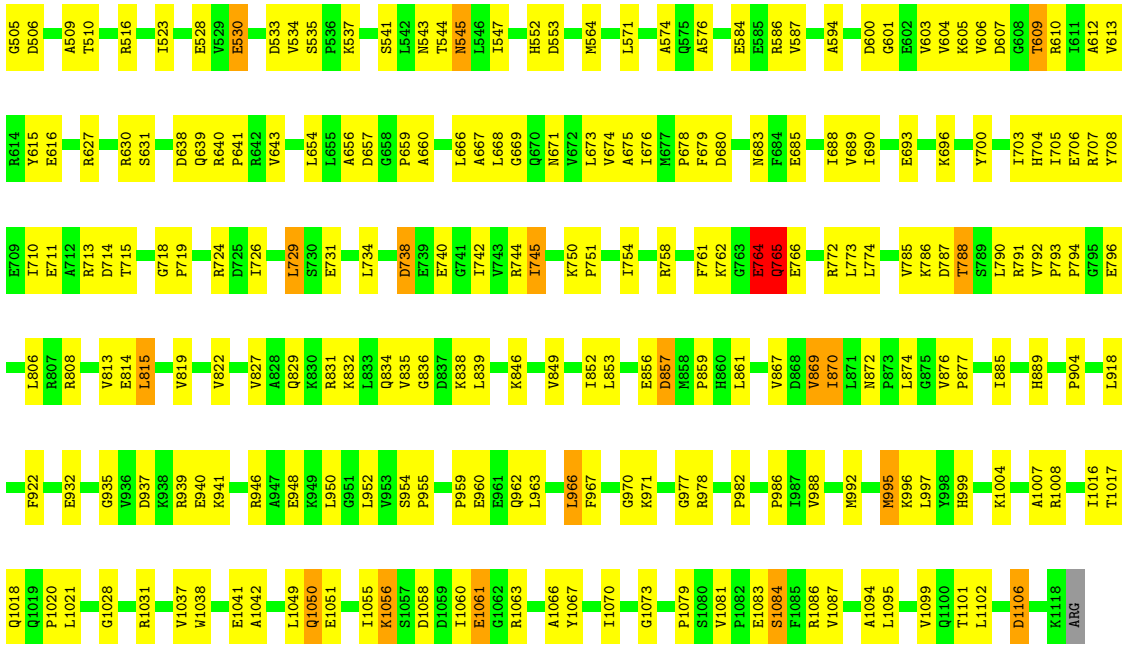
Chain H:



