



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:00 AM UTC

PDB ID : 8U6B / pdb_00008u6b
Title : Crystal Structure of HIV-1 Reverse Transcriptase in Complex with N-(4-chloro-3-(3-chloro-5-cyanophenoxy)phenethyl)acrylamide (JLJ731), a non-nucleoside inhibitor
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Deposited on : 2023-09-13
Resolution : 2.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

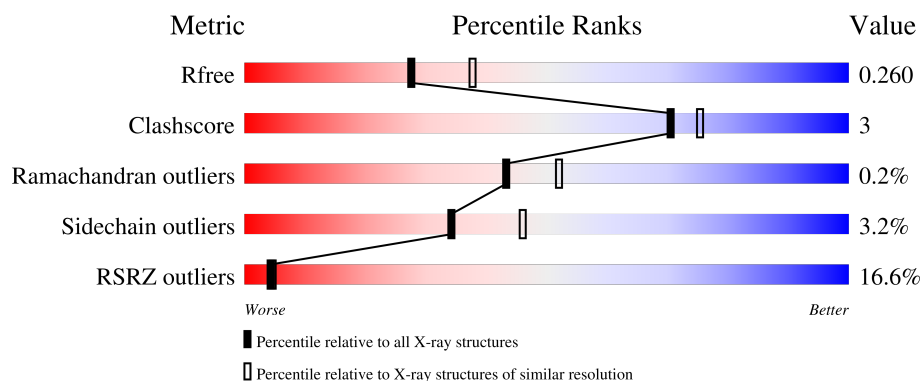
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	557	18% 84% 11% ••
2	B	428	13% 86% 7% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7382 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/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	2	0
			4085	2634	680	764	7			

There are 5 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	172	ALA	LYS	engineered mutation	UNP P03366
A	173	ALA	LYS	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

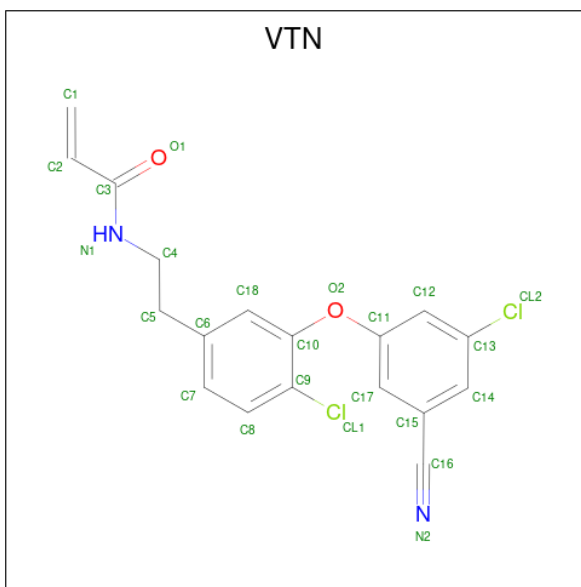
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	402	Total	C	N	O	S	0	2	0
			3201	2078	528	590	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is N-{2-[4-chloro-3-(3-chloro-5-cyanophenoxy)phenyl]ethyl}prop-2-enamide (CCD ID: VTN) (formula: C₁₈H₁₄Cl₂N₂O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	
			48	36	4	4	4	0
								1

