



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 25, 2024 – 08:16 PM EST

PDB ID : 9EFR
Title : Crystal structure of Danio rerio histone deacetylase 6 catalytic domain 2 complexed with TO-600
Authors : Erdogan, F.; Seo, H.-S.; Dhe-Paganon, S.
Deposited on : 2024-11-20
Resolution : 1.24 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 1.21
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

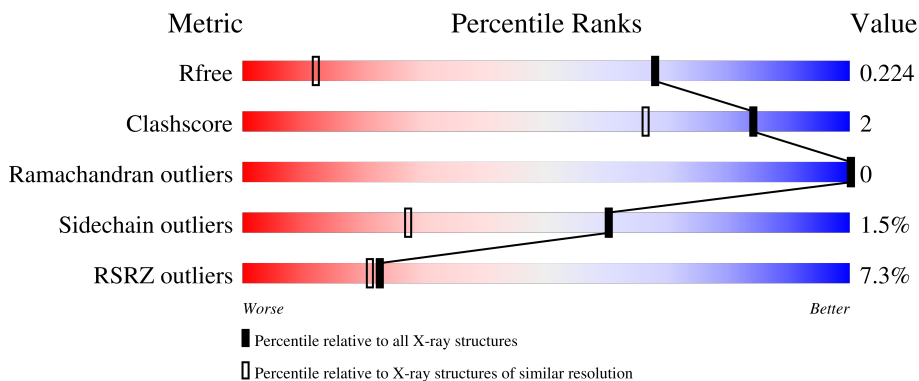
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

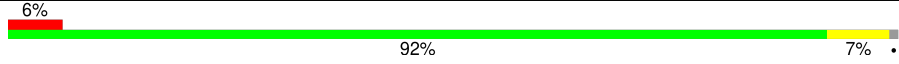
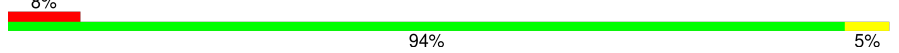
The reported resolution of this entry is 1.24 Å.

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}	164625	1389 (1.26-1.22)
Clashscore	180529	1509 (1.26-1.22)
Ramachandran outliers	177936	1478 (1.26-1.22)
Sidechain outliers	177891	1476 (1.26-1.22)
RSRZ outliers	164620	1389 (1.26-1.22)

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 $\leq 5\%$. 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	357	 6% 92% 7%
1	B	357	 8% 94% 5%

2 Entry composition [i](#)

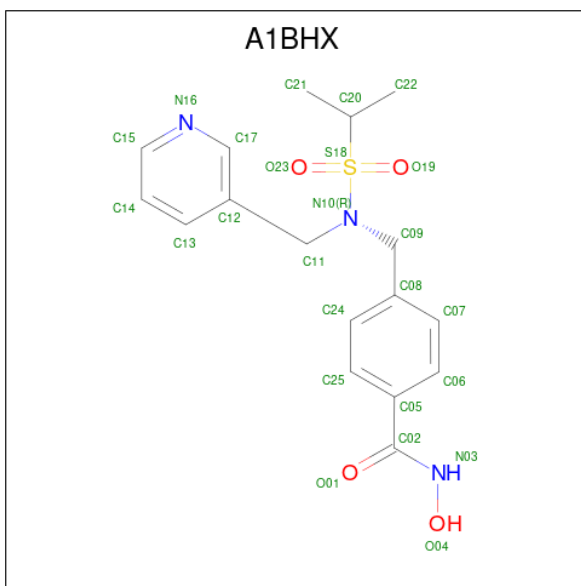
There are 5 unique types of molecules in this entry. The entry contains 6535 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Hdac6 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	354	Total 2834	C 1778	N 514	O 523	S 19	0	9	0
1	B	357	Total 2856	C 1792	N 516	O 529	S 19	0	9	0

