



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 11:58 PM UTC

PDB ID : 9EU0 / pdb_00009eu0
Title : Crystal structure of Danio rerio HDAC6 CD2 in complex with hydrolyzed DFMO-inhibitor (ITF7209)
Authors : Bebel, A.; Cellupica, E.; Stevenazzi, A.; Sandrone, G.; Vergani, B.; Caprini, G.
Deposited on : 2024-03-27
Resolution : 1.86 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

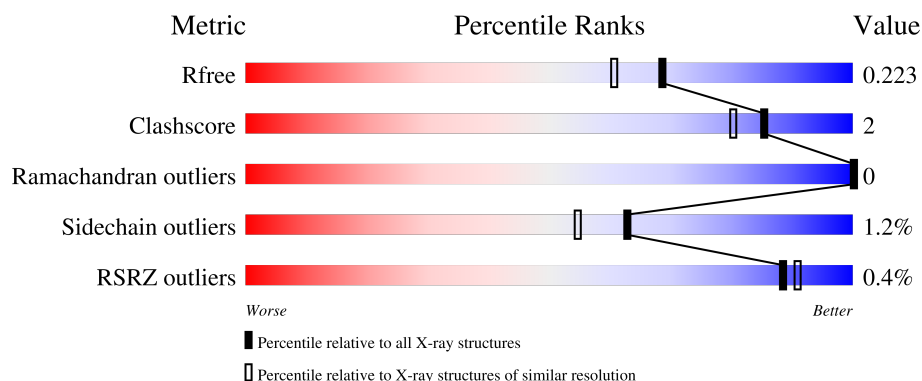
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

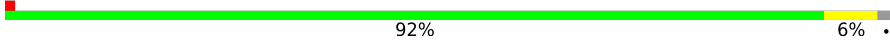
The reported resolution of this entry is 1.86 Å.

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}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	365	 90% 7% •
1	B	365	 92% 6% •

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11636 atoms, of which 5560 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	A	357	Total	C	H	N	O	S	109	6	0
			5583	1769	2765	510	521	18			
1	B	356	Total	C	H	N	O	S	109	4	0
			5543	1758	2743	505	519	18			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	434	GLY	-	cloning artifact	UNP F8W4B7
A	435	SER	-	cloning artifact	UNP F8W4B7
A	436	ASN	-	cloning artifact	UNP F8W4B7
A	437	ALA	-	cloning artifact	UNP F8W4B7
A	438	GLY	-	cloning artifact	UNP F8W4B7
A	439	GLY	-	cloning artifact	UNP F8W4B7
B	434	GLY	-	cloning artifact	UNP F8W4B7
B	435	SER	-	cloning artifact	UNP F8W4B7
B	436	ASN	-	cloning artifact	UNP F8W4B7
B	437	ALA	-	cloning artifact	UNP F8W4B7
B	438	GLY	-	cloning artifact	UNP F8W4B7
B	439	GLY	-	cloning artifact	UNP F8W4B7

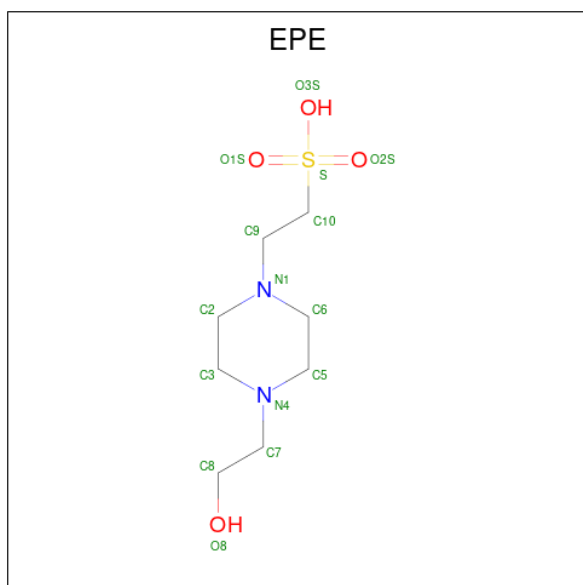
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

