Full wwPDB X-ray Structure Validation Report (i)

Nov 21, 2023 – 03:42 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 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 (i) 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 (i)) were used in the production of this report:

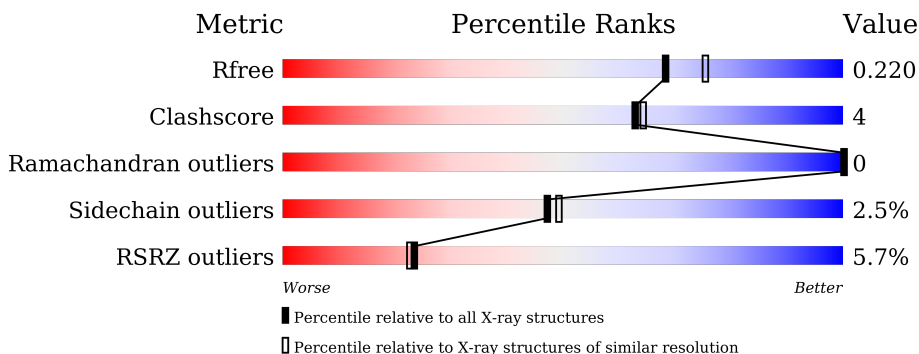|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
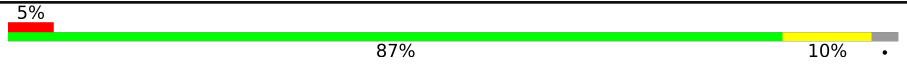*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	Percentile Ranks	Value
Rfree		0.220
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		2.5%
RSRZ outliers		5.7%

Worse   *Better*

▮ Percentile relative to all X-ray structures

◫ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	454	5% — 87% — 10% •
1	B	454	6% — 85% — 11% • •

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.

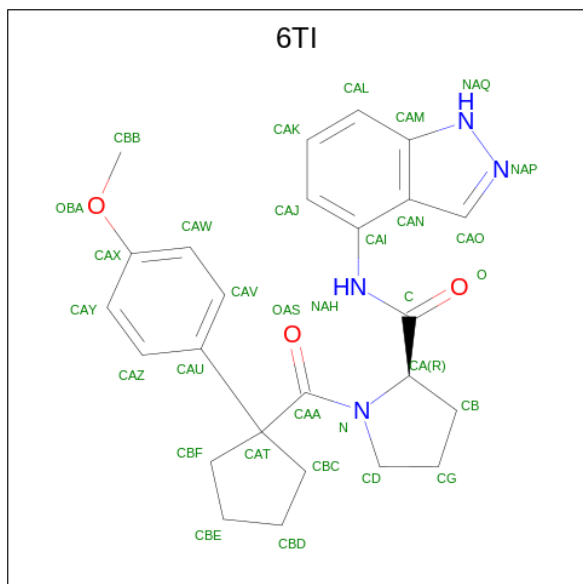| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total 3497	C 2222	N 599	O 648	S 28	0	0	0
1	B	437	Total 3473	C 2208	N 602	O 635	S 28	0	0	0

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 3	Zn 3	0	0
2	B	3	Total 3	Zn 3	0	0

