



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 09:39 AM UTC

PDB ID : 6BYU / pdb_00006byu
Title : X-ray crystal structure of Escherichia coli RNA polymerase (RpoB-H526Y) and ppApp complex
Authors : Murakami, K.S.; Molodtsov, V.
Deposited on : 2017-12-21
Resolution : 3.60 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

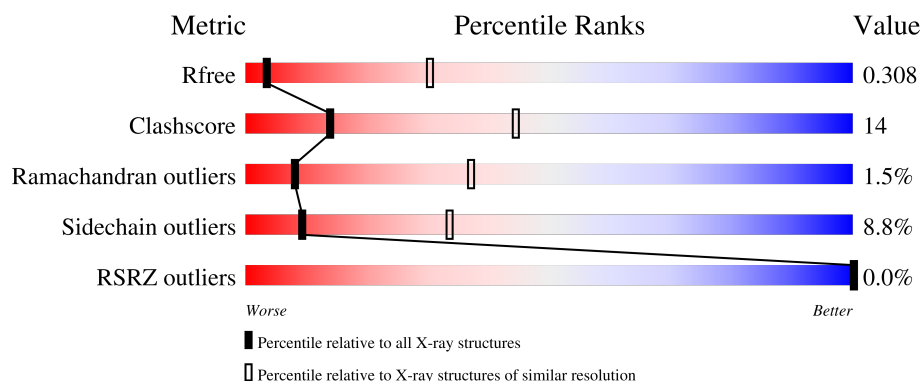
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	B	329	
1	G	329	
1	H	329	
2	C	1342	

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Mol	Chain	Length	Quality of chain
2	I	1342	63%32%5%
3	D	1407	51%27%5%17%
3	J	1407	51%27%.18%
4	E	91	64%32%. .
4	K	91	% 47%38%.13%
5	F	613	49%25%.24%
5	L	613	55%20%.23%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 54996 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	228	Total	C	N	O	S	0	0	0
			1768	1102	312	348	6			
1	B	217	Total	C	N	O	S	0	0	0
			1672	1044	295	327	6			
1	G	224	Total	C	N	O	S	0	0	0
			1730	1076	308	340	6			
1	H	217	Total	C	N	O	S	0	0	0
			1667	1041	293	327	6			

- 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	0	0	0
			10561	6626	1837	2055	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10557	6624	1836	2054	43			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	526	TYR	HIS	engineered mutation	UNP P0A8V2
I	526	TYR	HIS	engineered mutation	UNP P0A8V2

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1163	Total	C	N	O	S	0	0	0
			9063	5696	1622	1699	46			
3	J	1155	Total	C	N	O	S	0	0	0
			8998	5656	1612	1684	46			

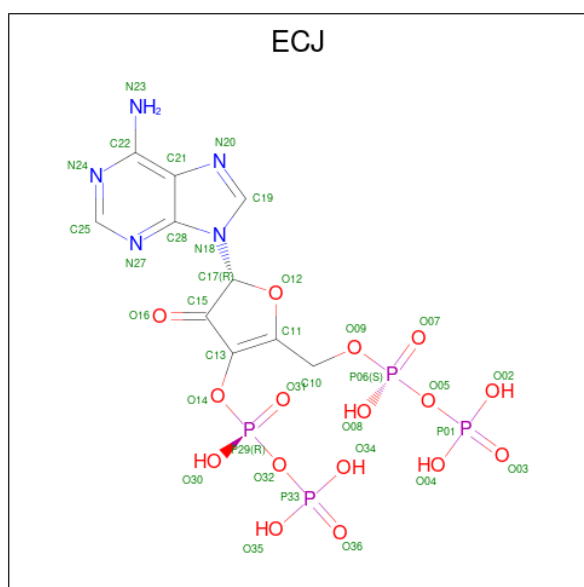
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	89	Total	C	N	O	S	0	0	0
			685	418	126	140	1			
4	K	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	467	Total	C	N	O	S	0	0	0
			3796	2379	677	717	23			
5	L	469	Total	C	N	O	S	0	0	0
			3796	2379	677	717	23			

- Molecule 6 is (5R)-5-(6-amino-9H-purin-9-yl)-2-([[(S)-hydroxy(phosphonooxy)phosphoryl]oxy}methyl)-4-oxo-4,5-dihydrofuran-3-yl trihydrogen diphosphate (CCD ID: ECJ) (formula: $C_{10}H_{13}N_5O_{16}P_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	P	0	0
			35	10	5	16	4		
6	J	1	Total	C	N	O	P	0	0
			35	10	5	16	4		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

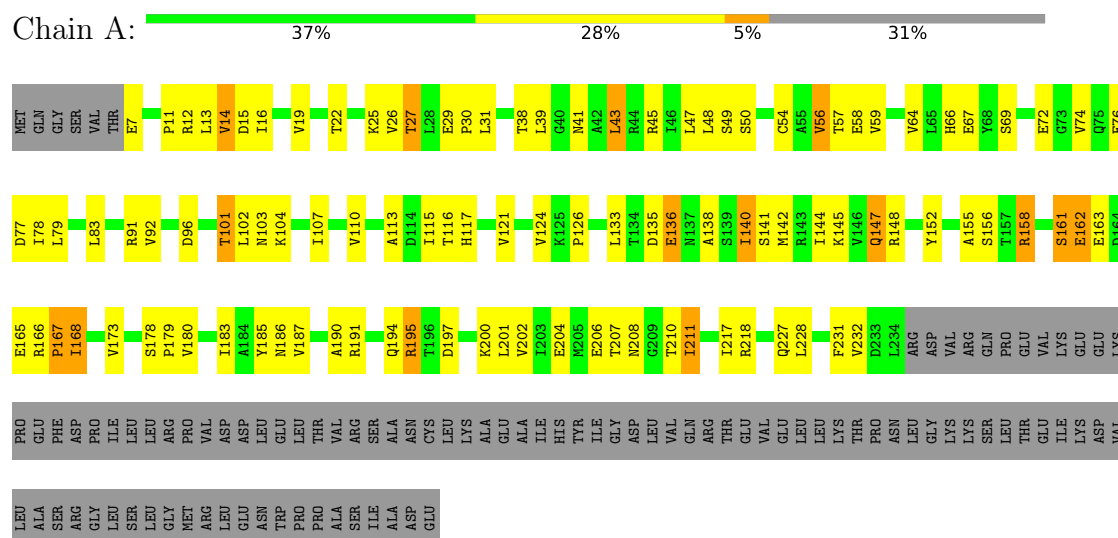
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

