



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 11:07 AM UTC

PDB ID : 5UAC / pdb_00005uac
Title : Escherichia coli RNA polymerase and Rifampin complex, wild-type
Authors : Molodtsov, V.; Scharf, N.T.; Stefan, M.A.; Garcia, G.A.; Murakami, K.S.
Deposited on : 2016-12-19
Resolution : 3.80 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

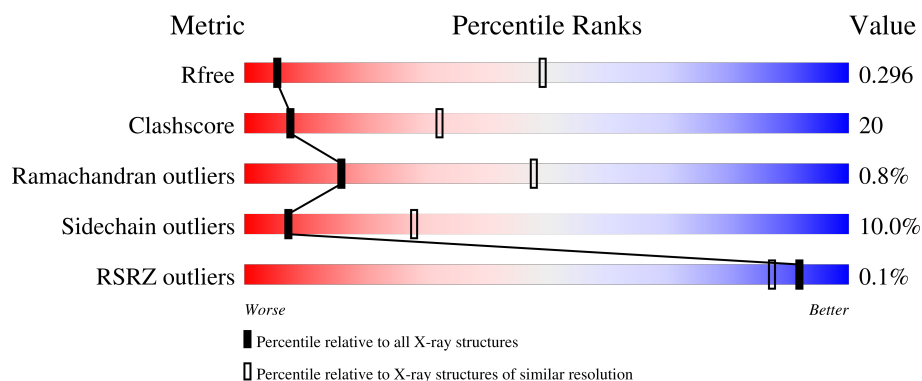
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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.



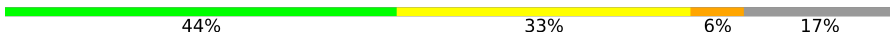
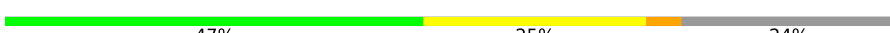
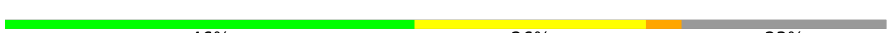
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	 58% 37% .
3	D	1407	 44% 33% 6% 17%
3	J	1407	 46% 31% 5% 18%
4	E	91	 67% 24% 7% .
4	K	91	 52% 34% . 13%
5	F	613	 47% 25% . 24%
5	L	613	 46% 26% . 23%

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
8	ZN	D	1503	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 55049 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	227	Total	C	N	O	S	0	0	0
			1753	1091	311	345	6			
1	B	214	Total	C	N	O	S	0	0	0
			1649	1029	290	324	6			
1	G	224	Total	C	N	O	S	0	0	0
			1730	1076	308	340	6			
1	H	215	Total	C	N	O	S	0	0	0
			1659	1037	291	325	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1342	Total	C	N	O	S	0	0	0
			10585	6641	1843	2057	44			
2	I	1340	Total	C	N	O	S	0	0	0
			10566	6629	1840	2054	43			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1166	Total	C	N	O	S	0	0	0
			9089	5714	1627	1702	46			
3	J	1155	Total	C	N	O	S	0	0	0
			9001	5659	1612	1684	46			

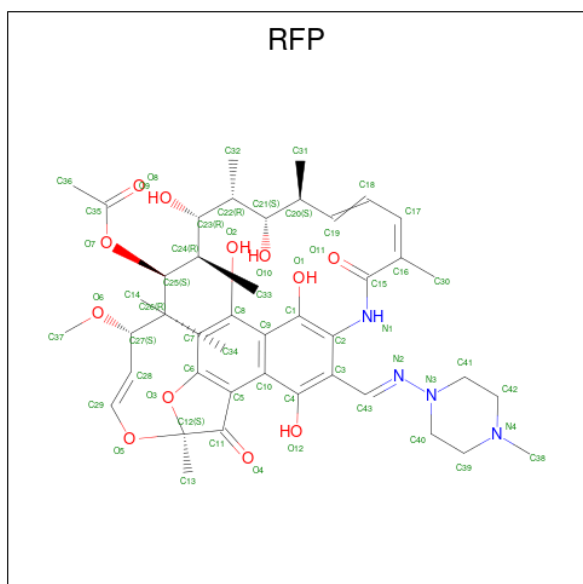
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	89	Total	C	N	O	S	0	0	0
			691	421	129	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	468	Total	C	N	O	S	0	0	0
			3813	2389	678	723	23			
5	L	469	Total	C	N	O	S	0	0	0
			3821	2393	679	726	23			

