



## Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2022 – 04:05 PM EDT

PDB ID : 8DV8  
Title : Estrogen Receptor Alpha Ligand Binding Domain in Complex with (6'-hydroxy-1'-(4-((2-(1-propylpyrrolidin-3-yl)ethyl)thio)phenyl)-1',4'-dihydro-2'-H</i>-spiro[cyclopropane-1,3'-isoquinolin]-2'-yl)(phenyl)methanone  
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Deposited on : 2022-07-28  
Resolution : 1.70 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](mailto: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>.

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The following versions of software and data (see [references](#) ①) 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	:	2.31.2
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)	:	2.31.2

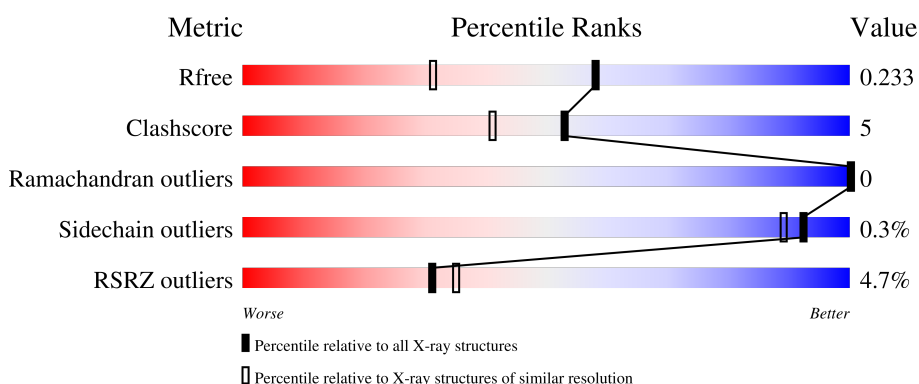
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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  $\geq 3$ , 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	255	<div> <div>3%</div> <div>74%</div> <div>8%</div> <div>18%</div> </div>
1	B	255	<div> <div>5%</div> <div>76%</div> <div>9%</div> <div>15%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3999 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.

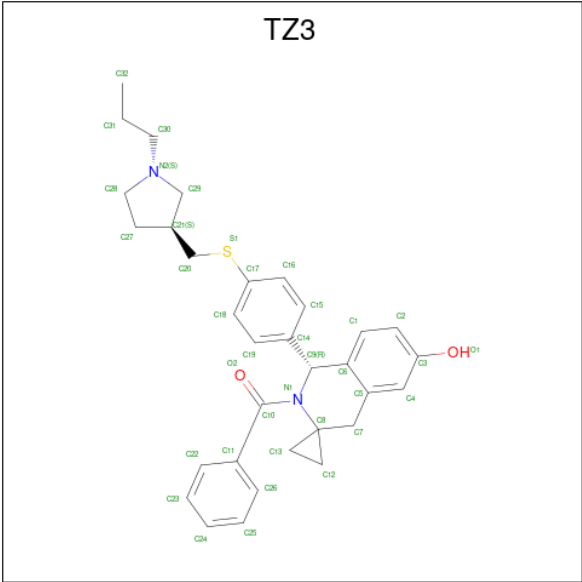
- Molecule 1 is a protein called Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	6	0
			1684	1080	287	303	14			
1	B	218	Total	C	N	O	S	0	9	0
			1775	1140	299	321	15			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	300	MET	-	initiating methionine	UNP P03372
A	381	SER	CYS	engineered mutation	UNP P03372
A	417	SER	CYS	engineered mutation	UNP P03372
A	530	SER	CYS	engineered mutation	UNP P03372
A	536	SER	LEU	engineered mutation	UNP P03372
B	300	MET	-	initiating methionine	UNP P03372
B	381	SER	CYS	engineered mutation	UNP P03372
B	417	SER	CYS	engineered mutation	UNP P03372
B	530	SER	CYS	engineered mutation	UNP P03372
B	536	SER	LEU	engineered mutation	UNP P03372

