



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:41 PM GMT

PDB ID : 4A0B  
Title : STRUCTURE OF HSDDDB1-DRDDB2 BOUND TO A 16 BP CPD-DUPLEX  
(PYRIMIDINE AT D-1 POSITION) AT 3.8 Å RESOLUTION (CPD 4)  
Authors : Scrima, A.; Fischer, E.S.; Iwai, S.; Gut, H.; Thoma, N.H.  
Deposited on : 2011-09-08  
Resolution : 3.80 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtrriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

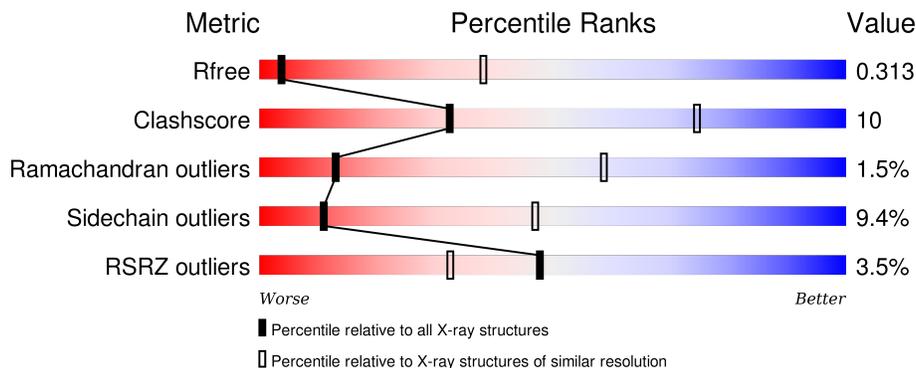
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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))
$R_{free}$	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	1159	 6% 65% 25% • 6%
1	C	1159	 3% 65% 27% • 6%
2	B	382	 63% 26% • 7%
2	D	382	 65% 24% • 7%
3	G	15	 47% 47% 7%

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Mol	Chain	Length	Quality of chain
3	I	15	 60% 27% 6% 6%
4	H	16	 44% 38% 6% 13%
4	J	16	 75% 6% 6% 13%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 23938 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 DNA DAMAGE-BINDING PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1090	8543	5423	1443	1631	46	0	0	0
1	C	1095	8582	5447	1449	1639	47	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	EXPRESSION TAG	UNP Q16531
A	-17	HIS	-	EXPRESSION TAG	UNP Q16531
A	-16	HIS	-	EXPRESSION TAG	UNP Q16531
A	-15	HIS	-	EXPRESSION TAG	UNP Q16531
A	-14	HIS	-	EXPRESSION TAG	UNP Q16531
A	-13	HIS	-	EXPRESSION TAG	UNP Q16531
A	-12	HIS	-	EXPRESSION TAG	UNP Q16531
A	-11	VAL	-	EXPRESSION TAG	UNP Q16531
A	-10	ASP	-	EXPRESSION TAG	UNP Q16531
A	-9	GLU	-	EXPRESSION TAG	UNP Q16531
A	-8	ASN	-	EXPRESSION TAG	UNP Q16531
A	-7	LEU	-	EXPRESSION TAG	UNP Q16531
A	-6	TYR	-	EXPRESSION TAG	UNP Q16531
A	-5	PHE	-	EXPRESSION TAG	UNP Q16531
A	-4	GLN	-	EXPRESSION TAG	UNP Q16531
A	-3	GLY	-	EXPRESSION TAG	UNP Q16531
A	-2	GLY	-	EXPRESSION TAG	UNP Q16531
A	-1	GLY	-	EXPRESSION TAG	UNP Q16531
A	0	ARG	-	EXPRESSION TAG	UNP Q16531
A	224	SER	GLU	ENGINEERED MUTATION	UNP Q16531
C	-18	MET	-	EXPRESSION TAG	UNP Q16531
C	-17	HIS	-	EXPRESSION TAG	UNP Q16531
C	-16	HIS	-	EXPRESSION TAG	UNP Q16531
C	-15	HIS	-	EXPRESSION TAG	UNP Q16531
C	-14	HIS	-	EXPRESSION TAG	UNP Q16531

