



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 12:50 am BST

PDB ID : 5TLP
Title : Crystal Structure of the ER-alpha Ligand-binding Domain (Y537S) in Complex with the OBHS-BSC Analog, 3-fluorophenyl (1R,2R,4S)-5-(4-hydroxyphenyl)-6-(4-(2-(piperidin-1-yl)ethoxy)phenyl)-7-oxabicyclo[2.2.1]hept-5-ene-2-sulfonate and 3-methyl-6-phenyl-3H-imidazo[4,5-b]pyridin-2-amine
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Deposited on : 2016-10-11
Resolution : 2.08 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 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 : 2.11
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) : 2.11

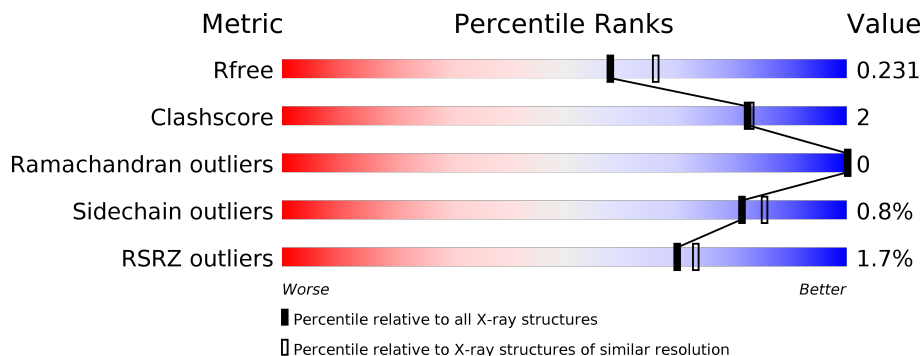
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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 on 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	257	
1	B	257	
2	C	13	
2	D	13	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3917 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	234	1847	1185	314	329	19	0	0	0
1	B	207	1615	1031	281	287	16	0	0	0

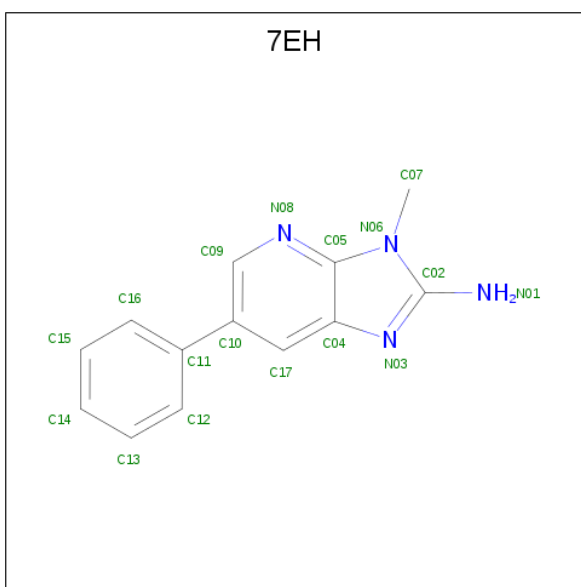
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	537	SER	TYR	engineered mutation	UNP P03372
B	537	SER	TYR	engineered mutation	UNP P03372

- Molecule 2 is a protein called NUCLEAR RECEPTOR COACTIVATOR 2.

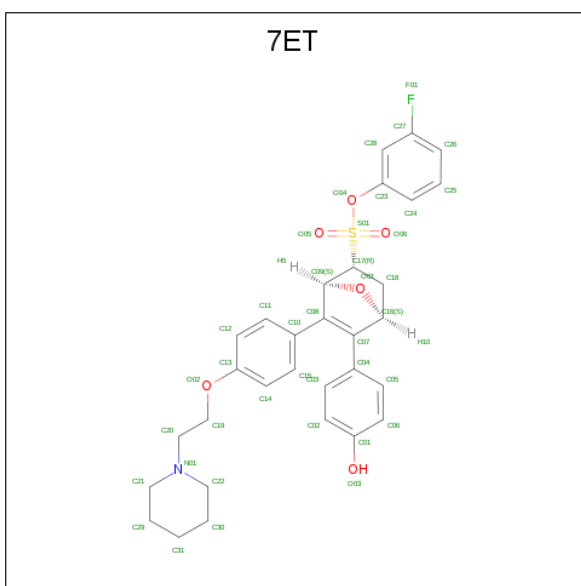
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	10	84	54	17	13	0	0	0
2	D	7	49	33	9	7	0	0	0