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



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

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

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

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

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

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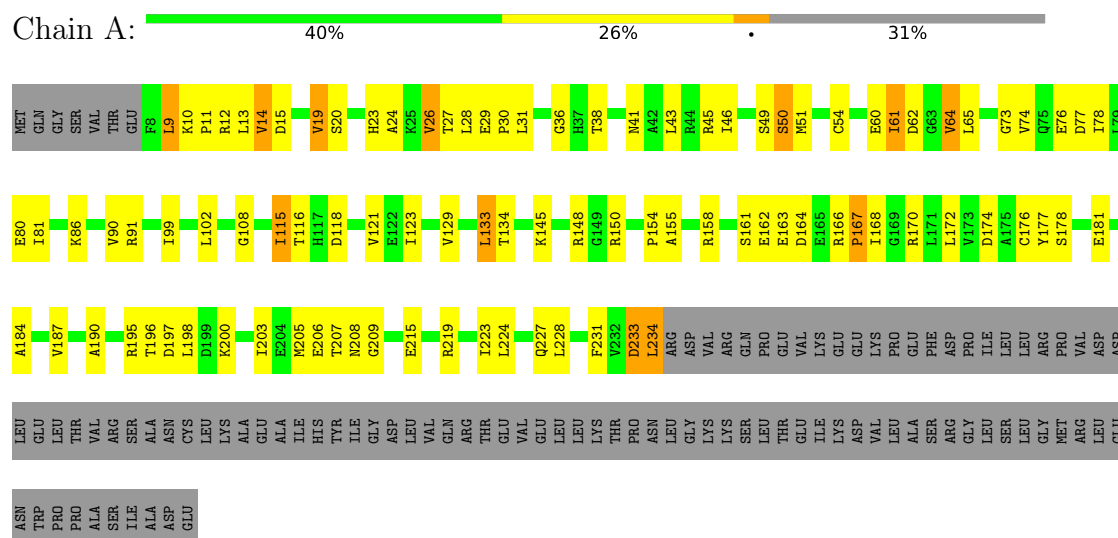
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	J	2	Total	Zn	0	0
			2	2		

