



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 28, 2020 – 12:40 PM EDT

PDB ID : 6VJS
Title : Escherichia coli RNA polymerase and ureidothiophene-2-carboxylic acid complex
Authors : Murakami, K.S.; Molodtsov, V.
Deposited on : 2020-01-17
Resolution : 4.02 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:

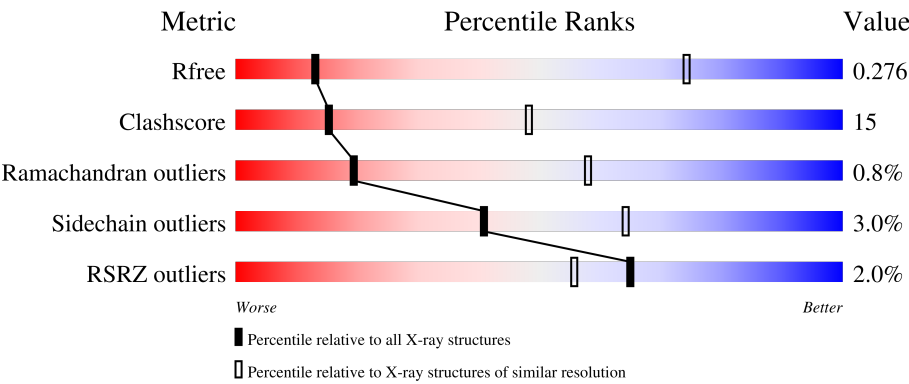
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.02 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	1098 (4.34-3.70)
Clashscore	141614	1159 (4.34-3.70)
Ramachandran outliers	138981	1118 (4.34-3.70)
Sidechain outliers	138945	1108 (4.34-3.70)
RSRZ outliers	127900	1034 (4.38-3.66)

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	A	329	<div><div></div><div><div></div><div>54%</div><div>17%</div><div>29%</div></div></div>
1	B	329	<div><div>2%</div><div></div><div><div></div><div>58%</div><div>33%</div><div>9%</div></div></div>
1	F	329	<div><div>2%</div><div></div><div><div></div><div>54%</div><div>16%</div><div>29%</div></div></div>
1	G	329	<div><div>5%</div><div></div><div><div></div><div>53%</div><div>16%</div><div>30%</div></div></div>
2	C	1342	<div><div></div><div><div></div><div>66%</div><div>31%</div><div></div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	1342	<p>3% 66% 31% .</p>
3	D	1407	<p>49% 32% . 17%</p>
3	I	1407	<p>2% 50% 32% . 18%</p>
4	E	91	<p>87% 12% .</p>
4	J	91	<p>9% 63% 20% . 16%</p>
5	X	613	<p>2% 51% 24% . 23%</p>
5	Y	613	<p>2% 54% 22% . 23%</p>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 56011 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	234	Total	C	N	O	S	0	0	0
			1809	1126	319	357	7			
1	B	301	Total	C	N	O	S	0	0	0
			2337	1462	411	456	8			
1	F	234	Total	C	N	O	S	0	0	0
			1809	1126	319	357	7			
1	G	229	Total	C	N	O	S	0	0	0
			1775	1106	313	350	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1336	Total	C	N	O	S	0	0	0
			10540	6614	1836	2047	43			
2	H	1336	Total	C	N	O	S	0	0	0
			10540	6614	1836	2047	43			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1164	Total	C	N	O	S	0	0	0
			9093	5717	1626	1704	46			
3	I	1160	Total	C	N	O	S	0	0	0
			9061	5698	1619	1698	46			

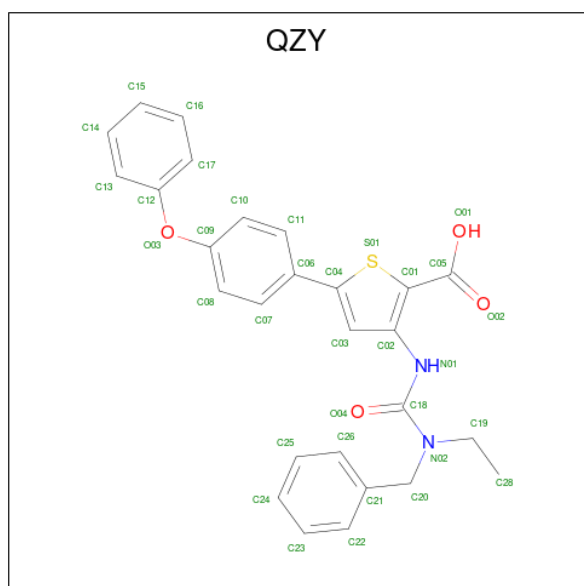
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	90	Total	C	N	O	S	0	0	0
			708	430	136	141	1			
4	J	76	Total	C	N	O	S	0	0	0
			605	368	115	121	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	X	471	Total	C	N	O	S	0	0	0
			3832	2398	687	724	23			
5	Y	475	Total	C	N	O	S	0	0	0
			3862	2413	692	734	23			

- Molecule 6 is 3-{[benzyl(ethyl)carbamoyl]amino}-5-(4-phenoxyphenyl)thiophene-2-carboxylic acid (three-letter code: QZY) (formula: C₂₇H₂₄N₂O₄S) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	N	O	S	0	0
			34	27	2	4	1		

