



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 24, 2023 – 07:31 AM EDT

PDB ID : 5UAH
Title : Escherichia coli RNA polymerase and Rifampin complex, RpoB D516V mutant
Authors : Molodtsov, V.; Scharf, N.T.; Stefan, M.A.; Garcia, G.A.; Murakami, K.S.
Deposited on : 2016-12-19
Resolution : 4.10 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 : 4.02b-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

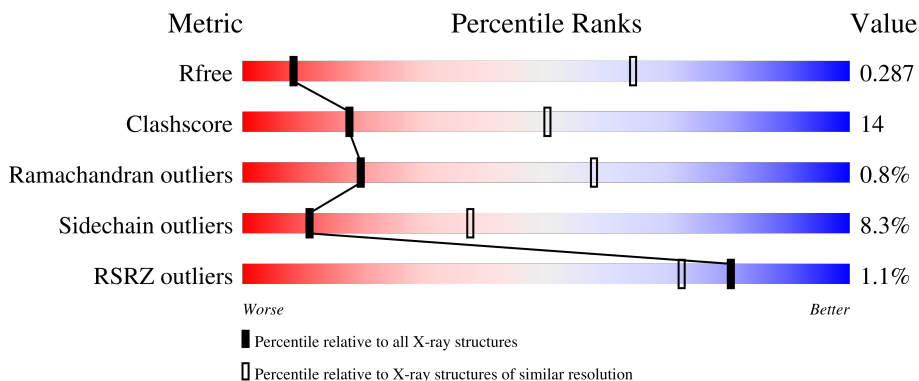
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 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	1193 (4.50-3.70)
Clashscore	141614	1003 (4.44-3.76)
Ramachandran outliers	138981	1005 (4.48-3.72)
Sidechain outliers	138945	1199 (4.50-3.70)
RSRZ outliers	127900	1034 (4.50-3.70)

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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	I	1342	
3	D	1407	
3	J	1407	
4	E	91	
4	K	91	
5	F	613	
5	L	613	

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
7	MG	C	3002	-	-	-	X
7	MG	I	1401	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 55125 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
			Total	C	N	O	S			
1	A	233	Total 1812	C 1127	N 323	O 356	S 6	0	0	0
1	B	217	Total 1677	C 1047	N 295	O 329	S 6	0	0	0
1	G	227	Total 1755	C 1093	N 311	O 345	S 6	0	0	0
1	H	216	Total 1662	C 1038	N 292	O 326	S 6	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	1340	Total 10569	C 6632	N 1841	O 2053	S 43	0	0	0
2	I	1340	Total 10565	C 6630	N 1840	O 2052	S 43	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	516	VAL	ASP	engineered mutation	UNP P0A8V2
I	516	VAL	ASP	engineered mutation	UNP P0A8V2

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	1167	Total 9065	C 5700	N 1622	O 1697	S 46	0	0	0
3	J	1155	Total 9001	C 5659	N 1612	O 1684	S 46	0	0	0

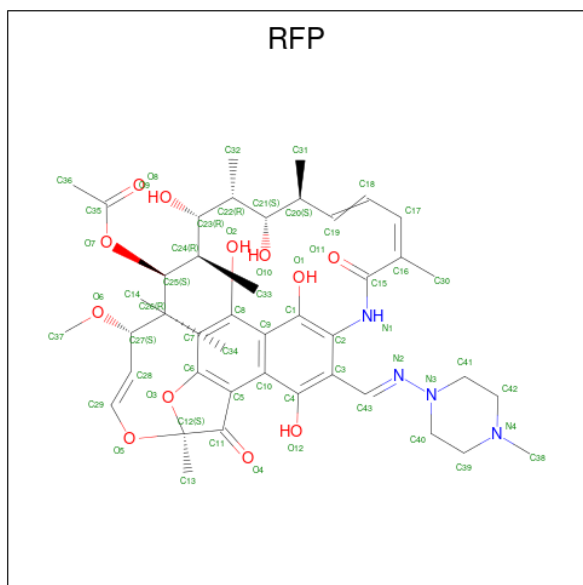
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	89	Total 691	C 421	N 129	O 140	S 1	0	0	0
4	K	79	Total 627	C 382	N 118	O 126	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	468	Total 3813	C 2389	N 678	O 723	S 23	0	0	0
5	L	469	Total 3821	C 2393	N 679	O 726	S 23	0	0	0

- Molecule 6 is RIFAMPICIN (three-letter code: RFP) (formula: $C_{43}H_{58}N_4O_{12}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	C	1	Total 59	C 43	N 4	O 12	0	0

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

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

Continued on next page...

Continued from previous page...

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

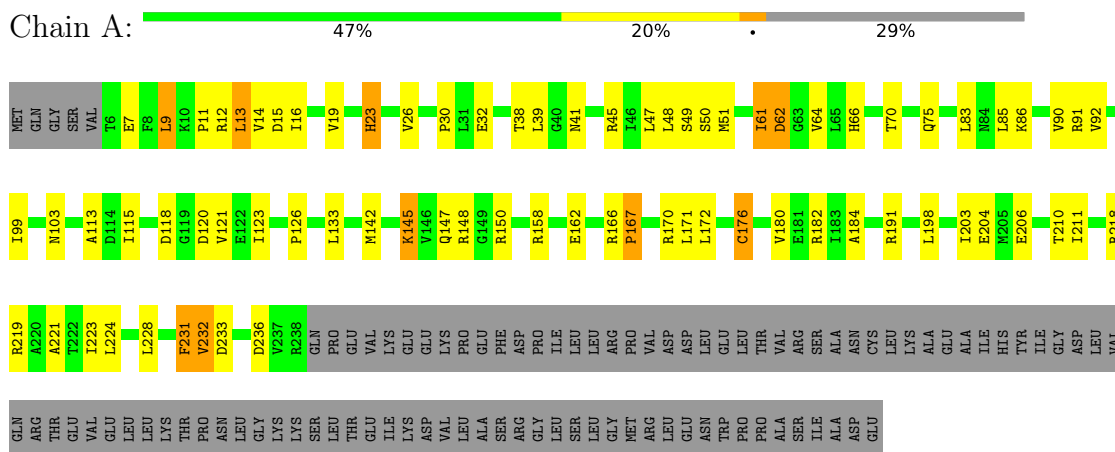
- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

