W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

May 22, 2020 – 12:09 am BST

PDB ID	:	4Q0B
Title	:	Crystal structure of HIV-1 reverse transcriptase in complex with gap-RNA/DNA and Nevirapine
Authors	:	Das, K.; Martinez, S.E.; Arnold, E.
Deposited on	:	2014-04-01
Resolution	:	3.30 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 (i) symbol.

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The following versions of software and data (see references (1)) were used in the production of this report:

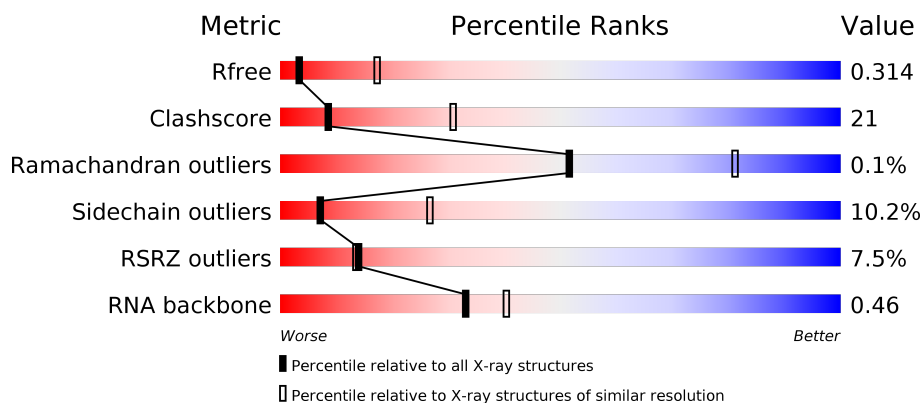|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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	Percentile Ranks	Value
Rfree		0.314
Clashscore		21
Ramachandran outliers		0.1%
Sidechain outliers		10.2%
RSRZ outliers		7.5%
RNA backbone		0.46

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

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 <=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	556	10% · 50% · 45% ·
1	C	556	12% · 58% · 38% ·
2	B	428	2% · 55% · 37% · ·
2	D	428	2% · 53% · 39% · 5% ·

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Mol	Chain	Length	Quality of chain
3	E	14	21% 14% 29% 36%
3	T	14	7% 29% 29% 36%
4	e	12	17% 33% 25% 17% 25%
4	t	12	17% 17% 67% 17%
5	F	21	24% 38% 38% 14% 10%
5	P	21	5% 52% 29% 10% 10%

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 17428 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 HIV-1 reverse transcriptase, p66 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total 4512	C 2920	N 751	O 833	S 8	0	0	0
1	C	555	Total 4506	C 2917	N 748	O 833	S 8	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	EXPRESSION TAG	UNP P03366
A	0	VAL	-	EXPRESSION TAG	UNP P03366
A	258	CYS	GLN	ENGINEERED MUTATION	UNP P03366
A	280	SER	CYS	ENGINEERED MUTATION	UNP P03366
A	498	ASN	ASP	ENGINEERED MUTATION	UNP P03366
C	-1	MET	-	EXPRESSION TAG	UNP P03366
C	0	VAL	-	EXPRESSION TAG	UNP P03366
C	258	CYS	GLN	ENGINEERED MUTATION	UNP P03366
C	280	SER	CYS	ENGINEERED MUTATION	UNP P03366
C	498	ASN	ASP	ENGINEERED MUTATION	UNP P03366

- Molecule 2 is a protein called HIV-1 reverse transcriptase, p51 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	412	Total 3400	C 2212	N 563	O 619	S 6	0	0	0
2	D	412	Total 3400	C 2212	N 563	O 619	S 6	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	ENGINEERED MUTATION	UNP P03366
D	280	SER	CYS	ENGINEERED MUTATION	UNP P03366

- Molecule 3 is a RNA chain called 5'-R(*AP*UP*GP*GP*UP*CP*GP*GP*CP*GP*CP*CP*CP*G)-3'.