- Molecule 2 is N-hydroxy-4-((propane-2-sulfonyl)[(pyridin-3-yl)methyl]amino)methyl)benzamide (three-letter code: A1BHX) (formula: C₁₇H₂₁N₃O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	Total 25	C 17	N 3	O 4	S 1	0	0
2	B	1	Total 25	C 17	N 3	O 4	S 1	0	0

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

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

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

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

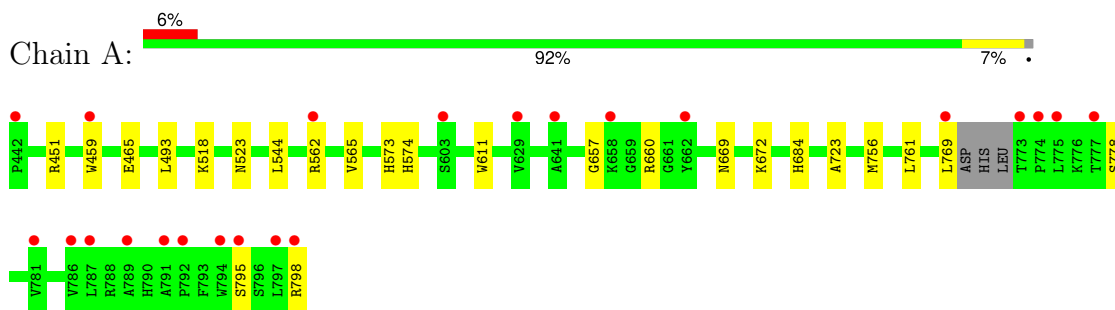
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	393	Total	O	0	0
			393	393		
5	B	395	Total	O	0	0
			395	395		

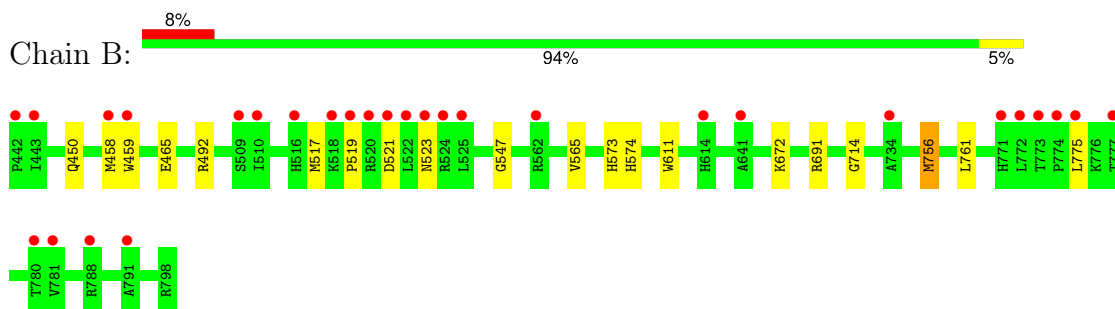
3 Residue-property plots [i](#)

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: Hdac6 protein



- Molecule 1: Hdac6 protein



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.14Å 92.60Å 96.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.28 – 1.24 59.28 – 1.24	Depositor EDS
% Data completeness (in resolution range)	82.5 (59.28-1.24) 82.5 (59.28-1.24)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 1.24Å)	Xtrriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.198 , (Not available) 0.199 , 0.224	Depositor DCC
R_{free} test set	41191 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	16.8	Xtrriage
Anisotropy	0.330	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.000 for -h,l,k	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6535	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.80 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.4191e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: ZN, A1BHX, 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	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.40	0/2906	0.60	0/3935
1	B	0.40	0/2930	0.62	0/3971
All	All	0.40	0/5836	0.61	0/7906