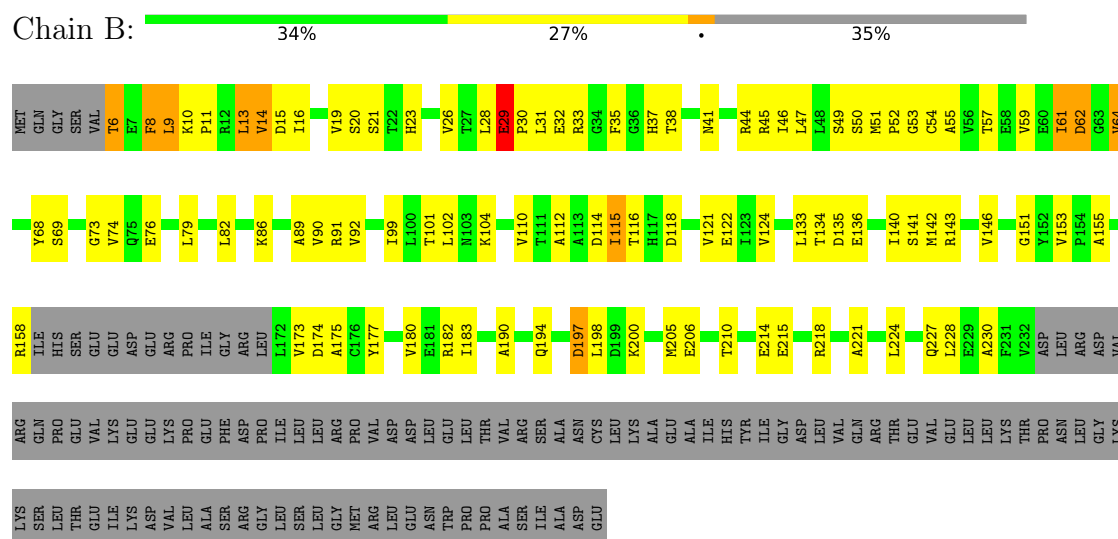
3 Residue-property plots

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



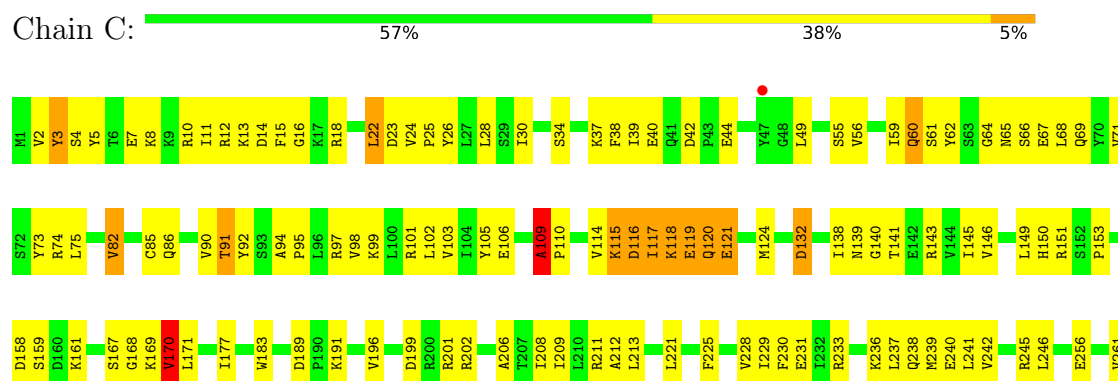
• Molecule 1: DNA-directed RNA polymerase subunit alpha

