wwPDB X-ray Structure Validation Summary Report (i)

Sep 26, 2023 – 03:04 PM EDT

PDB ID	:	6CCE
Title	:	Crystal structure of a Mycobacterium smegmatis RNA polymerase transcription initiation complex with inhibitor Kanglemycin A
Authors	:	Lilic, M.; Darst, S.A.; Campbell, E.A.
Deposited on	:	2018-02-07
Resolution	:	3.05 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 (i)) were used in the production of this report:

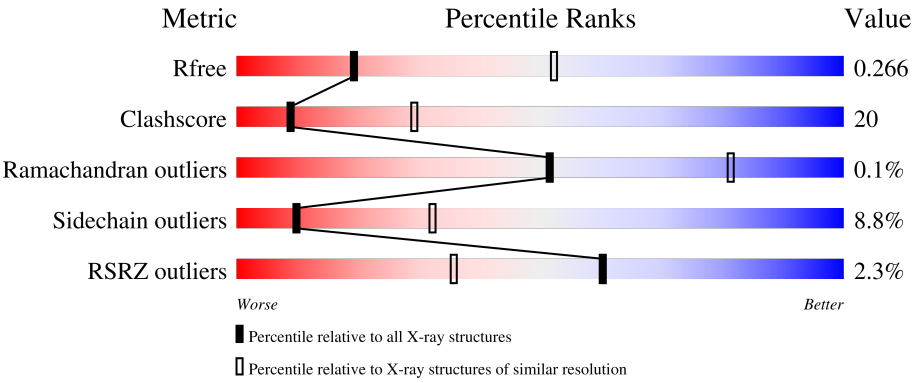
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.05 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.



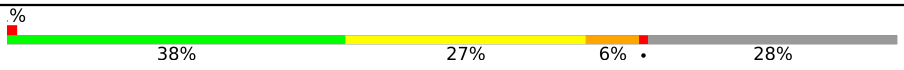
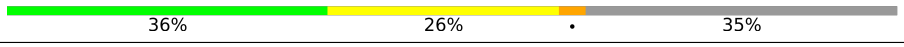
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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	J	114	% 22% 7% 68%
2	A	350	% 36% 24% 37%
2	B	350	2% 36% 26% 35%
3	C	1169	5% 57% 33% 6%
4	D	1317	% 56% 32% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	107	
6	F	466	
7	O	57	
8	G	19	

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	1202	-	-	X	-
10	SO4	C	1203	-	-	X	-
10	SO4	D	2004	-	-	X	-
10	SO4	D	2006	-	-	X	-
10	SO4	D	2007	-	-	X	-
13	GLU	D	2003	-	-	X	-

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 25375 atoms, of which 18 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	36	Total	C	N	O	S	0	0	0
			293	183	55	54	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	221	Total	C	N	O	S	0	0	0
			1615	1019	273	320	3			
2	B	226	Total	C	N	O	S	0	0	0
			1619	1015	278	324	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	1095	Total	C	N	O	S	0	0	0
			8269	5178	1448	1609	34			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	1195	Total	C	N	O	S	0	0	0
			9167	5746	1651	1734	36			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	77	Total	C	N	O	0	0	0
			593	379	100	114			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	302	Total	C	N	O	S	0	0	0
			2412	1511	434	460	7			

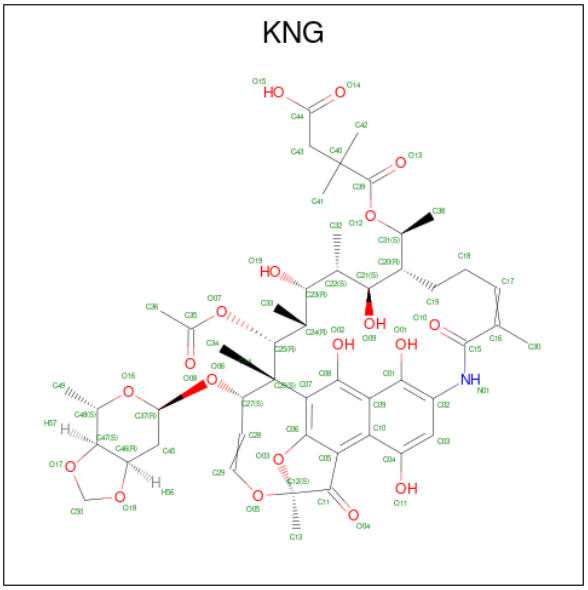
- Molecule 7 is a DNA chain called DNA (57-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	O	57	Total	C	N	O	P	0	0	0
			1161	560	208	338	55			

- Molecule 8 is a protein called poly(UNK).

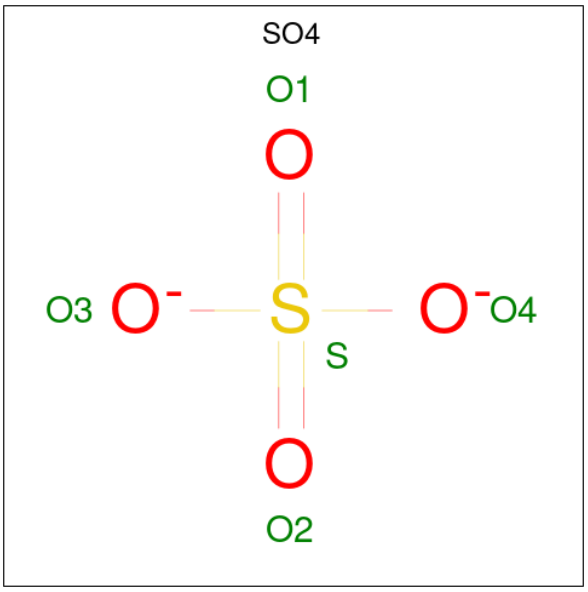
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	G	19	Total	C	N	O	0	0	0
			95	57	19	19			