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	2834	0	2754	14	0
1	B	2856	0	2769	11	0
2	A	25	0	0	1	0
2	B	25	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	2	0	0	0	0
4	B	3	0	0	0	0
5	A	393	0	0	4	0
5	B	395	0	0	3	0
All	All	6535	0	5523	25	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 (25) 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:451[A]:ARG:HD2	5:A:909:HOH:O	1.89	0.70
1:A:795[A]:SER:HA	1:A:798:ARG:HD2	1.81	0.63
1:A:795[B]:SER:HA	1:A:798:ARG:HD2	1.81	0.62
1:B:565[B]:VAL:HG23	1:B:761:LEU:HD12	1.82	0.62
1:A:684:HIS:HE1	5:A:1205:HOH:O	1.84	0.59
1:A:518:LYS:NZ	5:A:903:HOH:O	2.35	0.58
1:A:723:ALA:HB2	1:A:756[A]:MET:HG3	1.85	0.58
1:B:458:MET:HE1	1:B:519:PRO:HB3	1.85	0.58
1:B:756[B]:MET:HE1	5:B:943:HOH:O	2.06	0.55
1:A:565[B]:VAL:HG23	1:A:761:LEU:HD12	1.89	0.55
1:A:574:HIS:NE2	2:A:801:A1BHX:N03	2.56	0.53
1:B:574:HIS:NE2	2:B:801:A1BHX:N03	2.57	0.53
1:A:459:TRP:CZ2	1:A:523:ASN:HB2	2.48	0.48
1:B:450[A]:GLN:NE2	5:B:915:HOH:O	2.46	0.48
1:A:669:ASN:O	1:A:778:SER:OG	2.22	0.47
1:A:672:LYS:HB3	1:A:672:LYS:HE3	1.64	0.46
1:B:517:MET:HB3	1:B:521:ASP:HB2	1.98	0.46
1:B:459:TRP:CZ2	1:B:523:ASN:HB2	2.51	0.45
1:B:492:ARG:O	1:B:547:GLY:HA3	2.18	0.44
1:A:493:LEU:HD23	1:A:544:LEU:HG	1.99	0.44
1:B:672:LYS:HG3	1:B:714:GLY:O	2.18	0.43
1:A:562:ARG:NH1	5:A:912:HOH:O	2.50	0.43
1:B:691:ARG:HD3	5:B:1061:HOH:O	2.18	0.43
1:B:565[B]:VAL:HG23	1:B:761:LEU:CD1	2.49	0.41
1:A:657:GLY:O	1:A:660[A]:ARG:HG3	2.21	0.40

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	359/357 (101%)	349 (97%)	10 (3%)	0	100	100
1	B	364/357 (102%)	356 (98%)	8 (2%)	0	100	100
All	All	723/714 (101%)	705 (98%)	18 (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	306/301 (102%)	302 (99%)	4 (1%)	65	32
1	B	309/301 (103%)	303 (98%)	6 (2%)	52	17
All	All	615/602 (102%)	605 (98%)	10 (2%)	60	25

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	465	GLU
1	A	573	HIS
1	A	611	TRP
1	A	769	LEU
1	B	465	GLU
1	B	573	HIS
1	B	611	TRP
1	B	756[A]	MET
1	B	756[B]	MET
1	B	775	LEU

Sometimes 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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 7 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
2	A1BHX	A	801	3	24,26,26	2.37	4 (16%)	29,36,36	4.55	8 (27%)
2	A1BHX	B	801	3	24,26,26	2.96	4 (16%)	29,36,36	10.83	7 (24%)

