



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:24 AM UTC

PDB ID : 9Z55 / pdb\_00009z55  
Title : Isoreticular co-crystal 1 with asymmetrical expanded duplex (31mer) containing insert sequence CATGAGTCAT  
Authors : Shields, E.T.; Slaughter, C.K.; Magna, E.N.; Snow, C.D.  
Deposited on : 2025-11-11  
Resolution : 3.94 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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
Xtriage (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



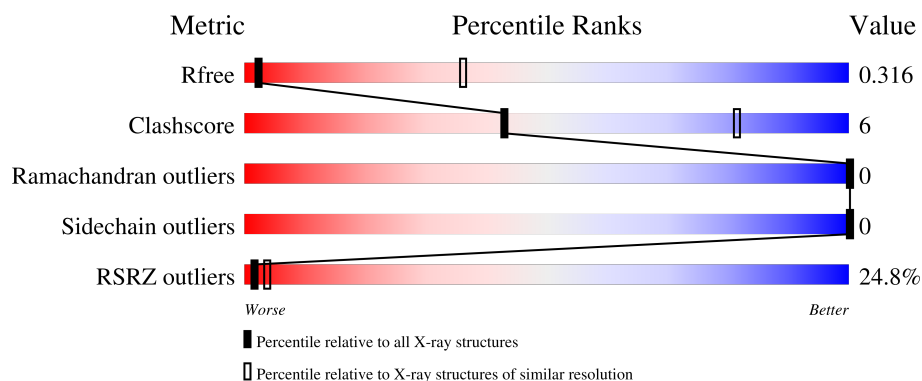
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.94 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	1022 (4.12-3.76)
Clashscore	190562	1000 (4.10-3.78)
Ramachandran outliers	187476	1009 (4.12-3.76)
Sidechain outliers	187428	1002 (4.12-3.76)
RSRZ outliers	180081	1022 (4.12-3.76)

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	31	<div> <div>3%</div> <div>48%</div> <div>52%</div> </div>
2	B	31	<div> <div>45%</div> <div>55%</div> </div>
3	C	263	<div> <div>26%</div> <div>78%</div> <div>•</div> <div>18%</div> </div>



## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2862 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 DNA (31-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	31	Total	C	N	O	P	0	0	0
			631	301	113	186	31			

- Molecule 2 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	31	Total	C	N	O	P	0	0	0
			640	304	119	186	31			

- Molecule 3 is a protein called Replication initiation protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	216	Total	C	N	O	S	0	3	0
			1591	998	282	306	5			

There are 13 discrepancies between the modelled and reference sequences:

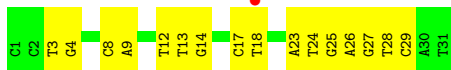
Chain	Residue	Modelled	Actual	Comment	Reference
C	-11	MET	-	initiating methionine	UNP P03856
C	-10	ARG	-	expression tag	UNP P03856
C	-9	GLY	-	expression tag	UNP P03856
C	-8	SER	-	expression tag	UNP P03856
C	-7	HIS	-	expression tag	UNP P03856
C	-6	HIS	-	expression tag	UNP P03856
C	-5	HIS	-	expression tag	UNP P03856
C	-4	HIS	-	expression tag	UNP P03856
C	-3	HIS	-	expression tag	UNP P03856
C	-2	HIS	-	expression tag	UNP P03856
C	-1	GLY	-	expression tag	UNP P03856
C	0	SER	-	expression tag	UNP P03856
C	118	PRO	ARG	conflict	UNP P03856