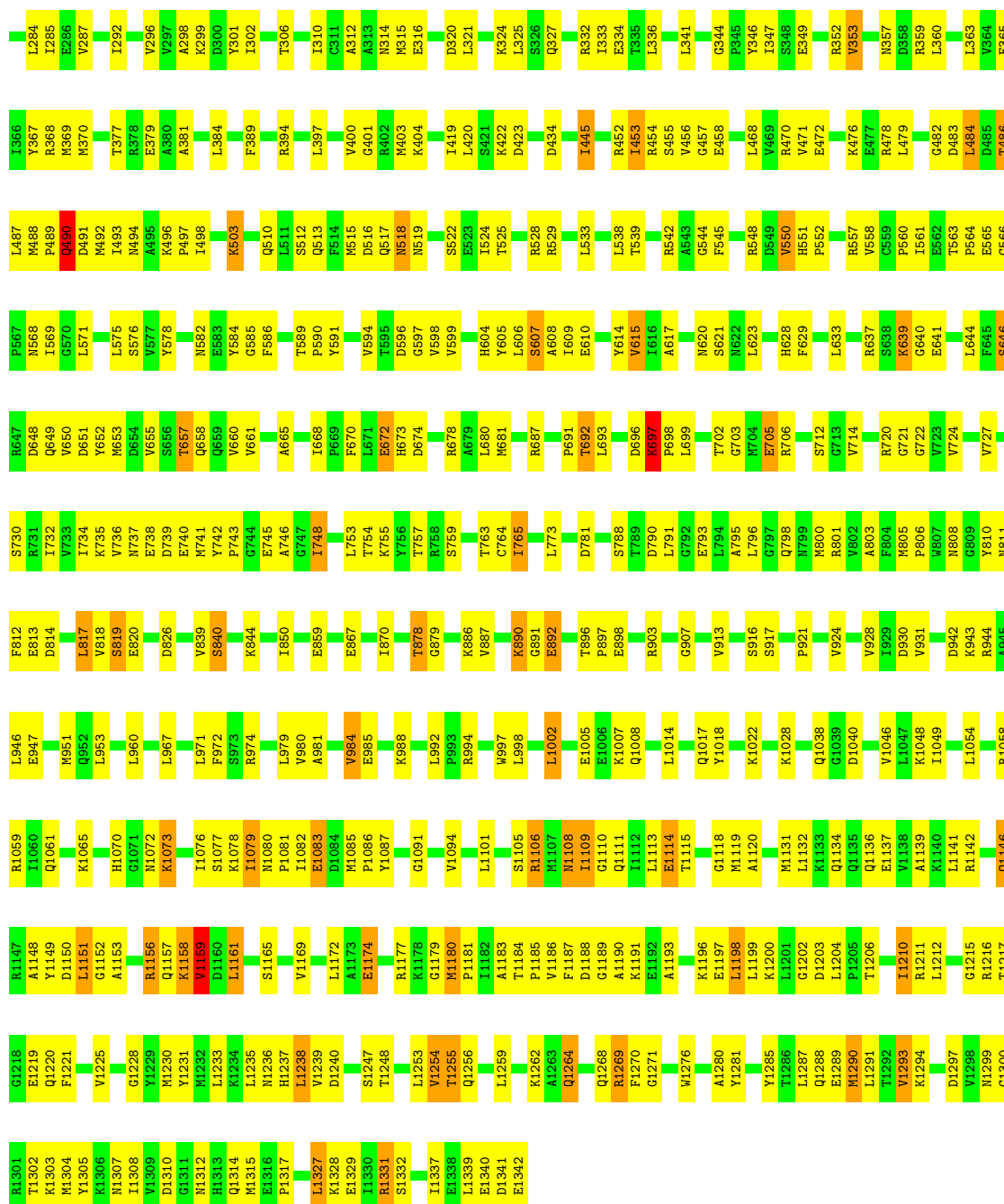


• Molecule 1: DNA-directed RNA polymerase subunit alpha

- Molecule 1: DNA-directed RNA polymerase subunit alpha

- Molecule 2: DNA-directed RNA polymerase subunit beta



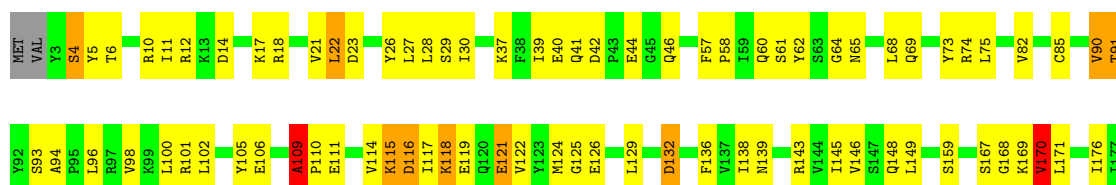


• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain I:

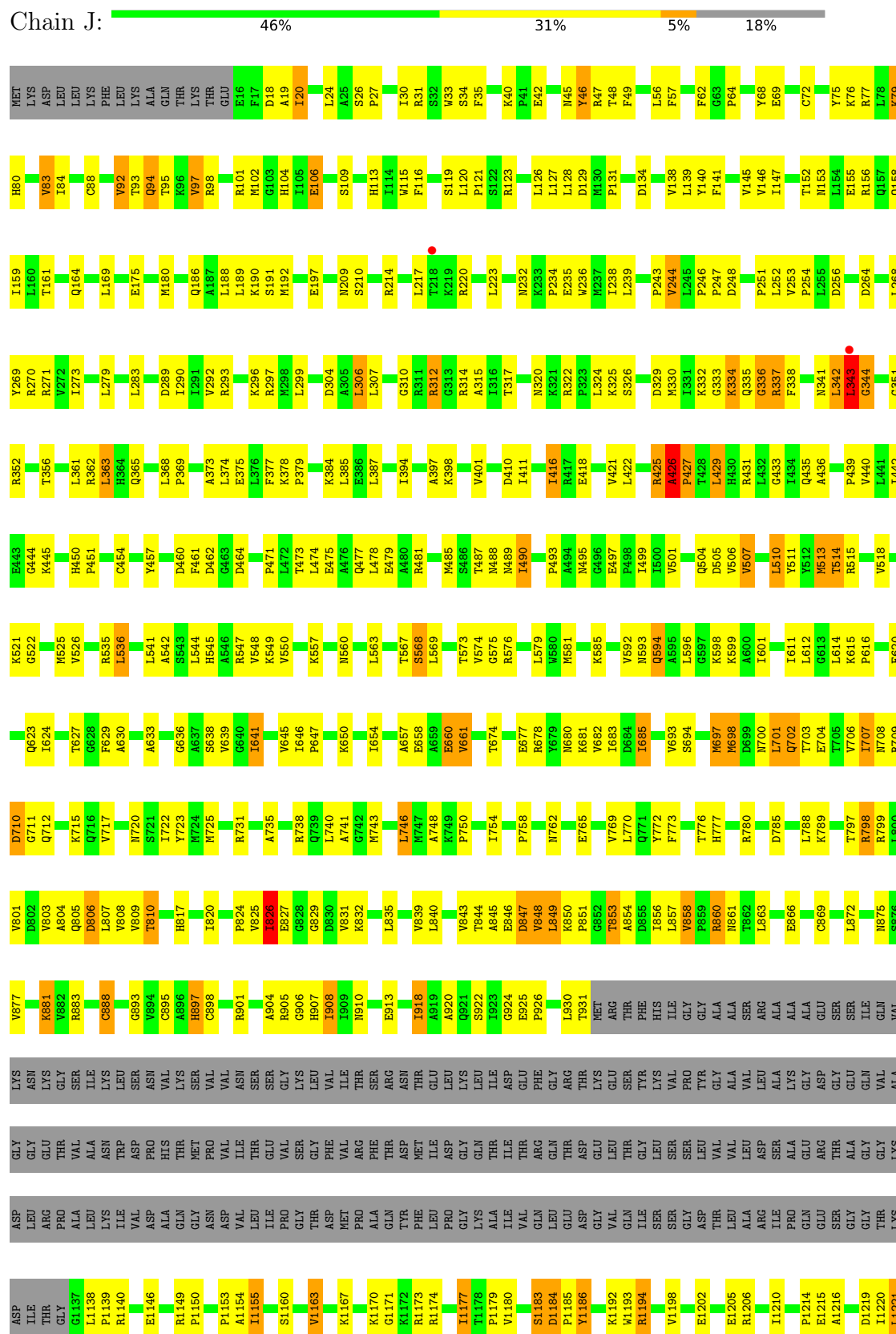
58%

37%

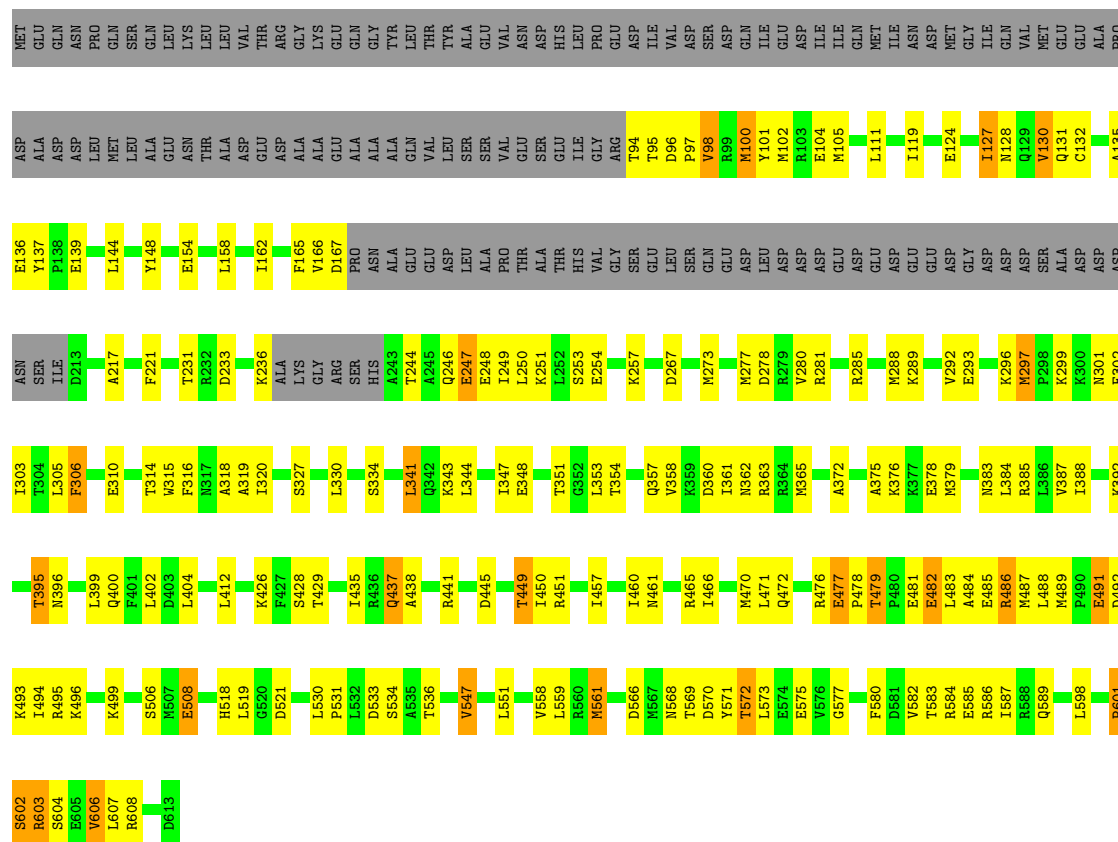




● Molecule 3: DNA-directed RNA polymerase subunit beta'







4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	188.96Å 204.43Å 313.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 3.80 29.98 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.98-3.80) 99.5 (29.98-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 3.75Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.248 , 0.295 0.252 , 0.296	Depositor DCC
R_{free} test set	1994 reflections (1.66%)	wwPDB-VP
Wilson B-factor (Å ²)	159.8	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 119.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	55049	wwPDB-VP
Average B, all atoms (Å ²)	188.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% 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: MG, RFP, ZN

