



wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2020 – 02:20 am BST

PDB ID : 1YNJ
Title : Taq RNA polymerase-Sorangicin complex
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Deposited on : 2005-01-24
Resolution : 3.20 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 : 2.11
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) : 2.11

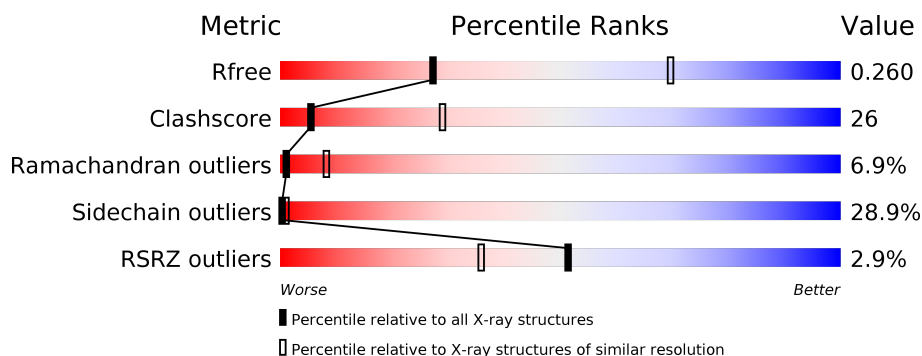
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	314	<div> <div>25%</div> <div>32%</div> <div>13%</div> <div>•</div> <div>27%</div> </div>
1	B	314	<div> <div>32%</div> <div>30%</div> <div>8%</div> <div>•</div> <div>28%</div> </div>
2	C	1119	<div> <div>39%</div> <div>42%</div> <div>15%</div> <div>•</div> </div>
3	D	1524	<div> <div>4%</div> <div>36%</div> <div>33%</div> <div>11%</div> <div>•</div> <div>19%</div> </div>
3	J	1524	<div> <div>7%</div> <div>7%</div> <div>•</div> <div>84%</div> </div>
4	K	99	<div> <div>2%</div> <div>42%</div> <div>35%</div> <div>17%</div> <div>• •</div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 24369 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 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1763	1126	300	334	3			
1	B	225	Total	C	N	O	S	0	0	0
			1750	1118	300	329	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1114	Total	C	N	O	S	0	0	0
			8578	5431	1516	1607	24			

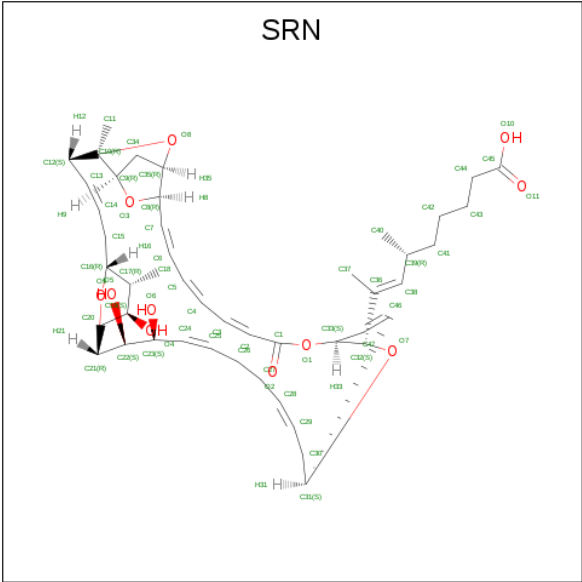
- Molecule 3 is a protein called DNA-directed RNA polymerase beta' chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1238	Total	C	N	O	S	0	0	0
			9602	6065	1703	1798	36			
3	J	249	Total	C	N	O	S	0	0	0
			1869	1191	320	356	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	95	Total	C	N	O	S	0	0	0
			747	476	134	132	5			

- Molecule 5 is SORANGICIN A (three-letter code: SRN) (formula: C₄₇H₆₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			58	47	11		