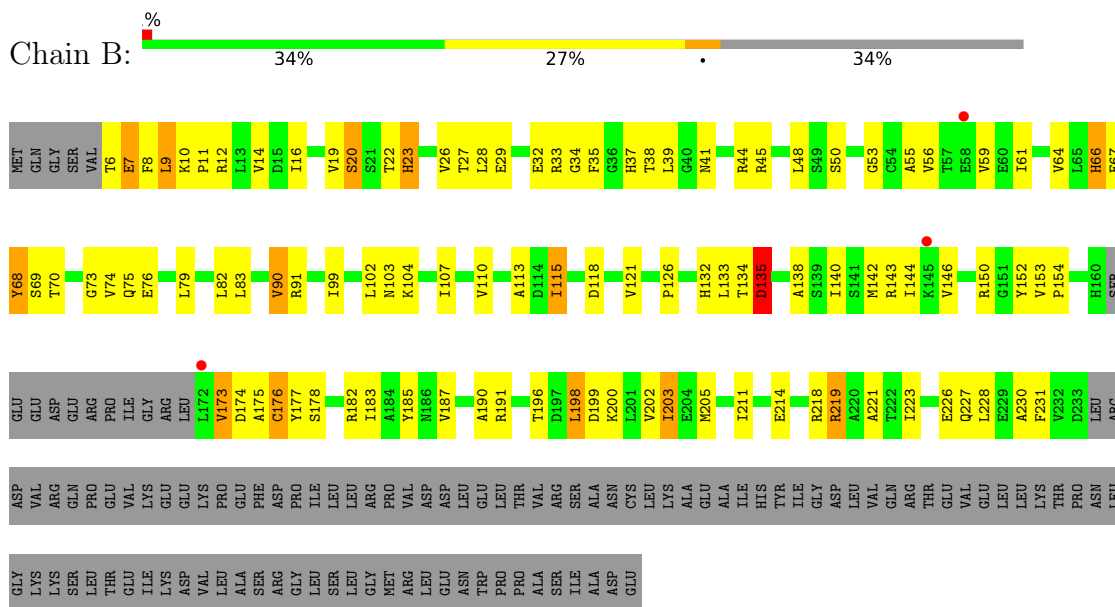
3 Residue-property plots [i](#)

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: DNA-directed RNA polymerase subunit alpha

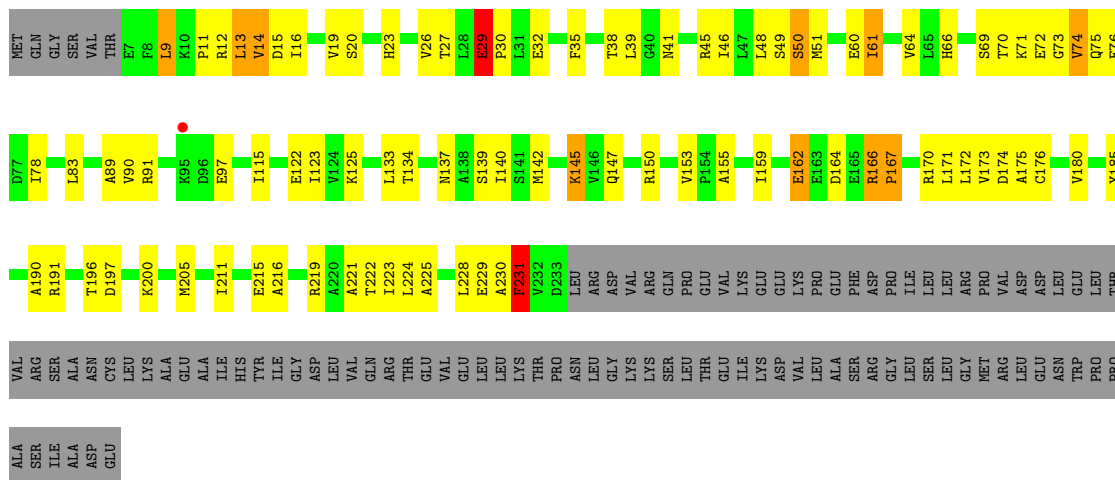


- Molecule 1: DNA-directed RNA polymerase subunit alpha

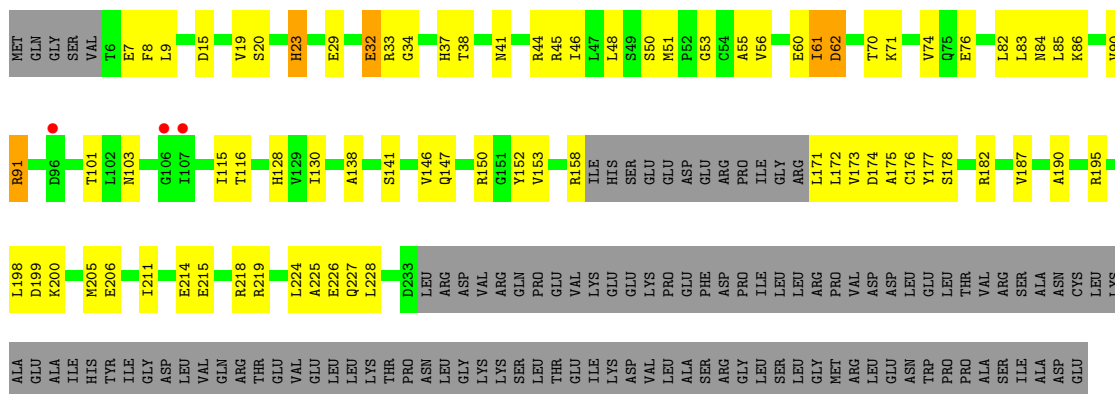
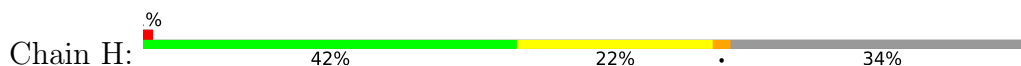