- Molecule 2: DNA-directed RNA polymerase subunit beta

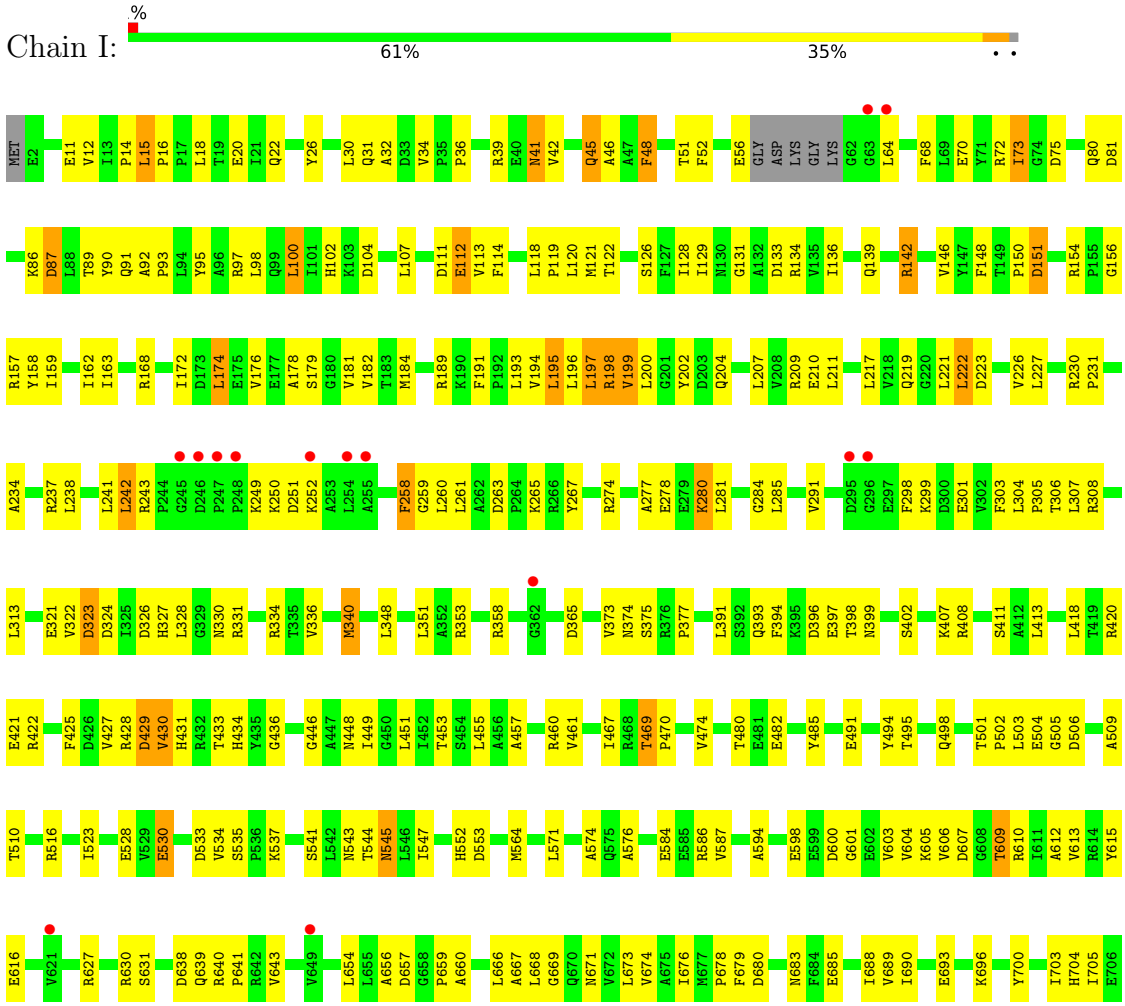
Chain C:

