



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 15, 2024 – 09:16 PM EST

PDB ID : 8U6H
Title : Crystal Structure of HIV-1 Reverse Transcriptase in Complex with 3-(2-(3-acryloyl-2-oxo-2,3-dihydro-1H-benzo[d]imidazol-1-yl)ethoxy)-4-chlorophenoxy)-5-chlorobenzonitrile (JLJ744), a non-nucleoside inhibitor
Authors : Prucha, G.; Carter, Z.; Jorgensen, W.L.; Anderson, K.S.
Deposited on : 2023-09-13
Resolution : 2.99 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

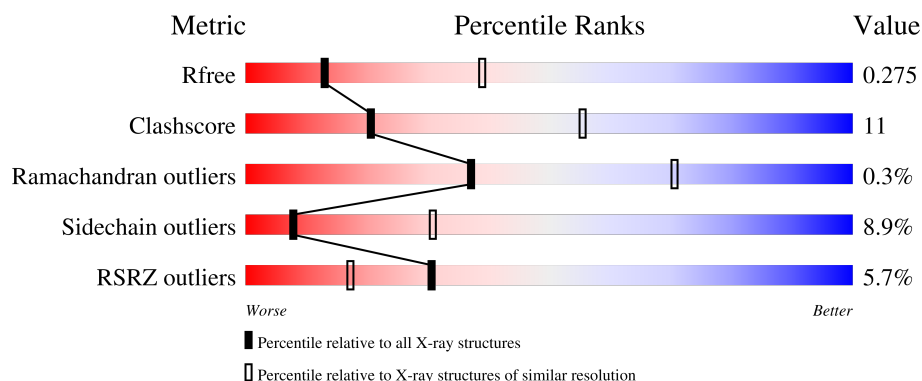
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	556	<div> <div>3%</div> <div>74%</div> <div>21%</div> <div>• •</div> </div>
1	C	556	<div> <div>9%</div> <div>70%</div> <div>23%</div> <div>• •</div> </div>
2	B	428	<div> <div>2%</div> <div>69%</div> <div>22%</div> <div>• 6%</div> </div>
2	D	428	<div> <div>7%</div> <div>72%</div> <div>19%</div> <div>• 8%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14102 atoms, of which 17 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	550	Total	C	N	O	S	0	0	0
			4192	2701	698	787	6			
1	C	531	Total	C	N	O	S	0	1	0
			3794	2418	645	727	4			

There are 10 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
C	-1	MET	-	expression tag	UNP P03366
C	0	VAL	-	expression tag	UNP P03366
C	172	ALA	LYS	engineered mutation	UNP P03366
C	173	ALA	LYS	engineered mutation	UNP P03366
C	280	SER	CYS	engineered mutation	UNP P03366

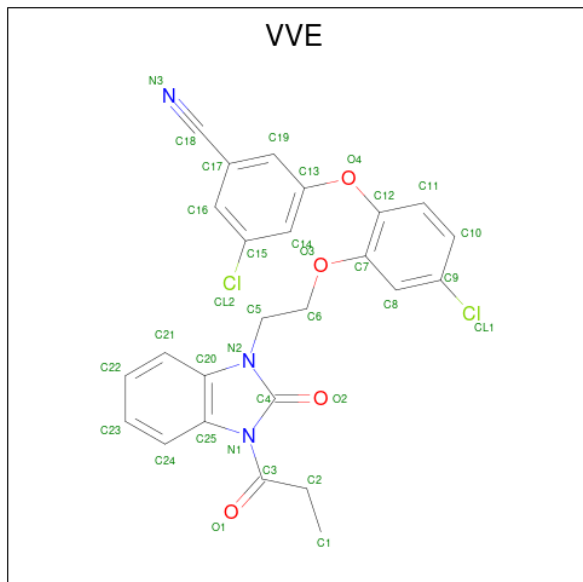
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	403	Total	C	N	O	S	0	0	0
			3230	2097	527	601	5			
2	D	395	Total	C	N	O	S	2	1	0
			2774	1775	472	524	3			

There are 2 discrepancies between the modelled and reference sequences:

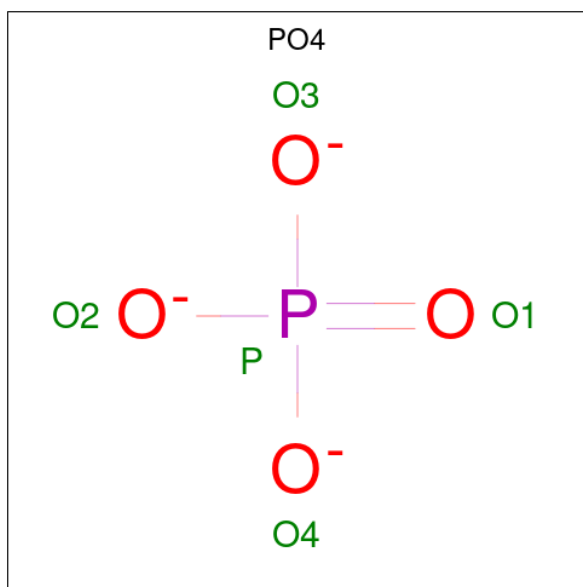
Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366
D	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is 3-chloro-5-{4-chloro-2-[2-(2-oxo-3-propanoyl-2,3-dihydro-1H-benzimidazol-1-yl)ethoxy]phenoxy}benzonitrile (three-letter code: VVE) (formula: $C_{25}H_{19}Cl_2N_3O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			34	25	2	3	4		
3	C	1	Total	C	Cl	H	N	O	0
			51	25	2	17	3	4	

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	9	Total	O	0	0
			9	9		
5	B	6	Total	O	0	0
			6	6		
5	C	2	Total	O	0	0
			2	2		

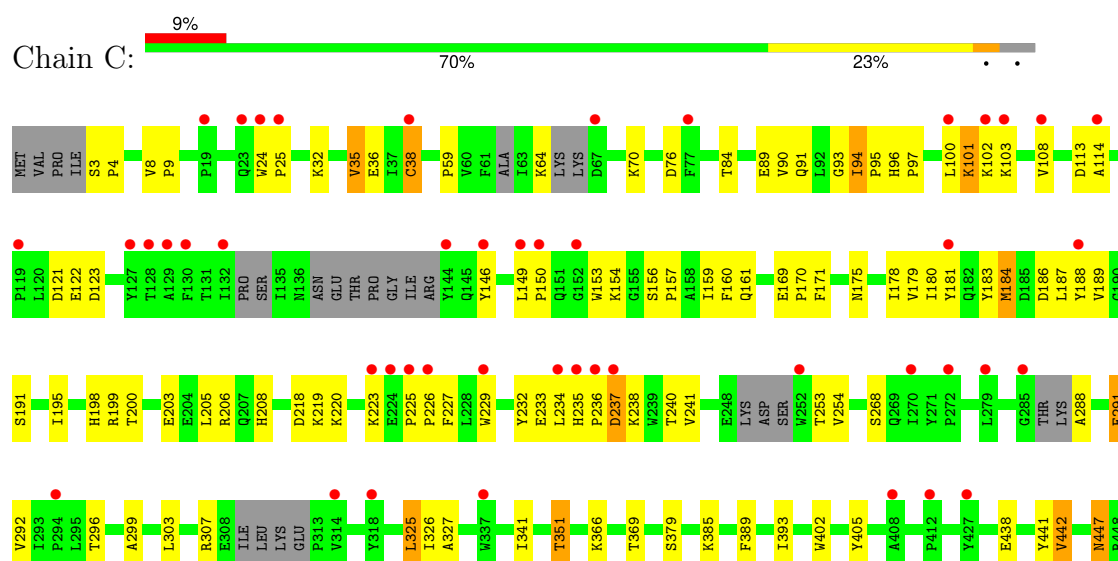
3 Residue-property plots

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.