- Molecule 1: DNA-directed RNA polymerase subunit alpha

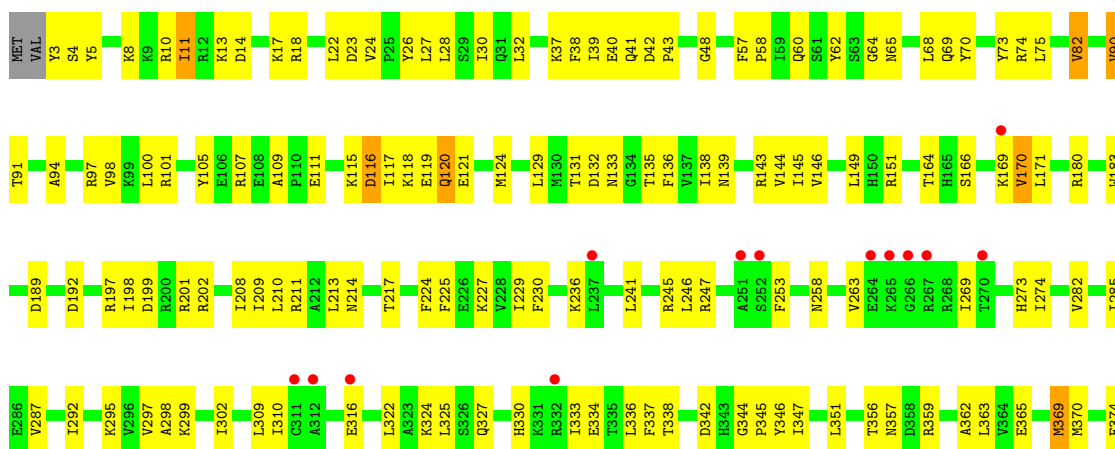


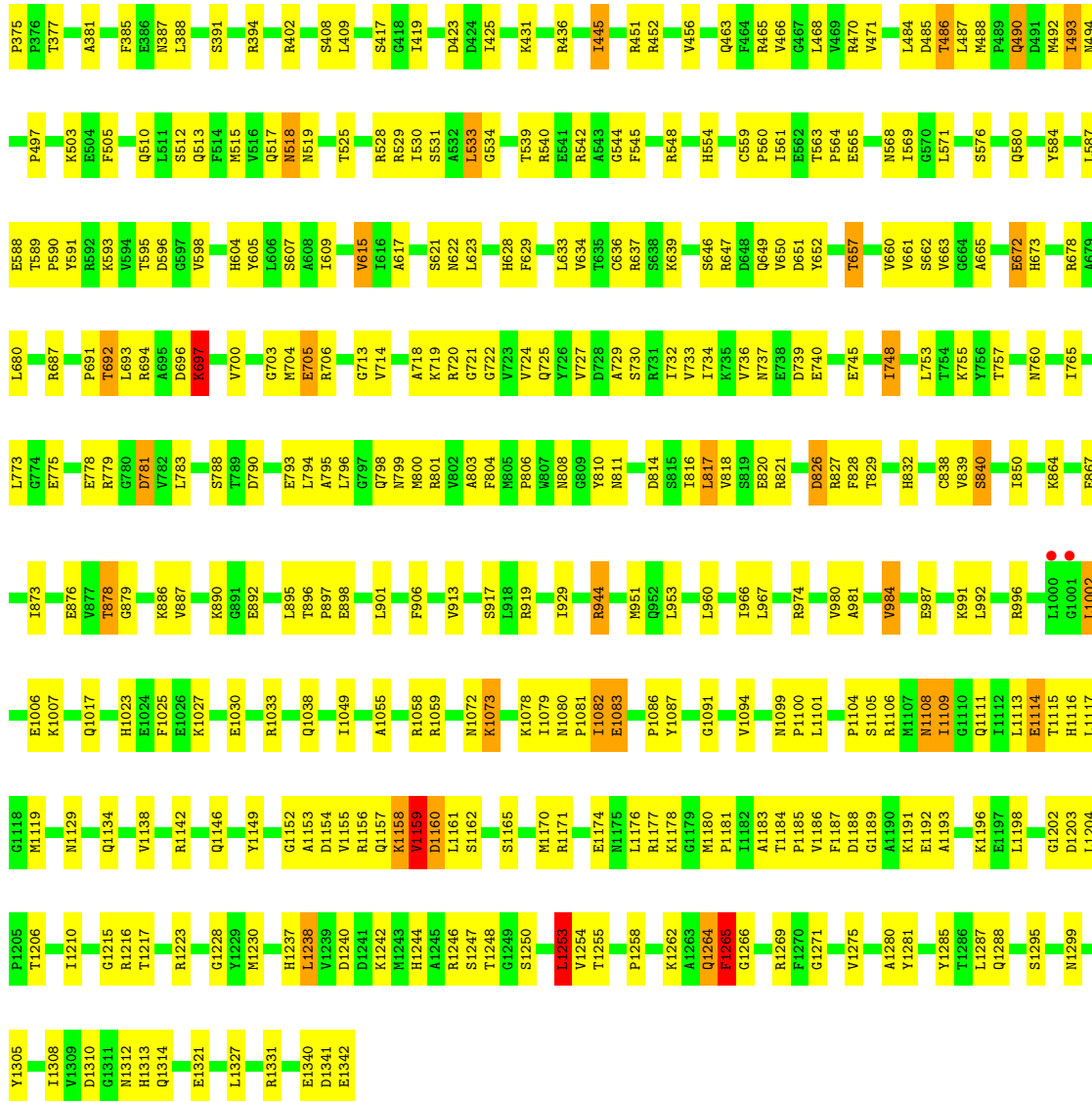


• Molecule 1: DNA-directed RNA polymerase subunit alpha

