



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 04:15 AM UTC

PDB ID : 3HVT / pdb_00003hvt
Title : STRUCTURAL BASIS OF ASYMMETRY IN THE HUMAN IMMUNODEFICIENCY VIRUS TYPE 1 REVERSE TRANSCRIPTASE HETEROODIMER
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Deposited on : 1994-07-25
Resolution : 2.90 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

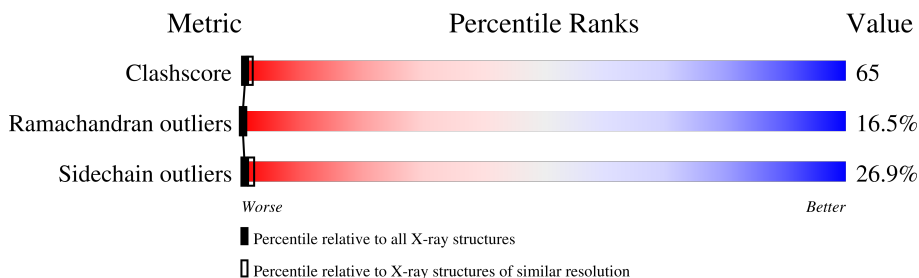
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

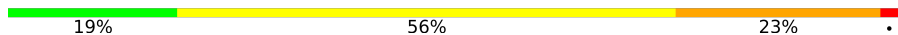
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	556	 19% 56% 23% •
2	B	428	 20% 37% 25% 11% 7%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7426 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.

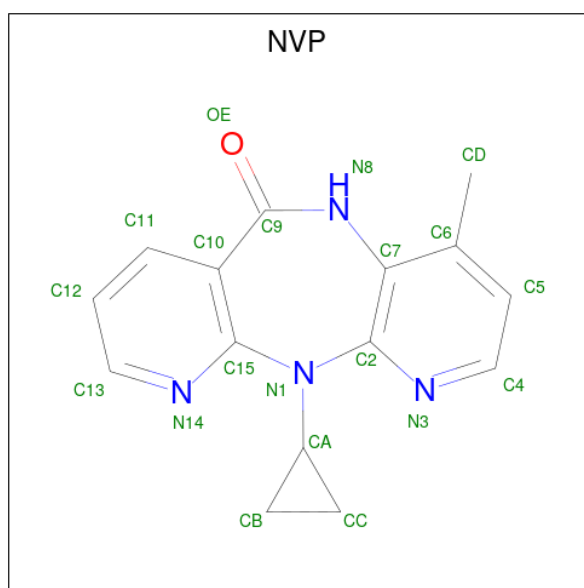
- Molecule 1 is a protein called HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P66).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	0	0
			4248	2744	709	787	8			

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P51).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	398	Total	C	N	O	S	0	0	0
			3158	2050	523	579	6			

- 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).