- Molecule 2 is {(1'R)-6'-hydroxy-1'-[4-({[(3S)-1-propylpyrrolidin-3-yl]methyl}sulfanyl)phenyl]-1',4'-dihydro-2'H-spiro[cyclopropane-1,3'-isoquinolin]-2'-yl}(phenyl)methanone (three-letter code: TZ3) (formula: C<sub>32</sub>H<sub>36</sub>N<sub>2</sub>O<sub>2</sub>S) (labeled as "Ligand of Interest" by depositor).



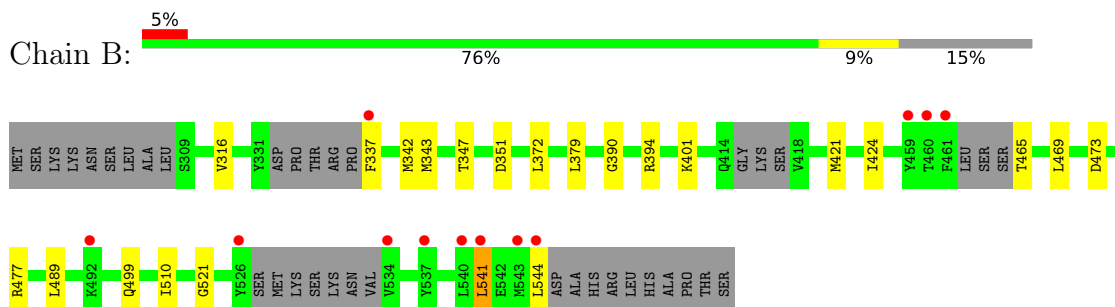
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			37	32	2	2	1		
2	B	1	Total	C	N	O	S	0	0
			37	32	2	2	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	237	Total	O	0	0
			237	237		
3	B	229	Total	O	0	0
			229	229		



- Molecule 1: Estrogen receptor



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.11Å 58.13Å 87.64Å 90.00° 102.79° 90.00°	Depositor
Resolution (Å)	41.41 – 1.70 42.74 – 1.70	Depositor EDS
% Data completeness (in resolution range)	92.7 (41.41-1.70) 92.8 (42.74-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.187 , 0.211 0.214 , 0.233	Depositor DCC
$R_{free}$ test set	2534 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.8	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 51.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3999	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.63% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: TZ3

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	0.40	0/1713	0.60	0/2315
1	B	0.44	0/1806	0.61	0/2436
All	All	0.42	0/3519	0.61	0/4751

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

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	1684	0	1699	16	0
1	B	1775	0	1792	23	0
2	A	37	0	0	2	0
2	B	37	0	0	1	0
3	A	237	0	0	3	0
3	B	229	0	0	5	0
All	All	3999	0	3491	38	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 5.