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	0.71	0/1774	0.90	0/2405
1	B	0.68	0/1668	1.11	4/2260 (0.2%)
1	G	0.56	1/1751 (0.1%)	0.83	2/2373 (0.1%)
1	H	0.54	0/1678	1.03	4/2274 (0.2%)
2	C	0.90	3/10754 (0.0%)	1.01	11/14509 (0.1%)
2	I	0.57	2/10735 (0.0%)	0.81	7/14484 (0.0%)
3	D	0.98	0/9229	1.08	12/12459 (0.1%)
3	J	0.75	1/9140 (0.0%)	0.93	5/12341 (0.0%)
4	E	0.72	0/693	0.85	0/935
4	K	0.28	0/629	0.63	0/847
5	F	0.52	0/3864	0.75	1/5194 (0.0%)
5	L	0.47	0/3872	0.70	1/5205 (0.0%)
All	All	0.75	7/55787 (0.0%)	0.93	47/75286 (0.1%)

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	B	0	1
2	C	0	6
2	I	0	2
3	D	0	6
3	J	0	2
4	E	0	1
5	F	0	1
5	L	0	1
All	All	0	20

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	343	LEU	CG-CD2	8.14	1.79	1.52
2	I	373	GLY	C-N	8.02	1.50	1.33
2	C	1079	ILE	C-N	-5.89	1.21	1.33
2	I	1271	GLY	C-N	5.76	1.41	1.33
2	C	764	CYS	CB-SG	-5.75	1.62	1.81

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	109	ALA	CA-C-N	15.69	136.72	119.93
2	C	109	ALA	C-N-CA	15.69	136.72	119.93
2	I	109	ALA	CA-C-N	15.03	136.01	119.93
2	I	109	ALA	C-N-CA	15.03	136.01	119.93
3	D	12	THR	N-CA-C	-8.47	104.96	114.62

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	29	GLU	Peptide
2	C	109	ALA	Peptide
2	C	1239	VAL	Mainchain
2	C	236	LYS	Peptide
2	C	646	SER	Mainchain

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	1753	0	1780	94	0
1	B	1649	0	1674	106	0
1	G	1730	0	1756	85	0
1	H	1659	0	1692	94	0
2	C	10585	0	10603	454	0
2	I	10566	0	10576	397	0
3	D	9089	0	9264	474	0
3	J	9001	0	9170	397	0
4	E	691	0	695	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	627	0	634	25	0
5	F	3813	0	3880	145	0
5	L	3821	0	3884	139	0
6	C	59	0	54	14	0
7	D	1	0	0	0	0
7	J	1	0	0	0	0
8	D	2	0	0	2	0
8	J	2	0	0	1	0
All	All	55049	0	55662	2236	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 2236 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:J:343:LEU:CD2	3:J:343:LEU:CG	1.79	1.59
3:D:426:ALA:CB	3:D:427:PRO:CD	2.12	1.26
3:J:426:ALA:CB	3:J:427:PRO:HD3	1.69	1.19
3:D:343:LEU:HD22	3:D:344:GLY:HA3	1.16	1.16
3:D:426:ALA:HB3	3:D:427:PRO:CD	1.70	1.13

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	225/329 (68%)	196 (87%)	25 (11%)	4 (2%)	6	33
1	B	210/329 (64%)	183 (87%)	22 (10%)	5 (2%)	4	29
1	G	222/329 (68%)	193 (87%)	25 (11%)	4 (2%)	6	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	211/329 (64%)	187 (89%)	17 (8%)	7 (3%)	3	24
2	C	1340/1342 (100%)	1233 (92%)	100 (8%)	7 (0%)	24	57
2	I	1338/1342 (100%)	1232 (92%)	101 (8%)	5 (0%)	30	62
3	D	1162/1407 (83%)	1072 (92%)	81 (7%)	9 (1%)	16	48
3	J	1151/1407 (82%)	1056 (92%)	80 (7%)	15 (1%)	9	38
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%)	422 (91%)	39 (8%)	1 (0%)	43	73
5	L	463/613 (76%)	424 (92%)	38 (8%)	1 (0%)	43	73
All	All	6948/8222 (84%)	6354 (92%)	536 (8%)	58 (1%)	16	48

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	GLU
1	A	167	PRO
1	B	13	LEU
2	C	1159	VAL
3	D	10	ALA

