



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 05:55 PM EDT

PDB ID : 1OFC / pdb_00001ofc
Title : nucleosome recognition module of ISWI ATPase
Authors : Grune, T.; Muller, C.W.
Deposited on : 2003-04-10
Resolution : 1.90 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	:	FAILED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

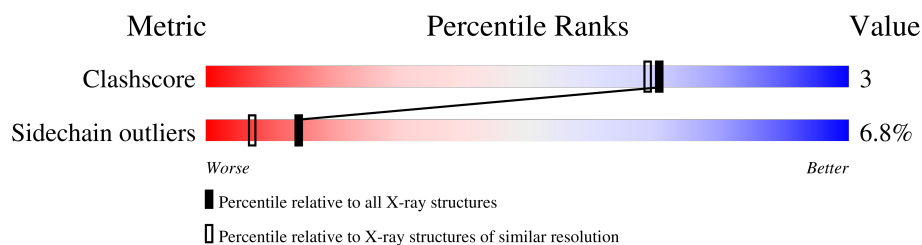
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
Clashscore	190562	8410 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	X	304	 79% 7% .. 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	G4D	X	1979	X	-	-	-

2 Entry composition [i](#)

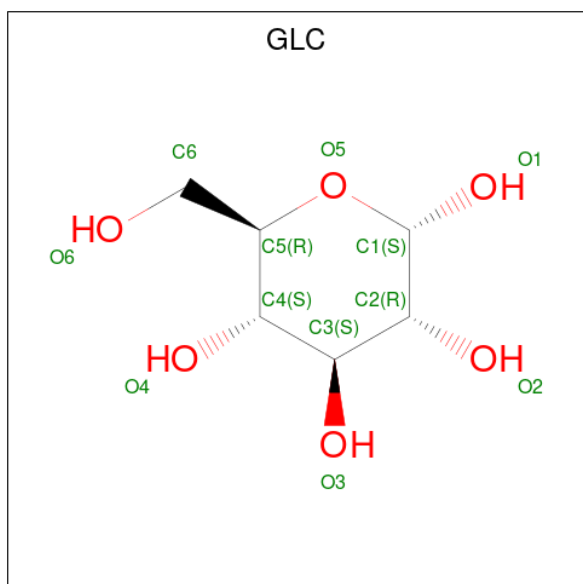
There are 5 unique types of molecules in this entry. The entry contains 2291 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ISWI PROTEIN.

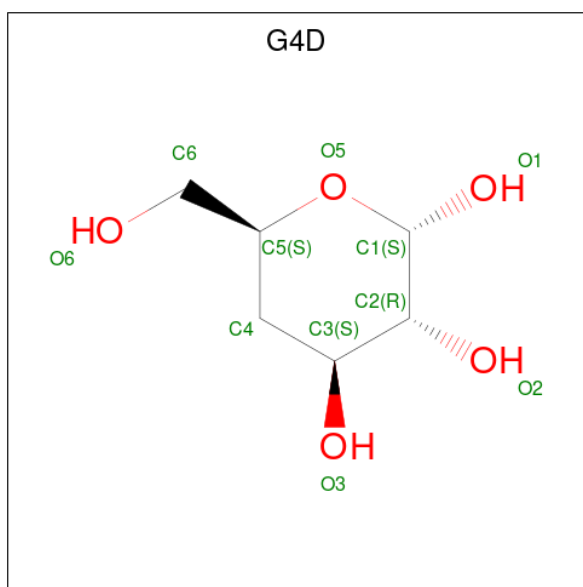
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	X	267	2214	1414	387	407	6	0	6	1

- Molecule 2 is alpha-D-glucopyranose (CCD ID: GLC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	X	1	12	6	6	0	0

- Molecule 3 is 4-deoxy-alpha-D-glucopyranose (CCD ID: G4D) (formula: C₆H₁₂O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	X	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	X	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	X	48	Total 48	O 48	0	0

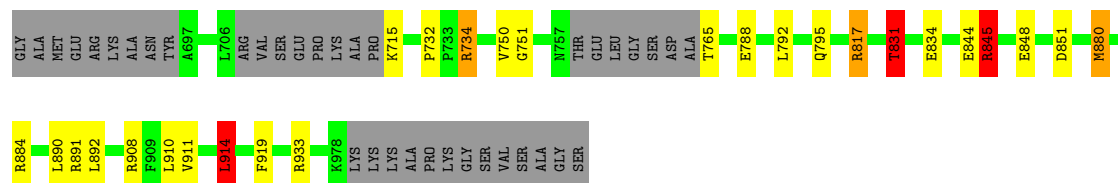
3 Residue-property plots [i](#)

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. 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. 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.

Note EDS failed to run properly.