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	A1BHX	A	801	3	-	4/26/26/26	0/2/2/2
2	A1BHX	B	801	3	-	6/26/26/26	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	A1BHX	C02-N03	9.95	1.45	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	A1BHX	C02-N03	9.89	1.45	1.32
2	B	801	A1BHX	O19-S18	8.14	1.50	1.43
2	B	801	A1BHX	O23-S18	-5.47	1.39	1.43
2	A	801	A1BHX	O23-S18	3.20	1.46	1.43
2	A	801	A1BHX	O19-S18	3.03	1.46	1.43
2	A	801	A1BHX	O01-C02	-2.75	1.16	1.23
2	B	801	A1BHX	O01-C02	-2.23	1.18	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	A1BHX	O23-S18-O19	-56.44	76.67	119.17
2	A	801	A1BHX	O23-S18-O19	-22.59	102.16	119.17
2	B	801	A1BHX	O23-S18-N10	12.37	119.93	107.44
2	A	801	A1BHX	O19-S18-N10	4.67	112.15	107.44
2	B	801	A1BHX	C22-C20-C21	-3.62	106.61	112.79
2	B	801	A1BHX	C15-N16-C17	3.42	122.83	116.85
2	A	801	A1BHX	C15-N16-C17	3.36	122.73	116.85
2	B	801	A1BHX	O01-C02-N03	-3.22	116.97	122.90
2	A	801	A1BHX	O01-C02-N03	-3.20	117.01	122.90
2	A	801	A1BHX	O23-S18-N10	3.12	110.59	107.44
2	A	801	A1BHX	C11-N10-C09	2.57	121.53	116.27
2	B	801	A1BHX	O19-S18-N10	-2.44	104.98	107.44
2	B	801	A1BHX	O04-N03-C02	2.29	125.46	119.73
2	A	801	A1BHX	C05-C02-N03	2.29	119.79	116.26
2	A	801	A1BHX	O04-N03-C02	2.23	125.32	119.73

There are no chirality outliers.

All (10) torsion outliers are listed below:

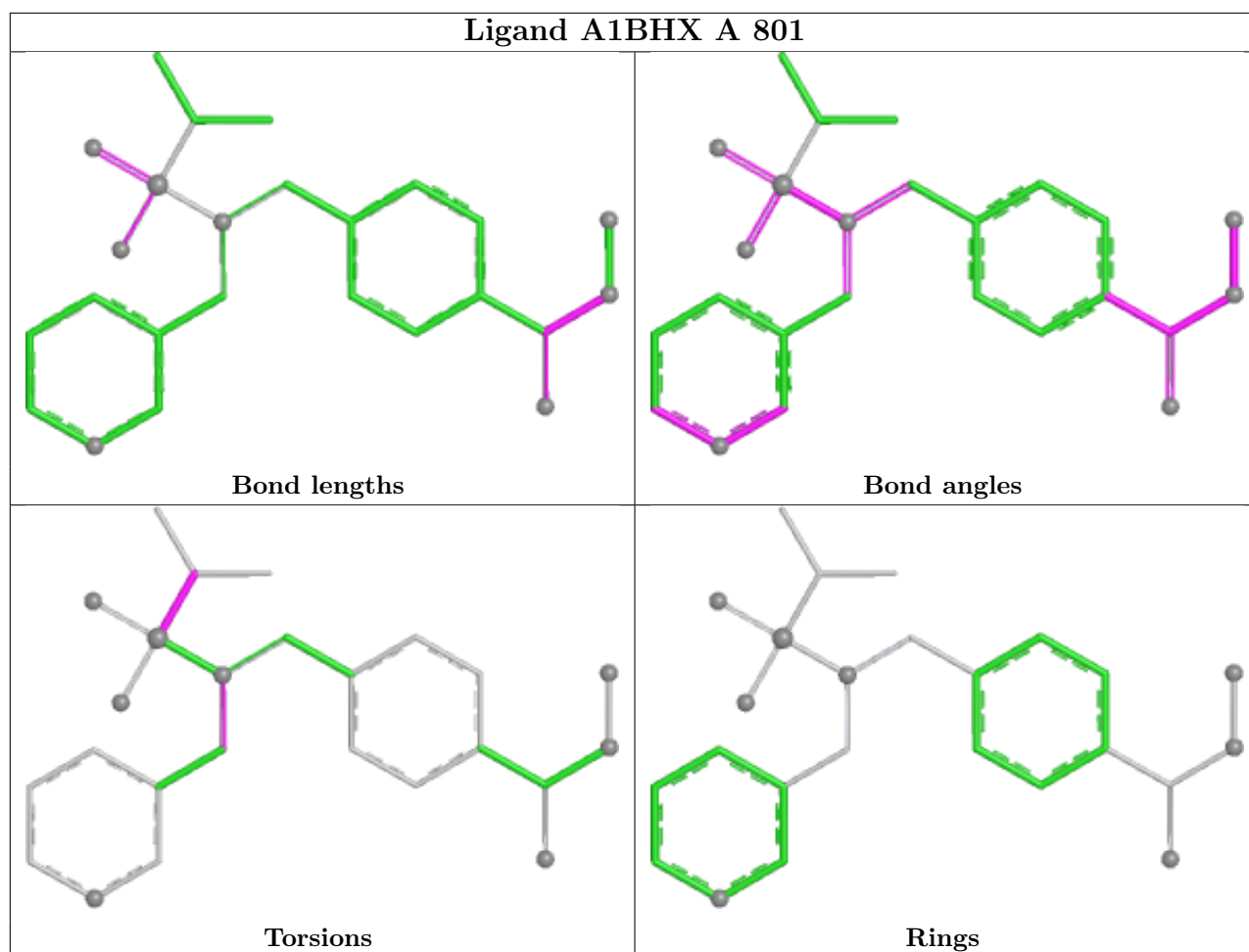
Mol	Chain	Res	Type	Atoms
2	A	801	A1BHX	C21-C20-S18-N10
2	B	801	A1BHX	C21-C20-S18-O23
2	B	801	A1BHX	C22-C20-S18-O23
2	B	801	A1BHX	C09-N10-S18-O23
2	B	801	A1BHX	C11-N10-S18-O23
2	B	801	A1BHX	C12-C11-N10-C09
2	A	801	A1BHX	C12-C11-N10-C09
2	A	801	A1BHX	C21-C20-S18-O19
2	A	801	A1BHX	C21-C20-S18-O23
2	B	801	A1BHX	C22-C20-S18-O19