- Molecule 3 is (2R)-N-(2H-indazol-4-yl)-1-[1-(4-methoxyphenyl)cyclopentyl]carbonyl-pyrroli dine-2-carboxamide (three-letter code: 6TI) (formula: $C_{25}H_{28}N_4O_3$) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	283	Total 283	O 283	0	0
4	B	256	Total 256	O 256	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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: Histone acetyltransferase p300
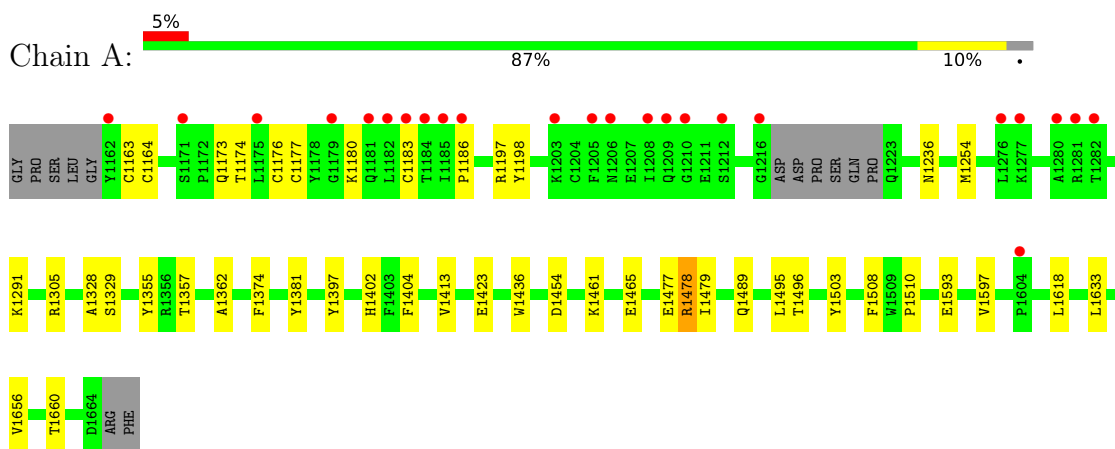
- Molecule 1: Histone acetyltransferase p300
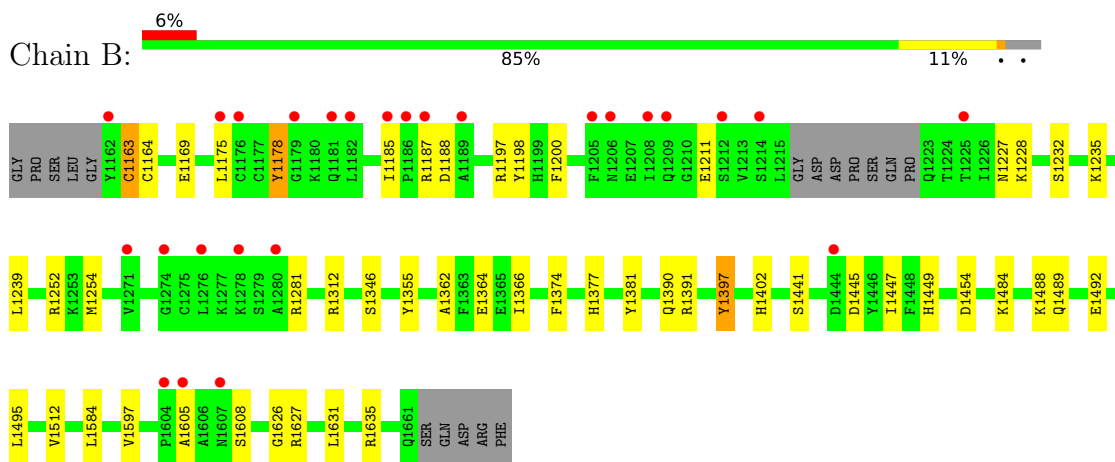
4 Data and refinement statistics ⓘ

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
$< I/\sigma(I) >$ [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]	$< |L| > = 0.49, < L^2 > = 0.32$	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.*

---

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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.