- Molecule 9 is Kanglemycin A (three-letter code: KNG) (formula: $C_{50}H_{67}NO_{19}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	C	1	Total	C	N	O	0	0
			70	50	1	19		

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

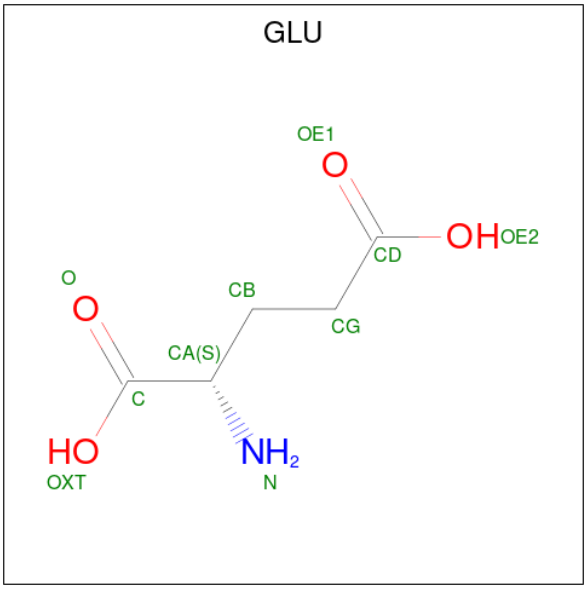
- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	D	1	Total Zn 1 1	0	0

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

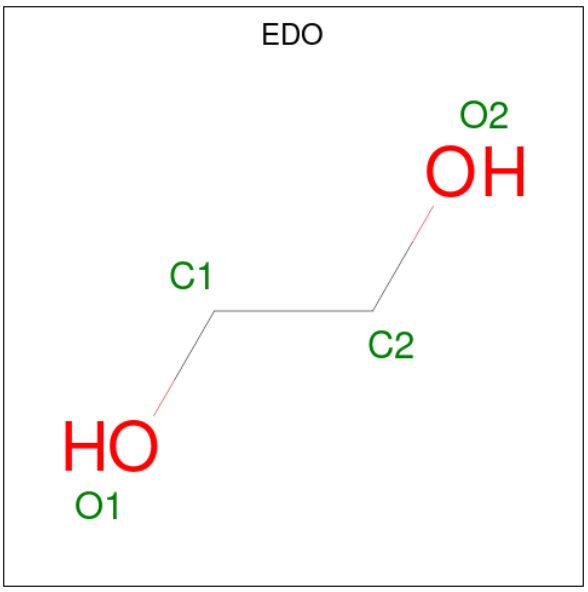
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	D	1	Total Mg 1 1	0	0

- 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 9 5 1 3	0	0

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



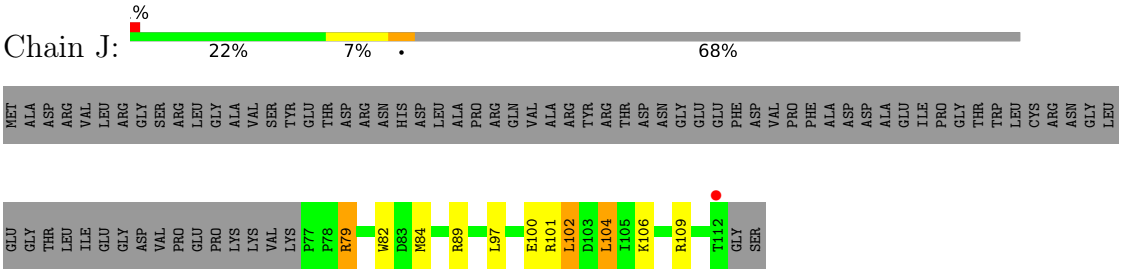
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	F	1	Total	C	H	O	0	0
			10	2	6	2		
14	F	1	Total	C	H	O	0	0
			10	2	6	2		
14	F	1	Total	C	H	O	0	0
			10	2	6	2		

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.

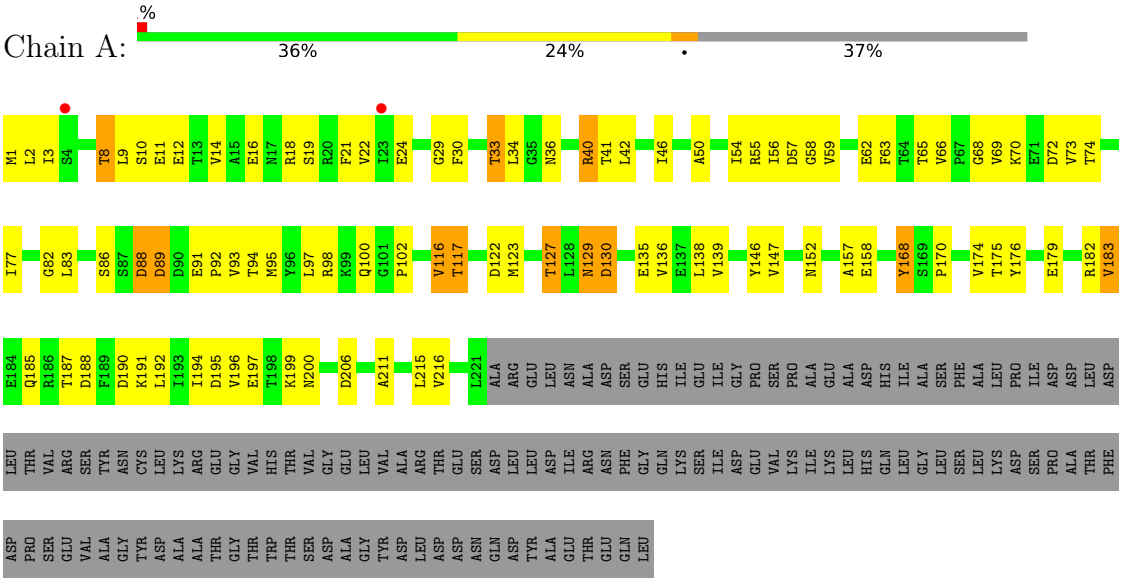
• Molecule 1: RNA polymerase-binding protein RbpA