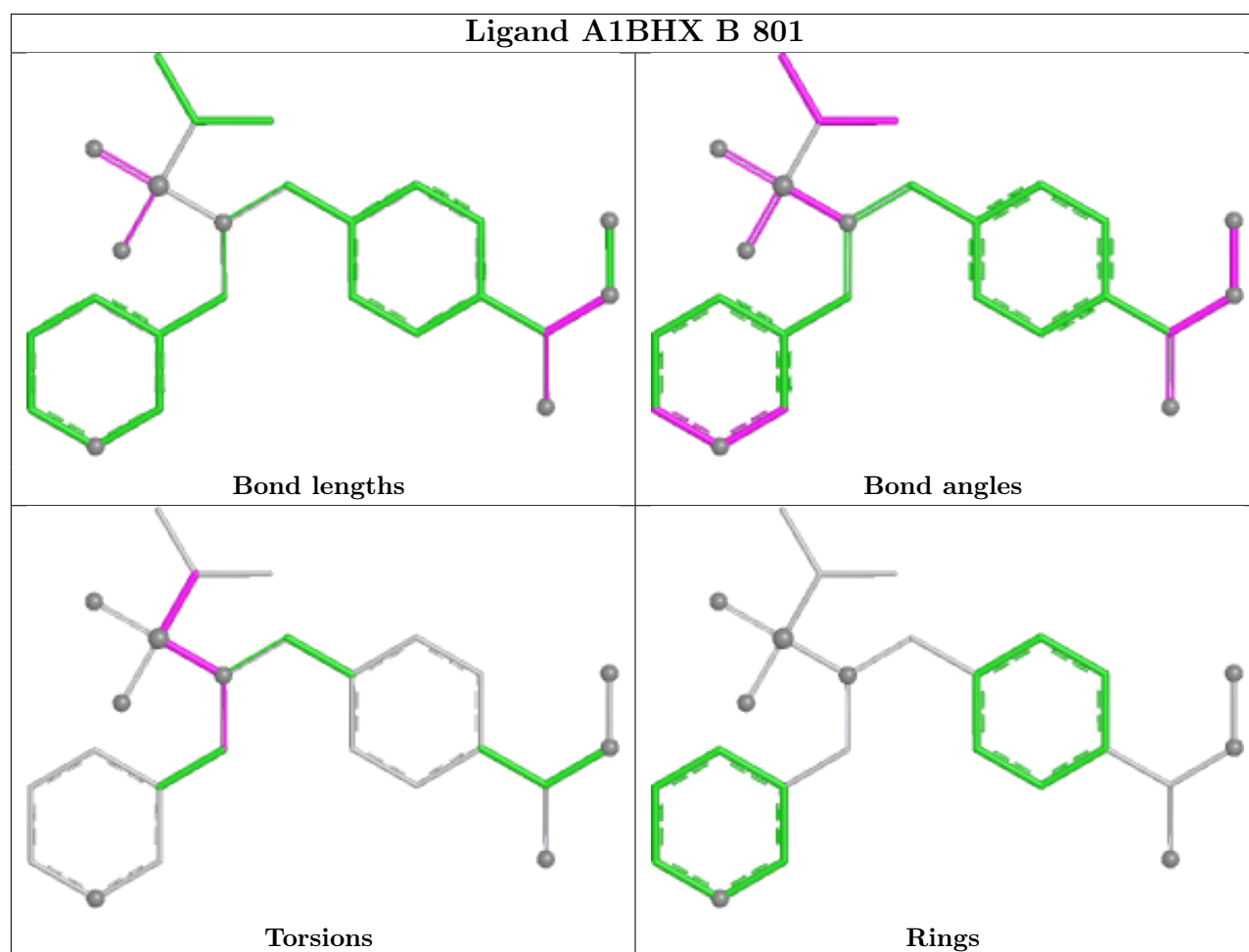
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	A1BHX	1	0
2	B	801	A1BHX	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