• Molecule 1: Reverse transcriptase/ribonuclease H

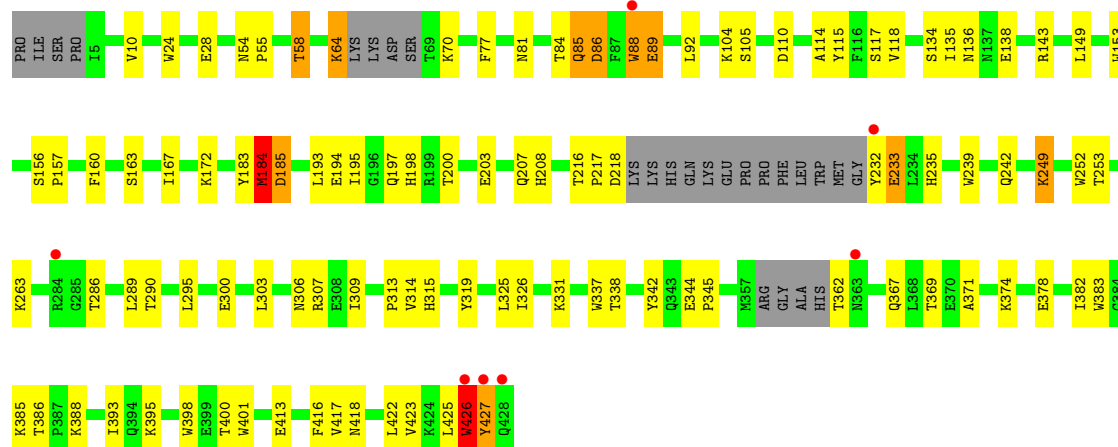


• Molecule 1: Reverse transcriptase/ribonuclease H

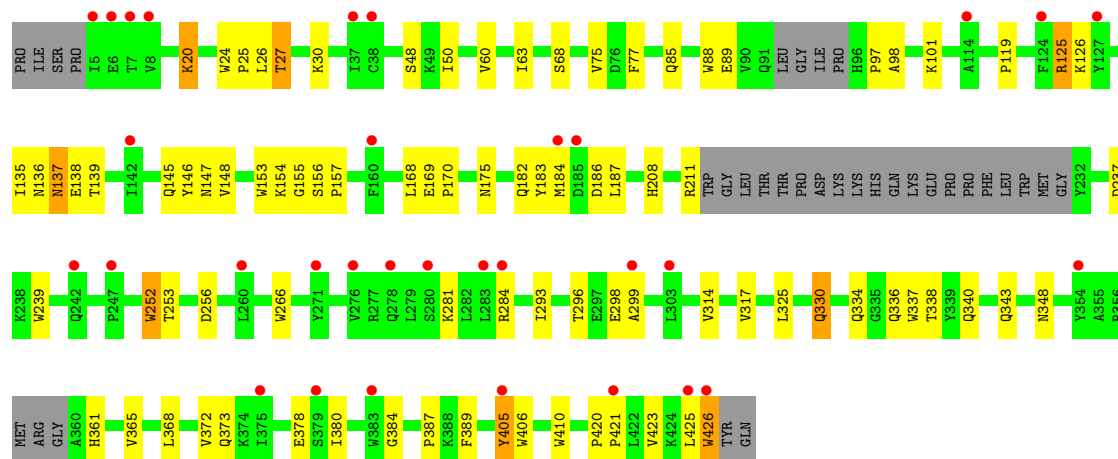




• Molecule 2: p51 RT



• Molecule 2: p51 RT



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	112.40Å 73.19Å 171.58Å 90.00° 97.51° 90.00°	Depositor
Resolution (Å)	170.11 – 2.99 170.11 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.6 (170.11-2.99) 99.5 (170.11-2.99)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.8.0405	Depositor
R, R_{free}	0.220 , 0.279 0.263 , 0.275	Depositor DCC
R_{free} test set	54455 reflections (3.56%)	wwPDB-VP
Wilson B-factor (Å ²)	87.5	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 92.5	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	0.92	EDS
Total number of atoms	14102	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: VVE, PO4

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	0.47	0/4303	0.75	1/5889 (0.0%)
1	C	0.43	0/3892	0.61	0/5346
2	B	0.48	0/3322	0.78	0/4538
2	D	0.45	0/2851	0.65	1/3940 (0.0%)
All	All	0.46	0/14368	0.70	2/19713 (0.0%)

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	D	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	544	GLY	N-CA-C	-5.40	99.59	113.10
2	D	348	ASN	CB-CA-C	5.26	120.92	110.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	97	PRO	Mainchain
2	D	98[A]	ALA	Mainchain
2	D	98[B]	ALA	Mainchain

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	4192	0	3936	88	0
1	C	3794	0	3243	103	0
2	B	3230	0	3113	60	0
2	D	2774	0	2275	48	0
3	A	34	0	0	8	0
3	C	34	17	0	6	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	9	0	0	0	0
5	B	6	0	0	0	0
5	C	2	0	0	0	0
All	All	14085	17	12567	293	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 11.