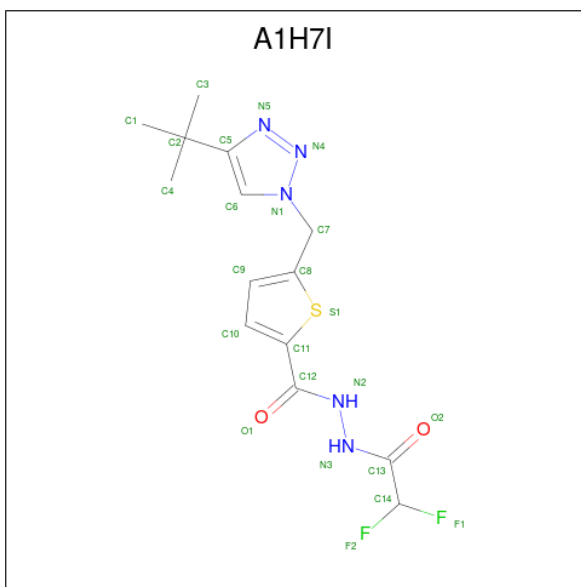
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total K 2 2	0	0
3	B	2	Total K 2 2	0	0

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	S	2	0
			33	8	18	2	4	1		

- Molecule 5 is {N}'-[2,2-bis(fluoranyl)ethanoyl]-5-[(4- {tert}-butyl-1,2,3-triazol-1-yl)methyl]thiophene-2-carbohydrazide (CCD ID: A1H7I) (formula: C₁₄H₁₇F₂N₅O₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
5	A	1	Total	C	F	H	N	O	S	0	0
			41	14	2	17	5	2	1		
5	B	1	Total	C	F	H	N	O	S	0	0
			41	14	2	17	5	2	1		

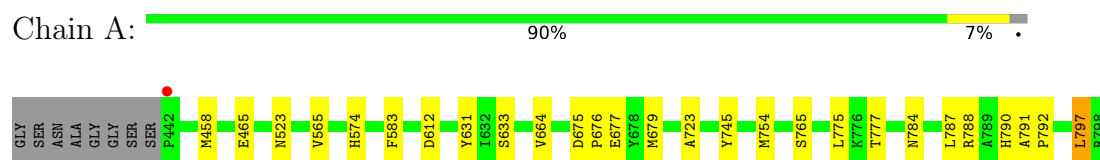
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	188	Total	O	0	0
			188	188		
6	B	201	Total	O	0	0
			201	201		

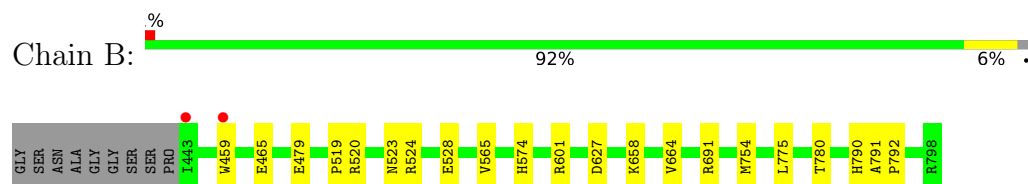
3 Residue-property plots [i](#)

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



- Molecule 1: Histone deacetylase 6



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.71Å 91.56Å 96.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.06 – 1.86 48.06 – 1.86	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.06-1.86) 99.9 (48.06-1.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.176 , 0.222 0.177 , 0.223	Depositor DCC
R_{free} test set	2801 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11636	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.83 % 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 7.0548e-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: EPE, A1H7I, ZN, 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	0.61	0/2909	1.03	3/3941 (0.1%)
1	B	0.63	0/2882	1.05	2/3906 (0.1%)
All	All	0.62	0/5791	1.04	5/7847 (0.1%)