Chain J:



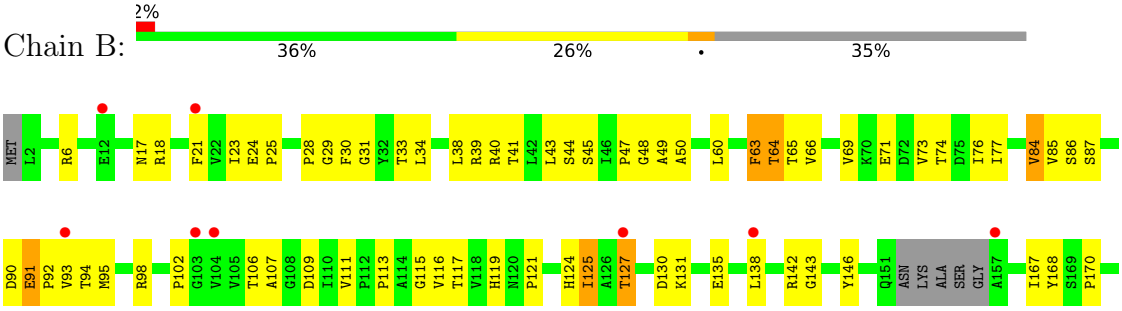
• Molecule 2: DNA-directed RNA polymerase subunit alpha

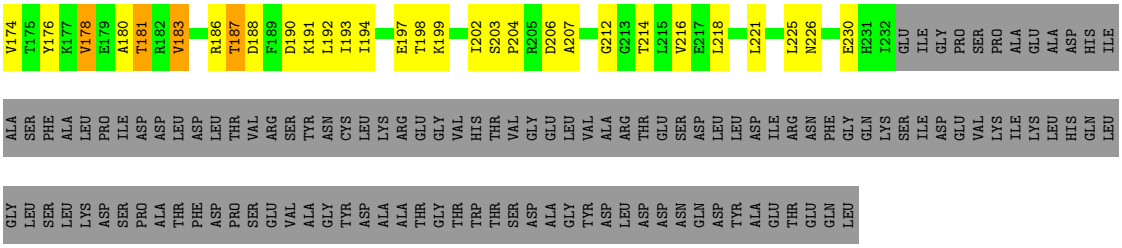
Chain A:



• Molecule 2: DNA-directed RNA polymerase subunit alpha

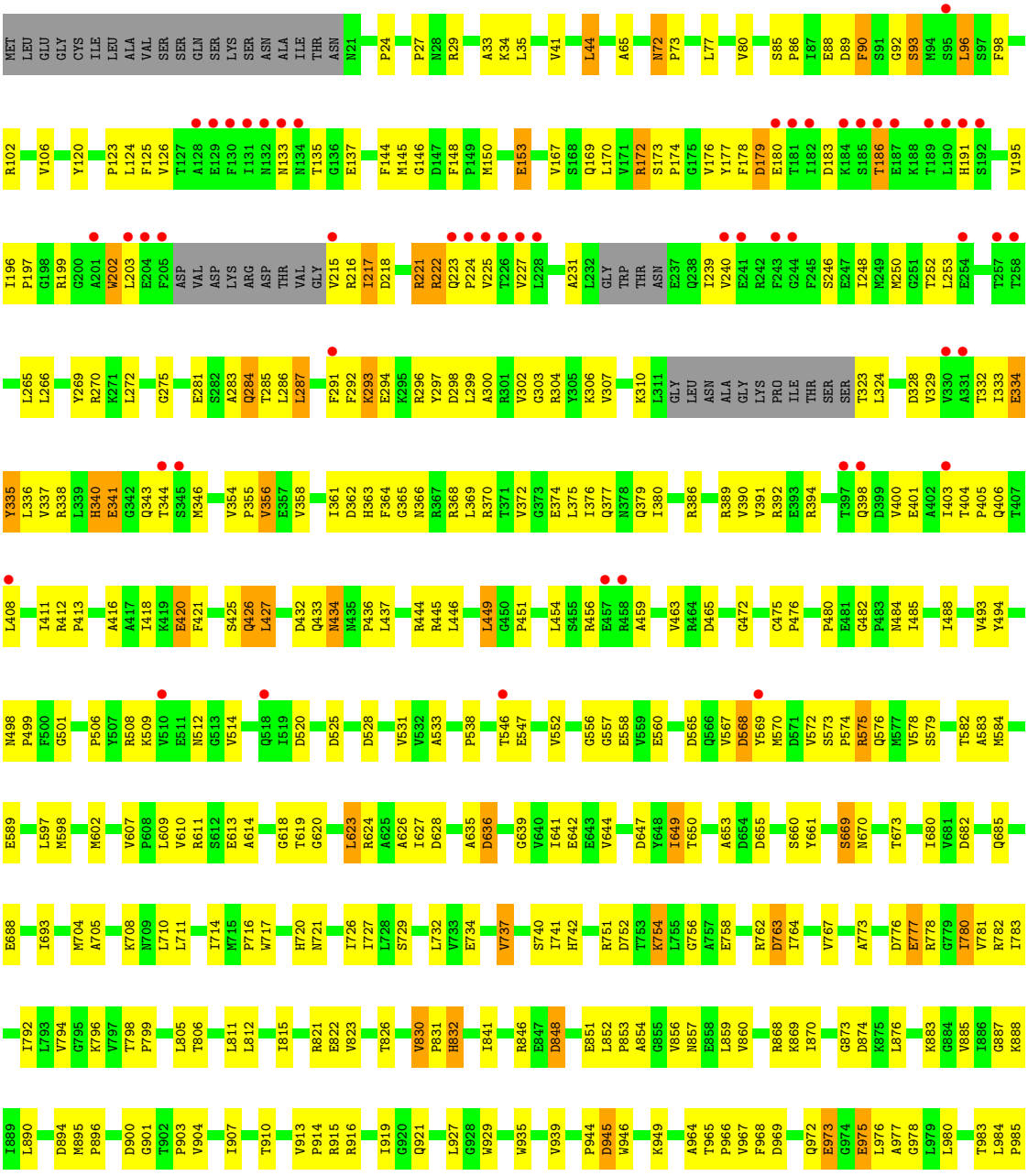
Chain B:

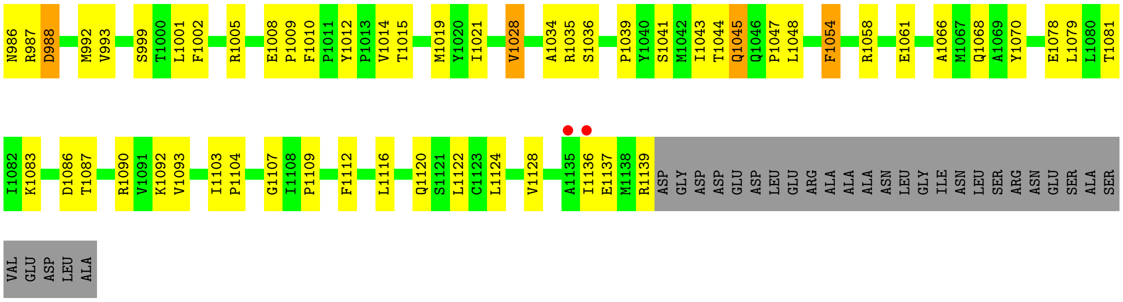




• Molecule 3: DNA-directed RNA polymerase subunit beta

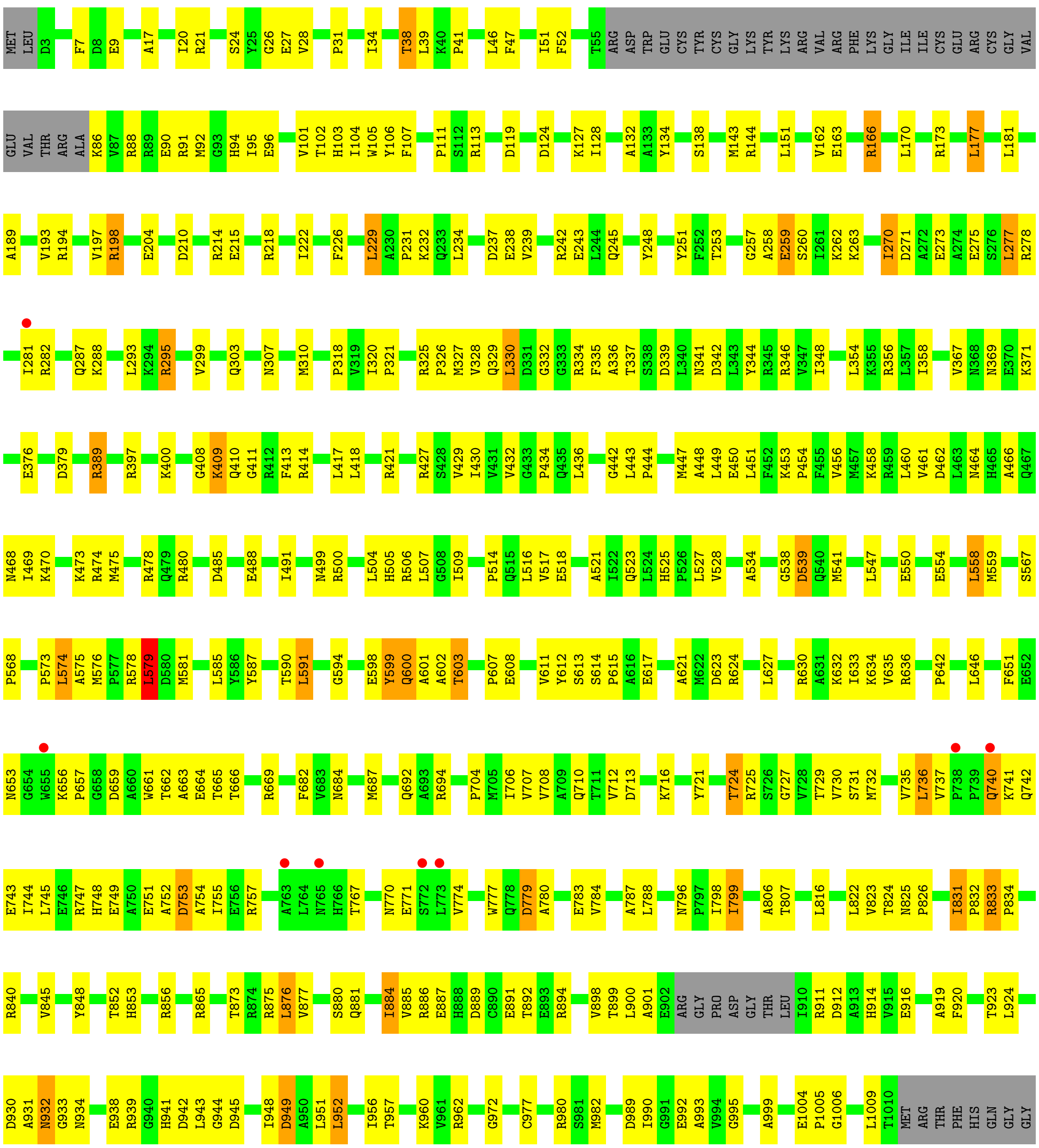
Chain C:

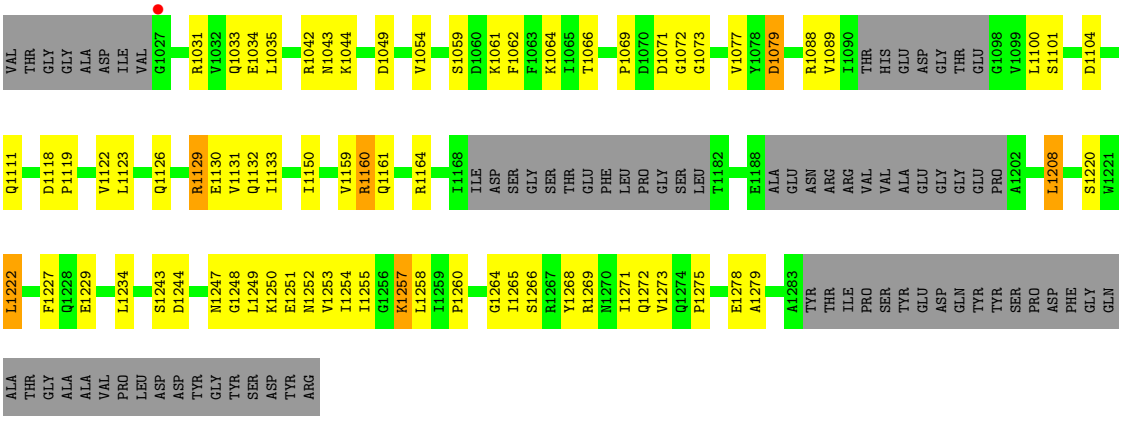




• Molecule 4: DNA-directed RNA polymerase subunit beta'

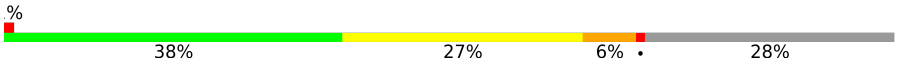
Chain D:

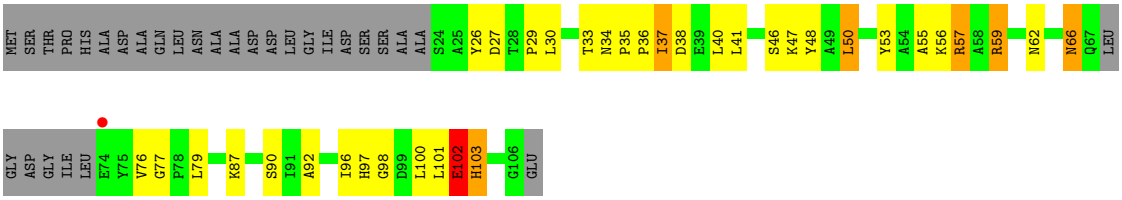




• Molecule 5: DNA-directed RNA polymerase subunit omega

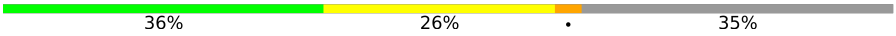
Chain E:

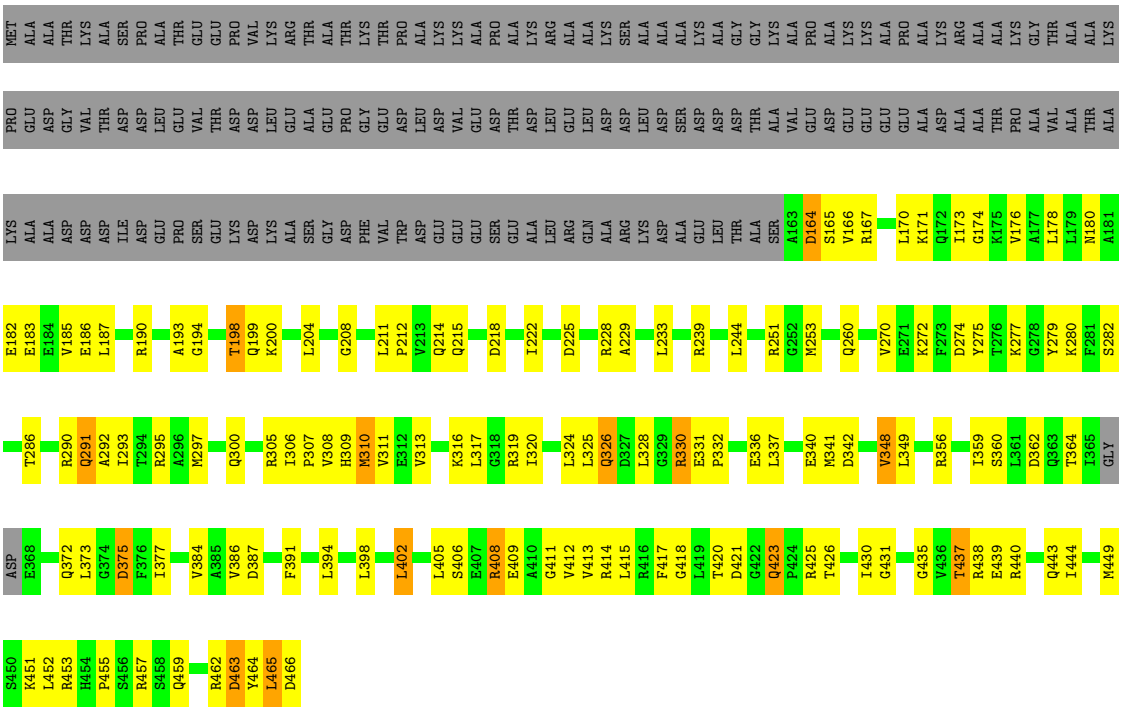




• Molecule 6: RNA polymerase sigma factor SigA

Chain F:



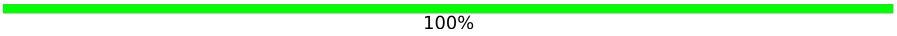


• Molecule 7: DNA (57-MER)

Chain O:

• Molecule 8: poly(UNK)

Chain G:



There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	130.56Å 161.58Å 135.14Å 90.00° 110.73° 90.00°	Depositor
Resolution (Å)	49.55 – 3.05 49.55 – 2.94	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.55-3.05) 96.9 (49.55-2.94)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.00 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.234 , 0.265 0.234 , 0.266	Depositor DCC
R_{free} test set	1951 reflections (1.81%)	wwPDB-VP
Wilson B-factor (Å^2)	105.6	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 61.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.020 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	25375	wwPDB-VP
Average B, all atoms (Å^2)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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: EDO, ZN, SO4, KNG, 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	J	0.22	0/297	0.38	0/399
2	A	0.24	0/1640	0.45	0/2241
2	B	0.24	0/1644	0.45	0/2250
3	C	0.24	0/8415	0.43	0/11431
4	D	0.24	0/9306	0.41	0/12596
5	E	0.24	0/605	0.42	0/824
6	F	0.23	0/2441	0.39	0/3290
7	O	0.49	0/1301	0.92	0/2004
All	All	0.26	0/25649	0.46	0/35035

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
4	D	0	1
5	E	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	270	ILE	Peptide
5	E	102	GLU	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	J	293	0	287	12	0
2	A	1615	0	1612	76	0
2	B	1619	0	1551	82	0
3	C	8269	0	8014	364	0
4	D	9167	0	9167	388	0
5	E	593	0	579	42	0
6	F	2412	0	2451	125	0
7	O	1161	0	650	35	0
8	G	95	0	21	0	0
9	C	70	0	0	1	0
10	C	10	0	0	4	0
10	D	20	0	0	9	0
10	F	10	0	0	0	0
11	D	1	0	0	0	0
12	D	1	0	0	0	0
13	D	9	0	5	10	0
14	F	12	18	18	4	0
All	All	25357	18	24355	1010	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 20.

The worst 5 of 1010 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:538:PRO:HB2	3:C:546:THR:HB	1.28	1.14
5:E:102:GLU:HA	5:E:103:HIS:HB3	1.09	1.07
4:D:636:ARG:HB3	4:D:662:THR:HG22	1.40	1.04
6:F:317:LEU:HA	6:F:341:MET:HE1	1.45	0.98
5:E:102:GLU:HA	5:E:103:HIS:CB	1.92	0.98

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	34/114 (30%)	34 (100%)	0	0	100 100
2	A	219/350 (63%)	216 (99%)	2 (1%)	1 (0%)	29 60
2	B	222/350 (63%)	203 (91%)	19 (9%)	0	100 100
3	C	1087/1169 (93%)	1057 (97%)	30 (3%)	0	100 100
4	D	1181/1317 (90%)	1146 (97%)	34 (3%)	1 (0%)	51 81
5	E	73/107 (68%)	67 (92%)	6 (8%)	0	100 100
6	F	298/466 (64%)	296 (99%)	2 (1%)	0	100 100
All	All	3114/3873 (80%)	3019 (97%)	93 (3%)	2 (0%)	51 81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	579	LEU
2	A	183	VAL

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	J	30/98 (31%)	26 (87%)	4 (13%)	4 14
2	A	175/297 (59%)	157 (90%)	18 (10%)	7 24
2	B	168/297 (57%)	146 (87%)	22 (13%)	4 15
3	C	865/984 (88%)	790 (91%)	75 (9%)	10 33

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	D	955/1095 (87%)	882 (92%)	73 (8%)	13 38
5	E	61/86 (71%)	53 (87%)	8 (13%)	4 15
6	F	256/379 (68%)	236 (92%)	20 (8%)	12 37
All	All	2510/3236 (78%)	2290 (91%)	220 (9%)	10 32

5 of 220 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	1028	VAL
4	D	464	ASN
6	F	465	LEU
5	E	103	HIS
4	D	7	PHE

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

Mol	Chain	Res	Type
4	D	692	GLN
6	F	215	GLN
4	D	796	ASN
5	E	66	ASN
3	C	467	HIS

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 15 ligands modelled in this entry, 2 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	$\#\|Z\| > 2$
14	EDO	F	505	-	3,3,3	0.48	0	2,2,2	0.35	0
10	SO4	D	2005	-	4,4,4	0.15	0	6,6,6	0.05	0
10	SO4	F	502	-	4,4,4	0.14	0	6,6,6	0.07	0
13	GLU	D	2003	-	7,8,9	0.90	0	4,9,11	1.09	0
10	SO4	D	2006	-	4,4,4	0.14	0	6,6,6	0.06	0
14	EDO	F	503	-	3,3,3	0.46	0	2,2,2	0.43	0
10	SO4	F	501	-	4,4,4	0.14	0	6,6,6	0.05	0
9	KNG	C	1201	-	75,75,75	2.59	17 (22%)	104,114,114	1.71	17 (16%)
10	SO4	C	1202	-	4,4,4	0.15	0	6,6,6	0.05	0
10	SO4	D	2007	-	4,4,4	0.14	0	6,6,6	0.06	0
14	EDO	F	504	-	3,3,3	0.49	0	2,2,2	0.37	0
10	SO4	D	2004	-	4,4,4	0.13	0	6,6,6	0.09	0
10	SO4	C	1203	-	4,4,4	0.14	0	6,6,6	0.04	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
14	EDO	F	505	-	-	0/1/1/1	-
13	GLU	D	2003	-	-	2/6/7/9	-
14	EDO	F	503	-	-	1/1/1/1	-
9	KNG	C	1201	-	-	15/76/113/113	0/5/6/6
14	EDO	F	504	-	-	1/1/1/1	-