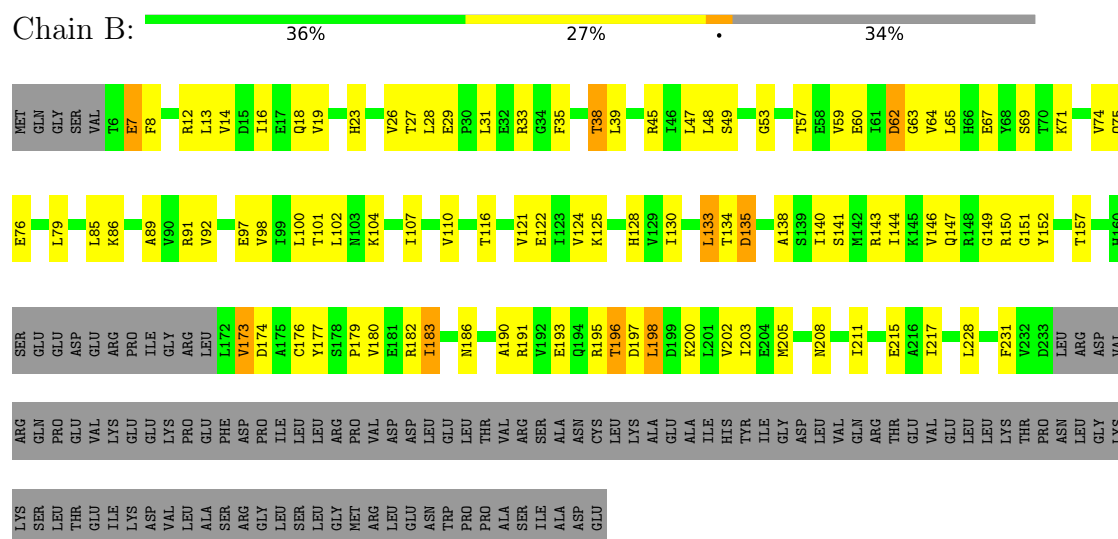
3 Residue-property plots

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

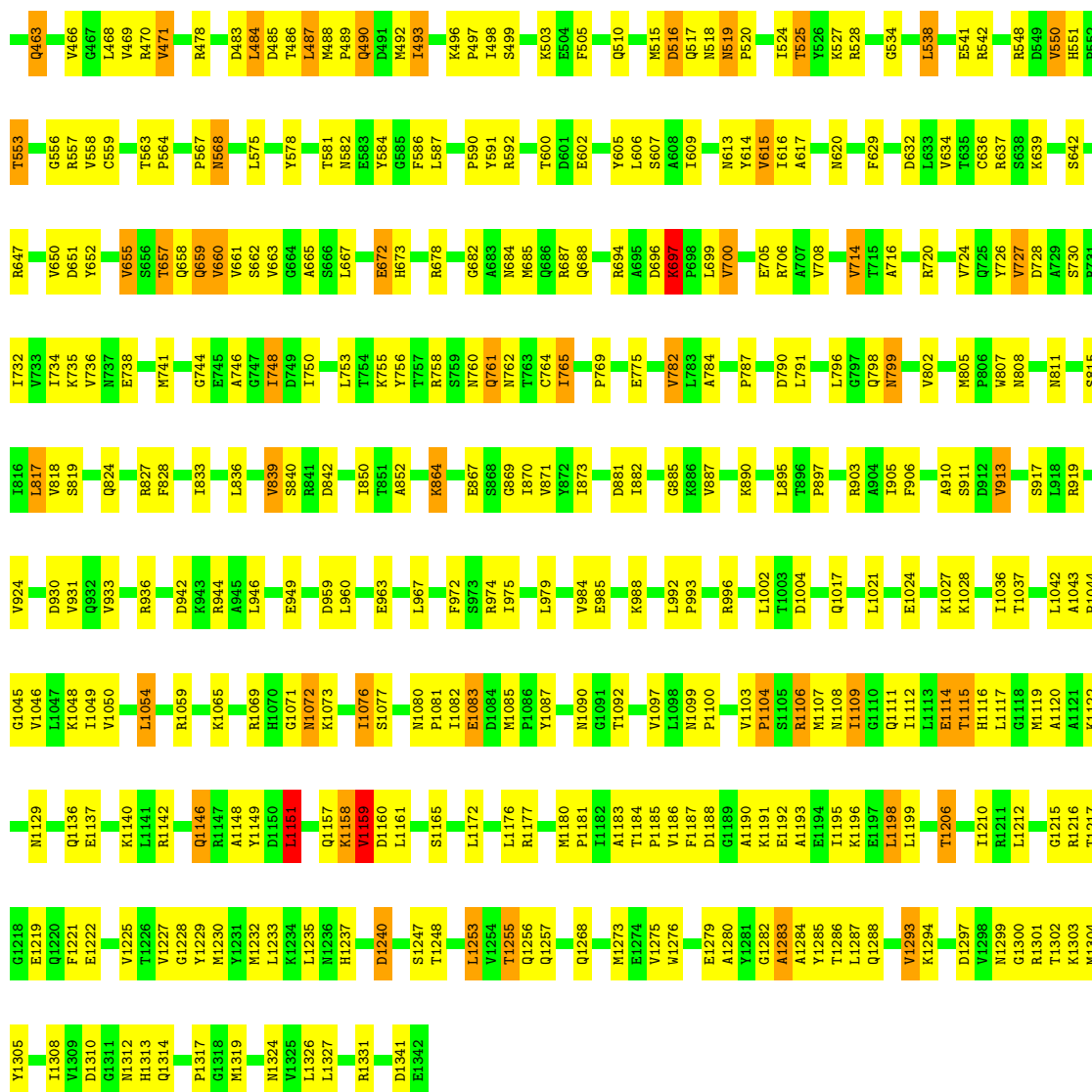


• Molecule 1: DNA-directed RNA polymerase subunit alpha



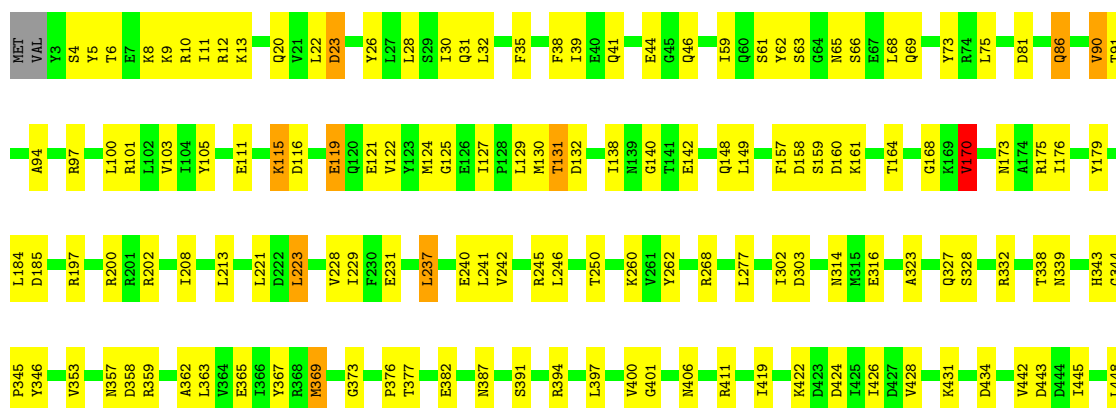
• Molecule 1: DNA-directed RNA polymerase subunit alpha