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	HIS	-	EXPRESSION TAG	UNP Q16531
C	-12	HIS	-	EXPRESSION TAG	UNP Q16531
C	-11	VAL	-	EXPRESSION TAG	UNP Q16531
C	-10	ASP	-	EXPRESSION TAG	UNP Q16531
C	-9	GLU	-	EXPRESSION TAG	UNP Q16531
C	-8	ASN	-	EXPRESSION TAG	UNP Q16531
C	-7	LEU	-	EXPRESSION TAG	UNP Q16531
C	-6	TYR	-	EXPRESSION TAG	UNP Q16531
C	-5	PHE	-	EXPRESSION TAG	UNP Q16531
C	-4	GLN	-	EXPRESSION TAG	UNP Q16531
C	-3	GLY	-	EXPRESSION TAG	UNP Q16531
C	-2	GLY	-	EXPRESSION TAG	UNP Q16531
C	-1	GLY	-	EXPRESSION TAG	UNP Q16531
C	0	ARG	-	EXPRESSION TAG	UNP Q16531
C	224	SER	GLU	ENGINEERED MUTATION	UNP Q16531

- Molecule 2 is a protein called DNA DAMAGE-BINDING PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	354	2839	1804	498	526	11	0	0	0
2	D	355	2843	1806	499	527	11	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	76	MET	-	EXPRESSION TAG	UNP Q2YDS1
B	77	HIS	-	EXPRESSION TAG	UNP Q2YDS1
B	78	HIS	-	EXPRESSION TAG	UNP Q2YDS1
B	79	HIS	-	EXPRESSION TAG	UNP Q2YDS1
B	80	HIS	-	EXPRESSION TAG	UNP Q2YDS1
B	81	HIS	-	EXPRESSION TAG	UNP Q2YDS1
B	82	HIS	-	EXPRESSION TAG	UNP Q2YDS1
B	83	ARG	-	EXPRESSION TAG	UNP Q2YDS1
B	84	ARG	-	EXPRESSION TAG	UNP Q2YDS1
B	85	LEU	-	EXPRESSION TAG	UNP Q2YDS1
B	86	VAL	-	EXPRESSION TAG	UNP Q2YDS1
B	87	PRO	-	EXPRESSION TAG	UNP Q2YDS1
B	88	ARG	-	EXPRESSION TAG	UNP Q2YDS1
B	89	GLY	-	EXPRESSION TAG	UNP Q2YDS1
B	90	SER	-	EXPRESSION TAG	UNP Q2YDS1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	91	GLY	-	EXPRESSION TAG	UNP Q2YDS1
B	92	GLY	-	EXPRESSION TAG	UNP Q2YDS1
B	93	ARG	-	EXPRESSION TAG	UNP Q2YDS1
B	180	GLN	LEU	VARIANT	UNP Q2YDS1
B	214	ARG	TRP	VARIANT	UNP Q2YDS1
D	76	MET	-	EXPRESSION TAG	UNP Q2YDS1
D	77	HIS	-	EXPRESSION TAG	UNP Q2YDS1
D	78	HIS	-	EXPRESSION TAG	UNP Q2YDS1
D	79	HIS	-	EXPRESSION TAG	UNP Q2YDS1
D	80	HIS	-	EXPRESSION TAG	UNP Q2YDS1
D	81	HIS	-	EXPRESSION TAG	UNP Q2YDS1
D	82	HIS	-	EXPRESSION TAG	UNP Q2YDS1
D	83	ARG	-	EXPRESSION TAG	UNP Q2YDS1
D	84	ARG	-	EXPRESSION TAG	UNP Q2YDS1
D	85	LEU	-	EXPRESSION TAG	UNP Q2YDS1
D	86	VAL	-	EXPRESSION TAG	UNP Q2YDS1
D	87	PRO	-	EXPRESSION TAG	UNP Q2YDS1
D	88	ARG	-	EXPRESSION TAG	UNP Q2YDS1
D	89	GLY	-	EXPRESSION TAG	UNP Q2YDS1
D	90	SER	-	EXPRESSION TAG	UNP Q2YDS1
D	91	GLY	-	EXPRESSION TAG	UNP Q2YDS1
D	92	GLY	-	EXPRESSION TAG	UNP Q2YDS1
D	93	ARG	-	EXPRESSION TAG	UNP Q2YDS1
D	180	GLN	LEU	VARIANT	UNP Q2YDS1
D	214	ARG	TRP	VARIANT	UNP Q2YDS1

