



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 14, 2020 – 01:10 AM BST

PDB ID : 6DCF
Title : Crystal structure of a Mycobacterium smegmatis transcription initiation complex with Rifampicin-resistant RNA polymerase and bound to kanglemycin A
Authors : Lilic, M.; Darst, S.A.; Campbell, E.A.
Deposited on : 2018-05-06
Resolution : 3.45 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.4.dev1
buster-report : 1.1.7 (2018)
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) : 2.14.4.dev1

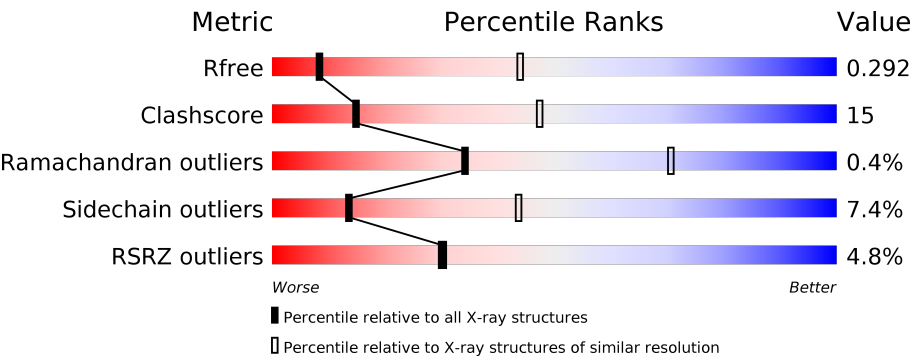
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	J	114	<div><div>4%</div><div><div></div><div>44%</div><div>25%</div><div>• •</div><div>25%</div></div></div>
2	A	350	<div><div>2%</div><div><div></div><div>42%</div><div>17%</div><div>•</div><div>37%</div></div></div>
2	B	350	<div><div>6%</div><div><div></div><div>47%</div><div>15%</div><div>•</div><div>36%</div></div></div>
3	C	1169	<div><div>5%</div><div><div></div><div>48%</div><div>22%</div><div>•</div><div>27%</div></div></div>
4	D	1317	<div><div>3%</div><div><div></div><div>62%</div><div>25%</div><div>•</div><div>11%</div></div></div>
5	E	107	<div><div>8%</div><div><div></div><div>43%</div><div>28%</div><div>6%</div><div>23%</div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	F	466	<div> <div>%</div> <div> <div></div> <div>49%</div> <div>14%</div> <div>36%</div> </div> </div>
7	O	31	<div> <div>61%</div> <div>39%</div> </div>
8	P	26	<div> <div>77%</div> <div>23%</div> </div>

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
10	SO4	C	1204	-	-	X	X
10	SO4	D	2006	-	-	X	-
10	SO4	D	2007	-	-	X	-
10	SO4	F	502	-	-	X	-
13	GLU	D	2008	-	-	X	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 23212 atoms, of which 12 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called RNA polymerase-binding protein RbpA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	J	85	Total	C	N	O	S	0	0	0
			662	416	120	124	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	219	Total	C	N	O	S	0	0	0
			1618	1022	276	318	2			
2	B	225	Total	C	N	O	S	0	0	0
			1604	1009	280	313	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	858	Total	C	N	O	S	0	0	0
			6237	3909	1094	1205	29			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	447	LEU	SER	engineered mutation	UNP P60281

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	1176	Total	C	N	O	S	0	0	0
			8792	5494	1582	1678	38			

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total	C	N	O	0	0	0
			624	396	107	121			

- Molecule 6 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	297	Total	C	N	O	S	0	0	0
			2360	1480	428	445	7			

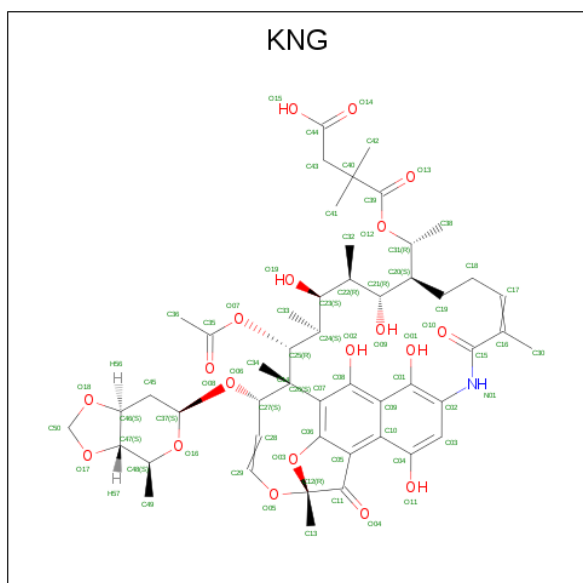
- Molecule 7 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	O	31	Total	C	N	O	P	0	0	0
			635	306	114	185	30			

- Molecule 8 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	P	26	Total	C	N	O	P	0	0	0
			526	254	94	153	25			

- Molecule 9 is Kanglemycin A (three-letter code: KNG) (formula: C₅₀H₆₇NO₁₉).



- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	O	S	0	0
			5	4	1		
10	C	1	Total	O	S	0	0
			5	4	1		
10	C	1	Total	O	S	0	0
			5	4	1		
10	D	1	Total	O	S	0	0
			5	4	1		
10	D	1	Total	O	S	0	0
			5	4	1		
10	D	1	Total	O	S	0	0
			5	4	1		
10	F	1	Total	O	S	0	0
			5	4	1		
10	F	1	Total	O	S	0	0
			5	4	1		

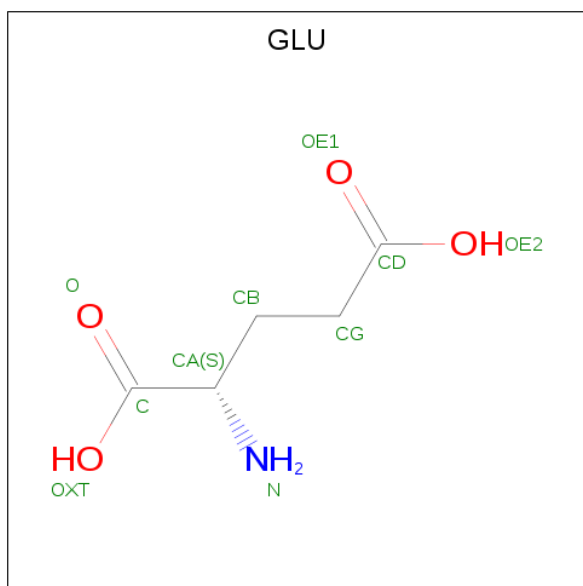
- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	2	Total	Zn	0	0
			2	2		

- Molecule 12 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

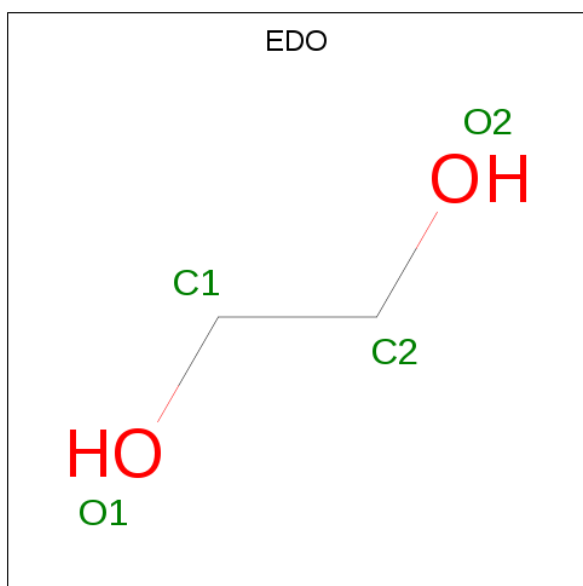
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	D	1	Total	Mg	0	0
			1	1		

- Molecule 13 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	D	1	Total	C	N	O	0	0
			9	5	1	3		

- Molecule 14 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	F	1	Total	C	H	O	0	0
			10	2	6	2		
14	F	1	Total	C	H	O	0	0
			10	2	6	2		

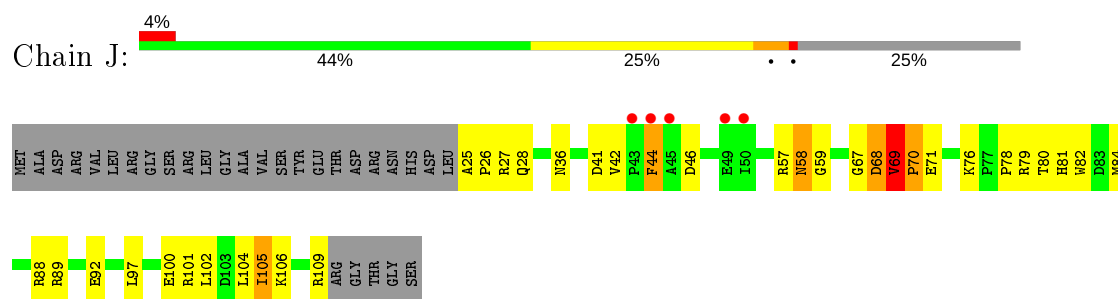
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	D	3	Total	O	0	0
			3	3		
15	F	2	Total	O	0	0
			2	2		
15	P	2	Total	O	0	0
			2	2		

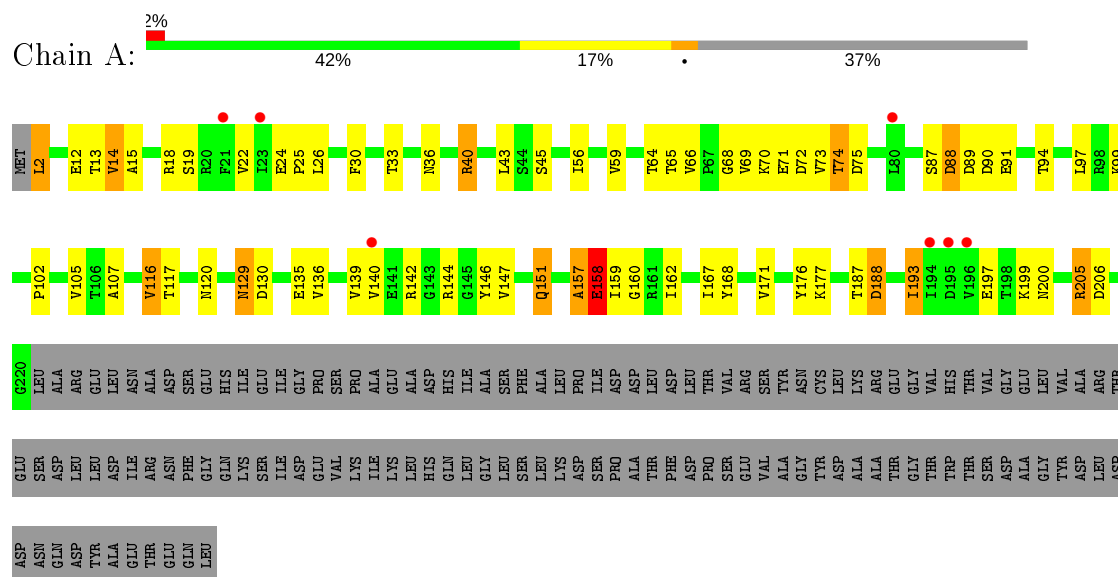
3 Residue-property plots [i](#)

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.

