

Full wwPDB X-ray Structure Validation Report (i)

Oct 9, 2023 – 04:16 pm BST

PDB ID : 8CJ7

Title: HDAC6 selective degraded (difluoromethyl)-1,3,4-oxadiazole substrate

inhibitor

Authors : Sandmark, J.; Ek, M.; Ripa, L.

Deposited on : 2023-02-12

Resolution : 1.51 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 (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.35.1

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

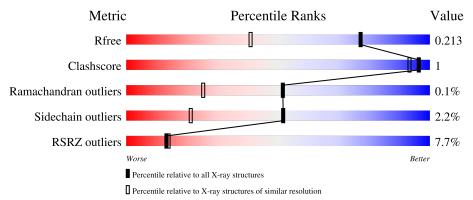
Validation Pipeline (wwPDB-VP) : 2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.51 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}({\rm \AA})) \end{array}$
R_{free}	130704	4009 (1.54-1.50)
Clashscore	141614	4249 (1.54-1.50)
Ramachandran outliers	138981	4148 (1.54-1.50)
Sidechain outliers	138945	4146 (1.54-1.50)
RSRZ outliers	127900	3943 (1.54-1.50)

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	Λ	364	2%		
1	А	304	93%	• • •	
1	В	364	93%		
			18%		
1	С	364	93%		



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9042 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 deacetylase 6.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	۸	356	Total	С	N	О	S	0	7	0
1	A	350	2807	1767	502	520	18	0	1	U
1	В	352	Total	С	N	О	S	0	5	0
1	Б	302	2764	1740	494	512	18	0		
1	С	352	Total	С	N	О	S	0	2	0
1		302	2756	1732	494	512	18	0)	

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	435	SER	-	expression tag	UNP F8W4B7
A	436	ASN	-	expression tag	UNP F8W4B7
A	437	ALA	-	expression tag	UNP F8W4B7
A	438	GLY	-	expression tag	UNP F8W4B7
A	439	GLY	-	expression tag	UNP F8W4B7
В	435	SER	-	expression tag	UNP F8W4B7
В	436	ASN	-	expression tag	UNP F8W4B7
В	437	ALA	-	expression tag	UNP F8W4B7
В	438	GLY	-	expression tag	UNP F8W4B7
В	439	GLY	-	expression tag	UNP F8W4B7
С	435	SER	-	expression tag	UNP F8W4B7
С	436	ASN	-	expression tag	UNP F8W4B7
С	437	ALA	-	expression tag	UNP F8W4B7
С	438	GLY	-	expression tag	UNP F8W4B7
С	439	GLY	-	expression tag	UNP F8W4B7

• Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

I	Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
	2	A	2	Total K 2 2	0	0



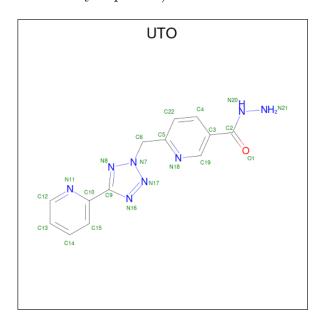
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	2	Total K 2 2	0	0
2	С	2	Total K 2 2	0	0

• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	В	1	Total Zn 1 1	0	0
3	С	1	Total Zn 1 1	0	0

• Molecule 4 is 6-[(5-pyridin-2-yl-1,2 4 ,3,4-tetrazacyclopenta-1,3-dien-2-yl)methyl]pyridin e-3-carbohydrazide (three-letter code: UTO) (formula: $C_{13}H_{12}N_8O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 22 13 8 1	0	0
4	В	1	Total C N O 44 26 16 2	0	1

• Molecule 5 is IODIDE ION (three-letter code: IOD) (formula: I).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total I 4 4	0	0
5	В	1	Total I 1 1	0	0
5	С	1	Total I 1 1	0	0

• Molecule 6 is water.