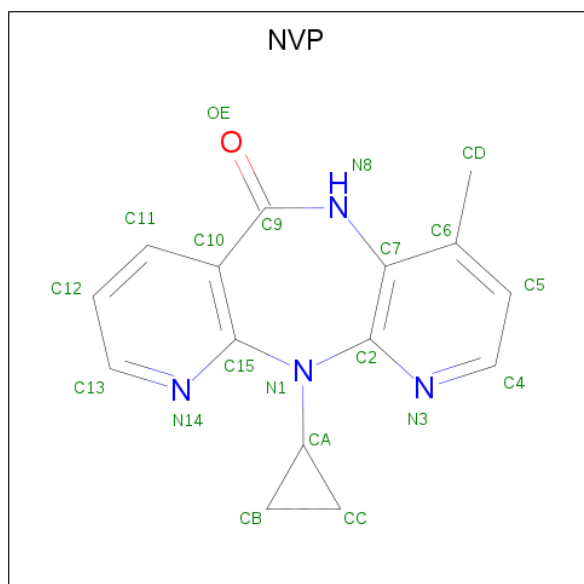| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	9	Total	C	N	O	P	0	0	0
			192	85	35	63	9			
3	E	9	Total	C	N	O	P	0	0	0
			192	85	35	63	9			

- Molecule 4 is a RNA chain called 5'-R(P*AP*CP*AP*GP*GP*GP*AP*CP*UP*GP*UP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	t	10	Total	C	N	O	P	0	0	0
			219	97	43	69	10			
4	e	9	Total	C	N	O	P	0	0	0
			196	87	38	62	9			

- Molecule 5 is a DNA chain called 5'-D(*A*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*GP*CP*GP*CP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	P	19	Total	C	N	O	P	0	0	0
			382	182	67	115	18			
5	F	19	Total	C	N	O	P	0	0	0
			382	182	67	115	18			

- Molecule 6 is 11-CYCLOPROPYL-5,11-DIHYDRO-4-METHYL-6H-DIPYRIDO[3,2-B:2',3'-E][1,4]DIAZEPIN-6-ONE (three-letter code: NVP) (formula: $C_{15}H_{14}N_4O$).
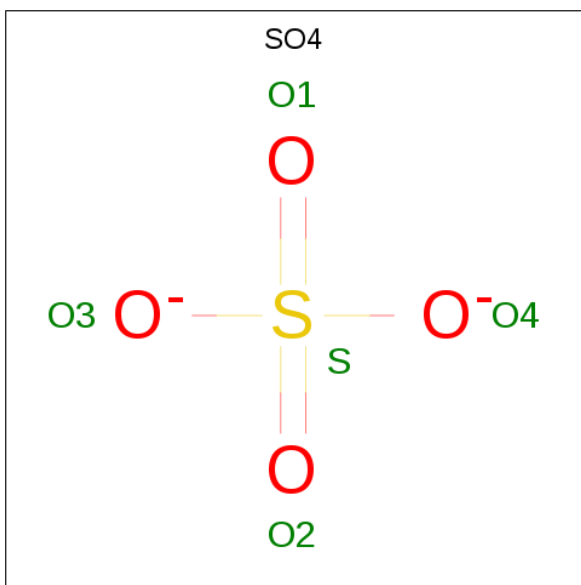
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			20	15	4	1		
6	C	1	Total	C	N	O	0	0
			20	15	4	1		

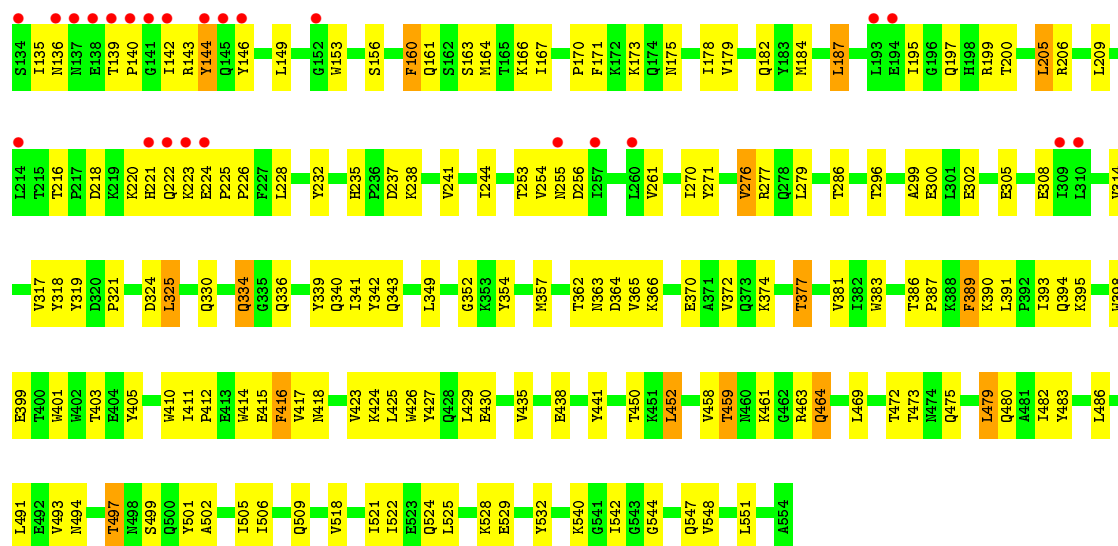- Molecule 7 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mn	0	0
			1	1		
7	C	1	Total	Mn	0	0
			1	1		