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	354/357 (99%)	0.53	23 (6%)	26 25	6, 18, 33, 60	10 (2%)
1	B	357/357 (100%)	0.65	29 (8%)	19 17	6, 19, 38, 63	11 (3%)
All	All	711/714 (99%)	0.59	52 (7%)	22 21	6, 18, 36, 63	21 (2%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	772	LEU	4.7
1	A	773	THR	4.7
1	B	459	TRP	4.6
1	B	775	LEU	4.2
1	A	769	LEU	4.2
1	A	629	VAL	4.0
1	B	774	PRO	3.9
1	B	771	HIS	3.8
1	A	777	THR	3.7
1	A	442	PRO	3.7
1	B	519	PRO	3.6
1	B	443	ILE	3.6
1	B	522	LEU	3.5
1	A	791	ALA	3.4
1	B	641	ALA	3.4
1	B	518	LYS	3.3
1	A	658	LYS	3.2
1	A	459	TRP	3.2
1	A	774	PRO	3.2
1	A	781	VAL	3.2
1	B	791	ALA	3.2
1	B	773	THR	3.1
1	B	523	ASN	3.0
1	B	524	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	516	HIS	3.0
1	B	525	LEU	2.9
1	B	442	PRO	2.9
1	B	781	VAL	2.9
1	B	777	THR	2.9
1	B	521	ASP	2.8
1	A	797	LEU	2.7
1	A	789	ALA	2.7
1	A	562	ARG	2.7
1	B	458	MET	2.7
1	B	562	ARG	2.6
1	B	780	THR	2.6
1	A	641	ALA	2.6
1	A	798	ARG	2.5
1	A	794	TRP	2.5
1	B	510	ILE	2.5
1	B	509	SER	2.4
1	B	520	ARG	2.4
1	A	795[A]	SER	2.3
1	B	614	HIS	2.3
1	A	775	LEU	2.2
1	A	662	TYR	2.2
1	B	788	ARG	2.1
1	B	734	ALA	2.0
1	A	792	PRO	2.0
1	A	603	SER	2.0
1	A	786	VAL	2.0
1	A	787	LEU	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.

