



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 6, 2022 – 04:10 PM EDT

PDB ID : 7UJW
Title : Estrogen Receptor Alpha Ligand Binding Domain Y537S Mutant in Complex with a Methylated Lasofoxifene Derivative that Possesses Selective Estrogen Receptor Degradation Activities
Authors : Hosfield, D.J.; Greene, G.L.; Fanning, S.W.
Deposited on : 2022-03-31
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 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) : 1.13
EDS : 2.28.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.28.1

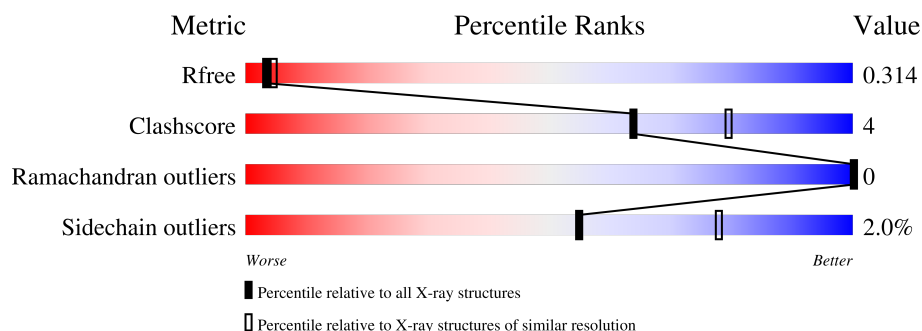
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	263	68% 11% 20%
1	B	263	72% 8% 19%
1	C	263	69% 10% 21%
1	D	263	75% 7% 17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6682 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
1	B	212	Total	C	N	O	S	0	0	0
			1621	1039	280	287	15			
1	D	218	Total	C	N	O	S	0	0	0
			1646	1052	285	294	15			
1	C	208	Total	C	N	O	S	0	0	0
			1589	1020	276	280	13			
1	A	210	Total	C	N	O	S	0	0	0
			1612	1034	278	286	14			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	292	HIS	-	expression tag	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	GLU	-	expression tag	UNP P03372
B	299	ASN	-	expression tag	UNP P03372
B	300	LEU	-	expression tag	UNP P03372
B	301	TYR	-	expression tag	UNP P03372
B	302	PHE	-	expression tag	UNP P03372
B	303	GLN	-	expression tag	UNP P03372
B	304	SER	-	expression tag	UNP P03372
B	305	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
D	292	HIS	-	expression tag	UNP P03372
D	293	HIS	-	expression tag	UNP P03372
D	294	HIS	-	expression tag	UNP P03372

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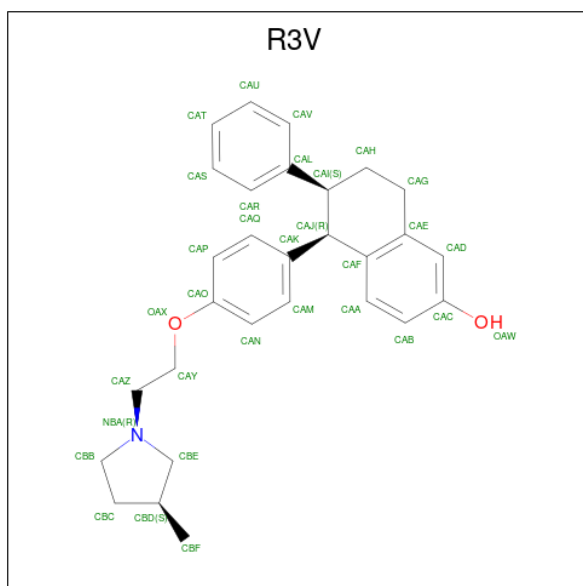
Chain	Residue	Modelled	Actual	Comment	Reference
D	295	HIS	-	expression tag	UNP P03372
D	296	HIS	-	expression tag	UNP P03372
D	297	HIS	-	expression tag	UNP P03372
D	298	GLU	-	expression tag	UNP P03372
D	299	ASN	-	expression tag	UNP P03372
D	300	LEU	-	expression tag	UNP P03372
D	301	TYR	-	expression tag	UNP P03372
D	302	PHE	-	expression tag	UNP P03372
D	303	GLN	-	expression tag	UNP P03372
D	304	SER	-	expression tag	UNP P03372
D	305	MET	-	expression tag	UNP P03372
D	381	SER	CYS	conflict	UNP P03372
D	417	SER	CYS	conflict	UNP P03372
D	530	SER	CYS	conflict	UNP P03372
D	537	SER	TYR	engineered mutation	UNP P03372
C	292	HIS	-	expression tag	UNP P03372
C	293	HIS	-	expression tag	UNP P03372
C	294	HIS	-	expression tag	UNP P03372
C	295	HIS	-	expression tag	UNP P03372
C	296	HIS	-	expression tag	UNP P03372
C	297	HIS	-	expression tag	UNP P03372
C	298	GLU	-	expression tag	UNP P03372
C	299	ASN	-	expression tag	UNP P03372
C	300	LEU	-	expression tag	UNP P03372
C	301	TYR	-	expression tag	UNP P03372
C	302	PHE	-	expression tag	UNP P03372
C	303	GLN	-	expression tag	UNP P03372
C	304	SER	-	expression tag	UNP P03372
C	305	MET	-	expression tag	UNP P03372
C	381	SER	CYS	conflict	UNP P03372
C	417	SER	CYS	conflict	UNP P03372
C	530	SER	CYS	conflict	UNP P03372
C	537	SER	TYR	engineered mutation	UNP P03372
A	292	HIS	-	expression tag	UNP P03372
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	GLU	-	expression tag	UNP P03372
A	299	ASN	-	expression tag	UNP P03372
A	300	LEU	-	expression tag	UNP P03372