- Molecule 3 is a DNA chain called 5'-D(\*DGP\*GP\*TP\*GP\*AP\*AP\*AP\*(TTD)P\*AP\*GP\*CP\*AP\*GP\*DGP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	G	14	312	149	61	88	14	0	0	0
3	I	13	290	139	56	82	13	0	0	0

- Molecule 4 is a DNA chain called 5'-D(\*CP\*CP\*TP\*GP\*CP\*TP\*CP\*CP\*TP\*TP\*TP\*CP\*AP\*CP\*CP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	H	14	274	133	44	84	13	0	0	0

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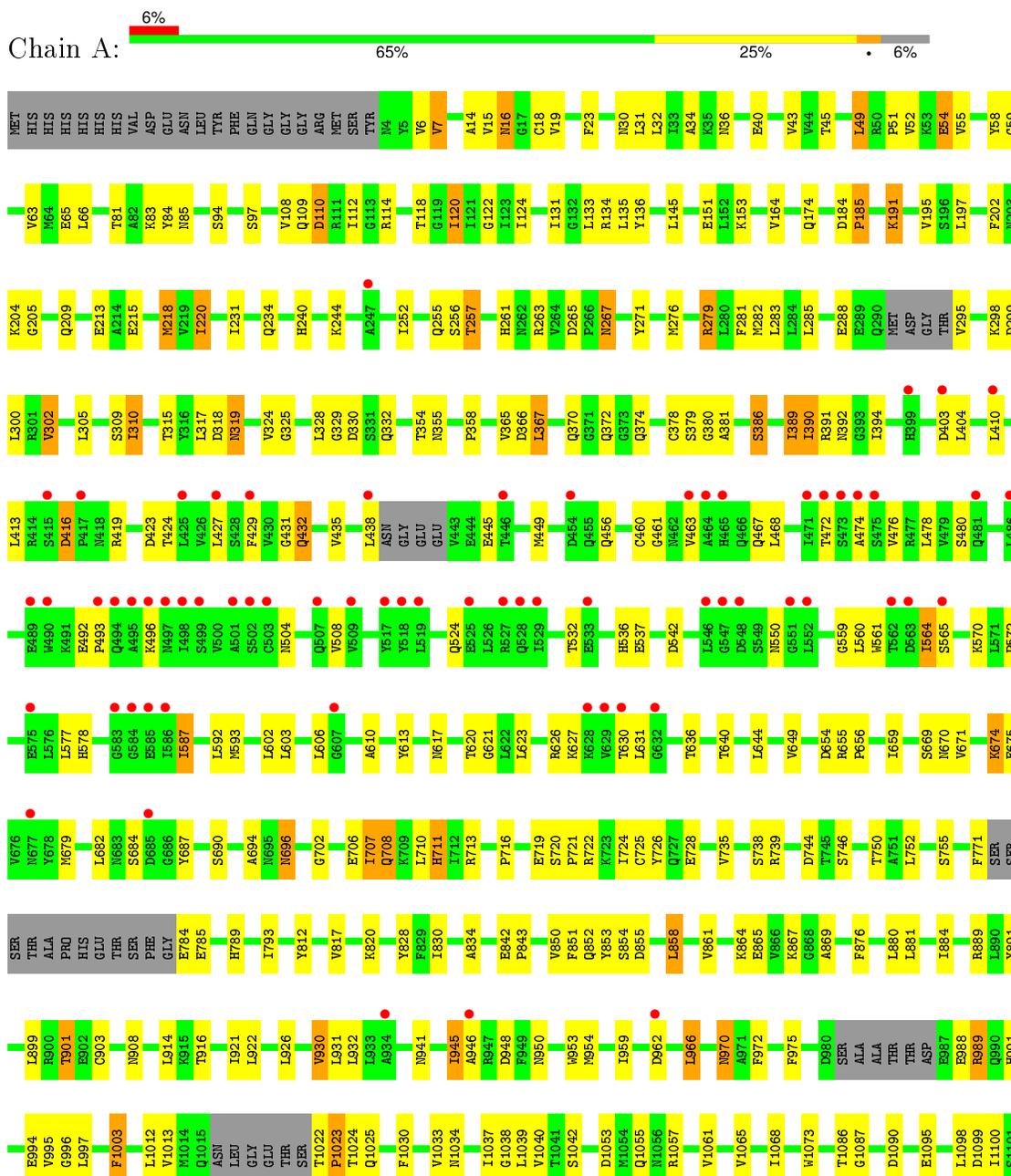
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	J	13	255	124	41	78	12	0	0	0