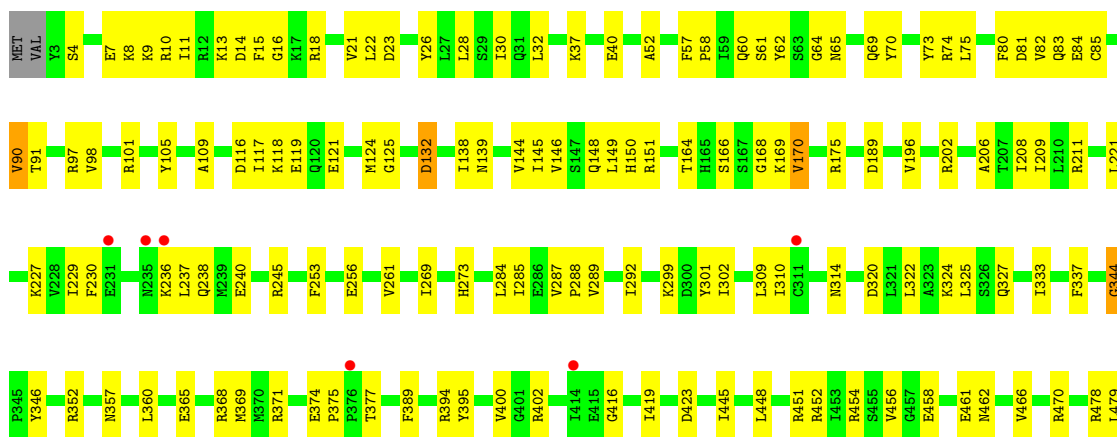


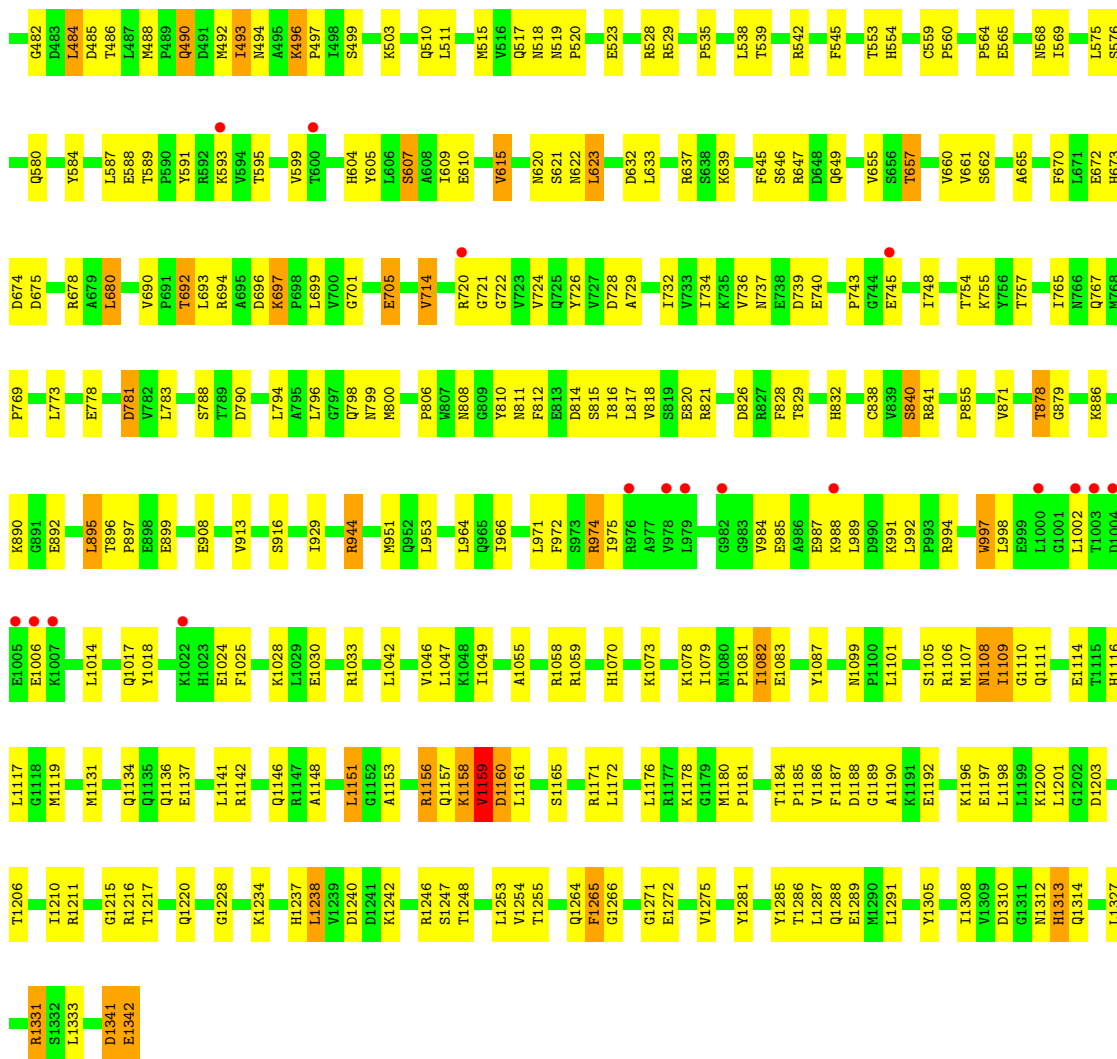
• Molecule 2: DNA-directed RNA polymerase subunit beta





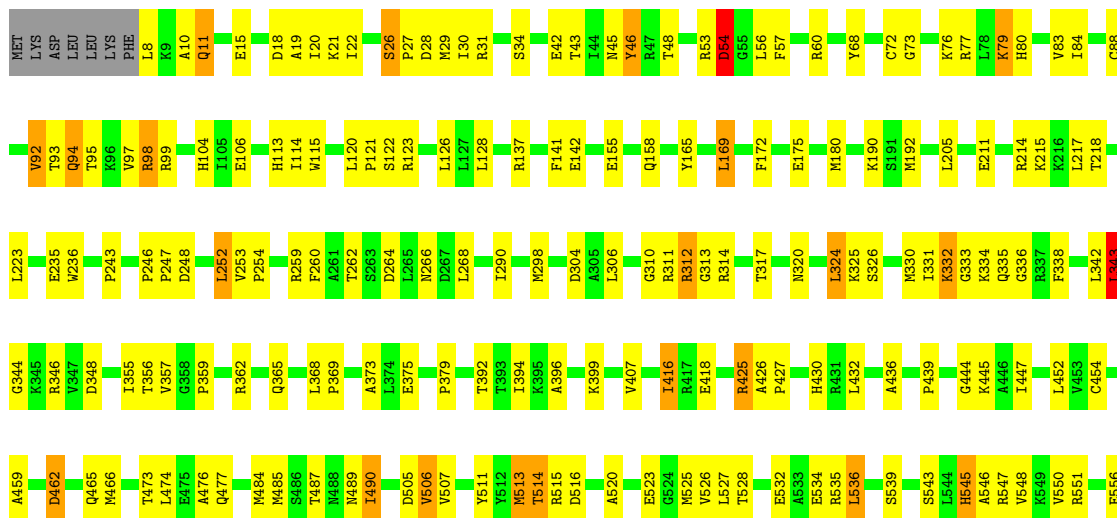
● Molecule 2: DNA-directed RNA polymerase subunit beta