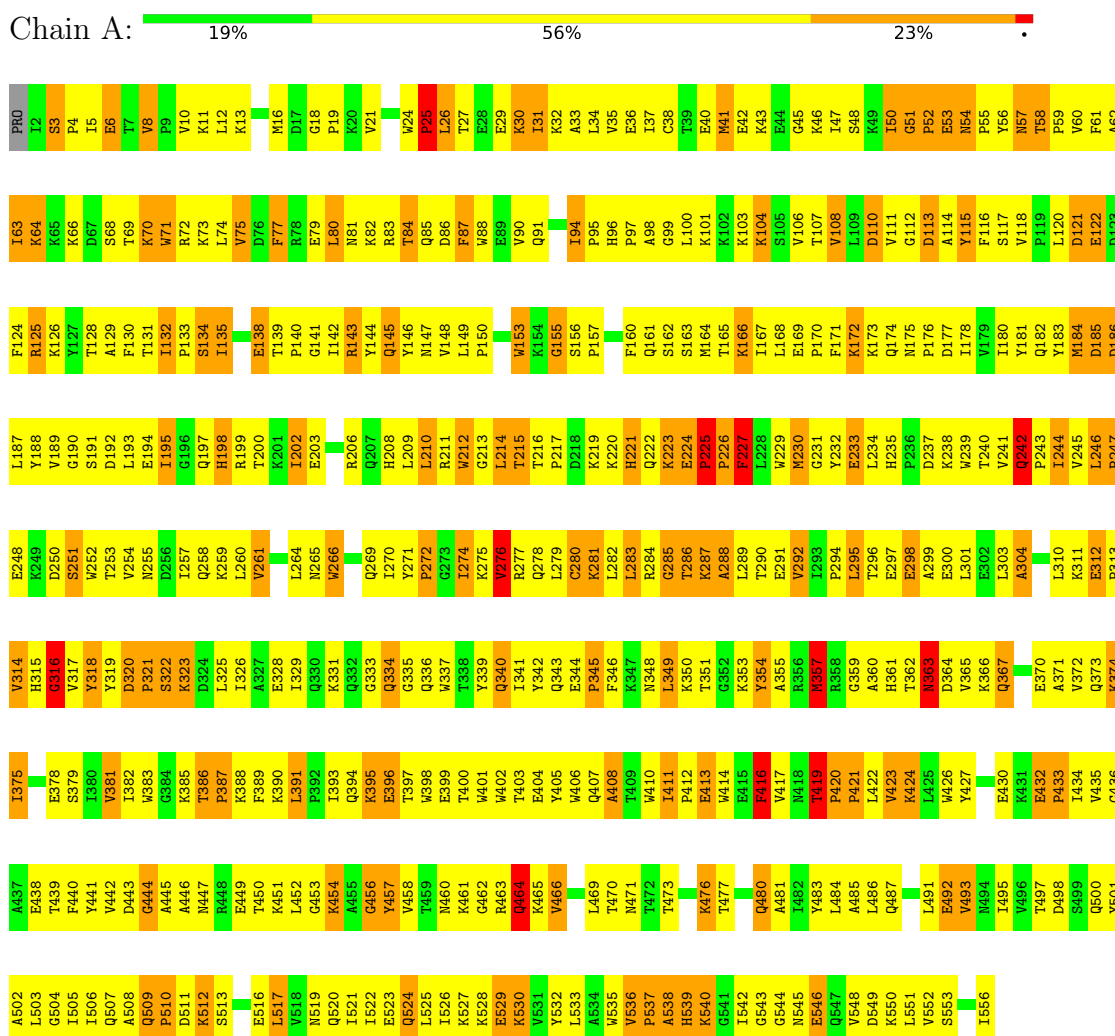
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			20	15	4	1		

3 Residue-property plots

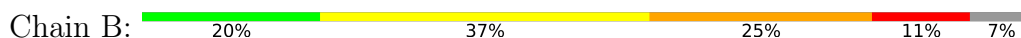
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P66)



• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P51)



L391	P392	I393	Q394	K395	T397	W398	W401	W402	T403	E404	Y405	W406	Q407	A408	T409	W410	I411	P412	E413	W414	E415	F416	V417	W418	T419	P420	P421	L422	V423	K424	L425	W426	Y427	Q428																									
H315	G316	V317	P321	S322	K323	Q332	Q333	Q334	G335	Q336	W337	Q340	E344	P345	F346	K347	K350	K353	Y354	A355	R358	GLY	ALA	HIS	THR	ASN	D364	V365	K366	Q367	L368	T369	E370	A371	V372	Q373	K374	T376	T377	E378	S379	I380	V381	I382	W383	T386	P387	K388	F389	K390									
V254	N255	D256	I257	Q258	K259	L260	V261	G262	K263	L264	N265	W266	A267	S268	Q269	I270	Y271	P272	G273	I274	K275	V276	R277	Q278	L279	C280	K281	L282	L283	R284	C285	T286	K287	A288	L289	T290	E291	V292	T293	P294	L295	T296	E297	E298	A299	E300	L301	E302	L303	A304	E305	N306	R307	E308	I309	E312	V314		
E194	I195	G196	Q197	H198	R199	T200	K201	L202	E203	E204	L205	R206	Q207	H208	L209	L210	R211	W212	G213	L214	T215	T216	P217	D218	K219	K220	H221	Q222	K223	E224	P225	PRO	PHE	LEU	TRP	MET	GLY	TYR	GLU	LEU	HIS	PRO	ASP	LYS	TRP	THR	VAL	GLN	PRO	ILE	VAL	LEU	PRO	GLU	LYS	D250	S251	W252	T253
T131	I132	P133	S134	D67	S68	T69	P140	G141	W142	R143	Y144	Y145	Y146	M147	V148	L149	P150	Q151	G152	W153	G154	G155	S156	P157	A158	I159	F160	Q161	S162	S163	M164	T165	K166	I167	L168	E169	P170	F171	K172	K173	Q174	M175	P176	D177	I178	V179	I180	Y183	M184	D185	D186	L187	Y188	V189	G190	S191	D192	L193	
PRO	I63	K64	K65	K66	D67	S68	T69	P78	W78	R78	M16	D17	Q21	K22	Q23	W24	P25	L26	T27	E28	E29	K30	I31	K32	A33	L34	V35	E36	I37	C38	T39	E40	M41	E42	K43	E44	G45	K46	I47	S48	K49	I50	G51	P52	E53	N54	P55	Y56	N57	T58	P59	V60	A61	A62					