### 3 Residue-property plots

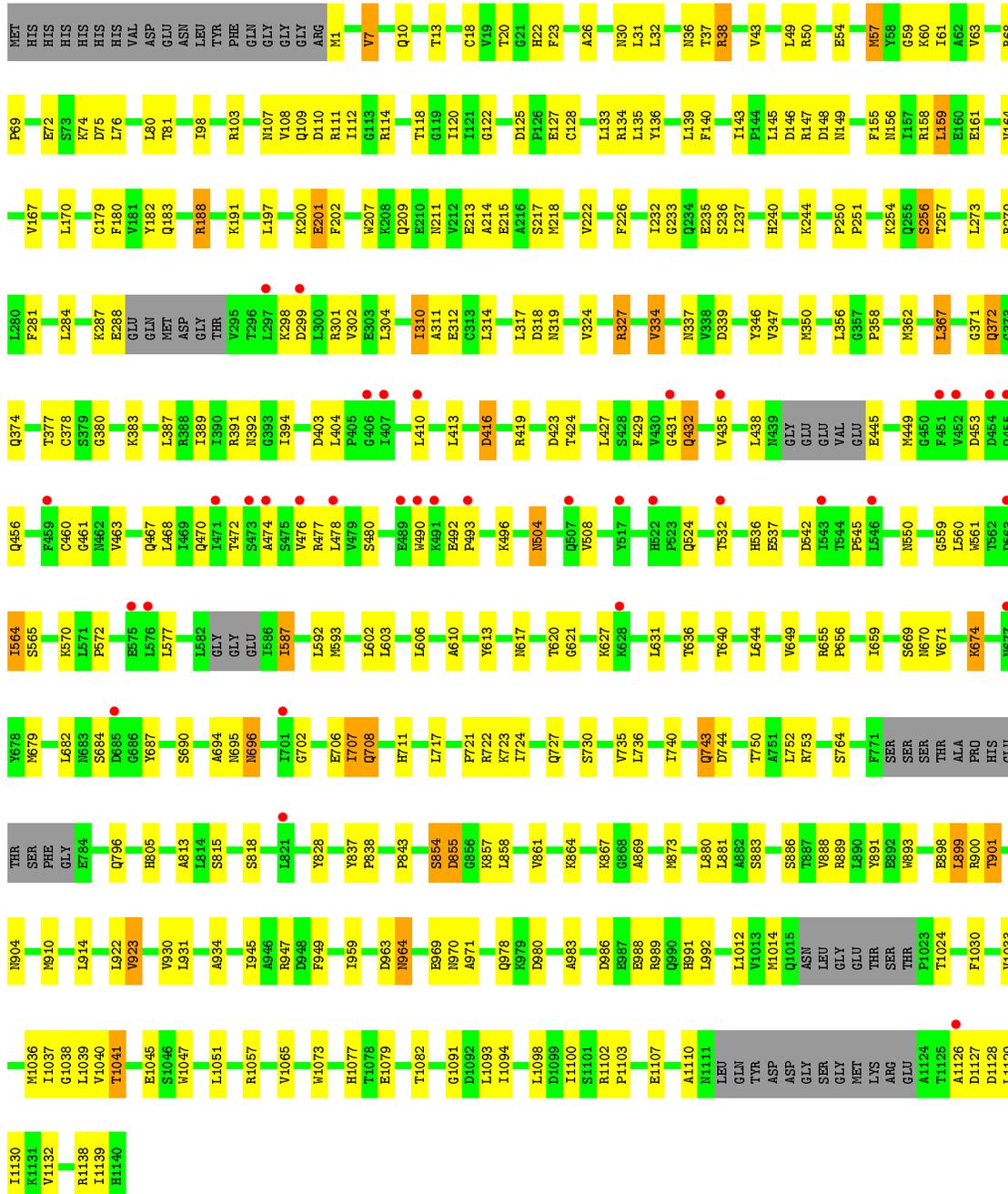
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: DNA DAMAGE-BINDING PROTEIN 1



