



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2022 – 06:24 PM JST

PDB ID : 7VHZ
Title : Crystal structure of EP300 HAT domain in complex with compound 7
Authors : Takahashi, M.; Hanzawa, H.
Deposited on : 2021-09-24
Resolution : 2.00 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:

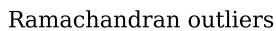
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.27
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

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X-RAY DIFFRACTION

A.

Metric	Percentile Banks	Value
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Ramachandran outliers

The numeric value for each fraction is indicated below the corresponding segment, with a dot

1

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7579 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 Histone acetyltransferase p300.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	0	0
			3497	2222	599	648	28			
1	B	437	Total	C	N	O	S	0	0	0
			3473	2208	602	635	28			

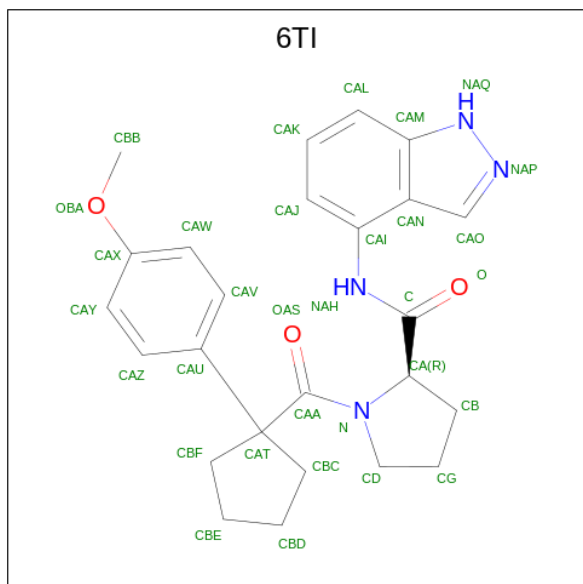
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1157	GLY	-	expression tag	UNP Q09472
A	1158	PRO	-	expression tag	UNP Q09472
A	1467	PHE	TYR	engineered mutation	UNP Q09472
A	1520	SER	-	linker	UNP Q09472
A	1521	GLY	-	linker	UNP Q09472
A	1578	GLY	-	linker	UNP Q09472
A	1579	SER	-	linker	UNP Q09472
A	1580	GLY	-	linker	UNP Q09472
B	1157	GLY	-	expression tag	UNP Q09472
B	1158	PRO	-	expression tag	UNP Q09472
B	1467	PHE	TYR	engineered mutation	UNP Q09472
B	1520	SER	-	linker	UNP Q09472
B	1521	GLY	-	linker	UNP Q09472
B	1578	GLY	-	linker	UNP Q09472
B	1579	SER	-	linker	UNP Q09472
B	1580	GLY	-	linker	UNP Q09472

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		
2	B	3	Total	Zn	0	0
			3	3		

- Molecule 3 is (2R)-N-(2H-indazol-4-yl)-1-[1-(4-methoxyphenyl)cyclopentyl]carbonyl-pyrrolidine-2-carboxamide (three-letter code: 6TI) (formula: C₂₅H₂₈N₄O₃) (labeled as "Ligand of Interest" by depositor).



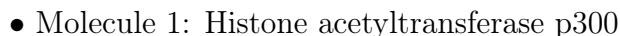
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			32	25	4	3		
3	B	1	Total	C	N	O	0	0
			32	25	4	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	283	Total	O	0	0
			283	283		
4	B	256	Total	O	0	0
			256	256		

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- Molecule 1: Histone acetyltransferase p300



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	43.68Å 89.22Å 91.13Å 114.99° 95.33° 92.02°	Depositor
Resolution (Å)	19.98 – 2.00 48.11 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.4 (19.98-2.00) 94.4 (48.11-2.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.191 , 0.219 0.193 , 0.220	Depositor DCC
R_{free} test set	3906 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	38.0	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7579	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.74% 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: 6TI, ZN

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	0.31	0/3590	0.51	0/4864
1	B	0.31	0/3566	0.53	0/4830
All	All	0.31	0/7156	0.52	0/9694