All (38) 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:372[B]:LEU:CD2	1:B:541:LEU:HD21	1.83	1.08
1:B:372[B]:LEU:HD21	1:B:541:LEU:CD2	1.83	1.07
1:B:372[B]:LEU:HD11	1:B:541:LEU:HD23	1.24	1.07
1:B:372[B]:LEU:HD21	1:B:541:LEU:HD21	0.90	0.79
1:B:372[B]:LEU:HD11	1:B:541:LEU:CD2	2.09	0.77
1:B:465:THR:O	1:B:469:LEU:HD23	1.92	0.68
1:A:459:TYR:OH	1:B:510:ILE:HG12	1.98	0.62
1:B:372[B]:LEU:CD1	1:B:541:LEU:HD23	2.15	0.62
1:B:499:GLN:NE2	3:B:701:HOH:O	2.33	0.61
1:A:498:GLN:HA	1:A:501:HIS:CE1	2.42	0.54
1:B:316:VAL:HG21	1:B:489:LEU:HD21	1.91	0.52
1:A:354:LEU:O	1:A:358:ILE:HG12	2.11	0.51
1:A:533:VAL:O	2:A:601:TZ3:C27	2.60	0.49
1:A:477:ARG:NE	3:A:709:HOH:O	2.46	0.48
1:B:337:PHE:HZ	1:B:342:MET:HG3	1.79	0.47
1:B:499:GLN:HG3	3:B:701:HOH:O	2.14	0.47
1:A:401:LYS:NZ	3:A:703:HOH:O	2.36	0.46
1:A:424:ILE:HD13	1:A:521:GLY:HA2	1.97	0.46
1:B:351:ASP:OD1	2:B:601:TZ3:N2	2.49	0.45
1:A:396:MET:HA	1:A:432:SER:OG	2.16	0.45
1:B:390:GLY:O	1:B:394:ARG:HG3	2.17	0.45
1:B:379:LEU:HD12	1:B:544:LEU:HD11	1.99	0.44
1:A:456:SER:HA	1:A:515:ARG:NH2	2.31	0.44
1:B:372[B]:LEU:CD1	1:B:541:LEU:CD2	2.87	0.44
1:B:499:GLN:CD	3:B:701:HOH:O	2.56	0.44
1:B:424:ILE:HD13	1:B:521:GLY:HA2	2.00	0.44
1:A:359:ASN:CG	3:A:702:HOH:O	2.56	0.43
1:A:451:ILE:HG13	1:A:482:ILE:HG21	2.00	0.43
1:A:342:MET:CE	1:A:410:LEU:HD13	2.48	0.43
1:B:343:MET:SD	1:B:421:MET:HE1	2.59	0.43
1:B:401:LYS:HE3	3:B:788:HOH:O	2.18	0.42
1:A:342:MET:HE2	1:A:410:LEU:HD13	2.01	0.42
1:B:343:MET:O	1:B:347[B]:THR:HG23	2.20	0.42
1:B:499:GLN:CG	3:B:701:HOH:O	2.66	0.42
1:A:396:MET:HE2	1:A:436:ARG:HA	2.02	0.42
1:A:533:VAL:HA	2:A:601:TZ3:C27	2.50	0.41
1:B:473:ASP:OD2	1:B:477:ARG:NE	2.54	0.41
1:A:436:ARG:HH11	1:A:436:ARG:HD2	1.76	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	203/255 (80%)	201 (99%)	2 (1%)	0	100	100
1	B	217/255 (85%)	216 (100%)	1 (0%)	0	100	100
All	All	420/510 (82%)	417 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	187/230 (81%)	187 (100%)	0	100	100
1	B	197/230 (86%)	196 (100%)	1 (0%)	88	83
All	All	384/460 (84%)	383 (100%)	1 (0%)	92	89

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	541	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA

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](#)

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	TZ3	B	601	-	40,42,42	4.58	12 (30%)	48,61,61	1.68	10 (20%)
2	TZ3	A	601	-	40,42,42	4.21	16 (40%)	48,61,61	1.45	8 (16%)

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	TZ3	B	601	-	-	3/20/52/52	0/6/6/6
2	TZ3	A	601	-	-	7/20/52/52	0/6/6/6