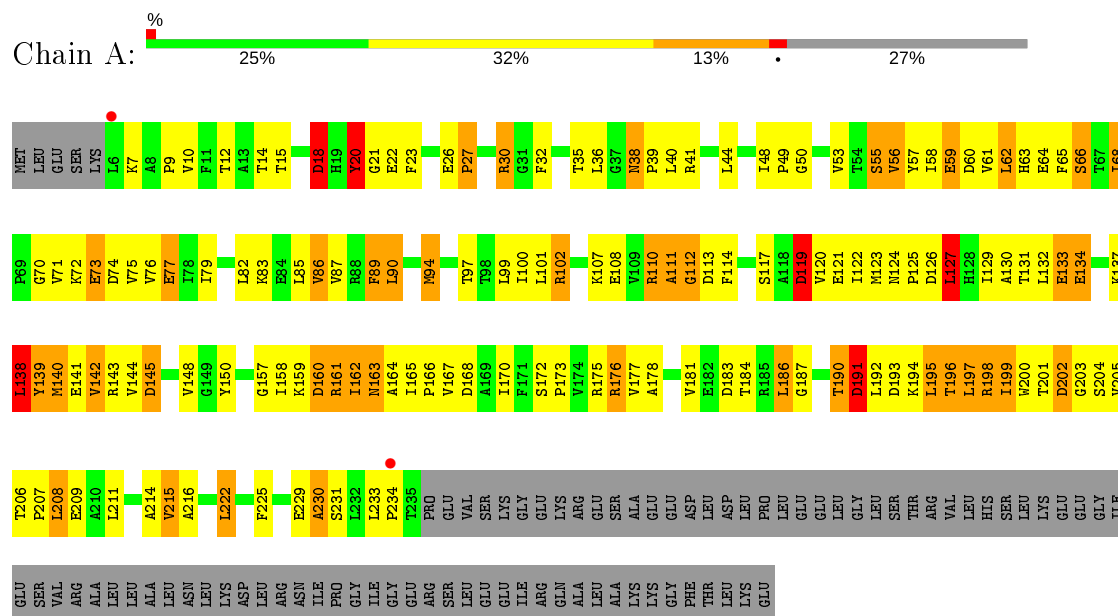
- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

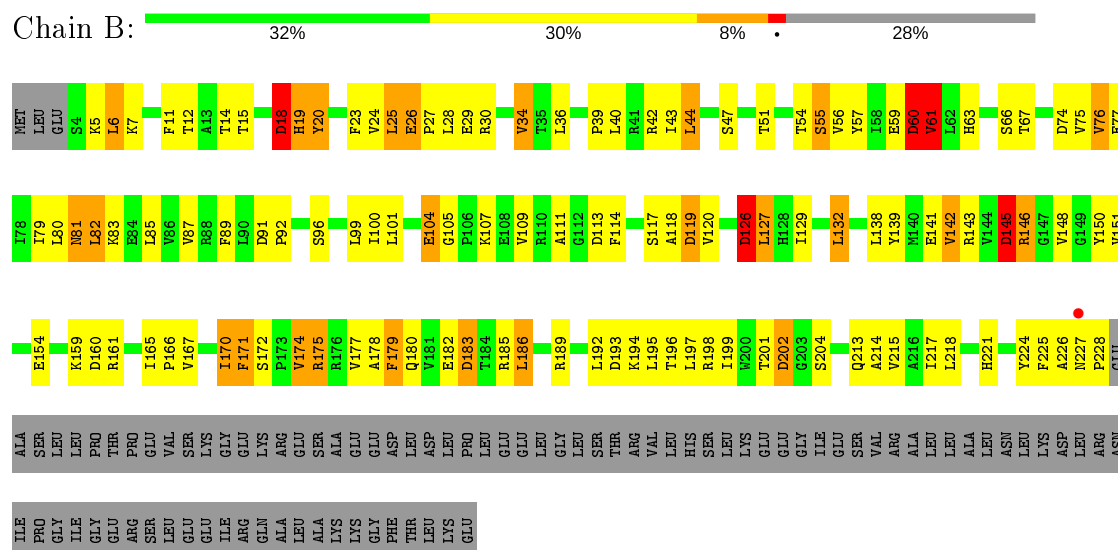
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 alpha chain