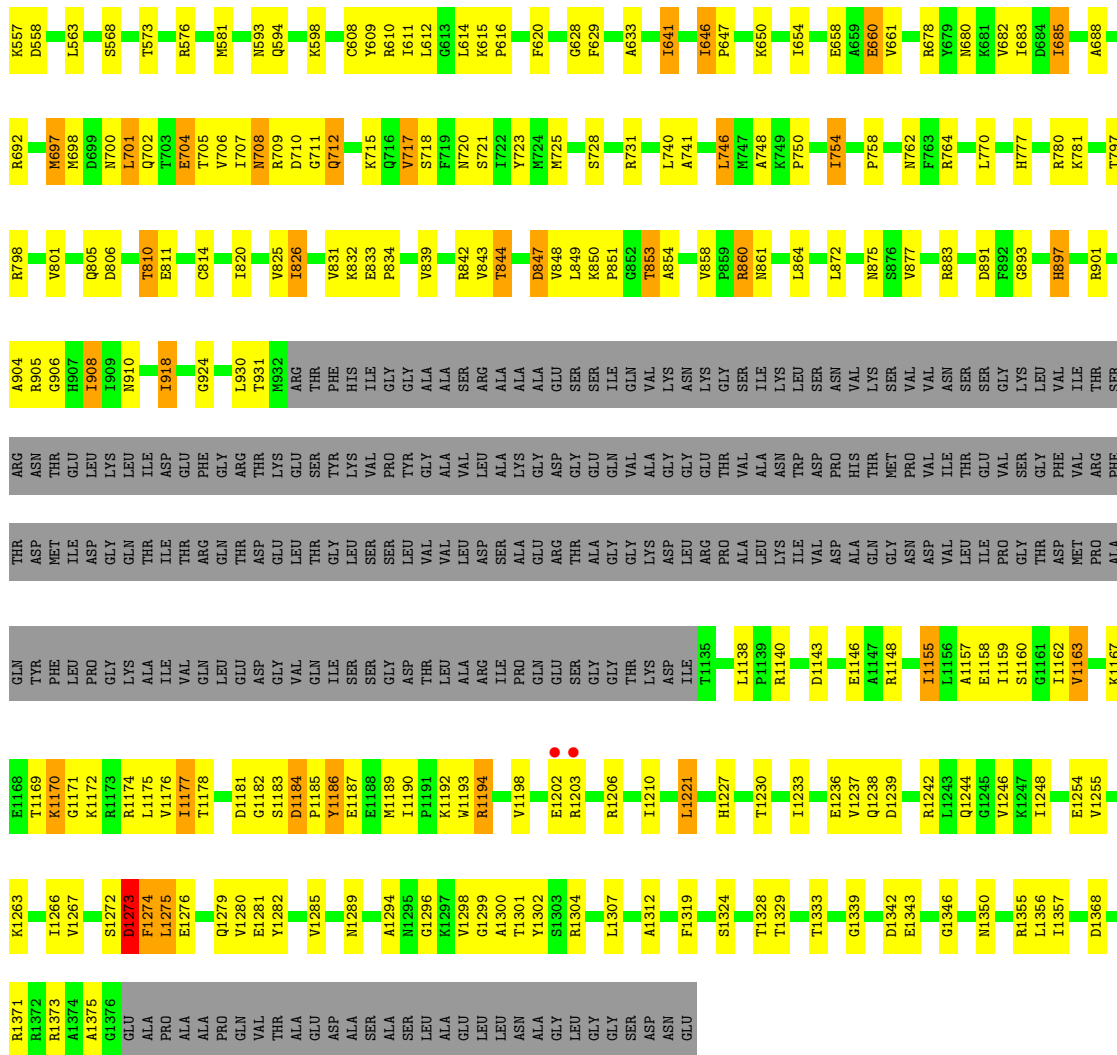




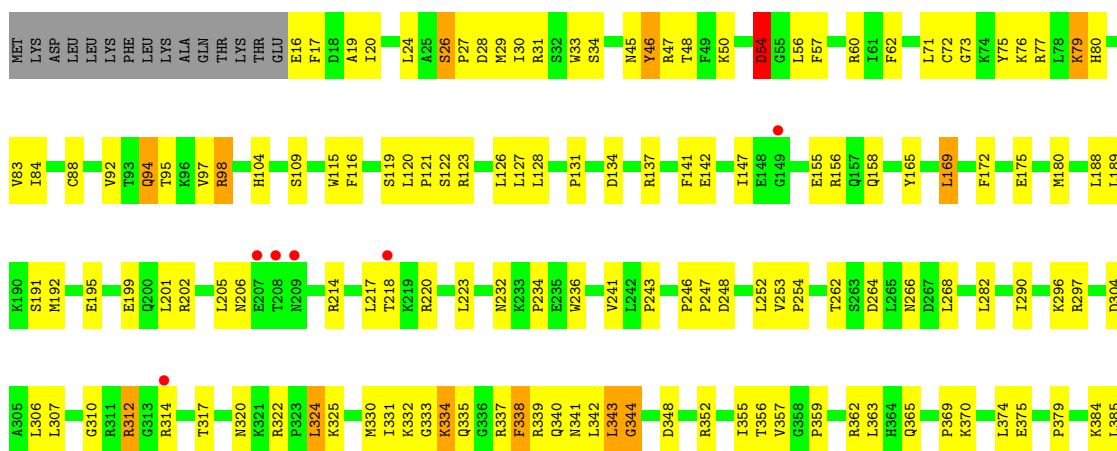
● Molecule 3: DNA-directed RNA polymerase subunit beta'

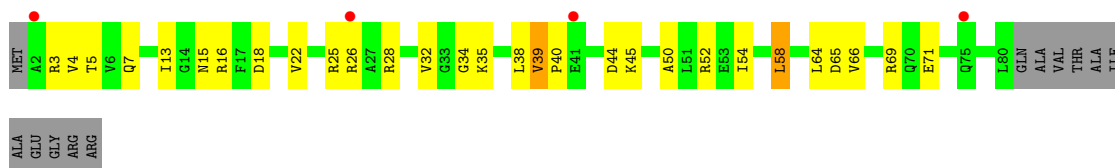
Chain D: 55% 24% 17%



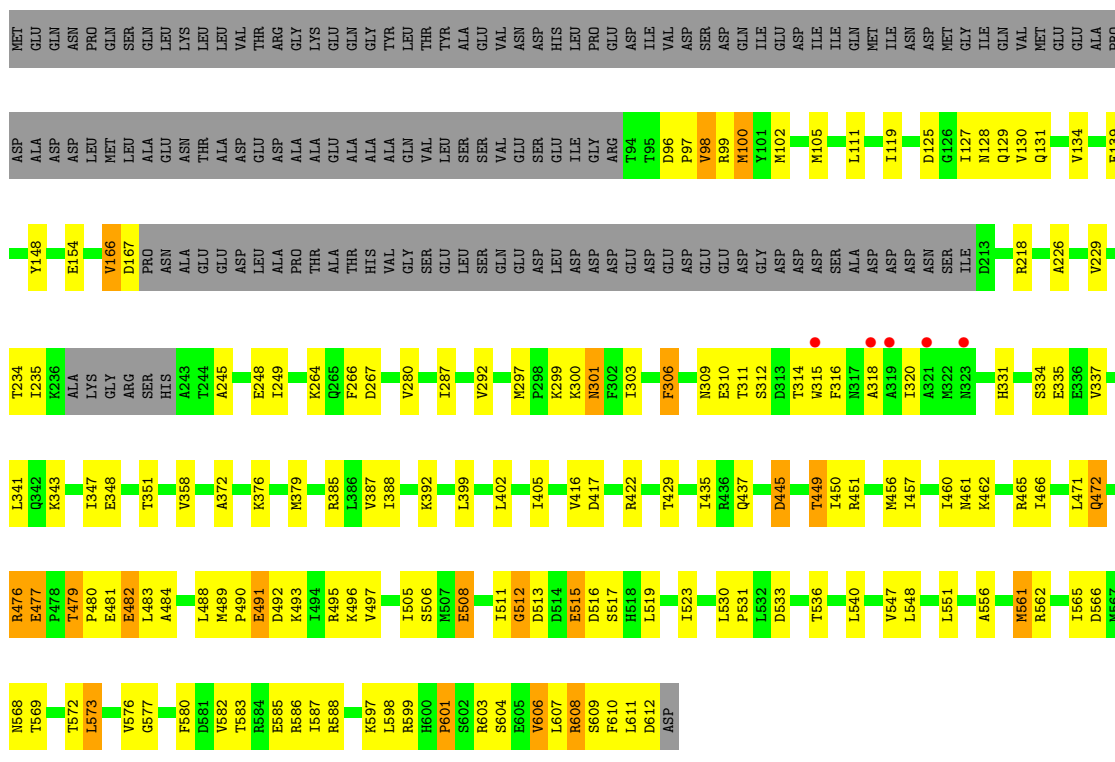


• Molecule 3: DNA-directed RNA polymerase subunit beta'