- Molecule 3 is 3-methyl-6-phenyl-3H-imidazo[4,5-b]pyridin-2-amine (three-letter code: 7EH) (formula: C₁₃H₁₂N₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
3	A	1	17	13	4	0	0

- Molecule 4 is 3-fluorophenyl (1S,2R,4S)-5-(4-hydroxyphenyl)-6-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-7-oxabicyclo[2.2.1]hept-5-ene-2-sulfonate (three-letter code: 7ET) (formula: $C_{31}H_{32}FNO_6S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	N	O			S
4	B	1	40	31	1	1	6	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	144	Total 144	O 144	0	0
5	B	117	Total 117	O 117	0	0
5	C	4	Total 4	O 4	0	0

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.94Å 83.26Å 58.65Å 90.00° 109.29° 90.00°	Depositor
Resolution (Å)	44.59 – 2.08 44.59 – 2.08	Depositor EDS
% Data completeness (in resolution range)	93.8 (44.59-2.08) 93.8 (44.59-2.08)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.88 (at 2.08Å)	Xtrriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.187 , 0.232 0.186 , 0.231	Depositor DCC
R_{free} test set	1947 reflections (6.50%)	wwPDB-VP
Wilson B-factor (Å ²)	20.6	Xtrriage
Anisotropy	0.122	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.024 for l,-k,h	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3917	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.75% 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: 7EH, 7ET

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	0.25	0/1881	0.41	0/2542
1	B	0.24	0/1642	0.39	0/2219
2	C	0.20	0/84	0.36	0/111
2	D	0.20	0/49	0.31	0/66
All	All	0.24	0/3656	0.40	0/4938

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
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	332	ASP	Peptide

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	1847	0	1875	12	0
1	B	1615	0	1631	7	0
2	C	84	0	90	1	0
2	D	49	0	45	0	0
3	A	17	0	0	0	0
4	B	40	0	0	1	0
5	A	144	0	0	0	0
5	B	117	0	0	0	0
5	C	4	0	0	0	0
All	All	3917	0	3641	18	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 2.

All (18) 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:308:LEU:HD21	1:A:477:ARG:HE	1.44	0.83
1:B:370:LEU:HD11	1:B:475:ILE:HD11	1.67	0.77
1:A:472:LYS:HE2	1:A:476:HIS:CD2	2.32	0.64
1:B:308:LEU:O	1:B:481:LYS:NZ	2.31	0.63
1:A:306:LEU:H	1:A:306:LEU:HD13	1.65	0.61
1:A:473:ASP:OD2	1:A:477:ARG:NH1	2.34	0.60
1:A:396:MET:O	1:A:436:ARG:NH1	2.35	0.56
1:A:316:VAL:HG21	1:A:489:LEU:HD21	1.90	0.54
1:A:331:TYR:CD2	1:A:333:PRO:HD3	2.43	0.54
1:A:330:GLU:OE1	1:A:330:GLU:N	2.40	0.50
1:B:456:SER:HA	1:B:515:ARG:NH2	2.25	0.50
1:A:376:VAL:HG13	2:C:690:LEU:HD23	1.94	0.49
1:A:539:LEU:O	1:A:543:MET:HG2	2.16	0.46
1:B:424:ILE:HG21	4:B:601:7ET:O06	2.19	0.43
1:A:497:LEU:HD11	1:B:497:LEU:HD21	2.01	0.42
1:B:496:THR:O	1:B:500:GLN:HG3	2.20	0.42
1:B:338:SER:N	1:B:341:SER:HG	2.19	0.41
1:A:490:MET:HB3	1:A:495:LEU:HD12	2.03	0.41

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	228/257 (89%)	225 (99%)	3 (1%)	0	100	100
1	B	201/257 (78%)	197 (98%)	4 (2%)	0	100	100
2	C	8/13 (62%)	8 (100%)	0	0	100	100
2	D	5/13 (38%)	5 (100%)	0	0	100	100
All	All	442/540 (82%)	435 (98%)	7 (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	205/232 (88%)	202 (98%)	3 (2%)	65	69
1	B	176/232 (76%)	176 (100%)	0	100	100
2	C	9/13 (69%)	9 (100%)	0	100	100
2	D	4/13 (31%)	4 (100%)	0	100	100
All	All	394/490 (80%)	391 (99%)	3 (1%)	81	85

