



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 2, 2026 – 01:58 AM UTC

PDB ID : 7E1B / pdb_00007e1b
Title : Crystal structure of VbrR-DNA complex
Authors : Hong, S.; Zhang, X.; Zhang, P.
Deposited on : 2021-02-01
Resolution : 4.59 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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
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

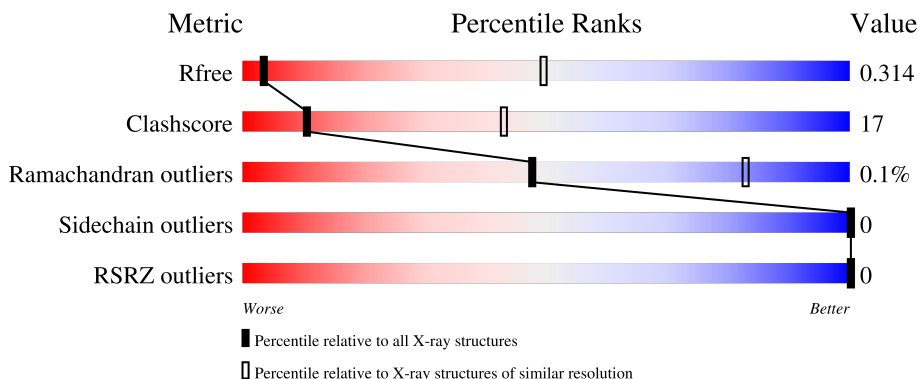
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.59 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.






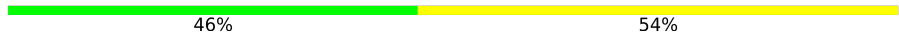
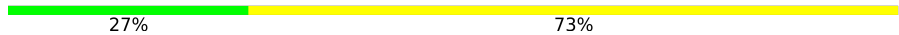


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1003 (5.22-3.92)
Clashscore	190562	1019 (5.22-3.94)
Ramachandran outliers	187476	1068 (5.26-3.90)
Sidechain outliers	187428	1050 (5.26-3.90)
RSRZ outliers	180081	1139 (5.26-3.90)

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	220	62% (green), 32% (yellow), 5% (grey)
1	B	220	60% (green), 32% (yellow), 5% (grey)
1	C	220	57% (green), 38% (yellow), 5% (grey)
1	D	220	58% (green), 36% (yellow), 5% (grey)
1	E	220	62% (green), 32% (yellow), 5% (grey)

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Mol	Chain	Length	Quality of chain
1	F	220	
1	G	220	
1	H	220	
2	I	26	
2	Y	26	
3	J	26	
3	Z	26	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15460 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 DNA-binding response regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	209	Total 1668	C 1064	N 288	O 313	S 3	0	0	0
1	B	208	Total 1664	C 1062	N 287	O 311	S 4	0	0	0
1	C	209	Total 1668	C 1064	N 288	O 313	S 3	0	0	0
1	D	208	Total 1664	C 1062	N 287	O 311	S 4	0	0	0
1	E	209	Total 1671	C 1066	N 288	O 313	S 4	0	0	0
1	F	208	Total 1661	C 1060	N 287	O 311	S 3	0	0	0
1	G	209	Total 1671	C 1066	N 288	O 313	S 4	0	0	0
1	H	208	Total 1661	C 1060	N 287	O 311	S 3	0	0	0

- Molecule 2 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	Y	26	Total 523	C 253	N 83	O 161	P 26	0	0	0
2	I	26	Total 523	C 253	N 83	O 161	P 26	0	0	0

- Molecule 3 is a DNA chain called DNA (26-MER).

