



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 06:56 AM EDT

PDB ID : 6V8T
Title : Estrogen Receptor Alpha Ligand Binding Domain Y537S in Complex with LSZ102
Authors : Fanning, S.W.; Greene, G.L.
Deposited on : 2019-12-12
Resolution : 2.10 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 : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : **FAILED**
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) : 2.35.1

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 2.10 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3511 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 Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	210	1633	1048	280	291	14	0	0	0
1	B	214	1669	1077	286	292	14	0	1	0

There are 36 discrepancies between the modelled and reference sequences:

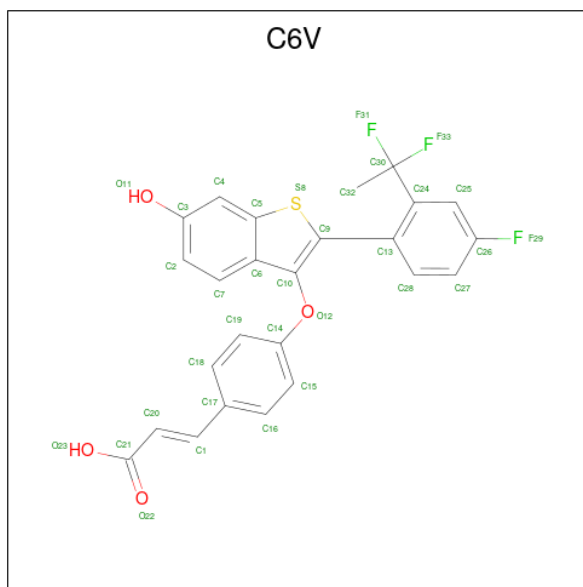
Chain	Residue	Modelled	Actual	Comment	Reference
A	293	HIS	-	expression tag	UNP P03372
A	294	HIS	-	expression tag	UNP P03372
A	295	HIS	-	expression tag	UNP P03372
A	296	HIS	-	expression tag	UNP P03372
A	297	HIS	-	expression tag	UNP P03372
A	298	HIS	-	expression tag	UNP P03372
A	299	GLU	-	expression tag	UNP P03372
A	300	ASN	-	expression tag	UNP P03372
A	301	LEU	-	expression tag	UNP P03372
A	302	TYR	-	expression tag	UNP P03372
A	303	PHE	-	expression tag	UNP P03372
A	304	GLN	-	expression tag	UNP P03372
A	305	SER	-	expression tag	UNP P03372
A	306	MET	-	expression tag	UNP P03372
A	381	SER	CYS	conflict	UNP P03372
A	417	SER	CYS	conflict	UNP P03372
A	530	SER	CYS	conflict	UNP P03372
A	537	SER	TYR	engineered mutation	UNP P03372
B	293	HIS	-	expression tag	UNP P03372
B	294	HIS	-	expression tag	UNP P03372
B	295	HIS	-	expression tag	UNP P03372
B	296	HIS	-	expression tag	UNP P03372
B	297	HIS	-	expression tag	UNP P03372
B	298	HIS	-	expression tag	UNP P03372
B	299	GLU	-	expression tag	UNP P03372

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Chain	Residue	Modelled	Actual	Comment	Reference
B	300	ASN	-	expression tag	UNP P03372
B	301	LEU	-	expression tag	UNP P03372
B	302	TYR	-	expression tag	UNP P03372
B	303	PHE	-	expression tag	UNP P03372
B	304	GLN	-	expression tag	UNP P03372
B	305	SER	-	expression tag	UNP P03372
B	306	MET	-	expression tag	UNP P03372
B	381	SER	CYS	conflict	UNP P03372
B	417	SER	CYS	conflict	UNP P03372
B	530	SER	CYS	conflict	UNP P03372
B	537	SER	TYR	engineered mutation	UNP P03372

- Molecule 2 is LSZ102 (three-letter code: C6V) (formula: C₂₅H₁₇F₃O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	O	S		
2	A	1	33	25	3	4	1	0	0
2	B	1	33	25	3	4	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	72	72	72	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	71	Total	O	0	0
			71	71		