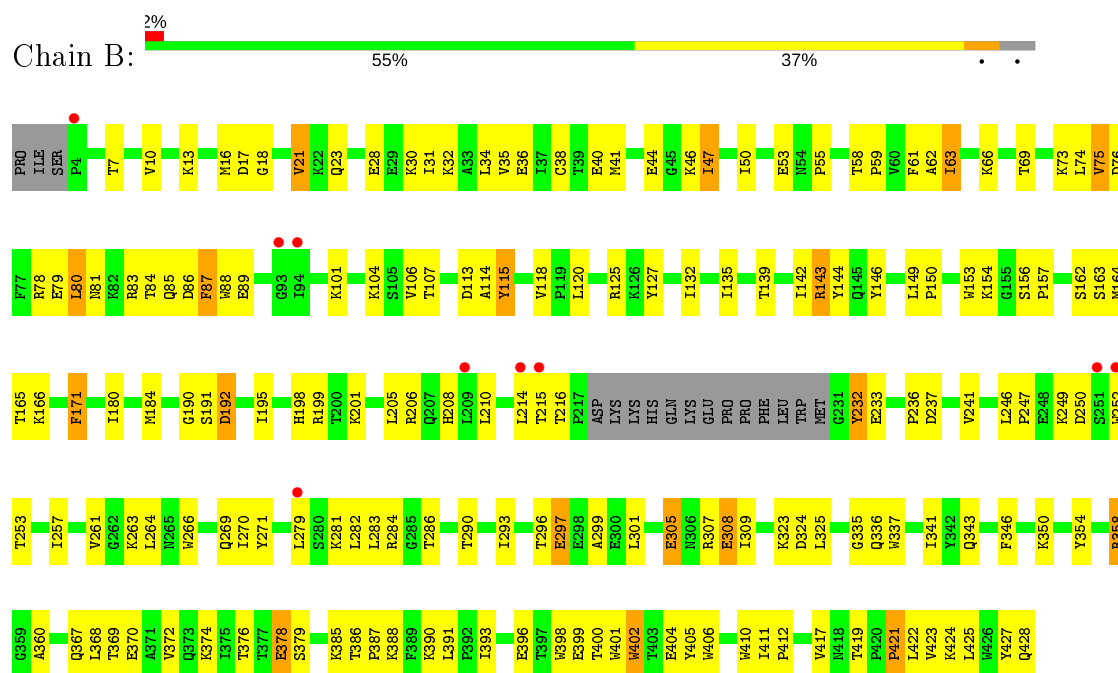- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	e	1	Total	O	S	0	0
			5	4	1		

3 Residue-property plots (i)

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: HIV-1 reverse transcriptase, p66 subunit
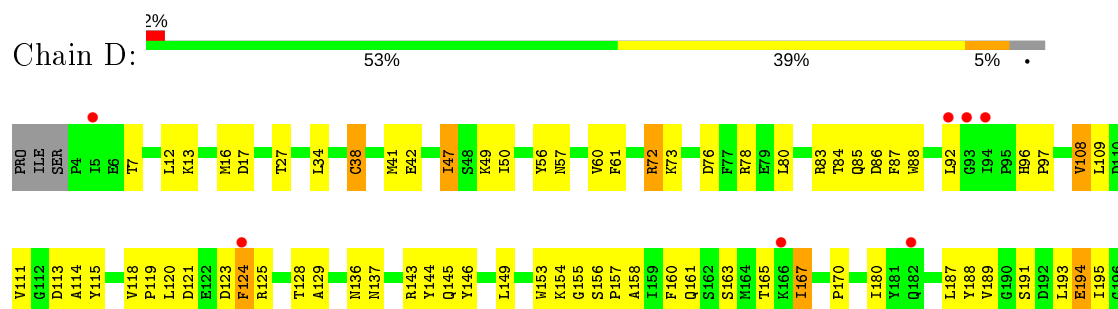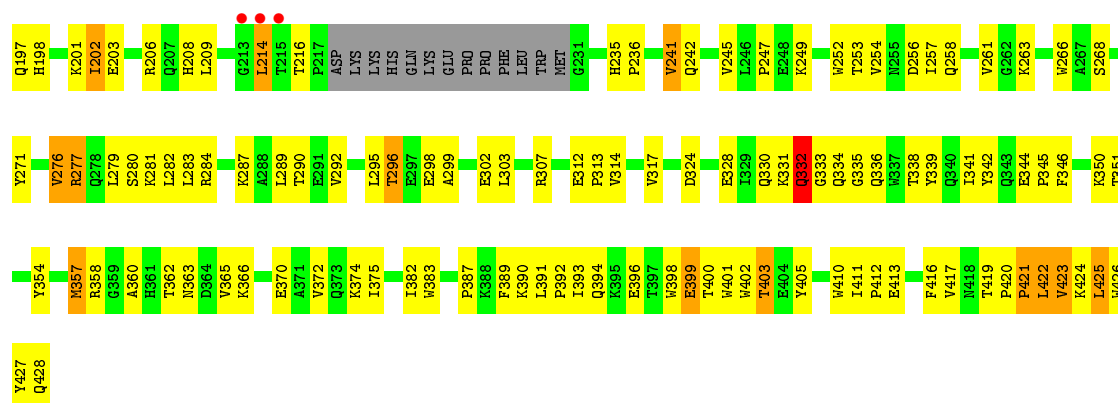