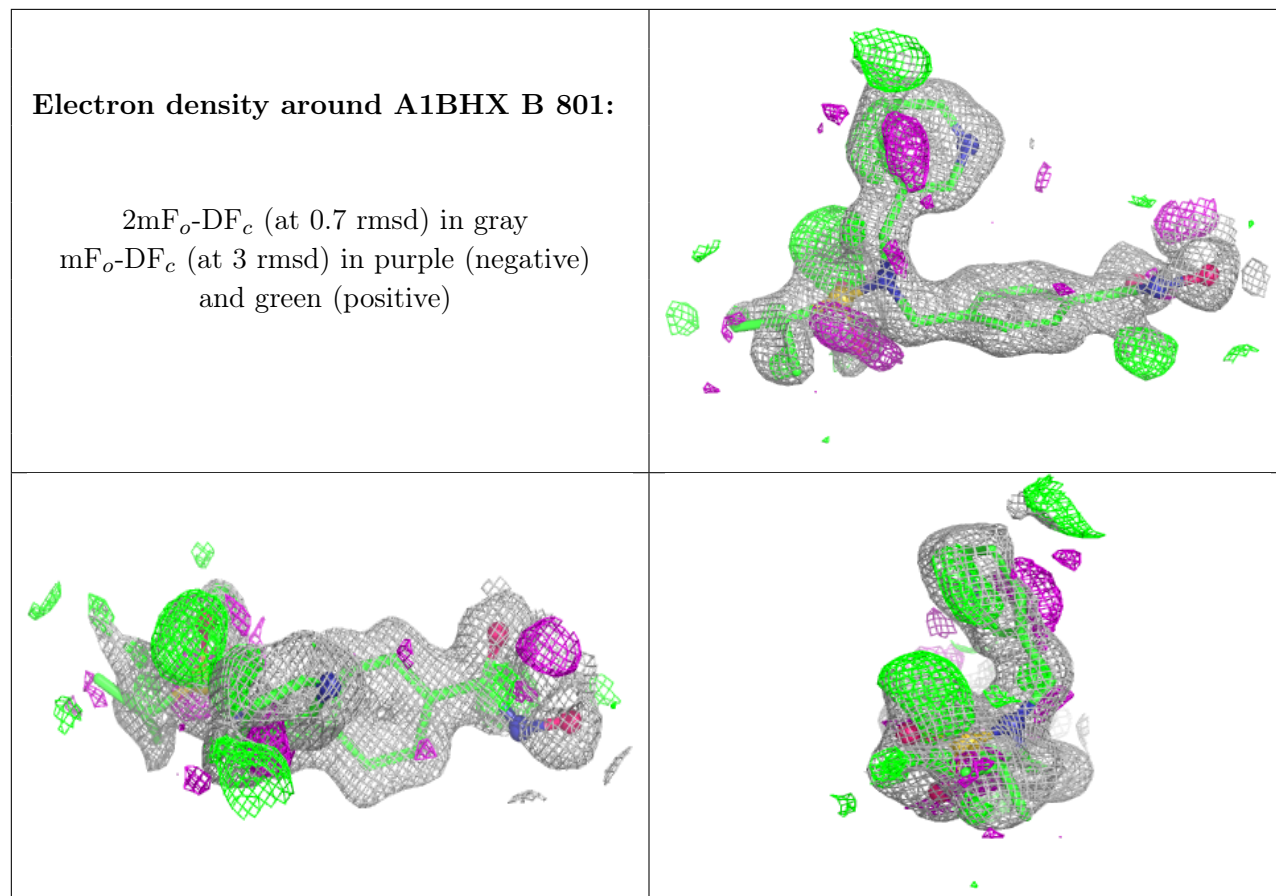
6.4 Ligands [i](#)