All (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
1:B:1377:HIS:CD2	1:B:1397:TYR:HE1	2.21	0.58
1:B:1227:ASN:OD1	1:B:1228:LYS:N	2.37	0.58
1:B:1484:LYS:NZ	1:B:1492:GLU:OE1	2.26	0.55
1:B:1377:HIS:CG	1:B:1397:TYR:CE1	2.96	0.54
1:B:1390:GLN:HG2	1:B:1391:ARG:HG3	1.89	0.54
1:B:1495:LEU:CD2	1:B:1584:LEU:HD21	2.40	0.51
1:A:1329:SER:HA	1:A:1618:LEU:HD22	1.91	0.51
1:A:1174:THR:HG22	1:A:1186:PRO:HA	1.92	0.51
1:A:1305:ARG:NH2	1:A:1477:GLU:OE2	2.39	0.51
1:B:1364:GLU:HG2	1:B:1366:ILE:HG12	1.92	0.51
1:B:1445:ASP:HB3	1:B:1631:LEU:HD22	1.93	0.50
1:B:1397:TYR:CE1	1:B:1627:ARG:HB3	2.48	0.49
1:B:1252:ARG:HG3	1:B:1252:ARG:NH1	2.25	0.48
1:B:1454:ASP:OD1	1:B:1454:ASP:N	2.45	0.48
1:B:1169:GLU:OE2	1:B:1239:LEU:HD23	2.15	0.47
1:B:1377:HIS:CD2	1:B:1397:TYR:CE1	3.01	0.47
1:A:1163:CYS:SG	1:A:1164:CYS:N	2.87	0.47
1:B:1397:TYR:OH	1:B:1627:ARG:N	2.48	0.46
1:A:1593:GLU:H	1:A:1593:GLU:CD	2.18	0.46
1:A:1173:GLN:O	1:A:1236:ASN:ND2	2.46	0.46
1:B:1355:TYR:HB3	1:B:1381:TYR:CE2	2.50	0.46
1:B:1489:GLN:HG2	1:B:1597:VAL:HG11	1.97	0.46
1:B:1163:CYS:HB2	1:B:1254:MET:SD	2.56	0.46
1:A:1163:CYS:HB3	1:A:1254:MET:HA	1.99	0.45
1:B:1312:ARG:NH2	4:B:1810:HOH:O	2.43	0.45
1:B:1188:ASP:HA	1:B:1235:LYS:HE2	1.98	0.45
1:B:1397:TYR:OH	1:B:1626:GLY:HA2	2.17	0.45
1:A:1355:TYR:HB3	1:A:1381:TYR:CE2	2.52	0.44
1:A:1503:TYR:CZ	1:A:1510:PRO:HB3	2.53	0.44
1:A:1656:VAL:O	1:A:1660:THR:HG23	2.17	0.44
1:A:1489:GLN:HG2	1:A:1597:VAL:HG11	2.00	0.43
1:B:1197:ARG:NH1	1:B:1198:TYR:OH	2.50	0.43
1:A:1197:ARG:HD3	1:A:1198:TYR:CE2	2.54	0.43
1:A:1362:ALA:HB3	1:A:1374:PHE:HB3	1.99	0.43
1:A:1461:LYS:O	1:A:1465:GLU:HG3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1478:ARG:HD3	1:B:1605:ALA:CB	2.48	0.43
1:B:1163:CYS:SG	1:B:1164:CYS:N	2.92	0.42
1:B:1488:LYS:H	1:B:1488:LYS:HG2	1.68	0.42
1:A:1495:LEU:HD23	1:A:1496:THR:N	2.35	0.41
1:B:1449:HIS:CE1	1:B:1635:ARG:HG2	2.55	0.41
1:B:1163:CYS:CB	1:B:1254:MET:HA	2.48	0.41
1:B:1175:LEU:HB2	1:B:1185:ILE:HB	2.01	0.41
1:A:1355:TYR:HB3	1:A:1381:TYR:CD2	2.55	0.41
1:B:1169:GLU:HG3	1:B:1239:LEU:HD23	2.01	0.41
1:B:1377:HIS:CG	1:B:1397:TYR:HE1	2.37	0.41
1:A:1423:GLU:HG3	1:A:1479:ILE:HG12	2.03	0.41
1:A:1454:ASP:OD1	1:A:1454:ASP:N	2.46	0.41
1:B:1495:LEU:HD21	1:B:1584:LEU:HD21	2.02	0.41
1:A:1436:TRP:CZ2	1:A:1508:PHE:HB2	2.55	0.41
1:B:1178:TYR:HB3	1:B:1200:PHE:CZ	2.56	0.41
1:B:1362:ALA:HB3	1:B:1374:PHE:HB3	2.03	0.41
1:A:1404:PHE:CZ	1:A:1413:VAL:HG21	2.56	0.40
1:A:1328:ALA:HA	1:A:1357:THR:O	2.21	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	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
1	B	373/407 (92%)	361 (97%)	12 (3%)	39	38
All	All	750/814 (92%)	731 (98%)	19 (2%)	47	49

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1176	CYS
1	A	1177	CYS
1	A	1291	LYS
1	A	1397	TYR
1	A	1402	HIS
1	A	1478	ARG
1	A	1633	LEU
1	B	1163	CYS
1	B	1178	TYR
1	B	1187	ARG
1	B	1211	GLU
1	B	1232	SER
1	B	1281	ARG
1	B	1346	SER
1	B	1397	TYR
1	B	1402	HIS
1	B	1441	SER
1	B	1512	VAL
1	B	1608	SER

