



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 06:50 AM UTC

PDB ID : 2INY / pdb\_00002iny  
Title : Nanoporous Crystals of Chicken Embryo Lethal Orphan (CELO) Adenovirus  
Major Coat Protein, Hexon  
Authors : Xu, L.; Benson, S.D.; Burnett, R.M.  
Deposited on : 2006-10-09  
Resolution : 3.90 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

<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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

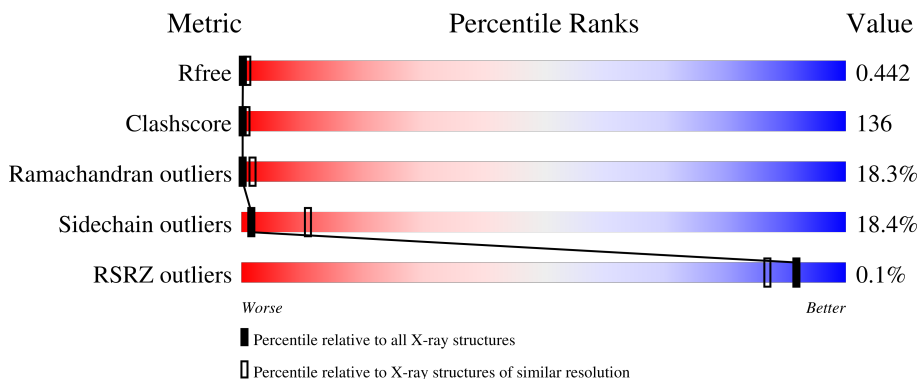
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.90 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))
$R_{free}$	180053	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	942	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7523 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.

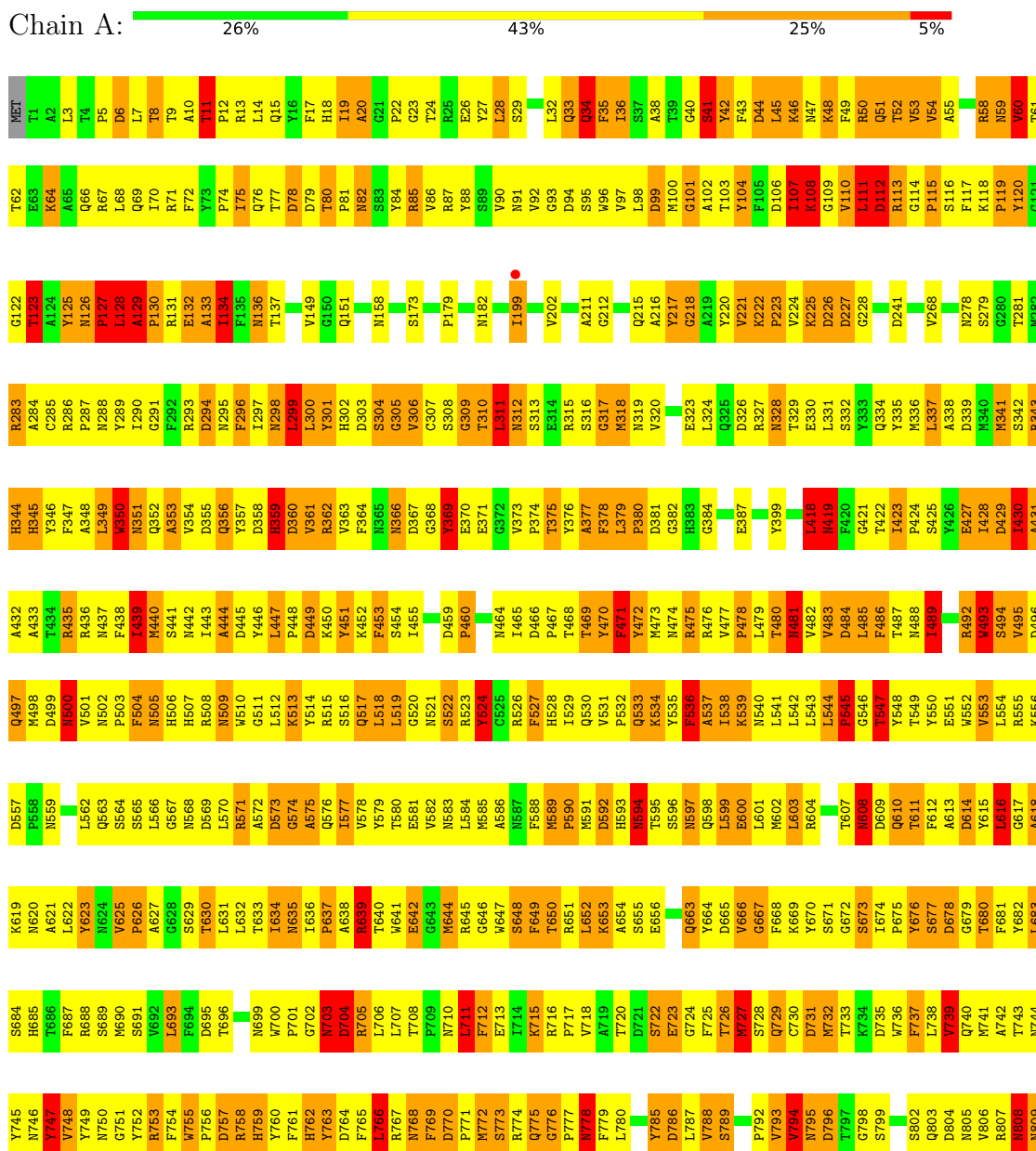
- Molecule 1 is a protein called Hexon protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	941	7523	4764	1281	1444	34	1667	0	0