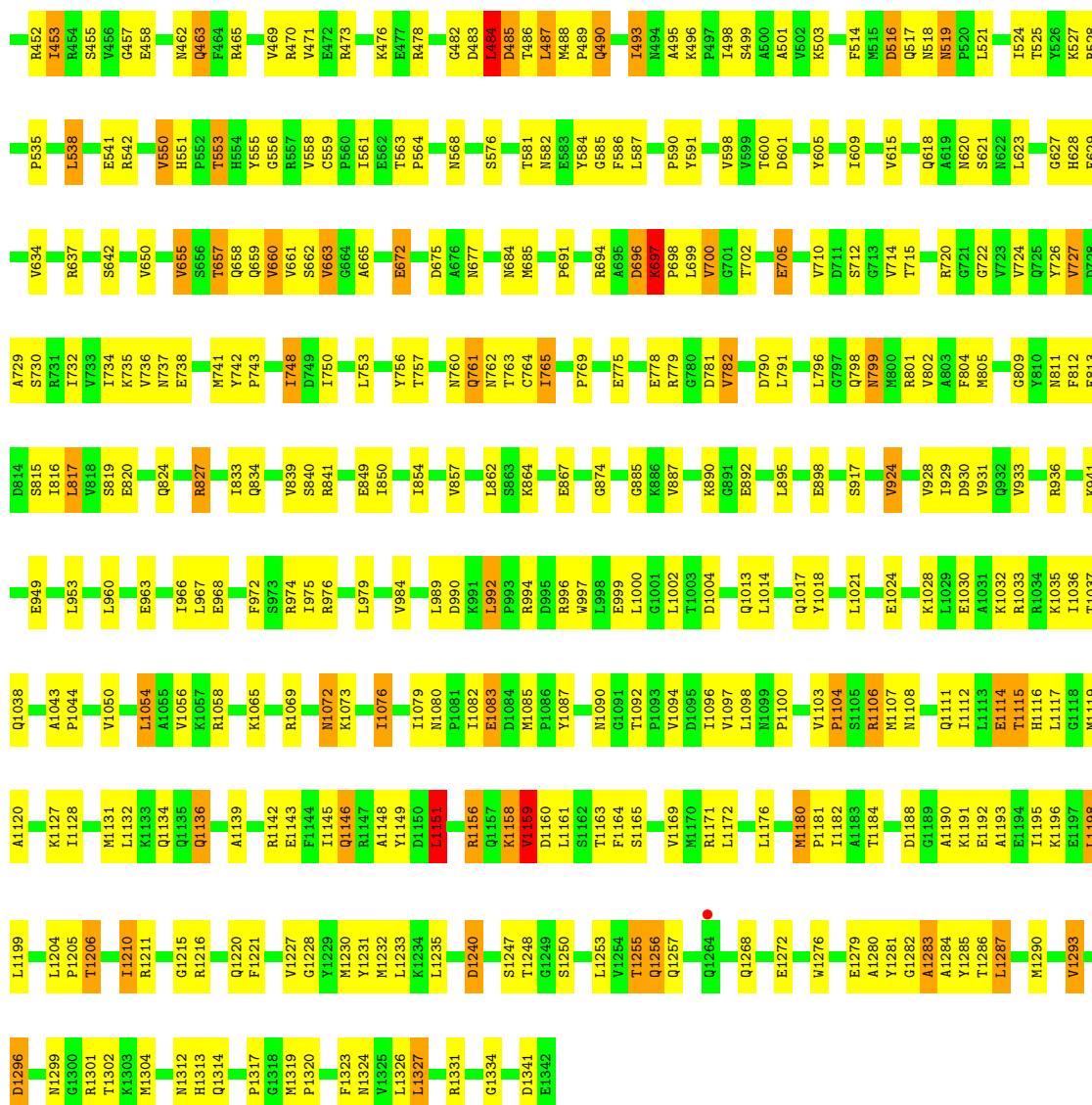




• Molecule 2: DNA-directed RNA polymerase subunit beta

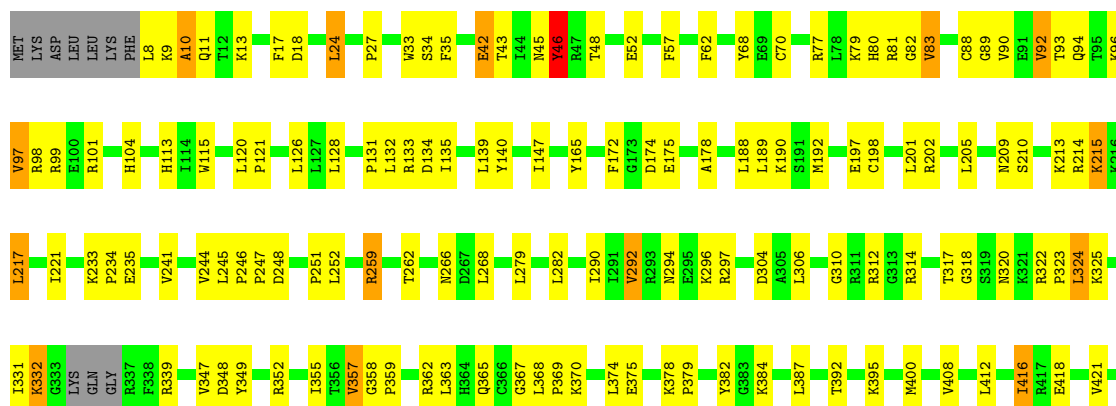
