



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 05:14 PM UTC

PDB ID : 1S1V / pdb_00001s1v
Title : Crystal structure of L100I mutant HIV-1 reverse transcriptase in complex with TNK-651
Authors : Ren, J.; Nichols, C.E.; Chamberlain, P.P.; Stammers, D.K.
Deposited on : 2004-01-07
Resolution : 2.60 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)	:	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

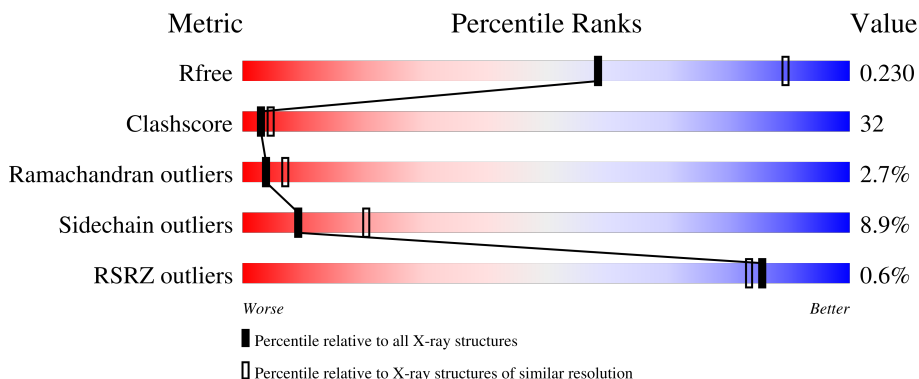
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	% 38% 48% 9% • 5%
2	B	440	 40% 44% 8% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7803 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 Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	534	Total	C	N	O	S	0	0	0
			4370	2830	727	805	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ILE	LEU	engineered mutation	UNP P04585
A	280	CSD	CYS	modified residue	UNP P04585

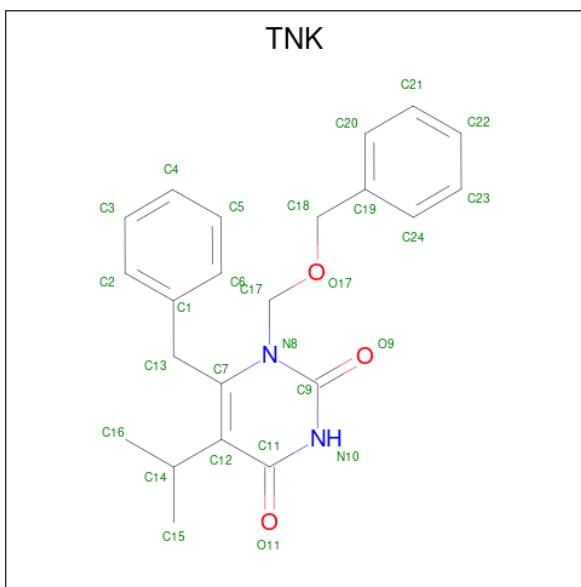
- Molecule 2 is a protein called Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	404	Total	C	N	O	S	0	0	0
			3339	2172	555	605	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	100	ILE	LEU	engineered mutation	UNP P04585

- Molecule 3 is 6-BENZYL-1-BENZYLOXYMETHYL-5-ISOPROPYL URACIL (CCD ID: TNK) (formula: C₂₂H₂₄N₂O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			27	22	2	3		