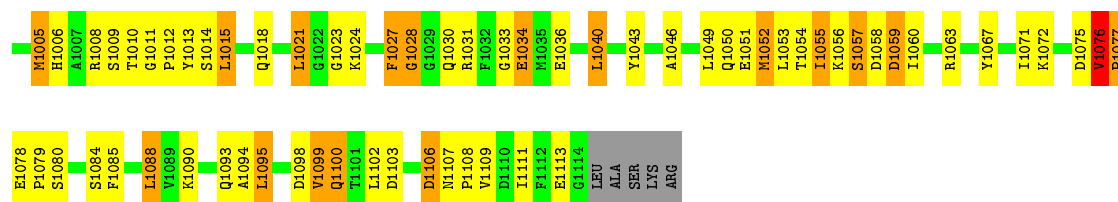


• Molecule 1: DNA-directed RNA polymerase alpha chain

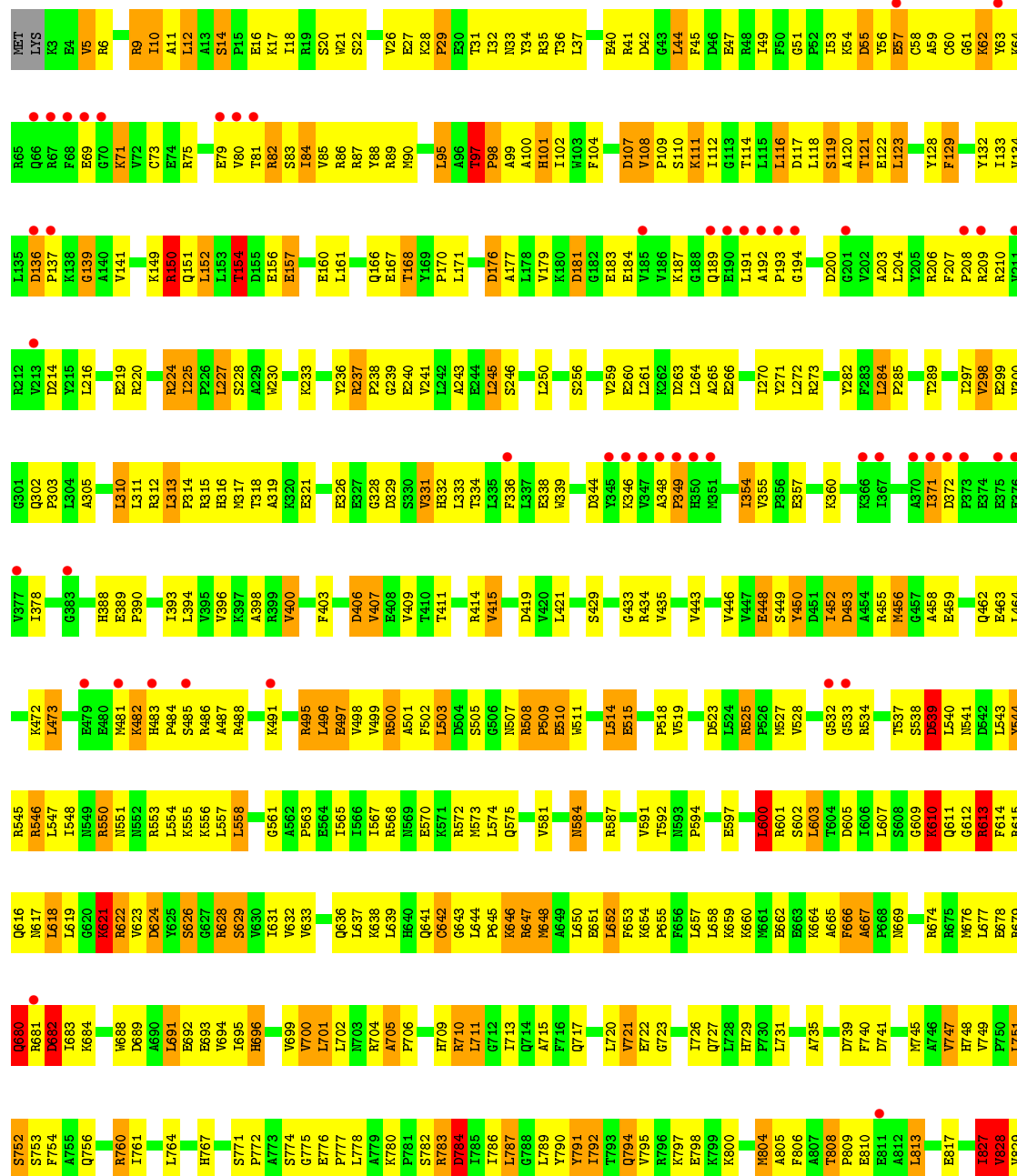


Chain C: ■ 39% ■ 42% ■ 15%

The treemap displays a hierarchical structure of 1000 items, categorized by color: Green (39%), Orange (42%), and Red (15%). The items are arranged in a grid-like structure, with rows and columns. The top row contains 10 items, and the bottom row contains 10 items. The items are labeled with numbers and letters, such as Q930, H860, K786, T715, R642, R573, T501, F425, K276, T206, S138, M1, Q930, F934, D863, G935, V936, D937, K938, R939, H868, V869, L944, A945, E948, K949, L940, L974, G951, H976, L952, P977, S988, R978, P959, E960, N980, L981, L986, K983, K964, E965, L966, P967, D968, L969, L897, K970, K971, V972, G973, D989, L974, L975, Y901, L902, R976, G977, S903, R978, R904, V905, V906, G980, E981, L907, F982, F983, E984, L987, K988, D989, E989, L994, L995, F996, L997, K998, L999, M1000.

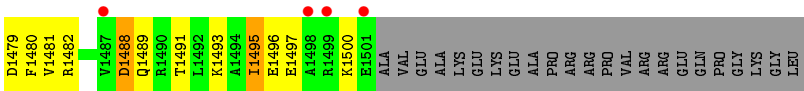


• Molecule 3: DNA-directed RNA polymerase beta' chain









• Molecule 4: DNA-directed RNA polymerase omega chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	199.19Å 199.19Å 289.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.20 39.84 – 3.18	Depositor EDS
% Data completeness (in resolution range)	93.1 (40.00-3.20) 92.3 (39.84-3.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.281 , 0.346 0.259 , 0.260	Depositor DCC
