wwPDB X-ray Structure Validation Summary Report (i)

Aug 22, 2020 – 08:18 AM BST

PDB ID	:	4MEX
Title	:	Crystal structure of Escherichia coli RNA polymerase in complex with salinamide A
Authors	:	Feng, Y.; Zhang, Y.; Arnold, E.; Ebright, R.H.
Deposited on	:	2013-08-27
Resolution	:	3.90 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 following versions of software and data (see references (1)) were used in the production of this report:

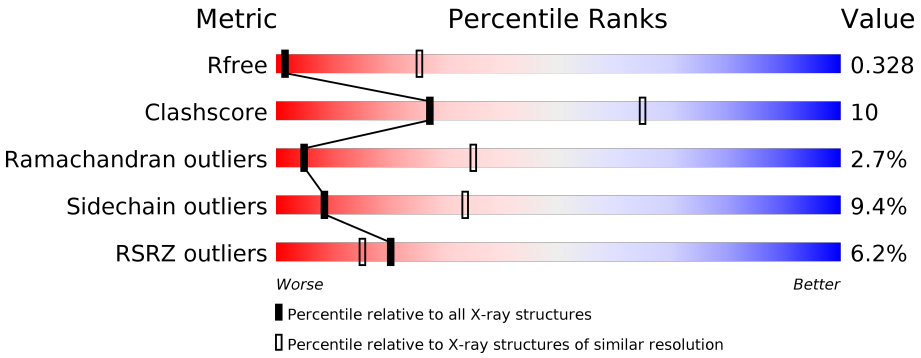
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 3.90 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	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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 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	335	6% 65% 19% 11%
1	B	335	7% 56% 26% 14%
1	G	335	8% 44% 19% 36%
1	H	335	10% 45% 15% 36%
2	C	1342	5% 81% 17%
2	I	1342	11% 79% 19%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	D	1407	2% 62% 17% 18%
3	J	1407	2% 60% 19% 19%
4	E	91	79% 15%
4	K	91	5% 68% 14% 18%
5	F	613	5% 51% 22% 24%
5	L	613	5% 50% 22% 24%
6	M	9	44% 44% 11%
6	N	9	44% 44% 11%

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
6	D4P	M	4	-	-	X	-
6	MEA	M	5	-	-	X	-
6	2TL	M	6	-	-	X	-
6	D4P	N	4	-	-	X	-
6	MEA	N	5	-	-	X	-
6	2TL	N	6	-	-	X	-
7	MG	J	2000	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 50018 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	298	Total	C	N	O	S	0	0	0
			2236	1405	391	432	8			
1	B	287	Total	C	N	O	S	0	0	0
			2160	1359	374	419	8			
1	G	216	Total	C	N	O	S	0	0	0
			1618	1013	282	317	6			
1	H	215	Total	C	N	O	S	0	0	0
			1605	1005	278	316	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	HIS	-	EXPRESSION TAG	UNP P0A7Z4
A	-3	HIS	-	EXPRESSION TAG	UNP P0A7Z4
A	-2	HIS	-	EXPRESSION TAG	UNP P0A7Z4
A	-1	HIS	-	EXPRESSION TAG	UNP P0A7Z4
A	0	HIS	-	EXPRESSION TAG	UNP P0A7Z4
A	1	HIS	-	EXPRESSION TAG	UNP P0A7Z4
B	-4	HIS	-	EXPRESSION TAG	UNP P0A7Z4
B	-3	HIS	-	EXPRESSION TAG	UNP P0A7Z4
B	-2	HIS	-	EXPRESSION TAG	UNP P0A7Z4
B	-1	HIS	-	EXPRESSION TAG	UNP P0A7Z4
B	0	HIS	-	EXPRESSION TAG	UNP P0A7Z4
B	1	HIS	-	EXPRESSION TAG	UNP P0A7Z4
G	-4	HIS	-	EXPRESSION TAG	UNP P0A7Z4
G	-3	HIS	-	EXPRESSION TAG	UNP P0A7Z4
G	-2	HIS	-	EXPRESSION TAG	UNP P0A7Z4
G	-1	HIS	-	EXPRESSION TAG	UNP P0A7Z4
G	0	HIS	-	EXPRESSION TAG	UNP P0A7Z4
G	1	HIS	-	EXPRESSION TAG	UNP P0A7Z4
H	-4	HIS	-	EXPRESSION TAG	UNP P0A7Z4
H	-3	HIS	-	EXPRESSION TAG	UNP P0A7Z4
H	-2	HIS	-	EXPRESSION TAG	UNP P0A7Z4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	HIS	-	EXPRESSION TAG	UNP P0A7Z4
H	0	HIS	-	EXPRESSION TAG	UNP P0A7Z4
H	1	HIS	-	EXPRESSION TAG	UNP P0A7Z4

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1340	Total	C	N	O	S	3	0	0
			9522	5999	1675	1829	19			
2	I	1340	Total	C	N	O	S	3	0	0
			9544	6013	1676	1835	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1150	Total	C	N	O	S	0	0	0
			7572	4771	1358	1415	28			
3	J	1143	Total	C	N	O	S	0	0	0
			7535	4748	1351	1408	28			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	89	Total	C	N	O	0	0	0
			482	299	93	90			
4	K	75	Total	C	N	O	0	0	0
			408	253	79	76			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	464	Total	C	N	O	S	0	0	0
			3592	2253	643	682	14			
5	L	464	Total	C	N	O	S	0	0	0
			3592	2253	643	682	14			

- Molecule 6 is a protein called Salinamide A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	M	9	Total	C	N	O	0	0	0
			73	51	7	15			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	N	9	Total C N O 73 51 7 15	0	0	0