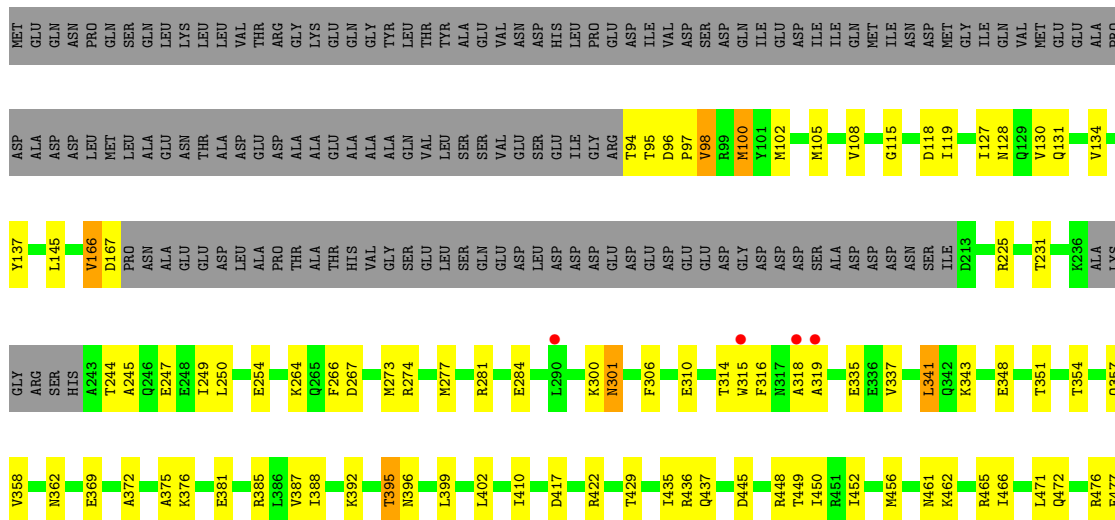


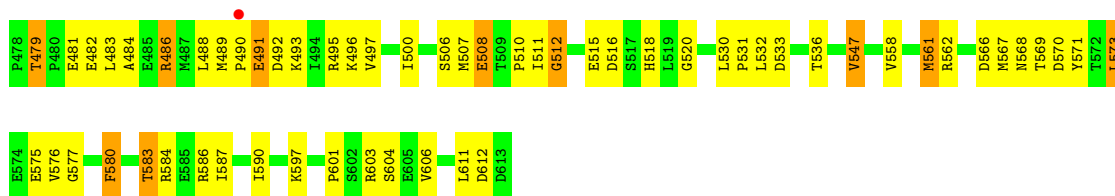


● Molecule 5: RNA polymerase sigma factor RpoD



● Molecule 5: RNA polymerase sigma factor RpoD





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	187.81Å 206.67Å 310.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.74 – 4.10 29.74 – 4.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.74-4.10) 99.4 (29.74-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 4.11Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.243 , 0.287 0.243 , 0.287	Depositor DCC
R_{free} test set	1946 reflections (2.06%)	wwPDB-VP
Wilson B-factor (Å ²)	184.9	Xtrriage
Anisotropy	0.260	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 155.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	55125	wwPDB-VP
Average B, all atoms (Å ²)	233.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% 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: RFP, 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	0.32	0/1834	0.62	0/2485
1	B	0.34	0/1697	0.79	3/2300 (0.1%)
1	G	0.30	0/1777	0.63	1/2408 (0.0%)
1	H	0.34	0/1681	0.79	2/2278 (0.1%)
2	C	0.32	0/10738	0.62	5/14488 (0.0%)
2	I	0.31	2/10734 (0.0%)	0.62	2/14483 (0.0%)
3	D	0.29	0/9205	0.61	2/12430 (0.0%)
3	J	0.29	0/9140	0.64	4/12341 (0.0%)
4	E	0.26	0/693	0.53	0/935
4	K	0.32	0/629	0.55	0/847
5	F	0.28	0/3864	0.61	0/5194
5	L	0.29	0/3872	0.61	2/5205 (0.0%)
All	All	0.30	2/55864 (0.0%)	0.63	21/75394 (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	A	0	1
1	B	0	1
2	C	0	3
2	I	0	3
3	D	0	2
3	J	0	3
5	F	0	1
All	All	0	14

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	344	GLY	C-N	-5.42	1.24	1.34
2	I	997	TRP	CB-CG	-5.04	1.41	1.50

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	425	ARG	NE-CZ-NH2	11.69	126.14	120.30
3	J	425	ARG	NE-CZ-NH1	-9.14	115.73	120.30
2	I	1137	GLU	CA-CB-CG	7.41	129.69	113.40
3	D	343	LEU	CB-CG-CD2	-7.04	99.03	111.00
1	B	135	ASP	CB-CG-OD1	-6.66	112.30	118.30

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	ASN	Sidechain
1	B	135	ASP	Sidechain
2	C	107	ARG	Peptide
2	C	109	ALA	Peptide
2	C	236	LYS	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	A	1812	0	1839	73	0
1	B	1677	0	1703	93	0
1	G	1755	0	1773	73	0
1	H	1662	0	1687	68	0
2	C	10569	0	10587	326	0
2	I	10565	0	10581	267	0
3	D	9065	0	9210	297	0
3	J	9001	0	9165	277	0
4	E	691	0	695	17	0
4	K	627	0	634	18	0
5	F	3813	0	3880	103	0
5	L	3821	0	3884	95	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	59	0	56	6	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	I	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	55125	0	55694	1519	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 14.