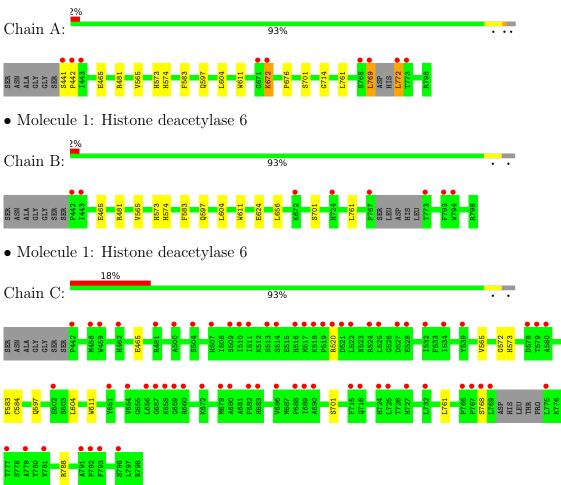
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	268	Total O 268 268	0	0
6	В	264	Total O 264 264	0	0
6	С	102	Total O 102 102	0	0



3 Residue-property plots (i)

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 deacetylase 6





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	95.98Å 84.06Å 96.13Å	Denogitor
a, b, c, α , β , γ	90.00° 110.25° 90.00°	Depositor
Resolution (Å)	90.19 - 1.51	Depositor
Resolution (A)	90.19 - 1.51	EDS
% Data completeness	51.8 (90.19-1.51)	Depositor
(in resolution range)	51.6 (90.19-1.51)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.00 (at 1.50Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.206 , 0.227	Depositor
it, itfree	0.213 , 0.213	DCC
R_{free} test set	5667 reflections $(4.86%)$	wwPDB-VP
Wilson B-factor (Å ²)	13.6	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.35, 41.0	EDS
L-test for twinning ²	$< L > = 0.49, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.014 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9042	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 13.61% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: ZN, UTO, IOD, K

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	
IVIOI		RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.55	0/2888	0.62	0/3914
1	В	0.52	0/2848	0.61	0/3860
1	С	0.47	0/2833	0.60	0/3838
All	All	0.51	0/8569	0.61	0/11612

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	2807	0	2739	8	0
1	В	2764	0	2693	5	0
1	С	2756	0	2677	3	0
2	A	2	0	0	0	0
2	В	2	0	0	0	0
2	С	2	0	0	0	0
3	A	1	0	0	0	0
3	В	1	0	0	0	0
3	С	1	0	0	0	0
4	A	22	0	0	1	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	В	44	0	0	1	0
5	A	4	0	0	1	0
5	В	1	0	0	1	0
5	С	1	0	0	0	0
6	A	268	0	0	0	0
6	В	264	0	0	0	0
6	С	102	0	0	0	0
All	All	9042	0	8109	16	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 1.

All (16) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:C:565:VAL:HG13	1:C:761:LEU:HD12	1.86	0.57
1:B:565[A]:VAL:HG13	1:B:761:LEU:HD12	1.87	0.57
1:A:565[A]:VAL:HG13	1:A:761:LEU:HD12	1.88	0.55
1:C:572:GLY:HA2	1:C:584:CYS:HB3	1.90	0.51
1:A:769:LEU:HD13	1:A:772:LEU:HD21	1.93	0.50
1:A:481:ARG:HA	5:A:808:IOD:I	2.82	0.50
1:B:574:HIS:NE2	4:B:804[B]:UTO:N20	2.60	0.50
1:B:481:ARG:HA	5:B:805:IOD:I	2.83	0.48
1:B:624:GLU:HG3	1:B:656:LEU:HD12	1.96	0.47
1:A:672[A]:LYS:HG3	1:A:714:GLY:O	2.16	0.45
1:B:597:GLN:HG2	1:B:604:LEU:HB3	1.99	0.44
1:A:574:HIS:NE2	4:A:804:UTO:N20	2.65	0.44
1:A:676:PRO:HG3	1:A:772:LEU:HB2	1.99	0.44
1:A:597:GLN:HG2	1:A:604:LEU:HB3	2.00	0.43
1:A:441:SER:CB	1:A:442:PRO:HD3	2.49	0.43
1:C:597:GLN:HG2	1:C:604:LEU:HB3	2.01	0.42

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	Percen	tiles
1	A	359/364 (99%)	352 (98%)	5 (1%)	2 (1%)	25	7
1	В	353/364 (97%)	347 (98%)	6 (2%)	0	100	100
1	С	351/364 (96%)	342 (97%)	9 (3%)	0	100	100
All	All	1063/1092 (97%)	1041 (98%)	20 (2%)	2 (0%)	51	23

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	672[A]	LYS
1	A	672[B]	LYS

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	Perce	ntiles
1	A	$304/305 \; (100\%)$	297 (98%)	7 (2%)	50	20
1	В	300/305~(98%)	295 (98%)	5 (2%)	60	32
1	С	298/305~(98%)	290 (97%)	8 (3%)	44	15
All	All	902/915 (99%)	882 (98%)	20 (2%)	52	21