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	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	780	THR	CA-CB-OG1	-6.04	100.54	109.60
1	B	479	GLU	CB-CA-C	-6.01	100.47	110.68
1	A	583	PHE	CA-CB-CG	5.84	119.64	113.80
1	A	612	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	523	ASN	CB-CA-C	5.13	119.56	110.85

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	601	ARG	Sidechain

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	2818	2765	2718	14	0
1	B	2800	2743	2706	10	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	15	18	18	0	0
5	A	24	17	0	3	0
5	B	24	17	0	1	0
6	A	188	0	0	1	0
6	B	201	0	0	1	0
All	All	6076	5560	5442	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:B:565:VAL:CG2	1:B:754:MET:HE2	2.32	0.59
1:B:691:ARG:HD3	6:B:930:HOH:O	2.00	0.59
1:B:574:HIS:NE2	5:B:804:A1H7I:O1	2.36	0.58
5:A:805:A1H7I:C13	5:A:805:A1H7I:O1	2.53	0.55
1:A:574:HIS:NE2	5:A:805:A1H7I:O1	2.42	0.52
1:B:459:TRP:CZ2	1:B:523:ASN:HB2	2.46	0.50
1:B:520:ARG:HH22	1:B:524:ARG:NH2	2.09	0.50
1:A:791:ALA:N	1:A:792:PRO:CD	2.74	0.50
1:A:565:VAL:CG2	1:A:754:MET:HE2	2.41	0.50
1:A:675:ASP:N	1:A:676:PRO:CD	2.75	0.49
1:B:565:VAL:HG22	1:B:754:MET:HE2	1.95	0.48
1:B:791:ALA:N	1:B:792:PRO:CD	2.77	0.47
1:A:677:GLU:HA	1:A:775:LEU:HD11	1.96	0.46
1:A:745:TYR:OH	5:A:805:A1H7I:N3	2.48	0.46
1:A:675:ASP:O	1:A:679:MET:HG2	2.18	0.43
1:A:784:ASN:HB3	1:A:788:ARG:HH22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:627:ASP:OD1	1:B:658:LYS:HE2	2.19	0.42
1:B:664:VAL:HG22	1:B:790:HIS:CE1	2.54	0.42
1:A:787:LEU:HD23	1:A:797:LEU:HG	2.02	0.41
1:A:664:VAL:HG22	1:A:790:HIS:CE1	2.56	0.41
1:A:458:MET:HE1	6:A:1035:HOH:O	2.21	0.40
1:B:524:ARG:O	1:B:528:GLU:HG3	2.21	0.40
1:A:631:TYR:CZ	1:A:633:SER:HB2	2.57	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	361/365 (99%)	345 (96%)	16 (4%)	0	100	100
1	B	358/365 (98%)	347 (97%)	11 (3%)	0	100	100
All	All	719/730 (98%)	692 (96%)	27 (4%)	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	306/305 (100%)	302 (99%)	4 (1%)	61	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	303/305 (99%)	300 (99%)	3 (1%)	68	60
All	All	609/610 (100%)	602 (99%)	7 (1%)	63	57

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	465	GLU
1	A	765	SER
1	A	777	THR
1	A	797	LEU
1	B	465	GLU
1	B	519	PRO
1	B	775	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	450	GLN
1	A	536	ASN
1	A	554	GLN
1	B	683	HIS
1	B	684	HIS
1	B	716	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 6 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	A1H7I	A	805	2	24,25,25	1.43	3 (12%)	32,36,36	1.12	4 (12%)
4	EPE	A	804	-	15,15,15	0.61	1 (6%)	19,20,20	0.76	0
5	A1H7I	B	804	2	24,25,25	1.42	2 (8%)	32,36,36	1.10	3 (9%)

