



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 09:06 am BST

PDB ID : 3HVT
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 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

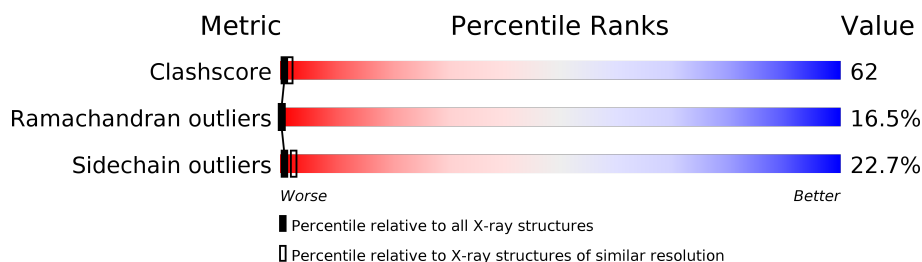
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	556	
2	B	428	

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.

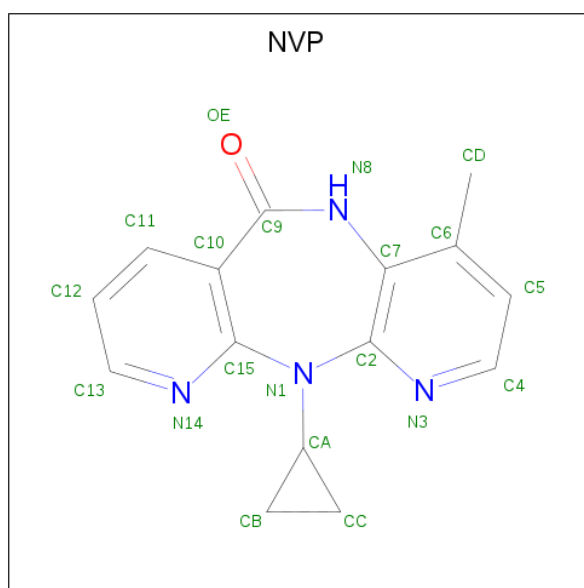
- Molecule 1 is a protein called HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P66).

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 (three-letter code: NVP) (formula: C₁₅H₁₄N₄O).



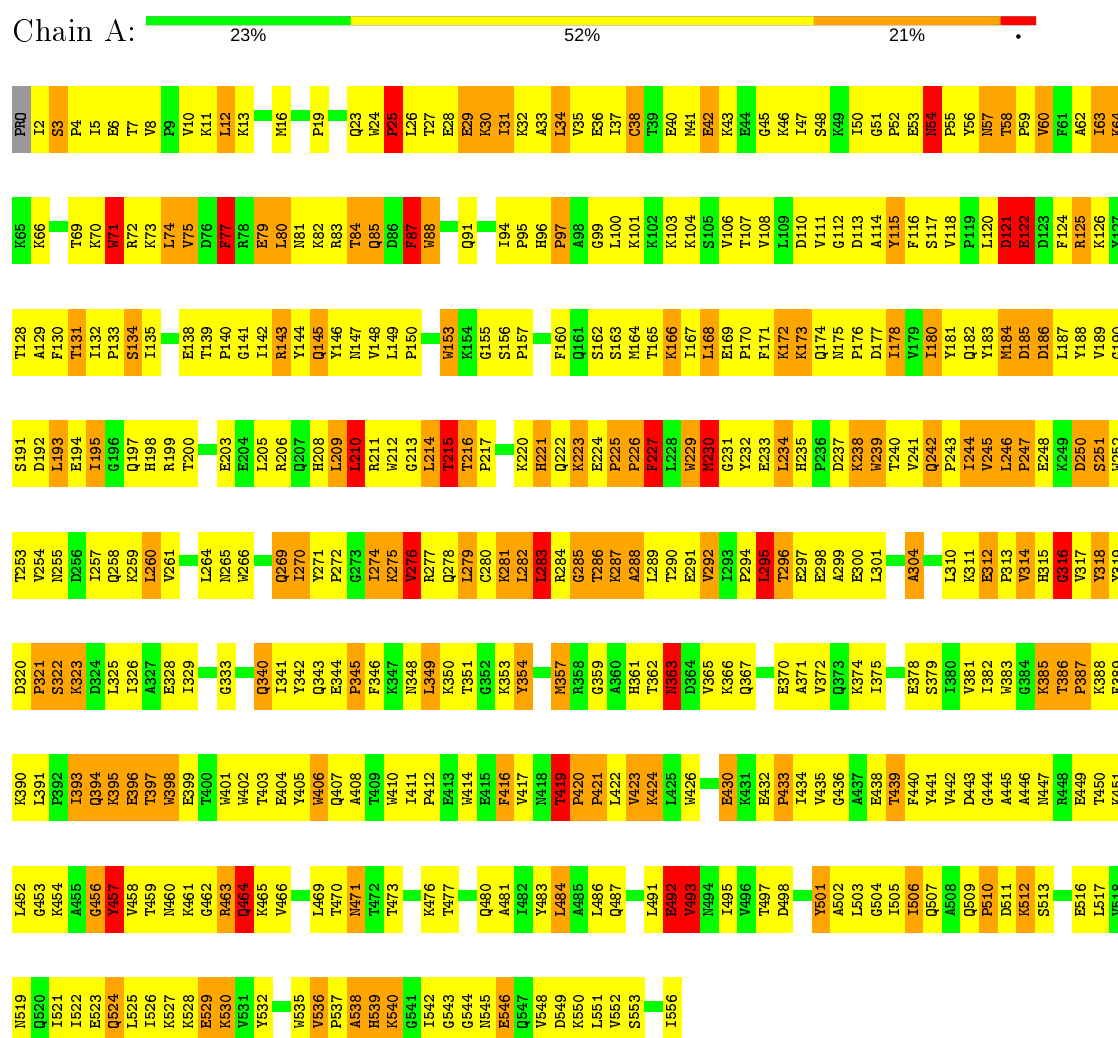
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			20	15	4	1		