The worst 5 of 293 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)
2:D:182:GLN:HA	2:D:187:LEU:HA	1.36	1.07
3:C:601:VVE:C1	3:C:601:VVE:O2	2.17	0.92
1:A:102:LYS:HD2	3:A:601:VVE:C2	2.04	0.86
1:C:225:PRO:HB2	1:C:226:PRO:HD3	1.58	0.85
1:C:451:LYS:HA	1:C:471:ASN:H	1.49	0.78

There are no symmetry-related clashes.

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	546/556 (98%)	512 (94%)	32 (6%)	2 (0%)	30	66
1	C	516/556 (93%)	465 (90%)	50 (10%)	1 (0%)	44	77
2	B	395/428 (92%)	374 (95%)	19 (5%)	2 (0%)	25	61
2	D	388/428 (91%)	339 (87%)	49 (13%)	0	100	100
All	All	1845/1968 (94%)	1690 (92%)	150 (8%)	5 (0%)	37	70

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	426	TRP
1	C	237	ASP
2	B	184	MET
1	A	226	PRO
1	A	225	PRO

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	417/495 (84%)	383 (92%)	34 (8%)	9	34
1	C	328/495 (66%)	303 (92%)	25 (8%)	11	37
2	B	340/390 (87%)	310 (91%)	30 (9%)	8	31
2	D	224/390 (57%)	197 (88%)	27 (12%)	4	18
All	All	1309/1770 (74%)	1193 (91%)	116 (9%)	8	31

5 of 116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	290	THR
2	D	340	GLN
1	C	161	GLN

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Mol	Chain	Res	Type
2	D	330	GLN
2	D	139	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	269	GLN
1	C	487	GLN
2	D	330	GLN
2	D	137	ASN
2	B	242	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
4	PO4	A	602	-	4,4,4	0.76	0	6,6,6	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	VVE	C	601	-	37,37,37	0.98	2 (5%)	49,52,52	1.16	1 (2%)
4	PO4	B	501	-	4,4,4	0.74	0	6,6,6	0.47	0
3	VVE	A	601	-	37,37,37	0.51	0	49,52,52	1.65	5 (10%)

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	VVE	C	601	-	-	6/18/18/18	0/4/4/4
3	VVE	A	601	-	-	4/18/18/18	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	VVE	C1-C2	-4.99	1.30	1.51
3	C	601	VVE	C2-C3	-2.18	1.47	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	VVE	C1-C2-C3	8.21	127.07	112.69
3	C	601	VVE	C1-C2-C3	6.73	124.48	112.69
3	A	601	VVE	O3-C7-C12	4.14	124.30	115.75
3	A	601	VVE	O3-C7-C8	-4.08	114.68	123.49
3	A	601	VVE	C6-O3-C7	2.34	123.34	117.69