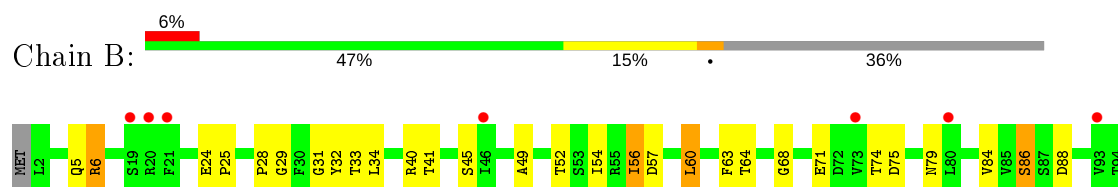
- Molecule 1: RNA polymerase-binding protein RbpA

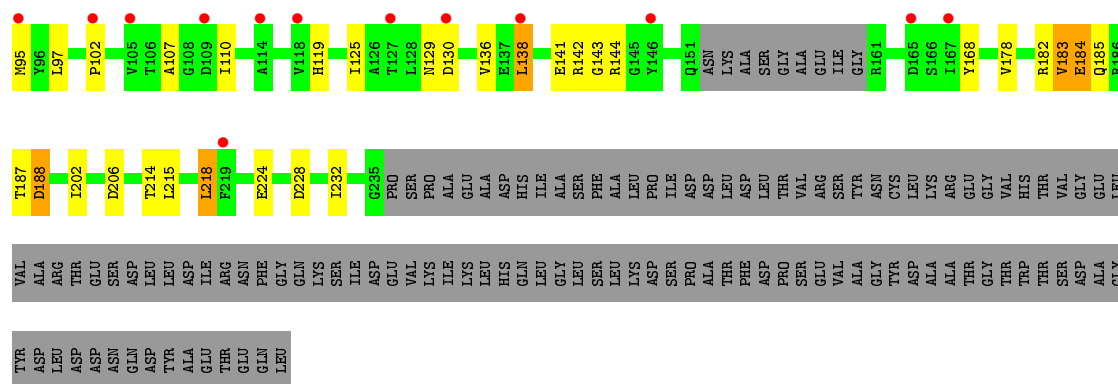


- Molecule 2: DNA-directed RNA polymerase subunit alpha

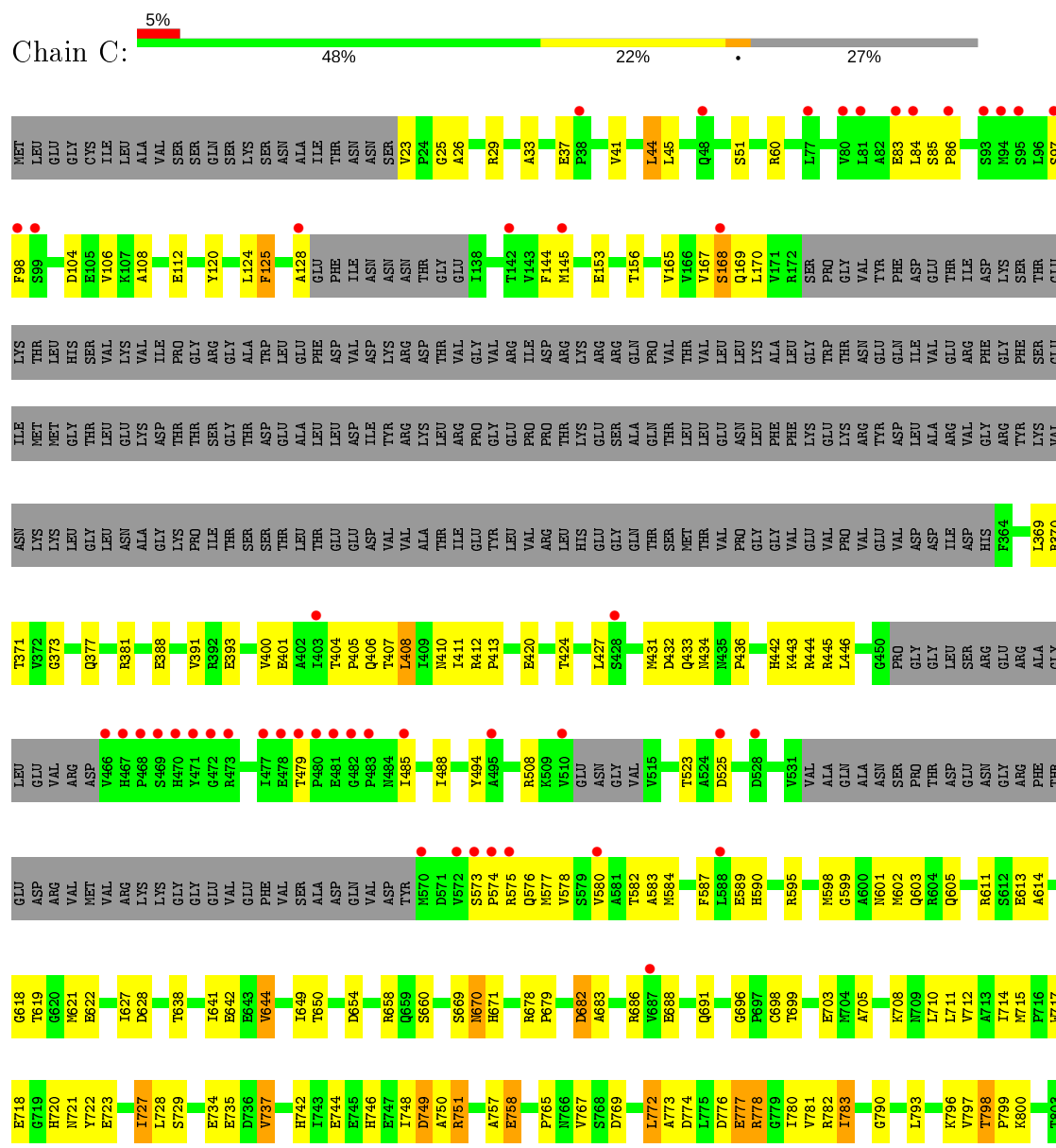


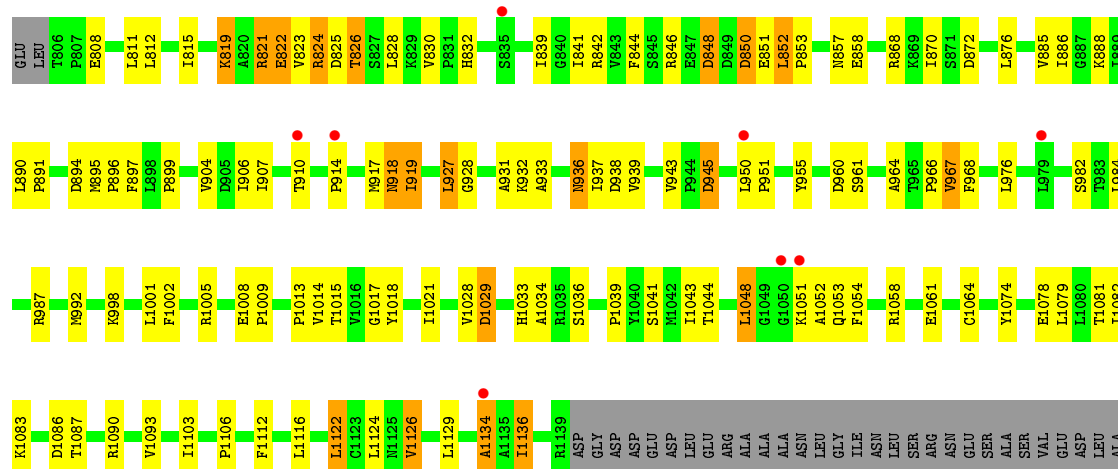
- Molecule 2: DNA-directed RNA polymerase subunit alpha



