



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 04:48 AM UTC

PDB ID : 1LWF / pdb_00001lwf
Title : CRYSTAL STRUCTURE OF A MUTANT HIV-1 REVERSE TRANSCRIPTASE (RTMQ+M184V: M41L/D67N/K70R/M184V/T215Y) IN COMPLEX WITH NEVIRAPINE
Authors : Ren, J.; Chamberlain, P.P.; Nichols, C.E.; Douglas, L.; Stuart, D.I.; Stammers, D.K.
Deposited on : 2002-05-31
Resolution : 2.80 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](#) ①) 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

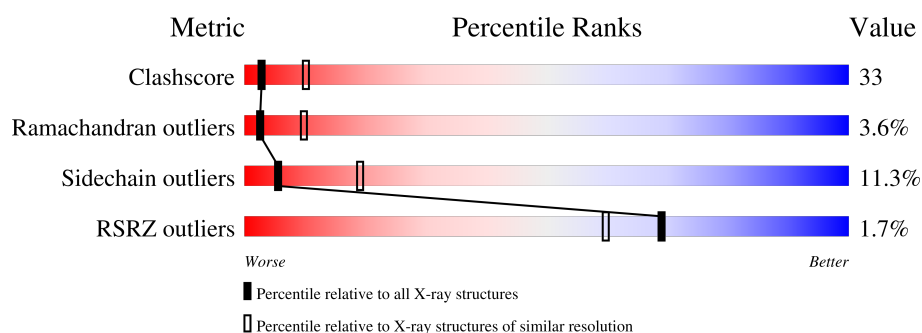
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	560	2% 40% 47% 9% . .
2	B	440	% 40% 39% 10% . 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7729 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	543	Total	C	N	O	S	0	0	0
			4424	2864	734	820	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	LEU	MET	engineered mutation	UNP P04585
A	67	ASN	ASP	engineered mutation	UNP P04585
A	70	ARG	LYS	engineered mutation	UNP P04585
A	184	VAL	MET	engineered mutation	UNP P04585
A	215	TYR	THR	engineered mutation	UNP P04585
A	280	CSD	CYS	modified residue	UNP P04585

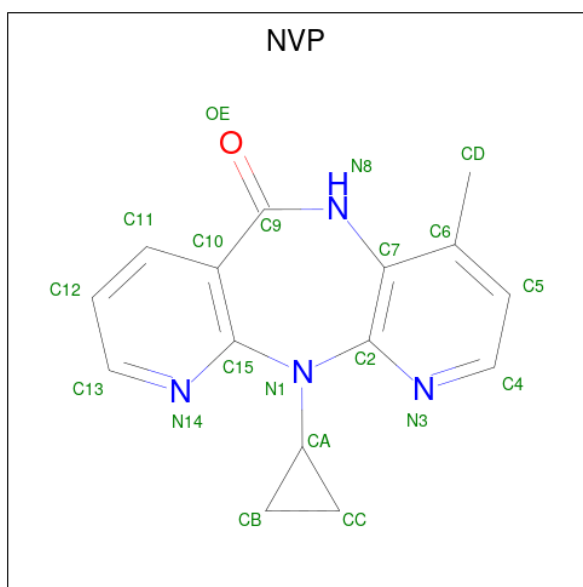
- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	395	Total	C	N	O	S	0	0	0
			3272	2125	549	593	5			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	41	LEU	MET	engineered mutation	UNP P04585
B	67	ASN	ASP	engineered mutation	UNP P04585
B	70	ARG	LYS	engineered mutation	UNP P04585
B	184	VAL	MET	engineered mutation	UNP P04585
B	215	TYR	THR	engineered mutation	UNP P04585

- Molecule 3 is 11-CYCLOPROPYL-5,11-DIHYDRO-4-METHYL-6H-DIPYRIDO[3,2-B:2',3'-E][1,4]DIAZEPIN-6-ONE (CCD ID: NVP) (formula: C₁₅H₁₄N₄O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			20	15	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total	O	0	0
			9	9		
4	B	4	Total	O	0	0
			4	4		

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.

