



wwPDB X-ray Structure Validation Summary Report i

Feb 26, 2014 – 07:35 PM GMT

PDB ID : 2VYF
Title : CRYSTAL STRUCTURE OF THE DNAC
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Deposited on : 2008-07-23
Resolution : 3.60 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

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

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

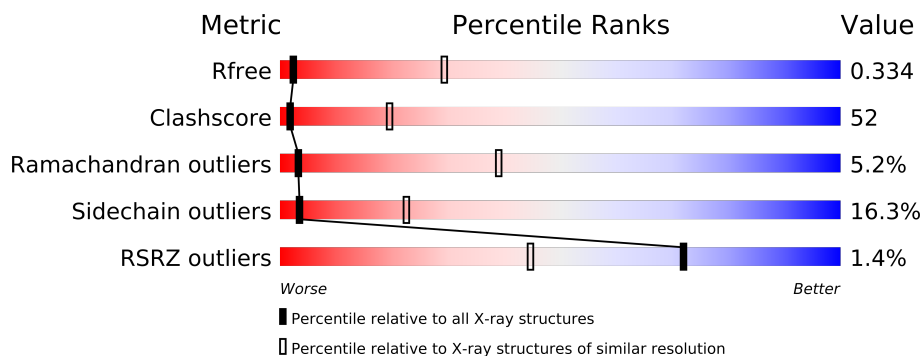
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.60 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}	66092	1020 (3.86-3.34)
Clashscore	79885	1155 (3.80-3.40)
Ramachandran outliers	78287	1109 (3.80-3.40)
Sidechain outliers	78261	1108 (3.80-3.40)
RSRZ outliers	66119	1000 (3.84-3.36)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	454	
1	B	454	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5946 atoms, of which 0 are hydrogen and 0 are deuterium.

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 REPLICATIVE DNA HELICASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	0	4
			3062	1912	539	599	12			
1	B	377	Total	C	N	O	S	0	0	6
			2880	1798	506	564	12			

- Molecule 2 is GOLD ION (three-letter code: AU) (formula: Au).

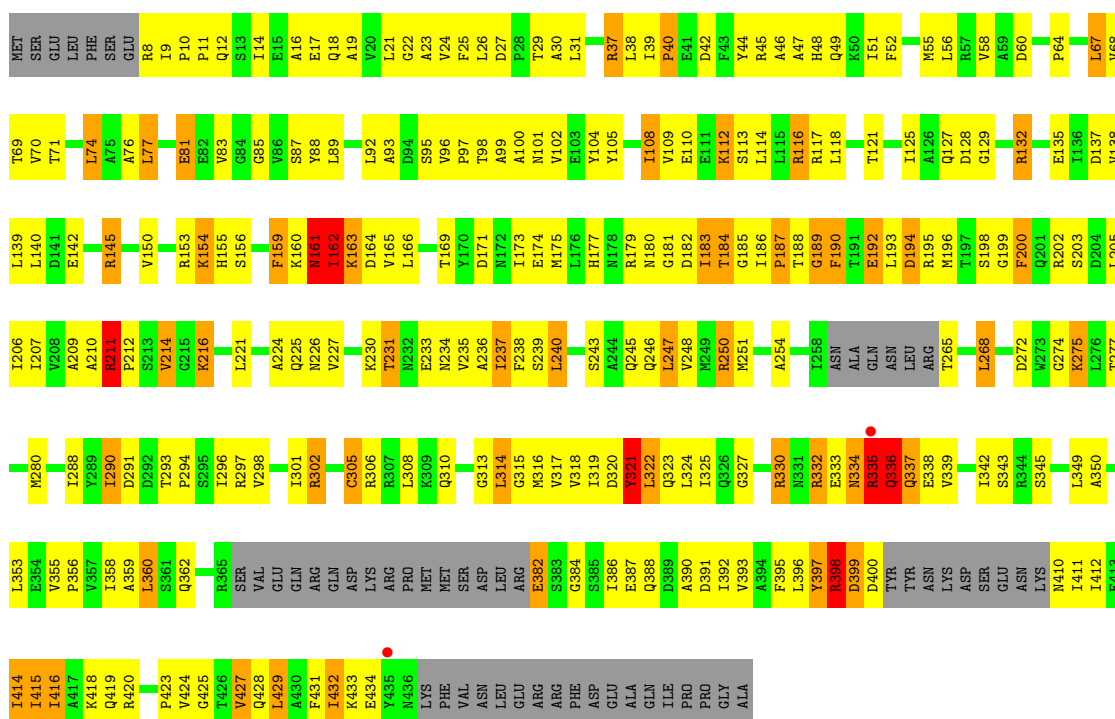
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Au	0	0
			2	2		
2	A	2	Total	Au	0	0
			2	2		

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.