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	465	GLU
1	A	573	HIS
1	A	583	PHE
1	A	611	TRP
1	A	701	SER
1	A	769	LEU
1	A	772	LEU
1	В	465	GLU



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Mol	Chain	Res	Type
1	В	573	HIS
1	В	583	PHE
1	В	611	TRP
1	В	701	SER
1	С	465	GLU
1	С	520	ARG
1	С	573	HIS
1	С	583	PHE
1	С	611	TRP
1	С	701	SER
1	С	768	SER
1	С	788	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	487	HIS
1	В	487	HIS

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)

Of 18 ligands modelled in this entry, 15 are monoatomic - leaving 3 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	Mol Type Chain Res		Link	Bond lengths			Bond angles			
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
4	UTO	В	804[B]	3	23,24,24	1.74	4 (17%)	25,32,32	2.19	8 (32%)
4	UTO	A	804	3	23,24,24	1.70	4 (17%)	25,32,32	2.53	7 (28%)
4	UTO	В	804[A]	3	23,24,24	1.80	4 (17%)	25,32,32	2.20	10 (40%)

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	UTO	В	804[B]	3	-	5/13/14/14	0/3/3/3
4	UTO	A	804	3	-	0/13/14/14	0/3/3/3
4	UTO	В	804[A]	3	-	0/13/14/14	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\mathring{\mathrm{A}})$	Ideal(A)
4	В	804[A]	UTO	O1-C2	6.23	1.36	1.23
4	В	804[B]	UTO	O1-C2	5.66	1.34	1.23
4	A	804	UTO	O1-C2	5.34	1.34	1.23
4	В	804[B]	UTO	C2-N20	-3.53	1.30	1.33
4	A	804	UTO	C2-N20	-3.23	1.30	1.33
4	В	804[A]	UTO	N17-N7	-3.12	1.29	1.34
4	В	804[A]	UTO	N16-N17	-3.09	1.28	1.34
4	A	804	UTO	N17-N7	-3.05	1.29	1.34
4	A	804	UTO	N16-N17	-2.78	1.29	1.34
4	В	804[A]	UTO	C2-N20	-2.73	1.31	1.33
4	В	804[B]	UTO	N17-N7	-2.70	1.29	1.34
4	В	804[B]	UTO	N16-N17	-2.56	1.29	1.34

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
4	A	804	UTO	C3-C2-N20	6.46	123.65	116.27
4	В	804[B]	UTO	N8-C9-N16	-6.29	107.02	111.85
4	В	804[A]	UTO	N8-C9-N16	-6.14	107.14	111.85
4	A	804	UTO	N8-C9-N16	-6.13	107.14	111.85



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
4	A	804	UTO	O1-C2-N20	-4.70	116.63	122.50
4	В	804[A]	UTO	C3-C2-N20	4.33	121.21	116.27
4	В	804[A]	UTO	C19-N18-C5	3.76	122.64	117.82
4	A	804	UTO	C19-N18-C5	3.73	122.61	117.82
4	В	804[B]	UTO	C3-C2-N20	3.69	120.48	116.27
4	В	804[A]	UTO	C12-N11-C10	3.42	122.03	117.23
4	В	804[B]	UTO	C19-N18-C5	3.19	121.92	117.82
4	В	804[B]	UTO	C6-N7-N17	3.13	126.72	117.77
4	В	804[B]	UTO	C12-N11-C10	2.99	121.42	117.23
4	В	804[B]	UTO	C9-C10-N11	2.96	120.14	116.75
4	В	804[B]	UTO	O1-C2-N20	-2.96	118.81	122.50
4	A	804	UTO	C12-N11-C10	2.89	121.28	117.23
4	В	804[A]	UTO	C5-C6-N7	-2.49	106.69	112.82
4	A	804	UTO	C6-N7-N17	2.48	124.88	117.77
4	В	804[A]	UTO	C6-N7-N17	2.31	124.39	117.77
4	В	804[B]	UTO	C22-C4-C3	-2.25	118.16	120.78
4	В	804[A]	UTO	C3-C19-N18	-2.24	120.54	123.67
4	В	804[A]	UTO	O1-C2-N20	-2.20	119.75	122.50
4	A	804	UTO	C5-C6-N7	-2.11	107.61	112.82
4	В	804[A]	UTO	C9-N16-N17	2.11	107.10	105.47
4	В	804[A]	UTO	C13-C12-N11	-2.10	120.00	123.43

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	В	804[B]	UTO	C15-C10-C9-N8
4	В	804[B]	UTO	N11-C10-C9-N8
4	В	804[B]	UTO	C15-C10-C9-N16
4	В	804[B]	UTO	N11-C10-C9-N16
4	В	804[B]	UTO	N20-C2-C3-C4

There are no ring outliers.