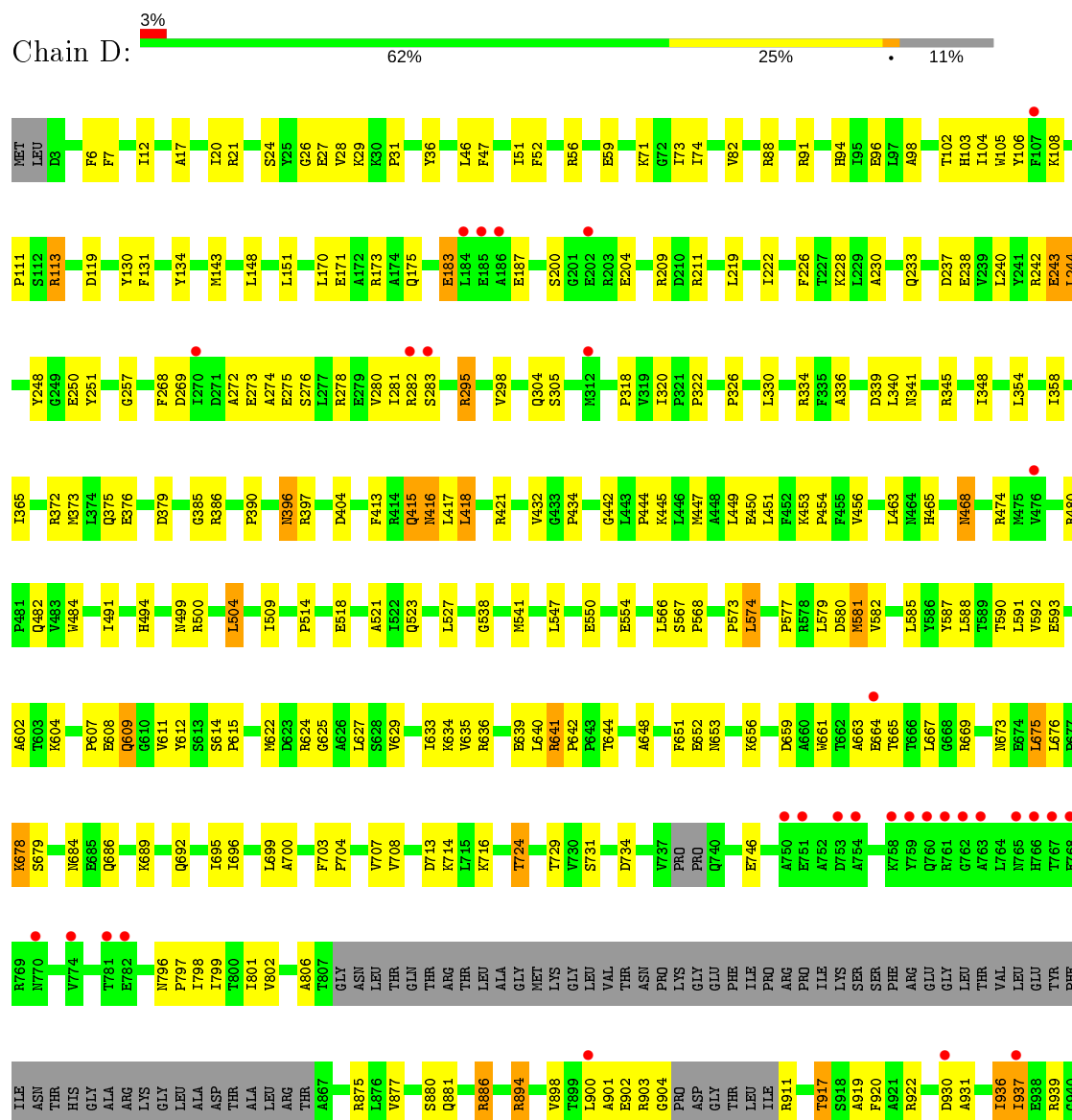


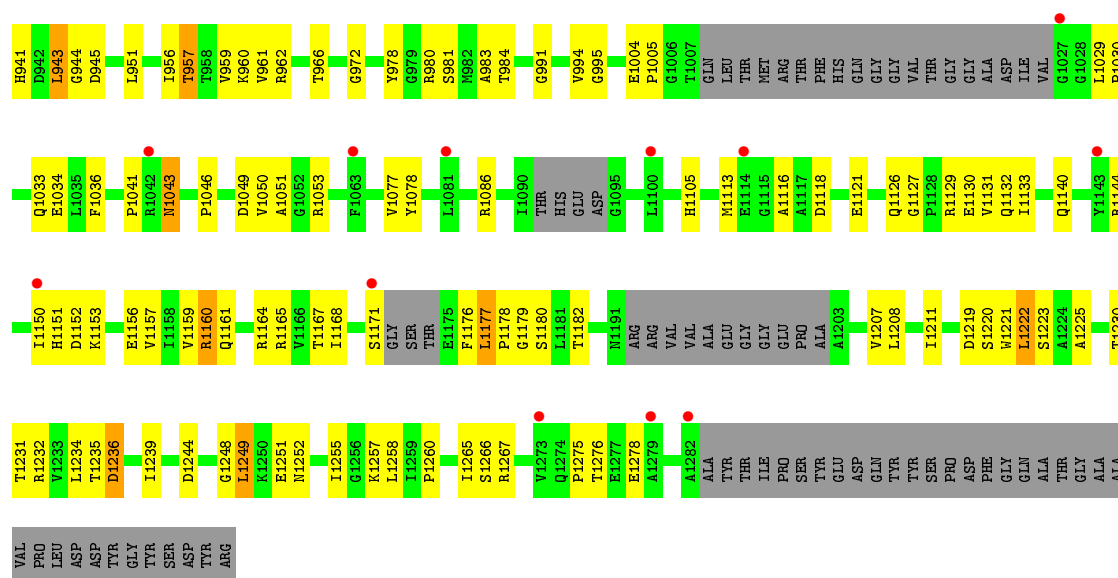
• Molecule 3: DNA-directed RNA polymerase subunit beta



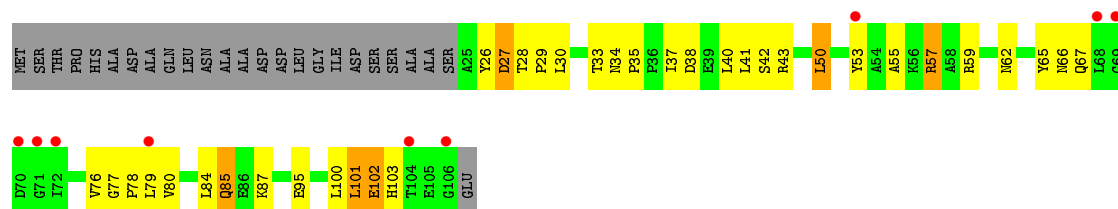
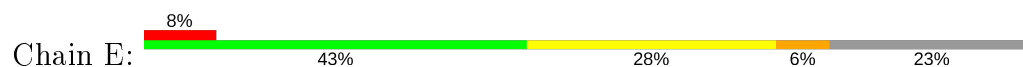


• Molecule 4: DNA-directed RNA polymerase subunit beta'