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

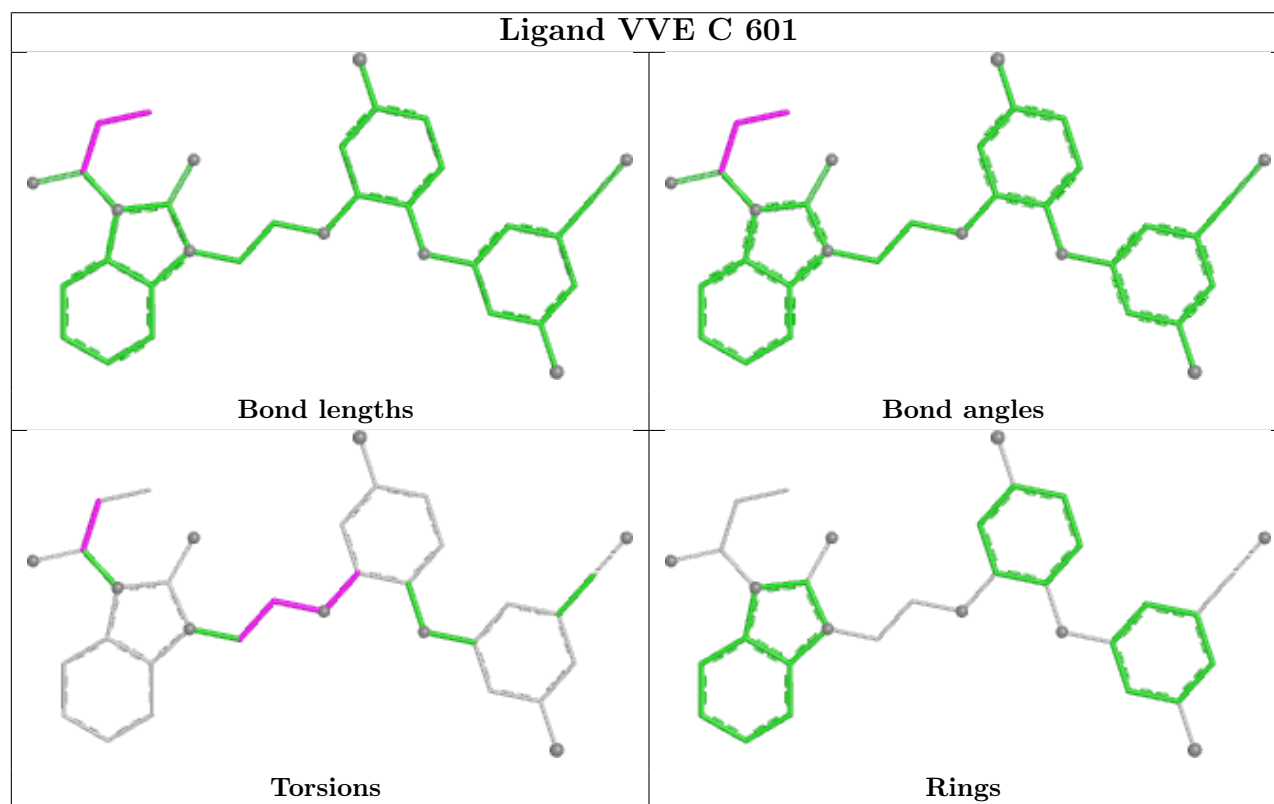
Mol	Chain	Res	Type	Atoms
3	C	601	VVE	C1-C2-C3-O1
3	C	601	VVE	C1-C2-C3-N1
3	A	601	VVE	C8-C7-O3-C6
3	A	601	VVE	C12-C7-O3-C6
3	C	601	VVE	N2-C5-C6-O3

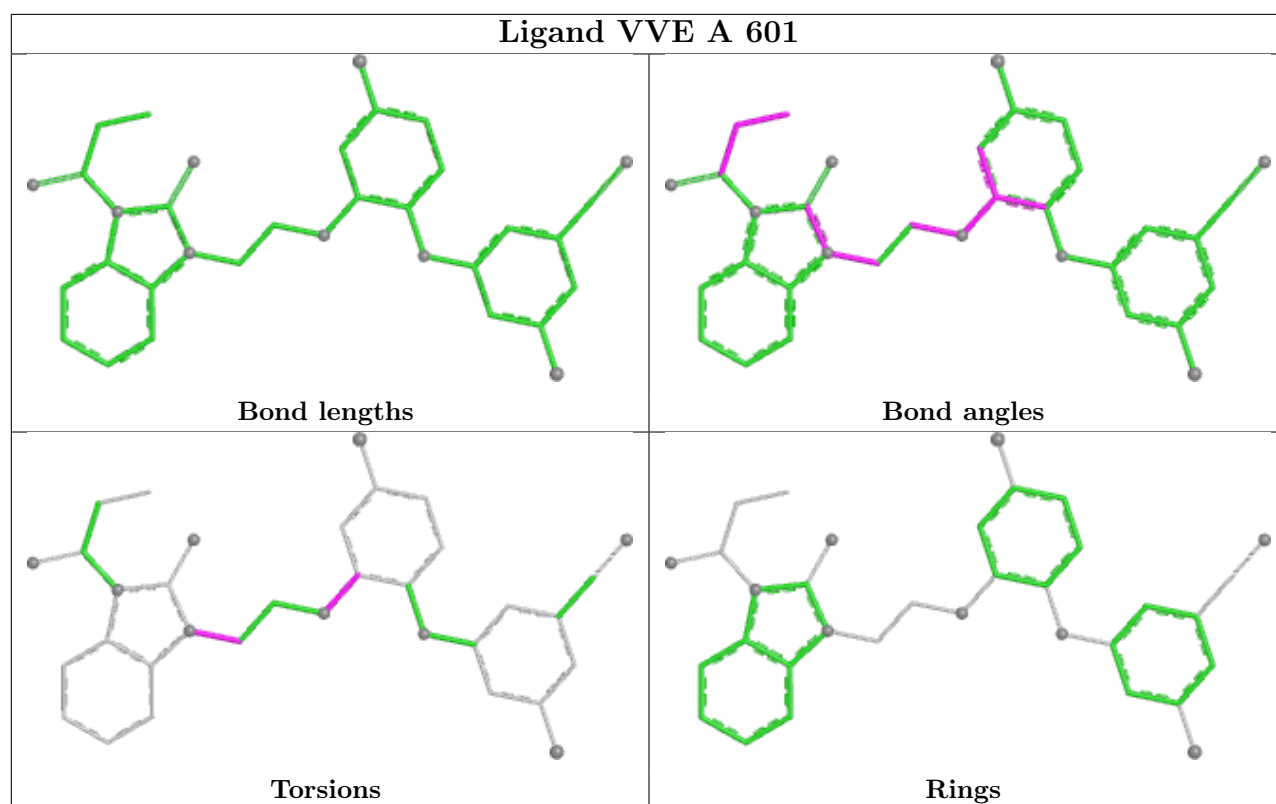
There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	601	VVE	6	0
3	A	601	VVE	8	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 ⓘ