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1201	KNG	O04-C11	11.51	1.40	1.21
9	C	1201	KNG	C17-C16	9.31	1.53	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1201	KNG	O03-C06	9.19	1.55	1.37
9	C	1201	KNG	C15-N01	4.50	1.45	1.35
9	C	1201	KNG	C12-C11	-3.93	1.39	1.54

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	C	1201	KNG	C18-C17-C16	-6.69	114.83	129.08
9	C	1201	KNG	O04-C11-C05	-5.08	122.12	131.81
9	C	1201	KNG	O07-C35-C36	4.87	120.06	111.09
9	C	1201	KNG	O03-C06-C07	4.58	129.01	121.14
9	C	1201	KNG	C12-C11-C05	4.25	115.63	107.30

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	1201	KNG	O07-C25-C26-C34
9	C	1201	KNG	C40-C43-C44-O14
9	C	1201	KNG	O07-C25-C26-C27
9	C	1201	KNG	C24-C25-C26-C34
9	C	1201	KNG	O12-C39-C40-C42

There are no ring outliers.

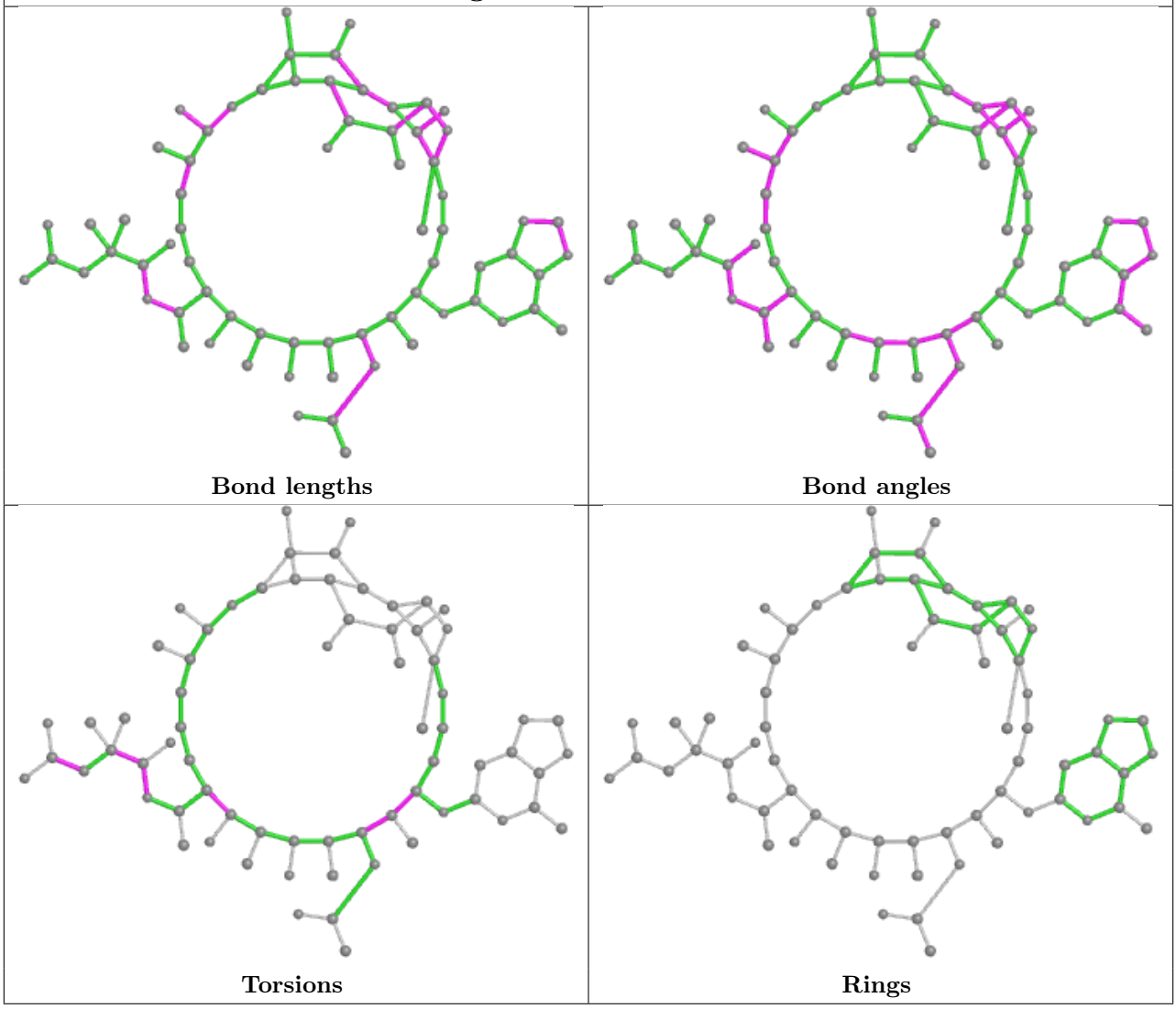
10 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	F	505	EDO	2	0
10	D	2005	SO4	1	0
13	D	2003	GLU	10	0
10	D	2006	SO4	2	0
14	F	503	EDO	2	0
9	C	1201	KNG	1	0
10	C	1202	SO4	2	0
10	D	2007	SO4	3	0
10	D	2004	SO4	3	0
10	C	1203	SO4	2	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 then 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.