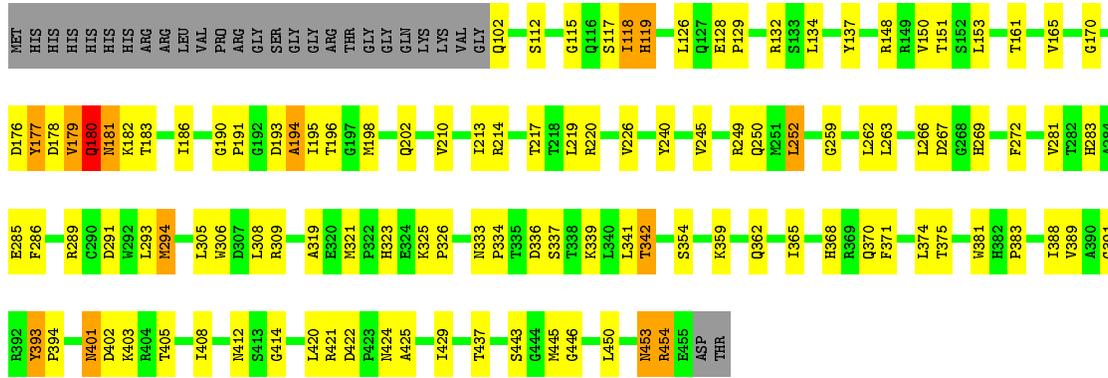


• Molecule 1: DNA DAMAGE-BINDING PROTEIN 1

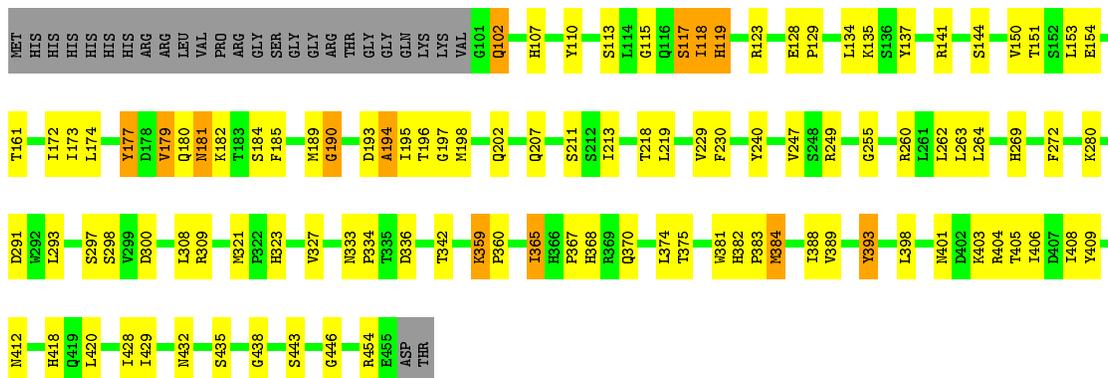


• Molecule 2: DNA DAMAGE-BINDING PROTEIN 2





• Molecule 2: DNA DAMAGE-BINDING PROTEIN 2



• Molecule 3: 5'-D(\*DGP\*GP\*TP\*GP\*AP\*AP\*AP\*(TTD)P\*AP\*GP\*CP\*AP\*GP\*DGP)-3'



• Molecule 3: 5'-D(\*DGP\*GP\*TP\*GP\*AP\*AP\*AP\*(TTD)P\*AP\*GP\*CP\*AP\*GP\*DGP)-3'



• Molecule 4: 5'-D(\*CP\*CP\*TP\*GP\*CP\*TP\*CP\*CP\*TP\*TP\*TP\*CP\*AP\*CP\*CP\*C)-3'



• Molecule 4: 5'-D(\*CP\*CP\*TP\*GP\*CP\*TP\*CP\*CP\*TP\*TP\*TP\*CP\*AP\*CP\*CP\*C)-3'

Chain J:  75% 6% 19%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.10Å 145.90Å 224.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.72 – 3.80 47.72 – 3.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.72-3.80) 99.8 (47.72-3.80)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.34 (at 3.77Å)	Xtrriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.243 , 0.319 0.240 , 0.313	Depositor DCC
$R_{free}$ test set	1862 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	102.6	Xtrriage