### 3 Residue-property plots

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: Hexon protein



S810	D877	Y941	S810
G811	L878		G811
F812	Q879		F812
I813	Q880		I813
A814	P881		A814
P815	M882		P815
	M883		
W818	Y884		W818
P819	T885		P819
W820	N886		W820
W821	N887		W821
T822	S888		T822
A823	H889		A823
Q824	S890		Q824
Q825	M891		Q825
G826	V892		G826
E827	I893		E827
A828	N894		A828
W829	F895		W829
	E896		
W833	L897		W833
P834	D898		P834
Y835	P899		Y835
P836	M900		P836
L837	D901		L837
I838	E902		I838
G839	N903		G839
N840	T904		N840
D841	Y905		D841
A842	V906		A842
I843	Y907		I843
S844	M908		S844
S845	L909		S845
N846	Y910		N846
Q847	G911		Q847
T848	V912		T848
	F913		
K853	D914		K853
F854	T915		F854
L855	V916		L855
C856	R917		C856
D857	V918		D857
N858	N919		N858
Y859	Q920		Y859
L860	P921		L860
W861	E922		W861
T862	R923		T862
V863	N924		V863
P864	V925		P864
F865	L926		F865
S866	A927		S866
S867	M928		S867
D868	A929		D868
F869	Y930		F869
	F931		
M872	R932		M872
G875	T933		G875
E874	P934		E874
L875	F935		L875
T876	A936		T876

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	157.77Å 157.77Å 114.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.06 – 3.90 47.06 – 3.90	Depositor EDS
% Data completeness (in resolution range)	92.3 (47.06-3.90) 92.3 (47.06-3.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.20	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.86 (at 3.88Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.372 , 0.416 0.350 , 0.442	Depositor DCC
$R_{free}$ test set	731 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.5	Xtrriage
Anisotropy	0.113	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 577.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.046 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.75	EDS
Total number of atoms	7523	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.79	7/7728 (0.1%)	1.22	97/10545 (0.9%)

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	A	0	2

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	847	GLN	CB-CG	30.75	2.44	1.52
1	A	524	TYR	CD2-CE2	14.10	1.80	1.38
1	A	524	TYR	CD1-CE1	12.00	1.74	1.38
1	A	524	TYR	CE2-CZ	10.35	1.63	1.38
1	A	524	TYR	CE1-CZ	9.44	1.60	1.38

The worst 5 of 97 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	500	ASN	N-CA-C	11.06	126.32	113.15
1	A	847	GLN	CA-CB-CG	10.51	135.12	114.10
1	A	367	ASP	N-CA-C	-10.43	100.22	113.16
1	A	439	ILE	N-CA-C	-10.33	100.80	110.82
1	A	876	THR	N-CA-C	9.93	125.90	110.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	301	TYR	Sidechain
1	A	747	TYR	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	A	7523	0	7147	1549	12
All	All	7523	0	7147	1549	12

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 136.

The worst 5 of 1549 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:524:TYR:CE2	1:A:524:TYR:CD2	1.80	1.65
1:A:524:TYR:CE1	1:A:524:TYR:CD1	1.74	1.64
1:A:376:TYR:HE2	1:A:427:GLU:HG2	1.08	1.18
1:A:433:ALA:HA	1:A:436:ARG:NH1	1.58	1.17
1:A:433:ALA:CA	1:A:436:ARG:HH12	1.57	1.16

The worst 5 of 12 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	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:ASN:ND2	1:A:635:ASN:ND2[6_555]	1.53	0.67
1:A:524:TYR:CE2	1:A:847:GLN:CG[3_455]	1.85	0.35
1:A:524:TYR:CZ	1:A:847:GLN:CG[3_455]	1.89	0.31
1:A:524:TYR:CD1	1:A:847:GLN:CB[3_455]	2.00	0.20
1:A:524:TYR:CD2	1:A:847:GLN:CB[3_455]	2.01	0.19

## 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	939/942 (100%)	508 (54%)	259 (28%)	172 (18%)	<b>0</b> <b>2</b>

5 of 172 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	ASP
1	A	11	THR
1	A	34	GLN
1	A	42	TYR
1	A	48	LYS

### 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	821/822 (100%)	670 (82%)	151 (18%)	<b>1</b> <b>11</b>

5 of 151 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	731	ASP
1	A	881	ASN
1	A	758	ARG
1	A	820	VAL
1	A	926	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	505	ASN
1	A	858	ASN
1	A	563	GLN
1	A	894	ASN
1	A	740	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](#)

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	719/942 (76%)	-0.62	1 (0%) <b>92</b> <b>87</b>	4, 30, 30, 30	4 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	199	ILE	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 oligosaccharides 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.