Chain A:

Position	Amino Acid	Category
P1	P1	Red
ARG	ARG	Green
SER	SER	Green
H208	H208	Green
Q278	Q278	Green
R358	R358	Green
G444	G444	Green
S514	S514	Green
S515	S515	Green
S516	S516	Green
S517	S517	Green
S518	S518	Green
S519	S519	Green
Q520	Q520	Green
L521	L521	Green
L522	L522	Green
L523	L523	Green
Q524	Q524	Green
E529	E529	Green
K530	K530	Green
W535	W535	Green
V536	V536	Green
F537	F537	Green
A538	A538	Green
L542	L542	Green
G543	G543	Green
G544	G544	Green
M545	M545	Green
E546	E546	Green
Q547	Q547	Green
V548	V548	Green
D549	D549	Green
V552	V552	Green
S553	S553	Green
G554	G554	Green
I555	I555	Green
I556	I556	Green
ARG	ARG	Green
LYS	LYS	Green
VAL	VAL	Green
LEU	LEU	Green

Chain B:

Category	Percentage
PRO	40%
ILE	39%
SER	10%
PRO	10%
ILE	0%

K73	L74	V75	D76	F77	R78	E79	L80	K81	K82	R83	T84	Q85	D86	F87	TRP	GLU	VAL	GLN	LEU	GLY	ILE	PRO	H96	P97	A98	G99	L100	K101	K102	K103	K104	S105	V106		D110	V111	G112	D113	A114	Y115	F116	S117	V118	P119	L120	D121	E122	D123	F124	A125		F130	T131	I132	P133	S134	I135	N136	N137
E138	T139	P140		R143	Y144	Q145	Y146		Q151	K154	G155	S156	P157	A158	I159	F160	Q161	S162	S163	M164	T165	K166	I167	L168	E169	P170	F171	R172	K173	Q174	M175	P176	D177	I178	V179	I180	Y183	V184	D185		Y188		S191	D192	L193	E194	I195	G196	Q197	H198	R199	T200	K201	I202		L205	R206		
	L210	F211	W212	GLY	LEU	TYR	THR	PRO	ASP	LYS	LYS	HIS	GLN	LYS	GLU	PRO	PRO	PHE	LEU	TRP	MET	GLY	TYR	E233	L234	H235	P236	D237	K238	W239		Q242	P243		D250		V254		I257	V261	G262	K263		W266		I270	Y271	V276	R277		C280	K281	L282	L283	R284	G285	T286		
K287	A288	L289	T290		L293	P294	L295	T296	E297	E298	A299	E300		E308		K311	E312		Y319	D320	P321		L325	L326		Q332		Q336	W337	T338		I341		E344	P345		L349	K350		Y354	A355	R356	M357	R358		H361	T362	N363	D364	V365	K366	Q367	L368		V372	Q373	K374	I375	T376
T377	E378	S379	I380	G384	P387	K388	F389	K390	E399	L391	P392	I393	Q394	K395		E399	T400	W401	W402	T403	E404	Q407		T411	F416	V417	N418	T419	P420	P421	L422	V423	K424	L425	W426	Y427	Q428	LEU	GLU	LYS	GLU	PRO	ILE	VAL	GLY	ALA	GLU	THR	PHE										

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	137.90Å 109.50Å 74.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.00 – 2.80 26.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.5 (26.00-2.80) 98.3 (26.00-2.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.76Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.234 , 0.289 0.213 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	68.0	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 91.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7729	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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: CSD, 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	0.66	1/4530 (0.0%)	1.18	35/6157 (0.6%)
2	B	0.64	0/3362	1.16	27/4566 (0.6%)
All	All	0.65	1/7892 (0.0%)	1.17	62/10723 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	375	ILE	CA-CB	-5.02	1.48	1.54

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	224	GLU	CA-C-N	11.56	128.10	119.66
1	A	224	GLU	C-N-CA	11.56	128.10	119.66
2	B	65	LYS	N-CA-C	-11.46	92.75	109.59
1	A	175	ASN	CA-C-N	11.23	130.92	119.24
1	A	175	ASN	C-N-CA	11.23	130.92	119.24

There are no chirality outliers.

There are no planarity outliers.

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	4424	0	4464	300	0
2	B	3272	0	3305	218	0
3	A	20	0	14	0	0
4	A	9	0	0	1	0
4	B	4	0	0	1	0
All	All	7729	0	7783	508	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 33.

