



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 03:44 AM UTC

PDB ID : 2YED / pdb_00002yed
Title : HSP90 inhibitors and drugs from fragment and virtual screening
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Deposited on : 2011-03-25
Resolution : 2.10 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 ⓘ 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
Mogul : 2022.3.0, CSD as543be (2022)
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

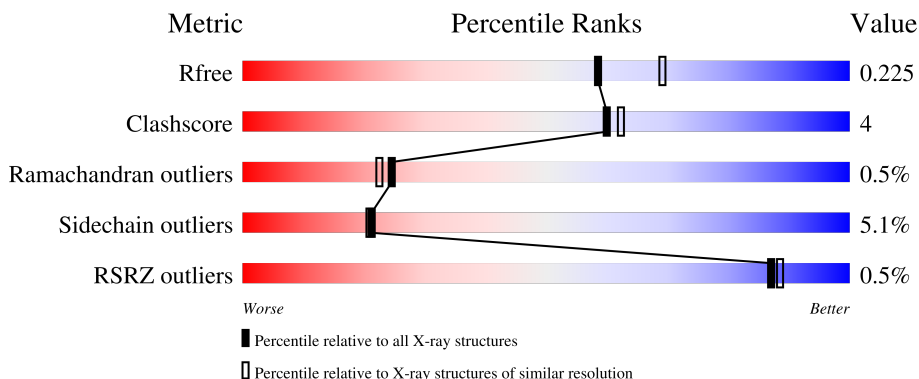
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 $\leq 5\%$. 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	252	 69% 13% 17%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1862 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 HEAT SHOCK PROTEIN HSP 90-ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	1
			1632	1036	270	321	5			

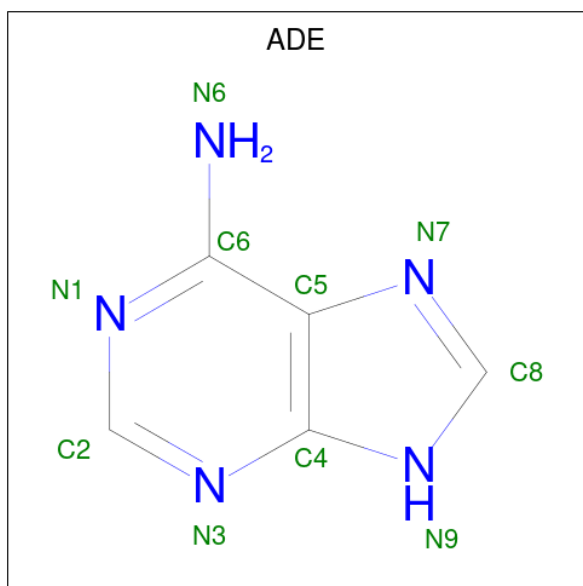
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	expression tag	UNP P07900
A	-14	GLY	-	expression tag	UNP P07900
A	-13	HIS	-	expression tag	UNP P07900
A	-12	HIS	-	expression tag	UNP P07900
A	-11	HIS	-	expression tag	UNP P07900
A	-10	HIS	-	expression tag	UNP P07900
A	-9	HIS	-	expression tag	UNP P07900
A	-8	HIS	-	expression tag	UNP P07900
A	-7	HIS	-	expression tag	UNP P07900
A	-6	HIS	-	expression tag	UNP P07900
A	-5	HIS	-	expression tag	UNP P07900
A	-4	HIS	-	expression tag	UNP P07900
A	-3	SER	-	expression tag	UNP P07900
A	-2	SER	-	expression tag	UNP P07900
A	-1	GLY	-	expression tag	UNP P07900
A	0	HIS	-	expression tag	UNP P07900
A	1	ILE	-	expression tag	UNP P07900
A	2	ASP	-	expression tag	UNP P07900
A	3	ASP	-	expression tag	UNP P07900
A	4	ALA	-	expression tag	UNP P07900
A	5	ASP	-	expression tag	UNP P07900
A	6	LYS	-	expression tag	UNP P07900
A	7	HIS	-	expression tag	UNP P07900
A	8	MET	-	expression tag	UNP P07900