Anisotropy	0.090	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 61.8	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Outliers	1 of 37280 reflections (0.003%)	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	23938	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	126.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.23% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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: TTD

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	0.37	0/8697	0.56	0/11777
1	C	0.37	0/8737	0.56	0/11831
2	B	0.37	0/2913	0.57	0/3957
2	D	0.37	0/2917	0.57	0/3962
3	G	0.63	0/306	1.13	2/470 (0.4%)
3	I	0.61	0/281	1.09	0/431
4	H	0.66	0/304	1.35	3/465 (0.6%)
4	J	0.65	0/283	1.17	1/433 (0.2%)
All	All	0.39	0/24438	0.61	6/33326 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	15	DG	P-O3'-C3'	5.89	126.77	119.70
4	J	12	DC	P-O3'-C3'	5.46	126.25	119.70
4	H	11	DT	C4-C5-C7	5.34	122.20	119.00
4	H	11	DT	C6-C5-C7	-5.21	119.77	122.90
4	H	12	DC	P-O3'-C3'	5.16	125.89	119.70

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	A	8543	0	8538	184	0
1	C	8582	0	8588	177	0
2	B	2839	0	2785	63	0
2	D	2843	0	2788	66	0
3	G	312	0	171	8	0
3	I	290	0	160	4	0
4	H	274	0	160	6	0
4	J	255	0	149	0	0
All	All	23938	0	23339	494	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 10.