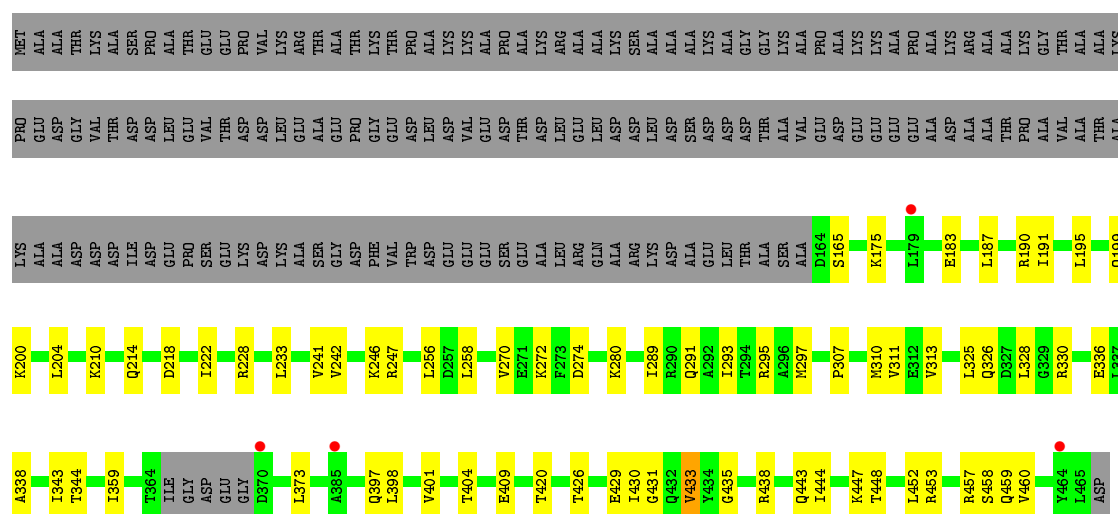




- Molecule 5: DNA-directed RNA polymerase subunit omega



- Molecule 6: RNA polymerase sigma factor SigA




- Molecule 7: DNA (31-MER)

Chain O:  61% 39%



● Molecule 8: DNA (26-MER)