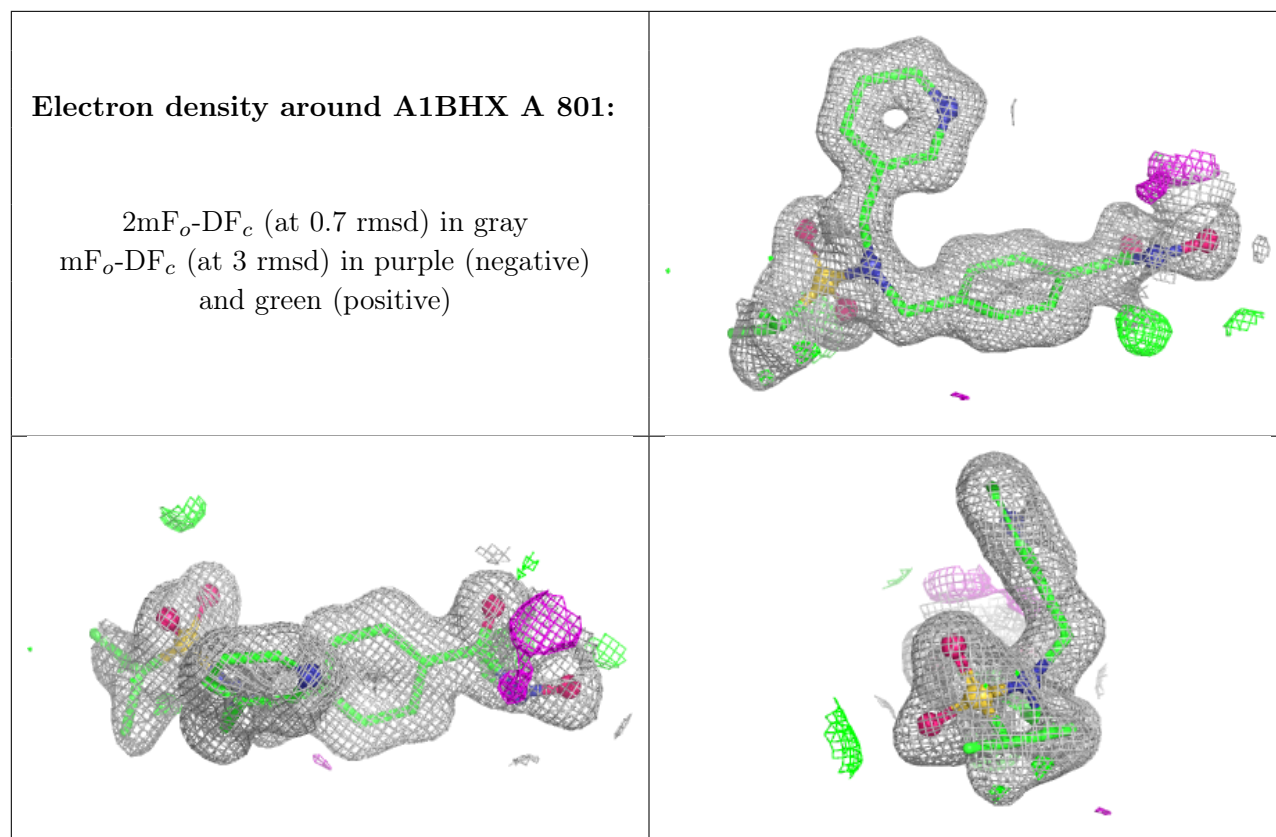
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 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	A1BHX	B	801	25/25	0.89	0.16	16,25,43,65	0
2	A1BHX	A	801	25/25	0.96	0.10	16,21,41,55	0
3	ZN	A	802	1/1	0.99	0.04	14,14,14,14	0
4	K	B	803	1/1	0.99	0.03	18,18,18,18	0
4	K	B	805	1/1	0.99	0.07	23,23,23,23	1
4	K	A	804	1/1	1.00	0.03	18,18,18,18	0
3	ZN	B	802	1/1	1.00	0.04	13,13,13,13	0
4	K	B	804	1/1	1.00	0.03	12,12,12,12	0
4	K	A	803	1/1	1.00	0.01	13,13,13,13	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 [i](#)

There are no such residues in this entry.