### 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.

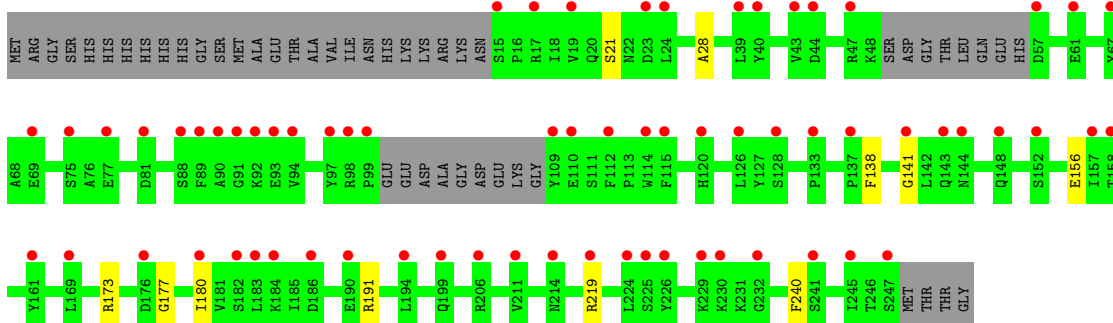
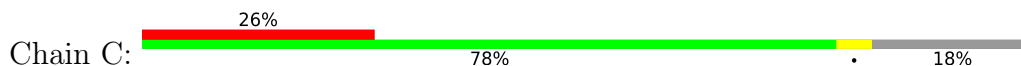
- Molecule 1: DNA (31-MER)



- Molecule 2: DNA (31-MER)



- Molecule 3: Replication initiation protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.48Å 129.88Å 73.32Å 90.00° 118.58° 90.00°	Depositor
Resolution (Å)	64.94 – 3.94 64.94 – 3.94	Depositor EDS
% Data completeness (in resolution range)	98.9 (64.94-3.94) 98.8 (64.94-3.94)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 3.89Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.297 , 0.316 0.297 , 0.316	Depositor DCC
$R_{free}$ test set	1066 reflections (6.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	189.6	Xtriage
Anisotropy	0.608	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 346.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.019 for k+l,h+l,-l 0.011 for -k+l,-h-l,-l 0.030 for -h-2*l,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	2862	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	299.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.40% 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	0.32	0/706	0.55	0/1086
2	B	0.33	0/718	0.56	0/1107
3	C	0.14	0/1630	0.43	0/2220
All	All	0.25	0/3054	0.49	0/4413

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	A	631	0	350	11	0
2	B	640	0	350	14	0
3	C	1591	0	1425	6	0
All	All	2862	0	2125	31	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 6.

All (31) 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:B:29:DG:H2''	2:B:30:DC:H5'	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:DT:H2'	1:A:14:DG:C8	2.27	0.69
1:A:28:DT:H2''	1:A:29:DC:C5	2.35	0.61
2:B:27:DG:H2'	2:B:28:DG:H8	1.67	0.59
1:A:23:DA:H2''	1:A:24:DT:C6	2.38	0.59
2:B:14:DT:H4'	2:B:15:DG:OP1	2.05	0.56
2:B:30:DC:H2''	2:B:31:DA:N7	2.23	0.54
2:B:27:DG:H2'	2:B:28:DG:C8	2.41	0.54
3:C:180:ILE:HA	3:C:240:PHE:O	2.08	0.53
3:C:28:ALA:HA	3:C:191:ARG:O	2.08	0.52
2:B:31:DA:H1'	2:B:32:DA:H5'	1.92	0.51
2:B:18:DT:H2''	2:B:19:DC:H5'	1.93	0.50
1:A:3:DT:H2'	1:A:4:DG:C8	2.48	0.49
2:B:14:DT:H2''	2:B:15:DG:C8	2.48	0.48
2:B:40:DC:H2''	2:B:41:DA:H8	1.79	0.47
1:A:26:DA:H2''	1:A:27:DG:C8	2.49	0.46
1:A:12:DT:H2''	1:A:13:DT:H72	1.97	0.46
3:C:21:SER:HB3	3:C:138:PHE:O	2.15	0.45
2:B:29:DG:H2'	2:B:30:DC:C6	2.50	0.45
1:A:27:DG:H1'	1:A:28:DT:H5'	1.98	0.45
2:B:20:DA:H2''	2:B:21:DT:C5	2.51	0.45
2:B:26:DA:H2''	2:B:27:DG:H8	1.81	0.45
3:C:173:ARG:HD2	3:C:177:GLY:HA2	1.97	0.45
2:B:12:DG:H2''	2:B:13:DA:C8	2.52	0.45
2:B:12:DG:H2''	2:B:13:DA:H8	1.84	0.43
1:A:8:DC:H2''	1:A:9:DA:H8	1.83	0.42
1:A:23:DA:H2''	1:A:24:DT:C5	2.54	0.42
3:C:156:GLU:O	3:C:219[B]:ARG:HD3	2.21	0.41
3:C:21:SER:HB2	3:C:141:GLY:HA3	2.02	0.40
1:A:17:DC:H1'	1:A:18:DT:H5'	2.04	0.40
1:A:24:DT:H1'	1:A:25:DG:C8	2.56	0.40