Chain I: 63% 32% 5%





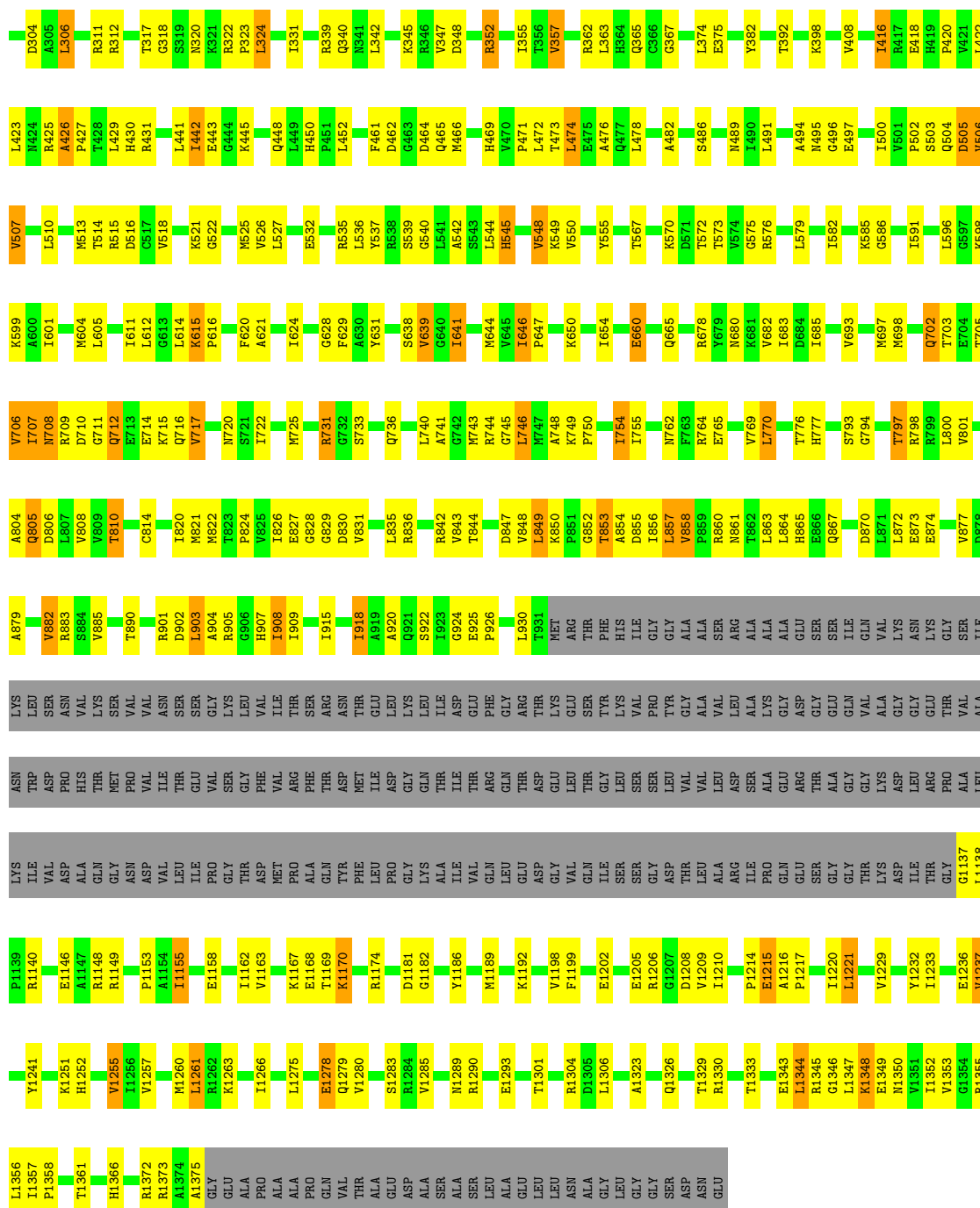
• Molecule 3: DNA-directed RNA polymerase subunit beta'

