wwPDB X-ray Structure Validation Summary Report (i)

Feb 20, 2024 – 06:02 AM EST

PDB ID	:	4LJZ
Title	:	Crystal Structure Analysis of the E.coli holoenzyme
Authors	:	Bae, B.; Darst, S.A.
Deposited on	:	2013-07-05
Resolution	:	3.59 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:

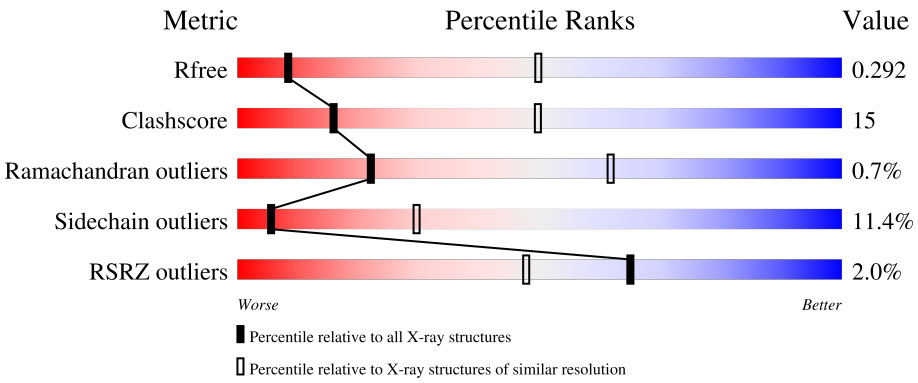
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.59 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	1094 (3.66-3.50)
Clashscore	141614	1181 (3.66-3.50)
Ramachandran outliers	138981	1143 (3.66-3.50)
Sidechain outliers	138945	1143 (3.66-3.50)
RSRZ outliers	127900	1012 (3.66-3.50)

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	239	60% 29% • 6%
1	B	239	4% 50% 38% • 8%
1	G	239	% 62% 29% • • 5%
1	H	239	5% 48% 38% 5% 9%
2	C	1342	62% 32% 5%

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Mol	Chain	Length	Quality of chain
2	I	1342	2%, 64%, 31%, 5%
3	D	1407	%, 50%, 28%, 17%
3	J	1407	4%, 56%, 33%, 5%, 6%
4	E	91	63%, 29%, 5%
4	K	91	53%, 26%, 8%, 13%
5	F	522	3%, 59%, 25%, 5%, 10%
5	L	522	2%, 57%, 26%, 6%, 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	ZN	J	1503	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 56339 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	224	1730	1076	308	340	6	0	0	0
1	B	220	1687	1053	298	330	6	0	0	0
1	G	228	1750	1088	312	344	6	0	0	0
1	H	217	1667	1041	293	327	6	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	GLU	-	expression tag	UNP C9QXI7
A	236	VAL	-	expression tag	UNP C9QXI7
A	237	LEU	-	expression tag	UNP C9QXI7
A	238	PHE	-	expression tag	UNP C9QXI7
A	239	GLN	-	expression tag	UNP C9QXI7
B	235	GLU	-	expression tag	UNP C9QXI7
B	236	VAL	-	expression tag	UNP C9QXI7
B	237	LEU	-	expression tag	UNP C9QXI7
B	238	PHE	-	expression tag	UNP C9QXI7
B	239	GLN	-	expression tag	UNP C9QXI7
G	235	GLU	-	expression tag	UNP C9QXI7
G	236	VAL	-	expression tag	UNP C9QXI7
G	237	LEU	-	expression tag	UNP C9QXI7
G	238	PHE	-	expression tag	UNP C9QXI7
G	239	GLN	-	expression tag	UNP C9QXI7
H	235	GLU	-	expression tag	UNP C9QXI7
H	236	VAL	-	expression tag	UNP C9QXI7
H	237	LEU	-	expression tag	UNP C9QXI7
H	238	PHE	-	expression tag	UNP C9QXI7
H	239	GLN	-	expression tag	UNP C9QXI7

- 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	1340	10570	6631	1841	2055	43	0	0	0
2	I	1340	10566	6629	1840	2054	43	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	1166	9107	5723	1634	1704	46	0	0	0
3	J	1325	10295	6470	1831	1945	49	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	89	691	421	129	140	1	0	0	0
4	K	79	627	382	118	126	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	470	3822	2394	680	725	23	0	0	0
5	L	469	3821	2393	679	726	23	0	0	0

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

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

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

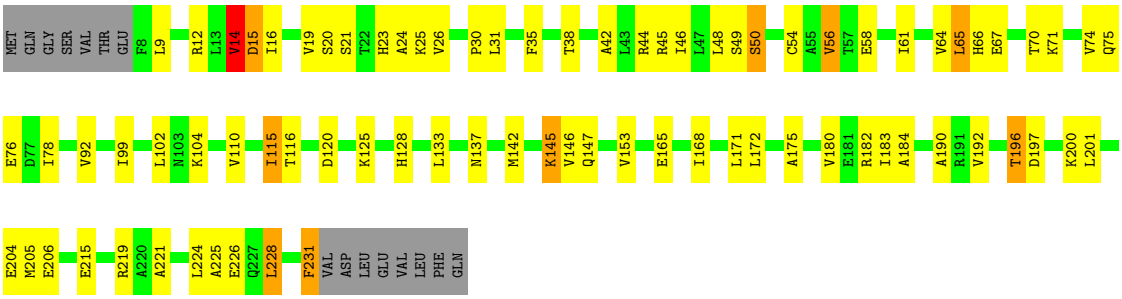
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
7	D	2	2	2	0	0
7	J	2	2	2	0	0

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.