R_{free} test set	4796 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	69.0	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	24369	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% 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, SRN

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	0.52	0/1798	0.88	10/2453 (0.4%)
1	B	0.52	0/1784	0.87	6/2428 (0.2%)
2	C	0.55	0/8744	0.88	35/11850 (0.3%)
3	D	0.52	0/9772	0.81	27/13234 (0.2%)
3	J	0.49	0/1897	0.81	7/2570 (0.3%)
4	K	0.52	0/762	0.79	1/1029 (0.1%)
All	All	0.53	0/24757	0.84	86/33564 (0.3%)

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	3
3	D	0	2
All	All	0	5

There are no bond length outliers.

The worst 5 of 86 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	680	ASP	CB-CG-OD2	7.16	124.74	118.30
2	C	554	ASP	CB-CG-OD2	6.96	124.56	118.30
3	D	860	LEU	CA-CB-CG	6.92	131.22	115.30
2	C	492	ASP	CB-CG-OD2	6.87	124.48	118.30
1	B	193	ASP	CB-CG-OD2	6.71	124.34	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	1076	VAL	Peptide
2	C	213	ALA	Peptide
2	C	671	ASN	Peptide
3	D	1207	TYR	Peptide
3	D	21	TRP	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	1763	0	1760	117	0
1	B	1750	0	1775	77	0
2	C	8578	0	8517	538	0
3	D	9602	0	9556	504	0
3	J	1869	0	1876	88	0
4	K	747	0	735	41	0
5	C	58	0	64	5	0
6	D	2	0	0	0	0
All	All	24369	0	24283	1265	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 26.