- Molecule 1: HIV-1 reverse transcriptase, p66 subunit

• Molecule 2: HIV-1 reverse transcriptase, p51 subunit

• Molecule 2: HIV-1 reverse transcriptase, p51 subunit

- Molecule 3: 5'-R(*AP*UP*GP*GP*UP*CP*GP*GP*CP*GP*CP*CP*CP*G)-3'

Chain T:
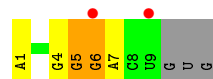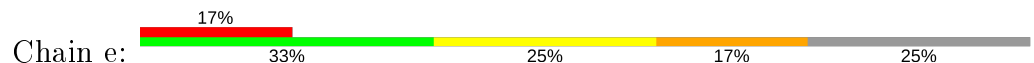

- Molecule 3: 5'-R(*AP*UP*GP*GP*UP*CP*GP*GP*CP*GP*CP*CP*CP*G)-3'

Chain E:

- Molecule 4: 5'-R(P*AP*CP*AP*GP*GP*GP*AP*CP*UP*GP*UP*G)-3'

Chain t:

- Molecule 4: 5'-R(P*AP*CP*AP*GP*GP*GP*AP*CP*UP*GP*UP*G)-3'

Chain e:
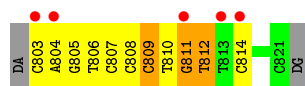

- Molecule 5: 5'-D(*A*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*GP*CP*GP*CP*CP*G)-3'

Chain P:

• Molecule 5: 5'-D(*A*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*GP*CP*GP
*CP*CP*G)-3'

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.72Å 131.05Å 141.63Å 90.00° 100.69° 90.00°	Depositor
Resolution (Å)	46.39 – 3.30 47.49 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.6 (46.39-3.30) 98.5 (47.49-3.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.68 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.235 , 0.317 0.237 , 0.314	Depositor DCC
R_{free} test set	1420 reflections (2.97%)	wwPDB-VP
Wilson B-factor (Å^2)	77.7	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 63.5	EDS
L-test for twinning[2]	$<|L|> = 0.43, <L^2> = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	17428	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ 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: MN, SO4, NVP

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	0.61	0/4630	0.78	1/6290 (0.0%)
1	C	0.63	1/4624 (0.0%)	0.78	1/6283 (0.0%)
2	B	0.65	0/3497	0.82	3/4751 (0.1%)
2	D	0.67	0/3497	0.83	4/4751 (0.1%)
3	E	0.39	0/213	1.07	0/330
3	T	0.37	0/213	1.01	0/330
4	e	0.93	1/219 (0.5%)	1.41	5/338 (1.5%)
4	t	0.77	1/245 (0.4%)	1.09	0/379
5	F	1.04	3/426 (0.7%)	1.14	3/655 (0.5%)
5	P	0.96	2/426 (0.5%)	1.05	3/655 (0.5%)
All	All	0.66	8/17990 (0.0%)	0.84	20/24762 (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	A	0	3
1	C	0	1
2	B	0	1
2	D	0	2
All	All	0	7

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	e	1	A	OP3-P	-11.16	1.47	1.61
4	t	1	A	OP3-P	-9.18	1.50	1.61
5	F	811	DG	C4'-O4'	7.68	1.52	1.45
5	F	809	DC	C4'-O4'	7.33	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	812	DT	C4'-O4'	-7.30	1.37	1.45