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
5	A1H7I	A	805	2	-	16/23/23/23	0/2/2/2
4	EPE	A	804	-	-	4/9/19/19	0/1/1/1
5	A1H7I	B	804	2	-	14/23/23/23	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	804	A1H7I	C11-S1	4.84	1.84	1.73
5	A	805	A1H7I	C11-S1	4.63	1.83	1.73
5	B	804	A1H7I	C8-S1	3.98	1.85	1.73
5	A	805	A1H7I	C8-S1	3.95	1.85	1.73
5	A	805	A1H7I	O1-C12	-2.15	1.19	1.23
4	A	804	EPE	O3S-S	2.09	1.55	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	804	A1H7I	O1-C12-C11	-3.68	113.93	120.62
5	A	805	A1H7I	C2-C5-C6	2.51	131.48	129.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	805	A1H7I	O1-C12-N2	-2.35	118.83	122.77
5	A	805	A1H7I	C13-N3-N2	2.35	123.29	120.06
5	A	805	A1H7I	C9-C10-C11	2.25	117.18	113.37
5	B	804	A1H7I	C12-N2-N3	2.16	122.56	119.49
5	B	804	A1H7I	C8-S1-C11	-2.09	90.13	92.63

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	804	EPE	C9-C10-S-O1S
5	A	805	A1H7I	C1-C2-C5-C6
5	A	805	A1H7I	C1-C2-C5-N5
5	A	805	A1H7I	C3-C2-C5-C6
5	A	805	A1H7I	C3-C2-C5-N5
5	A	805	A1H7I	C4-C2-C5-C6
5	A	805	A1H7I	C4-C2-C5-N5
5	A	805	A1H7I	C10-C11-C12-N2
5	A	805	A1H7I	S1-C11-C12-O1
5	A	805	A1H7I	S1-C11-C12-N2
5	A	805	A1H7I	C12-N2-N3-C13
5	A	805	A1H7I	O2-C13-N3-N2
5	A	805	A1H7I	C14-C13-N3-N2
5	A	805	A1H7I	N3-C13-C14-F2
5	B	804	A1H7I	C10-C11-C12-N2
5	B	804	A1H7I	S1-C11-C12-O1
5	B	804	A1H7I	S1-C11-C12-N2
5	B	804	A1H7I	C12-N2-N3-C13
5	B	804	A1H7I	O2-C13-N3-N2
5	B	804	A1H7I	C14-C13-N3-N2
5	B	804	A1H7I	N3-C13-C14-F1
5	A	805	A1H7I	C10-C11-C12-O1
5	B	804	A1H7I	C10-C11-C12-O1
5	B	804	A1H7I	C1-C2-C5-N5
5	B	804	A1H7I	C3-C2-C5-N5
4	A	804	EPE	S-C10-C9-N1
4	A	804	EPE	C9-C10-S-O3S
4	A	804	EPE	C9-C10-S-O2S
5	B	804	A1H7I	C4-C2-C5-N5
5	B	804	A1H7I	C3-C2-C5-C6
5	A	805	A1H7I	N1-C7-C8-S1
5	B	804	A1H7I	C1-C2-C5-C6