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	223.60 Å 69.90 Å 105.50 Å 90.00° 106.40° 90.00°	Depositor
Resolution (Å)	8.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.266 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7426	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.98	9/4358 (0.2%)	1.60	103/5951 (1.7%)
2	B	1.05	5/3242 (0.2%)	1.62	100/4411 (2.3%)
All	All	1.01	14/7600 (0.2%)	1.61	203/10362 (2.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	4

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	419	THR	CA-CB	11.80	1.60	1.52
2	B	142	ILE	CA-CB	8.52	1.62	1.54
1	A	357	MET	SD-CE	7.90	1.99	1.79
2	B	277	ARG	C-O	6.76	1.31	1.24
1	A	94	ILE	CA-CB	6.33	1.62	1.54

The worst 5 of 203 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	288	ALA	N-CA-C	17.82	133.10	110.65
2	B	178	ILE	N-CA-C	-14.56	87.15	108.12
1	A	24	TRP	CA-C-N	14.07	137.43	119.84
1	A	24	TRP	C-N-CA	14.07	137.43	119.84
1	A	51	GLY	CA-C-N	12.67	132.62	119.19

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	183	TYR	Sidechain
2	B	188	TYR	Sidechain
2	B	354	TYR	Sidechain
2	B	56	TYR	Sidechain

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	4248	0	4052	583	4
2	B	3158	0	3082	392	1
3	A	20	0	14	3	0
All	All	7426	0	7148	947	4

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 65.

The worst 5 of 947 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:441:TYR:HE2	2:B:286:THR:HG23	1.19	1.07
2:B:150:PRO:HD2	2:B:153:TRP:HE1	1.17	1.06
1:A:42:GLU:HA	1:A:46:LYS:HA	1.36	1.05
1:A:79:GLU:HG2	1:A:83:ARG:HH21	1.23	1.01
2:B:180:ILE:HG12	2:B:189:VAL:HG12	1.36	1.00

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ILE:CG1	1:A:449:GLU:OE2[4_647]	1.87	0.33
1:A:37:ILE:CD1	1:A:449:GLU:OE2[4_647]	1.99	0.21
1:A:4:PRO:CB	2:B:211:ARG:NH2[4_646]	2.08	0.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LYS:NZ	1:A:449:GLU:OE2[4_647]	2.09	0.11

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%)	338 (61%)	125 (23%)	90 (16%)	0	0
2	B	392/428 (92%)	264 (67%)	62 (16%)	66 (17%)	0	0
All	All	945/984 (96%)	602 (64%)	187 (20%)	156 (16%)	0	0

5 of 156 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	25	PRO
1	A	54	ASN
1	A	66	LYS
1	A	121	ASP

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	81/496 (16%)	64 (79%)	17 (21%)	1	4
2	B	328/390 (84%)	235 (72%)	93 (28%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	409/886 (46%)	299 (73%)	110 (27%)	0 1

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	192	ASP
2	B	254	VAL
2	B	428	GLN
2	B	393	ILE
2	B	195	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	373	GLN
2	B	428	GLN
2	B	57	ASN
2	B	147	ASN
2	B	198	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	557	-	23,23,23	1.77	3 (13%)	34,34,34	1.71	5 (14%)

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	557	-	-	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	557	NVP	C9-N8	6.97	1.41	1.35
3	A	557	NVP	OE-C9	-3.39	1.15	1.23
3	A	557	NVP	C7-N8	2.03	1.44	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	557	NVP	C10-C9-N8	-6.62	113.76	120.22
3	A	557	NVP	OE-C9-C10	4.57	124.19	119.61
3	A	557	NVP	C7-N8-C9	2.82	130.61	128.29
3	A	557	NVP	C15-N1-CA	-2.30	114.52	116.34
3	A	557	NVP	C15-C10-C9	2.10	126.06	124.01

There are no chirality outliers.