Warning: The R factor obtained from EDS is 0.2716, which does not match the depositor's R factor of 0.22. Please interpret the results in this section carefully.

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	550/556 (98%)	0.07	19 (3%)	47	28	30, 76, 143, 200	0
1	C	531/556 (95%)	0.65	49 (9%)	16	9	30, 125, 186, 235	1 (0%)
2	B	403/428 (94%)	-0.12	7 (1%)	69	47	38, 71, 120, 168	1 (0%)
2	D	395/428 (92%)	0.58	32 (8%)	19	11	30, 133, 183, 210	2 (0%)
All	All	1879/1968 (95%)	0.30	107 (5%)	30	17	30, 102, 173, 235	4 (0%)

The worst 5 of 107 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	7	THR	6.9
2	D	6	GLU	6.6
1	C	25	PRO	6.0
1	C	224	GLU	5.5
1	C	225	PRO	5.4

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands

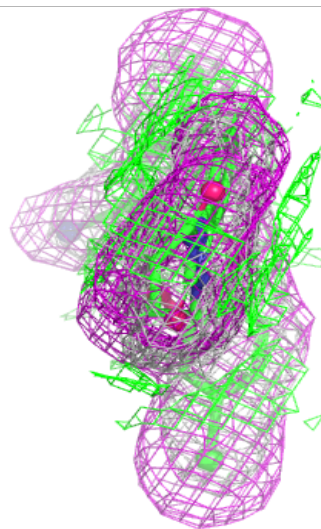
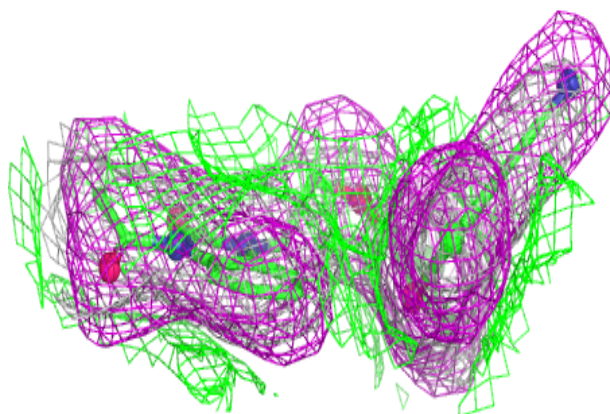
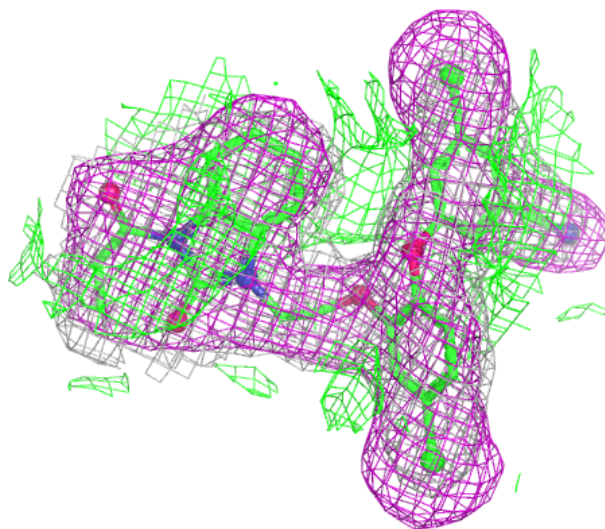
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