The worst 5 of 1519 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)
2:C:1271:GLY:HA2	3:D:343:LEU:HD21	1.23	1.11
2:C:1269:ARG:HG2	3:D:343:LEU:HD12	1.36	1.07
5:L:97:PRO:HA	5:L:100:MET:HG3	1.45	0.97
2:C:18:ARG:NH1	2:C:621:SER:O	2.04	0.91
2:I:1271:GLY:HA2	3:J:343:LEU:HD11	1.51	0.90

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	231/329 (70%)	198 (86%)	29 (13%)	4 (2%)	9	42
1	B	213/329 (65%)	187 (88%)	24 (11%)	2 (1%)	17	54
1	G	225/329 (68%)	191 (85%)	28 (12%)	6 (3%)	5	33
1	H	212/329 (64%)	187 (88%)	24 (11%)	1 (0%)	29	67

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	1338/1342 (100%)	1230 (92%)	102 (8%)	6 (0%)	34	71
2	I	1338/1342 (100%)	1230 (92%)	100 (8%)	8 (1%)	25	63
3	D	1163/1407 (83%)	1071 (92%)	83 (7%)	9 (1%)	19	58
3	J	1151/1407 (82%)	1060 (92%)	78 (7%)	13 (1%)	14	50
4	E	87/91 (96%)	82 (94%)	5 (6%)	0	100	100
4	K	77/91 (85%)	74 (96%)	3 (4%)	0	100	100
5	F	462/613 (75%)	421 (91%)	34 (7%)	7 (2%)	10	44
5	L	463/613 (76%)	424 (92%)	37 (8%)	2 (0%)	34	71
All	All	6960/8222 (85%)	6355 (91%)	547 (8%)	58 (1%)	19	58

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	170	VAL
2	C	484	LEU
2	C	1159	VAL
3	D	10	ALA
3	D	1274	PHE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	201/286 (70%)	190 (94%)	11 (6%)	21	50
1	B	186/286 (65%)	167 (90%)	19 (10%)	7	28
1	G	193/286 (68%)	178 (92%)	15 (8%)	12	39
1	H	183/286 (64%)	169 (92%)	14 (8%)	13	40
2	C	1155/1157 (100%)	1059 (92%)	96 (8%)	11	37
2	I	1154/1157 (100%)	1058 (92%)	96 (8%)	11	37
3	D	962/1168 (82%)	880 (92%)	82 (8%)	10	37
3	J	960/1168 (82%)	882 (92%)	78 (8%)	11	38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	72/75 (96%)	65 (90%)	7 (10%)	8	29
4	K	67/75 (89%)	63 (94%)	4 (6%)	19	47
5	F	417/540 (77%)	379 (91%)	38 (9%)	9	33
5	L	418/540 (77%)	384 (92%)	34 (8%)	11	38
All	All	5968/7024 (85%)	5474 (92%)	494 (8%)	11	37

5 of 494 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	449	THR
3	J	1186	TYR
2	I	82	VAL
3	J	918	ILE
5	L	422	ARG

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

Mol	Chain	Res	Type
3	J	716	GLN
3	J	910	ASN
5	L	472	GLN
3	D	929	GLN
3	D	910	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 8 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	RFP	C	3001	-	63,63,63	2.15	11 (17%)	94,94,94	2.00	22 (23%)

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	RFP	C	3001	-	-	10/60/85/85	0/5/5/5

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	3001	RFP	O3-C6	10.23	1.57	1.37
6	C	3001	RFP	C15-N1	6.63	1.49	1.35
6	C	3001	RFP	C12-C11	-4.41	1.37	1.54
6	C	3001	RFP	C3-C43	4.02	1.54	1.46
6	C	3001	RFP	C18-C17	3.69	1.54	1.43

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	3001	RFP	C2-C3-C43	-5.64	118.44	124.17
6	C	3001	RFP	C38-N4-C42	5.39	118.72	110.66
6	C	3001	RFP	O4-C11-C5	-5.06	122.15	131.81
6	C	3001	RFP	C41-N3-N2	4.97	139.53	113.86
6	C	3001	RFP	C38-N4-C39	4.93	118.03	110.66

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

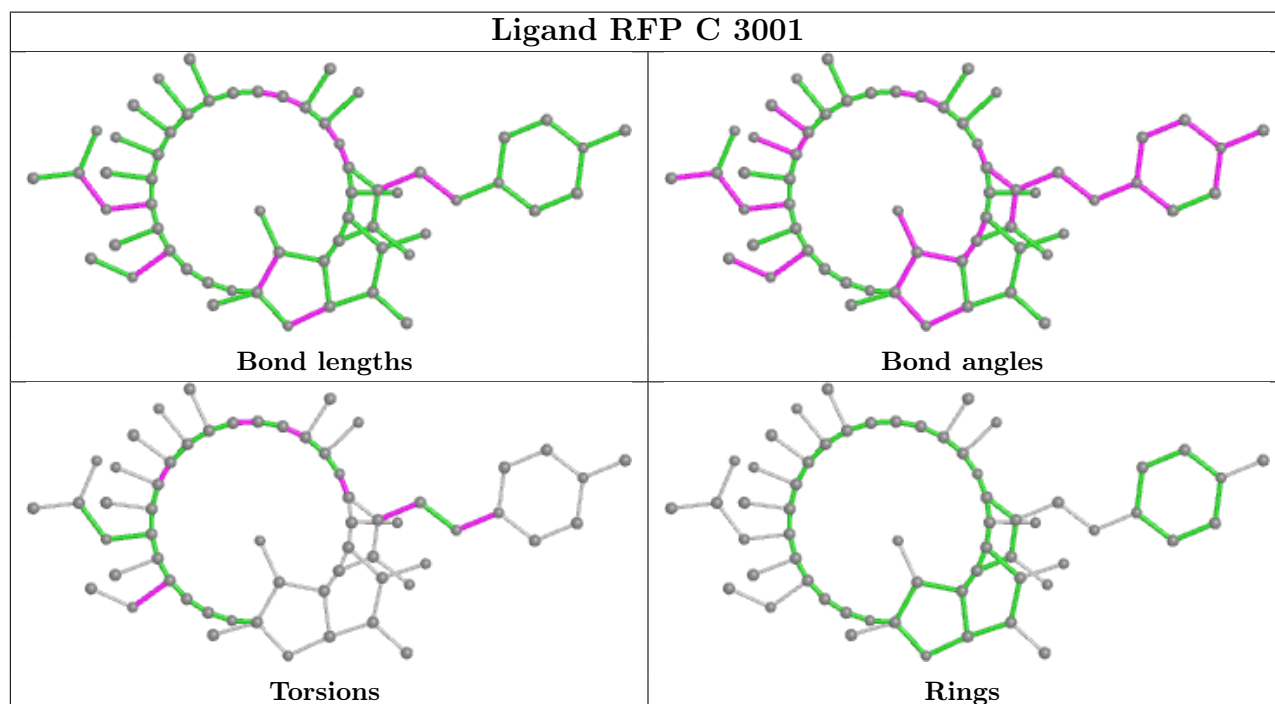
Mol	Chain	Res	Type	Atoms
6	C	3001	RFP	C2-C3-C43-N2
6	C	3001	RFP	C4-C3-C43-N2
6	C	3001	RFP	C43-N2-N3-C40
6	C	3001	RFP	C3-C2-N1-C15
6	C	3001	RFP	C43-N2-N3-C41