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	306	LEU
1	A	332	ASP
1	A	425	PHE

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

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 carbohydrates 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
4	7ET	B	601	-	44,45,45	2.30	16 (36%)	56,65,65	2.17	16 (28%)
3	7EH	A	601	-	17,19,19	1.83	2 (11%)	20,27,27	1.98	6 (30%)

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
4	7ET	B	601	-	-	7/23/57/57	0/7/6/6
3	7EH	A	601	-	-	3/4/4/4	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	7ET	C10-C08	-7.20	1.34	1.48
4	B	601	7ET	C04-C07	-6.63	1.36	1.48
3	A	601	7EH	C02-N01	5.57	1.45	1.33
4	B	601	7ET	O04-S01	4.13	1.67	1.60
4	B	601	7ET	C17-S01	3.27	1.86	1.79
4	B	601	7ET	O04-C23	-2.99	1.37	1.42
3	A	601	7EH	C17-C04	2.92	1.46	1.41
4	B	601	7ET	C25-C26	-2.43	1.33	1.38
4	B	601	7ET	C15-C10	-2.43	1.35	1.39
4	B	601	7ET	C11-C10	-2.34	1.35	1.39
4	B	601	7ET	C03-C02	-2.33	1.34	1.38
4	B	601	7ET	C28-C23	-2.30	1.34	1.38
4	B	601	7ET	C06-C05	-2.29	1.34	1.38
4	B	601	7ET	C12-C11	-2.22	1.34	1.38
4	B	601	7ET	C03-C04	-2.21	1.35	1.39
4	B	601	7ET	C15-C14	-2.20	1.34	1.38
4	B	601	7ET	C02-C01	-2.13	1.34	1.38
4	B	601	7ET	C05-C04	-2.03	1.35	1.39

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	601	7ET	O06-S01-C17	-6.90	100.35	109.33
4	B	601	7ET	O05-S01-C17	-5.98	101.54	109.33
3	A	601	7EH	C10-C09-N08	-4.51	121.38	125.55
3	A	601	7EH	C10-C17-C04	-4.37	117.62	121.44
4	B	601	7ET	C22-N01-C21	4.22	118.33	108.83
3	A	601	7EH	C09-N08-C05	3.67	121.41	116.73
4	B	601	7ET	C29-C21-N01	3.47	116.90	111.33
4	B	601	7ET	C14-C13-C12	-3.26	115.15	120.18
4	B	601	7ET	C24-C23-C28	-3.15	116.21	120.53
4	B	601	7ET	O04-S01-O06	3.12	116.44	106.82
4	B	601	7ET	O01-C16-C18	-2.98	98.79	104.64
4	B	601	7ET	C10-C08-C07	2.91	136.34	128.81
4	B	601	7ET	O04-S01-O05	2.86	115.64	106.82
4	B	601	7ET	C23-C28-C27	2.85	121.38	117.56
4	B	601	7ET	C23-O04-S01	-2.84	112.94	119.85
4	B	601	7ET	C30-C22-N01	2.80	115.81	111.33
4	B	601	7ET	C25-C24-C23	2.63	123.17	118.96
4	B	601	7ET	C15-C14-C13	2.49	122.78	119.73
3	A	601	7EH	C17-C04-C05	-2.30	118.81	121.12
4	B	601	7ET	C11-C12-C13	2.21	122.44	119.73
3	A	601	7EH	N01-C02-N03	2.14	126.07	123.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	7EH	C17-C10-C09	2.10	119.18	116.24

There are no chirality outliers.

All (10) torsion outliers are listed below:

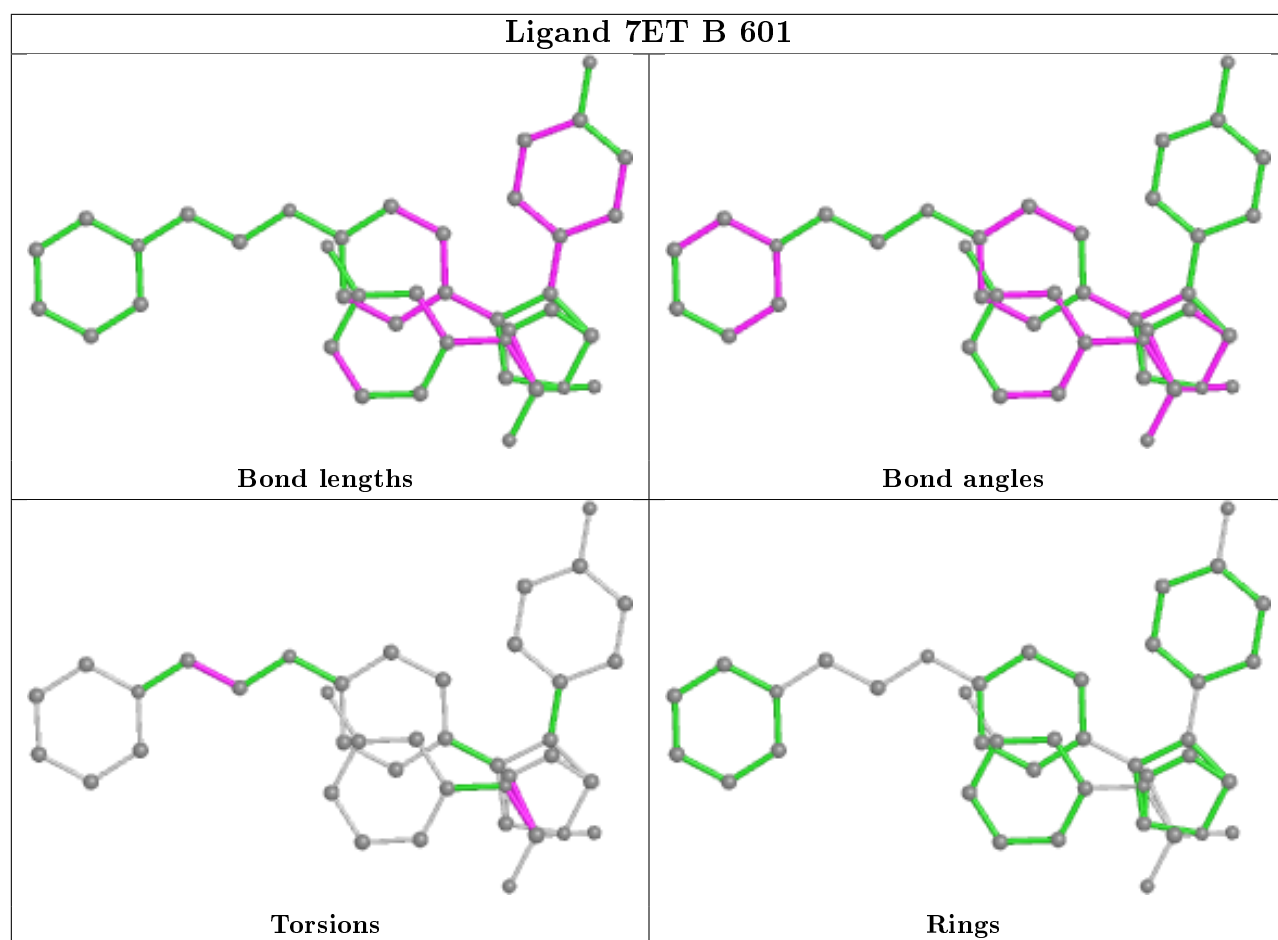
Mol	Chain	Res	Type	Atoms
4	B	601	7ET	C09-C17-S01-O06
4	B	601	7ET	O02-C19-C20-N01
4	B	601	7ET	C09-C17-S01-O05
4	B	601	7ET	C18-C17-S01-O05
4	B	601	7ET	C18-C17-S01-O06
4	B	601	7ET	C23-O04-S01-O06
3	A	601	7EH	C17-C10-C11-C12
3	A	601	7EH	C17-C10-C11-C16
4	B	601	7ET	C23-O04-S01-C17
3	A	601	7EH	C09-C10-C11-C12

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	601	7ET	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.