The worst 5 of 508 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:A:240:THR:HG22	1:A:315:HIS:HB3	1.34	1.09
1:A:132:ILE:HB	1:A:142:ILE:HB	1.36	1.06
1:A:270:ILE:HD11	1:A:314:VAL:HG11	1.41	1.03
2:B:175:ASN:HD21	2:B:201:LYS:NZ	1.59	1.00
2:B:103:LYS:HE3	2:B:179:VAL:HG23	1.42	0.98

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	536/560 (96%)	460 (86%)	59 (11%)	17 (3%)	3	11
2	B	389/440 (88%)	324 (83%)	49 (13%)	16 (4%)	2	8
All	All	925/1000 (92%)	784 (85%)	108 (12%)	33 (4%)	2	10

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	PRO
1	A	114	ALA
1	A	138	GLU
1	A	230	MET
1	A	543	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	483/499 (97%)	426 (88%)	57 (12%)	5	17
2	B	360/400 (90%)	322 (89%)	38 (11%)	6	22
All	All	843/899 (94%)	748 (89%)	95 (11%)	5	19

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	8	VAL
2	B	120	LEU
2	B	31	ILE
2	B	69	THR
2	B	162	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	524	GLN
2	B	85	GLN
2	B	361	HIS
2	B	57	ASN
2	B	147	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\# Z > 2$
1	CSD	A	280	1	4,7,8	2.76	1 (25%)	1,8,10	11.54	1 (100%)

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
1	CSD	A	280	1	-	2/2/6/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	CSD	OD1-SG	5.07	1.52	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CSD	OD1-SG-CB	11.54	126.86	105.60

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	280	CSD	N-CA-CB-SG
1	A	280	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

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	$\# Z > 2$
3	NVP	A	999	-	23,23,23	1.37	3 (13%)	34,34,34	1.83	6 (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
3	NVP	A	999	-	-	0/4/6/6	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	NVP	C15-N1	4.22	1.46	1.42
3	A	999	NVP	C2-N1	-2.38	1.39	1.42
3	A	999	NVP	C10-C9	2.17	1.52	1.49

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	NVP	C7-N8-C9	5.76	133.04	128.29
3	A	999	NVP	C7-C2-N1	-5.18	118.16	120.14
3	A	999	NVP	N14-C15-N1	3.25	119.12	116.67
3	A	999	NVP	N3-C2-N1	3.22	119.10	116.67
3	A	999	NVP	C2-N1-CA	-2.38	114.46	116.34

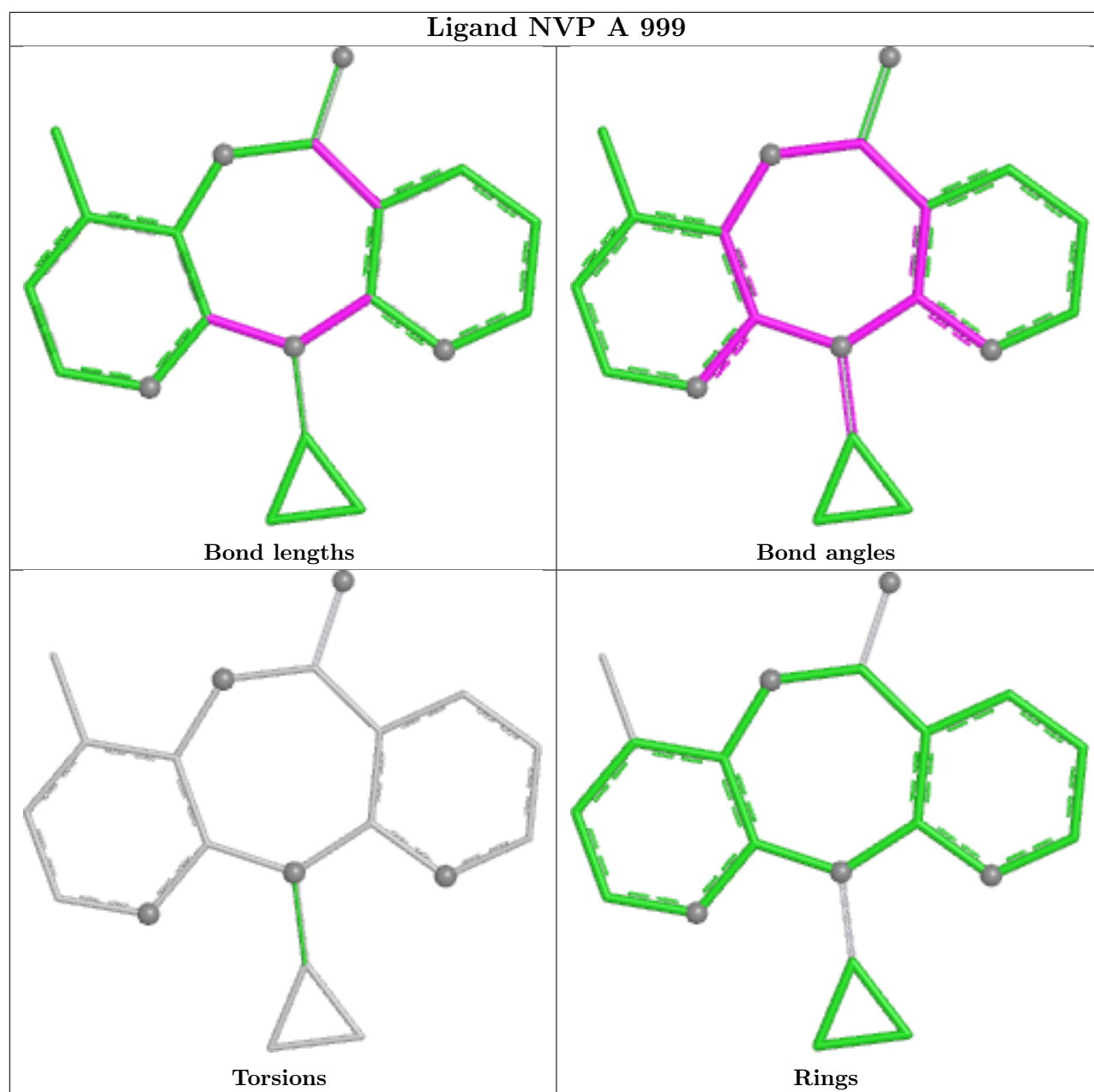
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	542/560 (96%)	-0.10	12 (2%) 62 52	32, 71, 124, 150	0
2	B	395/440 (89%)	-0.11	4 (1%) 79 72	38, 71, 124, 147	0
All	All	937/1000 (93%)	-0.10	16 (1%) 69 60	32, 71, 124, 150	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	116	PHE	2.9
2	B	202	ILE	2.8
1	A	33	ALA	2.7
1	A	402	TRP	2.7
1	A	50	ILE	2.6