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	811	DG	O4'-C4'-C3'	-8.96	100.62	106.00
4	e	4	G	OP1-P-O3'	8.70	124.34	105.20
4	e	6	G	OP1-P-O3'	8.42	123.72	105.20
4	e	5	G	OP1-P-O3'	7.81	122.37	105.20
5	F	809	DC	O4'-C4'-C3'	-7.49	101.50	104.50

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	ASP	Mainchain
1	A	35	VAL	Mainchain
1	A	389	PHE	Mainchain
2	B	421	PRO	Peptide
1	C	389	PHE	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	4512	0	4571	215	0
1	C	4506	0	4560	170	0
2	B	3400	0	3433	135	0
2	D	3400	0	3433	152	0
3	E	192	0	100	9	0
3	T	192	0	100	8	0
4	e	196	0	99	0	0
4	t	219	0	110	0	0
5	F	382	0	215	12	0
5	P	382	0	215	11	0
6	A	20	0	14	1	0
6	C	20	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	e	5	0	0	0	0
All	All	17428	0	16864	688	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 21.

The worst 5 of 688 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:C:416:PHE:HD1	1:C:417:VAL:N	1.53	1.06
1:C:21:VAL:H	1:C:57:ASN:HB2	1.23	1.01
1:C:416:PHE:CD1	1:C:417:VAL:N	2.30	0.98
1:A:416:PHE:CD1	1:A:417:VAL:N	2.38	0.92
1:A:416:PHE:HD1	1:A:417:VAL:N	1.69	0.91

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	553/556 (100%)	526 (95%)	26 (5%)	1 (0%)	47	77
1	C	553/556 (100%)	522 (94%)	30 (5%)	1 (0%)	47	77
2	B	408/428 (95%)	395 (97%)	13 (3%)	0	100	100
2	D	408/428 (95%)	397 (97%)	11 (3%)	0	100	100
All	All	1922/1968 (98%)	1840 (96%)	80 (4%)	2 (0%)	51	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	PRO
1	C	4	PRO

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	495/497 (100%)	443 (90%)	52 (10%)	7	25
1	C	494/497 (99%)	446 (90%)	48 (10%)	8	29
2	B	374/390 (96%)	336 (90%)	38 (10%)	7	27
2	D	374/390 (96%)	334 (89%)	40 (11%)	6	25
All	All	1737/1774 (98%)	1559 (90%)	178 (10%)	7	27

5 of 178 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	308	GLU
1	C	94	ILE
2	D	344	GLU
2	B	341	ILE
1	C	2	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	85	GLN
1	C	161	GLN
1	C	373	GLN
1	A	418	ASN
1	C	336	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	E	8/14 (57%)	3 (37%)	2 (25%)
3	T	8/14 (57%)	5 (62%)	1 (12%)
4	e	8/12 (66%)	3 (37%)	0
4	t	9/12 (75%)	7 (77%)	0
All	All	33/52 (63%)	18 (54%)	3 (9%)

5 of 18 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	T	9	C
3	T	11	C
3	T	12	C
3	T	13	C
3	T	14	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	T	11	C
3	E	11	C
3	E	13	C

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 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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
8	SO4	e	801	-	4,4,4	0.16	0	6,6,6	0.11	0
6	NVP	C	901	-	15,23,23	2.05	6 (40%)	13,34,34	2.13	7 (53%)
6	NVP	A	901	-	15,23,23	2.08	5 (33%)	13,34,34	2.11	6 (46%)

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	NVP	C	901	-	-	0/0/6/6	0/3/4/4
6	NVP	A	901	-	-	0/0/6/6	0/3/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	901	NVP	C4-N3	3.96	1.40	1.32
6	A	901	NVP	C4-N3	3.89	1.40	1.32
6	A	901	NVP	C2-N3	3.76	1.40	1.35
6	A	901	NVP	C13-N14	3.73	1.40	1.32
6	C	901	NVP	C13-N14	3.60	1.39	1.32

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	901	NVP	C11-C10-C15	3.70	121.67	117.11
6	C	901	NVP	C5-C4-N3	-3.14	119.72	124.58
6	A	901	NVP	CD-C6-C7	2.94	122.88	120.03
6	A	901	NVP	C10-C15-N14	-2.92	120.13	124.62
6	C	901	NVP	C10-C15-N14	-2.86	120.22	124.62