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	TZ3	C29-N2	-19.46	1.21	1.47
2	A	601	TZ3	C29-N2	-15.90	1.26	1.47
2	B	601	TZ3	C30-N2	-13.76	1.15	1.47
2	A	601	TZ3	C30-N2	-13.60	1.16	1.47
2	A	601	TZ3	C27-C28	-10.89	1.31	1.52
2	B	601	TZ3	C27-C28	-10.19	1.33	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	TZ3	C5-C6	-5.57	1.30	1.40
2	B	601	TZ3	O2-C10	-5.54	1.11	1.22
2	A	601	TZ3	O2-C10	-5.01	1.12	1.22
2	B	601	TZ3	C5-C6	-4.94	1.31	1.40
2	B	601	TZ3	C20-C21	-4.70	1.47	1.53
2	B	601	TZ3	C17-S1	3.92	1.84	1.76
2	B	601	TZ3	C10-N1	3.25	1.43	1.36
2	A	601	TZ3	C17-S1	3.23	1.83	1.76
2	B	601	TZ3	C22-C11	-2.97	1.34	1.39
2	B	601	TZ3	C28-N2	2.90	1.53	1.47
2	A	601	TZ3	C29-C21	2.82	1.61	1.53
2	A	601	TZ3	C1-C6	2.68	1.43	1.39
2	A	601	TZ3	C10-N1	2.63	1.42	1.36
2	A	601	TZ3	C11-C10	2.55	1.54	1.50
2	B	601	TZ3	C9-N1	-2.48	1.44	1.47
2	A	601	TZ3	C20-S1	2.48	1.86	1.81
2	A	601	TZ3	C28-N2	2.47	1.52	1.47
2	B	601	TZ3	C1-C6	2.30	1.42	1.39
2	A	601	TZ3	C27-C21	-2.27	1.41	1.53
2	A	601	TZ3	C15-C14	-2.27	1.35	1.39
2	A	601	TZ3	C12-C8	2.21	1.53	1.50
2	A	601	TZ3	C26-C11	-2.19	1.35	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	TZ3	C20-S1-C17	5.03	113.36	103.79
2	B	601	TZ3	C7-C5-C4	-3.65	114.10	121.23
2	B	601	TZ3	C30-N2-C29	-3.27	104.49	113.19
2	A	601	TZ3	C30-N2-C28	-3.09	104.71	113.29
2	A	601	TZ3	C22-C11-C10	-2.97	112.76	120.29
2	B	601	TZ3	C28-N2-C29	-2.92	101.16	104.02
2	A	601	TZ3	C2-C3-C4	-2.89	117.01	120.17
2	B	601	TZ3	C23-C22-C11	-2.89	116.92	120.34
2	A	601	TZ3	C27-C21-C29	-2.74	98.77	102.14
2	A	601	TZ3	C7-C5-C4	-2.70	115.95	121.23
2	B	601	TZ3	C16-C15-C14	-2.67	118.51	121.20
2	B	601	TZ3	C6-C9-N1	2.56	113.89	109.68
2	B	601	TZ3	C4-C5-C6	2.43	122.65	119.50
2	A	601	TZ3	C28-C27-C21	-2.42	98.97	104.50
2	A	601	TZ3	C11-C10-N1	2.40	122.14	117.86
2	B	601	TZ3	C26-C11-C10	-2.35	114.34	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	TZ3	C26-C11-C22	2.20	121.73	118.59
2	B	601	TZ3	C30-N2-C28	-2.14	107.35	113.29

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	TZ3	C11-C10-N1-C8
2	A	601	TZ3	O2-C10-N1-C8
2	A	601	TZ3	S1-C20-C21-C29
2	B	601	TZ3	C11-C10-N1-C8
2	B	601	TZ3	O2-C10-N1-C8
2	A	601	TZ3	N2-C30-C31-C32
2	B	601	TZ3	N2-C30-C31-C32
2	A	601	TZ3	C18-C17-S1-C20
2	A	601	TZ3	C16-C17-S1-C20
2	A	601	TZ3	S1-C20-C21-C27