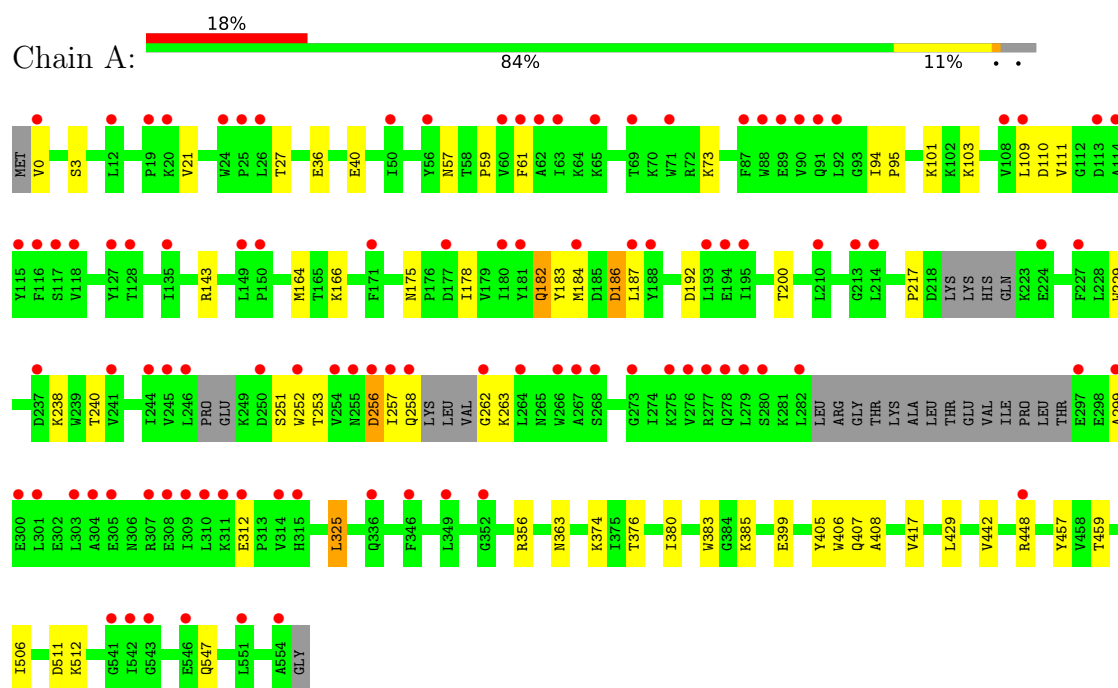
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	25	Total	O		
			25	25	0	0
4	B	23	Total	O		
			23	23	0	0

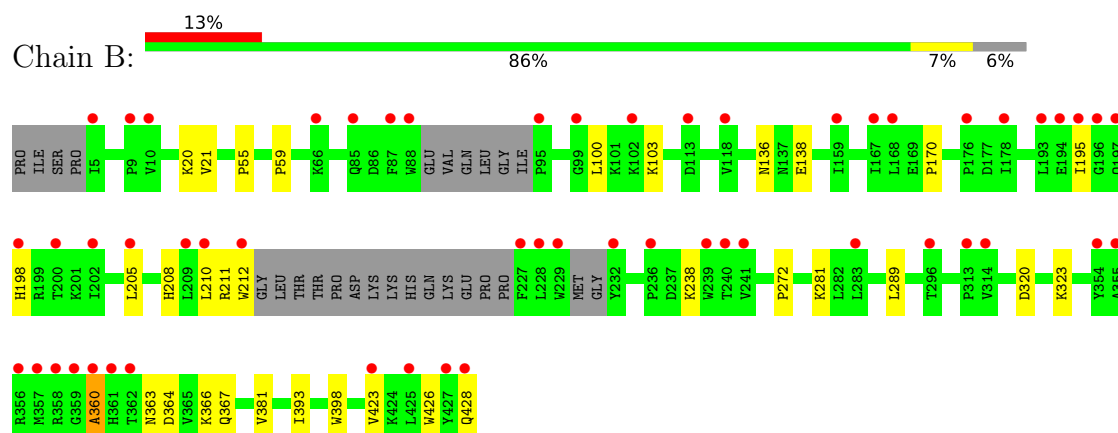
3 Residue-property plots [i](#)

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/ribonuclease H



- Molecule 2: p51 RT



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.24Å 73.84Å 108.78Å 90.00° 100.42° 90.00°	Depositor
Resolution (Å)	79.78 – 2.35 79.78 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.2 (79.78-2.35) 98.2 (79.78-2.35)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.34Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.230 , 0.264 0.229 , 0.260	Depositor DCC
R_{free} test set	2613 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	64.9	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.5	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	7382	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: VTN

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	0.30	0/4194	0.51	4/5729 (0.1%)
2	B	0.27	0/3292	0.50	2/4486 (0.0%)
All	All	0.29	0/7486	0.51	6/10215 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	263	LYS	N-CA-C	-5.60	106.21	113.16
2	B	210	LEU	N-CA-C	-5.58	105.19	111.28
1	A	256	ASP	N-CA-C	-5.34	105.99	112.88
1	A	184	MET	CB-CA-C	-5.24	110.56	116.63
1	A	252	TRP	N-CA-C	-5.18	106.66	112.87
2	B	360	ALA	N-CA-C	5.18	118.09	107.37

There are no chirality outliers.