There are no symmetry-related clashes.

## 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	
3	C	213/263 (81%)	205 (96%)	8 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	C	152/236 (64%)	152 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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

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, 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	31/31 (100%)	0.84	1 (3%) 50 36	203, 319, 442, 488	0
2	B	31/31 (100%)	0.68	0 100 100	210, 333, 400, 483	0
3	C	216/263 (82%)	1.55	68 (31%) 1 2	150, 264, 390, 509	3 (1%)
All	All	278/325 (85%)	1.37	69 (24%) 2 4	150, 276, 428, 509	3 (1%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	99	PRO	6.7
3	C	98	ARG	6.1
3	C	57	ASP	5.7
3	C	109	TYR	4.7
3	C	81	ASP	4.4
3	C	39	LEU	4.4
3	C	144	ASN	4.1
3	C	232	GLY	4.0
3	C	114	TRP	3.8
3	C	229	LYS	3.7
3	C	247	SER	3.7
3	C	199	GLN	3.7
3	C	23	ASP	3.6
3	C	19	VAL	3.5
3	C	148	GLN	3.5
3	C	224	LEU	3.4
3	C	211	VAL	3.3
3	C	69[A]	GLU	3.3
3	C	245	ILE	3.3
3	C	214	ASN	3.3
3	C	194	LEU	3.0
3	C	157	ILE	3.0
3	C	180	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
3	C	89	PHE	2.9
3	C	137	PRO	2.9
3	C	97	TYR	2.9
3	C	47	ARG	2.9
3	C	91	GLY	2.8
3	C	226	TYR	2.8
3	C	43	VAL	2.7
3	C	128	SER	2.7
3	C	230	LYS	2.7
3	C	61[A]	GLU	2.7
3	C	44	ASP	2.7
3	C	115	PHE	2.6
3	C	75	SER	2.6
3	C	152	SER	2.6
3	C	67	TYR	2.5
3	C	92	LYS	2.5
3	C	88	SER	2.5
3	C	186	ASP	2.5
3	C	126	LEU	2.5
3	C	15	SER	2.5
3	C	219[A]	ARG	2.4
3	C	133	PRO	2.4
3	C	158	THR	2.4
3	C	40	TYR	2.4
3	C	24	LEU	2.4
3	C	176	ASP	2.4
3	C	206	ARG	2.4
3	C	120	HIS	2.3
3	C	141	GLY	2.3
3	C	90	ALA	2.3
3	C	17	ARG	2.3
3	C	183	LEU	2.3
3	C	225	SER	2.2
1	A	18	DT	2.2
3	C	241	SER	2.2
3	C	161	TYR	2.1
3	C	112	PHE	2.1
3	C	169	LEU	2.1
3	C	94	VAL	2.1
3	C	93	GLU	2.1
3	C	182	SER	2.0
3	C	143	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
3	C	77	GLU	2.0
3	C	190	GLU	2.0
3	C	184	LYS	2.0
3	C	110	GLU	2.0

## 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.