

wwPDB X-ray Structure Validation Summary Report (i)

Jan 29, 2024 - 07:11 PM EST

PDB ID 1F0O: Title PVUII ENDONUCLEASE/COGNATE DNA COMPLEX (GLUTARALDEH : YDE-CROSSLINKED CRYSTAL) AT PH 7.5 WITH TWO CALCIUM IONS AT EACH ACTIVE SITE Authors Horton, J.R.; Cheng, X. : Deposited on 2000-05-16 Resolution 2.50 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:

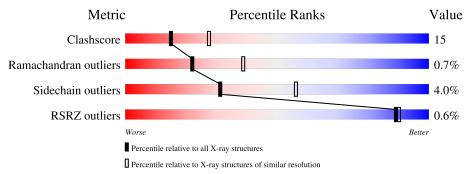
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.50 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	$5346 \ (2.50-2.50)$
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 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% 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	С	13	31%	69%			
1	D	13	8% 54%	46%			
2	А	157	62%	330	% • •		
2	В	157	.% • 7.	%	24% ••		



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3154 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(*TP*GP*AP*CP*CP*AP*GP*CP*TP*GP*GP*T P*C-3').

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	С	13	Total	С	Ν	Ο	Р	0	0	0
	U	10	263	126	48	77	12	0	0	0
1	Л	13	Total	С	Ν	Ο	Р	0	0	0
	D	15	248	117	45	74	12	0	0	0

• Molecule 2 is a protein called TYPE II RESTRICTION ENZYME PVUII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	Δ	154	Total	С	Ν	0	\mathbf{S}	0	0	0
	Л	104	1226	796	202	226	2	0	0	0
9	В	152	Total	С	Ν	0	S	0	0	0
2	D	152	1223	798	201	222	2	0	0	0

• Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

[Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
	3	А	2	Total Ca 2 2	0	0
	3	В	2	Total Ca 2 2	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	С	23	TotalO2323	0	0
4	D	20	TotalO2020	0	0
4	А	89	Total O 89 89	0	0

Continued on next page...



Continued from previous page...

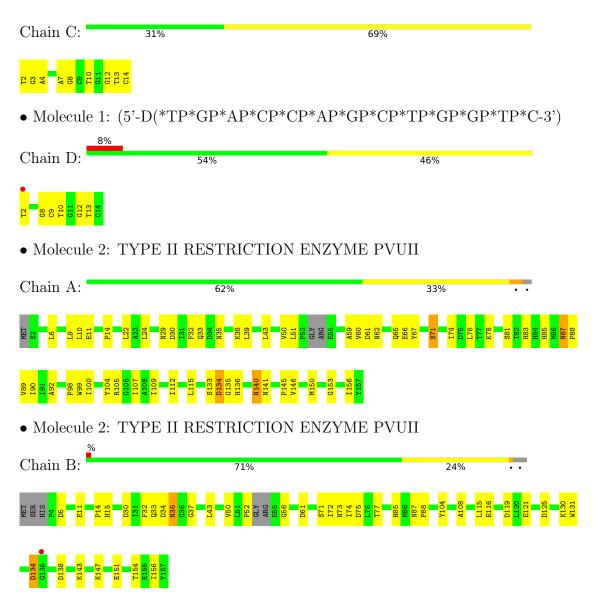
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	58	Total O 58 58	0	0



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 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: (5'-D(*TP*GP*AP*CP*CP*AP*GP*CP*TP*GP*GP*TP*C-3')





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	94.04Å 84.70Å 45.99Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 - 2.50	Depositor
Resolution (A)	22.19 - 2.50	EDS
% Data completeness	96.0 (30.00-2.50)	Depositor
(in resolution range)	96.1 (22.19-2.50)	EDS
R _{merge}	0.06	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.08 (at 2.50 \text{\AA})$	Xtriage
Refinement program	X-PLOR 3.851	Depositor
B B.	0.205 , 0.279	Depositor
R, R_{free}	0.191 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor $(Å^2)$	37.4	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.36 , 74.8	EDS
L-test for twinning ²	$ \langle L \rangle = 0.48, \langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3154	wwPDB-VP
Average B, all atoms $(Å^2)$	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.07% of the height of the origin peak. No significant pseudotranslation is detected.

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.



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: CA

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).

Mal	Mol Chain		lengths	Bond angles		
	lol l'hoin		# Z > 5	RMSZ	# Z > 5	
1	С	0.76	0/294	0.83	0/452	
1	D	0.88	0/277	0.93	0/427	
2	А	0.53	0/1260	0.72	1/1719~(0.1%)	
2	В	0.54	0/1258	0.72	0/1714	
All	All	0.60	0/3089	0.76	1/4312~(0.0%)	

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	С	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	105	ARG	N-CA-C	-5.54	96.04	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	С	8	DG	Sidechain
1	D	2	DT	Sidechain



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	С	263	0	148	11	0
1	D	248	0	136	4	0
2	А	1226	0	1157	49	0
2	В	1223	0	1167	33	0
3	А	2	0	0	0	0
3	В	2	0	0	0	0
4	А	89	0	0	2	0
4	В	58	0	0	5	0
4	С	23	0	0	1	0
4	D	20	0	0	0	0
All	All	3154	0	2608	84	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 15.

The worst 5 of 84 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)
2:A:60:VAL:HG12	2:A:66:GLU:HG2	1.37	1.05
2:B:43:LEU:HD11	2:B:50:VAL:HG13	1.49	0.94
2:B:130:LYS:O	2:B:134:ASP:HB2	1.70	0.90
1:C:7:DA:H62	2:A:140:ASN:HD21	1.28	0.82
1:D:10:DT:OP1	2:A:71:SER:HB2	1.81	0.81

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	А	150/157~(96%)	143~(95%)	6 (4%)	1 (1%)	22	39
2	В	148/157~(94%)	142 (96%)	5(3%)	1 (1%)	22	39
All	All	298/314~(95%)	285 (96%)	11 (4%)	2 (1%)	22	39

analysed, and the total number of residues.

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	В	56	GLY
2	А	134	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	Percentile	
2	А	126/139~(91%)	120~(95%)	6~(5%)	25 48	
2	В	126/139~(91%)	122 (97%)	4 (3%)	39 65	
All	All	252/278~(91%)	242 (96%)	10 (4%)	31 56	

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	В	116	GLU
2	В	125	ASP
2	В	134	ASP
2	А	134	ASP
2	А	136	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
2	В	15	HIS
2	В	35	ASN

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type
2	В	96	GLN
2	А	57	ASN
2	А	62	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 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.

No monomer is involved in short contacts.

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^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q < 0.9
1	\mathbf{C}	13/13~(100%)	-0.24	0 100 100	16, 29, 59, 60	0
1	D	13/13~(100%)	-0.17	1 (7%) 13 13	16, 28, 70, 86	0
2	А	154/157~(98%)	-0.38	0 100 100	11, 25, 41, 52	0
2	В	152/157~(96%)	-0.20	1 (0%) 87 89	12, 29, 41, 52	0
All	All	332/340~(97%)	-0.28	2 (0%) 89 90	11, 27, 46, 86	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2	DT	2.9
2	В	135	GLY	2.4

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (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. The B-factors column lists the minimum, median, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
3	CA	А	701	1/1	0.81	0.12	$51,\!51,\!51,\!51$	0
3	CA	В	761	1/1	0.91	0.10	45,45,45,45	0
3	CA	В	725	1/1	0.92	0.07	49,49,49,49	0
3	CA	А	784	1/1	0.95	0.14	76,76,76,76	0

6.5 Other polymers (i)

There are no such residues in this entry.