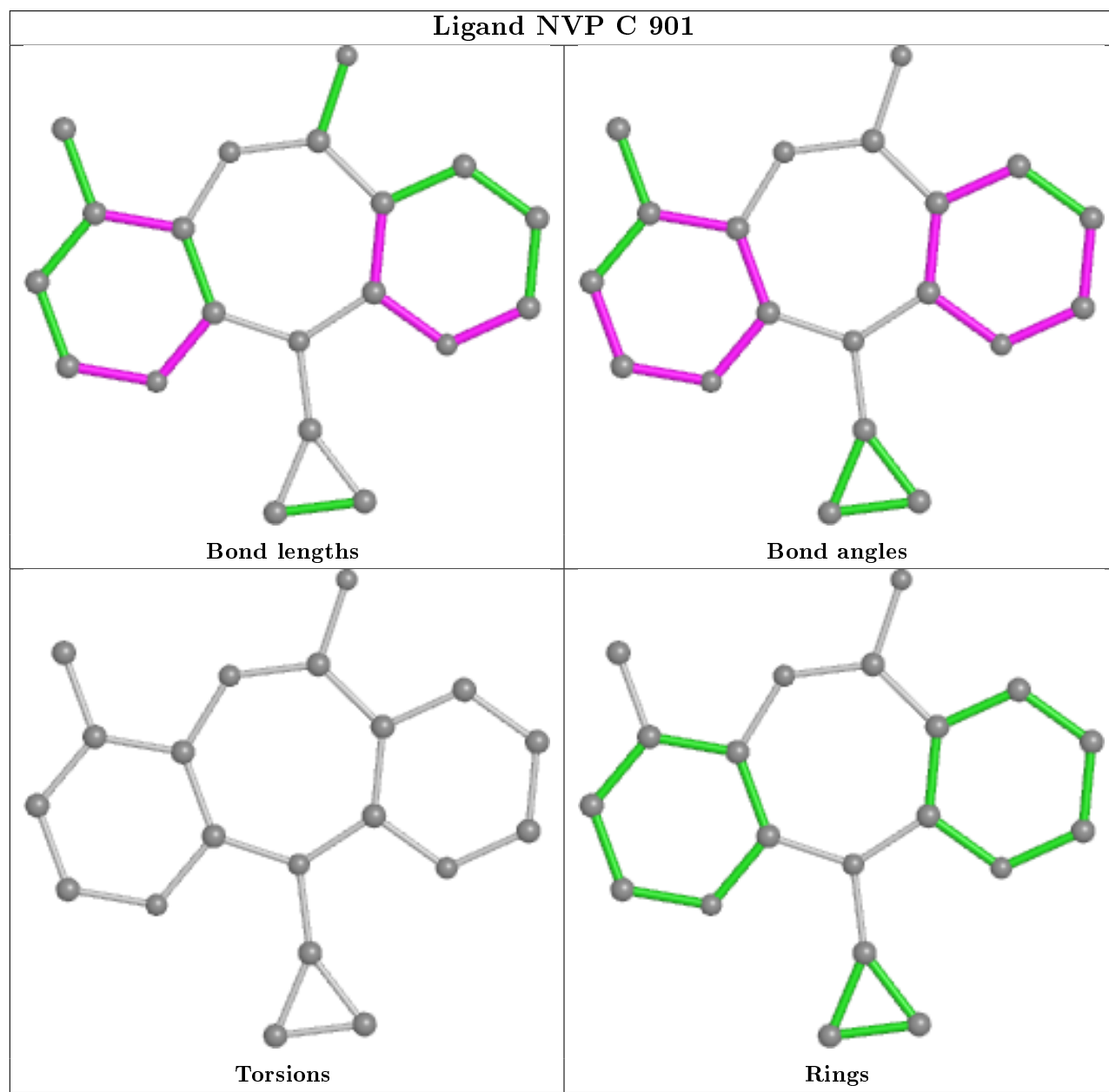There are no chirality outliers.