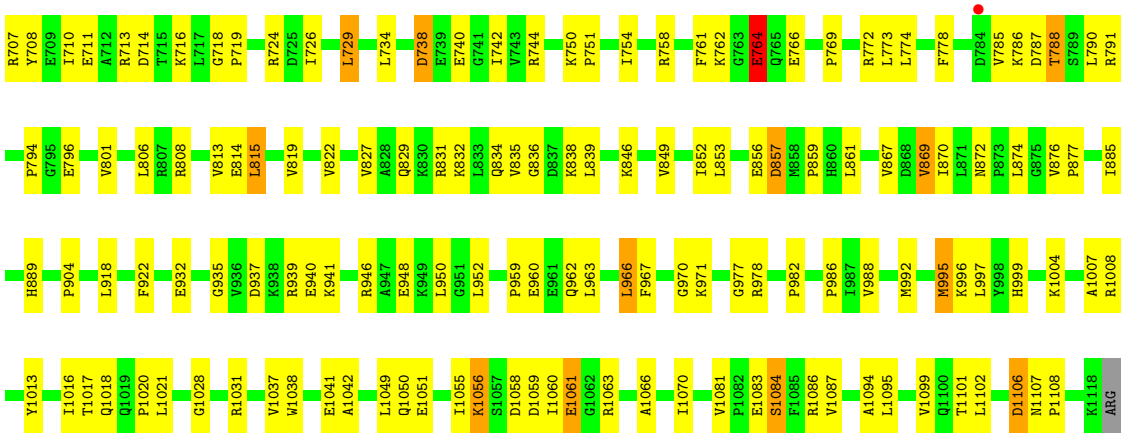




• Molecule 2: DNA-directed RNA polymerase subunit beta

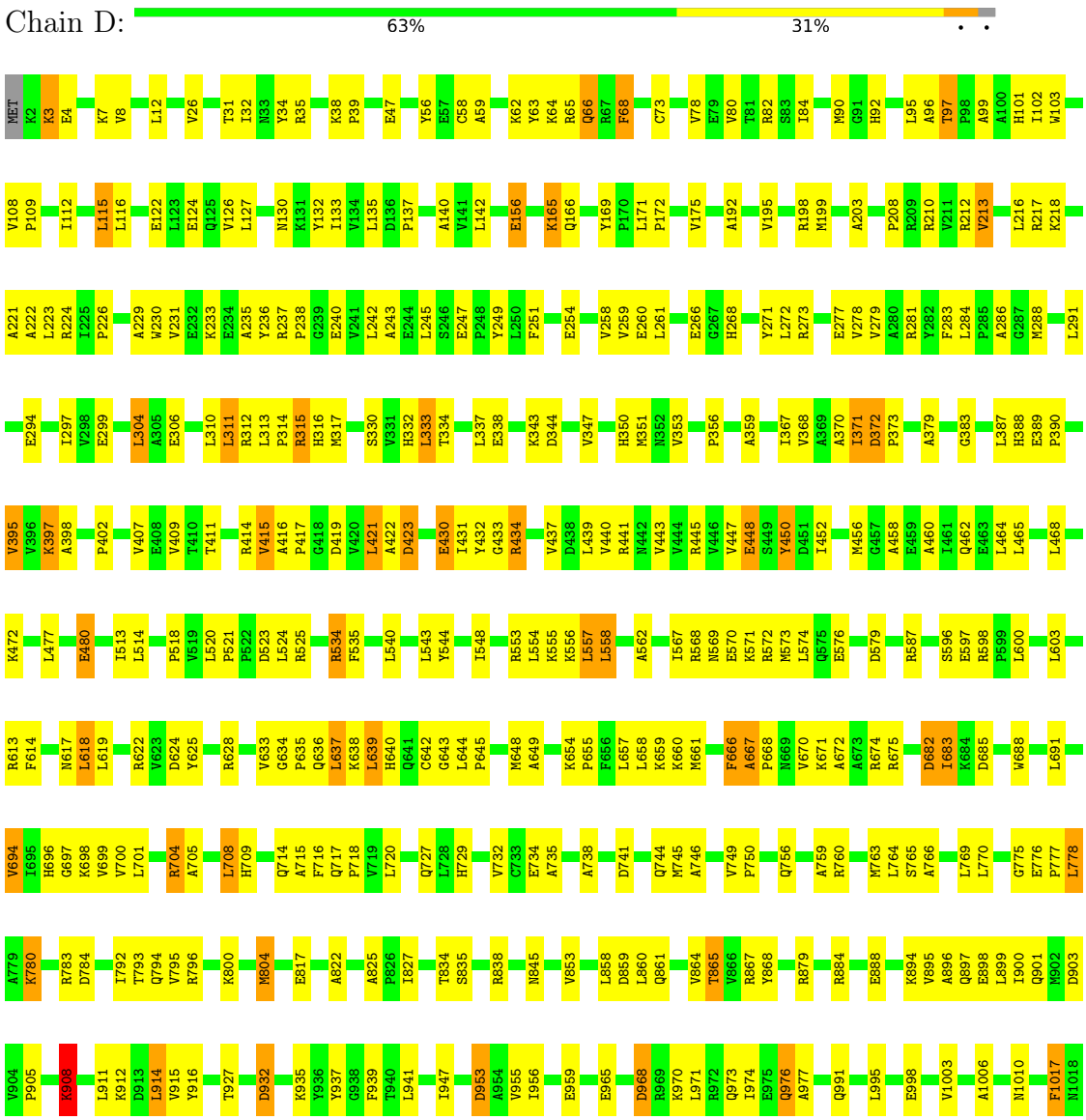
Chain I:





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

Chain D:



P1019 L1020 S1026 R1029 I1035 R1036 Q1037 M1041 R1042 K1047 P1048 T1052 F1053 V1057 S1060 F1061 R1062 E1063 G1064 L1065 L1068 E1069 Y1070 F1071 I1072 H1075 R1078 D1083 L1086 R1087 D1090 Y1093 L1098 V1099 H1103 V1106 V1107 R1108 Y1117 L1122

E1127 V1128 L1132 R1133 L1134 R1137 S1142 G1143 L1144 Y1145 L1149 R1158 R1159 L1160 E1161 Y1165 V1171 V1186 S1190 P1191 L1192 T1193 T1196 R1197 Y1198 C1201 Y1207 D1208 L1209 V1215 A1220 V1224 E1231 P1232 G1233 T1234 Q1235 L1236 T1237 M1238 ARG THR PHE