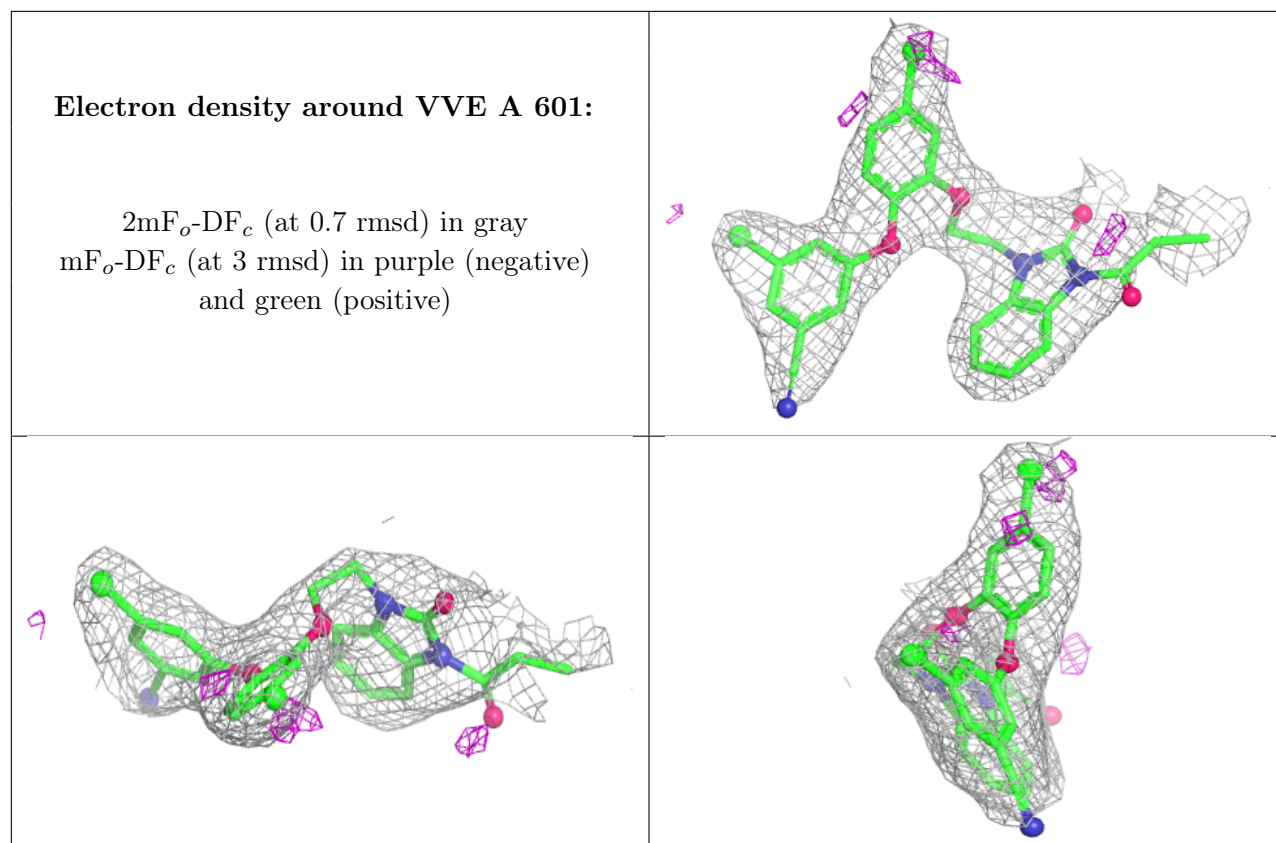
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	VVE	C	601	34/34	0.75	0.15	0,0,0,0	0
4	PO4	B	501	5/5	0.91	0.39	30,30,30,30	0
3	VVE	A	601	34/34	0.92	0.12	48,62,101,110	0
4	PO4	A	602	5/5	0.93	0.38	30,30,30,30	0

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 VVE C 601:

$2mF_o-DF_c$ (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.