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

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

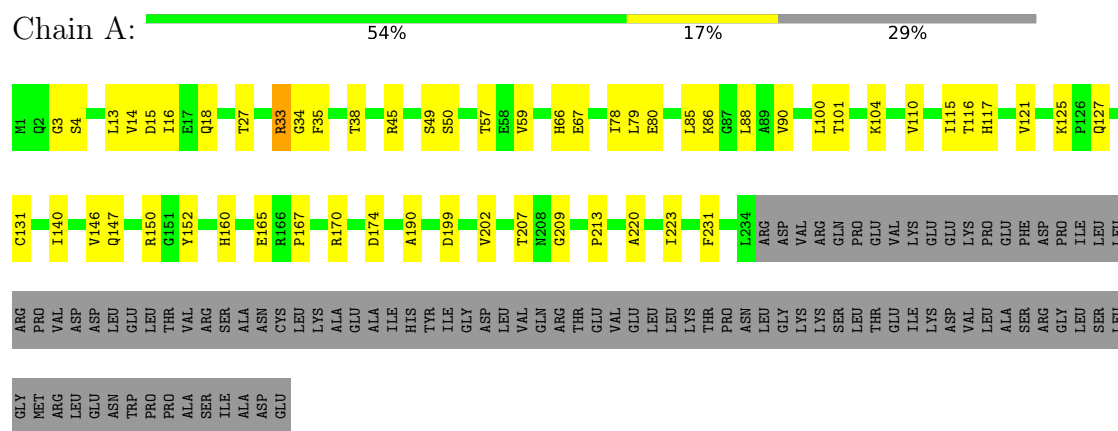
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	I	1	Total 1	Mg 1	0	0
8	D	1	Total 1	Mg 1	0	0