HIS THR GLY GLY VAL ALA VAL GLY THR ASP ILE T1253 Q1254 G1255 L1256 P1257 R1258 E1264 A1265 R1266 R1267 P1268 K1269 V1273 I1274 D1278 V1281 E1285 G1286 F1293 E1297 E1302 K1307 L1311 L1312 V1313 G1322 Q1323 P1324 L1325 H1333 Q1334 L1335 L1336 E1337 A1338 K1339

V1344 E1345 R1346 Y1347 L1348 E1351 I1352 Q1353 K1354 V1355 Y1356 H1364 D1365 K1366 H1367 I1368 E1369 I1370 R1373 Q1374 V1379 P1384 G1385 D1386 K1397 W1398 D1399 V1400 N1404 I1408 V1413 P1414 V1415 L1421 V1424 T1425 K1426 W1434 L1435 S1439 T1443 T1448 I1452

K1455 K1456 D1457 E1458 L1459 L1462 K1463 E1464 N1465 V1466 I1467 L1468 G1469 R1470 L1471 I1472 P1473 A1474 V1486 L1492 E1496 R1499 A1505 LYS GLU LYS GLU ALA PRO ARG ARG PRO VAL ARG ARG GLU GLN PRO GLY LYS GLY LEU

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

Chain J: 59% 28% • 10%

MET K2 K3 E4 K7 V8 L12 S22 V26 T31 I32 N33 Y34 R35 T36 L37 K38 P39 E47 Y56 E57 C58 A59 K62 Y63 K64 R65 Q66 R67 F68 C73 V78 E79 V80 T81 R82 S83 I84 M90 G91 H92 L95 A96 T97 P98 A99 A100 H101

I102 W103 V108 P109 I112 L115 L116 E122 L123 E124 Q125 V126 L127 Y128 F129 N130 K131 Y132 I133 V134 L135 D136 P137 L142 E156 E160 L161 R162 K165 Q166 E167 T168 Y169 P172 V175 L178 V179 E184 V185 V186 K187 L191 A192 P193 G194 V195

R198 M199 D200 G201 V202 A203 L204 Y205 P208 R209 R210 D214 Y215 L216 ARG LYS GLU ARG ALA ALA LEU ARG ILE PRO LEU SER ALA TRP VAL GLU LYS GLU ALA TYR ARG PRO GLY GLU VAL LEU ALA GLU LEU SER GLU PRO TYR LEU PHE ARG ALA GLU GLU SER GLY VAL VAL GLU

LEU LYS ASP LEU ALA GLU GLY HIS LEU ILE TYR LEU ARG GLN GLU GLU GLU VAL VAL ALA ARG TYR PHE LEU PRO ALA GLY MET THR PRO LEU VAL VAL GLU GLY GLU ILE VAL GLU VAL GLY GLN PRO LEU ALA GLU GLY LYS GLY LEU LEU ARG LEU PRO ARG HIS MET THR ALA LYS