Chain P:  77% 23%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	129.25Å 160.91Å 136.86Å 90.00° 110.75° 90.00°	Depositor
Resolution (Å)	43.89 – 3.45 59.56 – 3.14	Depositor EDS
% Data completeness (in resolution range)	97.8 (43.89-3.45) 89.2 (59.56-3.14)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 3.13Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.252 , 0.290 0.254 , 0.292	Depositor DCC
R_{free} test set	1890 reflections (2.32%)	wwPDB-VP
Wilson B-factor (Å ²)	106.1	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 68.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	23212	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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, 0.333 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: SO4, KNG, MG, ZN, EDO

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	J	0.23	0/676	0.44	0/918
2	A	0.24	0/1644	0.51	2/2245 (0.1%)
2	B	0.24	0/1628	0.45	1/2229 (0.0%)
3	C	0.24	0/6343	0.44	0/8636
4	D	0.24	0/8923	0.42	1/12103 (0.0%)
5	E	0.24	0/637	0.39	0/868
6	F	0.22	0/2390	0.37	0/3223
7	O	0.55	0/712	0.94	0/1098
8	P	0.56	0/589	0.92	0/906
All	All	0.27	0/23542	0.48	4/32226 (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	J	0	1
2	A	0	1
2	B	0	1
3	C	0	2
4	D	0	3
All	All	0	8

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	894	ARG	NE-CZ-NH2	-5.48	117.56	120.30
2	A	188	ASP	CB-CG-OD2	5.18	122.97	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	206	ASP	CB-CG-OD2	5.17	122.95	118.30
2	A	206	ASP	CB-CG-OD2	5.16	122.94	118.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	157	ALA	Peptide
2	B	183	VAL	Peptide
3	C	821	ARG	Peptide
3	C	822	GLU	Peptide
1	J	69	VAL	Peptide

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	J	662	0	631	31	0
2	A	1618	0	1624	53	0
2	B	1604	0	1552	46	0
3	C	6237	0	5937	230	0
4	D	8792	0	8499	286	0
5	E	624	0	604	25	0
6	F	2360	0	2388	59	0
7	O	635	0	354	14	0
8	P	526	0	296	10	0
9	C	70	0	0	2	0
10	C	15	0	0	4	0
10	D	20	0	0	13	0
10	F	10	0	0	3	0
11	D	2	0	0	0	0
12	D	1	0	0	0	0
13	D	9	0	5	14	0
14	F	8	12	12	1	0
15	D	3	0	0	0	0
15	F	2	0	0	0	0
15	P	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	23200	12	21902	680	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 15.

The worst 5 of 680 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)
3:C:819:LYS:HE3	3:C:819:LYS:HA	1.29	1.08
1:J:68:ASP:O	1:J:70:PRO:HD3	1.57	1.05
4:D:1129:ARG:NH1	10:D:2007:SO4:O2	1.92	1.01
4:D:1129:ARG:NH1	10:D:2007:SO4:S	2.33	1.00
3:C:800:LYS:CB	3:C:822:GLU:HB3	1.91	0.99

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	J	83/114 (73%)	74 (89%)	7 (8%)	2 (2%)	6	34
2	A	217/350 (62%)	207 (95%)	7 (3%)	3 (1%)	11	44
2	B	221/350 (63%)	211 (96%)	10 (4%)	0	100	100
3	C	844/1169 (72%)	804 (95%)	37 (4%)	3 (0%)	34	70
4	D	1160/1317 (88%)	1114 (96%)	43 (4%)	3 (0%)	41	75
5	E	80/107 (75%)	72 (90%)	8 (10%)	0	100	100
6	F	293/466 (63%)	293 (100%)	0	0	100	100
All	All	2898/3873 (75%)	2775 (96%)	112 (4%)	11 (0%)	34	70

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	68	ASP
2	A	90	ASP
3	C	751	ARG
2	A	158	GLU
3	C	918	ASN

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	J	66/98 (67%)	56 (85%)	10 (15%)	3	15
2	A	177/297 (60%)	162 (92%)	15 (8%)	10	38
2	B	165/297 (56%)	149 (90%)	16 (10%)	8	32
3	C	623/984 (63%)	576 (92%)	47 (8%)	13	43
4	D	876/1095 (80%)	817 (93%)	59 (7%)	16	48
5	E	63/86 (73%)	55 (87%)	8 (13%)	4	20
6	F	248/379 (65%)	239 (96%)	9 (4%)	35	66
All	All	2218/3236 (68%)	2054 (93%)	164 (7%)	13	43

5 of 164 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	890	LEU
4	D	148	LEU
5	E	85	GLN
3	C	927	LEU
3	C	1029	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	1057	GLN
4	D	304	GLN
5	E	103	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	165	GLN
4	D	207	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 3 are monoatomic - leaving 13 for Mogul analysis.

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	$\# Z > 2$
9	KNG	C	1201	-	72,75,75	2.64	19 (26%)	101,114,114	1.72	16 (15%)
10	SO4	D	2006	-	4,4,4	0.14	0	6,6,6	0.09	0
10	SO4	F	502	-	4,4,4	0.14	0	6,6,6	0.09	0
14	EDO	F	504	-	3,3,3	0.46	0	2,2,2	0.40	0
10	SO4	D	2005	-	4,4,4	0.14	0	6,6,6	0.06	0
10	SO4	C	1203	-	4,4,4	0.14	0	6,6,6	0.22	0
10	SO4	C	1204	-	4,4,4	0.14	0	6,6,6	0.13	0
13	GLU	D	2008	-	4,8,9	0.67	0	1,9,11	0.30	0
14	EDO	F	503	-	3,3,3	0.46	0	2,2,2	0.31	0
10	SO4	C	1202	-	4,4,4	0.14	0	6,6,6	0.05	0
10	SO4	D	2007	-	4,4,4	0.13	0	6,6,6	1.06	0
10	SO4	D	2004	-	4,4,4	0.14	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	SO4	F	501	-	4,4,4	0.14	0	6,6,6	0.05	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
9	KNG	C	1201	-	-	24/74/113/113	0/5/6/6
14	EDO	F	503	-	-	1/1/1/1	-
14	EDO	F	504	-	-	0/1/1/1	-
13	GLU	D	2008	-	-	0/4/7/9	-