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Chain	Residue	Modelled	Actual	Comment	Reference
A	301	TYR	-	expression tag	UNP P03372
A	302	PHE	-	expression tag	UNP P03372
A	303	GLN	-	expression tag	UNP P03372
A	304	SER	-	expression tag	UNP P03372
A	305	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

- Molecule 2 is (5R,6S)-5-(4-{2-[(3S)-3-methylpyrrolidin-1-yl]ethoxy}phenyl)-6-phenyl-5,6,7,8-tetrahydronaphthalen-2-ol (three-letter code: R3V) (formula: C₂₉H₃₃NO₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			32	29	1	2		
2	D	1	Total	C	N	O	0	0
			32	29	1	2		
2	C	1	Total	C	N	O	0	0
			32	29	1	2		
2	A	1	Total	C	N	O	0	0
			32	29	1	2		

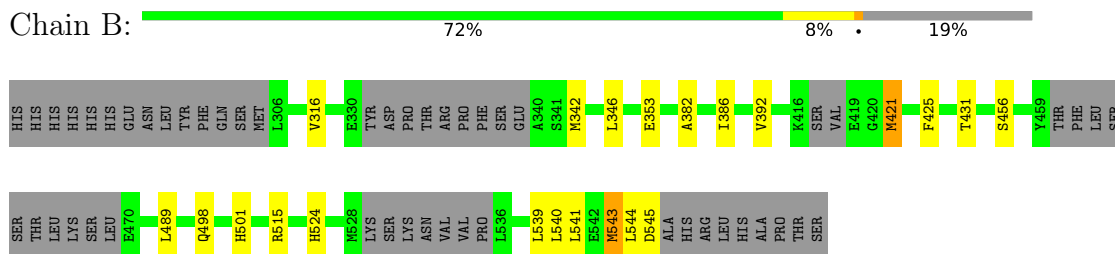
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	24	Total 24	O 24	0	0
3	D	19	Total 19	O 19	0	0
3	C	24	Total 24	O 24	0	0
3	A	19	Total 19	O 19	0	0

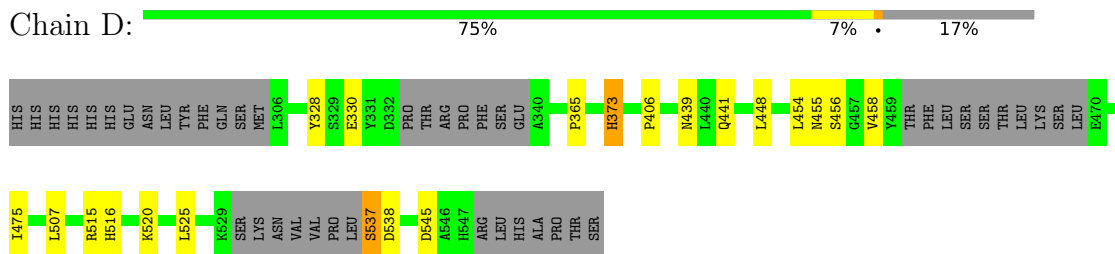
3 Residue-property plots

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.