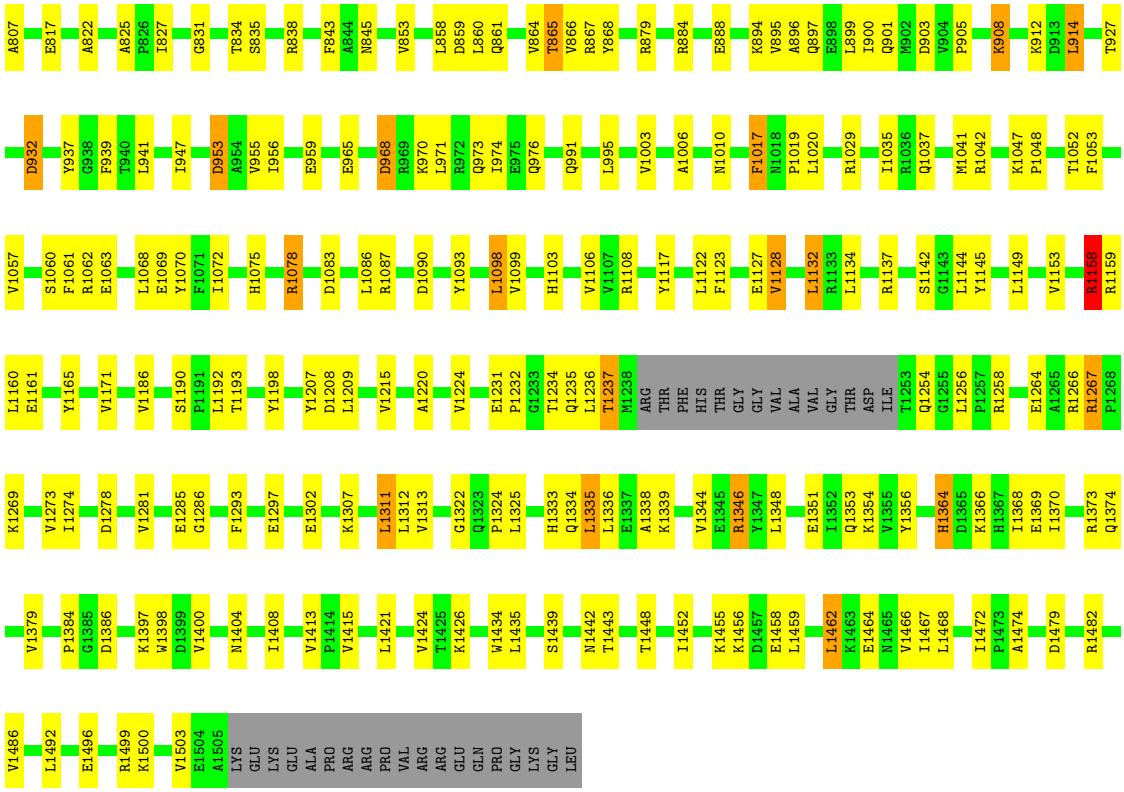
GLU VAL GLU ALA GLU GLU GLU GLY ASP SER VAL HIS LEU THR LEU PHE LEU GLU TRP T340 D344 V347 A348 P349 H350 M351 N352 V353 P356 V361 I367 V368 A369 A370 I371 D372 G383 L387 H388 E389 P390 I393 L394 V395 V396 K397 E404 D405 D406 V407 E408

V409 T410 T411 G412 D413 R414 V420 L421 A422 D423 G424 G425 R434 V437 R441 N442 V443 V444 R445 E448 I452 D453 A454 R455 M456 G457 A458 E459 A460 I461 Q462 E463 L464 L465 L468 K472 L477 E480 I513 L514 P518 V519 L520 P521 P522 D523 L524

V530 R534 F535 L540 L543 Y544 I548 R553 L554 K555 K556 L557 L558 A562 I565 I566 I567 R568 N569 E570 K571 R572 M573 L574 Q575 E576 D579 R587 S596 S597 R598 P599 L600 L603 R613 F614 N617 L618 L619 R622 V623 D624 Y625 R628

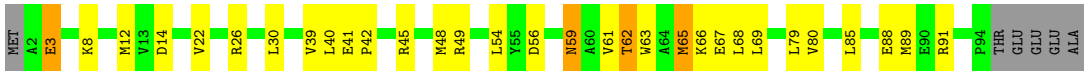
V633 G634 P635 Q636 L637 K638 L639 H640 Q641 C642 G643 L644 P645 M648 A649 K654 P655 F656 L657 L658 K659 K660 M661 F666 A667 K671 A672 R675 R679 D682 I683 K684 D685 E686 V687 W688 L691 V694 I695 H696 G697 K698 V699 V700 L701 R704 A705 L708 H709

Q714 A715 F716 Q717 P718 V719 L720 Q727 L728 H729 V732 C733 E734 A735 A738 D741 Q744 M745 A746 V749 P750 A759 R760 M763 L764 S765 A766 L769 L770 G775 E776 P777 L778 A779 K780 R783 D784 I792 T793 Q794 V795 R796 K800 M804



- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:

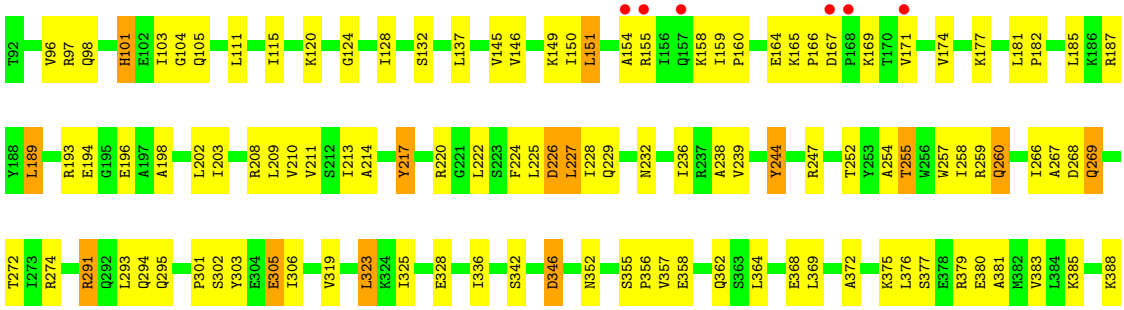


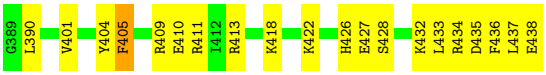
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain K:

- Molecule 5: RNA polymerase sigma factor SigA

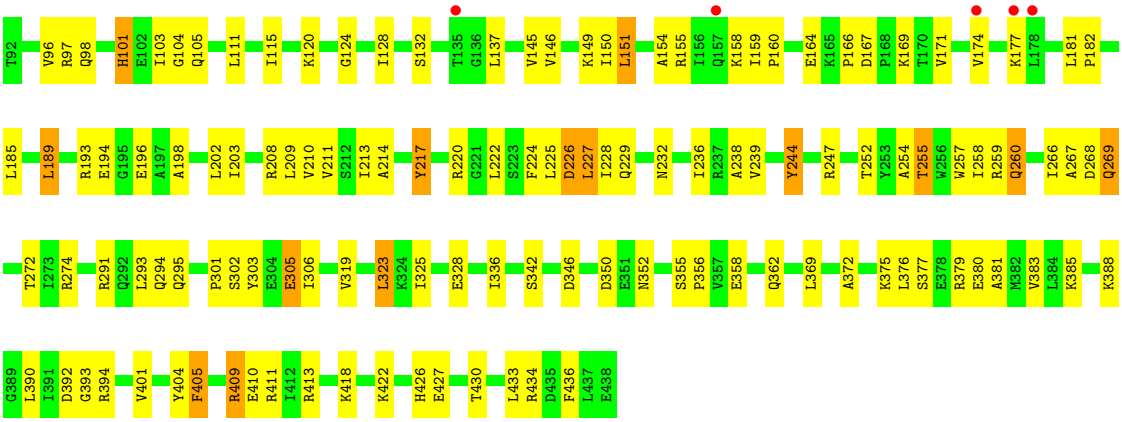
Chain F:





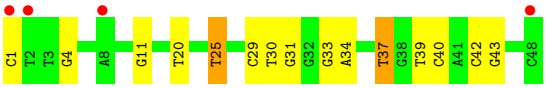
• Molecule 5: RNA polymerase sigma factor SigA

Chain L:



• Molecule 6: DNA (48-MER)

Chain O:

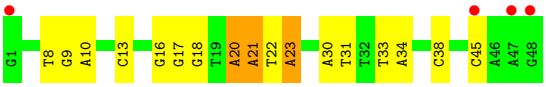


• Molecule 6: DNA (48-MER)

Chain R:

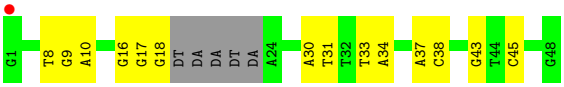
• Molecule 7: DNA (48-MER)

Chain P:



• Molecule 7: DNA (48-MER)

Chain S:



- Molecule 8: RNA (5'-D(P*UP*CP*GP*A)-3')

Chain Q: 75% 25%

- Molecule 8: RNA (5'-D(P*UP*CP*GP*A)-3')