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	3497	0	3315	24	0
1	B	3473	0	3305	36	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	32	0	0	0	0
3	B	32	0	0	0	0
4	A	283	0	0	0	0
4	B	256	0	0	1	0
All	All	7579	0	6620	58	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 58 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:1252:ARG:HH11	1:B:1252:ARG:HG3	1.55	0.71
1:A:1180:LYS:HB3	1:A:1183:CYS:HB2	1.73	0.70
1:B:1397:TYR:HD1	1:B:1447:ILE:HD11	1.64	0.63
1:A:1478:ARG:HD3	1:B:1605:ALA:HB1	1.81	0.63
1:B:1163:CYS:HB2	1:B:1254:MET:HA	1.82	0.61

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	437/454 (96%)	428 (98%)	9 (2%)	0	100	100
1	B	433/454 (95%)	422 (98%)	11 (2%)	0	100	100
All	All	870/908 (96%)	850 (98%)	20 (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	377/407 (93%)	370 (98%)	7 (2%)	57	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	373/407 (92%)	361 (97%)	12 (3%)	39	38
All	All	750/814 (92%)	731 (98%)	19 (2%)	47	49

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1397	TYR
1	B	1512	VAL
1	B	1608	SER
1	B	1441	SER
1	B	1178	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1402	HIS
1	A	1661	GLN
1	B	1402	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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
3	6TI	A	1704	-	34,36,36	3.49	11 (32%)	41,52,52	1.41	7 (17%)
3	6TI	B	1704	-	34,36,36	3.44	10 (29%)	41,52,52	1.52	7 (17%)

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	6TI	A	1704	-	-	0/26/45/45	0/5/5/5
3	6TI	B	1704	-	-	0/26/45/45	0/5/5/5

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1704	6TI	NAP-NAQ	-13.73	1.10	1.37
3	B	1704	6TI	NAP-NAQ	-13.34	1.11	1.37
3	B	1704	6TI	CAT-CAU	-8.79	1.39	1.53
3	A	1704	6TI	CAT-CAU	-8.65	1.39	1.53
3	A	1704	6TI	CAI-CAN	-5.26	1.32	1.43

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1704	6TI	CBC-CAT-CAU	-4.15	106.49	113.28
3	A	1704	6TI	CBC-CAT-CAU	-4.02	106.70	113.28
3	B	1704	6TI	CD-N-CAA	3.62	136.40	130.32
3	B	1704	6TI	CBB-OBA-CAX	-3.53	109.84	117.51
3	A	1704	6TI	CD-N-CAA	3.26	135.80	130.32

There are no chirality outliers.