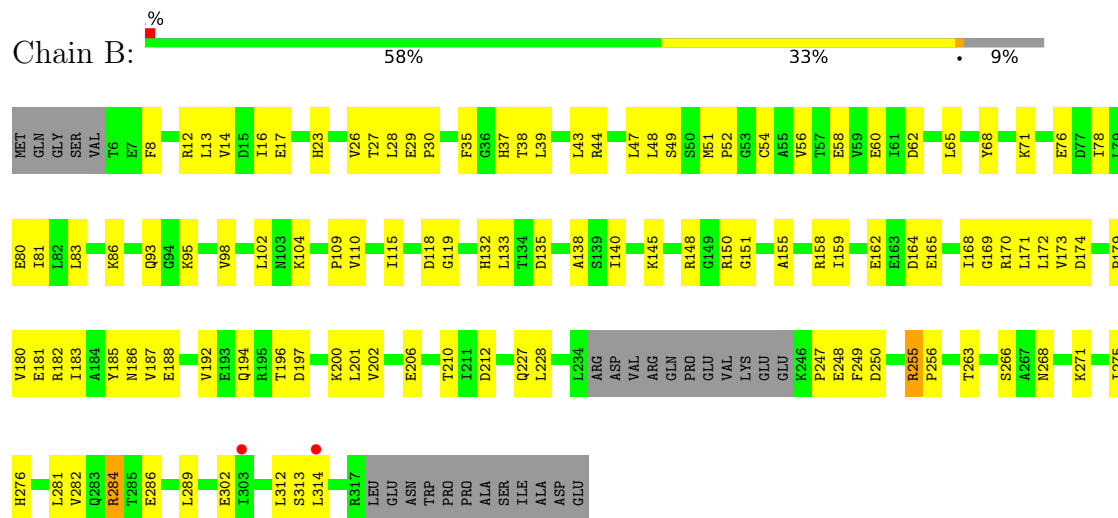
3 Residue-property plots

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

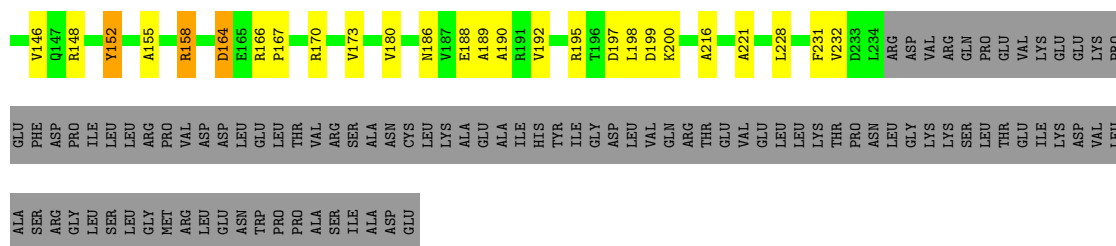


• Molecule 1: DNA-directed RNA polymerase subunit alpha

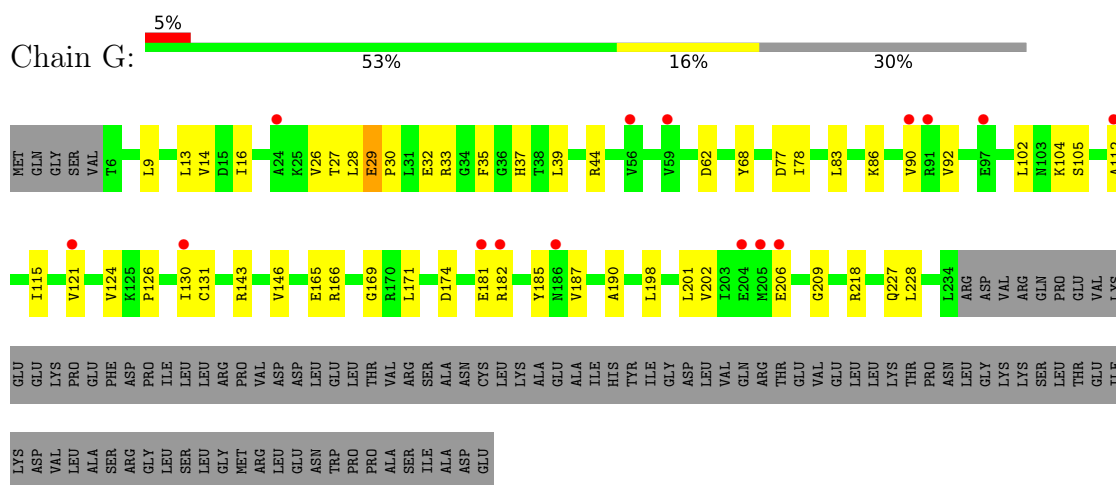