The worst 5 of 1265 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:D:705:ALA:CB	3:D:706:PRO:HD3	1.72	1.17
3:D:643:GLY:HA3	3:D:727:GLN:H	1.12	1.15
2:C:263:ASP:HB3	2:C:264:PRO:HD3	1.18	1.12
3:D:1110:ALA:HA	3:D:1202:GLN:HB3	1.33	1.09
3:D:551:ASN:O	3:D:555:LYS:HB2	1.51	1.08

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	228/314 (73%)	169 (74%)	45 (20%)	14 (6%)	1	12
1	B	223/314 (71%)	177 (79%)	33 (15%)	13 (6%)	1	13
2	C	1112/1119 (99%)	859 (77%)	168 (15%)	85 (8%)	1	7
3	D	1236/1524 (81%)	971 (79%)	186 (15%)	79 (6%)	1	10
3	J	247/1524 (16%)	190 (77%)	39 (16%)	18 (7%)	1	7
4	K	93/99 (94%)	66 (71%)	18 (19%)	9 (10%)	0	3
All	All	3139/4894 (64%)	2432 (78%)	489 (16%)	218 (7%)	1	8

5 of 218 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	TYR
1	A	111	ALA
1	A	139	TYR
1	A	187	GLY
1	A	203	GLY

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	189/270 (70%)	135 (71%)	54 (29%)	0	1
1	B	191/270 (71%)	138 (72%)	53 (28%)	0	1
2	C	889/936 (95%)	633 (71%)	256 (29%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	992/1281 (77%)	715 (72%)	277 (28%)	0	1
3	J	191/1281 (15%)	123 (64%)	68 (36%)	0	0
4	K	75/88 (85%)	53 (71%)	22 (29%)	0	1
All	All	2527/4126 (61%)	1797 (71%)	730 (29%)	0	1

5 of 730 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	963	LEU
3	D	216	LEU
3	J	1389	LEU
2	C	1010	THR
3	D	40	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	860	HIS
2	C	1030	GLN
3	J	1374	GLN
2	C	889	HIS
3	D	33	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 2 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
5	SRN	C	1120	-	57,62,62	1.34	4 (7%)	58,84,84	1.68	10 (17%)

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
5	SRN	C	1120	-	-	10/50/105/105	0/2/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1120	SRN	O1-C1	6.91	1.48	1.34
5	C	1120	SRN	C2-C1	-4.71	1.37	1.48
5	C	1120	SRN	C5-C6	-3.50	1.34	1.44
5	C	1120	SRN	C3-C4	-3.12	1.35	1.44

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1120	SRN	O1-C1-C2	5.25	123.29	111.38
5	C	1120	SRN	O1-C33-C47	-3.80	100.97	108.85
5	C	1120	SRN	C34-C9-C10	-3.53	106.16	114.05
5	C	1120	SRN	C35-O8-C12	3.22	118.53	112.81
5	C	1120	SRN	C8-C7-C6	-3.18	119.38	125.61