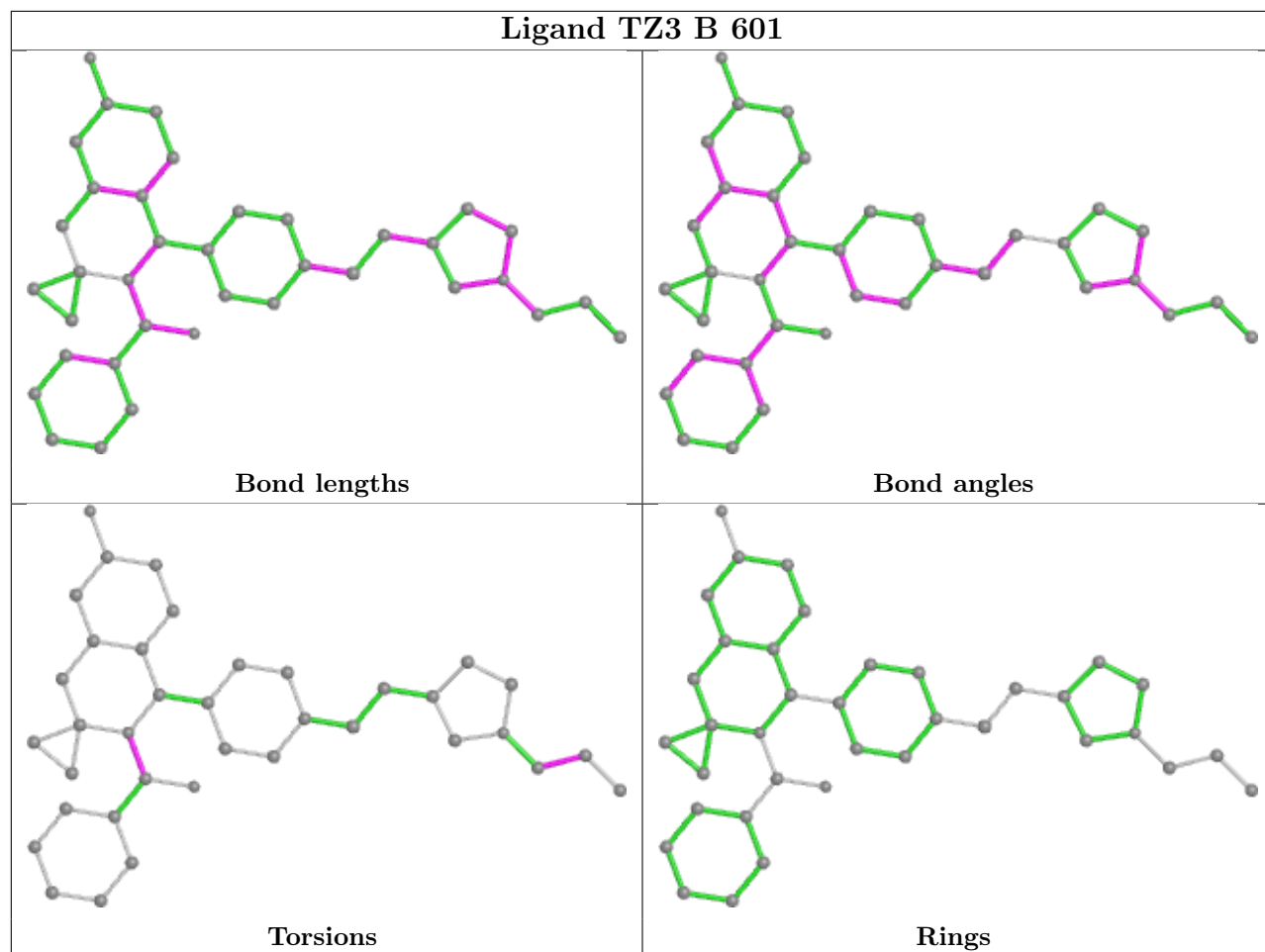
There are no ring outliers.