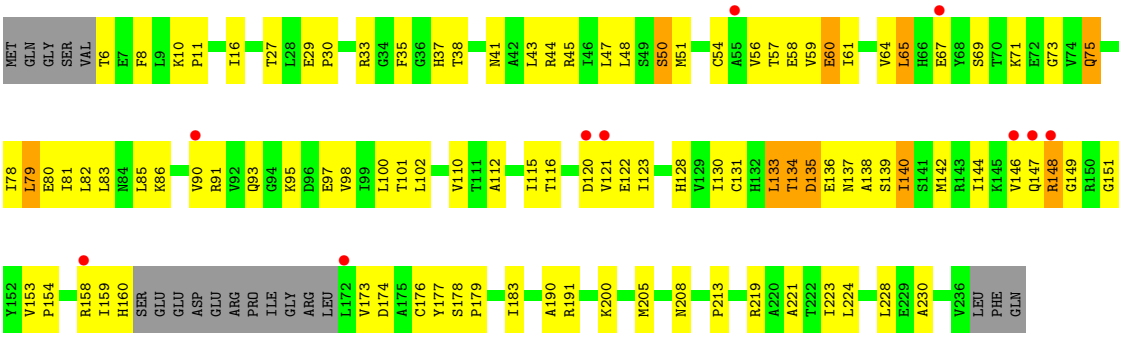
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



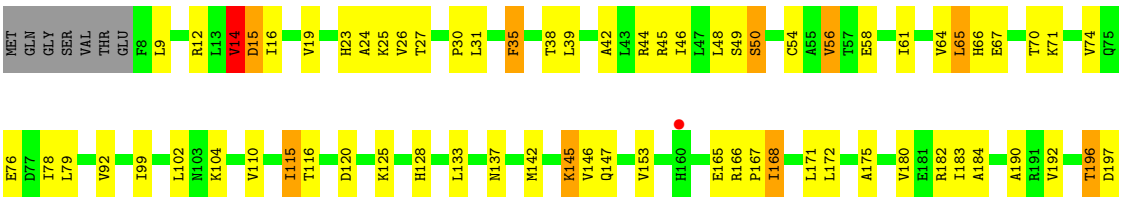
• Molecule 1: DNA-directed RNA polymerase subunit alpha

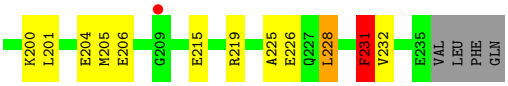
Chain B:



• Molecule 1: DNA-directed RNA polymerase subunit alpha

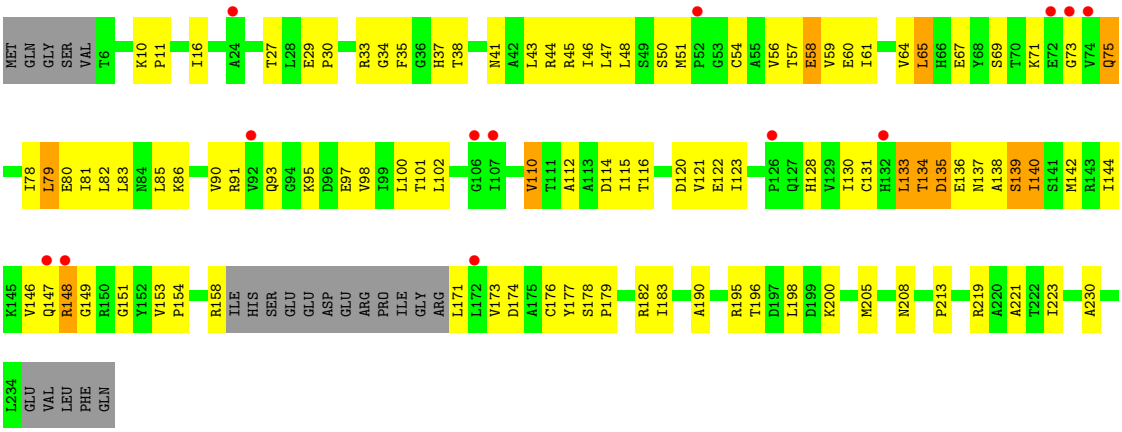
Chain G:





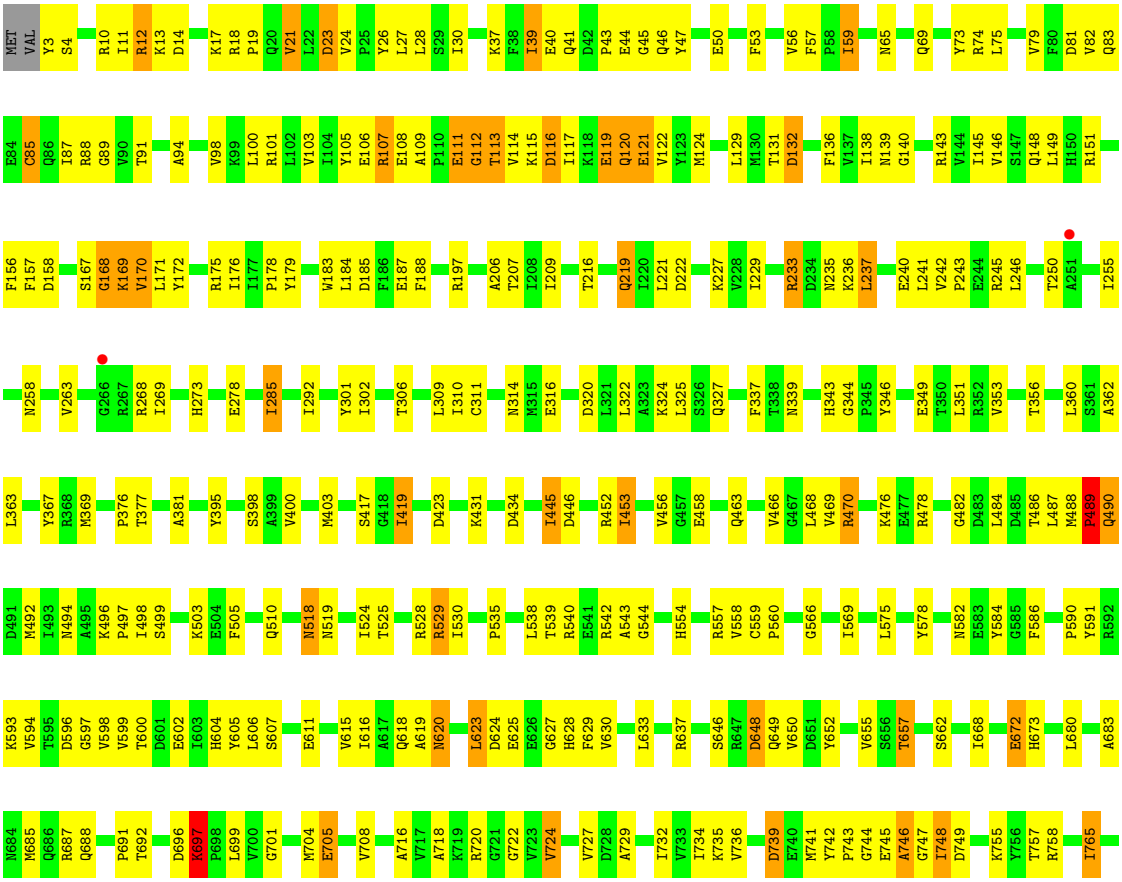
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain H:



• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C:



P769 L773 G774 E775 P776 V777 E778 V782 L783 A784 S788 T789 D790 L791 G792 E793 L794 A795 L796 G797 Q798 N799 M800 N808 E813 D814 S815 I816 L817 V818 R821 D826 R827 F828 T829 T830 I831 H832 I833 Q834 E835 L836 A837 C838 V839 S840 I850 T851 A852 D853 I854

V857 G858 E859 A860 A861 E867 I870 T878 G879 K886 V887 K890 G891 E892 T896 P897 E898 E899 K900 L901 L902 F906 S911 D912 V913 S917 P921 S925 D930 V931 K943 R944 A945 L946 S961 Q965 I966 L967 E968 L971 R974 I975

V978 L979 V980 A981 V984 E985 A986 E987 K988 K991 L1000 G1001 L1002 E1006 K1007 L1011 L1014 Q1017 Y1018 E1030 R1033 R1034 K1035 D1040 K1048 A1055 V1056 R1059 K1065 K1073 I1079 N1080 P1081 I1082 E1083 Y1087 G1091 P1100 L1101 P1104

S1105 R1106 M1107 N1108 I1109 G1110 Q1111 E1114 T1115 H1116 L1117 G1118 M1119 A1120 A1121 K1122 Q1134 Q1135 Q1136 E1137 K1140 L1141 R1142 Q1146 Y1149 D1150 L1151 G1152 A1153 D1154 V1155 R1156 Q1157 K1158 V1159 D1160 L1161 S1162 T1163 F1164 E1174 N1175 L1176 M1180 P1181 I1182 A1183 T1184 P1185 D1188 K1191

E1192 A1193 E1194 I1195 K1196 E1197 L1198 G1202 D1203 L1204 P1205 T1206 Q1209 I1210 G1215 R1216 E1222 R1223 P1224 G1228 Y1229 M1230 Y1231 V1239 D1240 M1243 R1246 S1247 T1248 Q1257 Q1264 F1265 E1272 V1275 W1276 A1280 Y1281 G1282 A1283 A1284 L1287 D1297 R1301

M1304 I1308 N1312 H1313 Q1314 P1320 F1323 L1327 R1331 D1341 E1342

- Molecule 2: DNA-directed RNA polymerase subunit beta

Chain I: 2% 64% 31% 5%

MET VAL Y3 S4 Y5 K8 K9 R10 I11 R12 K13 D14 V21 L22 D23 Y26 L27 L28 S29 I30 Q31 L32 K37 F38 I39 E40 Q41 D42 P43 E44 G45 Q46 Y47 E50 F53 V56 F57 P58 I59 N65 Q69 Y70 Y73 R74 L75 V79 F80 D81 V82

Q83 E84 C85 Q86 I87 T91 A94 R97 V98 K99 L100 R101 L102 V103 I104 Y105 E106 R107 E108 A109 P110 E111 G112 T113 V114 K115 D116 I117 K118 E119 Q120 E121 V122 Y123 M124 L129 M130 T131 D132 F136 V137 I138 N139 G140 I145 V146 L149 H150 R151 F156 F157 D158

K163 S167 G168 K169 V170 L171 Y172 R175 I176 I177 P178 W183 L184 D185 F186 E187 F188 R197 R202 A206 T207 I208 I209 T216 Q219 I220 L221 D222 K227 V228 I229 R233 D234 N235 K236 L237 E240 L241 V242 P243 E244 R245 L246 R247 T250 I255

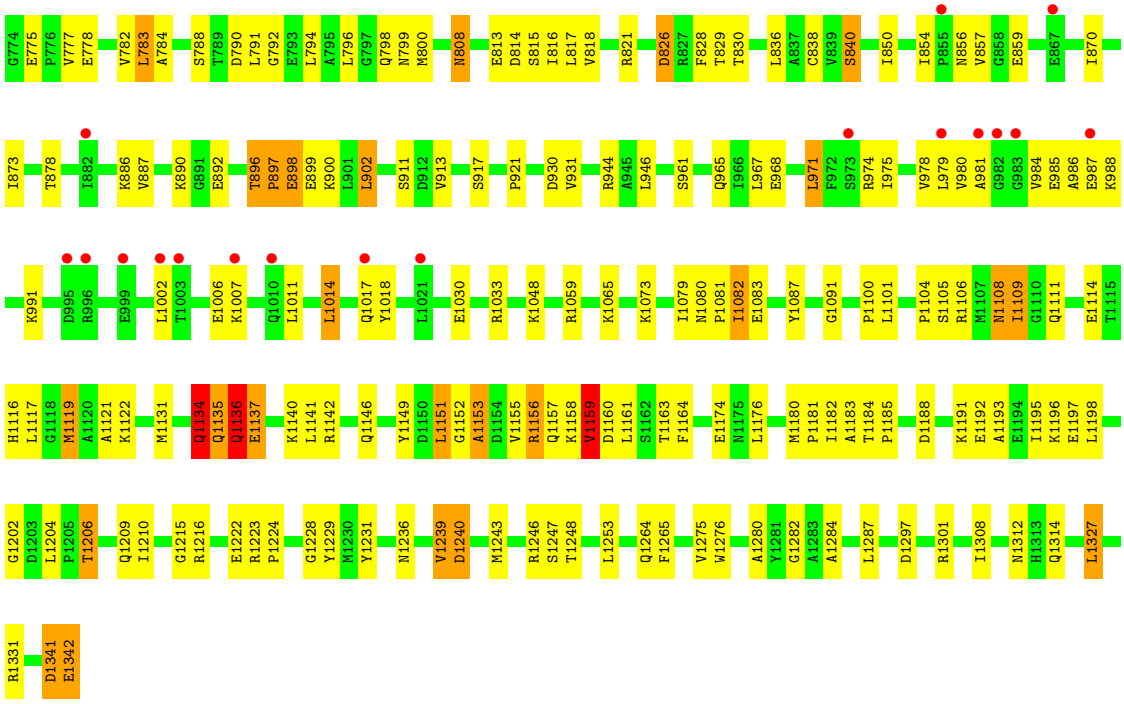
N258 V263 R268 I269 H273 E278 I285 I292 Y301 I302 T306 L309 I310 C311 N314 M315 E316 D320 L321 L322 A323 K324 L325 S326 Q327 F337 G344 P345 Y346 E349 T350 L351 R352 V353 T356 L360 S361 A362 L363 Y367 R368 M369