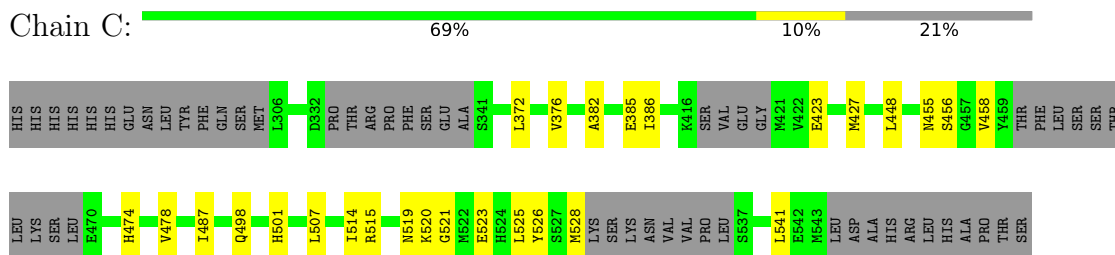
- Molecule 1: Estrogen receptor



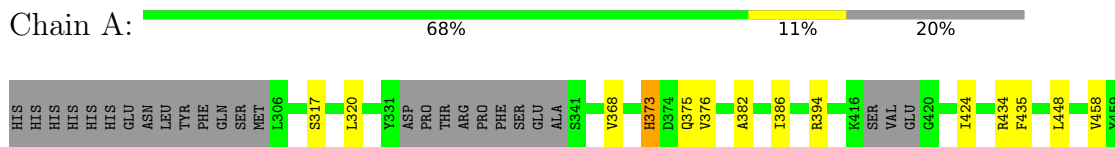
- Molecule 1: Estrogen receptor



- Molecule 1: Estrogen receptor



- Molecule 1: Estrogen receptor



THR	PHE	LEU	SER	SER	THR	LEU	LYS	SER	LEU	E470		D473	H474		V478		I487		L504		L507		I510		S527	MET	LYS	LYS	SER	SER	LYS	LYS	ASN	VAL	VAL	PRO	I536	S537	D538	L539	L540	L541	E542	M543	L544	D545	ALA	HIS	ARG	ARG	LEU	HIS	HIS	ALA	PRO	THR	SER
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.95Å 58.97Å 88.99Å 91.46° 102.06° 117.23°	Depositor
Resolution (Å)	47.59 – 2.60 47.59 – 2.60	Depositor EDS
% Data completeness (in resolution range)	87.1 (47.59-2.60) 87.2 (47.59-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.82	Depositor
R, R_{free}	0.215 , 0.263 0.292 , 0.314	Depositor DCC
R_{free} test set	1251 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	6682	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.23% 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: R3V

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	0/1637	0.45	0/2214
1	B	0.37	0/1645	0.46	0/2224
1	C	0.33	0/1614	0.48	0/2184
1	D	0.31	0/1671	0.45	0/2262
All	All	0.33	0/6567	0.46	0/8884

There are no bond length outliers.

There are no bond angle outliers.

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	1612	0	1594	17	0
1	B	1621	0	1601	14	0
1	C	1589	0	1562	15	0
1	D	1646	0	1611	11	0
2	A	32	0	0	1	0
2	B	32	0	0	1	0
2	C	32	0	0	1	0
2	D	32	0	0	1	0
3	A	19	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	0	0	0	0
3	C	24	0	0	0	0
3	D	19	0	0	0	0
All	All	6682	0	6368	55	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 4.