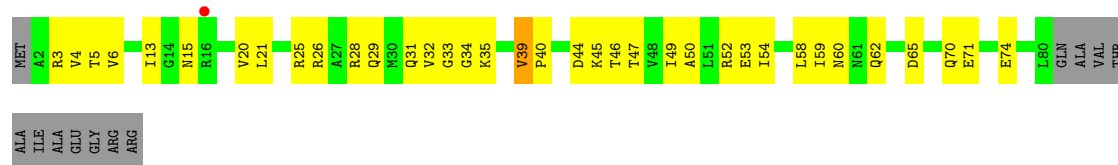
Chain D: 51% 27% 5% 17%





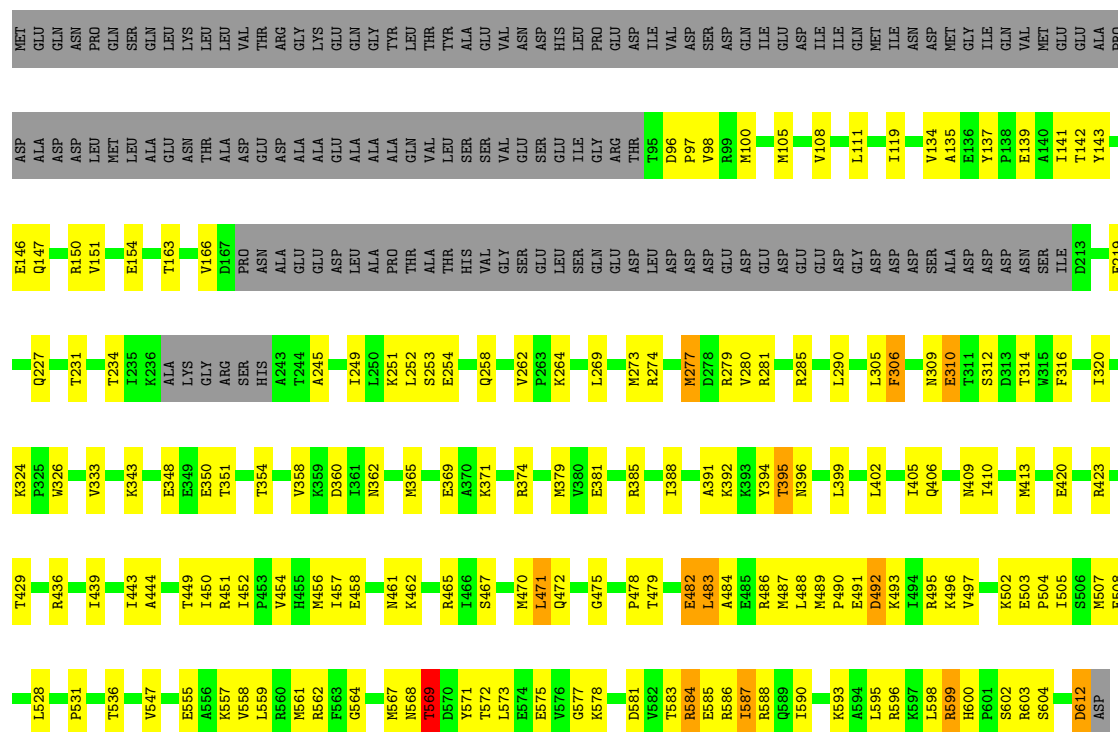
M192	M197	L201	L205	S210	K213	R214	K215	K216	L217	R220	I221	K222	N232	K233	P234	V241	L242	P243	L244	P246	P247	R250	P251	L252	V253	D256	T262	L265	D267	L268	V269	R270	R275	L279	L282	L283	I290	I291	V292	P298											
V97	R98	R101	H104	I105	E106		H113	T114	W115		P120	S122	R123	L126	L127	L128	P131	L132	R133	D134	I135		V138	L139	F140	F141	V145	V146	L147	E148		L154	E155	R156	I159	L160	T161		Q164		F172	G173	E174	E175	F176	D177	A178	M180		L189	
ASP	LEU	LVS	PHE	LEU	LVS	ALA	GLN	THR	LVS	THR	E16	F17	D18	L24	P27		R31		P41	E42		M45	R46	R47	T48		E52		F57		R60	I61	F62		C70	L71		R77	L78	K79	H80	G81	V83		C88	G89	V90	E91	V92	T93	Q94





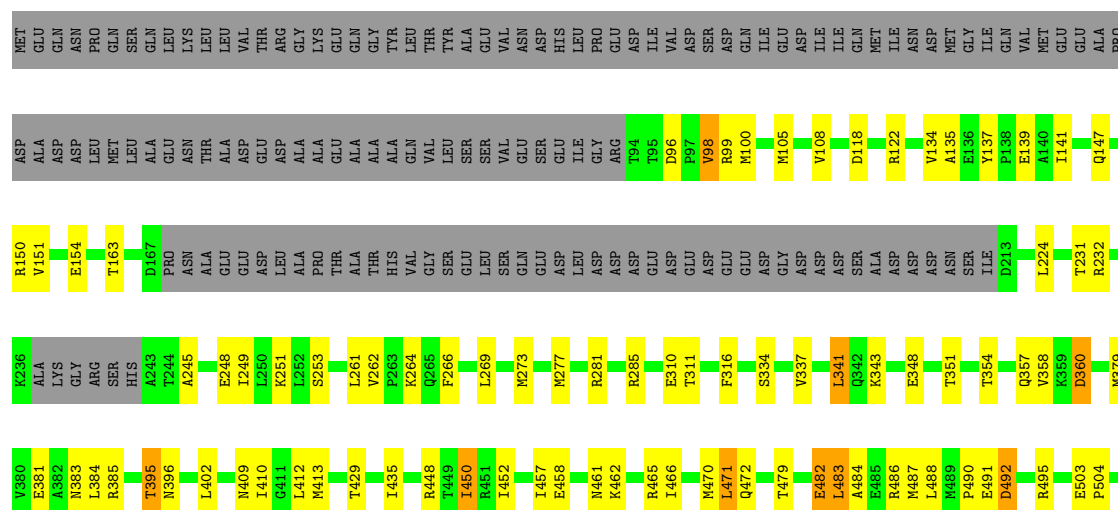
• Molecule 5: RNA polymerase sigma factor RpoD

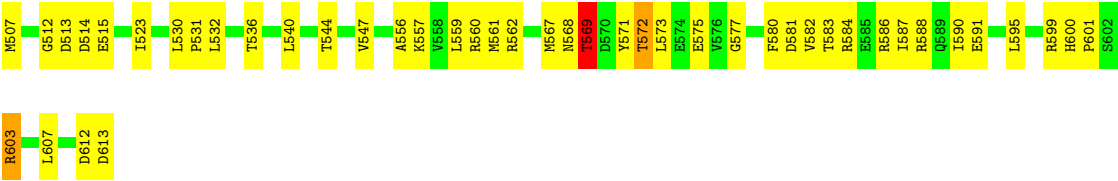
Chain F: 49% 25% • 24%



• Molecule 5: RNA polymerase sigma factor RpoD

Chain L: 55% 20% • 23%





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	186.25Å 203.66Å 308.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.60 30.00 – 3.60	Depositor EDS
% Data completeness (in resolution range)	98.5 (30.00-3.60) 98.3 (30.00-3.60)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 3.56Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.244 , 0.311 0.245 , 0.308	Depositor DCC
R_{free} test set	2000 reflections (1.47%)	wwPDB-VP
Wilson B-factor (Å ²)	119.5	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 121.6	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	0.94	EDS
Total number of atoms	54996	wwPDB-VP
Average B, all atoms (Å ²)	153.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% 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: ZN, ECJ, 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	0.20	0/1790	0.55	0/2426
1	B	0.18	0/1692	0.48	0/2293
1	G	0.20	0/1751	0.55	0/2373
1	H	0.19	0/1686	0.49	0/2285
2	C	0.16	0/10730	0.44	0/14479
2	I	0.15	0/10726	0.44	0/14474
3	D	0.17	0/9201	0.45	0/12420
3	J	0.16	0/9137	0.45	0/12337
4	E	0.18	0/687	0.47	0/928
4	K	0.14	0/629	0.44	0/847
5	F	0.15	0/3847	0.42	0/5171
5	L	0.15	0/3846	0.42	0/5171
All	All	0.16	0/55722	0.45	0/75204