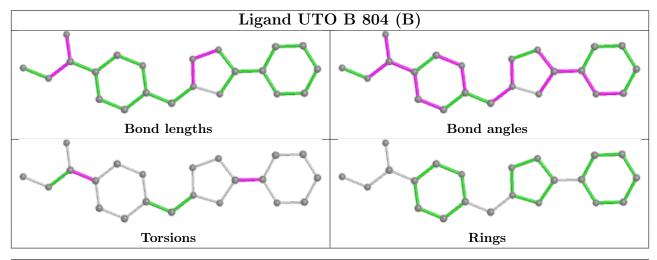
2 monomers are involved in 2 short contacts:

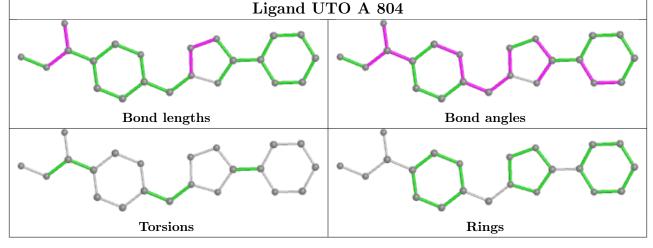
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	В	804[B]	UTO	1	0
4	A	804	UTO	1	0

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

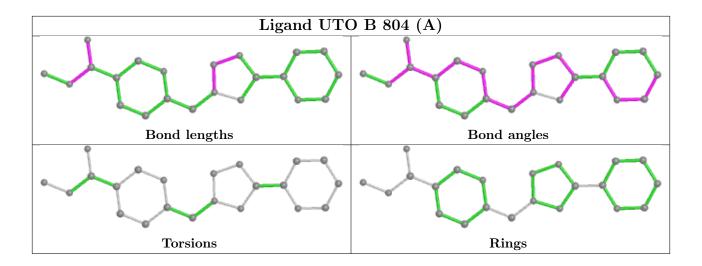


addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.









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, 95^{th} 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>	$\#\mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	A	356/364~(97%)	0.52	9 (2%) 57 62	6, 14, 31, 58	0
1	В	352/364~(96%)	0.47	8 (2%) 60 65	10, 18, 34, 50	0
1	С	352/364 (96%)	1.24	65 (18%) 1 1	19, 40, 72, 104	0
All	All	1060/1092 (97%)	0.75	82 (7%) 13 14	6, 20, 61, 104	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	769	LEU	11.7
1	A	772	LEU	8.5
1	С	442	PRO	8.0
1	С	767	PRO	7.8
1	В	442	PRO	7.6
1	A	442	PRO	7.4
1	A	441	SER	6.6
1	С	524	ARG	6.0
1	С	796	SER	5.5
1	С	768	SER	4.9
1	С	793	PHE	4.5
1	С	459	TRP	4.4
1	С	520	ARG	4.2
1	A	671[A]	GLY	4.1
1	С	518	LYS	4.0
1	С	510	ILE	3.9
1	A	769	LEU	3.9
1	В	767	PRO	3.9
1	С	791	ALA	3.6
1	С	725	LEU	3.6
1	С	528	GLU	3.5
1	С	580	ALA	3.5
1	A	773	THR	3.4



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Mol	nued fron Chain	$oxed{\mathbf{Res}}$	Type	RSRZ
1	С	724	HIS	3.4
1	C	658	LYS	3.3
1	C	683	HIS	3.3
1	C	715	PHE	3.3
1	C	688	PRO	3.2
1	C	679	MET	3.2
1	C C	509[A]	SER	3.1
1	C	519	PRO	3.1
1	C	654	VAL	3.1
1	C	680	ALA	3.1
1	C C A	672	LYS	3.0
1	Δ	672[A]	LYS	3.0
1	C	777	THR	3.0
1	C	792	PRO	3.0
1	C	775	LEU	2.9
1	C	481	ARG	2.8
1	C	516	HIS	2.8
1	C	682	PHE	2.8
1	C	458	MET	2.8
1	C	659	GLY	2.7
1	C		THR	2.7
1	C	579	ASP	2.6
1	C	527	LEU	2.6
1	C	732 578		2.6
1	C		ASP	
		521	ASP	2.5
1	В	773	THR	2.5
1	С	651	TYR	2.5
1	С	689	ILE	2.5
1	С	514	SER	2.4
1	С	781	VAL	2.4
1	В	443	ILE	2.4
1	С	534	ILE	2.3
1	С	513	SER	2.3
1	С	766	PRO	2.3
1	В	724	HIS	2.2
1	C	511	ILE	2.2
1	С	602	GLU	2.2
1	В	794	TRP	2.2
1	С	686	VAL	2.2
1	A	443	ILE	2.2
1	C	504	SER	2.2
1	С	507	HIS	2.2