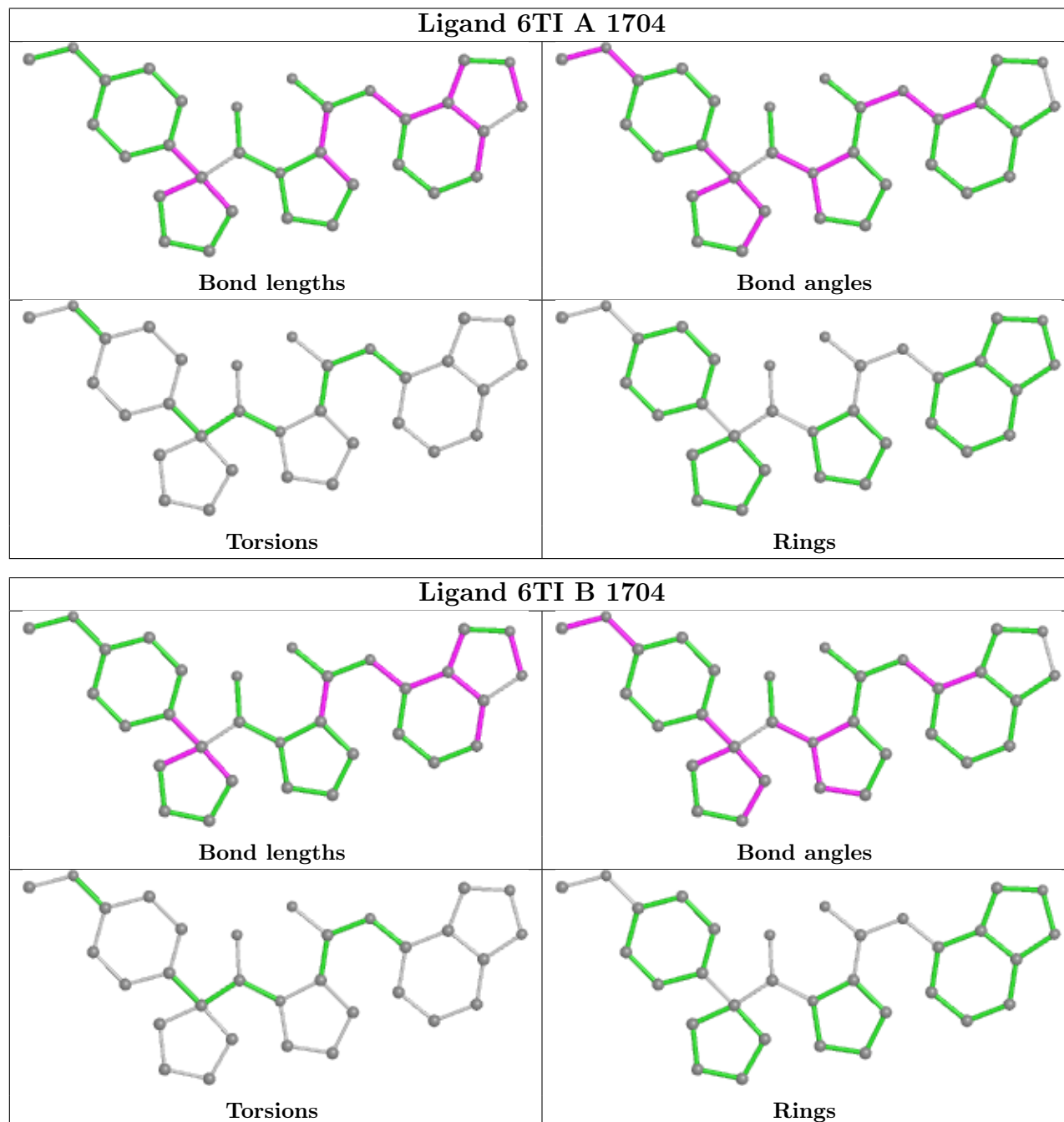
There are no torsion outliers.

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.



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	441/454 (97%)	-0.04	24 (5%) 25 24	27, 43, 88, 103	0
1	B	437/454 (96%)	-0.10	26 (5%) 22 21	26, 45, 88, 118	0
All	All	878/908 (96%)	-0.07	50 (5%) 23 23	26, 44, 88, 118	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1182	LEU	7.6
1	A	1181	GLN	5.1
1	B	1280	ALA	5.0
1	A	1208	ILE	4.8
1	B	1185	ILE	4.4

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](#)

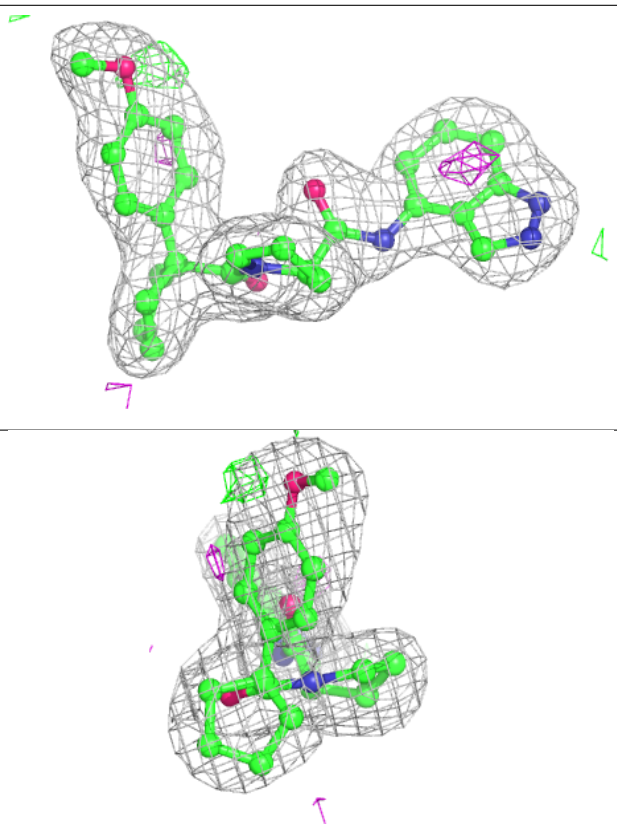
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