Chain T: 50% 50%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	289.26Å 289.26Å 536.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.96 – 4.00 34.96 – 4.00	Depositor EDS
% Data completeness (in resolution range)	98.9 (34.96-4.00) 99.0 (34.96-4.00)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.07 (at 3.99Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1839)	Depositor
R, R_{free}	0.280 , 0.315 0.280 , 0.315	Depositor DCC
R_{free} test set	9497 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	99.6	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 116.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	58255	wwPDB-VP
Average B, all atoms (Å^2)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.23	0/1804	0.46	0/2455
1	B	0.25	0/1804	0.50	1/2455 (0.0%)
1	G	0.24	0/1804	0.46	0/2455
1	H	0.24	0/1804	0.49	0/2455
2	C	0.25	1/8905 (0.0%)	0.48	3/12040 (0.0%)
2	I	0.26	1/8905 (0.0%)	0.48	2/12040 (0.0%)
3	D	0.24	0/11963	0.48	4/16165 (0.0%)
3	J	0.24	1/10959 (0.0%)	0.47	3/14802 (0.0%)
4	E	0.21	0/783	0.38	0/1054
4	K	0.21	0/783	0.38	0/1054
5	F	0.23	0/2843	0.53	4/3822 (0.1%)
5	L	0.23	0/2843	0.55	4/3822 (0.1%)
6	O	0.44	0/1109	1.07	4/1712 (0.2%)
6	R	0.44	0/1109	1.07	3/1712 (0.2%)
7	P	0.48	0/1106	1.11	5/1706 (0.3%)
7	S	0.44	0/989	1.01	0/1523
8	Q	0.15	0/94	0.67	0/144
8	T	0.16	0/94	0.67	0/144
All	All	0.26	3/59701 (0.0%)	0.55	33/81560 (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
1	B	0	2
2	C	0	2
2	I	0	1
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	764	GLU	CD-OE2	8.42	1.34	1.25
2	C	764	GLU	CB-CG	-6.22	1.40	1.52
3	J	597	GLU	CB-CG	5.05	1.61	1.52

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	291	ARG	NE-CZ-NH2	-12.83	113.89	120.30
5	L	291	ARG	NE-CZ-NH1	12.47	126.54	120.30
5	F	291	ARG	NE-CZ-NH1	-11.97	114.31	120.30
5	F	291	ARG	NE-CZ-NH2	11.77	126.18	120.30
2	I	764	GLU	C-N-CA	8.19	142.16	121.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	177	VAL	Mainchain,Peptide
2	C	178	ALA	Peptide
2	C	764	GLU	Peptide
2	I	178	ALA	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	57	0
1	B	1770	0	1799	55	0
1	G	1770	0	1799	59	0
1	H	1770	0	1799	55	0
2	C	8739	0	8841	295	0
2	I	8739	0	8841	282	0
3	D	11761	0	11976	343	0
3	J	10779	0	10993	314	0
4	E	768	0	784	18	0
4	K	768	0	784	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	2801	0	2881	97	0
5	L	2801	0	2881	87	0
6	O	988	0	544	17	0
6	R	988	0	544	16	0
7	P	985	0	543	17	0
7	S	882	0	487	14	0
8	Q	85	0	43	0	0
8	T	85	0	43	1	0
9	D	2	0	0	0	0
9	J	2	0	0	0	0
10	D	1	0	0	0	0
10	J	1	0	0	0	0
All	All	58255	0	57381	1567	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 14.

The worst 5 of 1567 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:14:THR:HB	1:G:22:GLU:HB2	1.54	0.90
1:A:14:THR:HB	1:A:22:GLU:HB2	1.54	0.89
2:C:630:ARG:HG3	2:C:705:ILE:HB	1.54	0.88
3:D:977:ALA:HB2	3:J:831:GLY:HA3	1.56	0.88
2:C:502:PRO:HG3	2:C:510:THR:HG22	1.56	0.85

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%)	206 (92%)	18 (8%)	1 (0%)	34	71
1	B	225/314 (72%)	205 (91%)	17 (8%)	3 (1%)	12	48
1	G	225/314 (72%)	205 (91%)	19 (8%)	1 (0%)	34	71
1	H	225/314 (72%)	205 (91%)	19 (8%)	1 (0%)	34	71
2	C	1108/1119 (99%)	1011 (91%)	94 (8%)	3 (0%)	41	75
2	I	1108/1119 (99%)	1012 (91%)	94 (8%)	2 (0%)	47	79
3	D	1486/1524 (98%)	1340 (90%)	141 (10%)	5 (0%)	41	75
3	J	1361/1524 (89%)	1235 (91%)	123 (9%)	3 (0%)	47	79
4	E	91/99 (92%)	83 (91%)	8 (9%)	0	100	100
4	K	91/99 (92%)	82 (90%)	9 (10%)	0	100	100
5	F	345/347 (99%)	316 (92%)	29 (8%)	0	100	100
5	L	345/347 (99%)	314 (91%)	31 (9%)	0	100	100
All	All	6835/7434 (92%)	6214 (91%)	602 (9%)	19 (0%)	41	75