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	3001	RFP	6	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	233/329 (70%)	-0.38	0 100 100	171, 206, 261, 301	0
1	B	217/329 (65%)	-0.12	3 (1%) 75 65	179, 243, 300, 333	0
1	G	227/329 (68%)	-0.26	1 (0%) 92 87	223, 269, 305, 330	0
1	H	216/329 (65%)	-0.13	3 (1%) 75 65	213, 288, 312, 327	0
2	C	1340/1342 (99%)	-0.30	15 (1%) 80 72	126, 197, 326, 418	0
2	I	1340/1342 (99%)	-0.08	23 (1%) 70 60	174, 254, 341, 465	0
3	D	1167/1407 (82%)	-0.29	2 (0%) 95 93	137, 186, 259, 335	0
3	J	1155/1407 (82%)	-0.20	12 (1%) 82 74	163, 218, 292, 350	0
4	E	89/91 (97%)	-0.34	1 (1%) 80 72	180, 221, 256, 264	0
4	K	79/91 (86%)	0.41	4 (5%) 28 24	244, 325, 377, 395	0
5	F	468/613 (76%)	-0.25	5 (1%) 80 72	185, 234, 373, 416	0
5	L	469/613 (76%)	-0.25	5 (1%) 80 72	219, 257, 379, 441	0
All	All	7000/8222 (85%)	-0.22	74 (1%) 80 72	126, 229, 321, 465	0

The worst 5 of 74 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	265	LYS	5.5
2	I	979	LEU	5.2
1	B	172	LEU	4.5
2	I	1000	LEU	4.5
2	C	316	GLU	3.9

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](#)

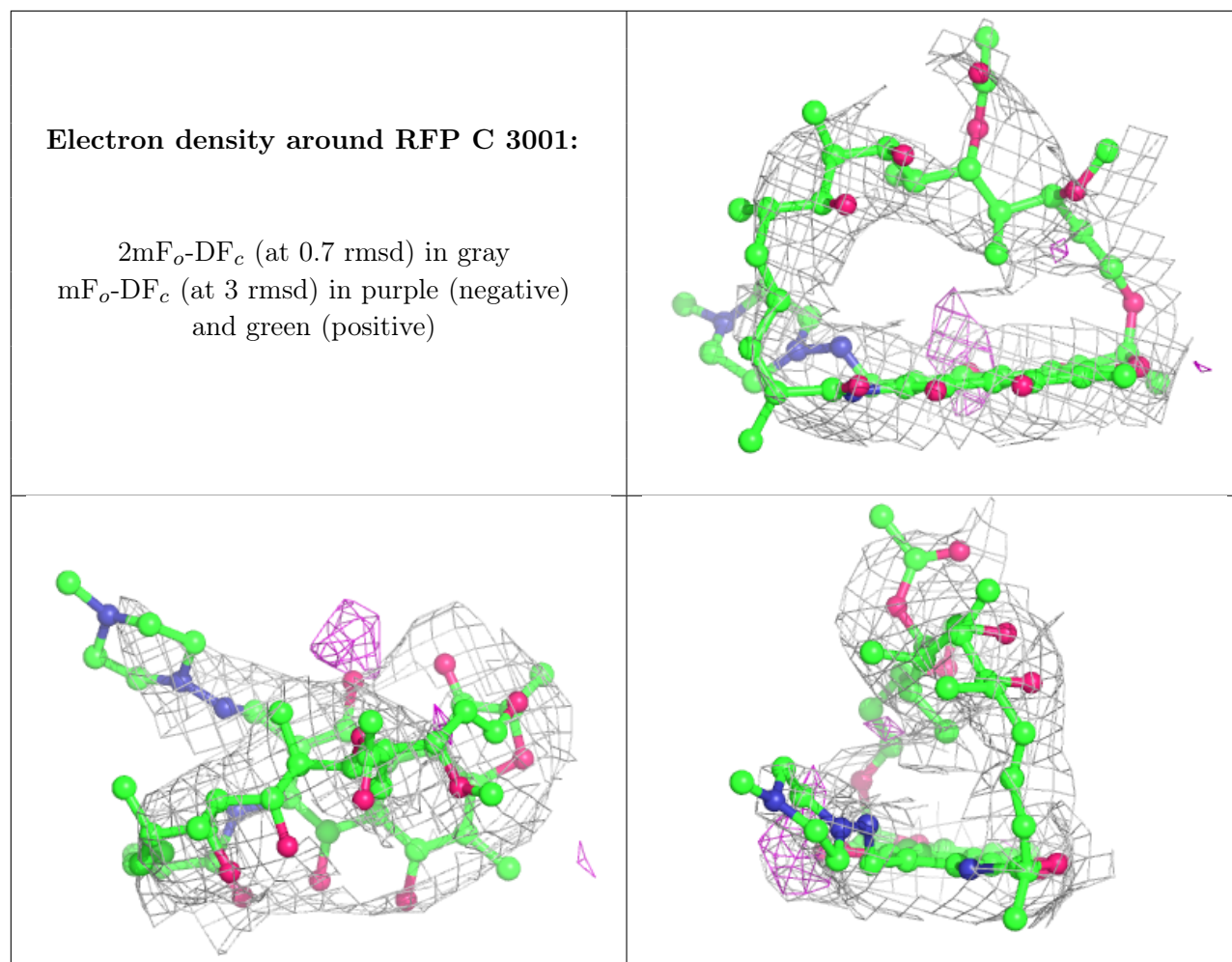
There are no monosaccharides in this entry.

6.4 Ligands [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(Å ²)	Q<0.9
7	MG	I	1401	1/1	0.23	0.47	216,216,216,216	0
7	MG	J	2001	1/1	0.46	0.21	216,216,216,216	0
7	MG	C	3002	1/1	0.61	0.57	216,216,216,216	0
7	MG	D	2001	1/1	0.68	0.14	216,216,216,216	0
8	ZN	D	2002	1/1	0.83	0.15	216,216,216,216	0
8	ZN	J	2002	1/1	0.84	0.10	222,222,222,222	0
8	ZN	D	2003	1/1	0.88	0.33	216,216,216,216	0
6	RFP	C	3001	59/59	0.91	0.32	136,178,213,228	0
8	ZN	J	2003	1/1	0.91	0.29	216,216,216,216	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.