

wwPDB X-ray Structure Validation Summary Report (i)

Aug 3, 2023 – 06:09 AM EDT

PDB ID : 1HU0

Title : CRYSTAL STRUCTURE OF AN HOGG1-DNA BOROHYDRIDE

TRAPPED INTERMEDIATE COMPLEX

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Deposited on : 2001-01-03

Resolution : 2.35 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 (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: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.34

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)

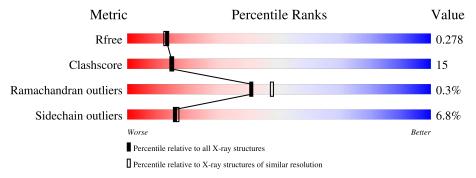
Validation Pipeline (wwPDB-VP) : 2.34

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 2.35 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	Similar resolution
Wietrie	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)

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%

Mol	Chain	Length	Quality of chain						
1	D	15	33%	67%					
2	Е	15	60%		40%				
3	A	324		71%	22%				



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3200 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 DNA chain called 5'-D(*GP*GP*TP*AP*GP*AP*CP*CP*TP*GP*GP*AP*CP*GP*C)-3'.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	D	15	Total 308	C 146	N 61	O 87	P 14	0	0	0

• Molecule 2 is a DNA chain called 5'-D(*GP*CP*GP*TP*CP*CP*AP*(PED)P*GP*TP*C P*TP*AP*CP*C)-3'.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	Е	15	Total 290	C 139	N 49	O 88	P 14	0	0	0

• Molecule 3 is a protein called 8-OXOGUANINE DNA GLYCOSYLASE 1.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
3	A	314	Total 2491	C 1579	N 448	O 453	S 11	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

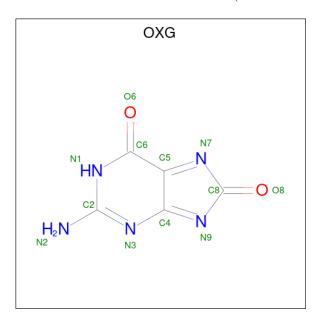
Chain	Residue	Modelled	Actual	Comment	Reference
A	4	ALA	-	cloning artifact	UNP O15527
A	5	MET	-	cloning artifact	UNP O15527
A	6	ALA	-	cloning artifact	
A	7	ASP	-	cloning artifact	UNP O15527
A	8	ILE	-	cloning artifact	UNP O15527
A	9	GLY	-	cloning artifact	UNP O15527
A	10	SER	_	cloning artifact	UNP O15527
A	11	GLU	-	cloning artifact	UNP O15527

• Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total Ca 1 1	0	0

 \bullet Molecule 5 is 8-OXOGUANINE (three-letter code: OXG) (formula: $\mathrm{C}_5\mathrm{H}_3\mathrm{N}_5\mathrm{O}_2).$



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 12	C 5	N 5	O 2	0	0

• Molecule 6 is water.

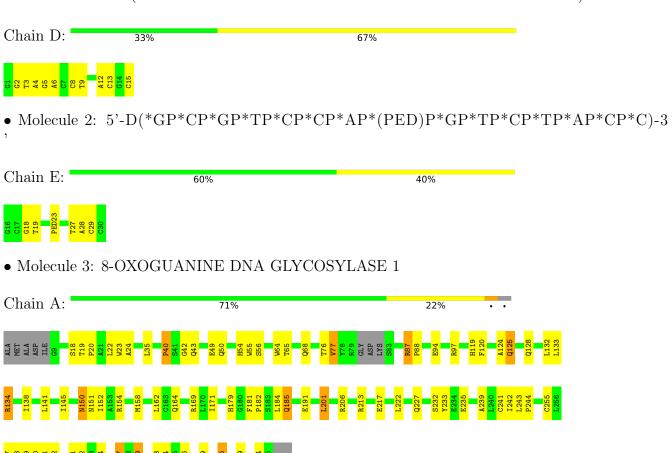
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	2	Total O 2 2	0	0
6	E	5	Total O 5 5	0	0
6	A	91	Total O 91 91	0	0



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.

 $\bullet \ \mathrm{Molecule} \ 1: \ 5'-\mathrm{D}(\mathrm{^*GP^*GP^*TP^*AP^*GP^*AP^*CP^*TP^*GP^*AP^*CP^*GP^*A}) - 3'$





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants	91.99Å 91.99Å 211.62Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.14 - 2.35	Depositor
Resolution (A)	42.18 - 2.33	EDS
% Data completeness	81.5 (42.14-2.35)	Depositor
(in resolution range)	90.0 (42.18-2.33)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) > 1$	3.75 (at 2.34Å)	Xtriage
Refinement program	CNS	Depositor
P. P.	0.210 , 0.245	Depositor
R, R_{free}	0.253 , 0.278	DCC
R_{free} test set	1860 reflections (8.13%)	wwPDB-VP
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34, 38.9	EDS
L-test for twinning ²	$ < L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3200	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.95% 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: OXG, CA, PED

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	D	0.29	0/346	0.65	0/533	
2	Е	0.28	0/310	0.64	0/473	
3	A	0.37	0/2559	0.62	0/3482	
All	All	0.36	0/3215	0.63	0/4488	

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	D	308	0	169	5	1
2	Е	290	0	167	4	0
3	A	2491	0	2423	82	1
4	Е	1	0	0	0	0
5	A	12	0	3	1	0
6	A	91	0	0	2	0
6	D	2	0	0	0	0
6	Е	5	0	0	0	0
All	All	3200	0	2762	90	2

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 15.

The worst 5 of 90 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	Clash overlap (Å)
3:A:87:ARG:NE	3:A:87:ARG:HA	1.65	1.09
3:A:87:ARG:NH2	3:A:88:PRO:HD3	1.80	0.96
3:A:87:ARG:CZ	3:A:88:PRO:HD3	2.07	0.84
3:A:185:GLN:NE2	3:A:185:GLN:H	1.75	0.82
3:A:76:THR:HA	3:A:87:ARG:HH22	1.46	0.78

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:D:15:DC:O3'	1:D:15:DC:O3'[11_655]	0.81	1.39
3:A:213:ARG:NH1	3:A:217:GLU:OE2[11_555]	1.88	0.32

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
3	A	310/324 (96%)	297 (96%)	12 (4%)	1 (0%)	41 47

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	40	PRO

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
3	A	264/271 (97%)	246 (93%)	18 (7%)	16 16

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	287	GLN
3	A	315	GLN
3	A	299	LEU
3	A	169	ARG
3	A	241	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	276	GLN
3	A	273	HIS
3	A	172	GLN
3	A	227	GLN
3	A	150	ASN

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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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).

Mal	Type	Chain	Pog	Link	Bond lengths			В	ond ang	les
MIOI	Type	Chain	rtes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	OXG	A	328	-	13,13,13	0.99	1 (7%)	14,19,19	1.20	2 (14%)

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	OXG	A	328	-	-	-	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
5	A	328	OXG	C8-N7	-2.82	1.30	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^{o})$	$\mathbf{Ideal}(^o)$
5	A	328	OXG	C5-C4-N3	2.75	128.64	123.28
5	A	328	OXG	C5-C4-N9	-2.09	105.36	110.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	328	OXG	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)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