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	1
2	I	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
2	C	1159	VAL	Peptide
2	I	1159	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	A	1768	0	1793	76	0
1	B	1672	0	1694	65	0
1	G	1730	0	1756	74	0
1	H	1667	0	1689	60	0
2	C	10561	0	10555	325	0
2	I	10557	0	10549	316	0
3	D	9063	0	9234	297	0
3	J	8998	0	9154	299	0
4	E	685	0	684	19	0
4	K	627	0	634	20	0
5	F	3796	0	3858	106	1
5	L	3796	0	3848	84	1
6	C	35	0	0	0	0
6	J	35	0	0	1	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	54996	0	55448	1588	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

The worst 5 of 1588 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)
1:G:45:ARG:HG2	1:H:38:THR:HB	1.49	0.94
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.51	0.92
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.53	0.91
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:418:GLU:HG3	4:E:45:LYS:H	1.42	0.85

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:219:GLU:OE1	5:L:232:ARG:NH2[1_565]	2.18	0.02

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	226/329 (69%)	202 (89%)	16 (7%)	8 (4%)	3	23
1	B	213/329 (65%)	195 (92%)	16 (8%)	2 (1%)	14	46
1	G	222/329 (68%)	196 (88%)	20 (9%)	6 (3%)	4	27
1	H	213/329 (65%)	194 (91%)	17 (8%)	2 (1%)	14	46
2	C	1338/1342 (100%)	1203 (90%)	114 (8%)	21 (2%)	7	36
2	I	1338/1342 (100%)	1203 (90%)	112 (8%)	23 (2%)	7	35
3	D	1157/1407 (82%)	1038 (90%)	101 (9%)	18 (2%)	7	36
3	J	1151/1407 (82%)	1036 (90%)	100 (9%)	15 (1%)	9	39
4	E	87/91 (96%)	81 (93%)	4 (5%)	2 (2%)	5	30
4	K	77/91 (85%)	72 (94%)	4 (5%)	1 (1%)	9	39
5	F	461/613 (75%)	432 (94%)	25 (5%)	4 (1%)	14	46
5	L	463/613 (76%)	426 (92%)	33 (7%)	4 (1%)	14	46
All	All	6946/8222 (84%)	6278 (90%)	562 (8%)	106 (2%)	8	37

5 of 106 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	PRO
1	A	195	ARG
2	C	62	TYR
2	C	170	VAL
2	C	516	ASP

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	196/286 (68%)	177 (90%)	19 (10%)	8	31
1	B	184/286 (64%)	167 (91%)	17 (9%)	8	33
1	G	191/286 (67%)	178 (93%)	13 (7%)	14	42
1	H	183/286 (64%)	165 (90%)	18 (10%)	7	31
2	C	1152/1157 (100%)	1049 (91%)	103 (9%)	9	33
2	I	1151/1157 (100%)	1041 (90%)	110 (10%)	8	32
3	D	968/1168 (83%)	875 (90%)	93 (10%)	8	32
3	J	959/1168 (82%)	868 (90%)	91 (10%)	8	32
4	E	71/75 (95%)	66 (93%)	5 (7%)	14	41
4	K	67/75 (89%)	62 (92%)	5 (8%)	12	39
5	F	413/540 (76%)	389 (94%)	24 (6%)	18	46
5	L	410/540 (76%)	384 (94%)	26 (6%)	16	44
All	All	5945/7024 (85%)	5421 (91%)	524 (9%)	9	33

5 of 524 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	770	LEU
3	J	1155	ILE
3	J	769	VAL
5	L	599	ARG
3	D	720	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 111 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	464	ASN
5	L	461	ASN
2	I	613	ASN
5	L	446	GLN
3	J	762	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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	ECJ	C	1401	-	32,37,37	2.95	10 (31%)	42,59,59	3.00	12 (28%)
6	ECJ	J	1501	-	32,37,37	2.94	9 (28%)	42,59,59	3.30	12 (28%)

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	ECJ	C	1401	-	-	5/25/43/43	0/3/3/3
6	ECJ	J	1501	-	-	5/25/43/43	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1401	ECJ	O16-C15	9.99	1.39	1.22
6	J	1501	ECJ	O16-C15	9.86	1.39	1.22
6	C	1401	ECJ	C13-C11	7.23	1.49	1.35
6	J	1501	ECJ	C13-C11	7.10	1.49	1.35
6	J	1501	ECJ	P29-O32	5.86	1.65	1.59

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	1501	ECJ	O16-C15-C13	-13.92	109.93	126.89
6	C	1401	ECJ	O16-C15-C13	-12.82	111.27	126.89
6	J	1501	ECJ	C15-C13-C11	-8.53	100.82	109.40
6	C	1401	ECJ	C15-C13-C11	-7.30	102.06	109.40
6	J	1501	ECJ	C21-C28-N27	-5.99	118.46	126.72

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1401	ECJ	O09-C10-C11-C13
6	J	1501	ECJ	O09-C10-C11-C13
6	J	1501	ECJ	P01-O05-P06-O09
6	J	1501	ECJ	C10-O09-P06-O05
6	J	1501	ECJ	C10-O09-P06-O08