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

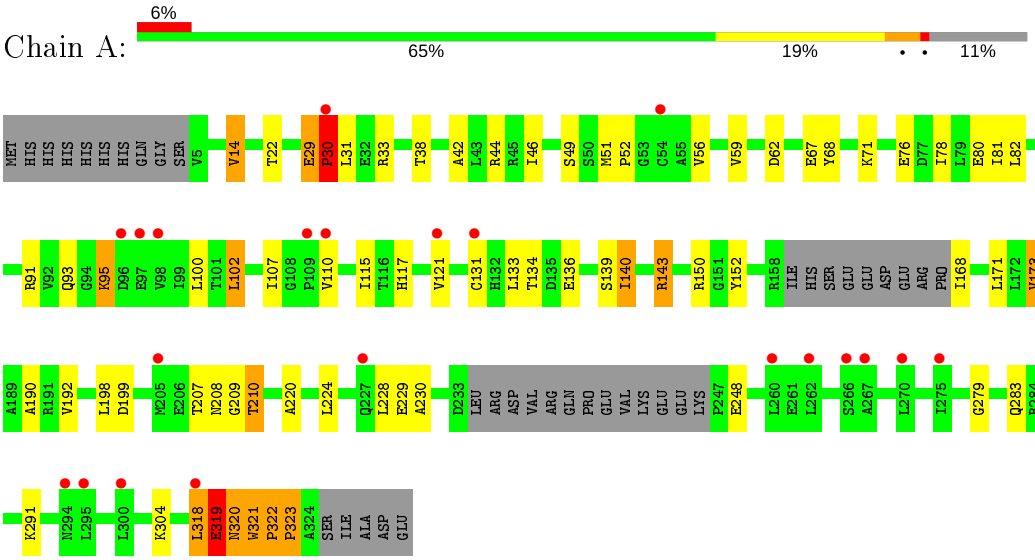
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	J	2	Total Zn 2 2	0	0
8	D	2	Total Zn 2 2	0	0

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.

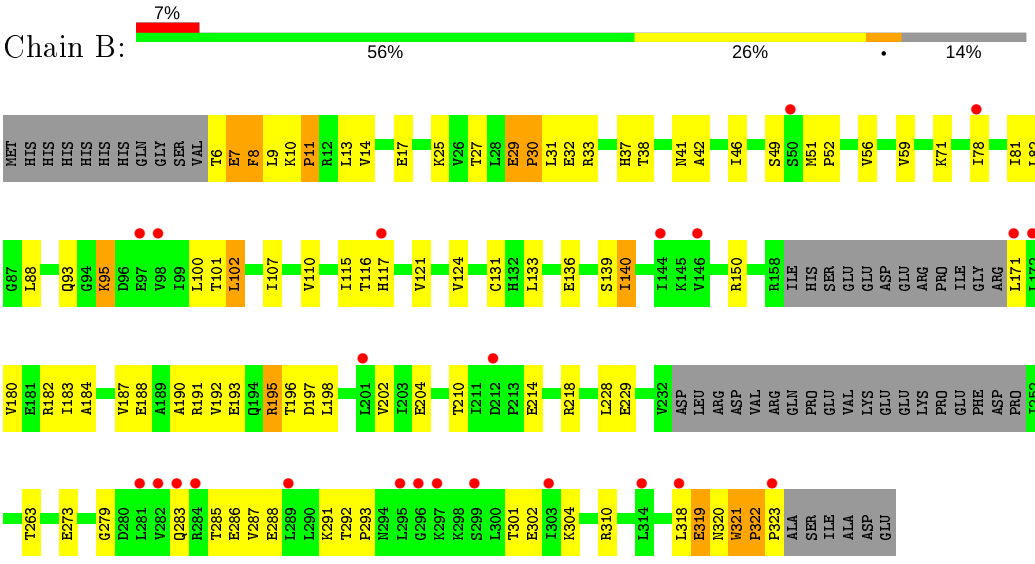
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:

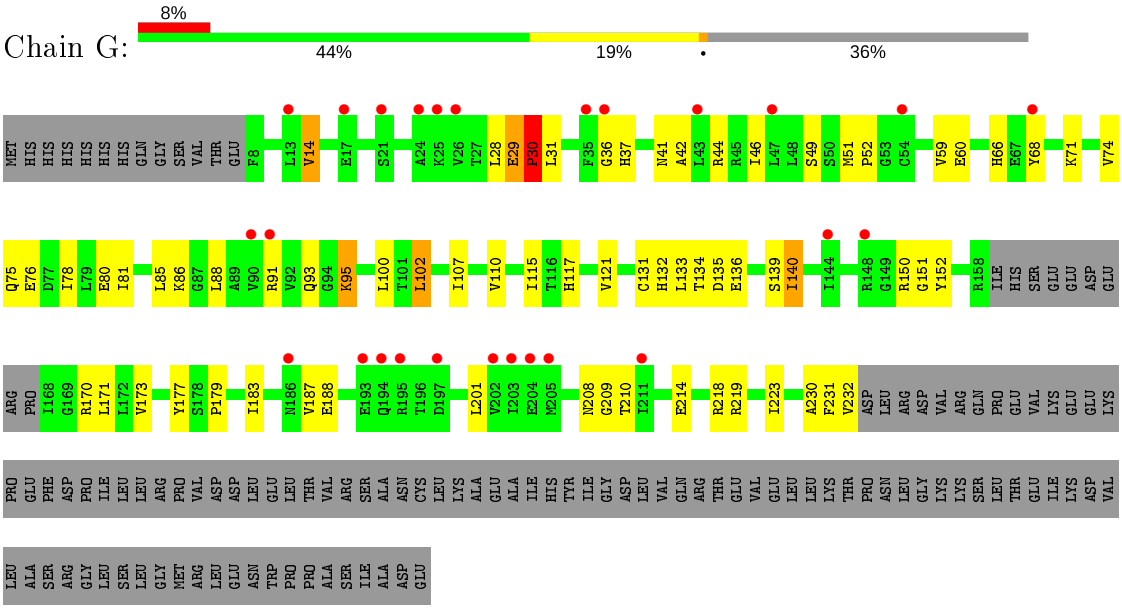


- Molecule 1: DNA-directed RNA polymerase subunit alpha

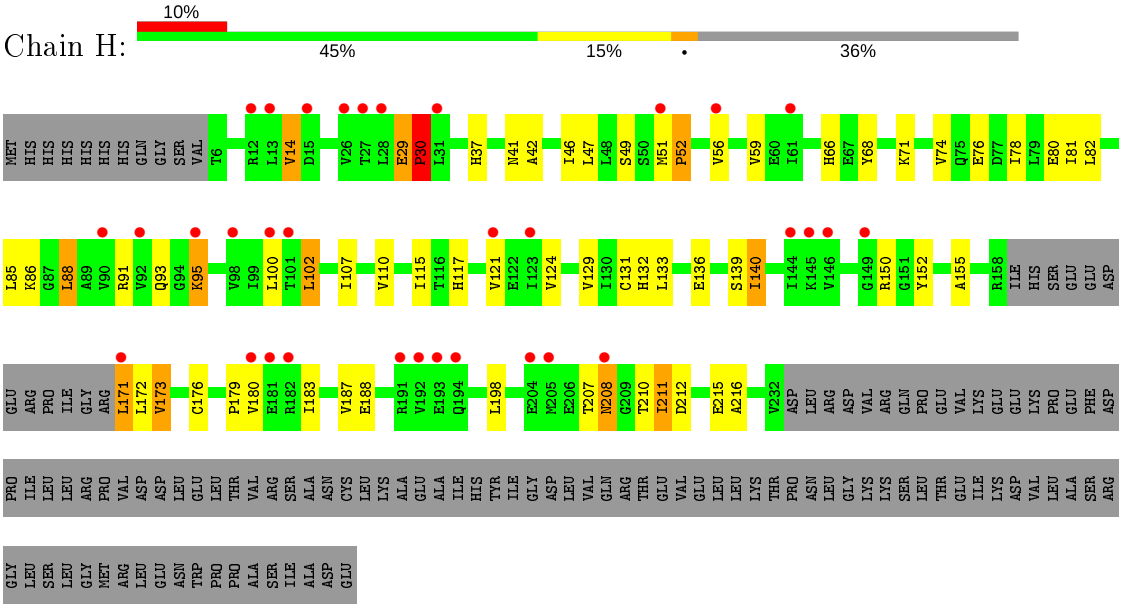
Chain B:



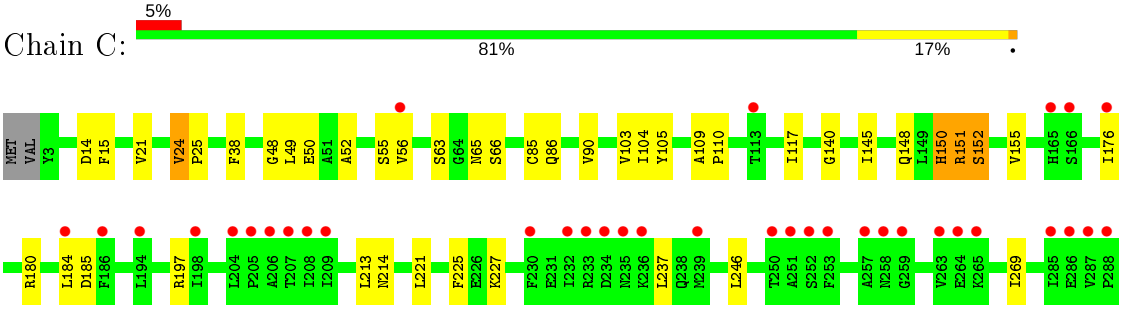
- Molecule 1: DNA-directed RNA polymerase subunit alpha