• Molecule 1: DNA-directed RNA polymerase subunit alpha

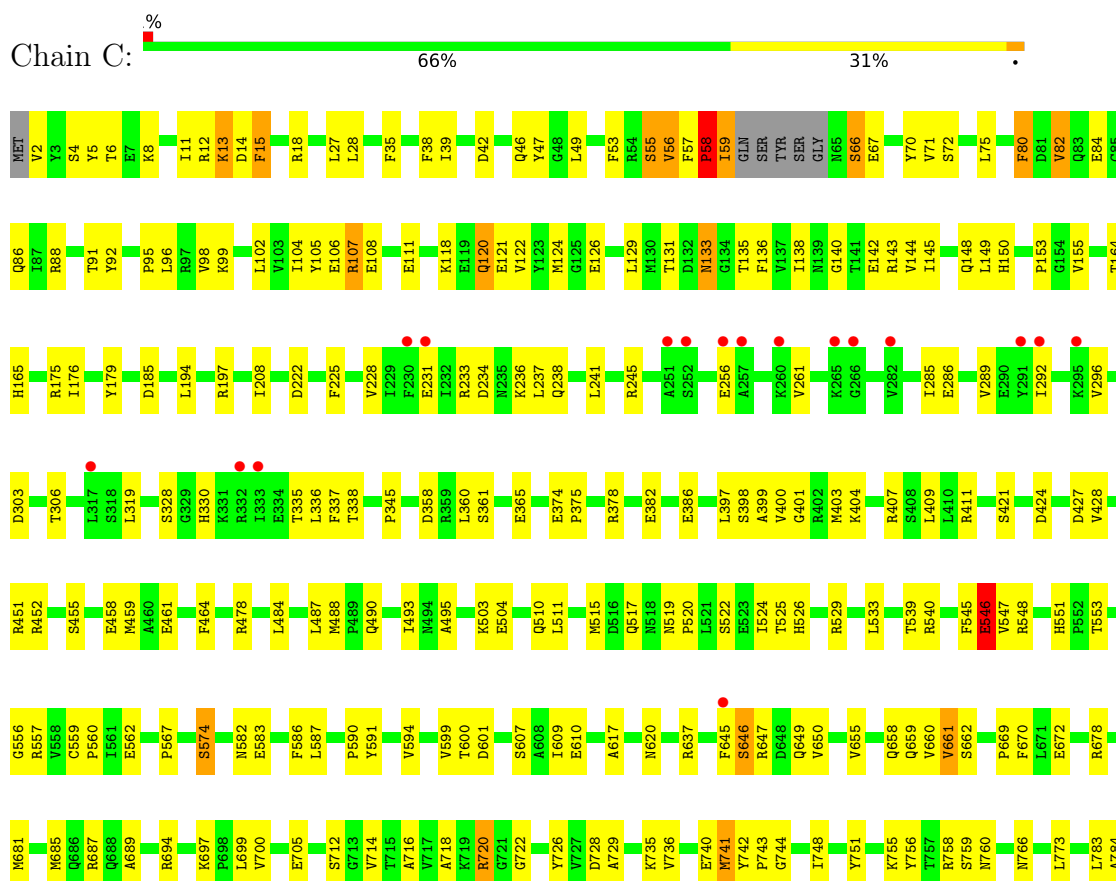


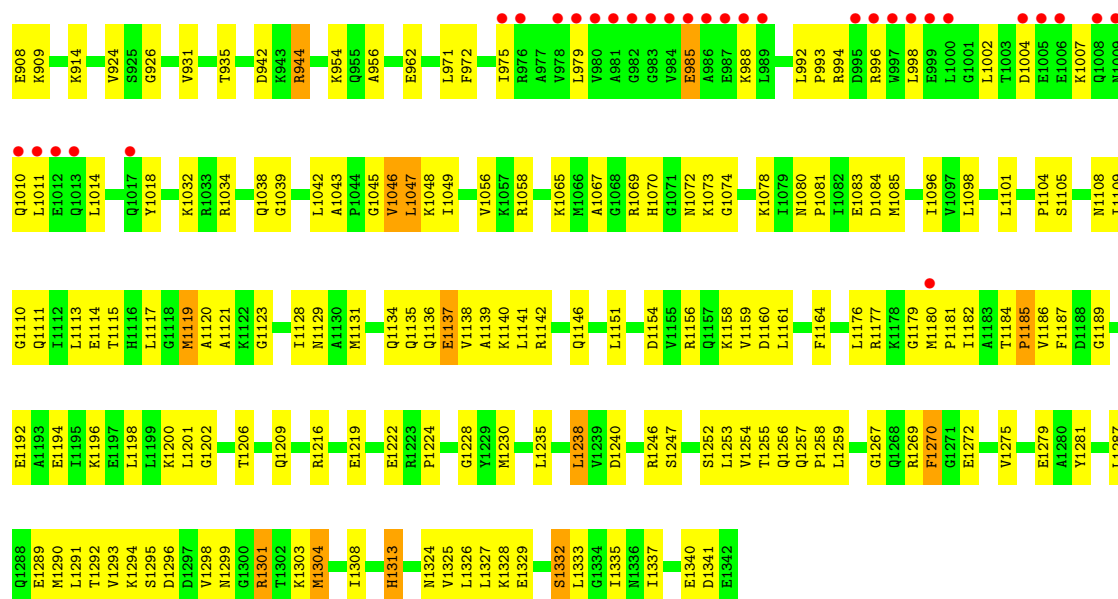


• Molecule 1: DNA-directed RNA polymerase subunit alpha



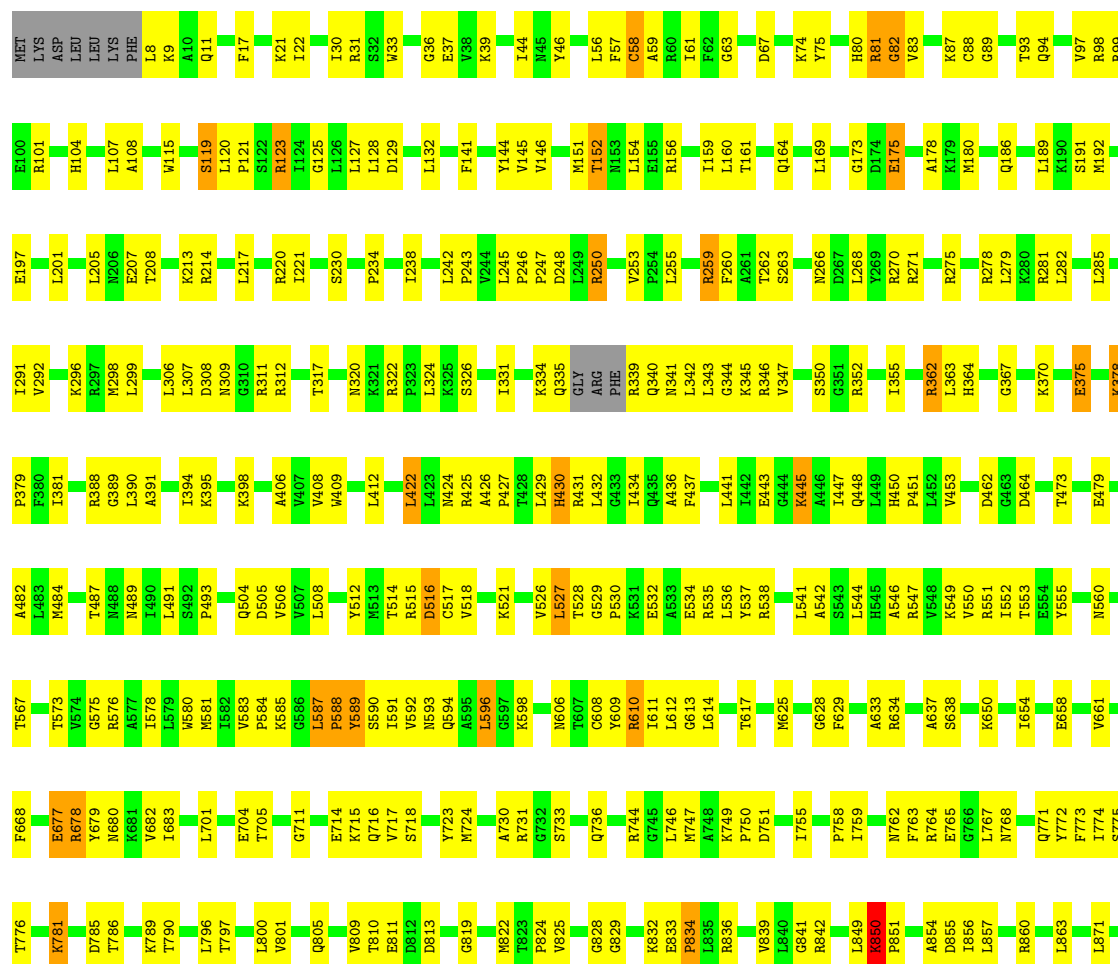
• Molecule 2: DNA-directed RNA polymerase subunit beta