3 Residue-property plots

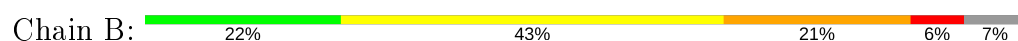
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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



W398	V317	N255	I195	I132	I63	PRO
W401	P321	D256	G196	P133	K64	I2
W402	S322	I257	Q197	S134	K65	S3
T403	K323	Q258	H198	I135	K66	P4
E404	K323	K259	R199	N136	D67	I5
Y405	Q332	L260	T200	S68	S68	E6
W406	G333	V261	K201	T69	T69	T7
Q407	G334	Q262	L202	P140	K70	V8
A408	Q334	K263	E203	G141	W71	P9
T409	Q336	L264	L205	I142	R72	V10
W410	Q337	N265	L205	R143	K73	K11
I411	K337	V266	R206	Y144	R73	K12
P412	P345	A267	Q207	Q145	L74	L13
E413	F346	S268	E208	Y146	V75	K13
W414	K347	Q269	L209	N147	D76	P14
E415	K347	I270	L210	V148	F77	G15
F416	K350	Y271	R211	L149	E79	M16
V417	K350	P272	W212	P150	E80	D17
M418	K354	G273	G213	Q151	L80	D17
T419	A355	V276	L214	G152	N81	
P420	R358	R277	T215	M153	K82	V21
L422	GLY	Q278	T216	K154	R83	K22
Y423	ALA	L279	D218	G155	Q23	Q23
K424	HIS	K280	K219	T84	W24	W24
L425	THR	L282	H221	S156	P25	P25
W426	ASN	R284	K222	Q157	D86	L26
Y427	D364	G285	E224	A158	F87	T27
Q428	V365	T286	P225	F157	W88	E28
	K366	K287	PRO	A158	E89	E29
	Q367	A288	PHE	F160	V90	K30
	L368	L289	LEU	Q161	Q91	I31
	T369	T290	TRP	S162	L92	K32
	E370	T291	GLY	M164	G93	A33
	A371	E291	MET	T165	I94	L34
	V372	V292	GLY	I167	P95	E36
	Q373	L293	TYR	L168	G99	I37
	K374	P294	GLU	E169	L100	C38
	I375	L295	LEU	P170	K101	T39
	T376	T296	HIS	F171	K102	E40
	T377	E297	PRO	K172	K103	M41
	E378	E298	ASP	R173	K104	E42
	S379	A299	LYS	Q174	S105	K43
	I380	E300	TRP	N175	S105	E44
	I381	L301	THR	D177	V108	G45
	W383	L303	GLN	I178	Y115	K46
	T386	A304	PRO	I180	F116	I47
	P387	E305	ILE	Y183	S117	S48
	K388	N306	VAL	M184	K49	K49
	F389	R307	LEU	D185	V118	I50
	K390	E308	PRO	D186	P119	G51
		I309	GLU	L187	L120	P52
			LYS	Y188	D121	E53
			D250	F124	E122	N54
			S251	Y189	D123	P55
			W252	V189	F124	Y56
			T253	G190	N57	N57
			G316	S191	R125	T58
				I192	T128	P59
				L193	A129	V60
				T193	F130	F61
					T131	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	0.76	1/4358 (0.0%)	1.06	15/5951 (0.3%)
2	B	0.81	0/3242	1.10	21/4411 (0.5%)
All	All	0.78	1/7600 (0.0%)	1.08	36/10362 (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	B	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	250	ASP	CB-CG	5.37	1.63	1.51

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	51	GLY	C-N-CD	-9.27	100.21	120.60
2	B	419	THR	C-N-CD	-8.95	100.92	120.60
2	B	178	ILE	N-CA-C	-8.83	87.15	111.00
1	A	420	PRO	C-N-CD	-8.65	101.56	120.60
2	B	288	ALA	N-CA-C	8.18	133.10	111.00

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	553	4
2	B	3158	0	3082	380	1
3	A	20	0	14	3	0
All	All	7426	0	7148	905	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 62.