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	765	GLN
3	D	1128	VAL
3	J	1128	VAL
1	A	53	VAL
1	B	178	ALA

5.3.2 Protein sidechains (i)

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%)	186 (96%)	8 (4%)	30	57
1	B	194/270 (72%)	179 (92%)	15 (8%)	13	40
1	G	194/270 (72%)	186 (96%)	8 (4%)	30	57
1	H	194/270 (72%)	179 (92%)	15 (8%)	13	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	931/936 (100%)	837 (90%)	94 (10%)	7	29
2	I	931/936 (100%)	838 (90%)	93 (10%)	7	29
3	D	1252/1281 (98%)	1128 (90%)	124 (10%)	8	29
3	J	1150/1281 (90%)	1048 (91%)	102 (9%)	9	34
4	E	83/88 (94%)	77 (93%)	6 (7%)	14	42
4	K	83/88 (94%)	77 (93%)	6 (7%)	14	42
5	F	297/299 (99%)	269 (91%)	28 (9%)	8	31
5	L	297/299 (99%)	269 (91%)	28 (9%)	8	31
All	All	5800/6288 (92%)	5273 (91%)	527 (9%)	9	33

5 of 527 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	1070	TYR
3	J	1267	ARG
3	J	1053	PHE
5	L	346	ASP
3	D	865	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
3	J	762	GLN
3	J	991	GLN
5	L	229	GLN
3	D	991	GLN
3	D	794	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	Q	3/4 (75%)	1 (33%)	0
8	T	3/4 (75%)	1 (33%)	0
All	All	6/8 (75%)	2 (33%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	Q	2	C
8	T	2	C

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 monosaccharides 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 (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	227/314 (72%)	-0.33	0	100	100	68, 121, 176, 228	0
1	B	227/314 (72%)	-0.49	0	100	100	42, 95, 150, 180	0
1	G	227/314 (72%)	-0.01	2 (0%)	84	77	96, 156, 194, 223	0
1	H	227/314 (72%)	-0.29	0	100	100	80, 131, 171, 192	0
2	C	1112/1119 (99%)	-0.30	6 (0%)	91	85	30, 123, 203, 260	0
2	I	1112/1119 (99%)	-0.17	15 (1%)	77	68	60, 146, 214, 259	0
3	D	1490/1524 (97%)	-0.42	1 (0%)	95	94	22, 88, 155, 231	0
3	J	1367/1524 (89%)	-0.33	1 (0%)	95	94	29, 112, 177, 240	0
4	E	93/99 (93%)	-0.41	0	100	100	23, 89, 154, 187	0
4	K	93/99 (93%)	-0.24	0	100	100	67, 126, 181, 236	0
5	F	347/347 (100%)	-0.20	6 (1%)	70	60	52, 131, 221, 275	0
5	L	347/347 (100%)	-0.12	5 (1%)	75	65	81, 151, 225, 270	0
6	O	48/48 (100%)	0.40	4 (8%)	11	10	86, 193, 267, 293	0
6	R	48/48 (100%)	0.08	1 (2%)	63	54	109, 184, 277, 300	0
7	P	48/48 (100%)	0.61	4 (8%)	11	10	77, 199, 251, 283	0
7	S	43/48 (89%)	0.14	1 (2%)	60	51	100, 195, 234, 248	0
8	Q	4/4 (100%)	0.06	0	100	100	116, 124, 128, 150	0
8	T	4/4 (100%)	0.05	0	100	100	122, 130, 143, 154	0
All	All	7064/7634 (92%)	-0.28	46 (0%)	87	82	22, 120, 200, 300	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	187	GLY	5.3
5	L	177	LYS	4.4
2	I	246	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
3	D	1253	THR	3.6
7	P	48	DG	3.2

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 monosaccharides 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(Å^2)	Q<0.9
10	MG	D	2003	1/1	0.94	0.07	180,180,180,180	0
9	ZN	J	2002	1/1	0.95	0.07	166,166,166,166	0
10	MG	J	2003	1/1	0.95	0.25	188,188,188,188	0
9	ZN	D	2002	1/1	0.96	0.07	79,79,79,79	0
9	ZN	D	2001	1/1	0.97	0.12	79,79,79,79	0
9	ZN	J	2001	1/1	0.99	0.12	97,97,97,97	0

6.5 Other polymers (i)

There are no such residues in this entry.