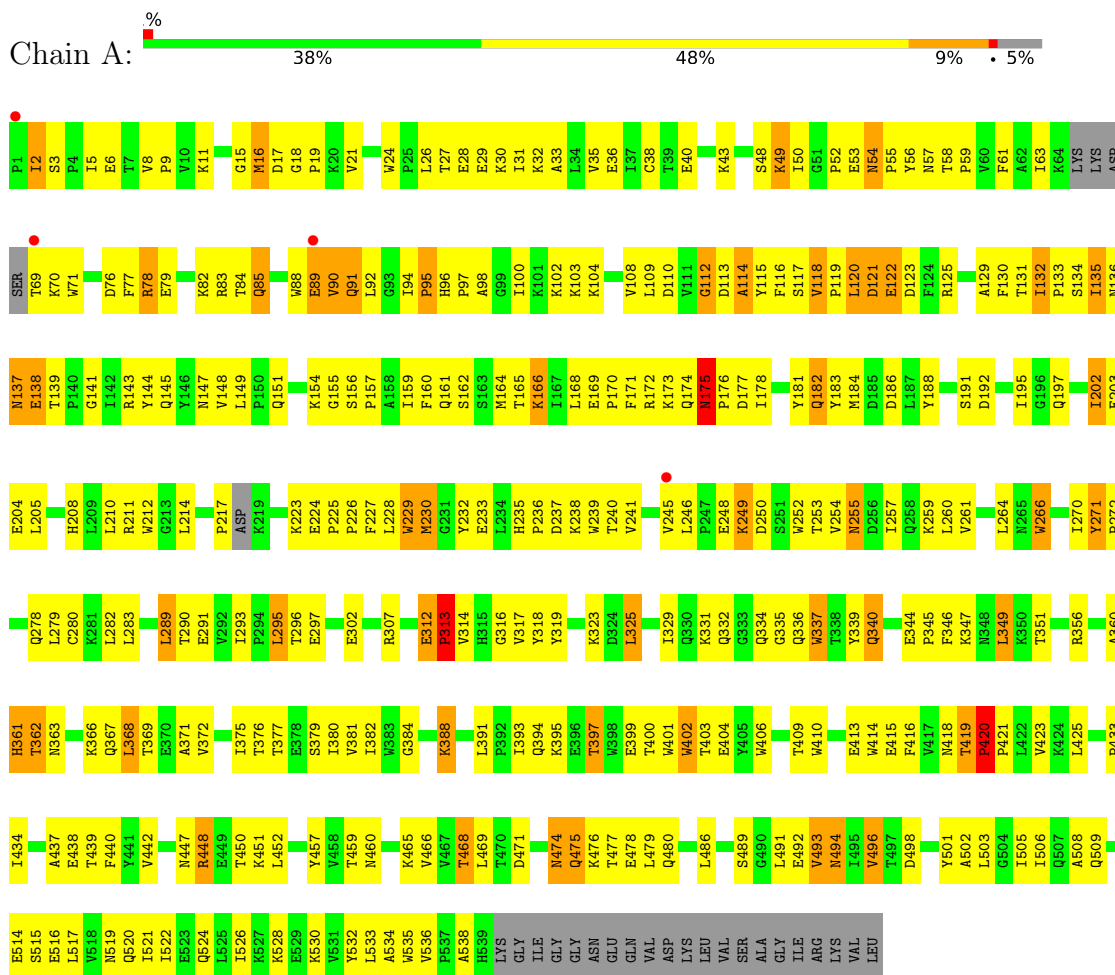
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	39	Total	O	0	0
			39	39		
4	B	28	Total	O	0	0
			28	28		

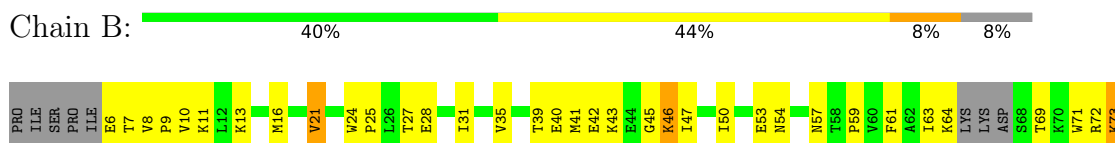
3 Residue-property plots

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 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: Reverse transcriptase