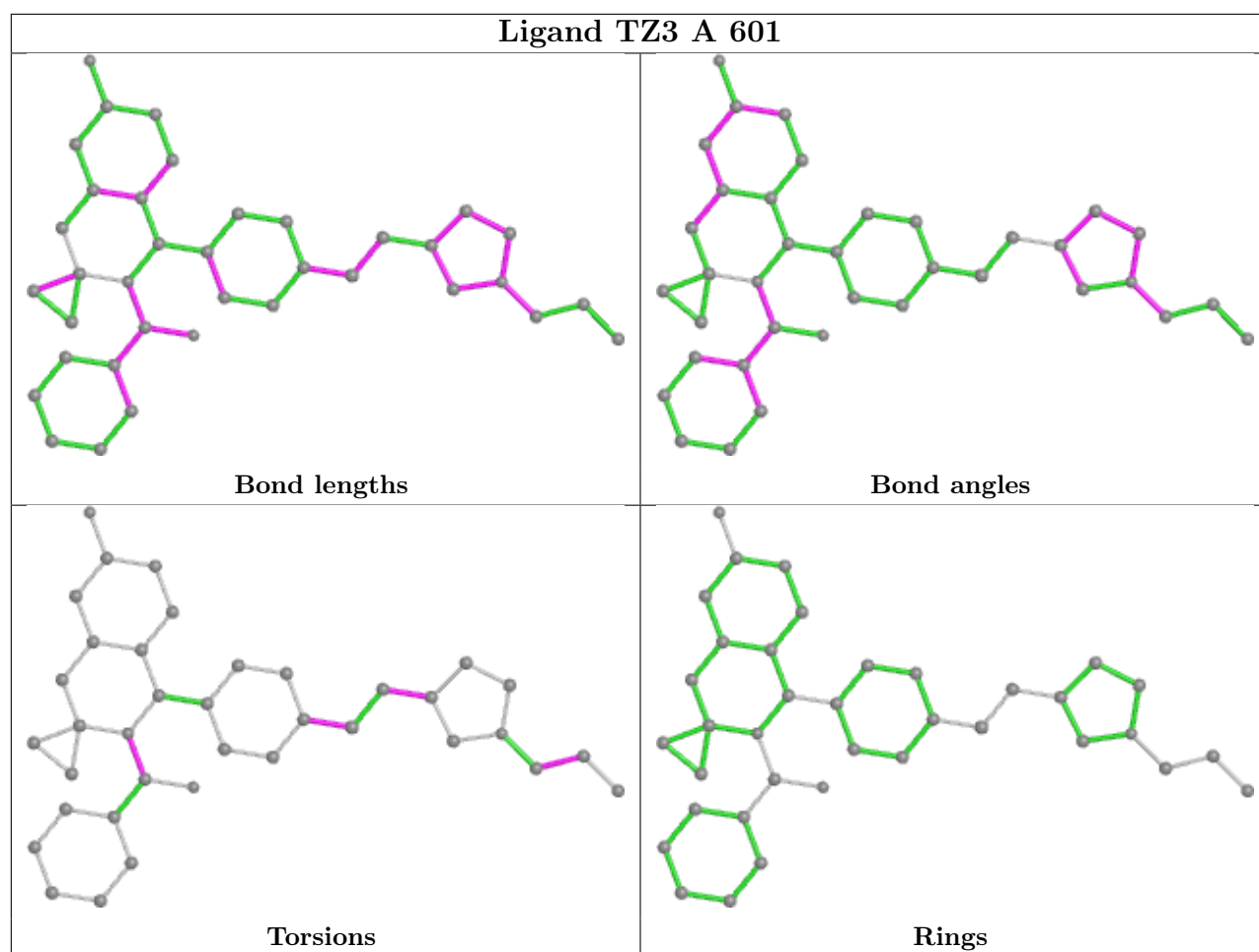
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	TZ3	1	0
2	A	601	TZ3	2	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 TZ3 B 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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	208/255 (81%)	0.11	8 (3%) 40 45	8, 19, 41, 58	1 (0%)
1	B	218/255 (85%)	0.12	12 (5%) 25 27	7, 15, 45, 57	0
All	All	426/510 (83%)	0.12	20 (4%) 31 35	7, 17, 43, 58	1 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	526	TYR	4.8
1	A	526	TYR	4.5
1	A	308	LEU	4.1
1	B	537	TYR	3.9
1	A	460	THR	3.6
1	A	547	HIS	3.4
1	B	337	PHE	3.2
1	A	437	MET	3.1
1	B	534	VAL	3.0
1	A	343	MET	2.9
1	A	309	SER	2.9
1	B	544	LEU	2.7
1	B	540	LEU	2.6
1	B	543	MET	2.6
1	B	459	TYR	2.5
1	B	460	THR	2.5
1	B	541	LEU	2.5
1	B	461	PHE	2.3
1	A	307	ALA	2.2
1	B	492	LYS	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