The worst 5 of 55 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:B:540:LEU:O	1:B:544:LEU:HD12	1.81	0.81
1:A:373:HIS:O	1:A:373:HIS:ND1	2.16	0.79
1:C:376:VAL:HG21	1:C:541:LEU:HG	1.70	0.74
1:B:539:LEU:O	1:B:543:MET:HB2	1.89	0.73
1:A:538:ASP:O	1:A:542:GLU:HG3	1.92	0.69

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	200/263 (76%)	196 (98%)	4 (2%)	0	100	100
1	B	202/263 (77%)	201 (100%)	1 (0%)	0	100	100
1	C	198/263 (75%)	195 (98%)	3 (2%)	0	100	100
1	D	210/263 (80%)	204 (97%)	6 (3%)	0	100	100
All	All	810/1052 (77%)	796 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	168/238 (71%)	164 (98%)	4 (2%)	49	74
1	B	167/238 (70%)	163 (98%)	4 (2%)	49	74
1	C	163/238 (68%)	162 (99%)	1 (1%)	86	95
1	D	168/238 (71%)	164 (98%)	4 (2%)	49	74
All	All	666/952 (70%)	653 (98%)	13 (2%)	55	78

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	537	SER
1	C	520	LYS
1	A	458	VAL
1	A	424	ILE
1	A	434	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	359	ASN
1	B	501	HIS
1	D	373	HIS
1	C	414	GLN
1	A	359	ASN

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 monosaccharides 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
2	R3V	C	601	-	36,36,36	0.78	2 (5%)	46,50,50	1.25	4 (8%)
2	R3V	D	601	-	36,36,36	0.79	2 (5%)	46,50,50	0.82	1 (2%)
2	R3V	B	601	-	36,36,36	0.84	1 (2%)	46,50,50	1.05	4 (8%)
2	R3V	A	601	-	36,36,36	3.42	17 (47%)	46,50,50	2.55	16 (34%)

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	R3V	C	601	-	-	2/14/36/36	0/5/5/5
2	R3V	D	601	-	-	5/14/36/36	0/5/5/5
2	R3V	B	601	-	-	3/14/36/36	0/5/5/5
2	R3V	A	601	-	-	3/14/36/36	0/5/5/5

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	R3V	CAA-CAF	8.39	1.50	1.39
2	A	601	R3V	CAB-CAC	7.12	1.52	1.38
2	A	601	R3V	CAM-CAN	6.92	1.51	1.38
2	A	601	R3V	CAQ-CAK	5.93	1.48	1.39
2	A	601	R3V	CAF-CAJ	-5.67	1.43	1.51

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	R3V	CAC-CAD-CAE	-8.17	111.75	120.83
2	C	601	R3V	CAK-CAJ-CAF	-6.33	103.30	112.86
2	A	601	R3V	CAD-CAE-CAF	6.07	127.38	119.50
2	A	601	R3V	CAG-CAE-CAD	-5.93	108.03	119.91
2	A	601	R3V	CAK-CAJ-CAF	-4.61	105.90	112.86

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	601	R3V	CAY-CAZ-NBA-CBB
2	C	601	R3V	CAJ-CAI-CAL-CAV
2	D	601	R3V	OAX-CAY-CAZ-NBA
2	C	601	R3V	CAJ-CAI-CAL-CAR
2	B	601	R3V	OAX-CAY-CAZ-NBA

