



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 09:30 PM UTC

PDB ID : 9YZQ / pdb_00009yzq
Title : Isoreticular co-crystal 1 with asymmetrical expanded duplex (31mer) containing insert sequence TGATGAGCAG and loaded with Engrailed homeodomain enhanced Green fluorescent protein fusion
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Deposited on : 2025-10-30
Resolution : 3.75 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 ⓘ 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 ⓘ](#)) 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

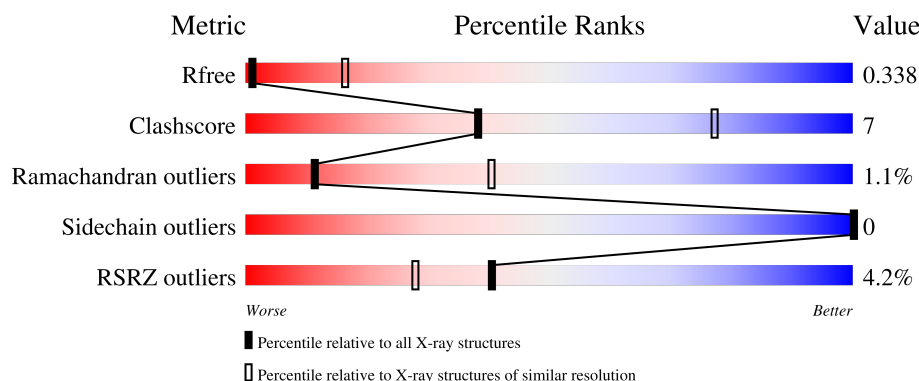
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.75 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	1029 (3.90-3.62)
Clashscore	190562	1061 (3.90-3.62)
Ramachandran outliers	187476	1014 (3.90-3.62)
Sidechain outliers	187428	1009 (3.90-3.62)
RSRZ outliers	180081	1028 (3.90-3.62)

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 $\leq 5\%$. 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	 45% 55%
2	B	31	 58% 42%
3	C	263	 5% 73% 8% 18%
4	D	313	 16% 82%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3198 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
			633	302	115	185	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
			638	304	116	187	31			

- Molecule 3 is a protein called Replication initiation protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	215	Total	C	N	O	S	0	1	0
			1614	1014	285	309	6			

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

- Molecule 4 is a protein called Segmentation polarity homeobox protein engrailed, Green fluorescent protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	57	Total	C	N	O	0	0	0
			311	187	60	64			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	initiating methionine	UNP P02836
D	61	THR	-	linker	UNP P02836
D	62	SER	-	linker	UNP P02836
D	63	GLN	-	linker	UNP P02836
D	64	PHE	-	linker	UNP P02836
D	65	TYR	-	linker	UNP P02836
D	66	LEU	-	linker	UNP P02836
D	67	ASN	-	linker	UNP P02836
D	68	GLU	-	linker	UNP P02836
D	70	VAL	-	insertion	UNP P42212
D	133	LEU	PHE	conflict	UNP P42212
D	134	THR	SER	conflict	UNP P42212
D	300	LEU	HIS	conflict	UNP P42212
D	308	HIS	-	expression tag	UNP P42212
D	309	HIS	-	expression tag	UNP P42212
D	310	HIS	-	expression tag	UNP P42212
D	311	HIS	-	expression tag	UNP P42212
D	312	HIS	-	expression tag	UNP P42212
D	313	HIS	-	expression tag	UNP P42212

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

ALA	ASP	GLN	LYS	ASN	GLY	ILE	LYS	VAL	ASN	PHE	LYS	ILE	ARG	HIS	ASN	ILE	GLY	ASP	GLY	SER	VAL	GLN	LEU	ALA	ASP	HIS	TYR	GLN	ASN	THR	PRO	ILE	GLY	ASP	GLY	PRO	VAL	LEU	LEU	PRO	ASP	ASN	HIS	TYR	LEU	SER	THR	GLN	SER	ALA	LEU	SER	LYS	ASP	PRO	ASN	GLU			
LYS	ARG	ASP	HIS	MET	VAL	LEU	LEU	GLU	PHE	VAL	THR	ALA	ALA	GLY	ILE	THR	LEU	GLY	MET	ASP	GLU	LEU	TYR	LYS	HIS	HIS	HIS	HIS	HIS	HIS	GLN	ASN	THR	PRO	ILE	GLY	ASP	GLY	PRO	VAL	LEU	LEU	PRO	ASP	ASN	HIS	TYR	LEU	SER	THR	GLN	SER	ALA	LEU	SER	LYS	ASP	PRO	ASN	GLU

4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	74.12Å 122.40Å 140.44Å 90.00° 90.38° 90.00°	Depositor
Resolution (Å)	46.92 – 3.75 46.92 – 3.75	Depositor EDS
% Data completeness (in resolution range)	97.7 (46.92-3.75) 97.6 (46.92-3.75)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.295 , 0.338 0.295 , 0.338	Depositor DCC
R_{free} test set	1267 reflections (9.77%)	wwPDB-VP
Wilson B-factor (Å ²)	135.0	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 160.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.099 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3198	wwPDB-VP
Average B, all atoms (Å ²)	221.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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: MG

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	0.35	0/709	0.51	0/1091
2	B	0.49	0/715	0.75	0/1102
3	C	0.32	0/1650	0.59	0/2241
4	D	0.49	0/312	0.72	0/432
All	All	0.38	0/3386	0.63	0/4866

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	633	0	350	12	0
2	B	638	0	351	8	0
3	C	1614	0	1450	14	0
4	D	311	0	174	2	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
All	All	3198	0	2325	36	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 7.

The worst 5 of 36 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)
3:C:185:ILE:HG21	3:C:201:MET:HE1	1.64	0.80
4:D:59:LYS:O	4:D:60:SER:CB	2.34	0.75
1:A:10:DA:H2''	1:A:11:DA:H5''	1.79	0.65
1:A:3:DT:H2'	1:A:4:DG:C8	2.36	0.60
3:C:35:GLN:HG3	3:C:85:ALA:HB1	1.85	0.59

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	
3	C	208/263 (79%)	203 (98%)	4 (2%)	1 (0%)	24	56
4	D	55/313 (18%)	51 (93%)	2 (4%)	2 (4%)	2	21
All	All	263/576 (46%)	254 (97%)	6 (2%)	3 (1%)	11	40

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	143	GLN
4	D	6	ARG
4	D	9	PHE

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	158/236 (67%)	158 (100%)	0	100	100
4	D	9/278 (3%)	9 (100%)	0	100	100
All	All	167/514 (32%)	167 (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 ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 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 ⓘ

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 [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, 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	31/31 (100%)	-0.26	0	100 100	215, 233, 312, 328	0
2	B	31/31 (100%)	-0.21	0	100 100	192, 239, 326, 402	0
3	C	215/263 (81%)	0.03	12 (5%)	30 22	87, 179, 282, 413	1 (0%)
4	D	57/313 (18%)	0.03	2 (3%)	47 32	131, 256, 433, 572	0
All	All	334/638 (52%)	-0.02	14 (4%)	40 28	87, 211, 326, 572	1 (0%)

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	45	GLN	7.7
3	C	63	HIS	5.2
3	C	76	ALA	5.2
3	C	62	ILE	4.1
3	C	65	ALA	3.7

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](#)

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, 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	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MG	A	101	1/1	0.94	0.06	69,69,69,69	0
5	MG	C	301	1/1	0.97	0.03	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.