• Molecule 2: Reverse transcriptase



L74	Q145	H208	K281	V365
V75	Y146	L209	L281	K366
D76	M147	L210	L282	Q367
F77	V148	R211	L283	L368
R78	L149	Q212	T286	T369
E79	P150	GLY	K287	E370
	Q151	LEU	A288	A371
K82	G152	THR	L289	V372
R83	W153	PRO		
T84	P157	ASP	T296	E378
Q85	A158	LYS	E297	
D86	I159	LYS	E298	V383
F87	F160	HIS	E302	G384
W88	Q161	GLN	L303	K385
GLU	S162	LYS	A304	T386
VAL	M163	PRO	E305	P387
GLN	M164	PRO	K306	K388
LEU	T165	PHE	R307	F389
G93	K166	LEU	E308	K390
I94	I167	TRP	I309	L391
P97	L168	MET	L310	P392
A98	E169	GLY	K311	T393
G99	P170	TYR	G316	Q394
I100	F171	E233	Y319	W401
K101	R172	L234	D320	W402
	K104	H235	P321	T403
K105	S105	P236	K323	E404
V106	P176	D237	D324	E405
T107	I177	K238	L325	W406
V108	I178	W239	E328	
L109	V179	T240	Q332	P412
V111	I180	Q242	G333	E413
	Q182	P243	Q336	W414
A114	Y183	T244	T338	E415
Y115	M184	V245	Y339	F416
F116	D185		Q340	W417
S117	L186	E248	I341	W418
V118	L187	K249	Y342	T419
P119	Y188	D250	Q343	P420
L120	V189	T253	L349	W423
D121	G190	V254	K350	K424
E122	S191	N255	K353	L425
	D192	D256	G359	W426
R125	L193	I257	A360	W427
K126	E194	Q258	R361	Q428
	I195		D364	
T131	G196	W266		K431
I135	R199	A267		
N136	T200	Y271		T434
N137	K201	I274		W435
F138	I202	K275		C436
T139	E203	V276		ALA
P140	E204	R277		GLU
	L205	Q278		THR
R143	R206			PHE
Y144	Q207			

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	138.10Å 110.30Å 72.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.51 – 2.60 29.51 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.1 (29.51-2.60) 94.0 (29.51-2.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.57Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.233 , 0.313 0.218 , 0.230	Depositor DCC
R_{free} test set	1632 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	69.1	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 73.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7803	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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, TNK

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	0.53	0/4477	1.07	30/6085 (0.5%)
2	B	0.54	1/3432 (0.0%)	1.04	19/4661 (0.4%)
All	All	0.54	1/7909 (0.0%)	1.06	49/10746 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	94	ILE	CA-CB	5.72	1.58	1.54

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	417	VAL	N-CA-C	8.66	119.39	108.82
1	A	137	ASN	N-CA-C	-7.89	102.47	113.20
1	A	114	ALA	N-CA-C	-7.83	103.19	112.89
1	A	349	LEU	N-CA-C	-7.72	103.47	113.12
1	A	250	ASP	N-CA-C	-7.62	103.55	112.92

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	4370	0	4413	284	1
2	B	3339	0	3367	220	0
3	A	27	0	24	5	0
4	A	39	0	0	2	1
4	B	28	0	0	0	0
All	All	7803	0	7804	493	1

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 32.

The worst 5 of 493 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:182:GLN:HE21	1:A:182:GLN:C	1.68	1.01
2:B:57:ASN:HD22	2:B:143:ARG:NH1	1.59	1.01
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.44	0.98
2:B:169:GLU:HB2	2:B:170:PRO:HD3	1.44	0.96
1:A:270:ILE:HG22	1:A:314:VAL:HG21	1.48	0.96

All (1) 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:28:GLU:OE1	4:A:1057:HOH:O[1_556]	2.15	0.05

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	527/560 (94%)	460 (87%)	49 (9%)	18 (3%)	3 4
2	B	396/440 (90%)	344 (87%)	45 (11%)	7 (2%)	6 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	923/1000 (92%)	804 (87%)	94 (10%)	25 (3%)	4 7

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	138	GLU
1	A	272	PRO
1	A	16	MET
1	A	85	GLN

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	478/499 (96%)	429 (90%)	49 (10%)	7 15
2	B	367/400 (92%)	341 (93%)	26 (7%)	13 31
All	All	845/899 (94%)	770 (91%)	75 (9%)	9 20

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	189	VAL
2	B	368	LEU
2	B	194	GLU
2	B	283	LEU
1	A	255	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	475	GLN
2	B	361	HIS
2	B	57	ASN

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Mol	Chain	Res	Type
2	B	428	GLN
2	B	269	GLN

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	1.22	0	1,8,10	4.13	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	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CSD	OD1-SG-CB	4.13	113.21	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 [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	TNK	A	999	-	29,29,29	1.91	9 (31%)	32,39,39	0.96	2 (6%)

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	TNK	A	999	-	-	3/14/14/14	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	TNK	C7-C12	5.53	1.41	1.35
3	A	999	TNK	C13-C7	3.23	1.54	1.50
3	A	999	TNK	C17-N8	2.80	1.51	1.46
3	A	999	TNK	C3-C2	2.59	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	TNK	C14-C12	2.52	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	TNK	C1-C13-C7	2.61	120.02	114.78
3	A	999	TNK	C14-C12-C7	2.23	126.08	120.21

There are no chirality outliers.