There are no planarity outliers.

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	4085	0	3867	32	0
2	B	3201	0	3099	18	0
3	A	48	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	25	0	0	0	0
4	B	23	0	0	1	0
All	All	7382	0	6966	49	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 3.

All (49) 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:61:PHE:CE2	1:A:61:PHE:CE1	2.39	1.03
2:B:360:ALA:O	2:B:367:GLN:NE2	2.37	0.58
1:A:256:ASP:C	1:A:258:GLN:H	2.13	0.57
1:A:111:VAL:HG11	1:A:187:LEU:HD12	1.88	0.56
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.07	0.55
1:A:183:TYR:CD2	1:A:229:TRP:HD1	2.24	0.54
1:A:258:GLN:CA	1:A:262:GLY:HA3	2.40	0.51
1:A:253:THR:CB	1:A:299:ALA:H	2.24	0.51
1:A:164:MET:CE	1:A:187:LEU:HD11	2.40	0.51
1:A:182:GLN:HA	1:A:187:LEU:HD23	1.94	0.50
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.93	0.50
1:A:258:GLN:C	1:A:262:GLY:HA3	2.37	0.49
1:A:256:ASP:C	1:A:258:GLN:N	2.72	0.48
1:A:258:GLN:HA	1:A:262:GLY:HA3	1.96	0.48
1:A:186:ASP:OD1	1:A:186:ASP:N	2.45	0.48
1:A:175:ASN:O	1:A:178:ILE:HG13	2.14	0.48
2:B:195:ILE:HA	2:B:198:HIS:HB3	1.95	0.47
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.49	0.47
2:B:20:LYS:HE2	2:B:55:PRO:HB2	1.96	0.47
2:B:320:ASP:HB3	2:B:323:LYS:HE2	1.95	0.47
1:A:376:THR:O	1:A:380:ILE:HG12	2.15	0.47
1:A:36:GLU:O	1:A:40:GLU:HG2	2.15	0.46
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.98	0.46
2:B:136:ASN:HB3	2:B:138:GLU:HG3	1.97	0.46
2:B:360:ALA:HB1	2:B:363:ASN:HB3	1.98	0.46
1:A:94:ILE:HD12	1:A:95:PRO:O	2.15	0.45
1:A:109:LEU:O	1:A:186:ASP:HA	2.17	0.45
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.97	0.45
1:A:442:VAL:HG12	1:A:457:TYR:HB3	1.99	0.45
1:A:101:LYS:HE2	1:A:101:LYS:HB2	1.78	0.44
2:B:360:ALA:HB2	2:B:366:LYS:HD3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:ILE:HD13	2:B:398:TRP:HB2	2.00	0.44
2:B:423:VAL:HG22	2:B:426:TRP:HD1	1.82	0.43
2:B:170:PRO:HB2	2:B:208:HIS:HE1	1.83	0.43
1:A:325:LEU:HB2	1:A:385:LYS:HE2	1.99	0.43
2:B:211:ARG:O	2:B:212:TRP:C	2.61	0.43
1:A:325:LEU:HD11	1:A:383:TRP:CE3	2.54	0.43
1:A:57:ASN:OD1	1:A:143:ARG:NH1	2.52	0.42
2:B:428:GLN:O	4:B:501:HOH:O	2.21	0.42
2:B:423:VAL:HA	2:B:426:TRP:CD1	2.55	0.42
1:A:110:ASP:HB3	1:A:217:PRO:HG3	2.02	0.41
1:A:406:TRP:CE2	1:A:407:GLN:HG3	2.55	0.41
1:A:251:SER:C	1:A:253:THR:N	2.78	0.41
1:A:325:LEU:HA	1:A:325:LEU:HD23	1.81	0.41
2:B:208:HIS:HA	2:B:211:ARG:NH1	2.36	0.41
1:A:103:LYS:HA	1:A:192:ASP:OD1	2.21	0.41
1:A:429:LEU:HD11	1:A:506:ILE:HG22	2.03	0.41
2:B:289:LEU:HD23	2:B:289:LEU:HA	1.93	0.41
2:B:100:LEU:HG	2:B:381:VAL:HG13	2.03	0.40