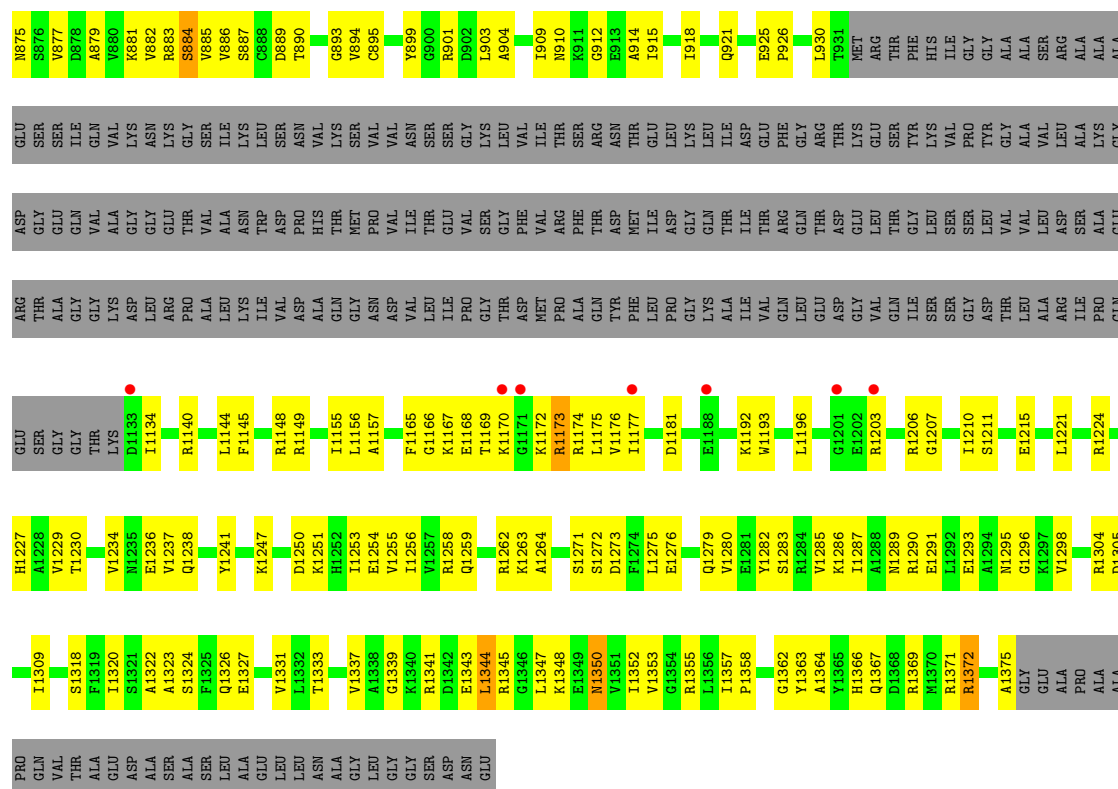




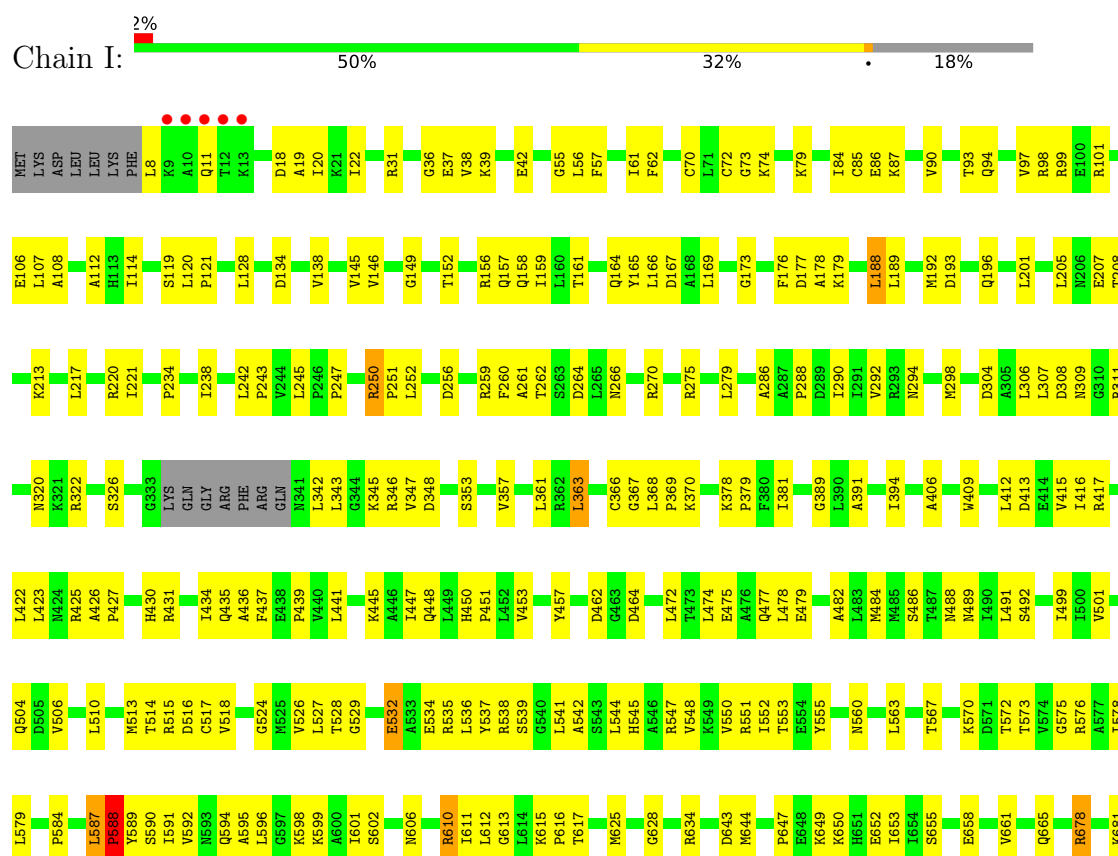
• Molecule 3: DNA-directed RNA polymerase subunit beta'