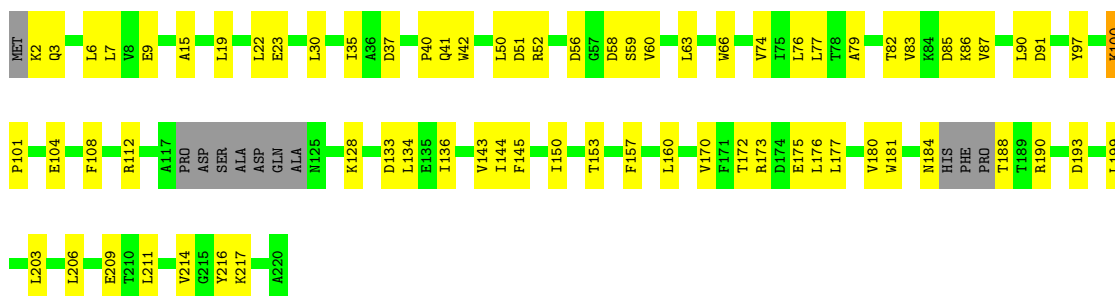
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	Z	26	Total 543	C 258	N 108	O 151	P 26	0	0	0
3	J	26	Total 543	C 258	N 108	O 151	P 26	0	0	0

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.

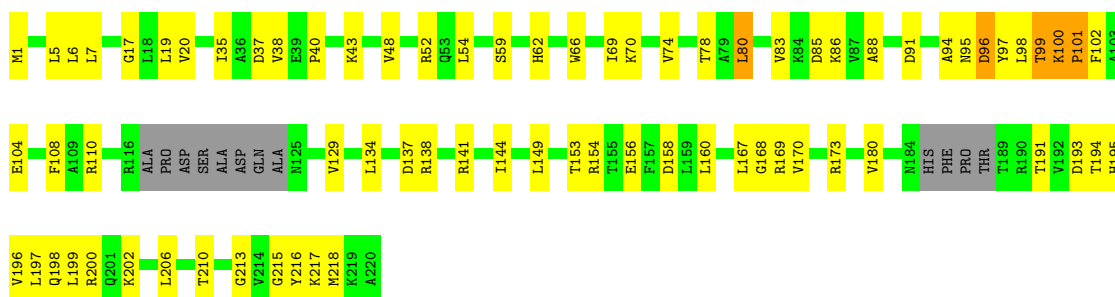
- Molecule 1: DNA-binding response regulator

Chain A: 



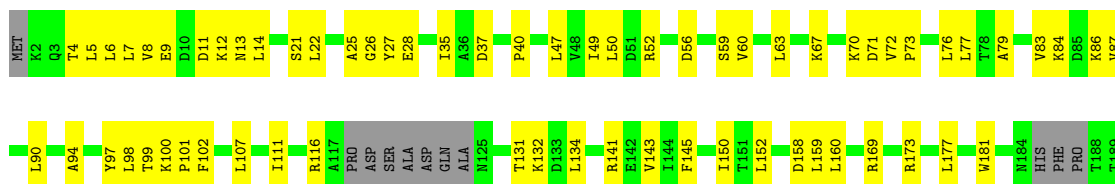
- Molecule 1: DNA-binding response regulator

Chain B: 



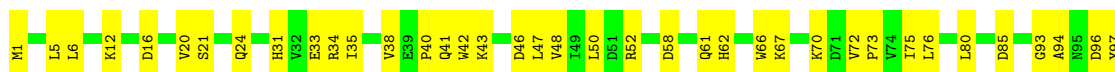
- Molecule 1: DNA-binding response regulator

Chain C: 

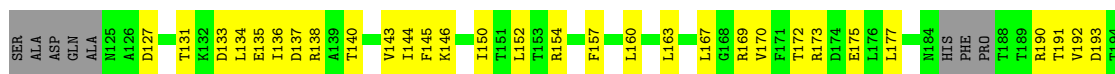
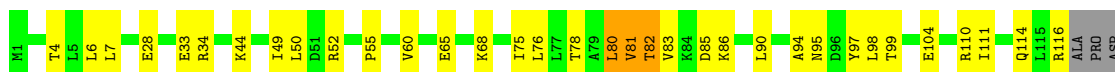