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	523/557 (94%)	514 (98%)	8 (2%)	1 (0%)	43	52
2	B	396/428 (92%)	386 (98%)	9 (2%)	1 (0%)	36	43
All	All	919/985 (93%)	900 (98%)	17 (2%)	2 (0%)	43	52

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	272	PRO
1	A	257	ILE

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	410/495 (83%)	390 (95%)	20 (5%)	22	28
2	B	333/390 (85%)	329 (99%)	4 (1%)	63	77
All	All	743/885 (84%)	719 (97%)	24 (3%)	34	46

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	VAL
1	A	3	SER
1	A	27	THR
1	A	73	LYS
1	A	166	LYS
1	A	182	GLN
1	A	186	ASP
1	A	200	THR
1	A	238	LYS
1	A	240	THR
1	A	312	GLU
1	A	325	LEU
1	A	356	ARG
1	A	374	LYS
1	A	399	GLU
1	A	417	VAL
1	A	448	ARG
1	A	459	THR
1	A	512	LYS
1	A	547	GLN
2	B	103	LYS
2	B	205	LEU

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Mol	Chain	Res	Type
2	B	238	LYS
2	B	281	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	GLN
1	A	197	GLN
1	A	520	GLN
1	A	545	ASN
1	A	547	GLN
2	B	182	GLN
2	B	208	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](#)

2 ligands are 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	VTN	A	601[A]	-	25,25,25	0.40	0	32,33,33	0.71	0
3	VTN	A	601[B]	-	25,25,25	0.25	0	32,33,33	0.64	0

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	VTN	A	601[A]	-	-	2/14/14/14	0/2/2/2
3	VTN	A	601[B]	-	-	1/14/14/14	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

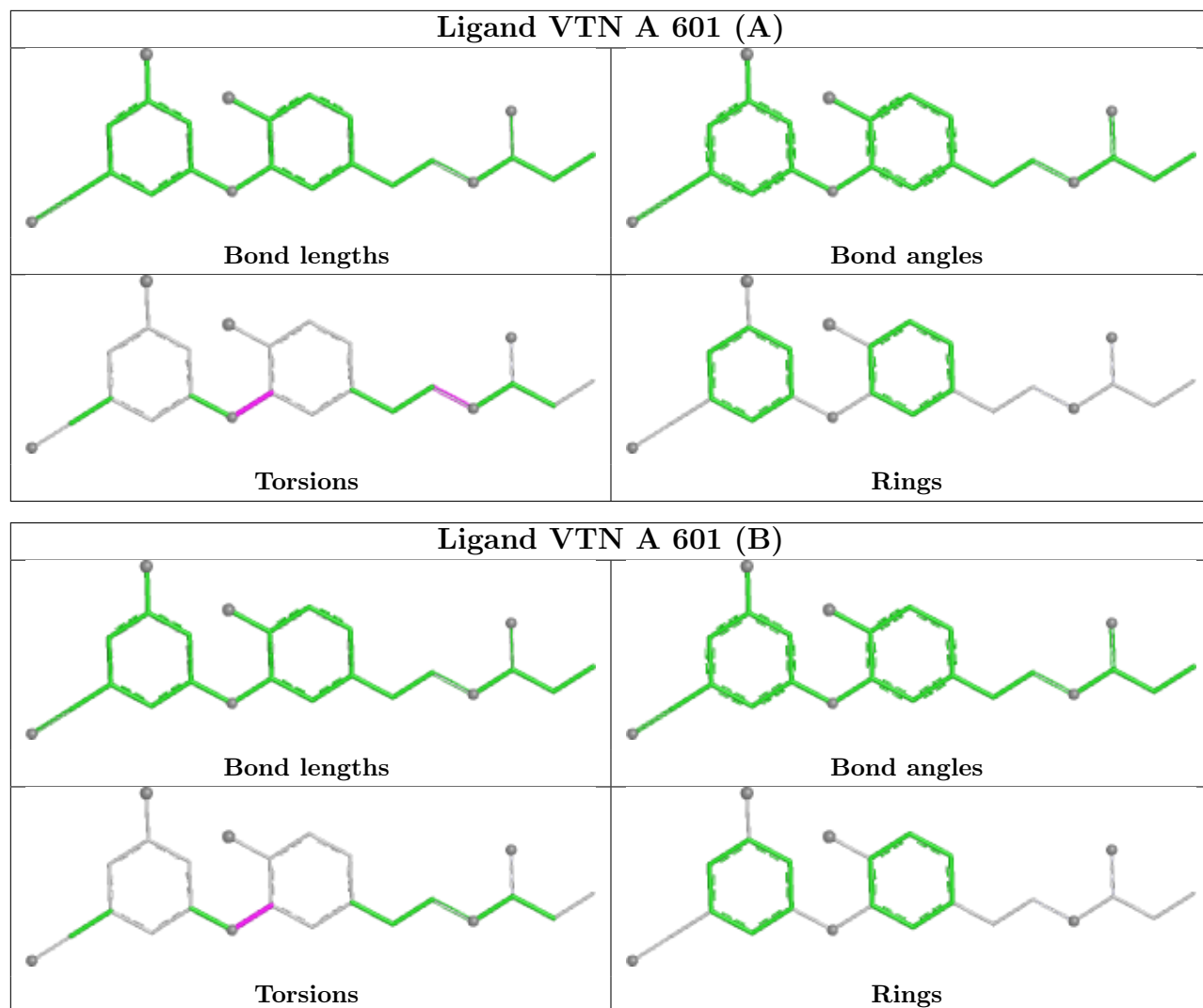
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601[A]	VTN	C5-C4-N1-C3
3	A	601[A]	VTN	C9-C10-O2-C11
3	A	601[B]	VTN	C9-C10-O2-C11