All (3) torsion outliers are listed below:

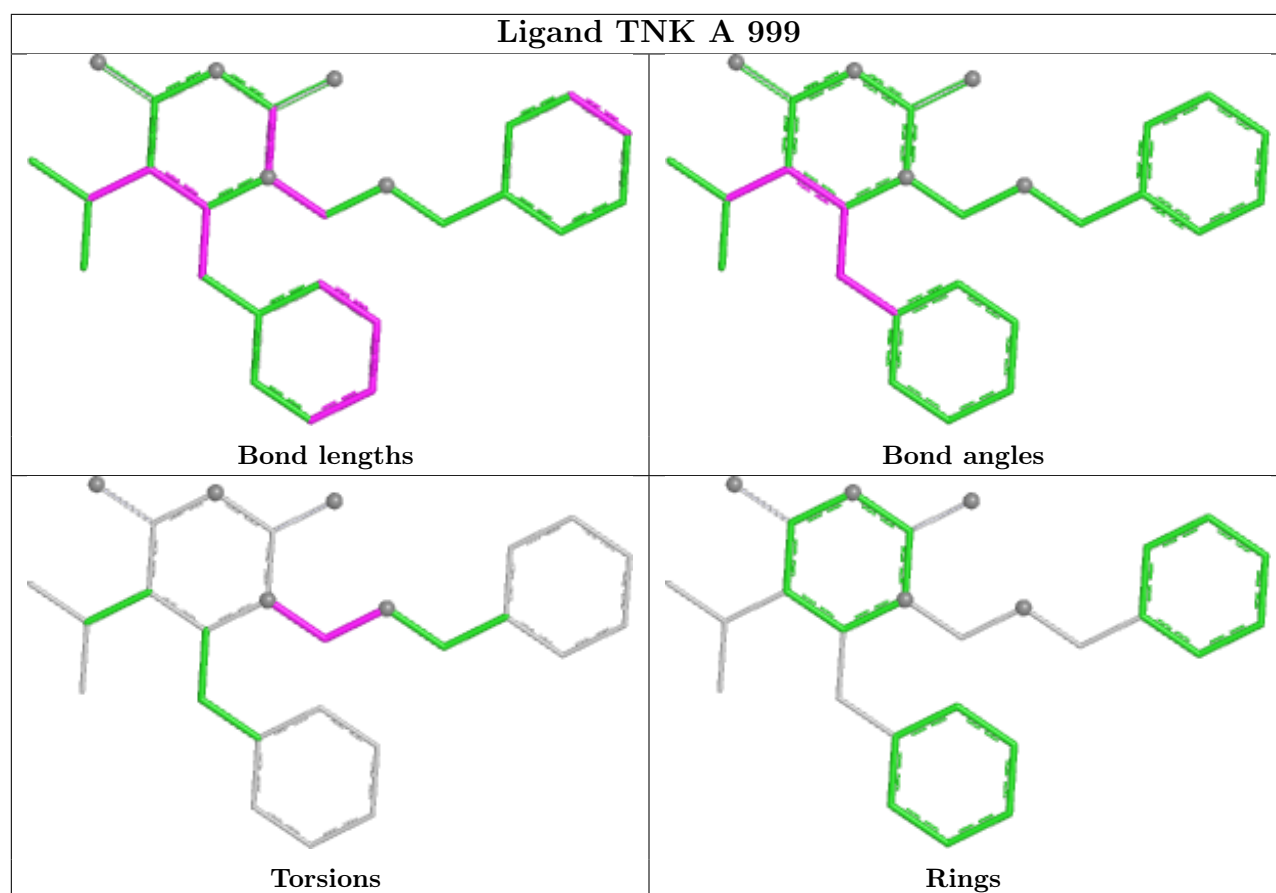
Mol	Chain	Res	Type	Atoms
3	A	999	TNK	O17-C17-N8-C7
3	A	999	TNK	O17-C17-N8-C9
3	A	999	TNK	N8-C17-O17-C18