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

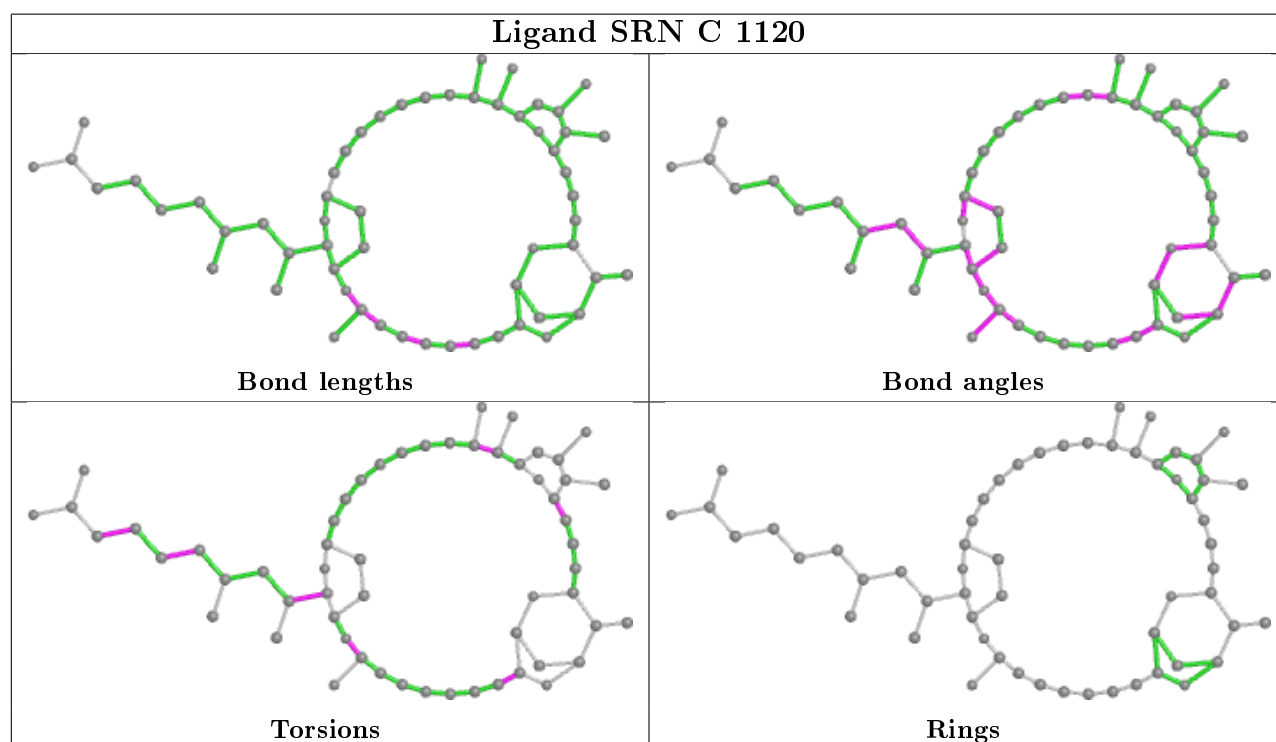
Mol	Chain	Res	Type	Atoms
5	C	1120	SRN	C42-C43-C44-C45
5	C	1120	SRN	O7-C32-C36-C37
5	C	1120	SRN	O2-C1-O1-C33
5	C	1120	SRN	C2-C1-O1-C33
5	C	1120	SRN	C39-C41-C42-C43

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1120	SRN	5	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 ⓘ

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	230/314 (73%)	-0.27	2 (0%) 84 75	22, 43, 76, 112	0
1	B	225/314 (71%)	-0.33	1 (0%) 92 89	24, 51, 81, 86	0
2	C	1114/1119 (99%)	-0.28	13 (1%) 79 67	19, 50, 90, 115	0
3	D	1238/1524 (81%)	-0.10	59 (4%) 30 18	18, 49, 94, 139	0
3	J	249/1524 (16%)	0.02	15 (6%) 21 12	24, 51, 125, 139	0
4	K	95/99 (95%)	-0.24	2 (2%) 63 49	27, 64, 149, 162	0
All	All	3151/4894 (64%)	-0.19	92 (2%) 51 36	18, 50, 95, 162	0

The worst 5 of 92 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	191	LEU	8.9
3	D	193	PRO	7.3
3	D	346	LYS	5.3
3	D	1240	THR	5.3
3	D	373	PRO	5.0