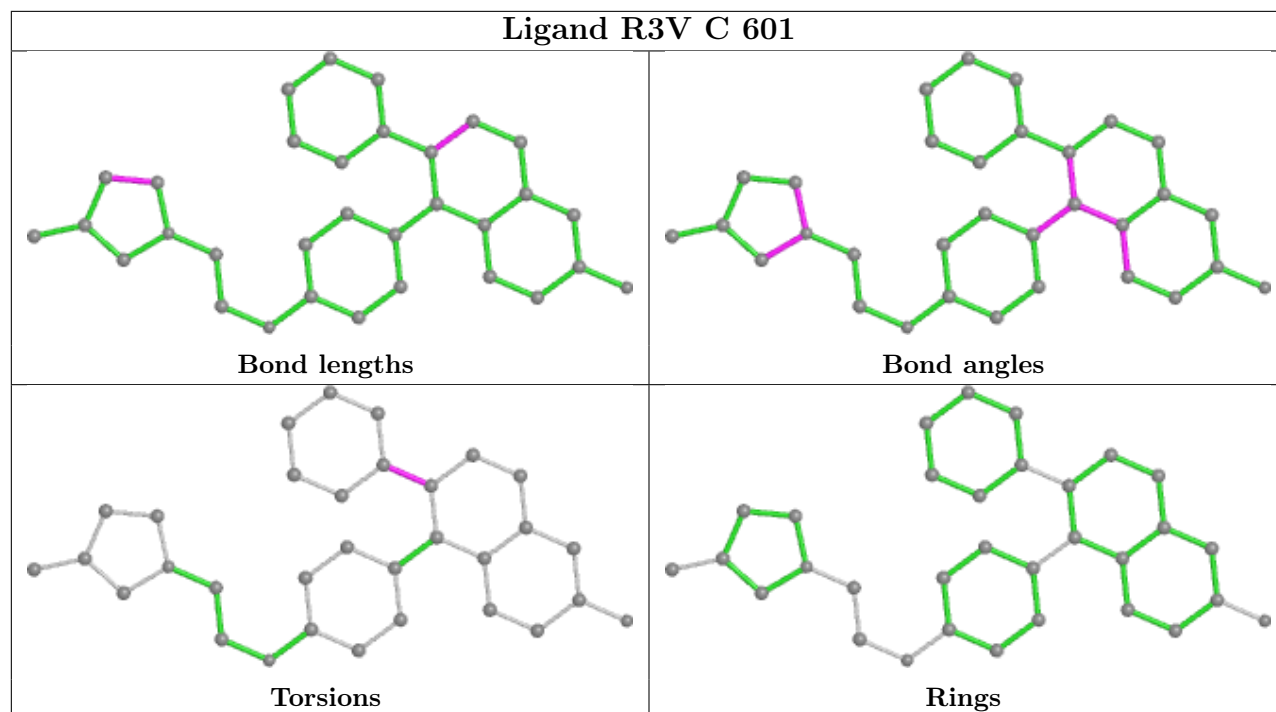
There are no ring outliers.

4 monomers are involved in 4 short contacts:

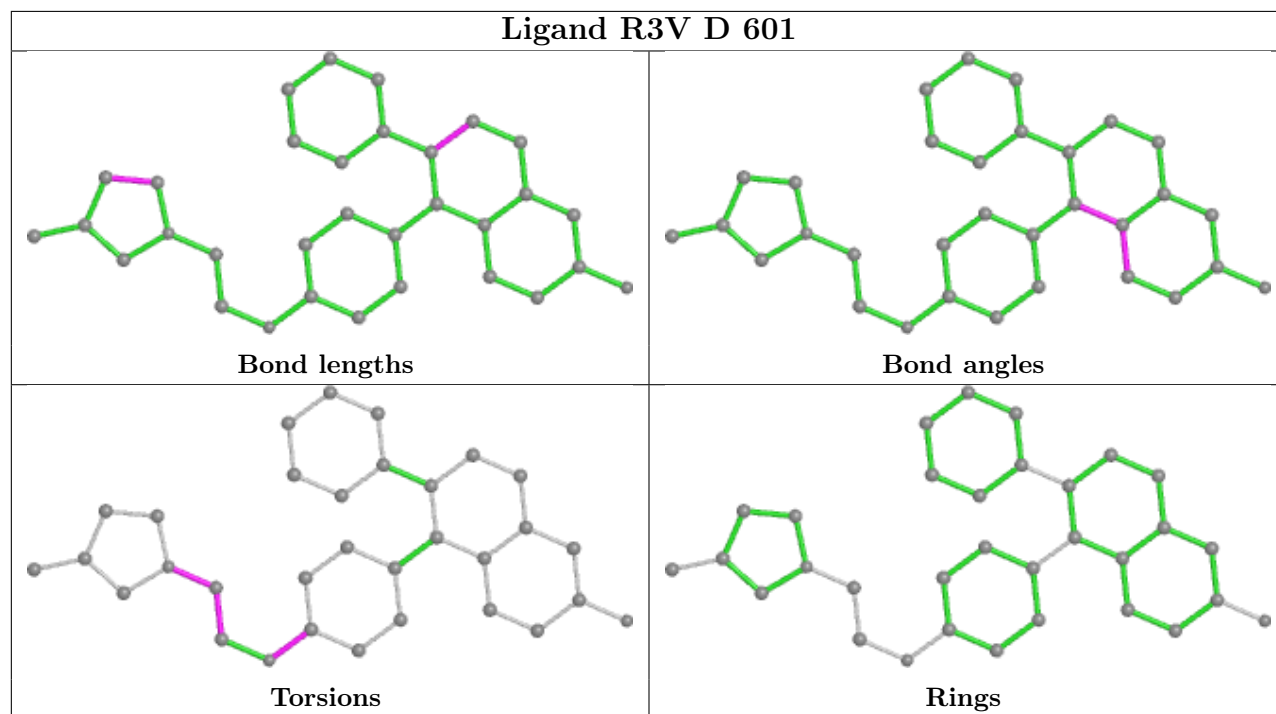
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	R3V	1	0
2	D	601	R3V	1	0
2	B	601	R3V	1	0
2	A	601	R3V	1	0