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	105.37Å 53.68Å 96.85Å 90.00° 113.74° 90.00°	Depositor
Resolution (Å)	42.17 – 2.10	Depositor
% Data completeness (in resolution range)	81.1 (42.17-2.10)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.48 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.9_1692+SVN	Depositor
R, R_{free}	0.207 , 0.256	Depositor
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.162	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3511	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.84% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 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
2	C6V	A	601	-	31,36,36	4.36	12 (38%)	37,53,53	2.52	10 (27%)
2	C6V	B	601	-	31,36,36	4.36	14 (45%)	37,53,53	2.29	9 (24%)

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
2	C6V	A	601	-	-	5/14/19/19	0/4/4/4
2	C6V	B	601	-	-	5/14/19/19	0/4/4/4

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	C6V	C2-C3	12.79	1.63	1.38
2	B	601	C6V	C2-C3	12.58	1.62	1.38
2	B	601	C6V	C25-C26	9.95	1.54	1.37
2	A	601	C6V	C25-C26	9.60	1.53	1.37
2	B	601	C6V	C13-C24	9.53	1.54	1.41
2	A	601	C6V	C13-C24	9.11	1.53	1.41
2	A	601	C6V	C28-C27	7.56	1.52	1.38
2	A	601	C6V	C4-C3	7.37	1.50	1.37
2	B	601	C6V	C28-C27	7.20	1.51	1.38
2	B	601	C6V	C4-C3	7.14	1.50	1.37
2	A	601	C6V	C20-C1	7.03	1.51	1.33
2	B	601	C6V	C20-C1	6.95	1.51	1.33
2	A	601	C6V	C13-C9	4.15	1.54	1.48
2	B	601	C6V	C13-C9	3.64	1.54	1.48
2	A	601	C6V	C4-C5	3.36	1.45	1.38
2	A	601	C6V	C7-C2	3.12	1.43	1.36
2	B	601	C6V	F33-C30	-3.09	1.34	1.37
2	B	601	C6V	C7-C2	3.02	1.43	1.36
2	B	601	C6V	C4-C5	2.87	1.44	1.38
2	B	601	C6V	F31-C30	-2.76	1.34	1.37
2	A	601	C6V	F33-C30	-2.71	1.34	1.37
2	B	601	C6V	C30-C24	2.57	1.55	1.51
2	A	601	C6V	C30-C24	2.30	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	C6V	C10-C6	2.30	1.43	1.40
2	A	601	C6V	C28-C13	-2.15	1.36	1.40
2	B	601	C6V	C28-C13	-2.14	1.36	1.40

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	C6V	C14-O12-C10	-10.39	100.08	118.54
2	B	601	C6V	C14-O12-C10	-8.85	102.81	118.54
2	A	601	C6V	C17-C1-C20	-6.04	113.08	126.91
2	B	601	C6V	C17-C1-C20	-5.98	113.22	126.91
2	B	601	C6V	C4-C5-S8	-3.76	117.58	125.10
2	A	601	C6V	C2-C3-C4	-3.71	115.65	120.39
2	B	601	C6V	C1-C20-C21	-3.19	113.67	122.28
2	A	601	C6V	C1-C20-C21	-3.04	114.08	122.28
2	B	601	C6V	C28-C13-C24	2.91	120.91	118.47
2	A	601	C6V	C4-C5-S8	-2.86	119.39	125.10
2	B	601	C6V	C7-C2-C3	-2.57	117.20	120.15
2	A	601	C6V	C15-C16-C17	-2.48	118.02	121.25
2	A	601	C6V	C18-C17-C16	2.44	121.25	117.64
2	A	601	C6V	C27-C26-C25	-2.36	120.23	123.29
2	A	601	C6V	C2-C7-C6	-2.33	117.90	121.13
2	B	601	C6V	C18-C17-C16	2.31	121.06	117.64
2	B	601	C6V	C19-C18-C17	-2.25	118.31	121.25
2	A	601	C6V	C24-C25-C26	2.18	120.56	117.56
2	B	601	C6V	C2-C3-C4	-2.08	117.74	120.39

There are no chirality outliers.