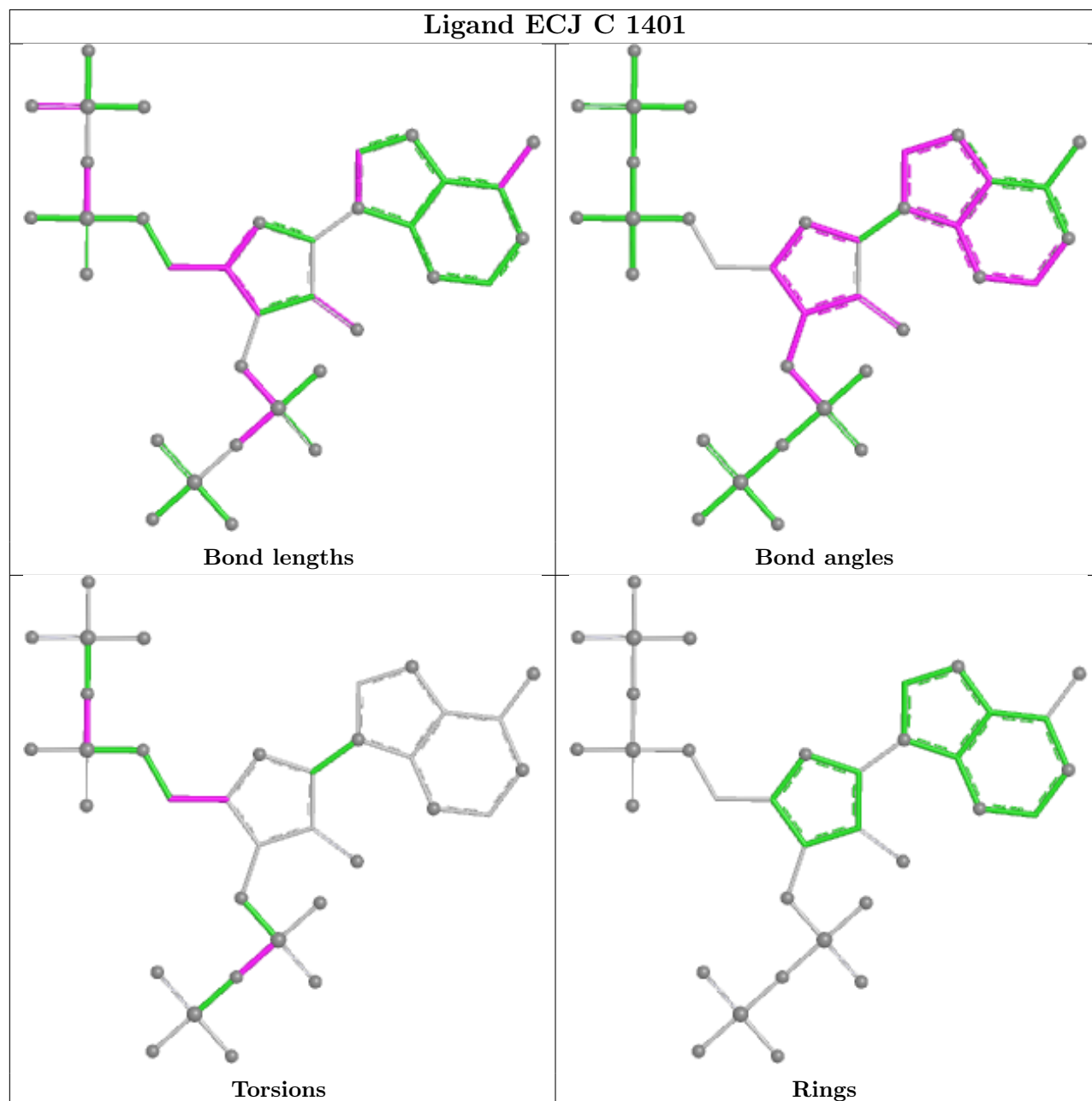
There are no ring outliers.

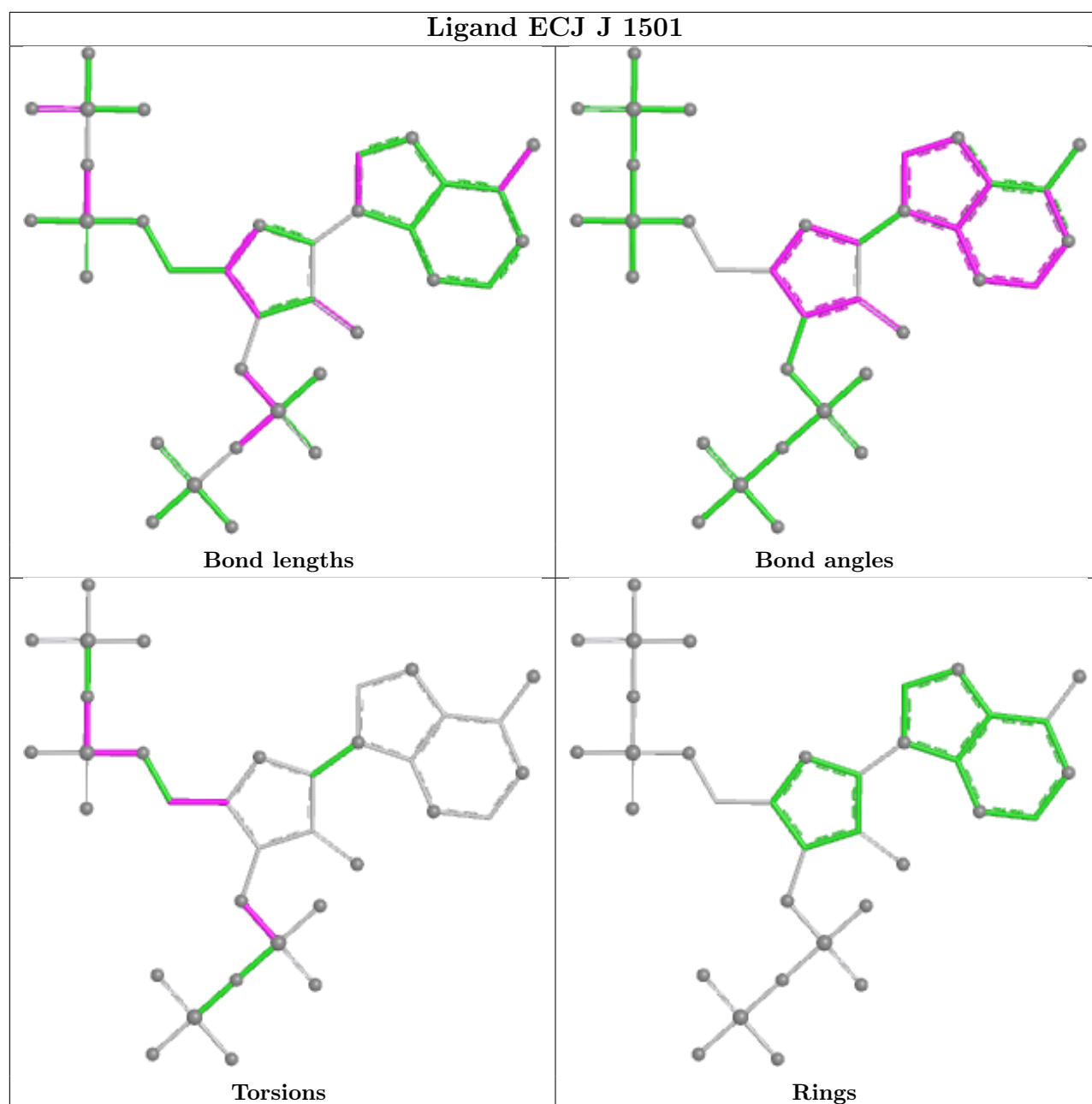
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	1501	ECJ	1	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	A	228/329 (69%)	-0.61	0 100 100	90, 124, 199, 234	0
1	B	217/329 (65%)	-0.48	0 100 100	85, 176, 231, 252	0
1	G	224/329 (68%)	-0.53	0 100 100	137, 176, 229, 280	0
1	H	217/329 (65%)	-0.43	0 100 100	150, 198, 235, 274	0
2	C	1340/1342 (99%)	-0.55	0 100 100	67, 119, 204, 265	0
2	I	1340/1342 (99%)	-0.53	1 (0%) 92 85	100, 147, 231, 373	0
3	D	1163/1407 (82%)	-0.56	1 (0%) 92 85	63, 114, 199, 265	0
3	J	1155/1407 (82%)	-0.54	0 100 100	82, 145, 217, 279	0
4	E	89/91 (97%)	-0.46	0 100 100	107, 148, 174, 186	0
4	K	79/91 (86%)	-0.35	1 (1%) 75 48	182, 265, 298, 321	0
5	F	467/613 (76%)	-0.49	0 100 100	97, 182, 330, 392	0
5	L	469/613 (76%)	-0.54	0 100 100	121, 192, 300, 372	0
All	All	6988/8222 (84%)	-0.53	3 (0%) 100 100	63, 145, 240, 392	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	K	16	ARG	2.6
2	I	1264	GLN	2.3
3	D	898	CYS	2.2