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

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

6.3 Carbohydrates ⓘ

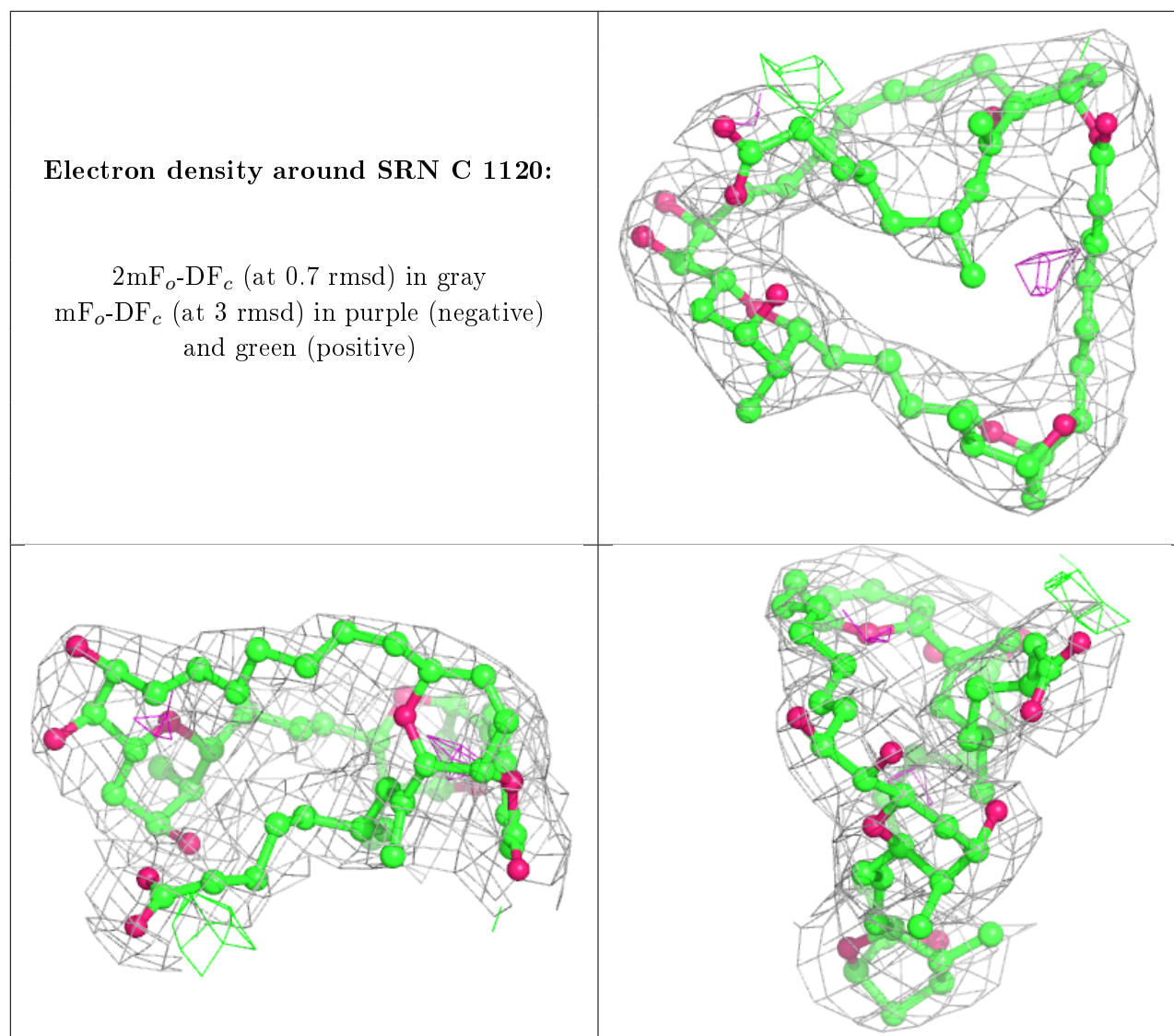
There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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
5	SRN	C	1120	58/58	0.92	0.27	33,45,56,59	0
6	ZN	D	1526	1/1	0.93	0.13	64,64,64,64	0
6	ZN	D	1525	1/1	0.96	0.03	77,77,77,77	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.