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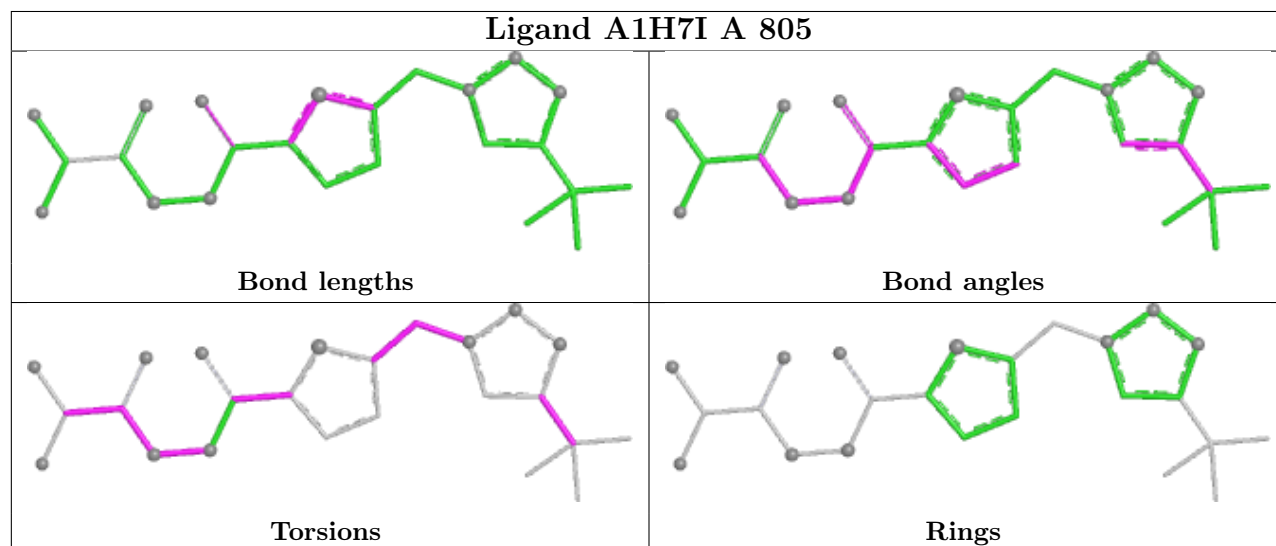
Mol	Chain	Res	Type	Atoms
5	B	804	A1H7I	C4-C2-C5-C6
5	A	805	A1H7I	C8-C7-N1-N4

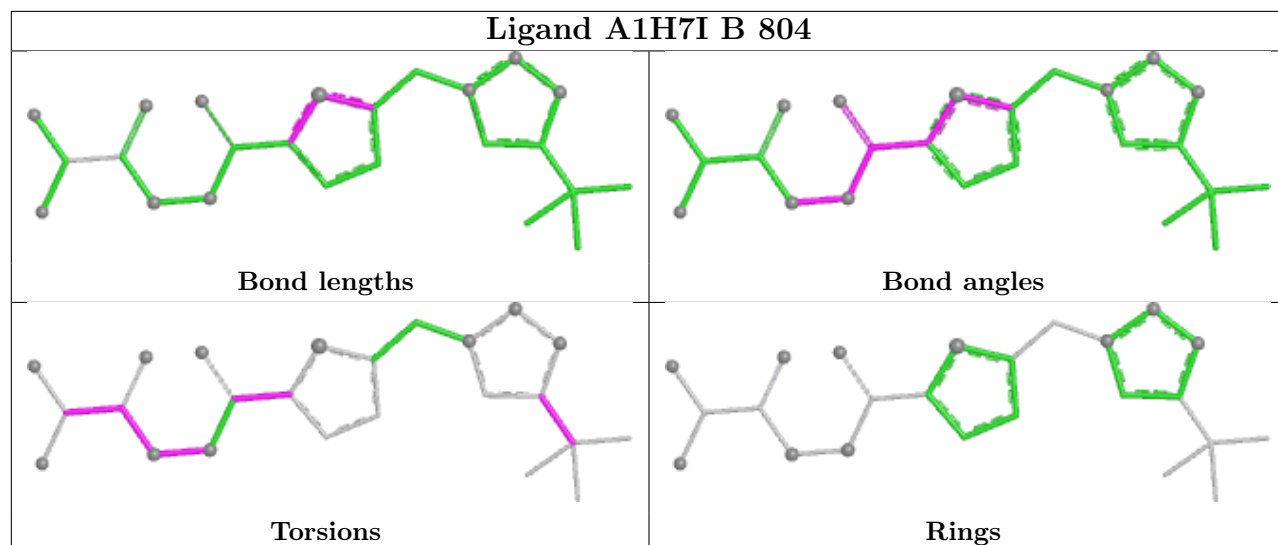
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	805	A1H7I	3	0
5	B	804	A1H7I	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	357/365 (97%)	-0.39	1 (0%) 90 92	9, 26, 44, 66	3 (0%)
1	B	356/365 (97%)	-0.42	2 (0%) 85 88	9, 25, 45, 78	2 (0%)
All	All	713/730 (97%)	-0.40	3 (0%) 88 91	9, 25, 44, 78	5 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	442	PRO	2.6
1	B	459	TRP	2.3
1	B	443	ILE	2.2