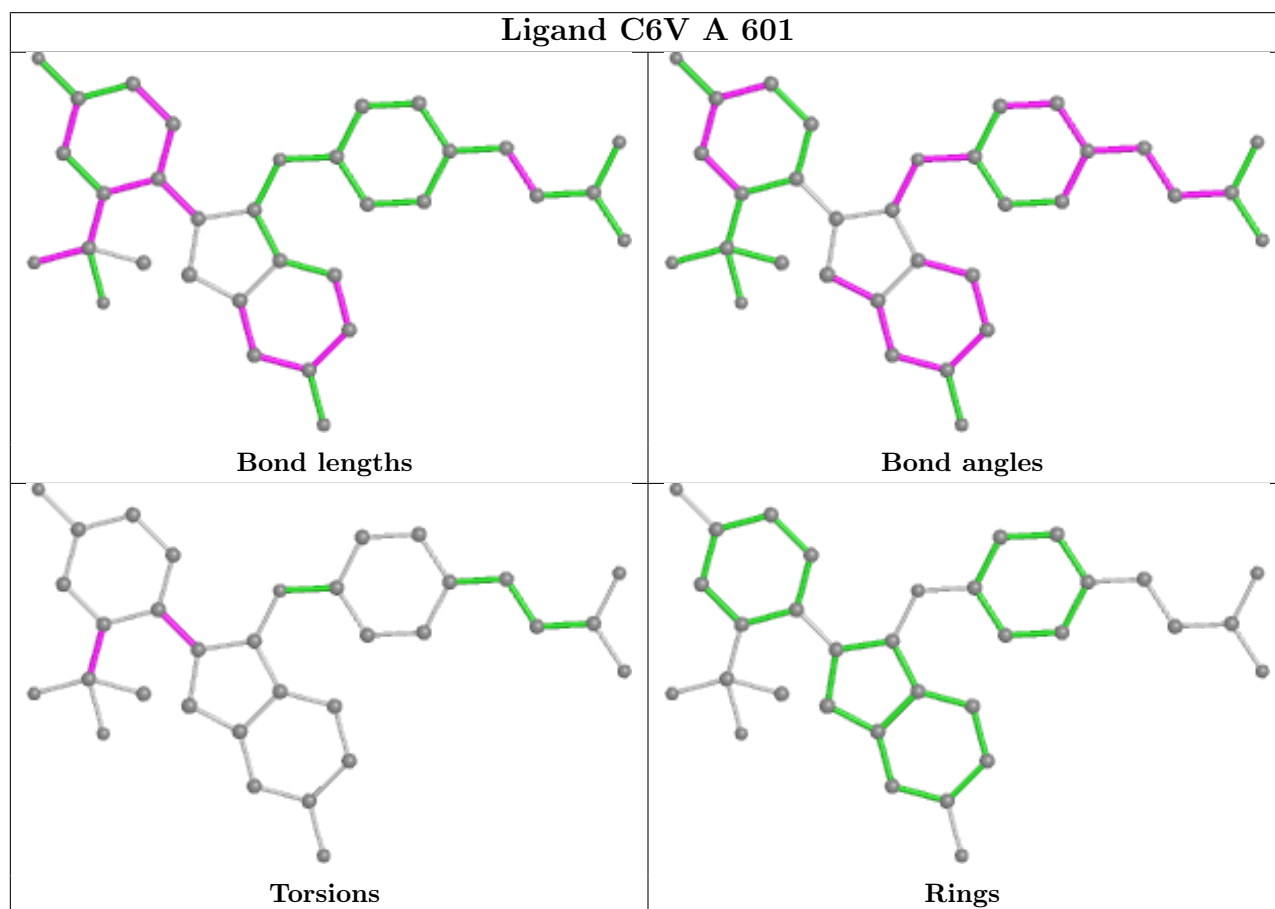
All (10) torsion outliers are listed below:

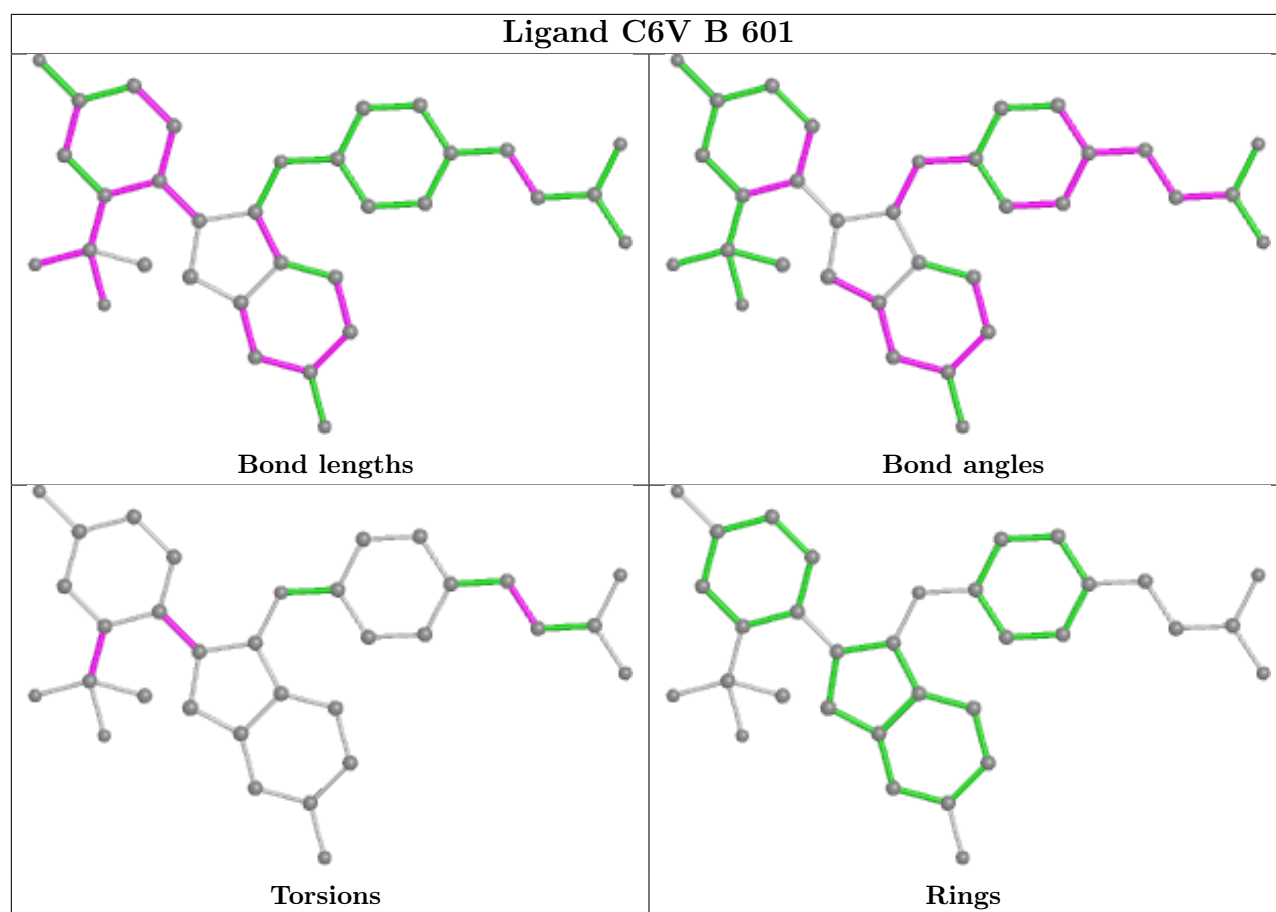
Mol	Chain	Res	Type	Atoms
2	A	601	C6V	C28-C13-C9-S8
2	B	601	C6V	C28-C13-C9-S8
2	B	601	C6V	C13-C24-C30-F33
2	B	601	C6V	C25-C24-C30-F33
2	B	601	C6V	C17-C1-C20-C21
2	A	601	C6V	C25-C24-C30-F31
2	A	601	C6V	C25-C24-C30-F33
2	A	601	C6V	C13-C24-C30-F31
2	A	601	C6V	C13-C24-C30-F33
2	B	601	C6V	C25-C24-C30-F31

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.





4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.