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

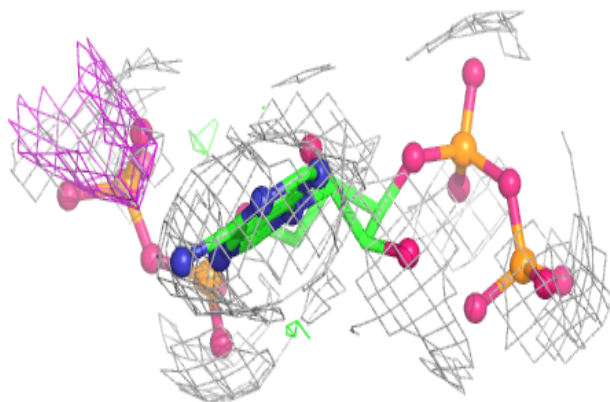
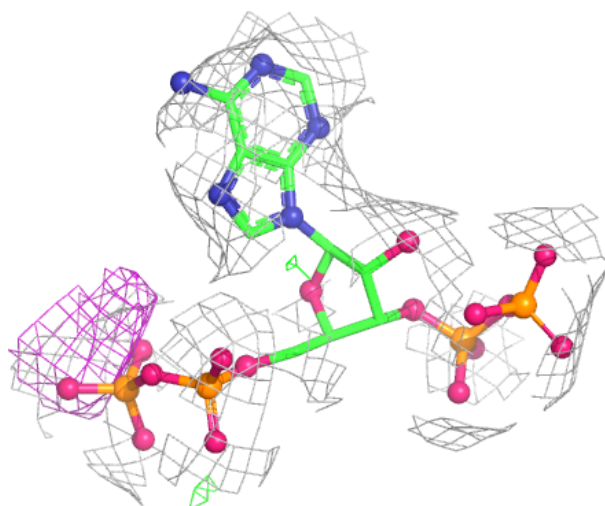
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	ECJ	J	1501	35/35	0.84	0.08	63,90,174,177	35
8	ZN	D	2003	1/1	0.86	0.31	377,377,377,377	0
6	ECJ	C	1401	35/35	0.89	0.08	74,99,183,185	35
7	MG	J	1502	1/1	0.96	0.05	81,81,81,81	0
8	ZN	D	2002	1/1	0.99	0.06	152,152,152,152	0
7	MG	D	2001	1/1	0.99	0.03	47,47,47,47	0
8	ZN	J	1504	1/1	0.99	0.03	128,128,128,128	0
8	ZN	J	1503	1/1	1.00	0.01	155,155,155,155	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.

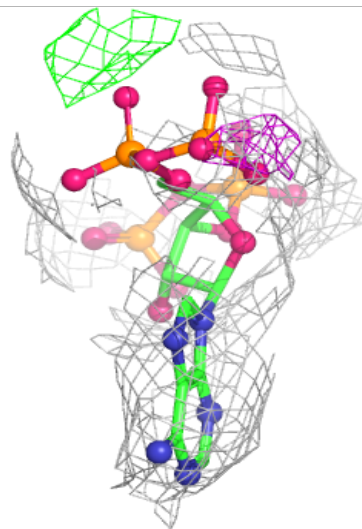
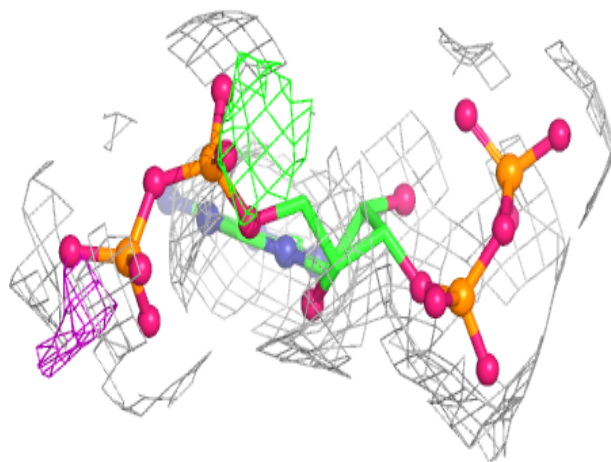
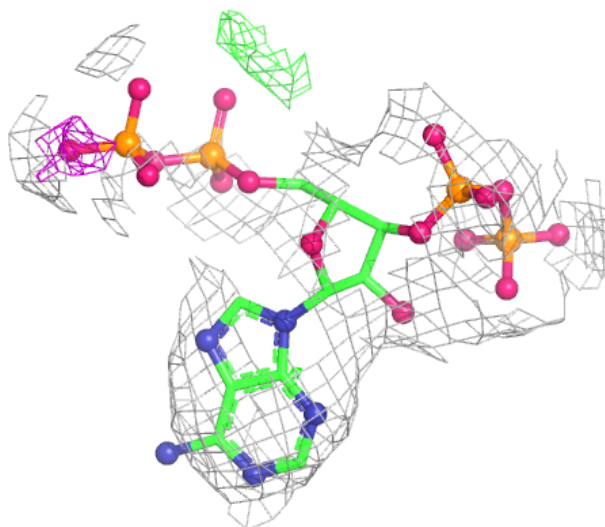
Electron density around ECJ J 1501:

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



Electron density around ECJ C 1401:

$2mF_o-DF_c$ (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.