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1201	KNG	O04-C11	11.43	1.40	1.21
9	C	1201	KNG	C17-C16	9.22	1.53	1.33
9	C	1201	KNG	O03-C06	9.15	1.55	1.37
9	C	1201	KNG	C15-N01	4.71	1.45	1.35
9	C	1201	KNG	C12-C11	-3.93	1.39	1.54

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	1201	KNG	C18-C17-C16	-8.39	111.22	129.08
9	C	1201	KNG	O04-C11-C05	-4.99	122.30	131.81
9	C	1201	KNG	O07-C35-C36	4.61	119.57	111.09
9	C	1201	KNG	O03-C06-C07	4.52	128.92	121.14
9	C	1201	KNG	C12-C11-C05	4.14	115.41	107.30

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

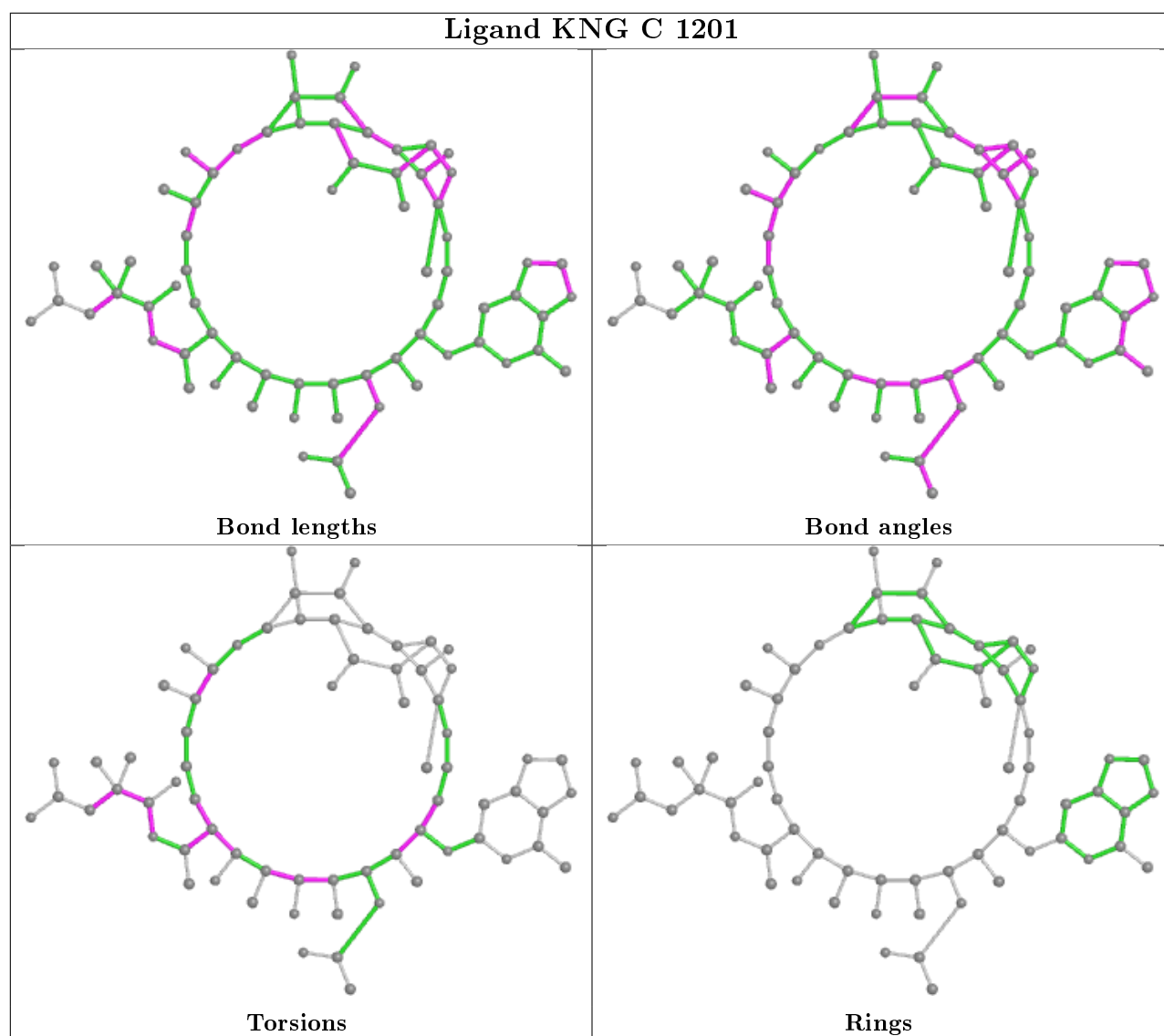
Mol	Chain	Res	Type	Atoms
9	C	1201	KNG	C18-C19-C20-C21
9	C	1201	KNG	O06-C27-C28-C29
9	C	1201	KNG	C39-C40-C43-C44
9	C	1201	KNG	C41-C40-C43-C44
9	C	1201	KNG	C42-C40-C43-C44

There are no ring outliers.

