wwPDB X-ray Structure Validation Summary Report (i)

May 3, 2025 – 08:22 AM EDT

PDB ID	:	3VOX / pdb_00003vox
Title	:	X-ray Crystal Structure of Wild Type HrtR in the Apo Form
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Deposited on	:	2012-02-23
Resolution	:	3.10 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 (i)) were used in the production of this report:

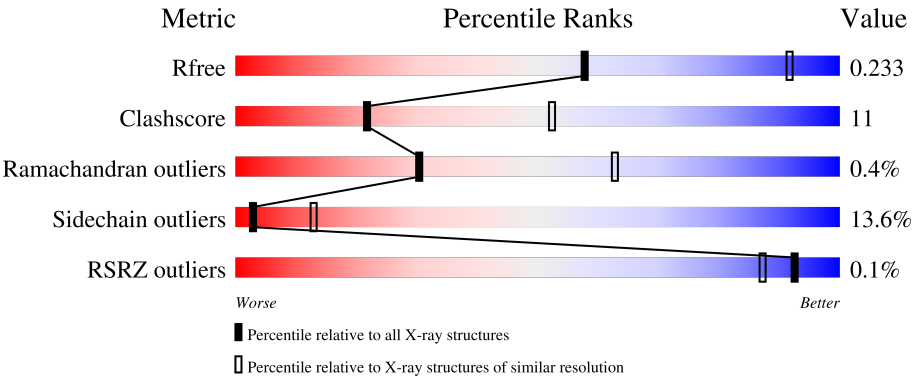
MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	164625	1351 (3.10-3.10)
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (3.10-3.10)

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	A	189	% 58% 29% 9% .
1	B	189	65% 24% 5% 6%
1	C	189	61% 29% . 7%
1	D	189	60% 28% 6% 6%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6136 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 Transcriptional regulator.

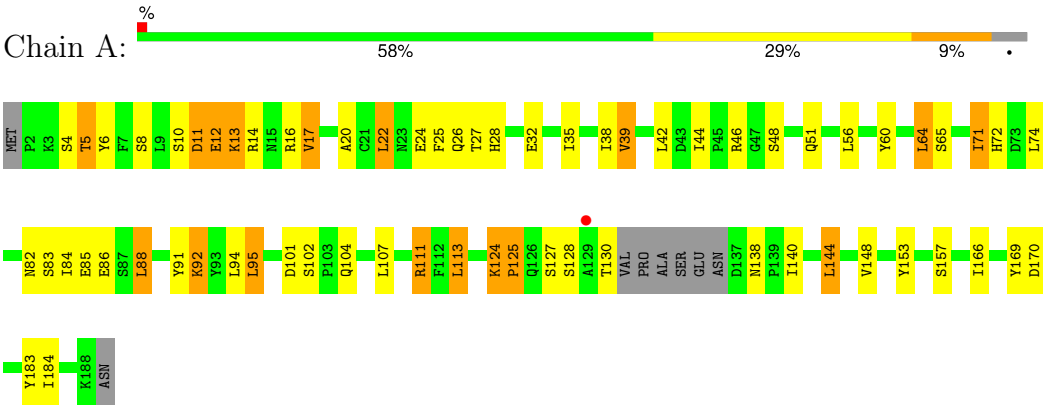
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	0	1	0
			1563	1015	250	296	2			
1	B	177	Total	C	N	O	S	0	1	0
			1530	996	242	290	2			
1	C	175	Total	C	N	O	S	0	0	0
			1510	983	237	288	2			
1	D	177	Total	C	N	O	S	0	1	0
			1533	997	243	291	2			

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.

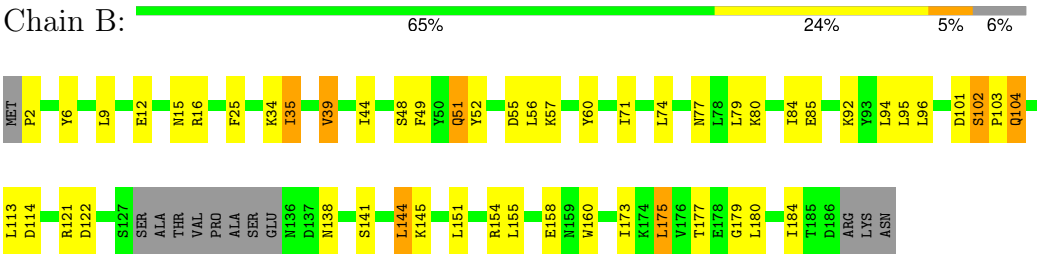
• Molecule 1: Transcriptional regulator

Chain A:



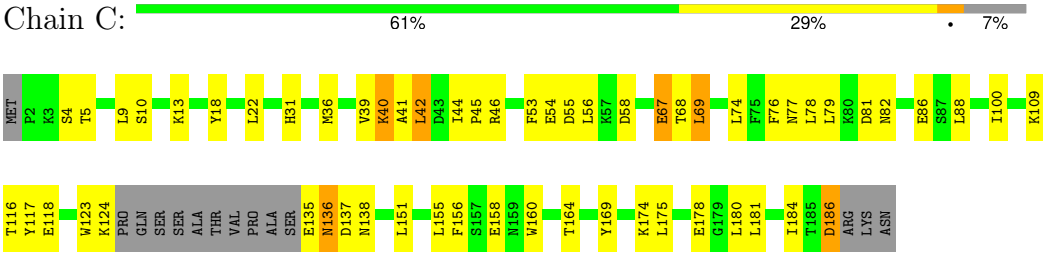
• Molecule 1: Transcriptional regulator

Chain B:



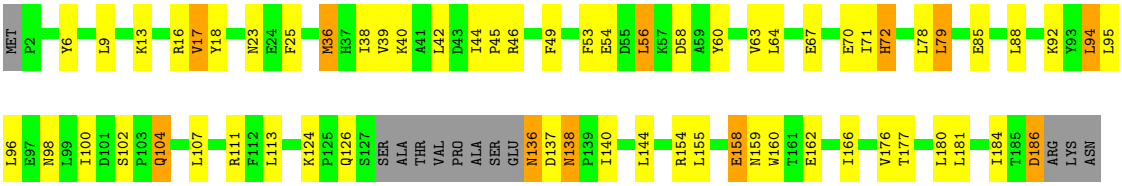
• Molecule 1: Transcriptional regulator

Chain C:



• Molecule 1: Transcriptional regulator

Chain D:


MET P2 Y6 L9 K13 R16 V17 Y18 N23 E24 F25 M36 H37 I38 V39 K40 A41 L42 D43 I44 P45 R46 F49 F53 E54 D55 L56 K57 D58 A59 Y60 V63 L64 E67 E70 I71 H72 L78 L79 E85 L88 K92 Y93 L94 L95
L96 E97 N98 L99 I100 D101 S102 P103 Q104 L107 R111 F112 L113 K124 P125 Q126 S127 SER ALA THR VAL PRO ALA SER GLU N136 D137 N138 P139 I140 L144 R154 L155 E158 N159 W160 T161 E162 I166 V176 T177 L180 L181 I184 T185 D186 ARG LYS ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	90.84Å 190.18Å 152.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 – 3.10 29.90 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.90-3.10) 99.7 (29.90-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	4.38 (at 3.06Å)	Xtriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.184 , 0.241 0.178 , 0.233	Depositor DCC
R_{free} test set	1249 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	79.6	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 78.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6136	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.62	0/1604	0.95	6/2168 (0.3%)
1	B	0.65	0/1574	0.97	4/2129 (0.2%)
1	C	0.51	0/1549	0.88	2/2094 (0.1%)
1	D	0.56	0/1574	0.92	5/2129 (0.2%)
All	All	0.59	0/6301	0.93	17/8520 (0.2%)

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	127	SER	N-CA-C	7.52	119.79	107.23
1	D	49	PHE	N-CA-C	-7.13	103.51	111.28
1	B	114	ASP	N-CA-C	6.30	118.00	110.44
1	C	137	ASP	N-CA-C	-6.17	105.80	113.15
1	A	6	TYR	N-CA-C	-6.15	105.91	113.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1563	0	1511	41	0
1	B	1530	0	1475	30	0
1	C	1510	0	1454	26	0
1	D	1533	0	1474	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6136	0	5914	128	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 11.

The worst 5 of 128 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:D:39:VAL:HG11	1:D:46:ARG:HA	1.61	0.83
1:A:111:ARG:HG2	1:A:111:ARG:HH11	1.47	0.77
1:A:140:ILE:HG23	1:B:180:LEU:HD11	1.72	0.71
1:D:44:ILE:HG12	1:D:45:PRO:HD2	1.72	0.70
1:C:136:ASN:HB3	1:C:138:ASN:H	1.57	0.70

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
1	A	178/189 (94%)	166 (93%)	10 (6%)	2 (1%)	12 39
1	B	174/189 (92%)	162 (93%)	12 (7%)	0	100 100
1	C	171/189 (90%)	166 (97%)	5 (3%)	0	100 100
1	D	174/189 (92%)	166 (95%)	7 (4%)	1 (1%)	22 53
All	All	697/756 (92%)	660 (95%)	34 (5%)	3 (0%)	30 63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	71	ILE

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Mol	Chain	Res	Type
1	A	125	PRO
1	A	11	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	175/181 (97%)	149 (85%)	26 (15%)	2	10
1	B	172/181 (95%)	152 (88%)	20 (12%)	4	18
1	C	169/181 (93%)	146 (86%)	23 (14%)	3	13
1	D	172/181 (95%)	148 (86%)	24 (14%)	3	12
All	All	688/724 (95%)	595 (86%)	93 (14%)	3	13

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	78	LEU
1	D	36	MET
1	C	81	ASP
1	C	136	ASN
1	D	56	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	66	GLN
1	C	159	ASN
1	D	136	ASN
1	D	126	GLN
1	B	142	GLN

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

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^{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	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	181/189 (95%)	-0.65	1 (0%) 85 72	30, 94, 143, 185	1 (0%)
1	B	177/189 (93%)	-0.85	0 100 100	37, 76, 128, 171	1 (0%)
1	C	175/189 (92%)	-0.68	0 100 100	72, 108, 154, 190	0
1	D	177/189 (93%)	-0.60	0 100 100	37, 96, 140, 166	1 (0%)
All	All	710/756 (93%)	-0.69	1 (0%) 92 87	30, 94, 143, 190	3 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	129	ALA	2.6

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides 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.