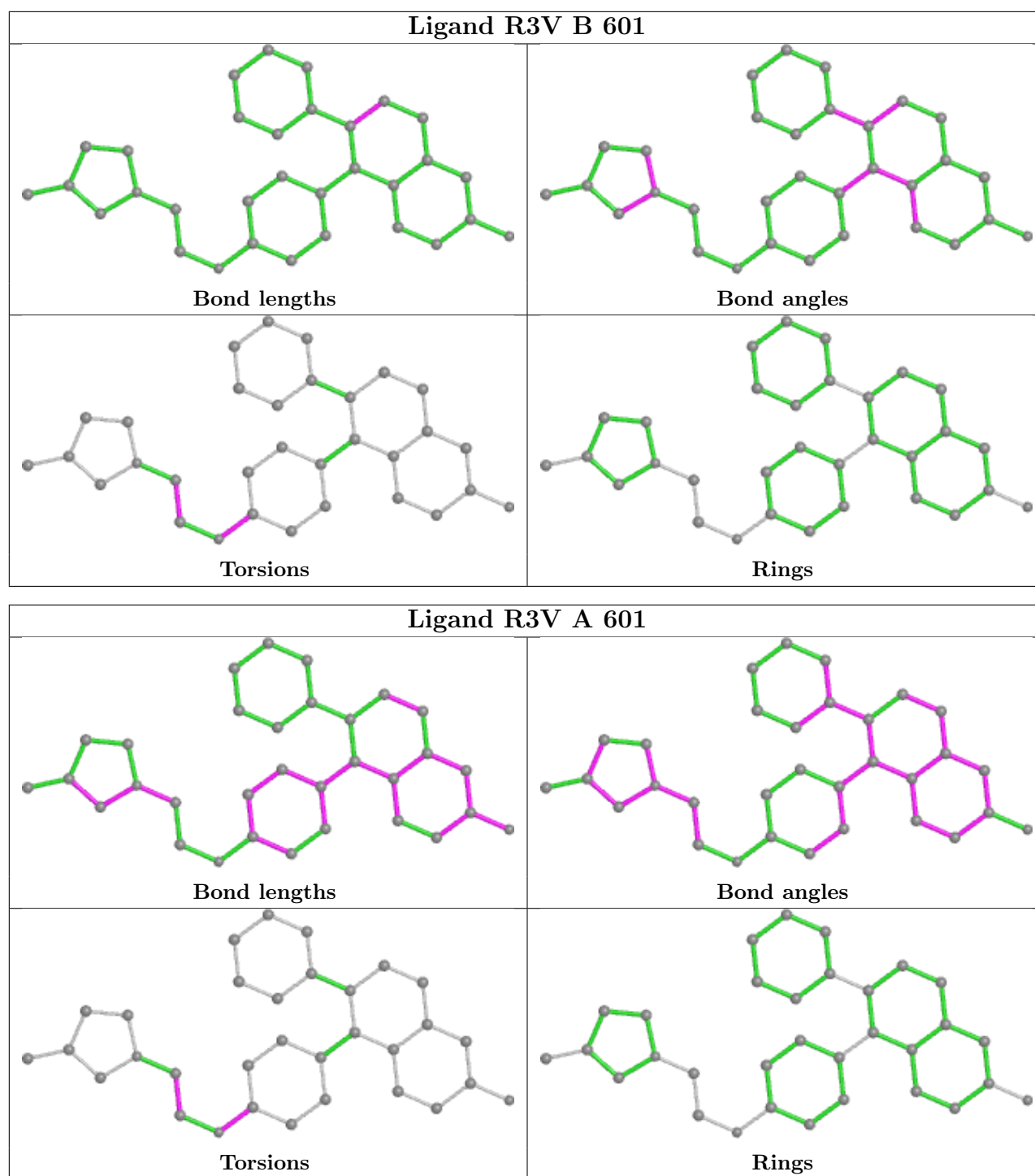
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand R3V C 601