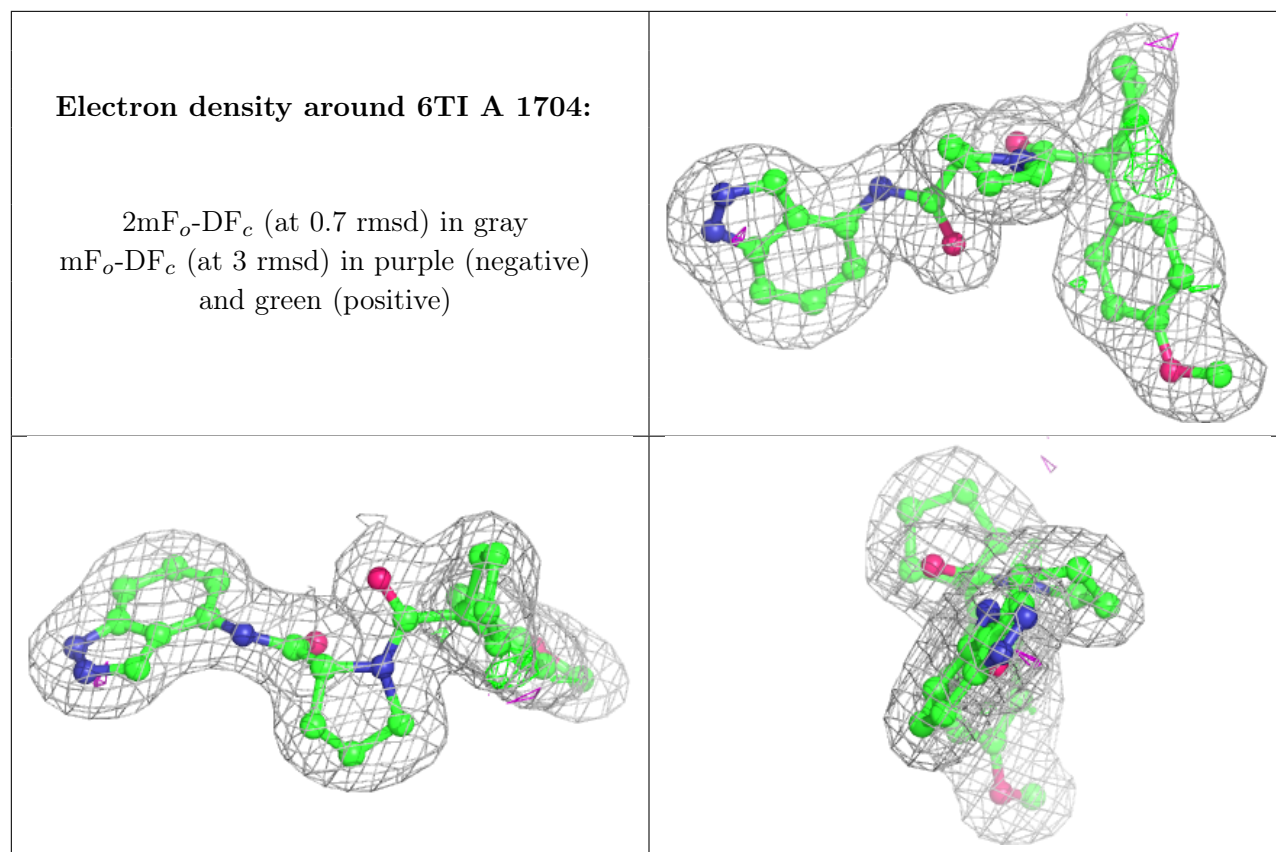
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZN	A	1703	1/1	0.82	0.08	87,87,87,87	0
2	ZN	B	1703	1/1	0.88	0.03	85,85,85,85	0
2	ZN	A	1702	1/1	0.89	0.05	76,76,76,76	0
3	6TI	B	1704	32/32	0.91	0.10	34,42,48,51	0
3	6TI	A	1704	32/32	0.95	0.12	25,31,36,38	0
2	ZN	B	1702	1/1	0.95	0.04	77,77,77,77	0
2	ZN	A	1701	1/1	0.98	0.11	52,52,52,52	0
2	ZN	B	1701	1/1	0.99	0.10	50,50,50,50	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 6TI B 1704:

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.