P376 T377 A381 Y395 R402 S408 S417 G418 I419 K422 D423 K431 D434 I445 D446 R452 I453 V456 Q463 V466 G467 L468 V469 R470 K476 E477 R478 G482 D483 L484 D485 T486 L487 M488 P489 Q490 D491 M492 I493 N494 A495 K496 P497 I498

S499 K503 E504 F505 Q510 L511 S512 D516 Q517 N518 N519 P520 I524 T525 R528 R529 I530 L538 T539 R540 E541 R542 A543 G544 H554 R557 V558 C559 P560 G566 I569 L575 Y578 N582 E583 Y584 G585 F586 P590 Y591 R592 K593 V594 T595 D596 G597

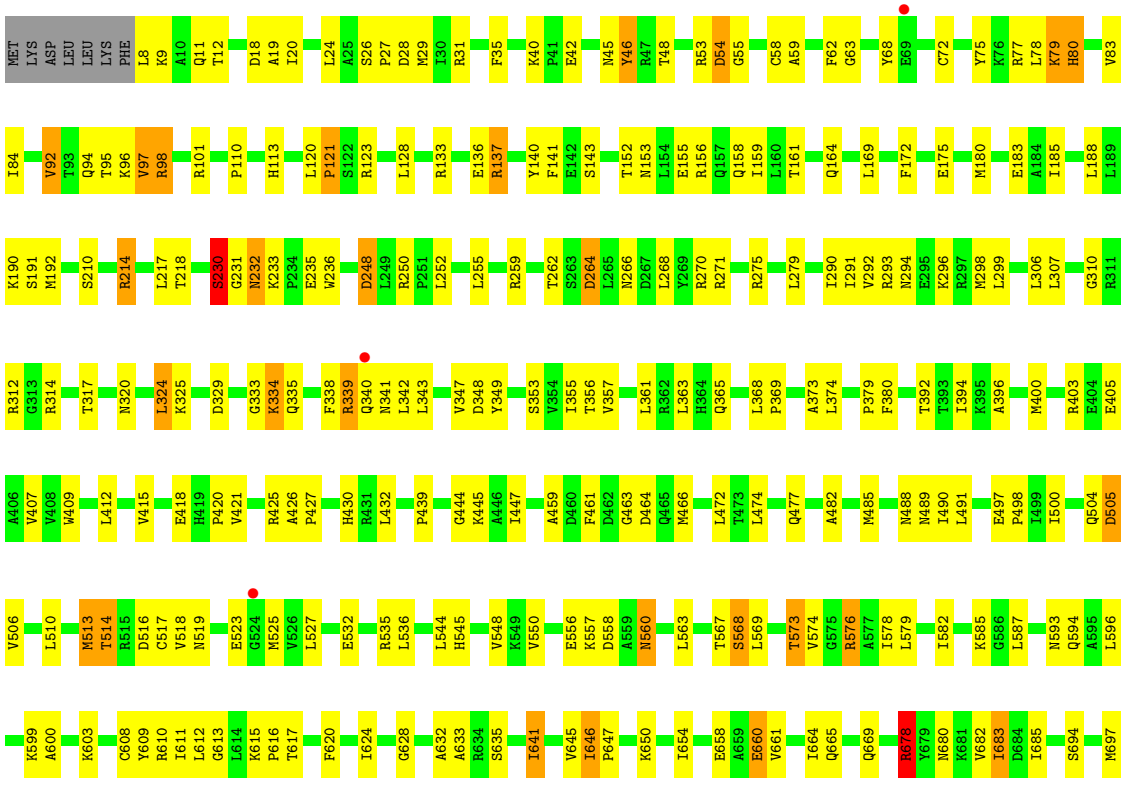
V598 V599 T600 D601 E602 T603 H604 Y605 L606 S607 E611 V615 I616 A617 Q618 A619 N620 L623 D624 E625 E626 G627 H628 F629 V630 L633 R637 S646 R647 D648 Q649 V650 D651 Y652 V655 S656 T657 S662 I668 E672 H673 L680 A683 N684 M685 Q686 R687 Q688