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

All (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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
3	B	1704	6TI	CAI-CAN	-5.18	1.32	1.43
3	A	1704	6TI	CAL-CAM	-5.09	1.33	1.41
3	B	1704	6TI	CAL-CAM	-5.03	1.33	1.41
3	B	1704	6TI	CA-C	-4.91	1.41	1.52
3	B	1704	6TI	CAO-CAN	-4.53	1.31	1.40
3	A	1704	6TI	CA-C	-4.52	1.42	1.52
3	A	1704	6TI	CAO-CAN	-4.48	1.31	1.40
3	A	1704	6TI	CAN-CAM	-3.89	1.32	1.42
3	B	1704	6TI	CAN-CAM	-3.81	1.32	1.42
3	A	1704	6TI	CBC-CAT	-3.53	1.50	1.55
3	B	1704	6TI	CBC-CAT	-3.46	1.50	1.55
3	A	1704	6TI	CBF-CAT	-3.30	1.50	1.55
3	B	1704	6TI	CBF-CAT	-2.97	1.50	1.55
3	A	1704	6TI	CAI-NAH	-2.49	1.34	1.41
3	B	1704	6TI	CAI-NAH	-2.26	1.35	1.41
3	A	1704	6TI	CB-CA	-2.16	1.48	1.53

All (14) bond angle outliers are listed below:

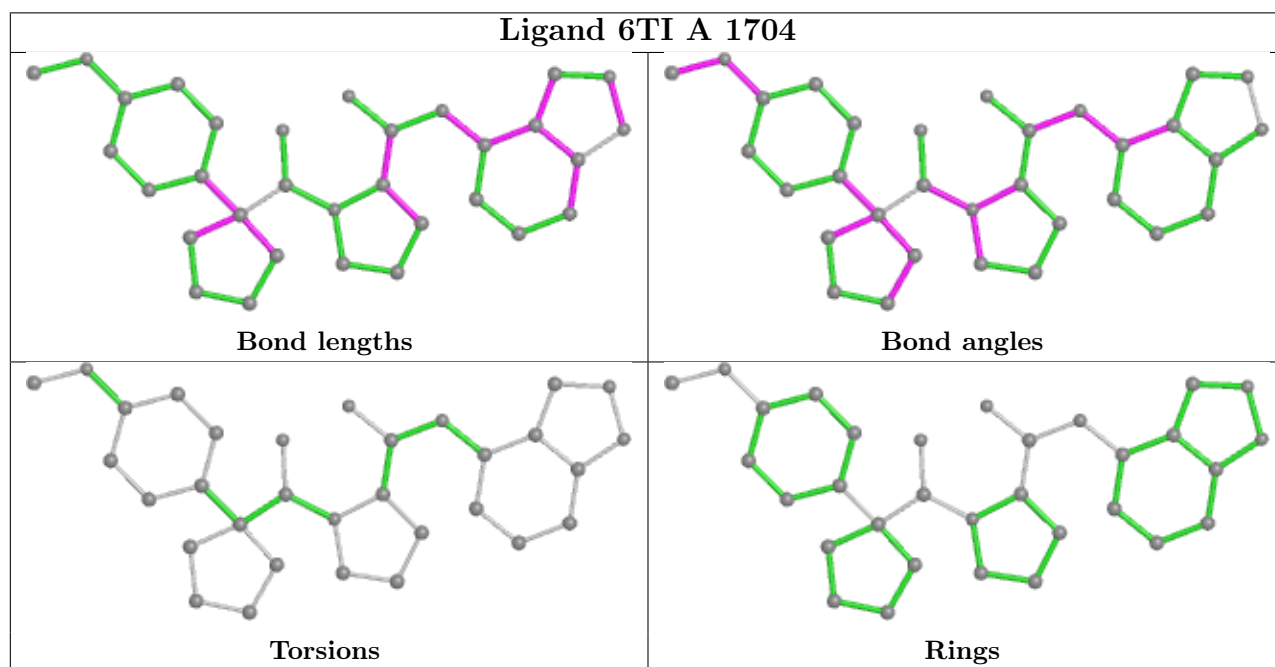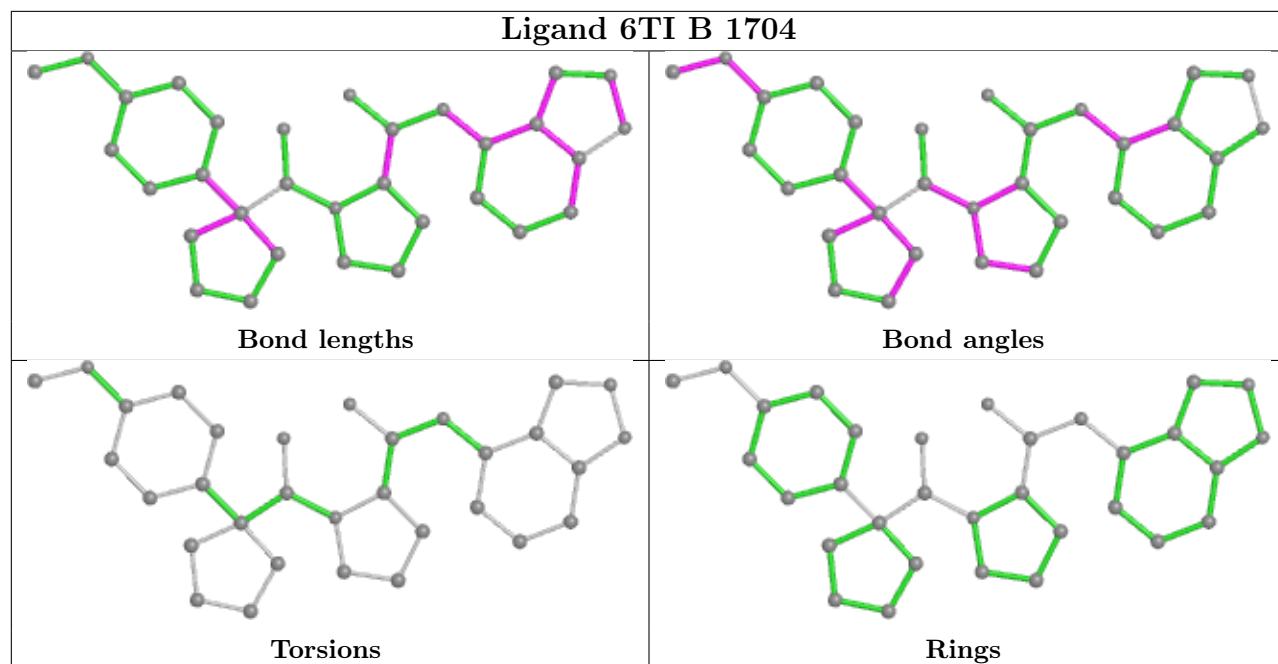| Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1704	6TI	CBC-CAT-CAU	-4.15	106.49	113.28
3	A	1704	6TI	CBC-CAT-CAU	-4.02	106.70	113.28
3	B	1704	6TI	CD-N-CAA	3.62	136.40	130.32
3	B	1704	6TI	CBB-OBA-CAX	-3.53	109.84	117.51
3	A	1704	6TI	CD-N-CAA	3.26	135.80	130.32
3	B	1704	6TI	CD-N-CA	-2.78	107.58	112.00
3	A	1704	6TI	CBE-CBF-CAT	-2.78	101.47	104.85
3	B	1704	6TI	CBE-CBF-CAT	-2.58	101.71	104.85
3	A	1704	6TI	CAN-CAI-NAH	-2.44	114.24	118.36
3	A	1704	6TI	CBB-OBA-CAX	-2.36	112.39	117.51
3	B	1704	6TI	CAN-CAI-NAH	-2.29	114.49	118.36
3	A	1704	6TI	CD-N-CA	-2.10	108.68	112.00
3	A	1704	6TI	CAI-NAH-C	-2.06	124.29	127.73
3	B	1704	6TI	CG-CD-N	2.05	106.85	103.25

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 then 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 6TI A 1704

Bond lengths

Bond angles

Torsions

Rings

Ligand 6TI B 1704

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 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