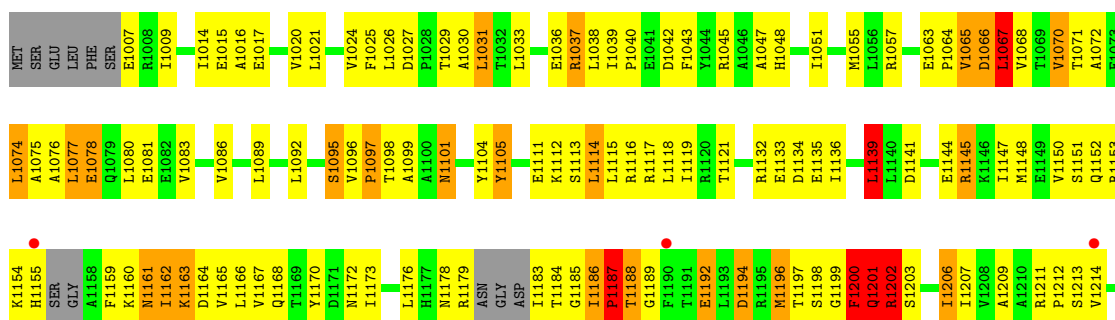
• Molecule 1: REPLICATIVE DNA HELICASE

Chain A:



• Molecule 1: REPLICATIVE DNA HELICASE

Chain B:



VAL	GLN	SER	R1365	GLN	LEU	VAL	S1295	T1217
	ALA	VAL	R1297		L1221			
	PHE	GLU	S1298		N1222			
	ILE	GLN	S1299		I1223			
	LYS	ARG	D1300		A1224			
	GLU	GLN	I1301		Q1225			
	TYR	ASP	R1302		N1226			
	ASN	LYS	A1303		V1227			
	ASN	ARG	K1304		A1228			
	LYS	PRO	C1305		T1229			
PHE	MET	R1306	K1230					
VAL	MET	R1307	T1231					
ASN	SER	L1308	N1232					
LEU	ASP	K1309	E1233					
GLU	LEU	ARG	N1234					
ARG	ARG	E1382	G1313	GLN	LEU	V1235	H1294	
PHE	ARG		L1314		V1236	I1237		
ASP	ASP	I1386	G1315		A1236			
GLU	GLU	E1387	M1316		F1238			
ALA	ALA	Q1388	V1318		S1239			
GLN	GLN	D1389	I1319		L1240			
ILE	ILE	A1390	D1320		M1242			
PRO	PRO	D1391	Y1321		S1243			
PRO	PRO	I1392	L1322		A1244			
GLY	GLY	V1393	GLN		Q1245			
ALA	ALA	A1394	LEU	Q1246				
GLN	LEU	F1395	L1247	V1248				
	LYS	L1396	GLN	V1248				
	ASP	L1397	GLY					
	ARG	ARG	SER	M1251				
	ASP	ASP	GLY	L1252				
	TYR	TYR	R1332	C1253				
	ASN	ASN	E1333					
	LYS	LYS	N1334	N1257				
	ASP	ASP		I1258				
	SER	SER		N1259				
GLU	GLU	E1341	A1260					
ASN	ASN	I1342	Q1261					
LYS	LYS	S1343	N1262					
ASN	ASN	R1344	L1263					
ASN	ASN		R1264					
ASN	ASN		T1265					
ASN	ASN	K1347	G1266					
ASP	ASP	I1412	F1267					
ALA	ALA	E1413	L1268					
GLN	GLN	I1414	T1269					
ILE	ILE	I1415	E1270					
GLN	GLN	I1416	P1271					
TYR	TYR	A1417	V1355					
ASN	ASN	K1418	P1356					
GLN	GLN	Q1419	V1357					
ALA	ALA	R1420	I1358					
GLN	GLN	M1421	A1359					
GLN	GLN	G1422	L1360					
GLN	GLN	P1423	S1361					
GLN	GLN	V1424	Q1362					
GLN	GLN	G1425	L1363					
GLN	GLN	T1426	S1364					