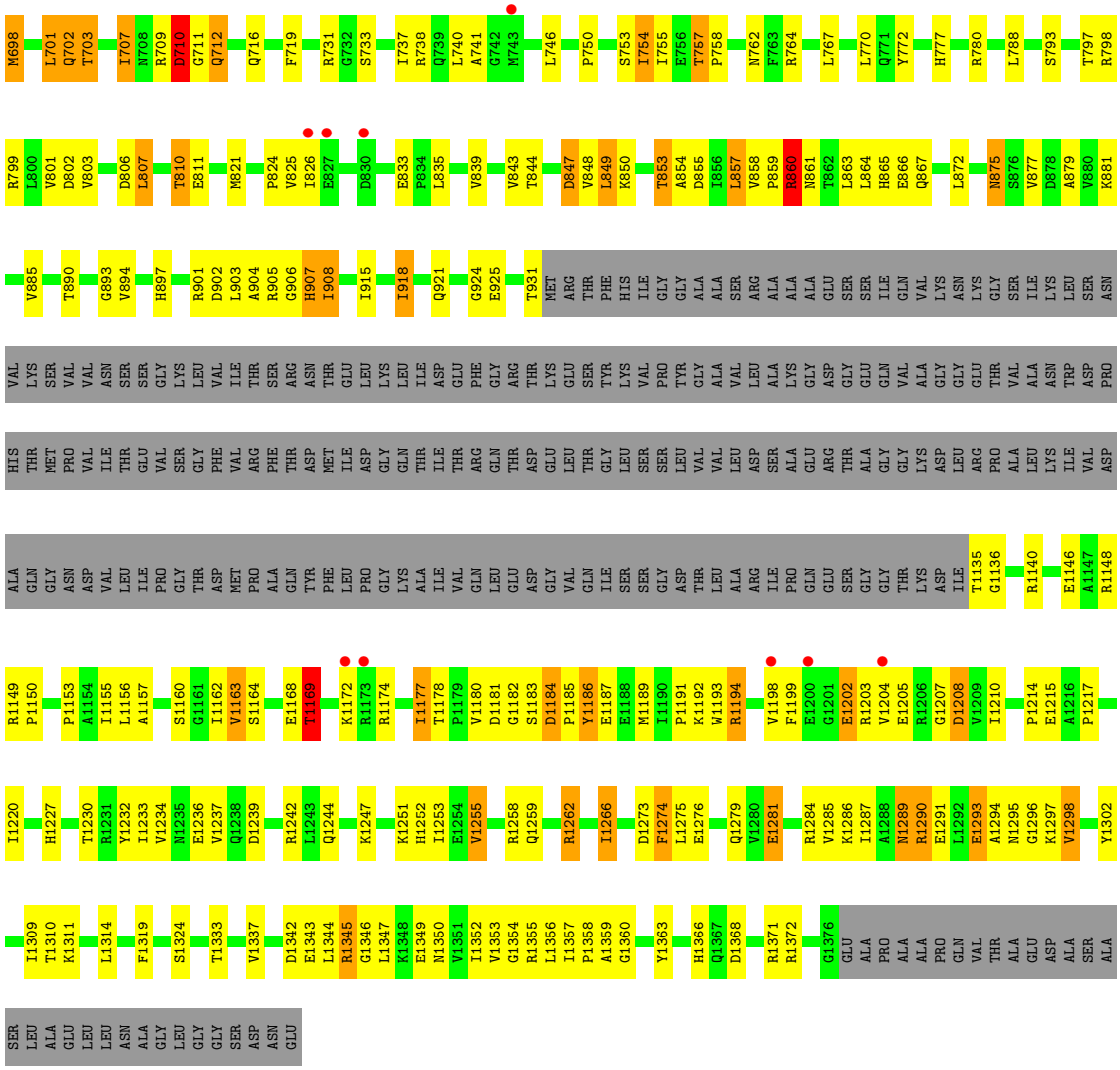
P691 T692 L693 D696 K697 P698 L699 V700 G701 E705 V708 A709 V710 V714 T715 A716 V717 A718 K719 R720 G721 G722 V723 V724 G725 Y726 V727 I732 V733 I734 K735 V736 D739 E740 M741 Y742 P743 G744 E745 A746 G747 T748 D749 K755 Y756 T757 I765 P769 L773



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

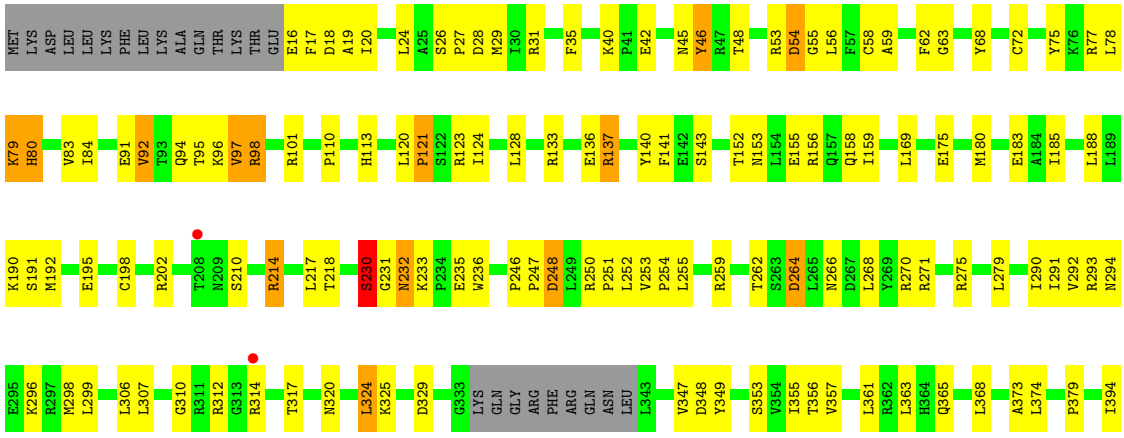
Chain D:

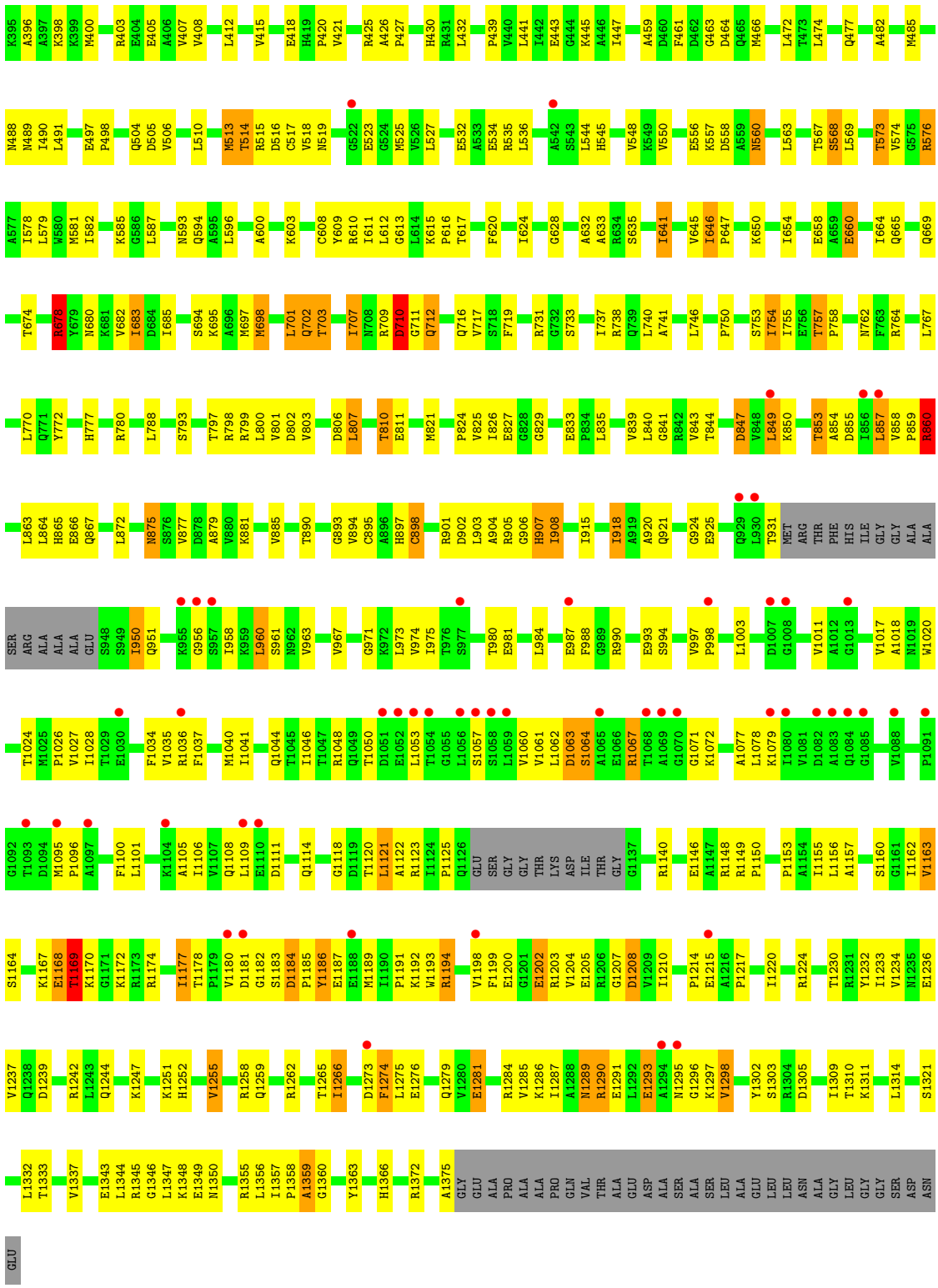




• Molecule 3: DNA-directed RNA polymerase subunit beta'

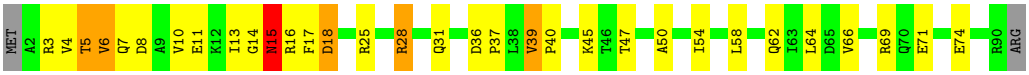
Chain J:





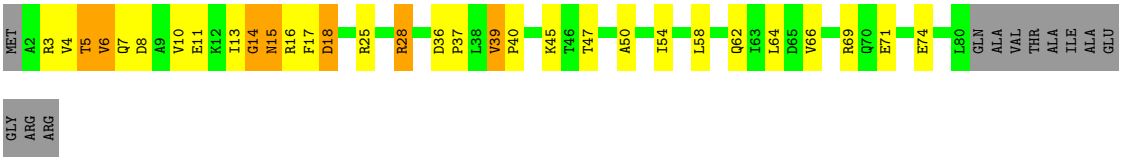
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:



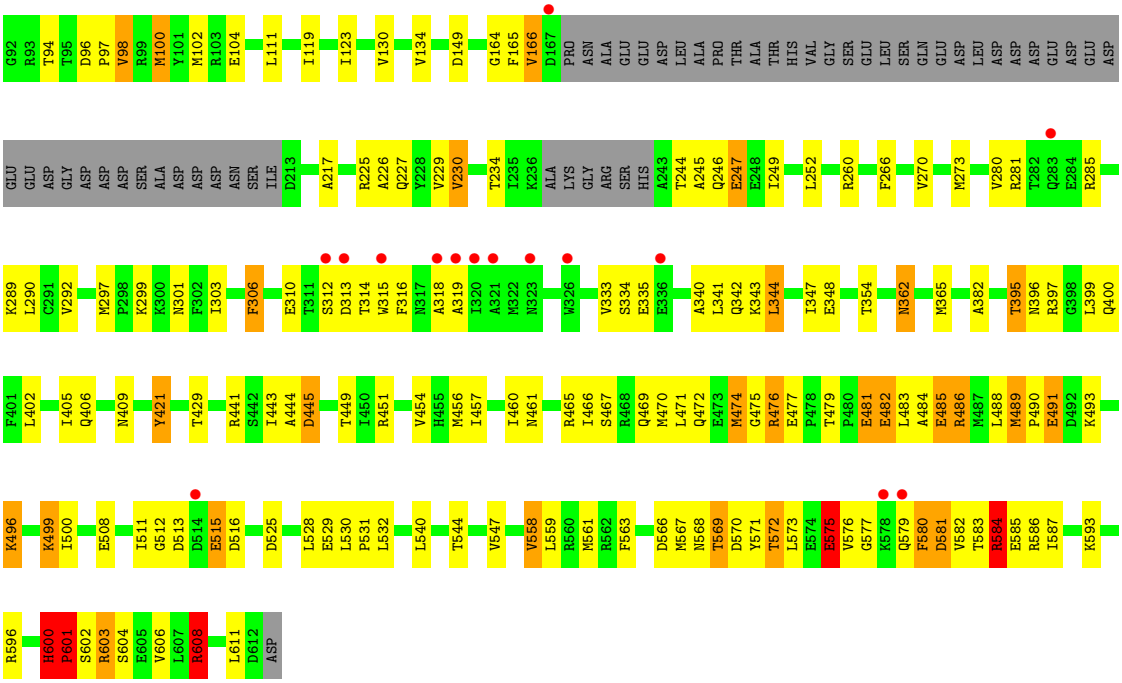
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain K:



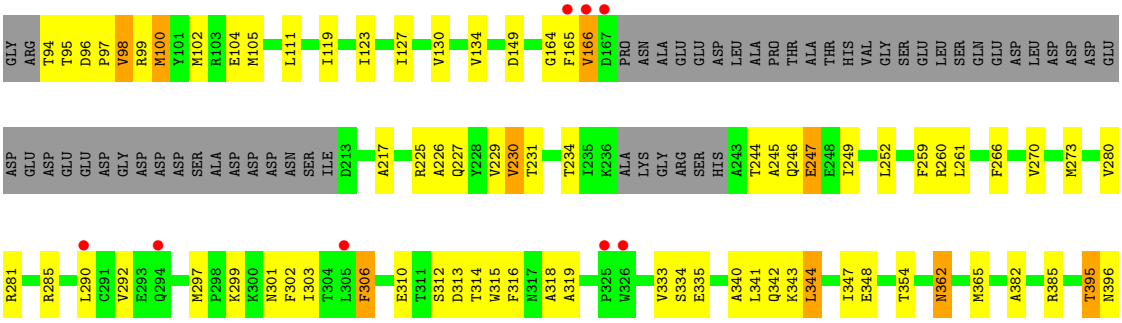
• Molecule 5: RNA polymerase sigma factor RpoD

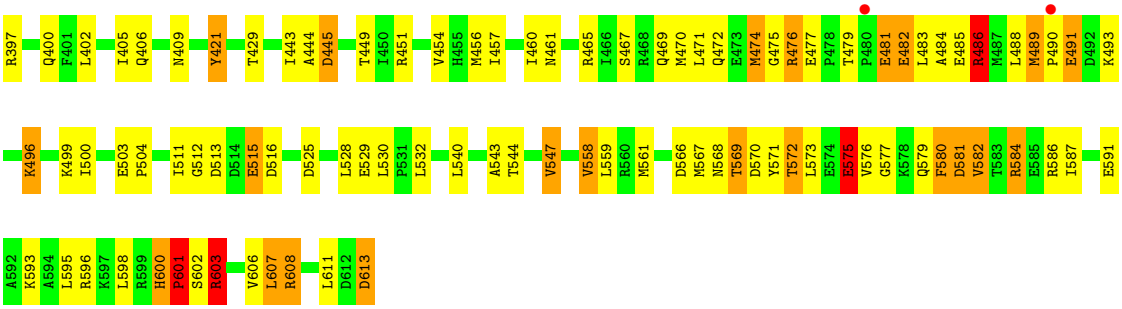
Chain F:



• Molecule 5: RNA polymerase sigma factor RpoD

Chain L:




R397
Q400
F401
L402
I405
Q406
N409
Y421
T429
I443
A444
D445
T449
I450
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V454
H455
M456
I457
I460
N461
R465
I466
S467
R468
Q469
M470
L471
Q472
E473
M474
G475
R476
E477
P478
T479
P480
E481
E482
L483
A484
E485
R486
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L488
M489
P490
E491
D492
K493
K496
K499
I500
E503
P504
I511
G512
D513
D514
E515
D516
D525
L528
E529
L530
P531
L532
L540
A543
T544
V547
V558
L559
R560
M561
D566
M567
N568
T569
D570
Y571
T572
L573
E574
E575
V576
G577
K578
Q579
F580
D581
V582
T583
R584
E585
R586
I587
E591
A592
K593
A594
L595
R596
K597
L598
R599
H600
P601
S602
R603
V606
L607
R608
L611
D612
D613

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	186.37Å 206.74Å 309.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 3.59 29.88 – 3.59	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.88-3.59) 99.3 (29.88-3.59)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 3.56Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.246 , 0.288 0.247 , 0.292	Depositor DCC
R_{free} test set	6971 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	122.5	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 48.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	56339	wwPDB-VP
Average B, all atoms (Å^2)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% 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: 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	0.28	0/1751	0.59	1/2373 (0.0%)
1	B	0.28	0/1707	0.58	1/2314 (0.0%)
1	G	0.30	0/1771	0.61	2/2401 (0.1%)
1	H	0.28	0/1686	0.59	1/2285 (0.0%)
2	C	0.30	0/10739	0.59	6/14489 (0.0%)
2	I	0.30	0/10735	0.58	7/14484 (0.0%)
3	D	0.28	0/9246	0.59	5/12478 (0.0%)
3	J	0.28	0/10450	0.56	2/14112 (0.0%)
4	E	0.27	0/693	0.58	1/935 (0.1%)
4	K	0.28	0/629	0.54	0/847
5	F	0.36	1/3873 (0.0%)	0.62	7/5206 (0.1%)
5	L	0.35	0/3872	0.63	6/5205 (0.1%)
All	All	0.30	1/57152 (0.0%)	0.59	39/77129 (0.1%)

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	1
1	G	0	1
1	H	0	1
2	C	0	14
2	I	0	15
3	D	0	5
3	J	0	6
4	K	0	1
5	F	0	4
5	L	0	2
All	All	0	50

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	600	HIS	N-CA	5.34	1.57	1.46

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	747	GLY	N-CA-C	14.60	149.61	113.10
2	I	747	GLY	N-CA-C	11.86	142.76	113.10
3	D	1262	ARG	NE-CZ-NH1	-7.19	116.70	120.30
2	I	112	GLY	N-CA-C	6.85	130.22	113.10
3	D	860	ARG	NE-CZ-NH1	6.80	123.70	120.30

There are no chirality outliers.