There are no torsion outliers.

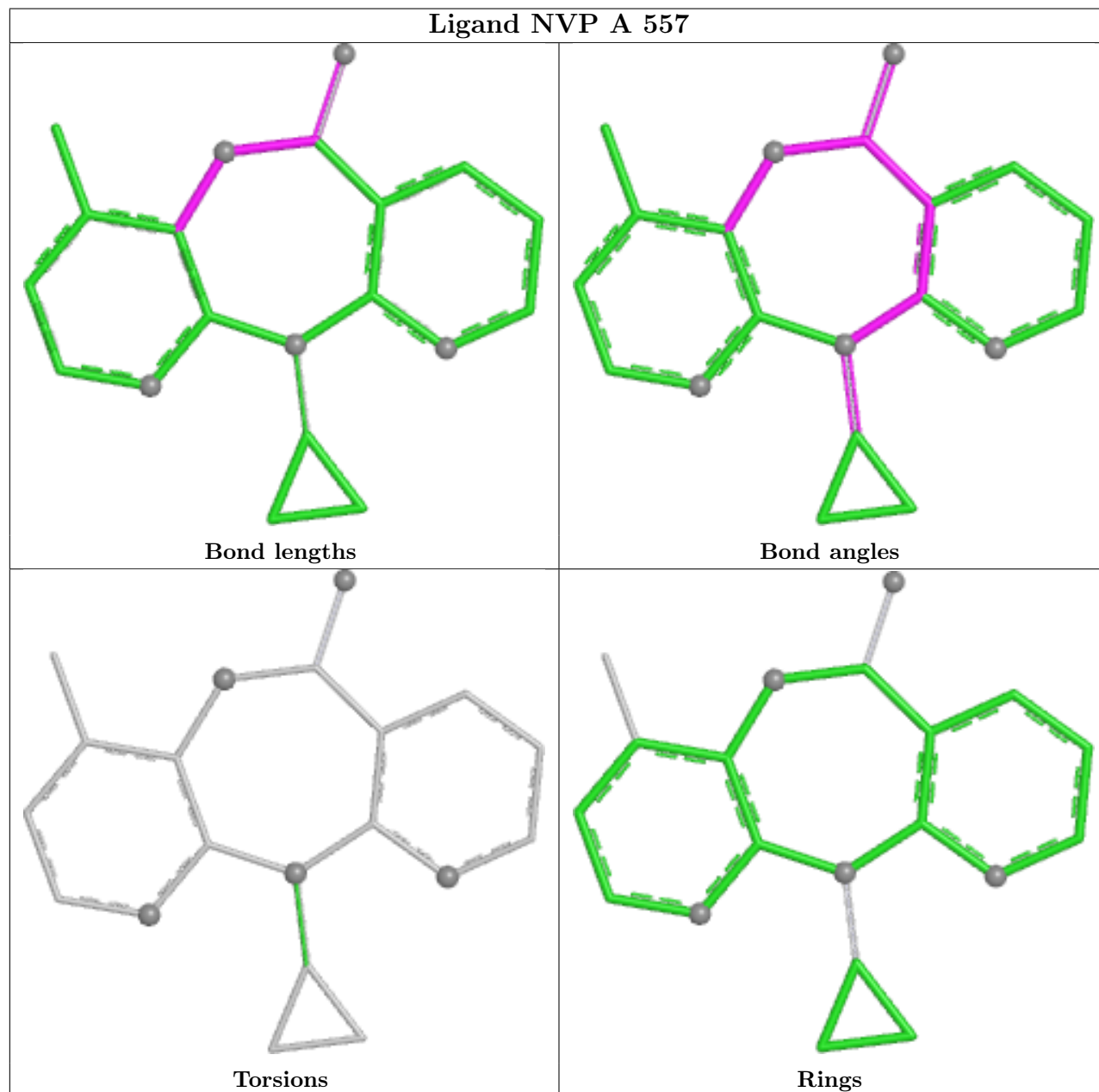
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	557	NVP	3	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.