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	TNK	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 [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	533/560 (95%)	-0.21	4 (0%) 82 80	39, 75, 120, 150	0
2	B	404/440 (91%)	-0.26	2 (0%) 87 85	38, 74, 125, 150	0
All	All	937/1000 (93%)	-0.23	6 (0%) 85 83	38, 74, 122, 150	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	93	GLY	2.5
1	A	69	THR	2.3
1	A	1	PRO	2.3
1	A	245	VAL	2.1
1	A	89	GLU	2.0

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	0.95	0.08	74,75,88,95	0

6.3 Carbohydrates [i](#)

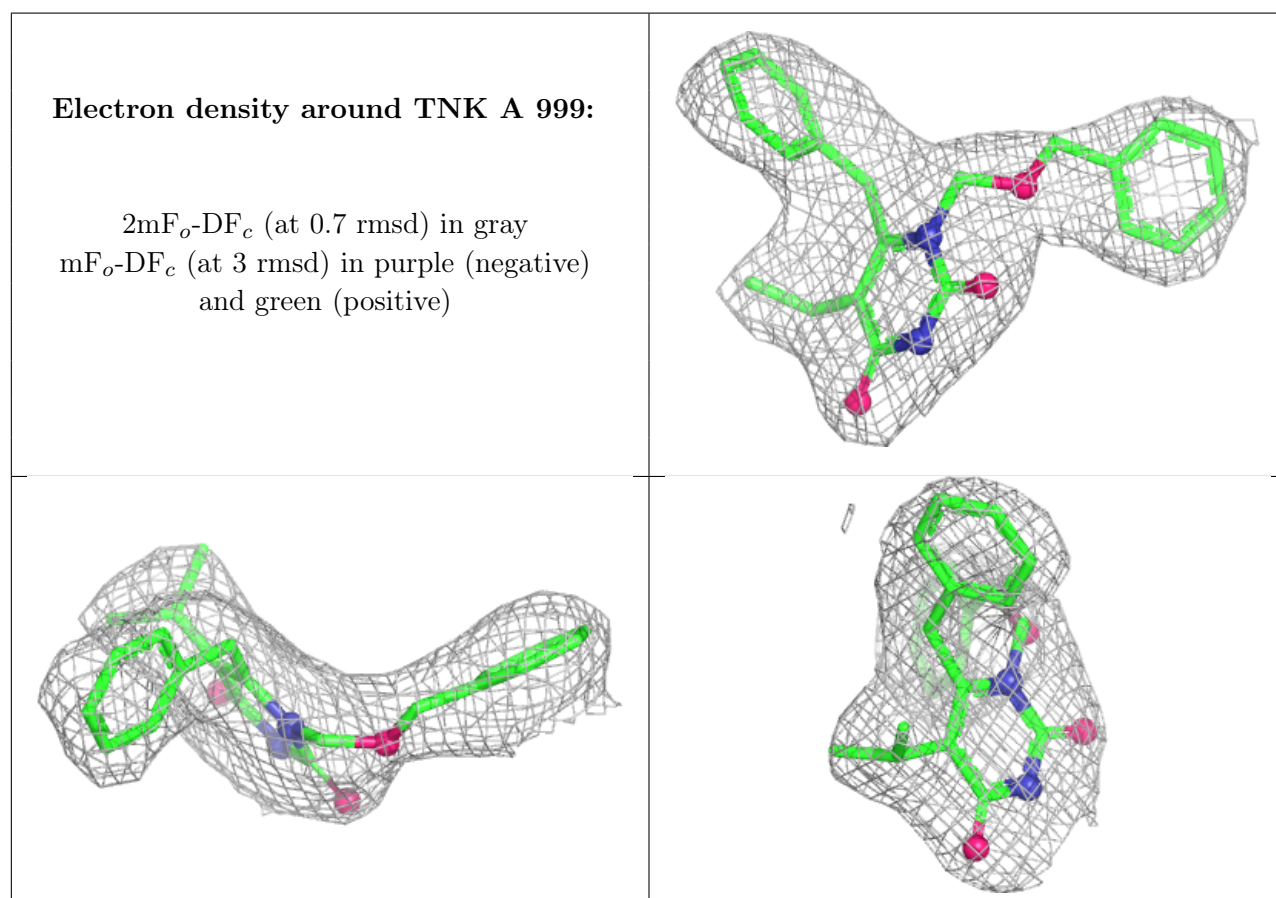
There are no oligosaccharides in this entry.

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	TNK	A	999	27/27	0.95	0.08	42,61,82,86	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.