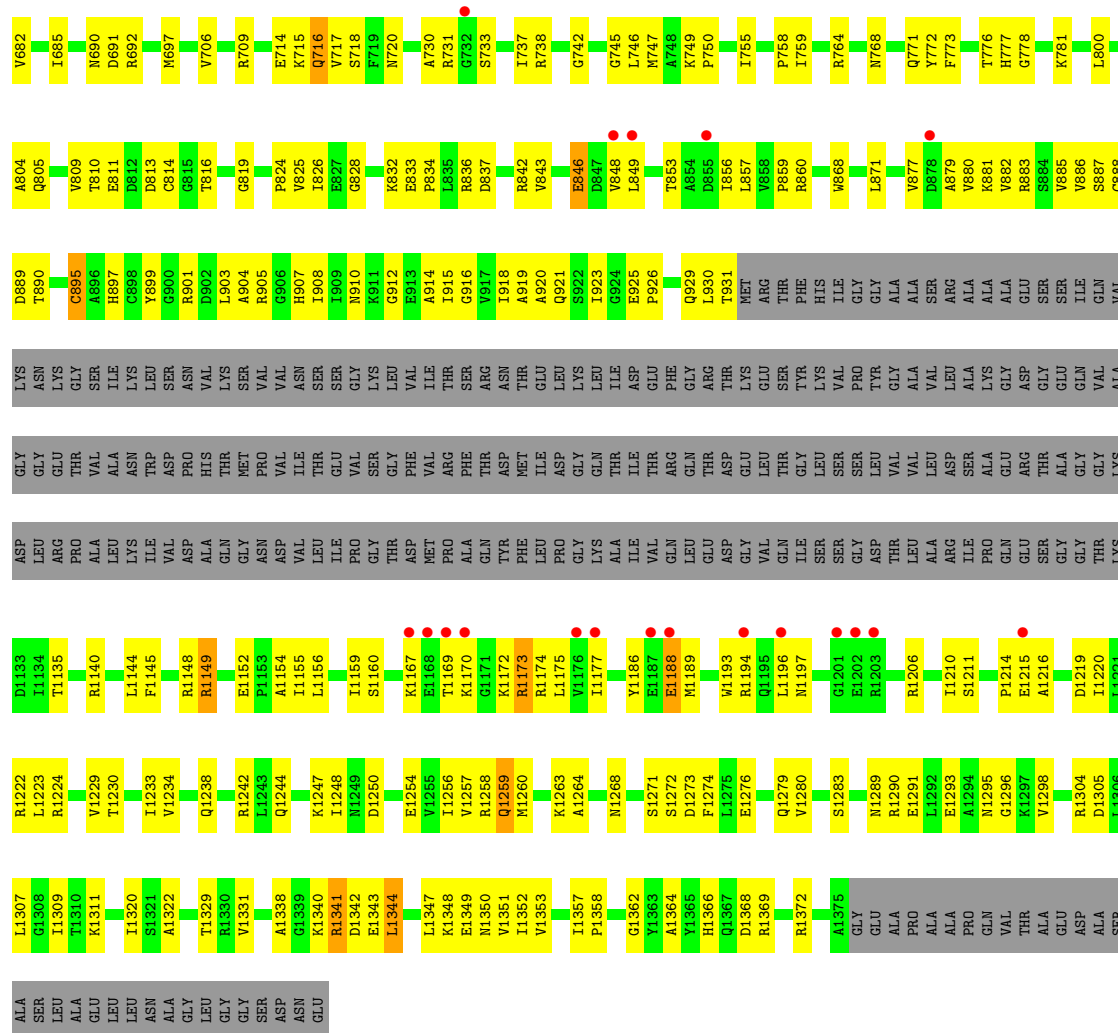
Chain D: 49% 32% 17%





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





- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 87% 12%



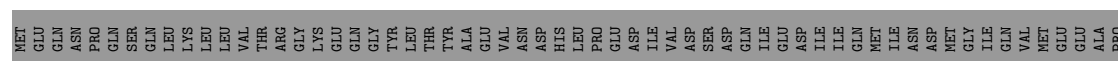
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain J: 9% 63% 20% 16%



- Molecule 5: RNA polymerase sigma factor RpoD

Chain X: 2% 51% 24% 23%





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	187.08Å 205.50Å 309.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.09 – 4.02 50.09 – 4.02	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.09-4.02) 99.3 (50.09-4.02)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 4.00Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.230 , 0.276 0.229 , 0.276	Depositor DCC
R_{free} test set	1999 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	157.4	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 154.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	56011	wwPDB-VP
Average B, all atoms (Å ²)	205.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: QZY, 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	0.26	0/1831	0.50	0/2481
1	B	0.24	0/2365	0.48	1/3202 (0.0%)
1	F	0.25	0/1830	0.47	0/2478
1	G	0.24	0/1797	0.47	0/2436
2	C	0.27	0/10708	0.55	1/14448 (0.0%)
2	H	0.26	0/10708	0.51	2/14448 (0.0%)
3	D	0.26	0/9231	0.52	2/12459 (0.0%)
3	I	0.25	0/9199	0.50	0/12417
4	E	0.23	0/710	0.46	0/956
4	J	0.22	0/607	0.44	0/817
5	X	0.28	0/3884	0.51	3/5220 (0.1%)
5	Y	0.25	0/3914	0.47	3/5261 (0.1%)
All	All	0.26	0/56784	0.51	12/76623 (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
2	C	0	8
2	H	0	5
3	D	0	9
3	I	0	8
5	Y	0	1
All	All	0	31

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1002	LEU	CA-CB-CG	8.35	134.50	115.30
3	D	711	GLY	N-CA-C	-6.24	97.51	113.10
5	X	259	PHE	CB-CG-CD2	6.21	125.15	120.80
1	B	228	LEU	CA-CB-CG	5.90	128.87	115.30
5	X	503	GLU	C-N-CD	-5.89	107.65	120.60

There are no chirality outliers.

5 of 31 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	13	LYS	Peptide
2	C	42	ASP	Peptide
2	C	546	GLU	Peptide
2	C	55	SER	Peptide
2	C	58	PRO	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	A	1809	0	1837	43	0
1	B	2337	0	2397	75	0
1	F	1809	0	1836	41	0
1	G	1775	0	1800	39	0
2	C	10540	0	10561	357	0
2	H	10540	0	10561	326	0
3	D	9093	0	9290	358	0
3	I	9061	0	9260	350	0
4	E	708	0	719	7	0
4	J	605	0	612	18	0
5	X	3832	0	3907	120	0
5	Y	3862	0	3926	113	0
6	D	34	0	0	2	0
7	D	2	0	0	0	0
7	I	2	0	0	0	0
8	D	1	0	0	0	0
8	I	1	0	0	0	0
All	All	56011	0	56706	1676	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 1676 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:I:1159:ILE:HD12	3:I:1186:TYR:CE2	1.82	1.13
5:X:166:VAL:H	5:X:259:PHE:HA	1.15	1.05
5:X:165:PHE:HB3	5:X:259:PHE:CD2	1.93	1.03
1:A:14:VAL:HG12	1:A:15:ASP:H	1.26	0.96
2:C:841:ARG:HA	2:C:1046:VAL:HG11	1.51	0.93

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	232/329 (70%)	201 (87%)	31 (13%)	0	100	100
1	B	297/329 (90%)	269 (91%)	28 (9%)	0	100	100
1	F	230/329 (70%)	203 (88%)	27 (12%)	0	100	100
1	G	227/329 (69%)	201 (88%)	26 (12%)	0	100	100
2	C	1334/1342 (99%)	1130 (85%)	186 (14%)	18 (1%)	12	48
2	H	1334/1342 (99%)	1127 (84%)	192 (14%)	15 (1%)	14	51
3	D	1158/1407 (82%)	983 (85%)	166 (14%)	9 (1%)	19	58
3	I	1154/1407 (82%)	955 (83%)	192 (17%)	7 (1%)	25	63
4	E	88/91 (97%)	75 (85%)	12 (14%)	1 (1%)	14	51
4	J	74/91 (81%)	64 (86%)	9 (12%)	1 (1%)	11	46
5	X	467/613 (76%)	425 (91%)	39 (8%)	3 (1%)	25	63
5	Y	471/613 (77%)	431 (92%)	37 (8%)	3 (1%)	25	63
All	All	7066/8222 (86%)	6064 (86%)	945 (13%)	57 (1%)	19	58