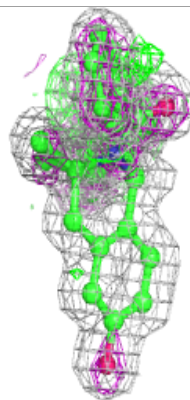
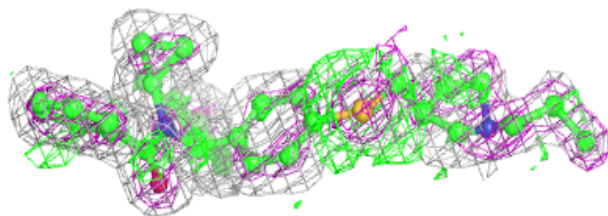
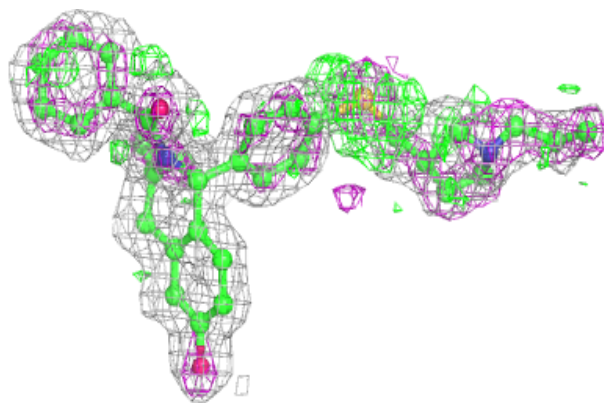
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	TZ3	B	601	37/37	0.90	0.19	0,0,0,0	0
2	TZ3	A	601	37/37	0.93	0.18	0,0,0,0	0

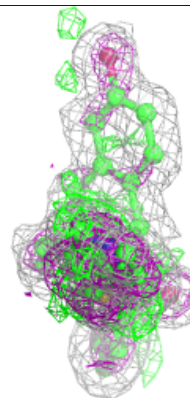
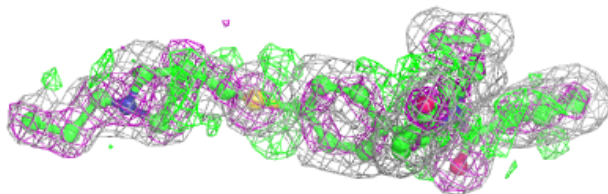
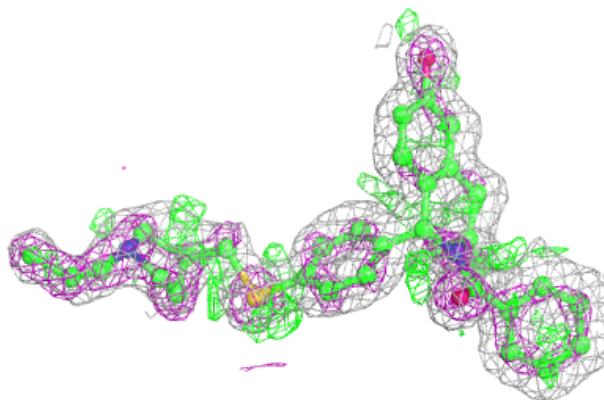
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around TZ3 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 TZ3 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](#)

There are no such residues in this entry.