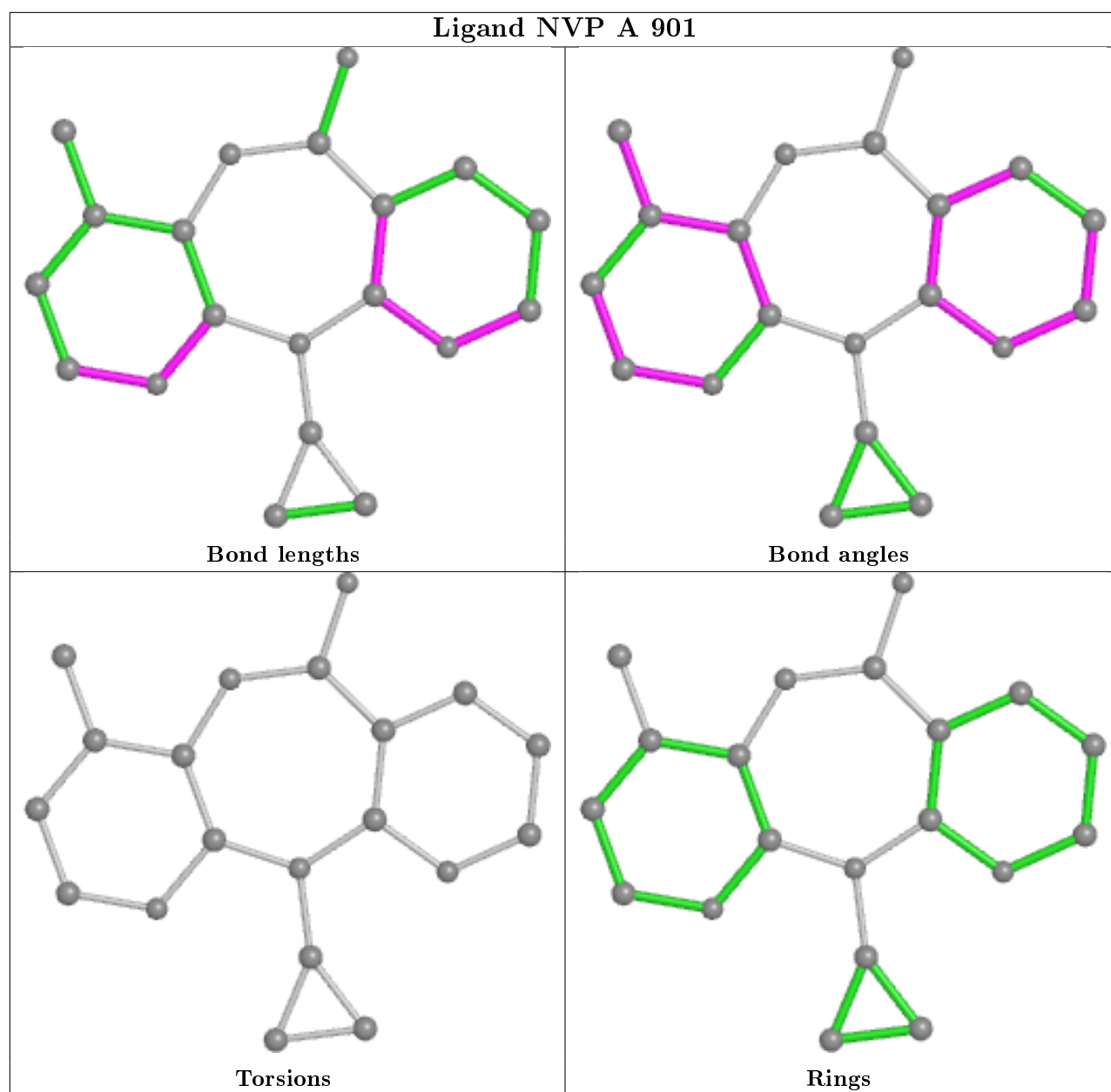There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	901	NVP	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 then 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.

Ligand NVP C 901

Bond lengths

Bond angles

Torsions

Rings

Ligand NVP A 901

Bond lengths

Bond angles

Torsions

Rings

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(Å²)	Q<0.9
1	A	555/556 (99%)	0.51	53 (9%)	8	8	21, 82, 195, 225	0
1	C	555/556 (99%)	0.65	69 (12%)	4	3	16, 93, 206, 228	0
2	B	412/428 (96%)	0.03	9 (2%)	62	60	23, 64, 113, 140	0
2	D	412/428 (96%)	0.06	10 (2%)	59	56	22, 68, 120, 150	0
3	E	9/14 (64%)	0.57	0	100	100	149, 156, 179, 197	0
3	T	9/14 (64%)	0.45	0	100	100	139, 144, 168, 201	0
4	e	9/12 (75%)	0.98	2 (22%)	0	1	127, 136, 165, 175	0
4	t	10/12 (83%)	0.52	2 (20%)	1	1	103, 124, 159, 172	0
5	F	19/21 (90%)	1.15	5 (26%)	0	0	96, 140, 198, 200	0
5	P	19/21 (90%)	0.39	1 (5%)	26	24	78, 125, 174, 176	0
All	All	2009/2062 (97%)	0.37	151 (7%)	14	13	16, 76, 185, 228	0

The worst 5 of 151 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	133	PRO	21.2
1	C	31	ILE	12.8
1	A	62	ALA	12.3
1	A	61	PHE	10.8
1	C	62	ALA	10.4