The worst 5 of 905 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
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	422/496 (85%)	332 (79%)	90 (21%)	1	3
2	B	328/390 (84%)	248 (76%)	80 (24%)	0	2
All	All	750/886 (85%)	580 (77%)	170 (23%)	1	2

5 of 170 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	457	TYR

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Mol	Chain	Res	Type
2	B	23	GLN
2	B	367	GLN
1	A	464	GLN
1	A	523	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	428	GLN
1	A	524	GLN
2	B	407	GLN
1	A	447	ASN
1	A	487	GLN

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 carbohydrates 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	-	15,23,23	1.23	1 (6%)	13,34,34	1.08	1 (7%)

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	-	-	0/0/6/6	0/3/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	557	NVP	OE-C9	-3.62	1.15	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	557	NVP	CD-C6-C7	2.69	122.64	120.03

There are no chirality outliers.

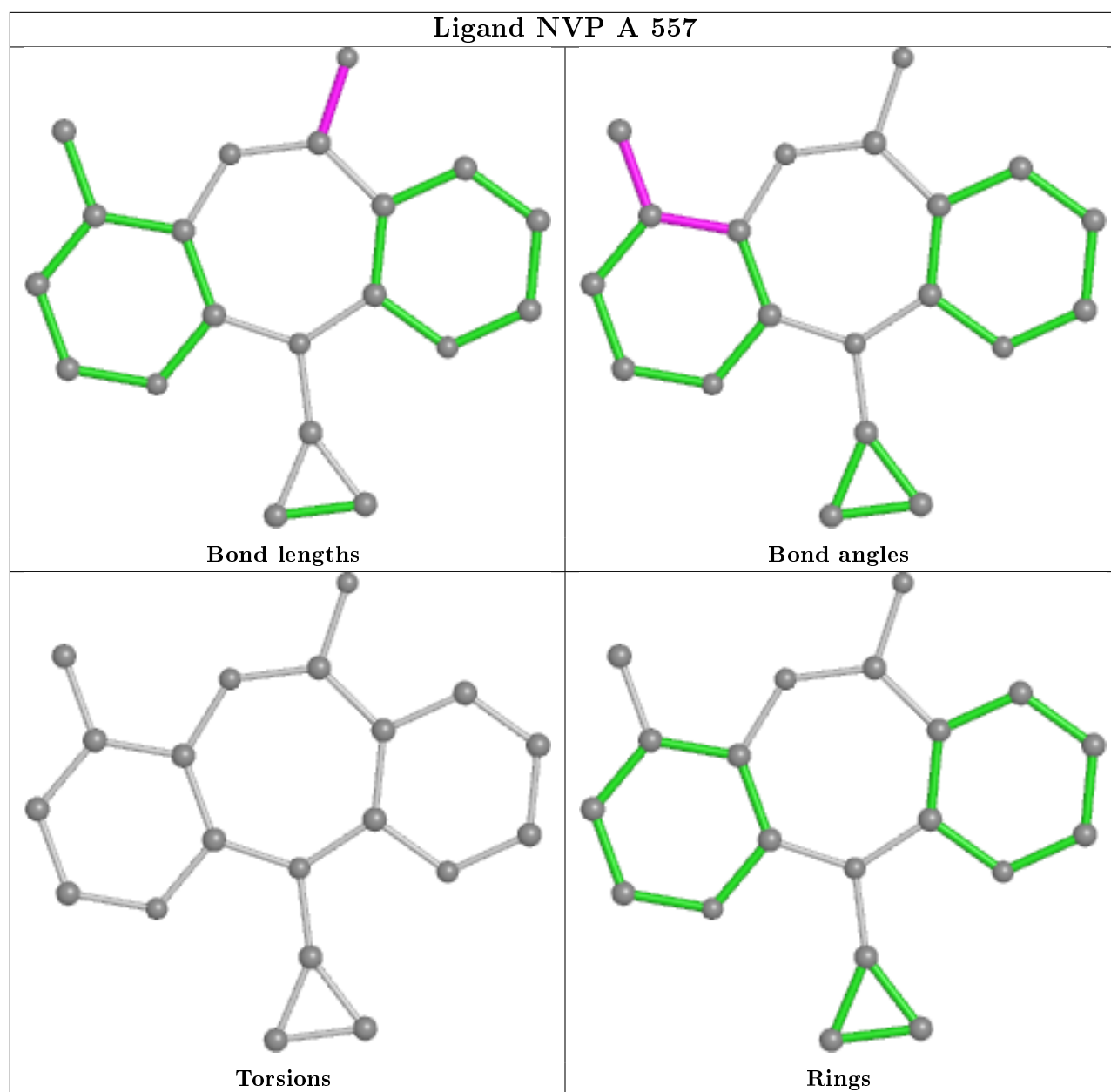
There are no torsion outliers.

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.