Ligand R3V D 601





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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

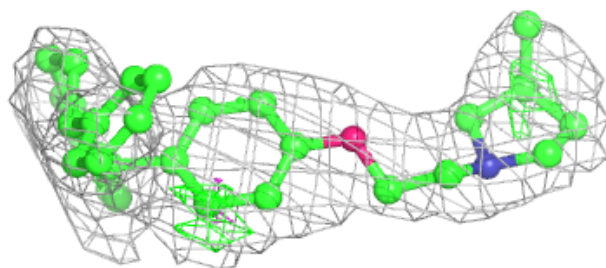
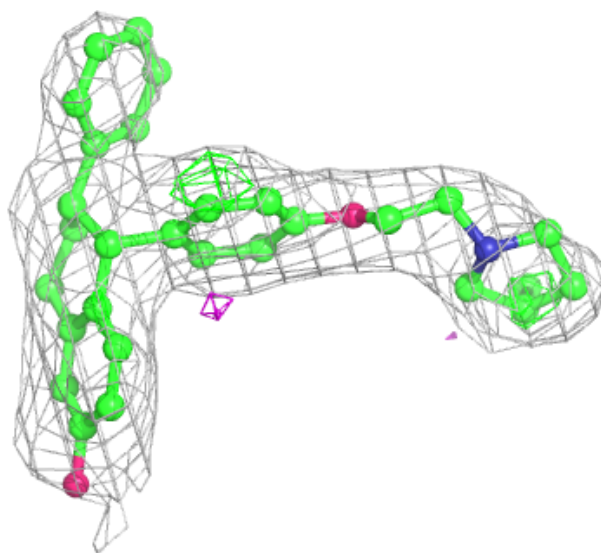
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

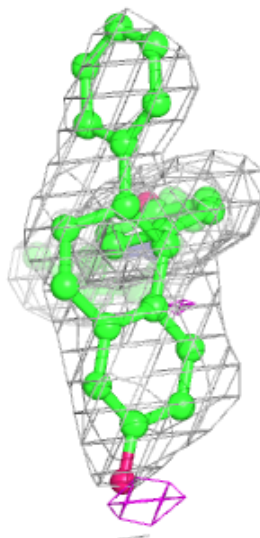
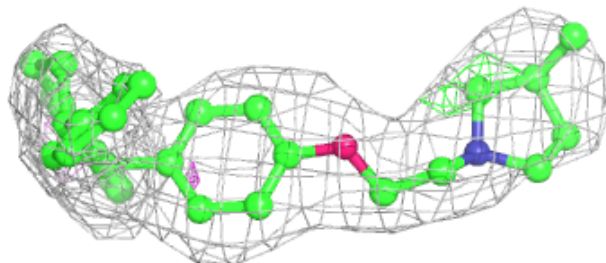
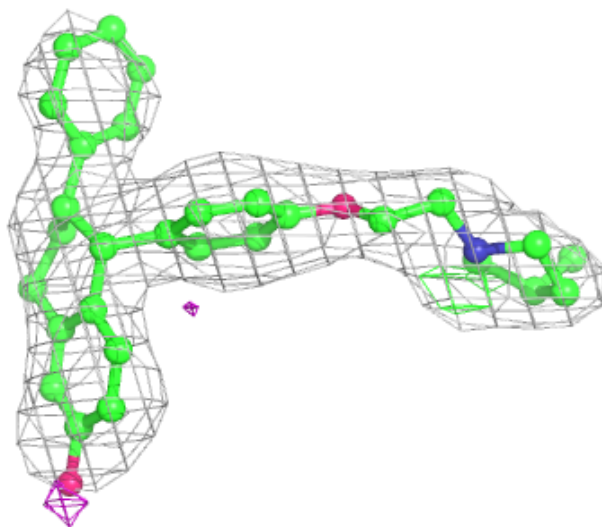
Electron density around R3V B 601:

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



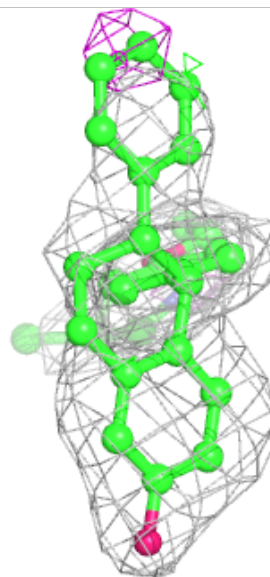
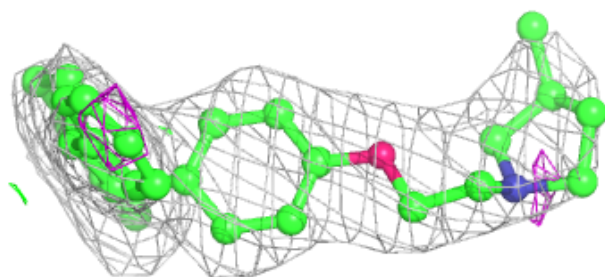
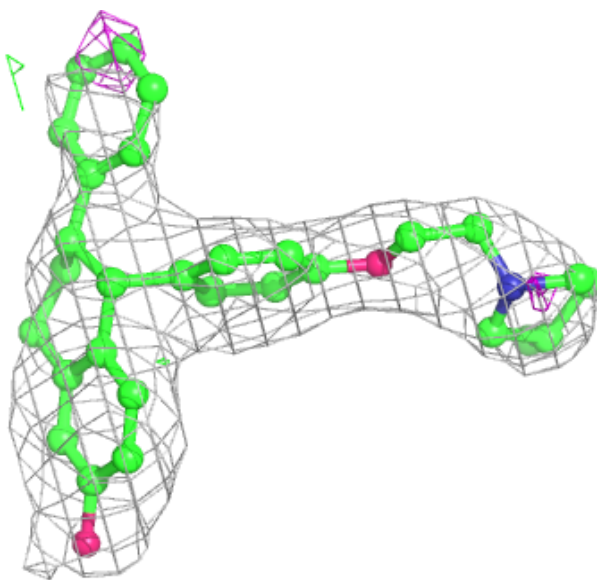
Electron density around R3V D 601:

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



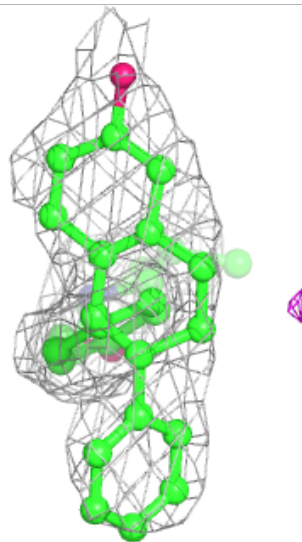
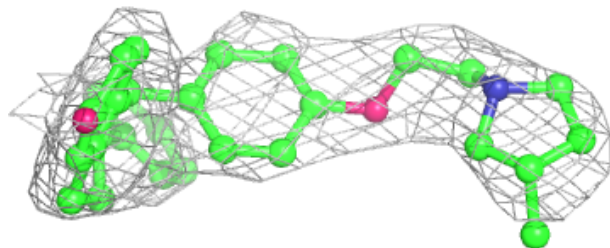
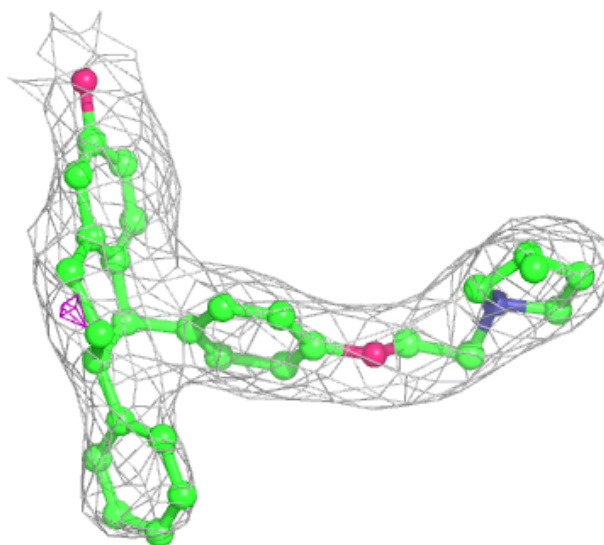
Electron density around R3V C 601:

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



Electron density around R3V A 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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.