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 carbohydrates 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
8	SO4	e	801	5/5	0.67	0.15	173,175,182,185	0
6	NVP	A	901	20/20	0.91	0.42	64,72,79,79	0
6	NVP	C	901	20/20	0.93	0.38	79,85,91,93	0
7	MN	A	902	1/1	0.95	0.24	73,73,73,73	0
7	MN	C	902	1/1	0.97	0.11	63,63,63,63	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.
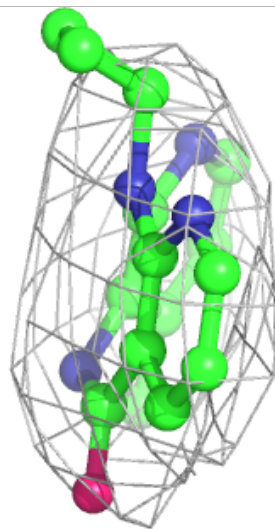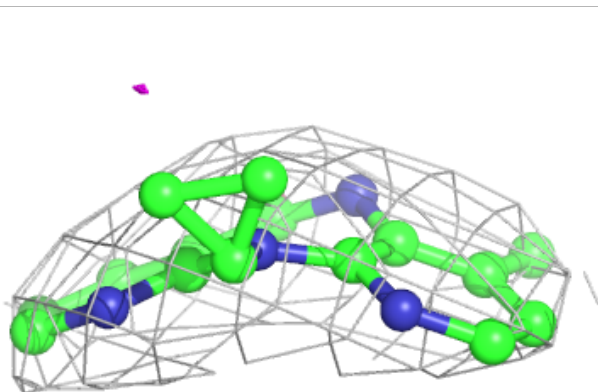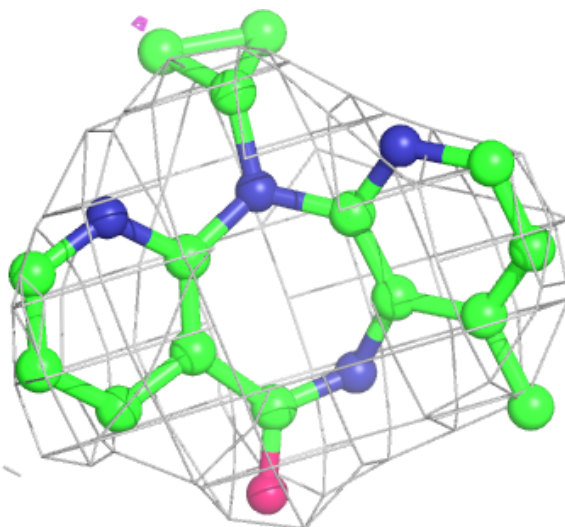
Electron density around NVP A 901:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
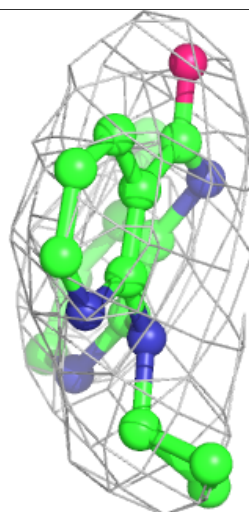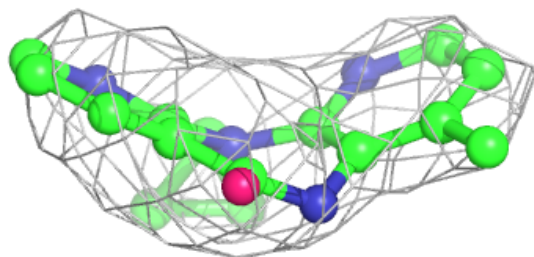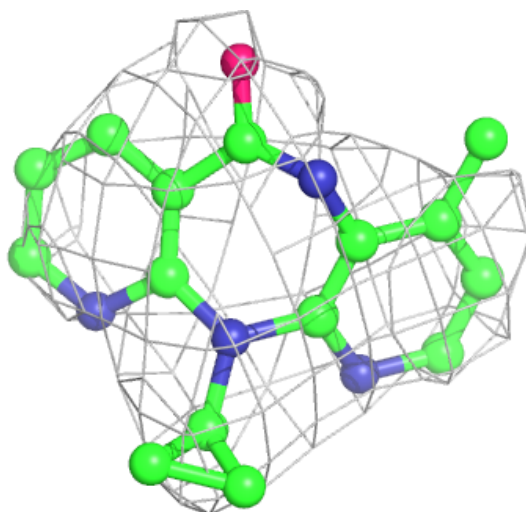
Electron density around NVP C 901:

$2mF_o$-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.