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	15	PHE
2	C	66	SER
2	C	547	VAL
2	C	661	VAL
2	C	1005	GLU

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	A	201/286 (70%)	198 (98%)	3 (2%)	65	80
1	B	261/286 (91%)	251 (96%)	10 (4%)	33	59
1	F	201/286 (70%)	195 (97%)	6 (3%)	41	64
1	G	197/286 (69%)	194 (98%)	3 (2%)	65	80
2	C	1152/1157 (100%)	1121 (97%)	31 (3%)	44	67
2	H	1152/1157 (100%)	1122 (97%)	30 (3%)	46	67
3	D	975/1168 (84%)	928 (95%)	47 (5%)	25	53
3	I	972/1168 (83%)	944 (97%)	28 (3%)	42	65
4	E	74/75 (99%)	73 (99%)	1 (1%)	67	81
4	J	65/75 (87%)	65 (100%)	0	100	100
5	X	418/540 (77%)	409 (98%)	9 (2%)	52	71
5	Y	422/540 (78%)	409 (97%)	13 (3%)	40	63
All	All	6090/7024 (87%)	5909 (97%)	181 (3%)	41	64

5 of 181 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	884	SER
2	H	70	TYR
5	X	580	PHE
3	D	1193	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	E	80	LEU

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

Mol	Chain	Res	Type
1	G	37	HIS
2	H	688	GLN
4	J	31	GLN
1	G	84	ASN
1	G	227	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 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 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
6	QZY	D	1501	-	31,37,37	4.21	5 (16%)	36,50,50	1.77	6 (16%)

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	QZY	D	1501	-	-	4/20/26/26	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1501	QZY	C03-C02	21.50	1.59	1.39
6	D	1501	QZY	C03-C04	5.19	1.44	1.37
6	D	1501	QZY	C18-N02	4.83	1.45	1.36
6	D	1501	QZY	C18-N01	4.56	1.45	1.37
6	D	1501	QZY	O04-C18	-2.22	1.19	1.23

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1501	QZY	C03-C02-N01	-6.10	122.34	130.12
6	D	1501	QZY	N01-C18-N02	4.57	121.12	115.89
6	D	1501	QZY	C02-N01-C18	-4.37	114.21	125.52
6	D	1501	QZY	C09-O03-C12	-3.24	111.23	118.80
6	D	1501	QZY	C20-N02-C19	3.15	120.22	116.54

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	1501	QZY	C03-C04-C06-C11
6	D	1501	QZY	C03-C04-C06-C07
6	D	1501	QZY	C28-C19-N02-C18
6	D	1501	QZY	C28-C19-N02-C20

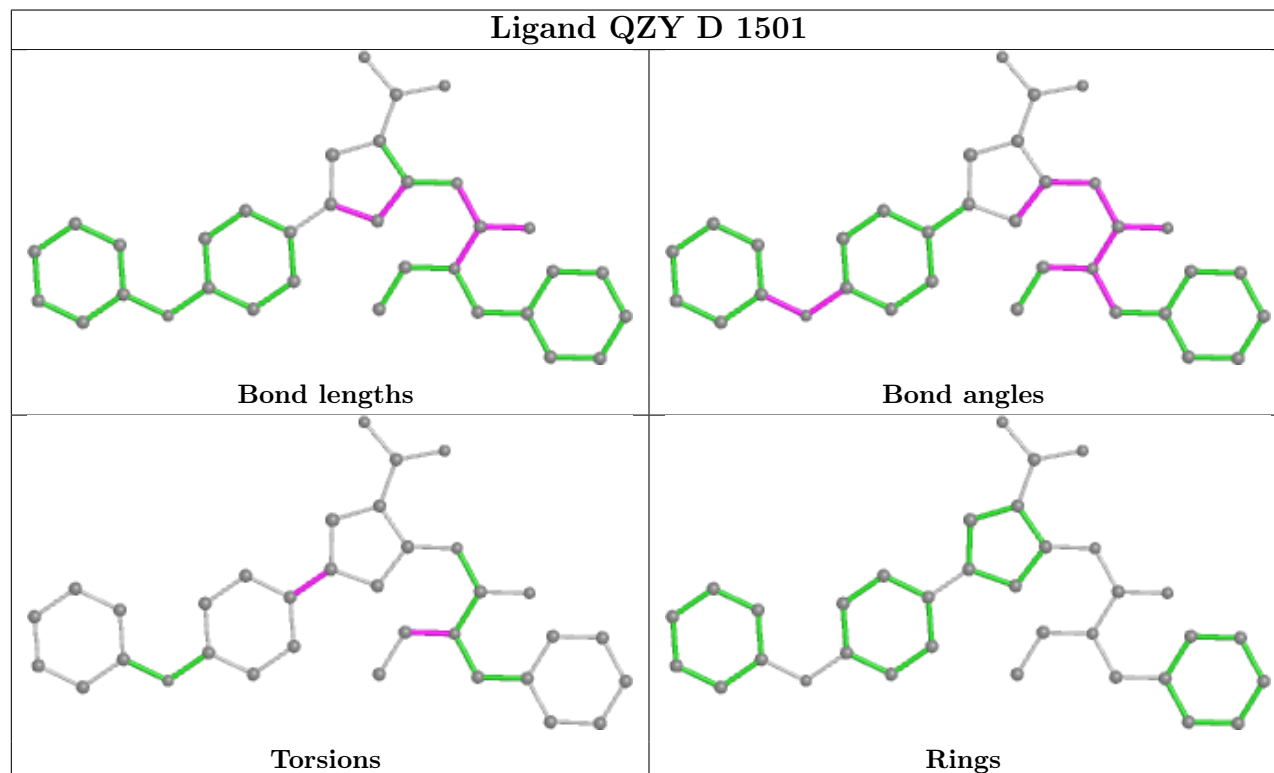
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	1501	QZY	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 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	2:GLN	C	3:GLY	N	3.61