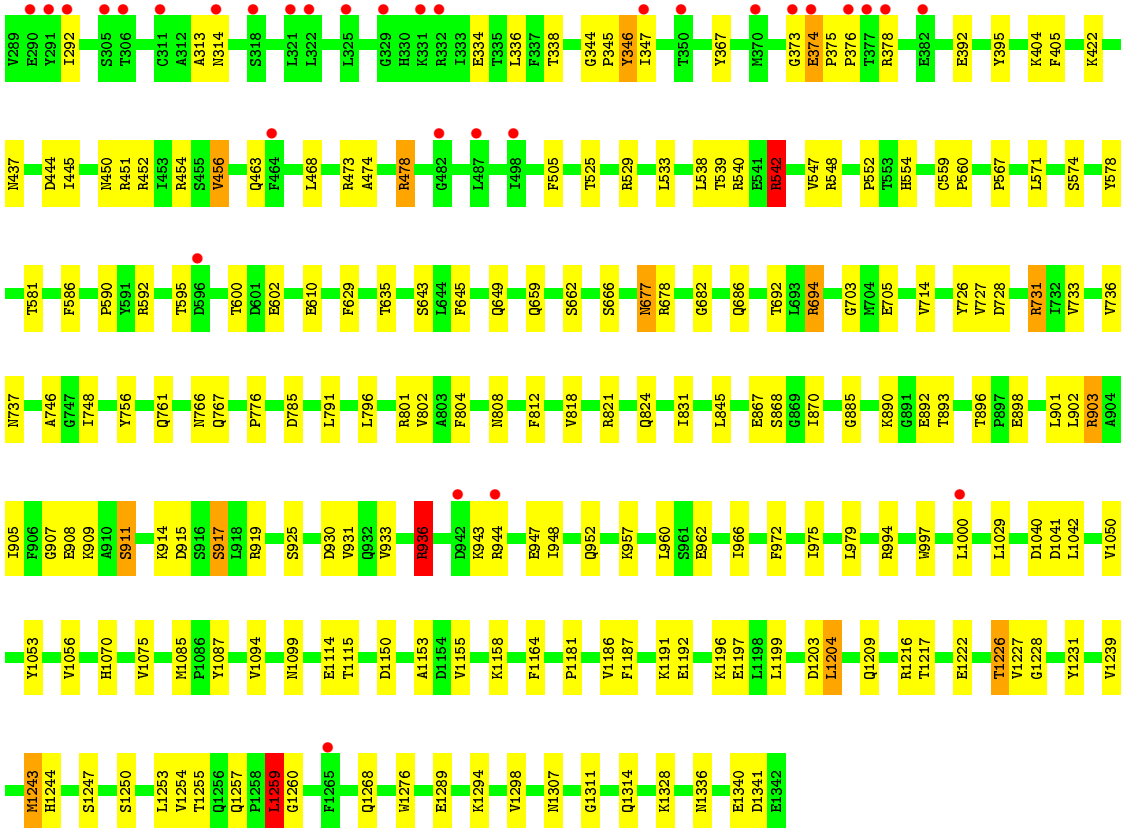


• Molecule 1: DNA-directed RNA polymerase subunit alpha



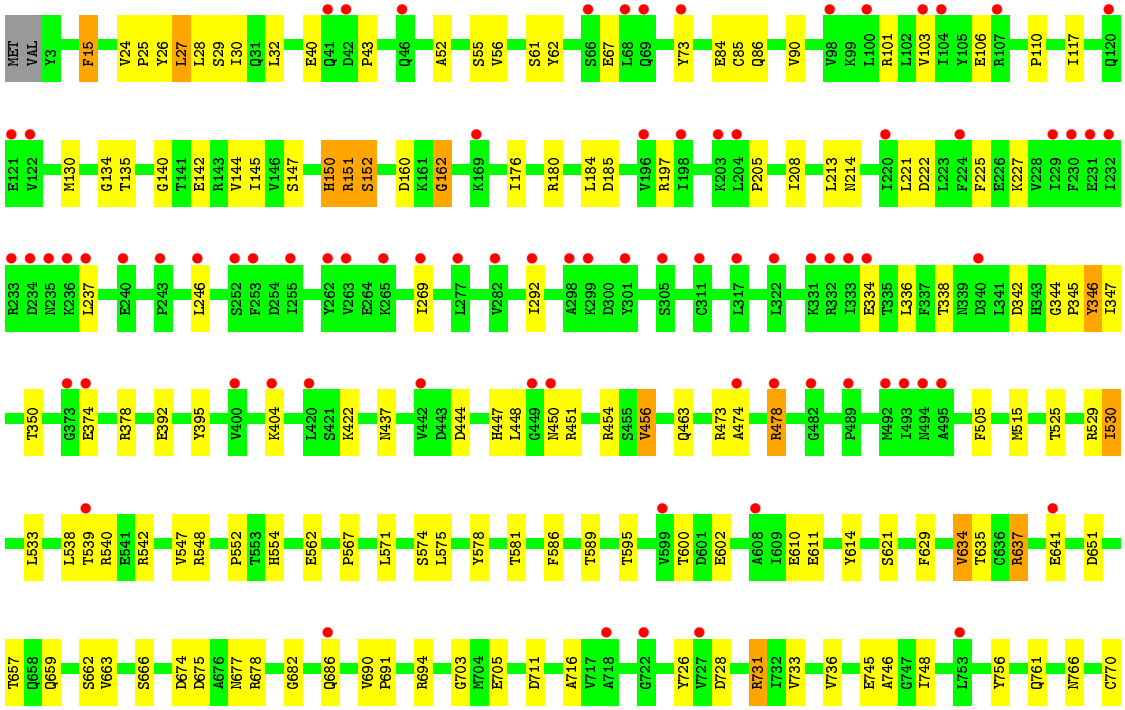
• Molecule 2: DNA-directed RNA polymerase subunit beta

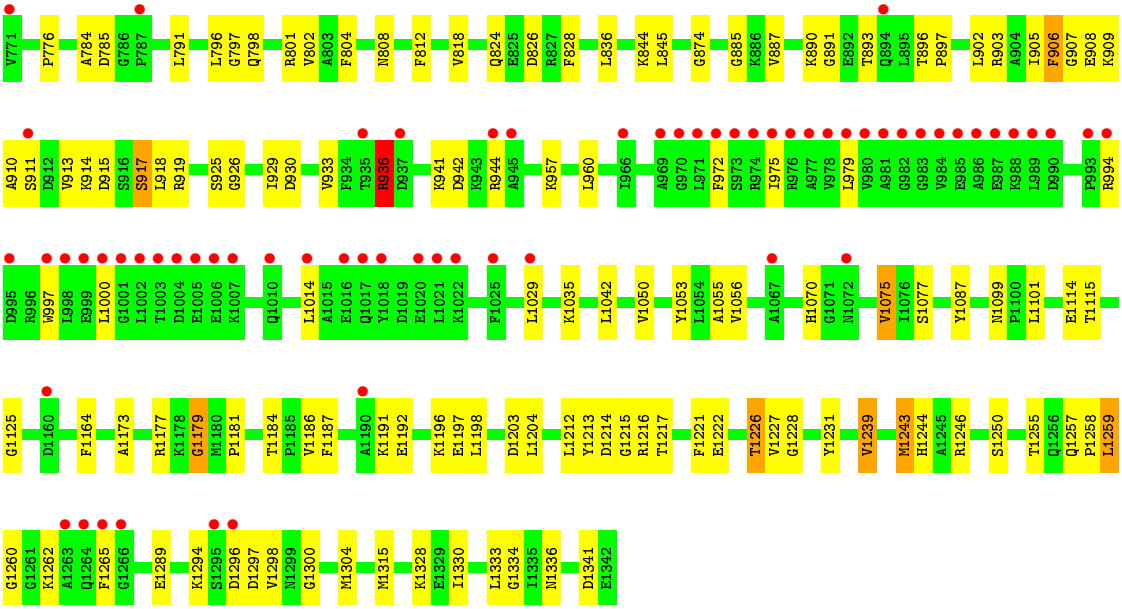




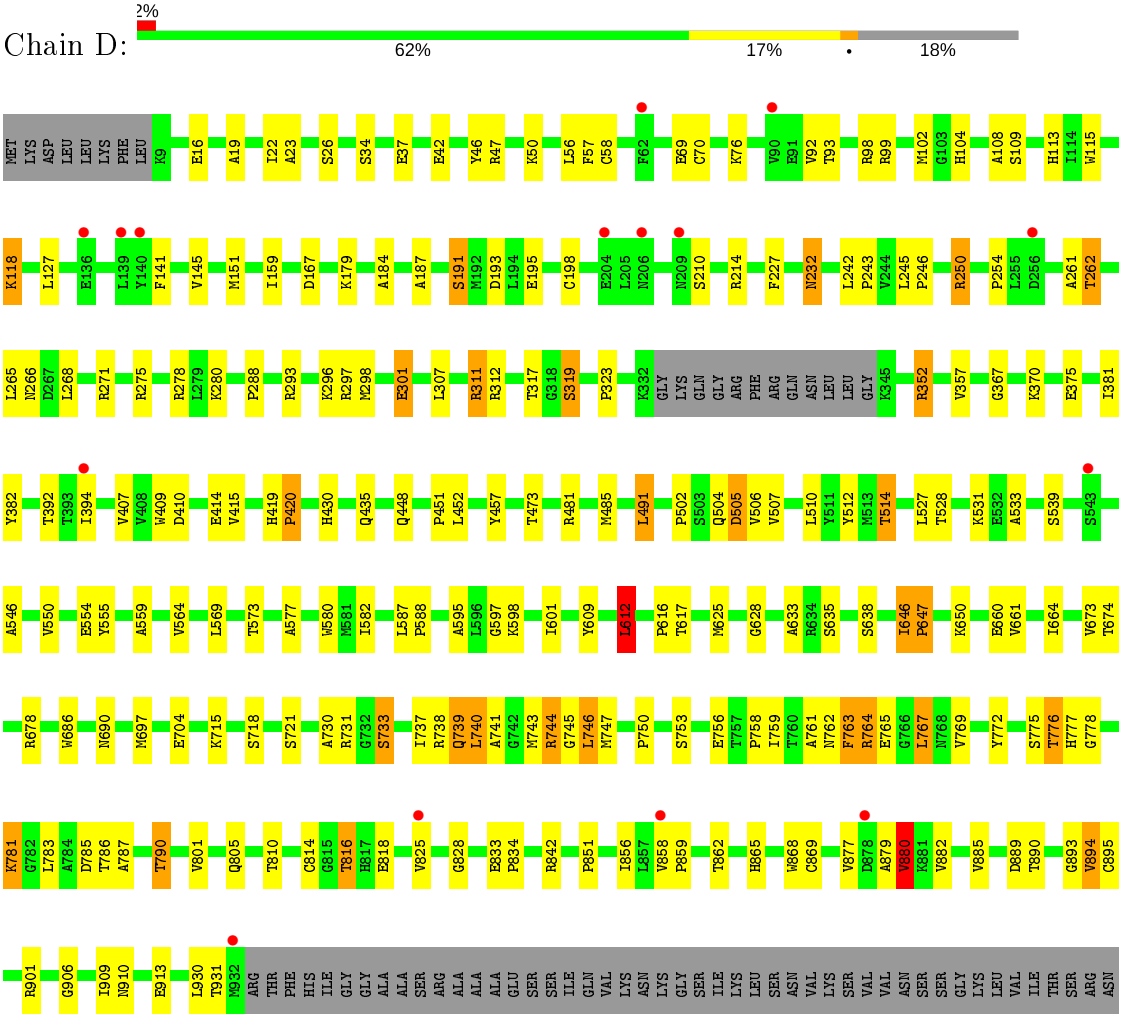
• Molecule 2: DNA-directed RNA polymerase subunit beta