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	194/286 (68%)	179 (92%)	15 (8%)	12	37
1	B	182/286 (64%)	171 (94%)	11 (6%)	17	43
1	G	191/286 (67%)	177 (93%)	14 (7%)	13	39
1	H	184/286 (64%)	176 (96%)	8 (4%)	26	50
2	C	1157/1157 (100%)	1042 (90%)	115 (10%)	7	28
2	I	1154/1157 (100%)	1039 (90%)	115 (10%)	7	28
3	D	970/1168 (83%)	861 (89%)	109 (11%)	6	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	J	960/1168 (82%)	850 (88%)	110 (12%)	5	23
4	E	72/75 (96%)	64 (89%)	8 (11%)	6	24
4	K	67/75 (89%)	62 (92%)	5 (8%)	12	38
5	F	417/540 (77%)	375 (90%)	42 (10%)	7	27
5	L	418/540 (77%)	376 (90%)	42 (10%)	7	28
All	All	5966/7024 (85%)	5372 (90%)	594 (10%)	7	28

5 of 594 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	394	ILE
5	L	472	GLN
3	J	536	LEU
3	J	374	LEU
3	J	897	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 114 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	518	HIS
5	L	406	GLN
2	I	688	GLN
5	L	383	ASN
3	J	1259	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	RFP	C	3001	-	63,63,63	2.54	23 (36%)	94,94,94	2.62	37 (39%)

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	-	-	15/60/85/85	0/5/5/5

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	3001	RFP	O3-C6	9.51	1.55	1.37
6	C	3001	RFP	O7-C25	-8.32	1.32	1.44
6	C	3001	RFP	C12-C11	-5.64	1.32	1.54
6	C	3001	RFP	C15-N1	5.07	1.46	1.35
6	C	3001	RFP	C18-C17	4.13	1.56	1.43

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	3001	RFP	C32-C22-C23	-7.43	96.82	111.43
6	C	3001	RFP	C33-C24-C23	-7.11	97.45	111.43
6	C	3001	RFP	O7-C25-C26	-6.64	92.21	107.52
6	C	3001	RFP	O4-C11-C5	-5.64	121.23	131.63
6	C	3001	RFP	C31-C20-C19	-5.44	97.59	109.91

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

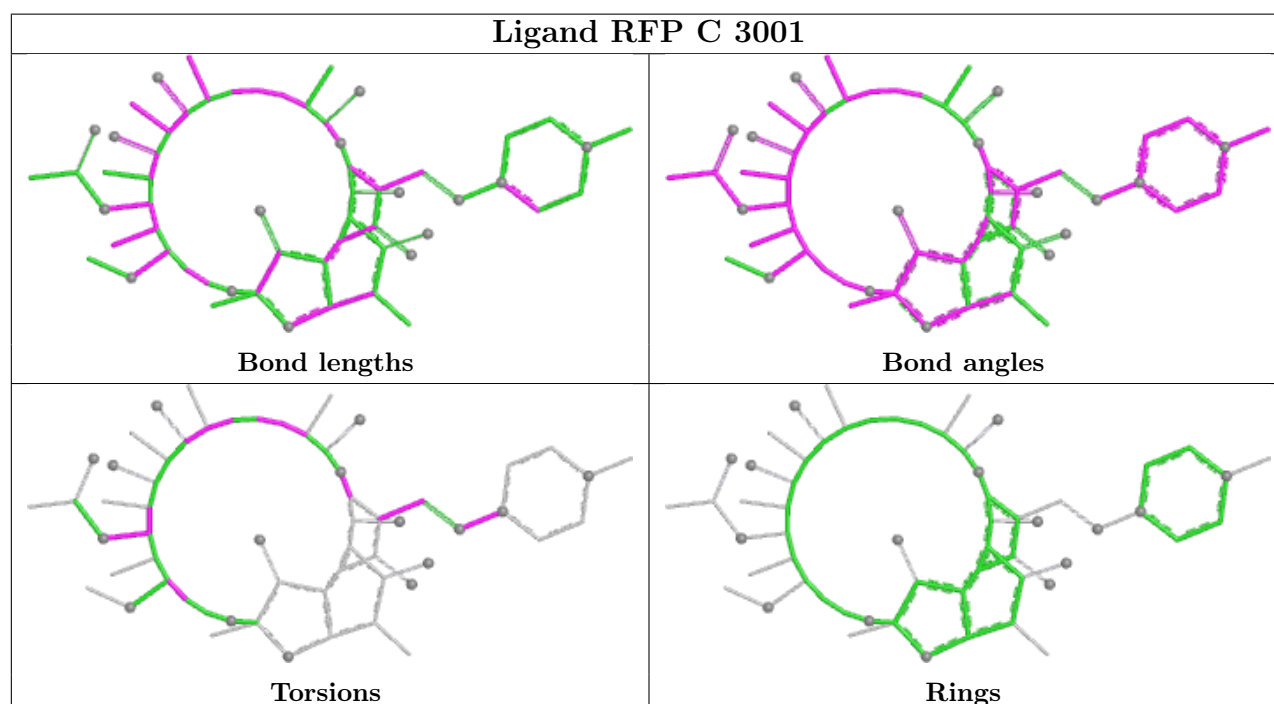
Mol	Chain	Res	Type	Atoms
6	C	3001	RFP	C3-C2-N1-C15
6	C	3001	RFP	C4-C3-C43-N2
6	C	3001	RFP	C19-C20-C21-O10
6	C	3001	RFP	O6-C27-C28-C29
6	C	3001	RFP	C43-N2-N3-C40