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Mol	Chain	Res	Type	RSRZ
1	С	539	TYR	2.2
1	С	525	LEU	2.1
1	С	727	HIS	2.1
1	В	672	LYS	2.1
1	A	768	SER	2.1
1	С	660	ARG	2.1
1	С	462	HIS	2.1
1	С	500	ALA	2.1
1	С	532	ILE	2.1
1	С	517	MET	2.1
1	С	656	LEU	2.1
1	С	690	ALA	2.1
1	С	716	GLN	2.0
1	С	779	ALA	2.0
1	В	793	PHE	2.0
1	С	522	LEU	2.0
1	С	657	GLY	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^{th} 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.

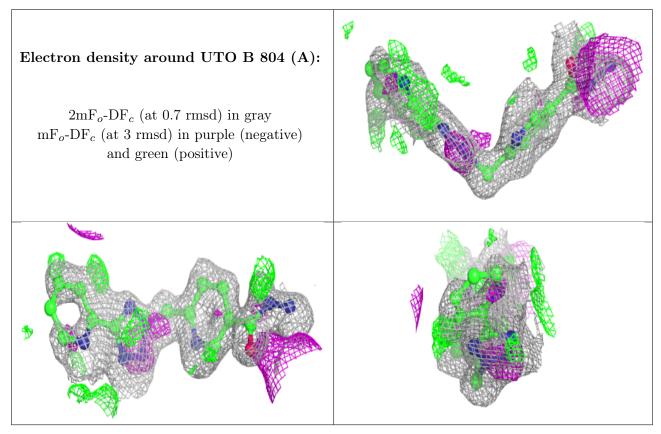
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
3	ZN	С	803	1/1	0.84	0.11	89,89,89,89	0
4	UTO	В	804[A]	22/22	0.87	0.20	24,26,27,28	22
4	UTO	В	804[B]	22/22	0.87	0.20	4,22,36,36	22
4	UTO	A	804	22/22	0.88	0.15	12,25,40,42	0
5	IOD	В	805	1/1	0.94	0.07	71,71,71,71	0
5	IOD	A	808	1/1	0.96	0.08	46,46,46,46	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$ m B ext{-}factors(\AA^2)$	Q < 0.9
5	IOD	С	804	1/1	0.96	0.07	46,46,46,46	0
5	IOD	A	807	1/1	0.99	0.04	28,28,28,28	0
3	ZN	A	803	1/1	0.99	0.22	41,41,41,41	0
3	ZN	В	803	1/1	0.99	0.23	51,51,51,51	0
2	K	С	802	1/1	0.99	0.08	53,53,53,53	0
2	K	A	802	1/1	1.00	0.11	13,13,13,13	0
5	IOD	A	805	1/1	1.00	0.05	24,24,24,24	0
5	IOD	A	806	1/1	1.00	0.10	15,15,15,15	0
2	K	В	801	1/1	1.00	0.11	12,12,12,12	0
2	K	В	802	1/1	1.00	0.12	16,16,16,16	0
2	K	С	801	1/1	1.00	0.10	31,31,31,31	0
2	K	A	801	1/1	1.00	0.12	9,9,9,9	0

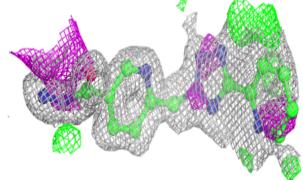
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

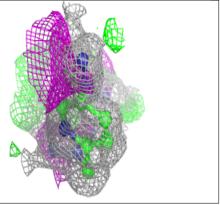




Electron density around UTO B 804 (B): 2mF_o-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive) Electron density around UTO A 804:

Electron density around UTO A 804: $2mF_o$ -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.