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	532/557 (95%)	1.08	101 (18%) 3 3	32, 77, 128, 146	1 (0%)
2	B	402/428 (93%)	0.95	54 (13%) 7 8	28, 70, 113, 134	2 (0%)
All	All	934/985 (94%)	1.02	155 (16%) 4 5	28, 74, 121, 146	3 (0%)

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	227	PHE	5.8
1	A	262	GLY	5.0
2	B	354	TYR	4.8
2	B	229	TRP	4.8
2	B	194	GLU	4.7
1	A	116	PHE	4.7
2	B	87	PHE	4.6
2	B	193	LEU	4.4
2	B	5	ILE	4.2
2	B	195	ILE	4.1
2	B	425	LEU	4.0
1	A	246	LEU	3.9
1	A	315	HIS	3.9
1	A	127	TYR	3.9
2	B	232	TYR	3.8
1	A	310	LEU	3.8
1	A	554	ALA	3.7
2	B	362	THR	3.7
2	B	197	GLN	3.6
1	A	280	SER	3.6
1	A	543	GLY	3.6
1	A	108	VAL	3.5
1	A	114	ALA	3.5
1	A	24	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	252	TRP	3.5
2	B	358	ARG	3.5
2	B	212	TRP	3.4
2	B	95	PRO	3.4
1	A	188	TYR	3.3
2	B	88	TRP	3.3
2	B	209	LEU	3.2
2	B	428	GLN	3.2
1	A	115	TYR	3.2
1	A	195	ILE	3.2
1	A	276	VAL	3.1
1	A	303	LEU	3.1
1	A	257	ILE	3.1
1	A	346	PHE	3.1
2	B	359	GLY	3.1
2	B	360	ALA	3.1
2	B	239	TRP	3.0
1	A	278	GLN	3.0
1	A	61	PHE	3.0
2	B	423	VAL	3.0
1	A	117	SER	3.0
1	A	264	LEU	3.0
2	B	202	ILE	3.0
1	A	177	ASP	3.0
1	A	551	LEU	2.9
2	B	118	VAL	2.9
1	A	546	GLU	2.9
1	A	309	ILE	2.9
1	A	279	LEU	2.9
2	B	427	TYR	2.9
1	A	118	VAL	2.9
2	B	361	HIS	2.8
1	A	241	VAL	2.8
1	A	254	VAL	2.8
2	B	241	VAL	2.8
1	A	69	THR	2.8
2	B	228	LEU	2.8
1	A	62	ALA	2.8
1	A	0	VAL	2.8
1	A	90	VAL	2.8
1	A	213	GLY	2.8
1	A	87	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	89	GLU	2.8
1	A	20	LYS	2.7
1	A	301	LEU	2.7
2	B	113	ASP	2.7
1	A	91	GLN	2.7
1	A	255	ASN	2.7
1	A	63	ILE	2.7
2	B	159	ILE	2.7
2	B	196	GLY	2.7
1	A	210	LEU	2.7
1	A	224	GLU	2.7
2	B	240	THR	2.7
1	A	19	PRO	2.7
2	B	210	LEU	2.7
1	A	256	ASP	2.6
1	A	312	GLU	2.6
2	B	313	PRO	2.6
2	B	357	MET	2.6
1	A	193	LEU	2.6
1	A	308	GLU	2.6
1	A	250	ASP	2.6
1	A	314	VAL	2.6
1	A	113	ASP	2.6
1	A	71	TRP	2.5
1	A	542	ILE	2.5
2	B	167	ILE	2.5
1	A	297	GLU	2.5
1	A	304	ALA	2.5
2	B	85	GLN	2.5
2	B	356	ARG	2.4
1	A	245	VAL	2.4
1	A	194	GLU	2.4
1	A	305	GLU	2.4
2	B	296	THR	2.4
1	A	275	LYS	2.4
1	A	311	LYS	2.4
1	A	12	LEU	2.4
1	A	214	LEU	2.4
2	B	283	LEU	2.4
1	A	273	GLY	2.4
2	B	168	LEU	2.4
1	A	258	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	355	ALA	2.4
1	A	227	PHE	2.4
1	A	187	LEU	2.4
2	B	205	LEU	2.4
1	A	277	ARG	2.4
1	A	541	GLY	2.3
1	A	149	LEU	2.3
2	B	200	THR	2.3
1	A	299	ALA	2.3
1	A	268	SER	2.3
2	B	10	VAL	2.3
2	B	102	LYS	2.3
1	A	171	PHE	2.2
2	B	99	GLY	2.2
1	A	56	TYR	2.2
1	A	88	TRP	2.2
1	A	244	ILE	2.2
1	A	352	GLY	2.2
1	A	336	GLN	2.2
1	A	135	ILE	2.2
1	A	282	LEU	2.2
1	A	307	ARG	2.2
2	B	176	PRO	2.2
1	A	65	LYS	2.2
1	A	448	ARG	2.1
1	A	26	LEU	2.1
1	A	50	ILE	2.1
2	B	9	PRO	2.1
2	B	198	HIS	2.1
1	A	181	TYR	2.1
1	A	109	LEU	2.1
1	A	60	VAL	2.1
2	B	236	PRO	2.1
2	B	66	LYS	2.1
1	A	128	THR	2.1
1	A	184	MET	2.1
2	B	178	ILE	2.1
1	A	25	PRO	2.1
2	B	314	VAL	2.1
1	A	266	TRP	2.1
1	A	267	ALA	2.0
1	A	300	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	92	LEU	2.0
1	A	349	LEU	2.0
1	A	180	ILE	2.0
1	A	150	PRO	2.0
1	A	237	ASP	2.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