5 of 50 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	140	ILE	Peptide
2	C	109	ALA	Peptide
2	C	111	GLU	Peptide
2	C	112	GLY	Peptide
2	C	43	PRO	Mainchain

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	1730	0	1756	54	0
1	B	1687	0	1700	70	0
1	G	1750	0	1764	52	0
1	H	1667	0	1689	71	0
2	C	10570	0	10582	305	1
2	I	10566	0	10576	284	1
3	D	9107	0	9308	331	0
3	J	10295	0	10511	386	0
4	E	691	0	695	21	0
4	K	627	0	634	18	0
5	F	3822	0	3885	98	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	3821	0	3884	106	0
6	D	1	0	0	0	0
6	J	1	0	0	0	0
7	D	2	0	0	0	0
7	J	2	0	0	0	0
All	All	56339	0	56984	1652	1

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 15.

The worst 5 of 1652 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:233:ARG:HH11	2:C:233:ARG:HG3	1.24	1.02
3:D:26:SER:HA	3:D:236:TRP:HE1	1.30	0.96
3:J:98:ARG:HG2	3:J:98:ARG:HH11	1.32	0.94
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.51	0.93
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.51	0.92

All (1) 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:108:GLU:OE2	2:I:422:LYS:NZ[3_554]	2.19	0.01

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	222/239 (93%)	195 (88%)	26 (12%)	1 (0%)	29 67
1	B	216/239 (90%)	192 (89%)	23 (11%)	1 (0%)	29 67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	226/239 (95%)	197 (87%)	27 (12%)	2 (1%)	17	57
1	H	213/239 (89%)	191 (90%)	21 (10%)	1 (0%)	29	67
2	C	1338/1342 (100%)	1224 (92%)	100 (8%)	14 (1%)	15	55
2	I	1338/1342 (100%)	1228 (92%)	97 (7%)	13 (1%)	15	55
3	D	1162/1407 (83%)	1078 (93%)	78 (7%)	6 (0%)	29	67
3	J	1317/1407 (94%)	1225 (93%)	87 (7%)	5 (0%)	34	71
4	E	87/91 (96%)	76 (87%)	10 (12%)	1 (1%)	14	53
4	K	77/91 (85%)	72 (94%)	4 (5%)	1 (1%)	12	49
5	F	464/522 (89%)	420 (90%)	41 (9%)	3 (1%)	25	64
5	L	463/522 (89%)	422 (91%)	36 (8%)	5 (1%)	14	53
All	All	7123/7680 (93%)	6520 (92%)	550 (8%)	53 (1%)	22	62

5 of 53 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	44	GLU
2	C	169	LYS
2	C	697	LYS
2	C	897	PRO
2	C	898	GLU

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	191/206 (93%)	169 (88%)	22 (12%)	5	29
1	B	184/206 (89%)	161 (88%)	23 (12%)	4	25
1	G	191/206 (93%)	169 (88%)	22 (12%)	5	29
1	H	183/206 (89%)	164 (90%)	19 (10%)	7	34
2	C	1155/1157 (100%)	1025 (89%)	130 (11%)	6	30
2	I	1154/1157 (100%)	1022 (89%)	132 (11%)	5	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	975/1168 (84%)	870 (89%)	105 (11%)	6	32
3	J	1110/1168 (95%)	996 (90%)	114 (10%)	7	34
4	E	72/75 (96%)	63 (88%)	9 (12%)	4	25
4	K	67/75 (89%)	58 (87%)	9 (13%)	4	23
5	F	417/462 (90%)	361 (87%)	56 (13%)	4	23
5	L	418/462 (90%)	359 (86%)	59 (14%)	3	21
All	All	6117/6548 (93%)	5417 (89%)	700 (11%)	5	29

5 of 700 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	778	GLU
3	J	710	ASP
2	I	890	LYS
2	I	773	LEU
3	J	54	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	579	GLN
5	L	383	ASN
2	I	688	GLN
5	L	246	GLN
5	L	579	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 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	224/239 (93%)	-0.35	0	100	100	59, 91, 130, 167	0
1	B	220/239 (92%)	0.12	10 (4%)	33	19	63, 125, 155, 166	0
1	G	228/239 (95%)	-0.15	2 (0%)	84	71	85, 121, 148, 164	0
1	H	217/239 (90%)	0.13	13 (5%)	21	11	90, 130, 156, 165	0
2	C	1340/1342 (99%)	-0.34	5 (0%)	92	86	33, 84, 134, 170	0
2	I	1340/1342 (99%)	-0.17	22 (1%)	72	55	48, 101, 149, 179	0
3	D	1166/1407 (82%)	-0.26	12 (1%)	82	69	28, 77, 137, 168	0
3	J	1325/1407 (94%)	-0.05	54 (4%)	37	22	40, 96, 152, 176	0
4	E	89/91 (97%)	-0.51	0	100	100	44, 84, 114, 133	0
4	K	79/91 (86%)	-0.31	0	100	100	63, 97, 136, 150	0
5	F	470/522 (90%)	-0.08	15 (3%)	47	31	53, 119, 159, 181	0
5	L	469/522 (89%)	-0.11	10 (2%)	63	46	61, 117, 159, 173	0
All	All	7167/7680 (93%)	-0.18	143 (1%)	65	48	28, 97, 150, 181	0

The worst 5 of 143 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	167	ASP	9.2
1	B	172	LEU	7.5
5	L	167	ASP	7.4
2	I	999	GLU	6.0
3	J	1054	THR	5.7

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 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
7	ZN	J	1503	1/1	0.40	0.43	316,316,316,316	0
6	MG	D	1501	1/1	0.83	0.41	78,78,78,78	0
6	MG	J	1501	1/1	0.87	0.22	89,89,89,89	0
7	ZN	D	1503	1/1	0.88	0.28	114,114,114,114	0
7	ZN	J	1502	1/1	0.91	0.30	314,314,314,314	0
7	ZN	D	1502	1/1	0.95	0.21	198,198,198,198	0

6.5 Other polymers (i)

There are no such residues in this entry.