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSD	A	280	8/9	0.94	0.08	53,62,80,84	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

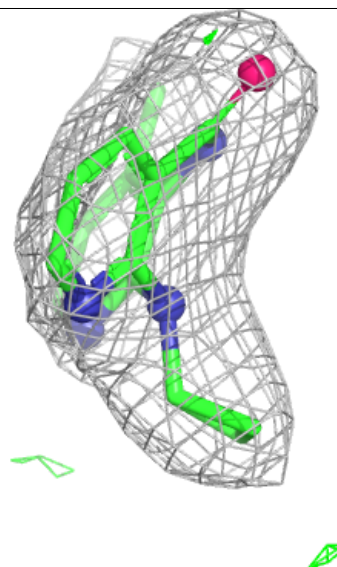
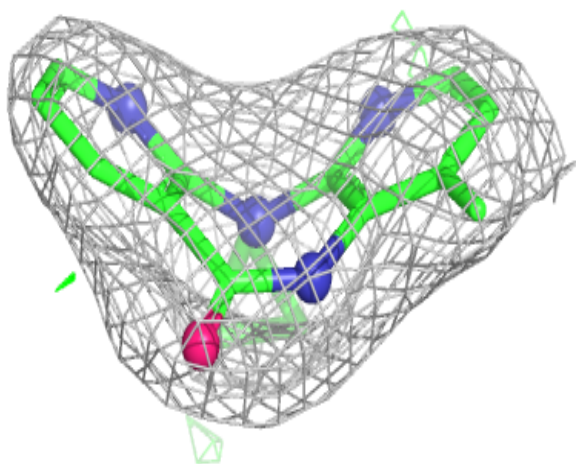
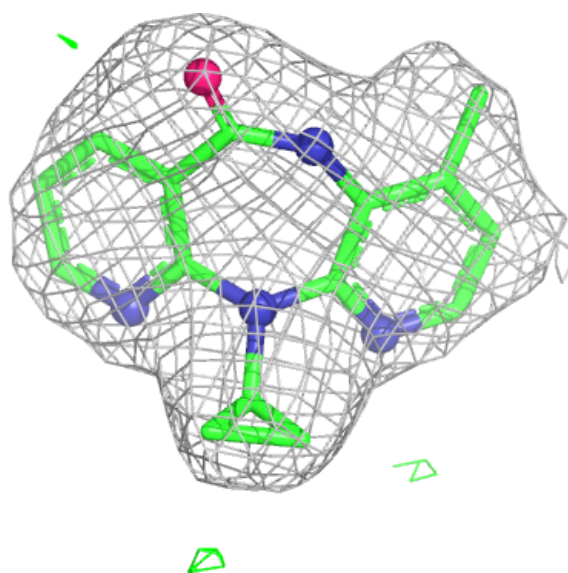
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	NVP	A	999	20/20	0.95	0.07	37,50,65,67	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 999:

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.