There are no ring outliers.

1 monomer is involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	3001	RFP	14	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	227/329 (68%)	-0.62	0 100 100	128, 159, 207, 262	0
1	B	214/329 (65%)	-0.46	0 100 100	115, 179, 246, 259	0
1	G	224/329 (68%)	-0.65	0 100 100	162, 193, 225, 245	0
1	H	215/329 (65%)	-0.48	0 100 100	165, 218, 246, 265	0
2	C	1342/1342 (100%)	-0.57	1 (0%) 92 87	96, 152, 303, 368	0
2	I	1340/1342 (99%)	-0.53	4 (0%) 90 78	129, 200, 287, 371	0
3	D	1166/1407 (82%)	-0.59	0 100 100	94, 140, 215, 278	0
3	J	1155/1407 (82%)	-0.58	2 (0%) 91 81	118, 164, 225, 300	0
4	E	89/91 (97%)	-0.65	0 100 100	131, 170, 200, 214	0
4	K	79/91 (86%)	-0.44	0 100 100	221, 276, 310, 318	0
5	F	468/613 (76%)	-0.46	0 100 100	139, 216, 432, 522	0
5	L	469/613 (76%)	-0.52	0 100 100	144, 239, 458, 518	0
All	All	6988/8222 (84%)	-0.55	7 (0%) 92 87	94, 176, 295, 522	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	47	TYR	3.4
2	I	998	LEU	2.9
3	J	218	THR	2.8
2	I	975	ILE	2.7
2	I	1018	TYR	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](#)

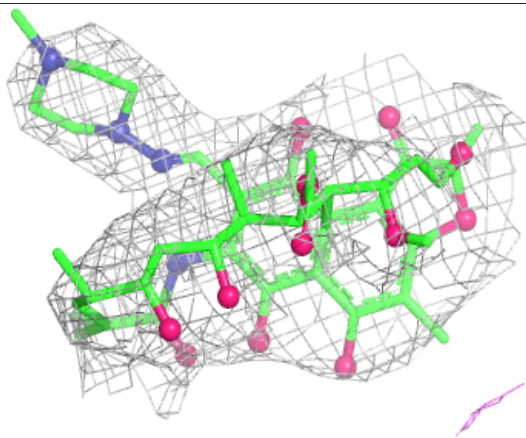
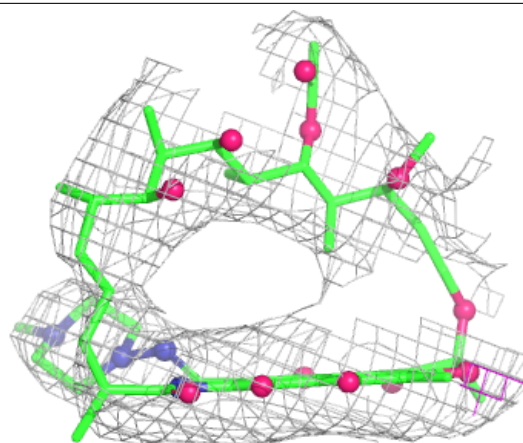
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
7	MG	D	1501	1/1	0.59	0.15	264,264,264,264	0
7	MG	J	1501	1/1	0.69	0.19	290,290,290,290	0
8	ZN	J	1502	1/1	0.81	0.15	322,322,322,322	0
8	ZN	D	1502	1/1	0.83	0.15	324,324,324,324	0
8	ZN	J	1503	1/1	0.89	0.16	281,281,281,281	0
8	ZN	D	1503	1/1	0.90	0.16	274,274,274,274	0
6	RFP	C	3001	59/59	0.94	0.08	88,136,160,162	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 RFP C 3001:

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.