



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 04:25 PM UTC

PDB ID : 6HA6 / pdb_00006ha6
Title : Factor Inhibiting HIF (FIH) in complex with zinc, NOG and TRPV3 (220-246)
Authors : Leissing, T.M.; Clifton, I.J.; Seward, B.G.; Lu, X.; Hopkinson, R.J.; Schofield, C.J.
Deposited on : 2018-08-07
Resolution : 1.98 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

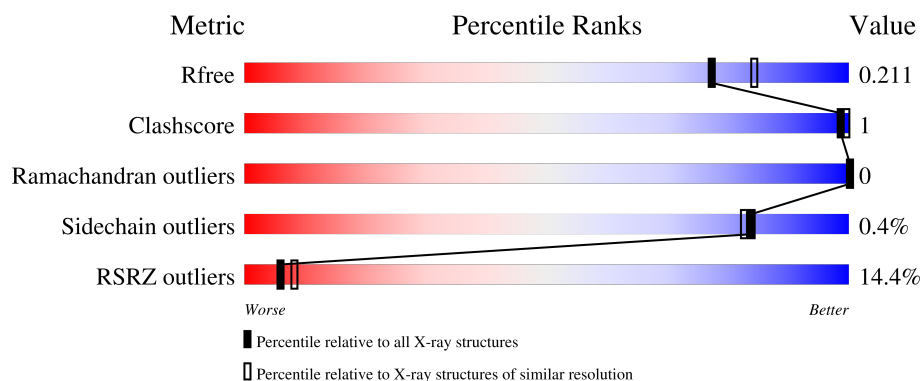
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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.



2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 3003 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 Hypoxia-inducible factor 1-alpha inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	5	0
			2754	1776	466	501	11			

- Molecule 2 is a protein called Transient receptor potential cation channel subfamily V member 3.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Zn	0	0
			1	1		

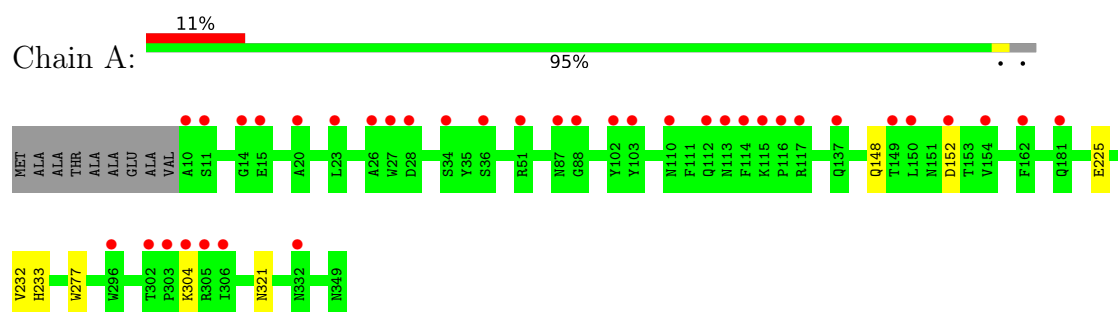
- Molecule 7 is water.

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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: Hypoxia-inducible factor 1-alpha inhibitor



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	87.08Å 87.08Å 149.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.58 – 1.98 61.58 – 1.98	Depositor EDS
% Data completeness (in resolution range)	100.0 (61.58-1.98) 100.0 (61.58-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 1.98Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.181 , 0.203 0.195 , 0.211	Depositor DCC
R_{free} test set	2027 reflections (4.97%)	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GOL, ZN, OGA

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	0.58	5/2838 (0.2%)	0.55	1/3865 (0.0%)
2	D	0.82	0/82	0.66	0/112
All	All	0.59	5/2920 (0.2%)	0.56	1/3977 (0.0%)

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2754	0	2575	2	0
2	D	83	0	77	2	0
3	A	10	0	3	0	0
4	A	20	0	0	1	0
5	A	18	0	24	0	0
6	A	1	0	0	0	0
7	A	115	0	0	0	0
7	D	2	0	0	0	0
All	All	3003	0	2679	3	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 (3) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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	280/304 (92%)	279 (100%)	1 (0%)	84	82
2	D	5/17 (29%)	5 (100%)	0	100	100
All	All	285/321 (89%)	284 (100%)	1 (0%)	84	82

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	225	GLU

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	GOL	A	407	-	5,5,5	0.38	0	5,5,5	0.20	0
4	SO4	A	403	-	4,4,4	0.23	0	6,6,6	0.08	0
3	OGA	A</								

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	408	GOL	O1-C1-C2-C3
5	A	408	GOL	O1-C1-C2-O2
5	A	406	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	405	SO4	1	0

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	340/349 (97%)	0.75	37 (10%) 10 15	22, 63, 103, 127	6 (1%)
2	D	14/27 (51%)	4.01	14 (100%) 0 0	94, 113, 146, 147	0
All	All	354/376 (94%)	0.88	51 (14%) 6 8	22, 64, 111, 147	6 (1%)

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	A	405	5/5	0.41	0.12	167,168,171,171	0
5	GOL	A	408	6/6	0.72	0.24	106,108,110,113	0
4	SO4	A	404	5/5	0.78	0.14	48,49,55,80	5
5	GOL	A	407	6/6	0.83	0.18	92,94,95,95	0
4	SO4	A	402	5/5	0.85	0.08	121,121,123,124	0
4	SO4	A	403	5/5	0.86	0.10	108,109,109,110	0
5	GOL	A	406	6/6	0.91	0.18	95,99,100,101	0
3	OGA							