- Molecule 1: ISWI PROTEIN

Chain X: 



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	109.47Å 66.34Å 82.83Å 90.00° 124.41° 90.00°	Depositor
Resolution (Å)	18.80 – 1.90	Depositor
% Data completeness (in resolution range)	98.6 (18.80-1.90)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 1.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.218 , 0.253	Depositor
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.022	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2291	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% of the height of the origin peak. No significant pseudotranslation is detected.*

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: GLC, G4D, GOL

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	X	1.08	3/2281 (0.1%)	1.05	4/3064 (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	X	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	817	ARG	CB-CG	-6.37	1.33	1.52
1	X	844	GLU	C-O	-5.94	1.17	1.24
1	X	880	MET	SD-CE	-5.74	1.65	1.79

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	817	ARG	CB-CA-C	-7.61	98.15	110.79
1	X	845	ARG	NE-CZ-NH2	-5.33	114.40	119.20
1	X	831	THR	N-CA-CB	-5.23	101.06	110.37
1	X	914	LEU	N-CA-C	-5.16	105.73	111.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	751	GLY	Peptide

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	X	2214	0	2141	14	0
2	X	12	0	12	0	0
3	X	11	0	12	1	0
4	X	6	0	8	1	0
5	X	48	0	0	1	0
All	All	2291	0	2173	15	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 3.

All (15) 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:X:845:ARG:HD2	1:X:848:GLU:OE2	1.80	0.81
1:X:734:ARG:HD3	1:X:788:GLU:OE1	1.89	0.72
1:X:831:THR:HG22	1:X:834:GLU:H	1.69	0.56
1:X:845:ARG:CD	1:X:848:GLU:OE2	2.51	0.55
3:X:1979:G4D:H5	5:X:2026:HOH:O	2.09	0.53
1:X:880:MET:CE	1:X:911:VAL:HG12	2.39	0.52
1:X:732:PRO:HG3	1:X:795:GLN:NE2	2.27	0.49
1:X:908:ARG:HH22	4:X:1980:GOL:H31	1.79	0.48
1:X:880:MET:HE1	1:X:911:VAL:HG12	1.97	0.46
1:X:845:ARG:HD2	1:X:848:GLU:CD	2.41	0.44
1:X:890:LEU:O	1:X:908:ARG:HD3	2.20	0.42
1:X:914:LEU:HD22	1:X:919:PHE:HA	2.02	0.41
1:X:792:LEU:HD23	1:X:792:LEU:HA	1.94	0.40
1:X:910:LEU:O	1:X:914:LEU:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains

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	X	181/268 (68%)	168 (93%)	13 (7%)	13 6

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	715	LYS
1	X	734	ARG
1	X	750	VAL
1	X	765	THR
1	X	817	ARG
1	X	831	THR
1	X	845	ARG
1	X	851	ASP
1	X	884[A]	ARG
1	X	884[B]	ARG
1	X	891	ARG
1	X	892	LEU
1	X	914	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	726	GLN
1	X	795	GLN
1	X	839	ASN
1	X	878	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 ⓘ

3 ligands are modelled in this entry.

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	G4D	X	1979	-	11,11,11	1.19	1 (9%)	15,15,15	2.57	9 (60%)
4	GOL	X	1980	-	5,5,5	0.75	0	5,5,5	1.98	3 (60%)
2	GLC	X	1978	-	12,12,12	0.82	0	17,17,17	1.08	0

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	G4D	X	1979	-	1/1/4/4	2/2/18/18	0/1/1/1
4	GOL	X	1980	-	-	0/4/4/4	-
2	GLC	X	1978	-	-	2/2/22/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	1979	G4D	O5-C5	-2.05	1.41	1.44

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	1979	G4D	O1-C1-C2	5.03	123.58	108.98
3	X	1979	G4D	O5-C1-C2	-4.13	103.03	110.30
3	X	1979	G4D	O5-C5-C6	-3.50	101.22	106.83
3	X	1979	G4D	C1-O5-C5	-3.49	106.95	113.65
3	X	1979	G4D	O6-C6-C5	-2.87	104.40	111.77
3	X	1979	G4D	O2-C2-C1	2.58	115.20	109.25
4	X	1980	GOL	O1-C1-C2	2.34	120.91	110.38
3	X	1979	G4D	C3-C4-C5	2.31	115.10	111.19
3	X	1979	G4D	O1-C1-O5	-2.28	103.64	110.41
4	X	1980	GOL	O2-C2-C1	2.23	118.43	109.18
4	X	1980	GOL	O2-C2-C3	-2.21	100.04	109.18
3	X	1979	G4D	O5-C5-C4	2.10	113.35	110.14

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	X	1979	G4D	C1

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	X	1979	G4D	C4-C5-C6-O6
3	X	1979	G4D	O5-C5-C6-O6
2	X	1978	GLC	O5-C5-C6-O6
2	X	1978	GLC	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	1979	G4D	1	0
4	X	1980	GOL	1	0

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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.