The worst 5 of 494 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:40:GLU:HG2	1:A:54:GLU:HG3	1.44	0.97
1:A:864:LYS:HG3	1:A:899:LEU:HB2	1.51	0.93
1:A:204:LYS:HG2	1:A:205:GLY:H	1.33	0.91
1:C:391:ARG:HH21	1:C:711:HIS:HD2	1.18	0.90
2:D:102:GLN:HG3	2:D:107:HIS:HB3	1.54	0.89

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	1076/1159 (93%)	960 (89%)	100 (9%)	16 (2%)	<b>13</b> 59
1	C	1081/1159 (93%)	953 (88%)	114 (10%)	14 (1%)	15 <b>61</b>
2	B	352/382 (92%)	307 (87%)	36 (10%)	9 (3%)	<b>7</b> 48
2	D	353/382 (92%)	318 (90%)	30 (8%)	5 (1%)	14 <b>59</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2862/3082 (93%)	2538 (89%)	280 (10%)	44 (2%)	13	59

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	118	ILE
2	B	183	THR
2	B	194	ALA
1	C	707	ILE
1	C	855	ASP

### 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	957/1015 (94%)	873 (91%)	84 (9%)	12	50
1	C	962/1015 (95%)	870 (90%)	92 (10%)	10	46
2	B	313/335 (93%)	278 (89%)	35 (11%)	7	38
2	D	313/335 (93%)	284 (91%)	29 (9%)	11	47
All	All	2545/2700 (94%)	2305 (91%)	240 (9%)	11	47

5 of 240 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	365	ILE
1	C	159	LEU
2	D	202	GLN
2	B	389	VAL
1	C	13	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	370	GLN
1	C	183	GLN
2	D	202	GLN
2	B	401	ASN
2	B	419	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

2 non-standard protein/DNA/RNA residues 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	TTD	G	9	3	40,45,46	1.63	7 (17%)	58,74,77	2.26	16 (27%)
3	TTD	I	9	3	40,45,46	1.55	7 (17%)	58,74,77	2.16	14 (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
3	TTD	G	9	3	-	0/22/109/110	0/3/6/6
3	TTD	I	9	3	-	0/22/109/110	0/3/6/6

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	9	TTD	C2T-N1T	2.26	1.41	1.36
3	G	9	TTD	C6T-N1T	2.29	1.50	1.46
3	I	9	TTD	O4'-C1'	2.37	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	9	TTD	C2T-N1T	2.64	1.42	1.36
3	I	9	TTD	C6T-N1T	2.80	1.51	1.46

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	9	TTD	O4-C4-C5	-3.87	119.76	122.92
3	I	9	TTD	O4-C4-C5	-3.53	120.04	122.92
3	I	9	TTD	O4T-C4T-C5T	-3.42	120.13	122.92
3	I	9	TTD	C4'-O4R-C1R	-3.33	101.04	109.46
3	G	9	TTD	C4-N3-C2	-3.26	120.97	126.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	9	TTD	5	0
3	I	9	TTD	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1090/1159 (94%)	0.15	68 (6%) 24 14	68, 109, 228, 265	0
1	C	1095/1159 (94%)	0.05	36 (3%) 50 34	70, 106, 215, 247	0
2	B	354/382 (92%)	-0.26	0 100 100	77, 98, 133, 144	0
2	D	355/382 (92%)	-0.19	0 100 100	74, 103, 147, 175	0
3	G	13/15 (86%)	-0.53	0 100 100	128, 164, 217, 229	0
3	I	12/15 (80%)	-0.31	0 100 100	167, 206, 232, 286	0
4	H	14/16 (87%)	-0.19	0 100 100	131, 154, 223, 232	0
4	J	13/16 (81%)	0.35	0 100 100	196, 230, 337, 374	0
All	All	2946/3144 (93%)	0.02	104 (3%) 48 32	68, 106, 219, 374	0

The worst 5 of 104 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	583	GLY	6.3
1	A	584	GLY	6.3
1	A	497	ASN	4.9
1	A	548	ASP	4.8
1	A	547	GLY	4.5

### 6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	TTD	G	9	40/41	0.89	0.23	-	128,141,161,167	0
3	TTD	I	9	40/41	0.83	0.28	-	164,193,226,236	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.