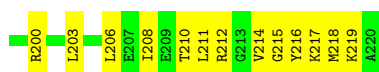
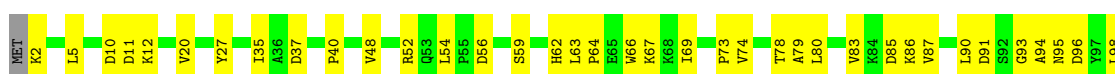
- Molecule 1: DNA-binding response regulator



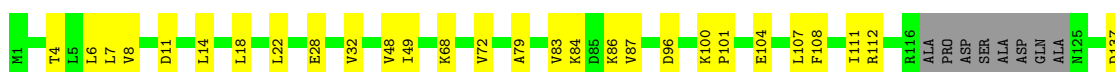
- Molecule 1: DNA-binding response regulator

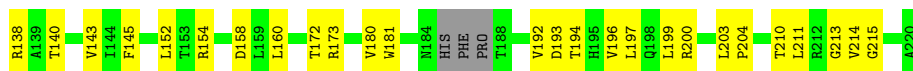


- Molecule 1: DNA-binding response regulator



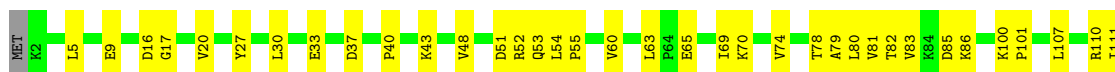
- Molecule 1: DNA-binding response regulator





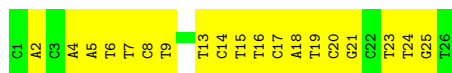
- Molecule 1: DNA-binding response regulator

Chain H: 65% 30% 5%



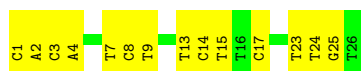
- Molecule 2: DNA (26-MER)

Chain Y: 27% 73%



- Molecule 2: DNA (26-MER)

Chain I: 46% 54%



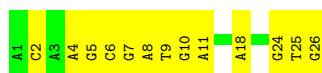
- Molecule 3: DNA (26-MER)

Chain Z: 54% 46%



- Molecule 3: DNA (26-MER)

Chain J: 50% 50%



4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	329.94Å 114.06Å 114.04Å 90.00° 110.02° 90.00°	Depositor
Resolution (Å)	46.01 – 4.59 46.01 – 4.59	Depositor EDS
% Data completeness (in resolution range)	71.1 (46.01-4.59) 65.4 (46.01-4.59)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 4.64Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.265 , 0.321 0.263 , 0.314	Depositor DCC
R_{free} test set	1597 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å ²)	78.2	Xtrriage
Anisotropy	0.259	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 207.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.389 for -h-k-l,l,k 0.398 for -h+k-l,-l,-k 0.408 for -h-2*l,-k,l	Xtrriage
Reported twinning fraction	0.450 for -h-k-l,l,k	Depositor
Outliers	0 of 15997 reflections	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15460	wwPDB-VP
Average B, all atoms (Å ²)	140.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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](#)

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	0.15	0/1691	0.46	1/2287 (0.0%)
1	B	0.35	0/1687	0.62	4/2280 (0.2%)
1	C	0.13	0/1691	0.34	0/2287
1	D	0.23	0/1687	0.51	2/2280 (0.1%)
1	E	0.19	0/1694	0.52	4/2290 (0.2%)
1	F	0.15	0/1684	0.44	2/2277 (0.1%)
1	G	0.13	0/1694	0.36	0/2290
1	H	0.14	0/1684	0.40	1/2277 (0.0%)
2	I	0.19	0/582	0.38	0/894
2	Y	0.18	0/582	0.38	0/894
3	J	0.21	0/612	0.38	0/944
3	Z	0.18	0/612	0.33	0/944
All	All	0.20	0/15900	0.45	14/21944 (0.1%)

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	1

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	99	THR	N-CA-C	8.07	120.64	108.46
1	E	82	THR	N-CA-C	-7.88	95.66	109.06
1	E	80	LEU	N-CA-C	-7.01	95.65	107.99
1	E	82	THR	N-CA-CB	6.88	123.44	111.13
1	B	101	PRO	CA-N-CD	-6.56	102.82	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	91	ASP	Peptide