10 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	1201	KNG	2	0
10	D	2006	SO4	2	0
10	F	502	SO4	3	0
14	F	504	EDO	1	0
10	D	2005	SO4	1	0
10	C	1203	SO4	1	0
10	C	1204	SO4	2	0
13	D	2008	GLU	14	0
10	C	1202	SO4	1	0
10	D	2007	SO4	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	J	85/114 (74%)	0.25	5 (5%)	22 23	76, 135, 173, 199	0
2	A	219/350 (62%)	0.15	7 (3%)	47 46	75, 115, 159, 186	0
2	B	225/350 (64%)	0.32	20 (8%)	9 12	88, 141, 164, 175	0
3	C	858/1169 (73%)	0.37	56 (6%)	18 19	49, 116, 175, 200	0
4	D	1176/1317 (89%)	0.26	44 (3%)	41 40	50, 104, 180, 218	0
5	E	82/107 (76%)	0.50	9 (10%)	5 7	73, 108, 188, 213	0
6	F	297/466 (63%)	0.14	4 (1%)	77 73	52, 101, 138, 168	0
7	O	31/31 (100%)	-0.70	0	100 100	76, 108, 149, 160	0
8	P	26/26 (100%)	-0.66	0	100 100	97, 109, 155, 169	0
All	All	2999/3930 (76%)	0.27	145 (4%)	30 30	49, 112, 171, 218	0

The worst 5 of 145 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	1027	GLY	7.5
3	C	38	PRO	6.5
4	D	763	ALA	6.5
5	E	71	GLY	6.0
3	C	482	GLY	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](#)

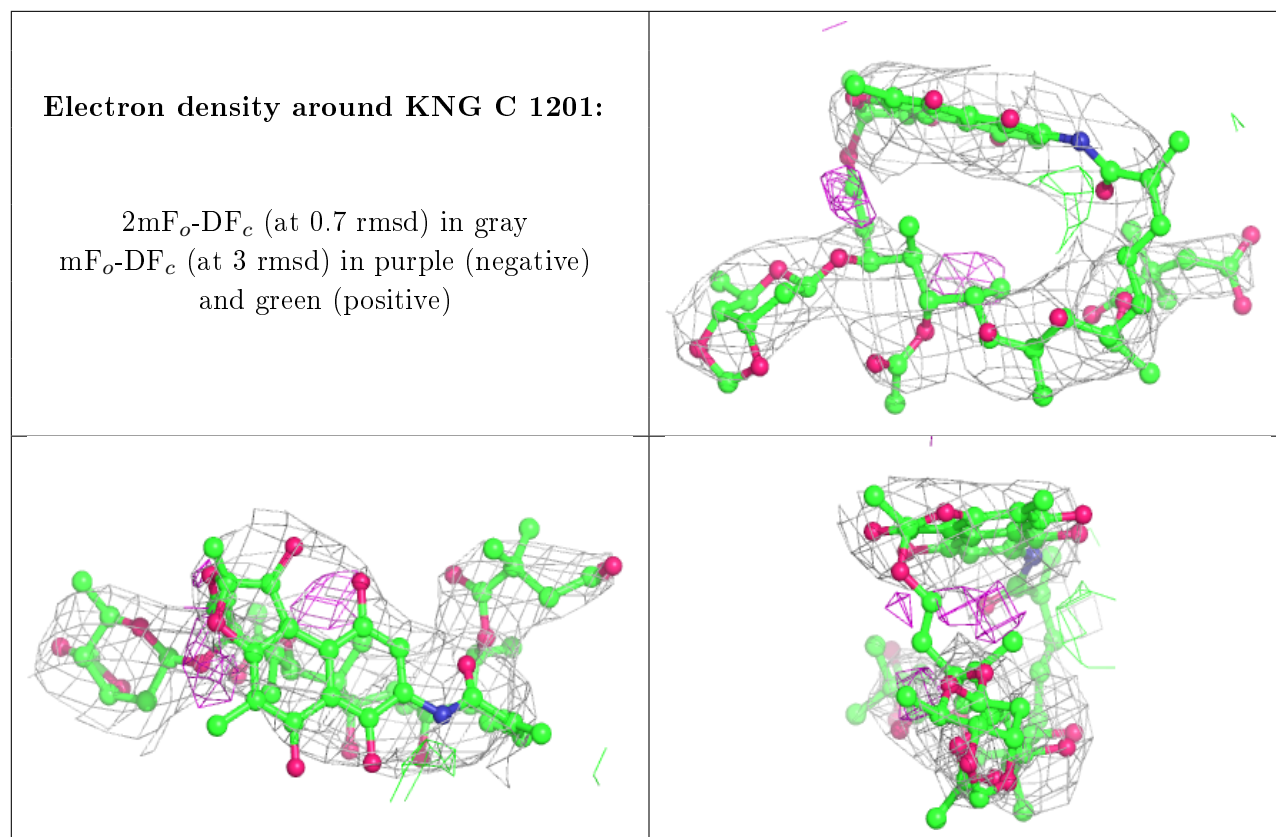
There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
14	EDO	F	504	4/4	0.62	0.35	84,105,126,126	0
13	GLU	D	2008	9/10	0.68	0.26	102,110,119,120	0
10	SO4	C	1203	5/5	0.74	0.19	176,177,184,205	0
10	SO4	C	1204	5/5	0.76	0.43	112,113,137,244	0
10	SO4	C	1202	5/5	0.79	0.38	130,139,157,159	0
10	SO4	F	501	5/5	0.80	0.18	120,120,137,146	0
9	KNG	C	1201	70/70	0.84	0.30	99,127,142,159	0
10	SO4	F	502	5/5	0.85	0.23	94,123,128,128	0
10	SO4	D	2007	5/5	0.86	0.16	180,186,220,337	0
14	EDO	F	503	4/4	0.87	0.76	83,100,114,121	0
10	SO4	D	2006	5/5	0.88	0.19	120,134,161,165	0
10	SO4	D	2004	5/5	0.90	0.25	117,122,130,130	0
10	SO4	D	2005	5/5	0.91	0.50	112,129,156,157	0
11	ZN	D	2002	1/1	0.91	0.17	118,118,118,118	0
12	MG	D	2003	1/1	0.97	0.57	151,151,151,151	0
11	ZN	D	2001	1/1	0.97	0.22	89,89,89,89	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.