All (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
1	B	1186	PRO	4.1
1	A	1182	LEU	4.0
1	A	1205	PHE	3.9
1	A	1179	GLY	3.8
1	A	1162	TYR	3.8
1	B	1179	GLY	3.7
1	A	1175	LEU	3.6
1	B	1176	CYS	3.5
1	A	1280	ALA	3.5
1	B	1604	PRO	3.3
1	B	1605	ALA	3.3
1	B	1175	LEU	3.2
1	A	1185	ILE	3.1
1	B	1162	TYR	3.1
1	B	1278	LYS	3.1
1	B	1208	ILE	3.0
1	A	1210	GLY	2.9
1	A	1604	PRO	2.7
1	B	1181	GLN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1209	GLN	2.7
1	B	1276	LEU	2.7
1	A	1186	PRO	2.6
1	A	1212	SER	2.6
1	B	1274	GLY	2.5
1	B	1271	VAL	2.5
1	A	1209	GLN	2.5
1	A	1171	SER	2.4
1	B	1444	ASP	2.4
1	B	1206	ASN	2.4
1	B	1607	ASN	2.4
1	B	1212	SER	2.4
1	A	1216	GLY	2.3
1	B	1189	ALA	2.3
1	A	1282	THR	2.3
1	A	1183	CYS	2.3
1	A	1206	ASN	2.3
1	A	1281	ARG	2.3
1	B	1214	SER	2.3
1	B	1187	ARG	2.2
1	B	1205	PHE	2.2
1	A	1277	LYS	2.2
1	B	1225	THR	2.1
1	A	1184	THR	2.0
1	A	1276	LEU	2.0
1	A	1203	LYS	2.0

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

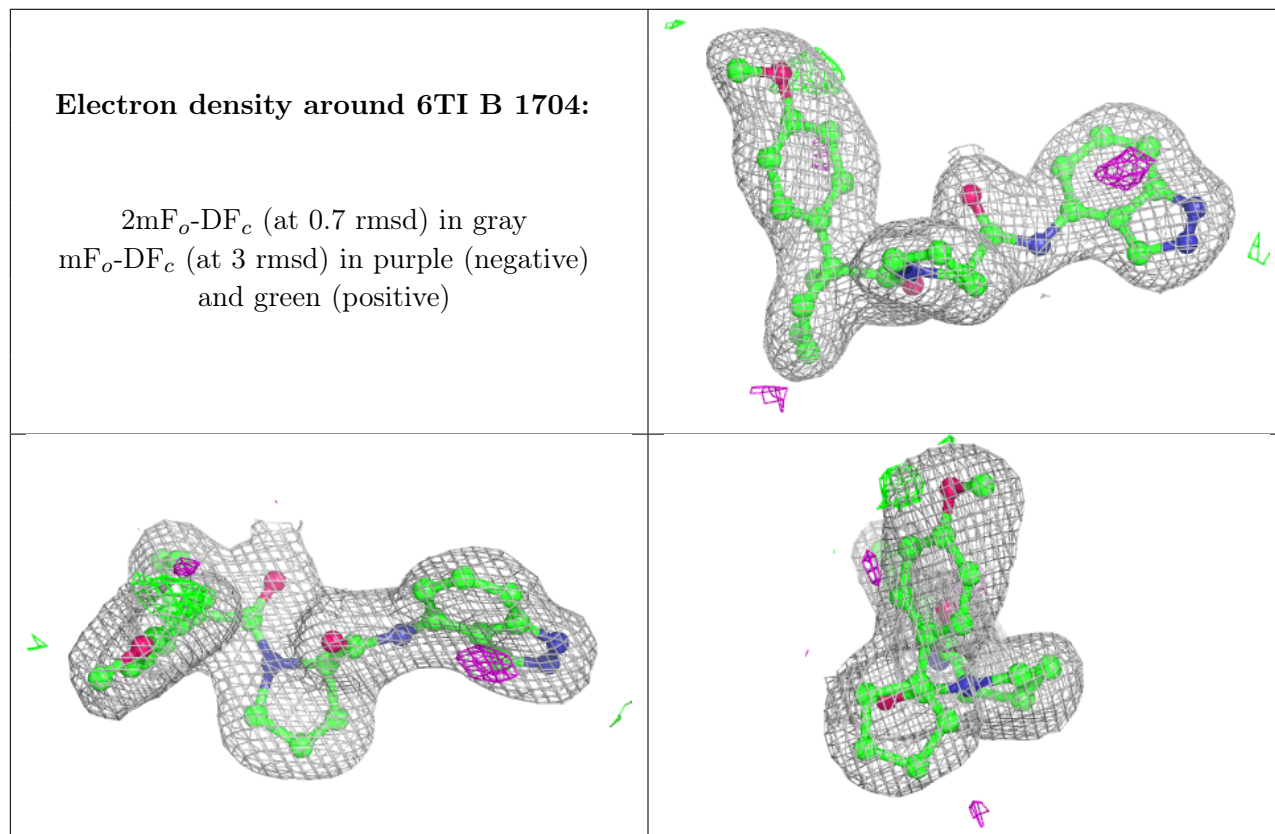There are no non-standard protein/DNA/RNA residues in this entry.