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, 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	234/329 (71%)	-0.30	0 100 100	118, 170, 244, 287	0
1	B	301/329 (91%)	-0.20	2 (0%) 87 82	127, 224, 319, 341	0
1	F	234/329 (71%)	-0.00	6 (2%) 56 45	188, 241, 284, 351	0
1	G	229/329 (69%)	0.36	15 (6%) 18 14	199, 303, 339, 363	0
2	C	1336/1342 (99%)	-0.22	17 (1%) 77 68	95, 160, 263, 327	0
2	H	1336/1342 (99%)	-0.13	38 (2%) 53 42	137, 195, 310, 420	0
3	D	1164/1407 (82%)	-0.25	7 (0%) 89 84	90, 154, 258, 314	0
3	I	1160/1407 (82%)	-0.06	24 (2%) 63 54	130, 203, 302, 360	0
4	E	90/91 (98%)	-0.16	0 100 100	141, 198, 256, 300	0
4	J	76/91 (83%)	0.93	8 (10%) 6 6	277, 333, 432, 451	0
5	X	471/613 (76%)	-0.07	12 (2%) 57 47	135, 226, 364, 410	0
5	Y	475/613 (77%)	-0.05	11 (2%) 60 51	149, 240, 364, 395	0
All	All	7106/8222 (86%)	-0.12	140 (1%) 65 56	90, 194, 319, 451	0

The worst 5 of 140 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	2	GLN	6.9
2	H	982	GLY	5.9
3	I	11	GLN	5.8
1	F	3	GLY	5.7
2	H	981	ALA	5.5

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 [i](#)

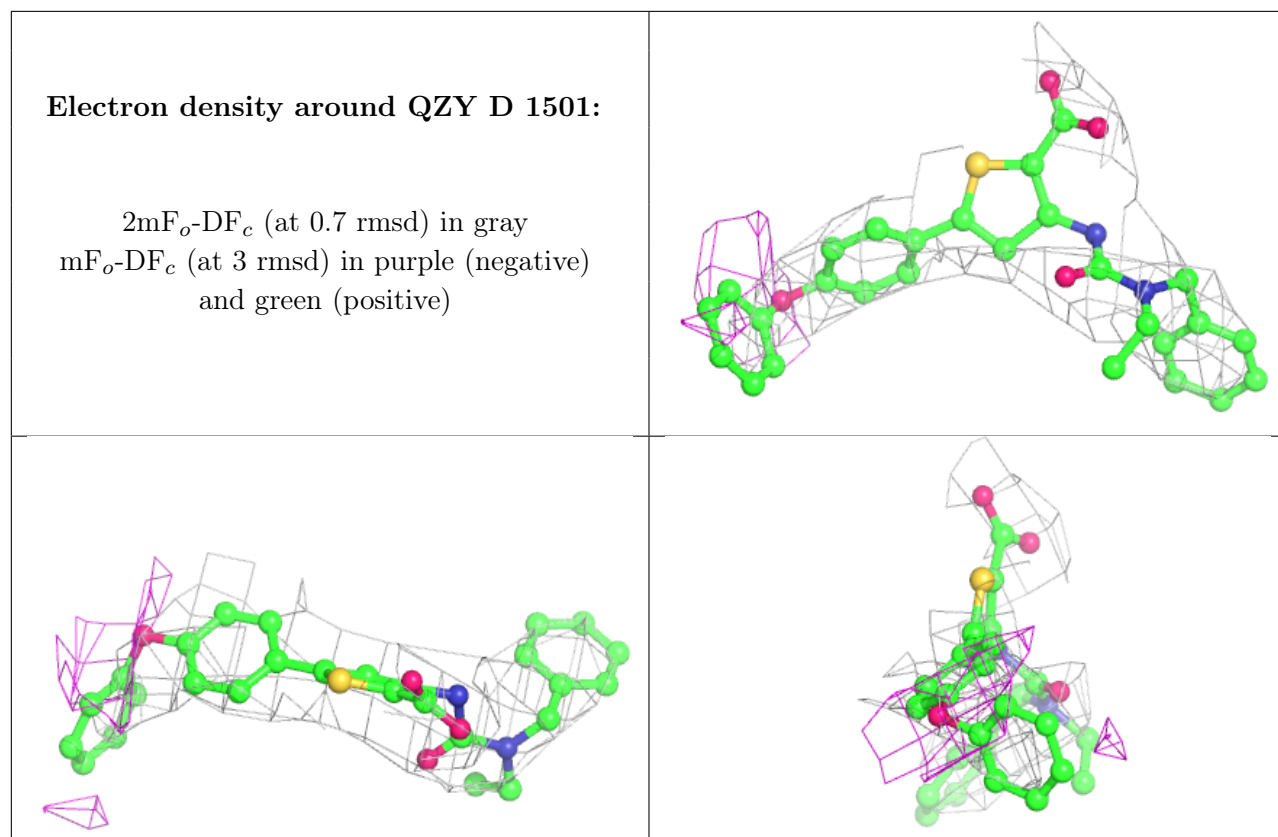
There are no monosaccharides in this entry.

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(\AA^2)	Q<0.9
6	QZY	D	1501	34/34	0.84	0.44	112,133,149,170	0
8	MG	I	1503	1/1	0.84	0.33	135,135,135,135	0
7	ZN	D	1503	1/1	0.96	0.37	179,179,179,179	0
7	ZN	I	1502	1/1	0.96	0.20	149,149,149,149	0
8	MG	D	1504	1/1	0.97	0.28	58,58,58,58	0
7	ZN	D	1502	1/1	0.97	0.12	171,171,171,171	0
7	ZN	I	1501	1/1	0.97	0.12	168,168,168,168	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.