4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	176.97Å 176.97Å 108.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.87 – 3.60 24.87 – 3.59	Depositor EDS
% Data completeness (in resolution range)	(Not available) (24.87-3.60) 91.9 (24.87-3.59)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 3.64Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.293 , 0.324 0.308 , 0.334	Depositor DCC
R_{free} test set	1637 reflections (8.51%)	DCC
Wilson B-factor (Å ²)	142.8	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 91.8	EDS
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 22531 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5946	wwPDB-VP
Average B, all atoms (Å ²)	167.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AU

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	0.40	0/3096	0.77	3/4184 (0.1%)
1	B	0.43	0/2908	0.95	18/3930 (0.5%)
All	All	0.42	0/6004	0.86	21/8114 (0.3%)

There are no bond length outliers.

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1297	ARG	N-CA-C	9.29	136.08	111.00
1	B	1260	ALA	N-CA-C	9.18	135.79	111.00
1	A	162	ILE	CG1-CB-CG2	-8.29	93.16	111.40
1	B	1411	ILE	N-CA-C	8.28	133.36	111.00
1	B	1419	GLN	N-CA-C	7.66	131.68	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3062	0	3098	343	2
1	B	2880	0	2922	299	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	0	0	0	0
2	B	2	0	0	0	0
All	All	5946	0	6020	621	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 52.

The worst 5 of 621 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:211:ARG:HD3	1:A:212:PRO:CD	1.49	1.41
1:A:297:ARG:HH22	1:B:1154:LYS:N	1.15	1.39
1:A:145:ARG:NH2	1:A:145:ARG:HB3	1.35	1.37
1:B:1145:ARG:NH2	1:B:1145:ARG:HB2	1.41	1.34
1:A:297:ARG:NH2	1:B:1154:LYS:H	1.24	1.33

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	Distance(Å)	Clash(Å)
1:A:154:LYS:O	1:B:1307:ARG:NH1[2_655]	1.77	0.43
1:A:87:SER:OG	1:B:1163:LYS:NZ[4_665]	1.89	0.31

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	390/454 (86%)	319 (82%)	54 (14%)	17 (4%)	4	45
1	B	365/454 (80%)	305 (84%)	38 (10%)	22 (6%)	2	34
All	All	755/908 (83%)	624 (83%)	92 (12%)	39 (5%)	3	39

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	PRO

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Mol	Chain	Res	Type
1	A	161	ASN
1	A	190	PHE
1	A	192	GLU
1	A	211	ARG

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	A	332/388 (86%)	274 (82%)	58 (18%)	3	18
1	B	313/388 (81%)	266 (85%)	47 (15%)	4	27
All	All	645/776 (83%)	540 (84%)	105 (16%)	3	22

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	360	LEU
1	B	1031	LEU
1	B	1341	GLU
1	A	362	GLN
1	A	414	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1101	ASN
1	B	1201	GLN
1	B	1419	GLN
1	B	1127	GLN
1	B	1152	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

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	398/454 (87%)	0.04	2 (0%)	88 71	112, 165, 187, 187	0
1	B	377/454 (83%)	0.09	9 (2%)	56 32	96, 175, 187, 187	0
All	All	775/908 (85%)	0.06	11 (1%)	72 45	96, 171, 187, 187	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1265	THR	3.8
1	A	435	TYR	2.6
1	B	1322	LEU	2.6
1	B	1155	HIS	2.5
1	B	1268	LEU	2.5

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	AU	B	2426	1/1	0.12	-1.92	186,186,186,186	0
2	AU	A	1436	1/1	0.03	-3.43	186,186,186,186	0
2	AU	B	2427	1/1	0.07	-4.45	186,186,186,186	0
2	AU	A	1437	1/1	0.09	-9.68	186,186,186,186	0

6.5 Other polymers

There are no such residues in this entry.