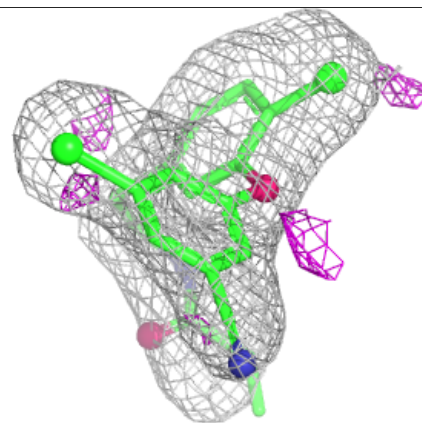
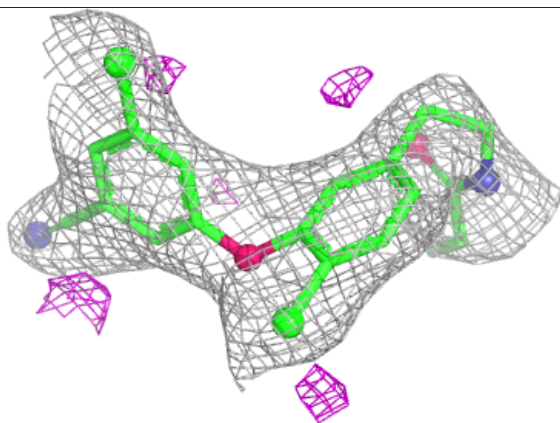
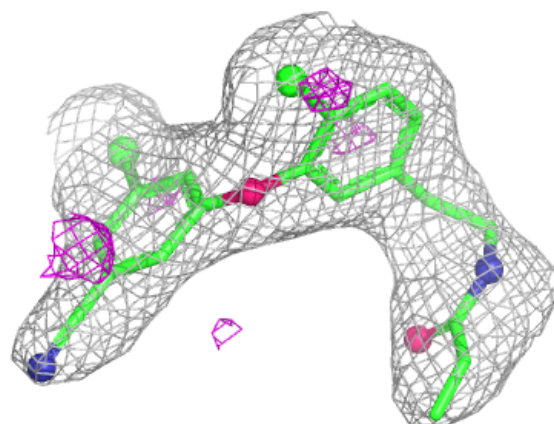
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	VTN	A	601[A]	24/24	0.92	0.15	77,81,84,85	24
3	VTN	A	601[B]	24/24	0.92	0.15	77,81,84,86	24

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.

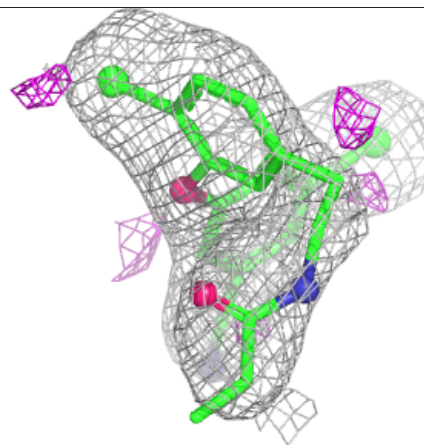
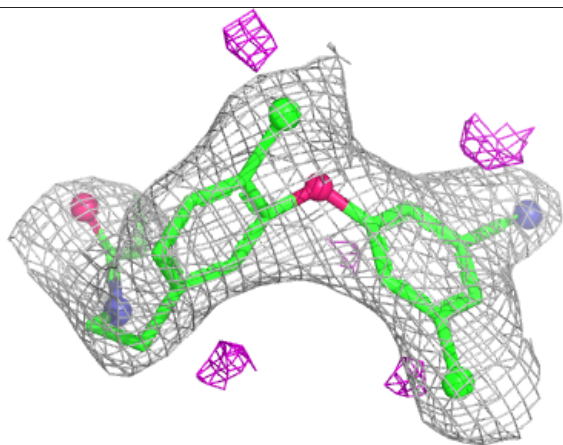
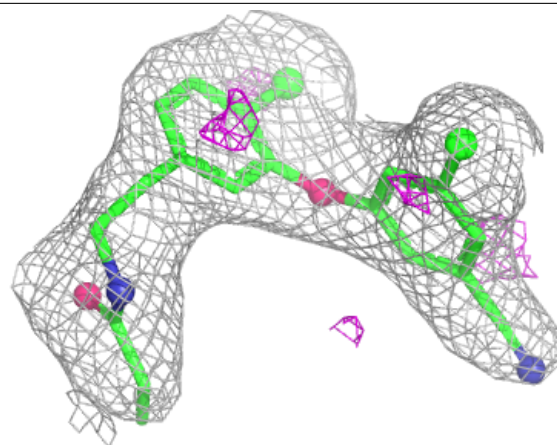
Electron density around VTN A 601 (A):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around VTN A 601 (B):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.