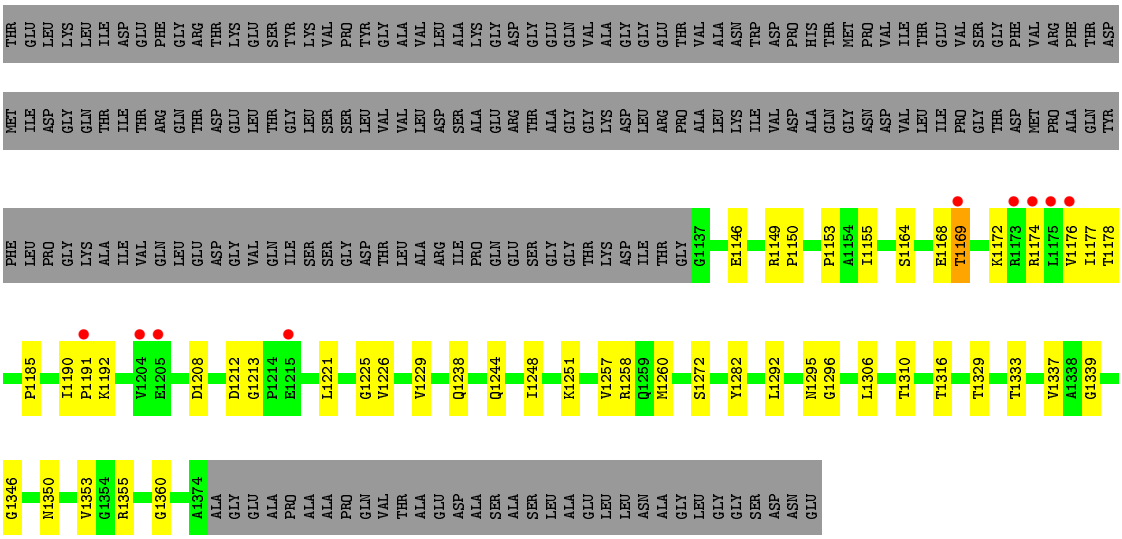
Chain I:

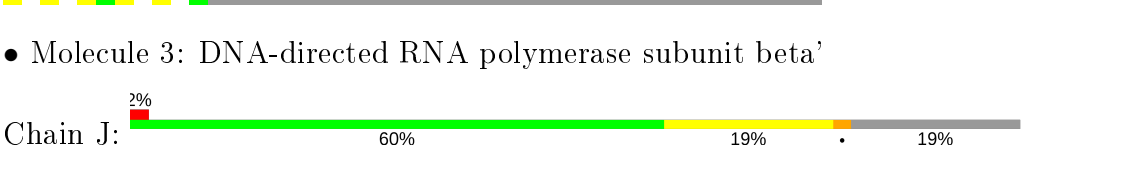




• Molecule 3: DNA-directed RNA polymerase subunit beta'

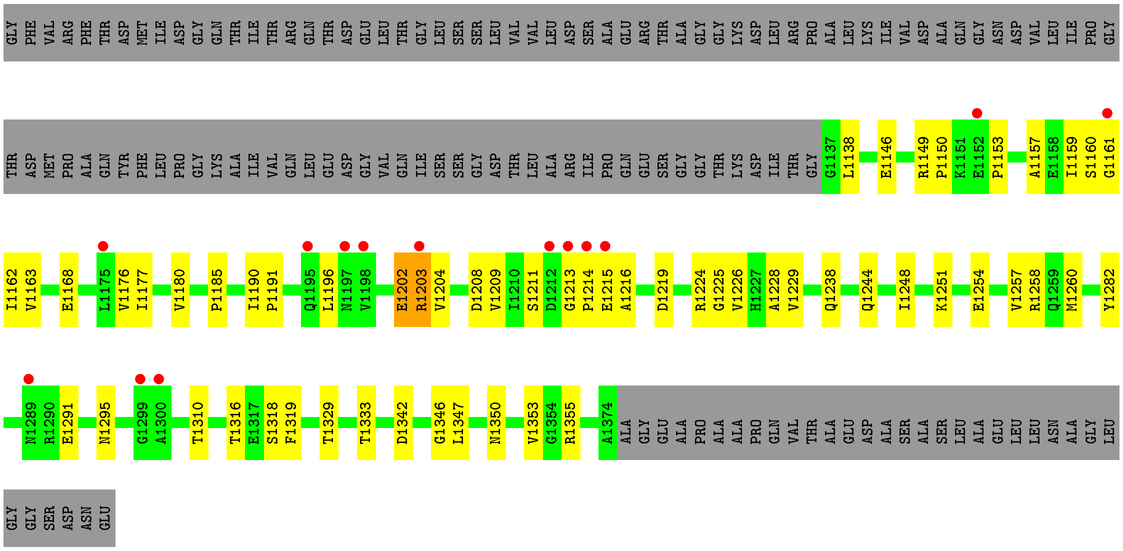






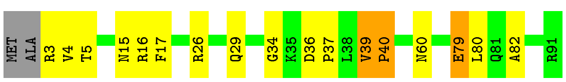
• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain J:



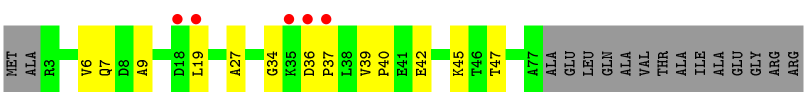
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:



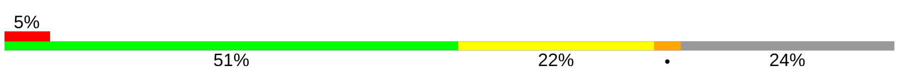
• Molecule 4: DNA-directed RNA polymerase subunit omega

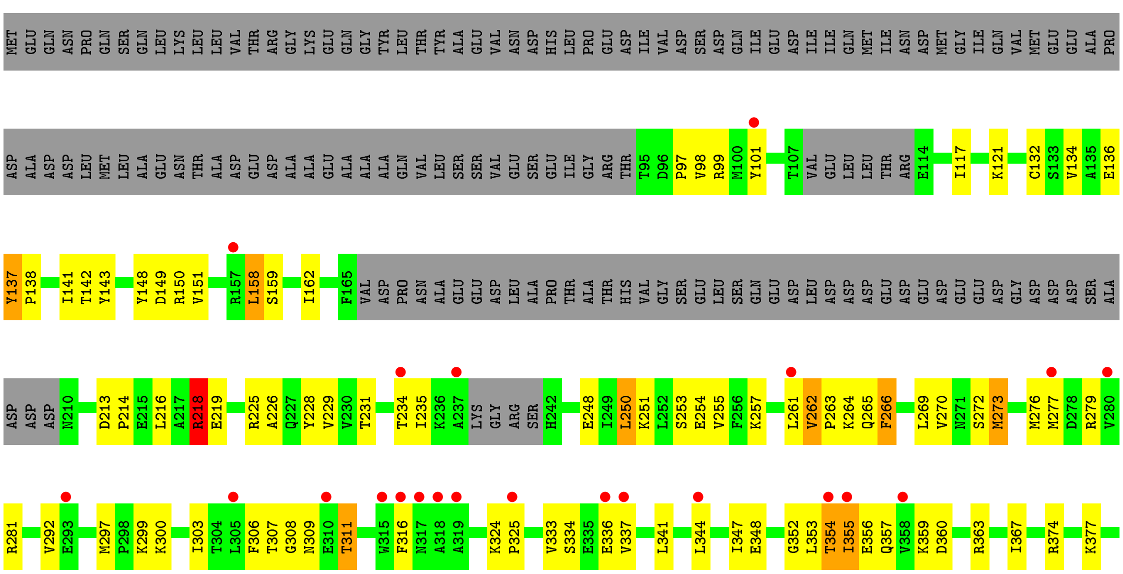
Chain K:

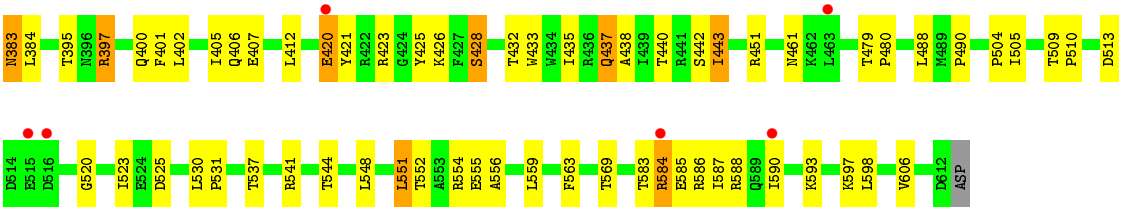


• Molecule 5: RNA polymerase sigma factor RpoD

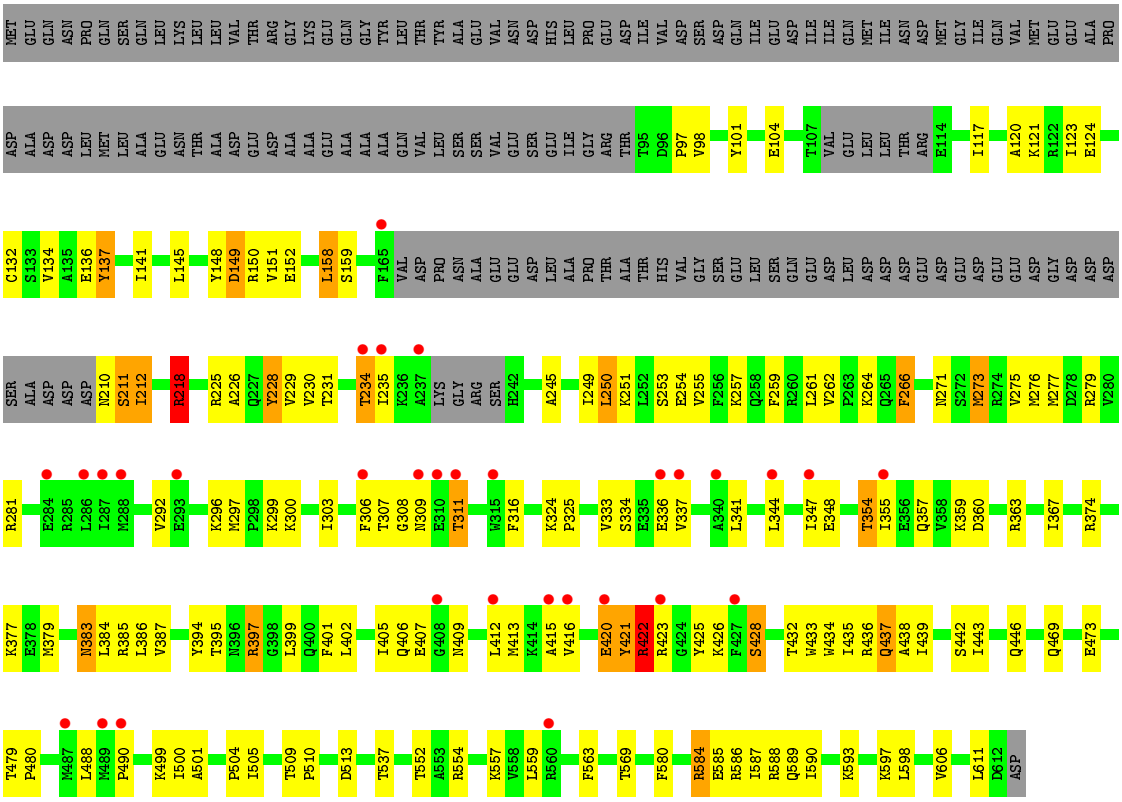
Chain F:







• Molecule 5: RNA polymerase sigma factor RpoD



• Molecule 6: Salinamide A

• Molecule 6: Salinamide A

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	185.80Å 208.19Å 308.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.87 – 3.90 49.87 – 3.90	Depositor EDS
% Data completeness (in resolution range)	98.0 (49.87-3.90) 97.6 (49.87-3.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 3.88Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.286 , 0.325 0.287 , 0.328	Depositor DCC
R_{free} test set	2174 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	151.0	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 156.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	50018	wwPDB-VP
Average B, all atoms (Å^2)	155.0	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 28H, MG, 28J, MEA, 2TL, ZN, 28K, D4P

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	0.25	0/2263	0.55	1/3073 (0.0%)
1	B	0.26	0/2185	0.58	0/2967
1	G	0.25	0/1636	0.55	0/2221
1	H	0.28	0/1623	0.53	0/2205
2	C	0.24	0/9653	0.50	3/13062 (0.0%)
2	I	0.24	0/9676	0.48	1/13089 (0.0%)
3	D	0.24	0/7667	0.51	1/10416 (0.0%)
3	J	0.24	0/7630	0.51	0/10365
4	E	0.25	0/482	0.68	1/662 (0.2%)
4	K	0.26	0/407	0.57	0/558
5	F	0.26	0/3636	0.54	2/4892 (0.0%)
5	L	0.26	0/3636	0.55	3/4892 (0.1%)
6	M	2.92	3/14 (21.4%)	0.80	0/14
6	N	2.92	3/14 (21.4%)	0.79	0/14
All	All	0.26	6/50522 (0.0%)	0.52	12/68430 (0.0%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	8	GLY	CA-C	-7.75	1.39	1.51
6	N	8	GLY	CA-C	-7.73	1.39	1.51
6	M	2	THR	CA-C	-5.17	1.39	1.52
6	N	2	THR	CA-C	-5.17	1.39	1.52
6	M	7	SER	CA-C	-5.16	1.39	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	39	VAL	C-N-CA	7.85	154.96	122.00
3	D	612	LEU	CA-CB-CG	7.73	133.07	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	936	ARG	NE-CZ-NH2	6.61	123.61	120.30
5	F	218	ARG	NE-CZ-NH1	6.54	123.57	120.30
2	C	936	ARG	NE-CZ-NH2	6.26	123.43	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2236	0	2254	49	0
1	B	2160	0	2184	59	1
1	G	1618	0	1622	41	0
1	H	1605	0	1599	44	1
2	C	9522	0	8569	149	0
2	I	9544	0	8601	156	0
3	D	7572	0	6293	156	0
3	J	7535	0	6272	162	0
4	E	482	0	301	7	0
4	K	408	0	255	4	0
5	F	3592	0	3433	89	1
5	L	3592	0	3433	94	1
6	M	73	0	64	34	0
6	N	73	0	64	31	0
7	D	1	0	0	0	0
7	J	1	0	0	0	0
8	D	2	0	0	0	0
8	J	2	0	0	0	0
All	All	50018	0	44944	955	2

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 10.

The worst 5 of 955 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)
6:N:4:D4P:C4	6:N:9:28K:H46	1.64	1.26
6:M:4:D4P:C4	6:M:9:28K:H46	1.64	1.25
6:N:4:D4P:C3	6:N:9:28K:H46	1.68	1.22
6:M:4:D4P:C5	6:M:9:28K:H46	1.68	1.22
6:M:4:D4P:C4	6:M:9:28K:CAF	2.37	0.99

All (2) 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)
5:F:218:ARG:NH2	5:L:149:ASP:OD1[1_545]	2.05	0.15
1:B:292:THR:O	1:H:68:TYR:OH[4_555]	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	292/335 (87%)	261 (89%)	19 (6%)	12 (4%)	3 27
1	B	281/335 (84%)	252 (90%)	13 (5%)	16 (6%)	1 21
1	G	212/335 (63%)	193 (91%)	14 (7%)	5 (2%)	6 37
1	H	211/335 (63%)	193 (92%)	13 (6%)	5 (2%)	6 37
2	C	1338/1342 (100%)	1265 (94%)	55 (4%)	18 (1%)	12 48
2	I	1338/1342 (100%)	1265 (94%)	54 (4%)	19 (1%)	11 46
3	D	1144/1407 (81%)	1027 (90%)	77 (7%)	40 (4%)	3 30
3	J	1137/1407 (81%)	1029 (90%)	60 (5%)	48 (4%)	3 26
4	E	87/91 (96%)	70 (80%)	8 (9%)	9 (10%)	0 9
4	K	73/91 (80%)	58 (80%)	10 (14%)	5 (7%)	1 18
5	F	456/613 (74%)	431 (94%)	19 (4%)	6 (1%)	12 48
5	L	456/613 (74%)	430 (94%)	18 (4%)	8 (2%)	8 42

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	7025/8246 (85%)	6474 (92%)	360 (5%)	191 (3%)	5 35

5 of 191 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	PRO
1	A	93	GLN
1	A	188	GLU
1	A	229	GLU
1	A	320	ASN

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	239/292 (82%)	220 (92%)	19 (8%)	12 41
1	B	233/292 (80%)	218 (94%)	15 (6%)	17 47
1	G	173/292 (59%)	161 (93%)	12 (7%)	15 45
1	H	171/292 (59%)	158 (92%)	13 (8%)	13 42
2	C	822/1157 (71%)	765 (93%)	57 (7%)	15 45
2	I	828/1157 (72%)	765 (92%)	63 (8%)	13 42
3	D	520/1168 (44%)	455 (88%)	65 (12%)	4 23
3	J	518/1168 (44%)	452 (87%)	66 (13%)	4 23
4	E	10/75 (13%)	10 (100%)	0	100 100
4	K	9/75 (12%)	8 (89%)	1 (11%)	6 27
5	F	348/540 (64%)	306 (88%)	42 (12%)	5 24
5	L	348/540 (64%)	305 (88%)	43 (12%)	4 24
6	M	2/2 (100%)	1 (50%)	1 (50%)	0 0
6	N	2/2 (100%)	1 (50%)	1 (50%)	0 0
All	All	4223/7052 (60%)	3825 (91%)	398 (9%)	8 33