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0

- Molecule 3 is ADENINE (CCD ID: ADE) (formula: $C_5H_5N_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 10 5 5	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	219	Total O 219 219	0	0

• Molecule 1: HEAT SHOCK PROTEIN HSP 90-ALPHA

Q123	A124	G125	V136	E188	Q159	Y160	T174	D175	G177	T176	M180	K185	E200	R201	V207	K208	K209	V222	E223	K224	GLU	ARG	ASP	LYS	GLU	VAL	SER	ASP	ASP	GLU	ALA	GLU							
Met	GLY	HIS	HIS	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	ILE	ASP	ALA	ASP	LVS	ASP	GLN	GLY	ASP	GLU	GLU	E16	V17	L32	S39	S50	T65	I81	R87	I96	K100	A101	V105	A111	K112	K116	M119	F120

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	65.33Å 89.19Å 99.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.94 – 2.10 65.94 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (65.94-2.10) 99.7 (65.94-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.206 , 0.258 (Not available) , 0.225	Depositor DCC
R_{free} test set	878 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	1862	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.07% 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: ADE, CL

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	1.28	3/1658 (0.2%)	1.23	7/2237 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	223	GLU	C-N	-5.57	1.25	1.33
1	A	81	ILE	CA-CB	5.56	1.61	1.54
1	A	176	THR	CA-CB	5.27	1.61	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	GLY	N-CA-C	6.38	122.55	114.25
1	A	209	LYS	N-CA-C	6.32	117.83	111.07
1	A	17	VAL	N-CA-C	5.81	116.22	107.80
1	A	105	ASN	CB-CA-C	-5.75	103.17	111.91
1	A	158	GLU	CB-CA-C	-5.57	99.52	111.78

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	1632	0	1630	14	0
2	A	1	0	0	0	0
3	A	10	0	4	0	0
4	A	219	0	0	7	0
All	All	1862	0	1634	14	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 4.

The worst 5 of 14 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:224:LYS:N	4:A:2214:HOH:O	2.23	0.71
1:A:100:LYS:HE2	4:A:2111:HOH:O	1.96	0.64
1:A:32:LEU:C	1:A:32:LEU:HD23	2.26	0.60
1:A:180:MET:HE1	1:A:185:LYS:HG3	1.84	0.58
1:A:111:ALA:HA	1:A:136:VAL:CG1	2.40	0.51

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	207/252 (82%)	195 (94%)	11 (5%)	1 (0%)	24 22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	GLY

5.3.2 Protein sidechains ⓘ

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	178/219 (81%)	169 (95%)	9 (5%)	21	21

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	201	ARG
1	A	222	VAL
1	A	105	ASN
1	A	119	MET
1	A	123	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	40	ASN
1	A	77	HIS
1	A	79	ASN
1	A	212	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

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADE	A	1225	-	11,11,11	2.09	3 (27%)	15,15,15	2.18	5 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADE	A	1225	-	-	-	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1225	ADE	C6-N6	5.19	1.47	1.34
3	A	1225	ADE	C5-N7	-3.24	1.33	1.39
3	A	1225	ADE	C4-N9	-2.32	1.33	1.36

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1225	ADE	N3-C2-N1	-4.38	121.94	128.58
3	A	1225	ADE	C5-C4-N3	-3.40	120.56	126.75
3	A	1225	ADE	C5-N7-C8	3.20	107.09	103.48
3	A	1225	ADE	N9-C4-N3	2.91	131.41	126.69
3	A	1225	ADE	N9-C8-N7	-2.67	109.81	113.87

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 [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	209/252 (82%)	-0.33	1 (0%) 87 88	23, 32, 48, 59	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	176	THR	3.2

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(Å ²)	Q<0.9
2	CL	A	1224	1/1	0.96	0.08	48,48,48,48	0
3	ADE	A	1225	10/10	0.96	0.05	23,25,29,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.