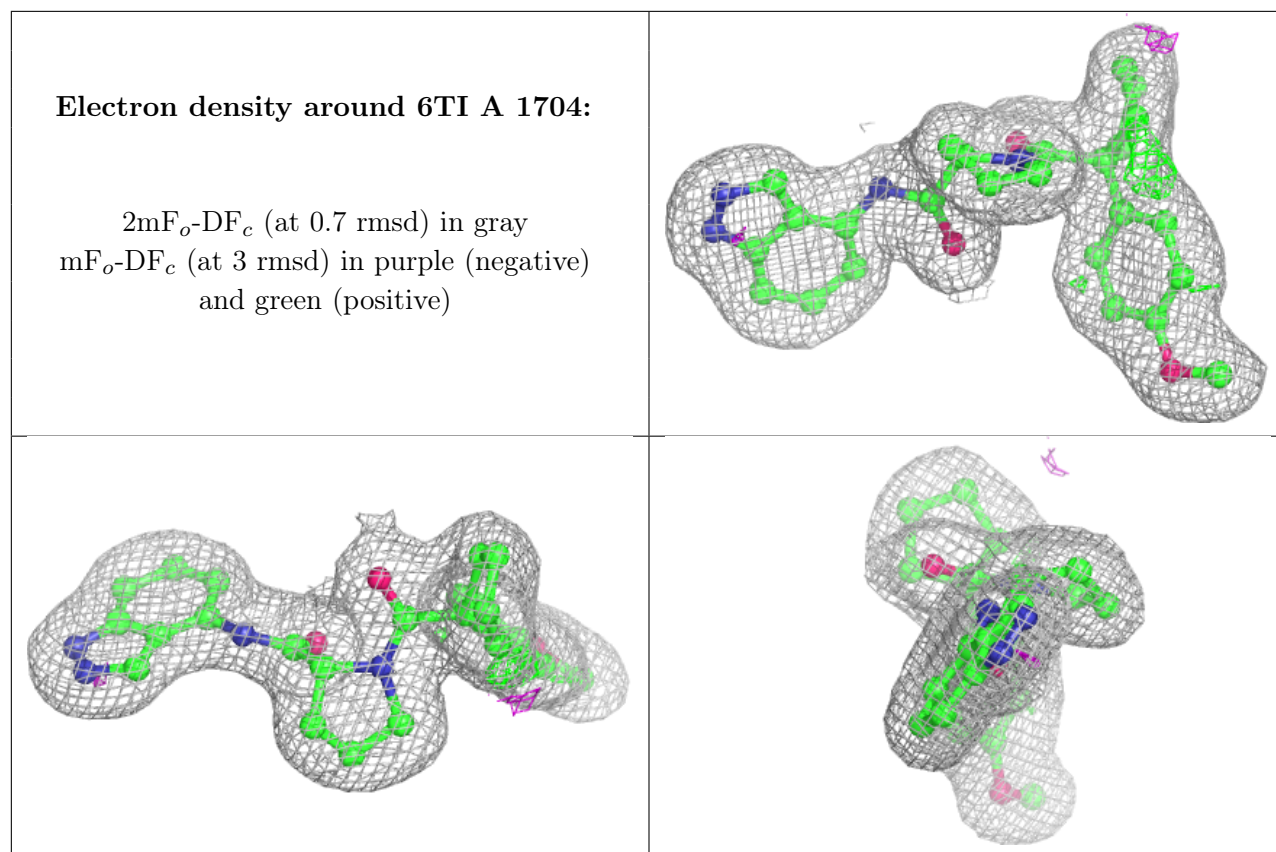## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
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)

Electron density around 6TI A 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.