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 oligosaccharides 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
4	EPE	A	804	15/15	0.74	0.18	66,77,83,87	2
5	A1H7I	B	804	24/24	0.76	0.24	34,83,95,98	0

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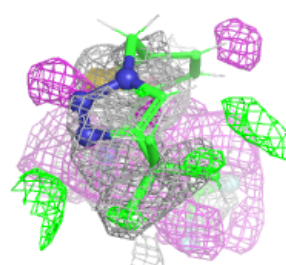
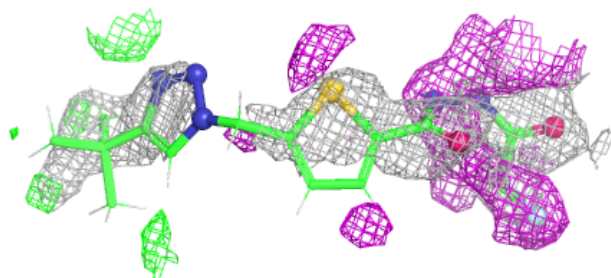
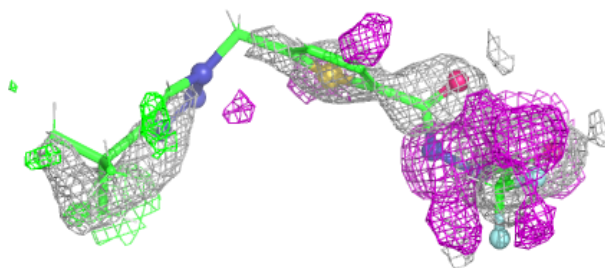
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	A1H7I	A	805	24/24	0.79	0.20	37,68,91,93	0
3	K	B	802	1/1	0.99	0.05	23,23,23,23	0
3	K	B	803	1/1	0.99	0.03	24,24,24,24	0
2	ZN	A	801	1/1	0.99	0.09	30,30,30,30	0
3	K	A	802	1/1	0.99	0.05	24,24,24,24	0
3	K	A	803	1/1	0.99	0.03	24,24,24,24	0
2	ZN	B	801	1/1	1.00	0.10	30,30,30,30	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.

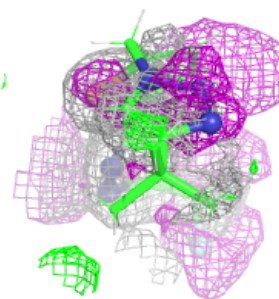
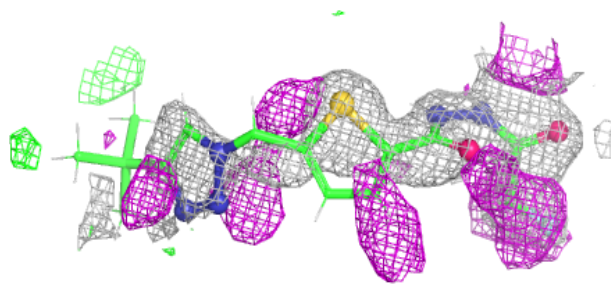
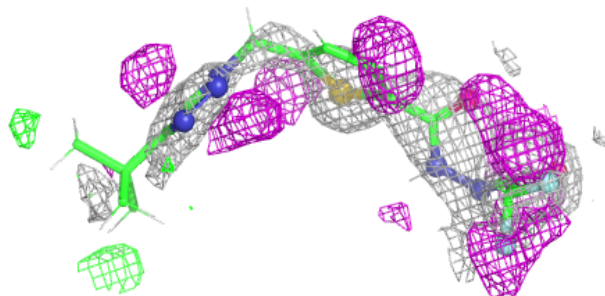
Electron density around A1H7I B 804:

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 A1H7I A 805:

$2mF_o-DF_c$ (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.