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	1668	0	1718	64	0
1	B	1664	0	1718	89	0
1	C	1668	0	1718	63	0
1	D	1664	0	1718	61	1
1	E	1671	0	1725	60	0
1	F	1661	0	1711	63	0
1	G	1671	0	1725	41	0
1	H	1661	0	1711	54	0
2	I	523	0	298	19	0
2	Y	523	0	298	20	0
3	J	543	0	293	16	1
3	Z	543	0	293	22	0
All	All	15460	0	14926	493	1

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 17.

The worst 5 of 493 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:B:78:THR:HG23	1:B:80:LEU:HD22	1.18	1.08
1:B:78:THR:HG23	1:B:80:LEU:CD2	1.84	1.06
1:F:98:LEU:HD23	1:F:99:THR:H	1.23	0.99
1:H:100:LYS:HG3	1:H:101:PRO:HD3	1.48	0.96
1:D:191:THR:HG1	3:Z:26:DG:H8	0.92	0.89

All (1) 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:D:212:ARG:NH2	3:J:8:DA:O3'[1_566]	2.08	0.12

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	203/220 (92%)	189 (93%)	14 (7%)	0	100	100
1	B	202/220 (92%)	190 (94%)	10 (5%)	2 (1%)	12	47
1	C	203/220 (92%)	189 (93%)	14 (7%)	0	100	100
1	D	202/220 (92%)	185 (92%)	17 (8%)	0	100	100
1	E	203/220 (92%)	190 (94%)	13 (6%)	0	100	100
1	F	202/220 (92%)	180 (89%)	22 (11%)	0	100	100
1	G	203/220 (92%)	189 (93%)	14 (7%)	0	100	100
1	H	202/220 (92%)	183 (91%)	19 (9%)	0	100	100
All	All	1620/1760 (92%)	1495 (92%)	123 (8%)	2 (0%)	48	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	100	LYS
1	B	96	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	Percentiles	
1	A	182/191 (95%)	182 (100%)	0	100	100
1	B	182/191 (95%)	182 (100%)	0	100	100
1	C	182/191 (95%)	182 (100%)	0	100	100
1	D	182/191 (95%)	182 (100%)	0	100	100
1	E	183/191 (96%)	183 (100%)	0	100	100
1	F	181/191 (95%)	181 (100%)	0	100	100
1	G	183/191 (96%)	183 (100%)	0	100	100
1	H	181/191 (95%)	181 (100%)	0	100	100
All	All	1456/1528 (95%)	1456 (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. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	166	ASN
1	G	195	HIS
1	E	114	GLN
1	E	13	ASN
1	E	198	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, 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	209/220 (95%)	-1.11	0 100 100	86, 96, 147, 151	0
1	B	208/220 (94%)	-1.10	0 100 100	84, 98, 137, 139	0
1	C	209/220 (95%)	-1.07	0 100 100	87, 100, 139, 142	0
1	D	208/220 (94%)	-1.05	0 100 100	81, 89, 132, 142	0
1	E	209/220 (95%)	-1.04	0 100 100	162, 168, 173, 174	0
1	F	208/220 (94%)	-1.00	0 100 100	150, 167, 172, 173	0
1	G	209/220 (95%)	-1.00	0 100 100	153, 167, 181, 183	0
1	H	208/220 (94%)	-1.00	0 100 100	147, 164, 168, 171	0
2	I	26/26 (100%)	-0.73	0 100 100	141, 164, 176, 178	0
2	Y	26/26 (100%)	-0.76	0 100 100	135, 140, 155, 161	0
3	J	26/26 (100%)	-0.77	0 100 100	141, 165, 178, 179	0
3	Z	26/26 (100%)	-0.76	0 100 100	135, 143, 159, 160	0
All	All	1772/1864 (95%)	-1.03	0 100 100	81, 149, 174, 183	0

There are no RSRZ outliers to report.

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.