Ligand KNG C 1201



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	J	36/114 (31%)	-0.33	1 (2%) 53 28	75, 99, 146, 158	0
2	A	221/350 (63%)	-0.23	2 (0%) 84 66	76, 106, 144, 170	0
2	B	226/350 (64%)	0.10	8 (3%) 44 22	101, 137, 164, 184	0
3	C	1095/1169 (93%)	0.19	54 (4%) 29 13	54, 110, 174, 200	0
4	D	1195/1317 (90%)	-0.13	9 (0%) 86 70	45, 96, 152, 196	0
5	E	77/107 (71%)	0.05	1 (1%) 77 56	76, 109, 153, 172	0
6	F	302/466 (64%)	-0.22	0 100 100	57, 98, 144, 165	0
7	O	57/57 (100%)	-0.74	0 100 100	74, 103, 133, 140	0
8	G	0/19	-	-	-	-
All	All	3209/3949 (81%)	-0.03	75 (2%) 60 36	45, 106, 167, 200	0

The worst 5 of 75 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	184	LYS	8.2
3	C	185	SER	6.9
5	E	74	GLU	6.7
3	C	226	THR	6.6
3	C	224	PRO	6.6

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

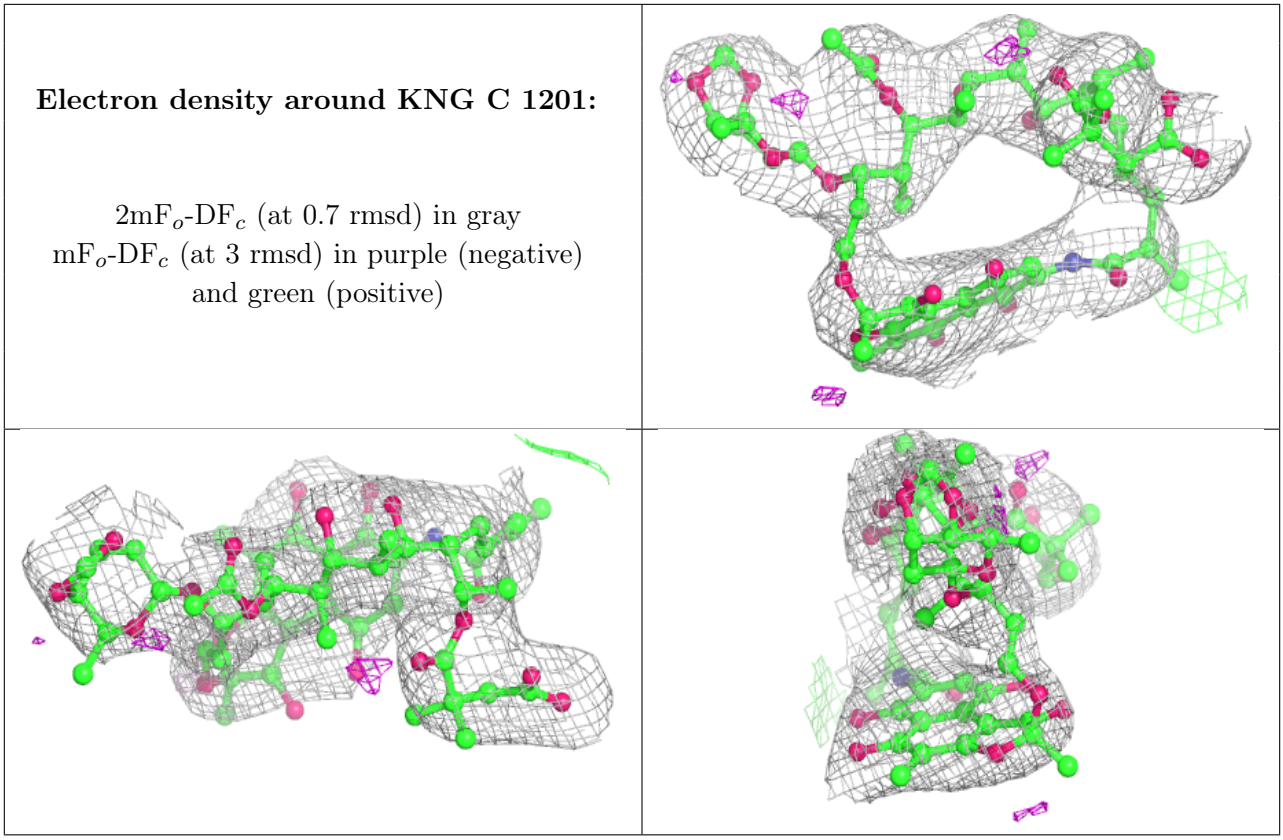
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
10	SO4	D	2007	5/5	0.63	0.28	135,138,154,236	0
10	SO4	C	1203	5/5	0.71	0.38	122,132,137,156	0
10	SO4	F	502	5/5	0.80	0.28	103,105,125,132	0
14	EDO	F	505	4/4	0.80	0.17	90,108,127,127	0
13	GLU	D	2003	9/10	0.81	0.19	96,108,115,117	0
10	SO4	D	2006	5/5	0.84	0.22	115,123,131,165	0
14	EDO	F	504	4/4	0.86	0.36	95,114,127,127	0
12	MG	D	2002	1/1	0.86	0.17	109,109,109,109	0
10	SO4	D	2004	5/5	0.89	0.13	120,136,154,158	0
10	SO4	D	2005	5/5	0.90	0.21	109,117,126,129	0
10	SO4	F	501	5/5	0.92	0.23	97,98,114,116	0
9	KNG	C	1201	70/70	0.92	0.24	75,100,119,136	0
14	EDO	F	503	4/4	0.93	0.38	73,88,103,104	0
10	SO4	C	1202	5/5	0.95	0.15	129,134,157,157	0
11	ZN	D	2001	1/1	0.98	0.28	116,116,116,116	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.

Electron density around KNG C 1201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.