5 of 398 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	425	TYR
1	H	211	ILE
5	L	309	ASN
5	F	479	THR
1	G	95	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	227	GLN
1	G	41	ASN
5	L	131	GLN
5	F	309	ASN
5	F	406	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)

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	28J	N	3	6	6,7,8	0.46	0	5,8,10	1.38	1 (20%)
6	28J	M	3	6	6,7,8	0.46	0	5,8,10	1.38	1 (20%)
6	MEA	M	5	6	11,12,13	1.55	1 (9%)	13,14,16	1.19	2 (15%)
6	D4P	N	4	6	10,11,12	4.30	2 (20%)	11,14,16	0.79	0
6	MEA	N	5	6	11,12,13	1.56	1 (9%)	13,14,16	1.18	2 (15%)
6	2TL	M	6	6	5,6,7	0.48	0	6,7,9	1.00	0
6	2TL	N	6	6	5,6,7	0.48	0	6,7,9	1.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	D4P	M	4	6	10,11,12	4.31	2 (20%)	11,14,16	0.78	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	28J	N	3	6	-	6/7/8/10	-
6	28J	M	3	6	-	6/7/8/10	-
6	MEA	M	5	6	-	4/5/8/10	0/1/1/1
6	D4P	N	4	6	-	2/4/6/8	0/1/1/1
6	MEA	N	5	6	-	4/5/8/10	0/1/1/1
6	2TL	M	6	6	-	2/5/6/8	-
6	2TL	N	6	6	-	2/5/6/8	-
6	D4P	M	4	6	-	2/4/6/8	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	4	D4P	C1-CA	-12.36	1.39	1.52
6	N	4	D4P	C1-CA	-12.35	1.39	1.52
6	M	4	D4P	CA-C	-5.59	1.39	1.51
6	N	4	D4P	CA-C	-5.56	1.39	1.51
6	N	5	MEA	CB-CG	-4.92	1.39	1.51

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	5	MEA	CG-CB-CA	-2.86	109.53	113.63
6	N	5	MEA	CG-CB-CA	-2.85	109.55	113.63
6	M	3	28J	CB-CA-C	-2.18	109.50	112.83
6	N	3	28J	CB-CA-C	-2.17	109.51	112.83
6	M	5	MEA	C1-N-CA	2.06	120.04	113.64

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	N	3	28J	N-CA-CB-CG2
6	N	3	28J	C-CA-CB-CG2
6	N	3	28J	C-CA-CB-CG1
6	M	3	28J	N-CA-CB-CG2
6	M	3	28J	C-CA-CB-CG2

There are no ring outliers.

8 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	N	3	28J	1	0
6	M	3	28J	1	0
6	M	5	MEA	10	0
6	N	4	D4P	7	0
6	N	5	MEA	9	0
6	M	6	2TL	6	0
6	N	6	2TL	6	0
6	M	4	D4P	7	0

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	N	1
6	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	7:SER	C	8:GLY	N	5.81
1	N	7:SER	C	8:GLY	N	5.81

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, 95^{th} 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	298/335 (88%)	0.28	21 (7%) 16 12	41, 129, 238, 393	0
1	B	287/335 (85%)	0.35	25 (8%) 10 8	58, 173, 336, 460	0
1	G	216/335 (64%)	0.56	26 (12%) 4 4	68, 183, 311, 358	0
1	H	215/335 (64%)	0.64	33 (15%) 2 2	79, 191, 326, 488	0
2	C	1340/1342 (99%)	0.08	68 (5%) 28 23	16, 113, 346, 550	1 (0%)
2	I	1340/1342 (99%)	0.46	146 (10%) 5 5	37, 162, 408, 550	1 (0%)
3	D	1150/1407 (81%)	-0.14	24 (2%) 63 53	19, 89, 227, 505	0
3	J	1143/1407 (81%)	-0.13	29 (2%) 57 47	31, 110, 251, 550	0
4	E	89/91 (97%)	-0.62	0 100 100	28, 105, 210, 326	0
4	K	75/91 (82%)	0.13	5 (6%) 17 13	91, 185, 373, 403	0
5	F	464/613 (75%)	0.15	28 (6%) 21 16	45, 151, 353, 550	0
5	L	464/613 (75%)	0.14	31 (6%) 17 13	53, 167, 378, 550	0
6	M	3/9 (33%)	-0.36	0 100 100	107, 107, 108, 111	0
6	N	3/9 (33%)	-0.68	0 100 100	130, 130, 134, 138	0
All	All	7087/8264 (85%)	0.13	436 (6%) 20 15	16, 134, 326, 550	2 (0%)

The worst 5 of 436 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	1000	LEU	26.0
2	I	981	ALA	18.1
2	I	231	GLU	16.2
2	I	332	ARG	12.1
2	I	1001	GLY	11.9

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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
6	MEA	N	5	12/13	0.83	0.31	109,123,128,130	0
6	2TL	N	6	7/8	0.90	0.18	124,127,132,147	0
6	MEA	M	5	12/13	0.91	0.27	79,91,106,106	0
6	D4P	N	4	11/12	0.93	0.16	133,140,153,159	0
6	D4P	M	4	11/12	0.93	0.18	102,118,135,137	0
6	28J	N	3	8/9	0.95	0.18	106,127,131,132	0
6	2TL	M	6	7/8	0.95	0.21	91,110,113,123	0
6	28J	M	3	8/9	0.97	0.28	97,105,111,114	0

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, 95^{th} 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	MG	J	2000	1/1	0.79	0.82	98,98,98,98	0
7	MG	D	2000	1/1	0.88	0.72	258,258,258,258	0
8	ZN	D	2001	1/1	0.93	0.10	87,87,87,87	0
8	ZN	J	2002	1/1	0.97	0.24	80,80,80,80	0
8	ZN	J	2001	1/1	0.97	0.08	106,106,106,106	0
8	ZN	D	2002	1/1	0.98	0.23	64,64,64,64	0

6.5 Other polymers (i)

There are no such residues in this entry.