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	234/257 (91%)	-0.16	1 (0%) 92 93	10, 29, 61, 102	0
1	B	207/257 (80%)	-0.07	7 (3%) 45 50	11, 31, 73, 98	0
2	C	10/13 (76%)	0.29	0 100 100	29, 43, 62, 75	0
2	D	7/13 (53%)	0.95	0 100 100	51, 59, 72, 73	0
All	All	458/540 (84%)	-0.09	8 (1%) 70 73	10, 30, 68, 102	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	526	TYR	4.6
1	B	417	CYS	3.5
1	B	331	TYR	2.9
1	B	308	LEU	2.4
1	A	332	ASP	2.2
1	B	528	MET	2.2
1	B	527	SER	2.1
1	B	340	ALA	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](#)

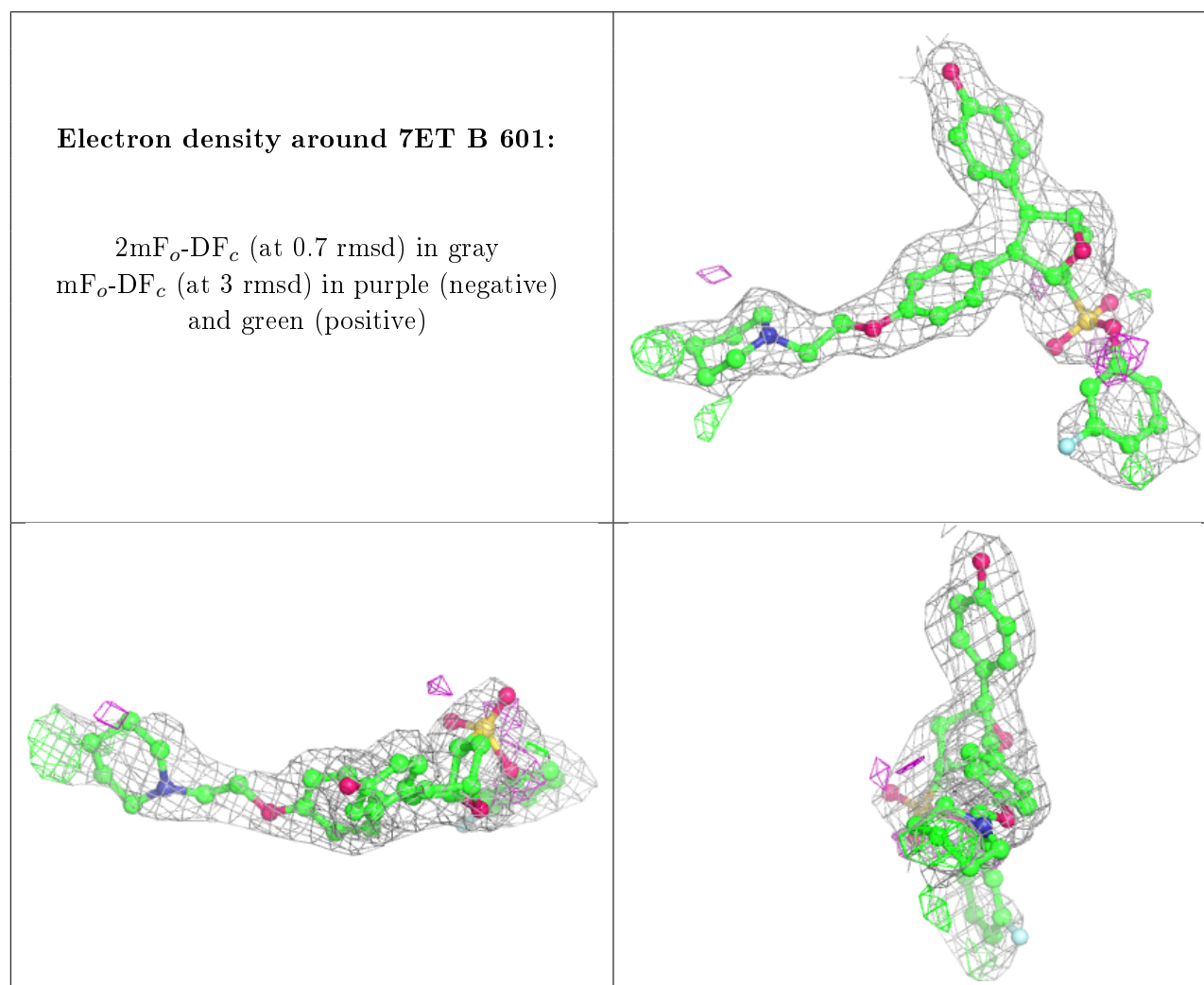
There are no carbohydrates in this entry.

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	7EH	A	601	17/17	0.77	0.24	38,46,65,71	0
4	7ET	B	601	40/40	0.87	0.18	22,42,73,74	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.



6.5 Other polymers

There are no such residues in this entry.