



# wwPDB X-ray Structure Validation Summary Report

Mar 5, 2026 – 10:13 AM UTC


PDB ID : 6DD7 / pdb\_00006dd7  
Title : Crystal structure of plant UVB photoreceptor UVR8 from in situ serial Laue diffraction  
Authors : Ren, Z.  
Deposited on : 2018-05-09  
Resolution : 2.00 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](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  
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

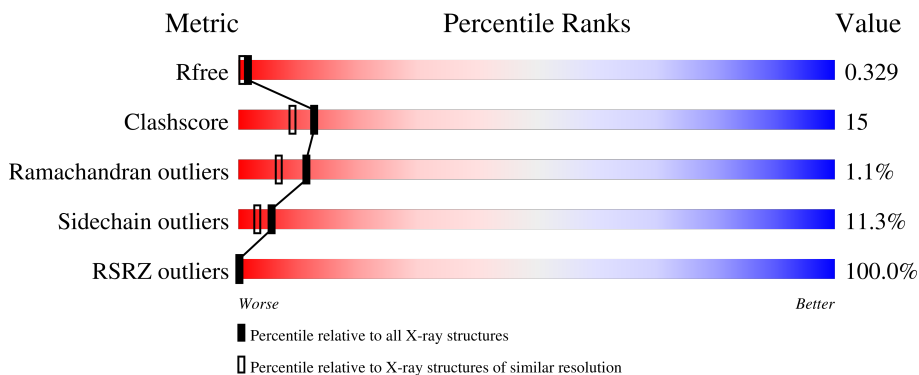
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

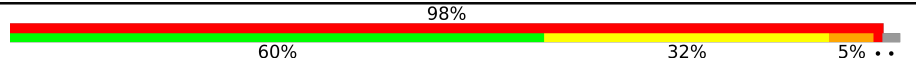
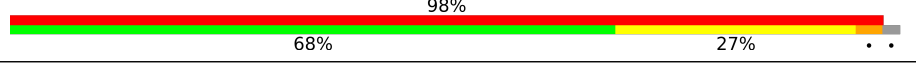
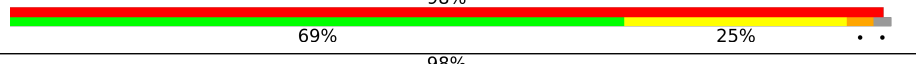

The reported resolution of this entry is 2.00 Å.

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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	377	
1	B	377	
1	C	377	
1	D	377	

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 12160 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 Ultraviolet-B receptor UVR8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	368	2793	1741	505	534	13	0	0	0
1	B	368	2793	1741	505	534	13	0	0	0
1	C	368	2793	1741	505	534	13	0	0	0
1	D	368	2793	1741	505	534	13	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	382	LEU	-	expression tag	UNP Q9FN03
A	383	GLU	-	expression tag	UNP Q9FN03
A	384	HIS	-	expression tag	UNP Q9FN03
A	385	HIS	-	expression tag	UNP Q9FN03
A	386	HIS	-	expression tag	UNP Q9FN03
A	387	HIS	-	expression tag	UNP Q9FN03
A	388	HIS	-	expression tag	UNP Q9FN03
A	389	HIS	-	expression tag	UNP Q9FN03
B	382	LEU	-	expression tag	UNP Q9FN03
B	383	GLU	-	expression tag	UNP Q9FN03
B	384	HIS	-	expression tag	UNP Q9FN03
B	385	HIS	-	expression tag	UNP Q9FN03
B	386	HIS	-	expression tag	UNP Q9FN03
B	387	HIS	-	expression tag	UNP Q9FN03
B	388	HIS	-	expression tag	UNP Q9FN03
B	389	HIS	-	expression tag	UNP Q9FN03
C	382	LEU	-	expression tag	UNP Q9FN03
C	383	GLU	-	expression tag	UNP Q9FN03
C	384	HIS	-	expression tag	UNP Q9FN03
C	385	HIS	-	expression tag	UNP Q9FN03
C	386	HIS	-	expression tag	UNP Q9FN03

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Chain	Residue	Modelled	Actual	Comment	Reference
C	387	HIS	-	expression tag	UNP Q9FN03
C	388	HIS	-	expression tag	UNP Q9FN03
C	389	HIS	-	expression tag	UNP Q9FN03
D	382	LEU	-	expression tag	UNP Q9FN03
D	383	GLU	-	expression tag	UNP Q9FN03
D	384	HIS	-	expression tag	UNP Q9FN03
D	385	HIS	-	expression tag	UNP Q9FN03
D	386	HIS	-	expression tag	UNP Q9FN03
D	387	HIS	-	expression tag	UNP Q9FN03
D	388	HIS	-	expression tag	UNP Q9FN03
D	389	HIS	-	expression tag	UNP Q9FN03

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	200	Total 200	O 200	0	0
2	B	306	Total 306	O 306	0	0
2	C	276	Total 276	O 276	0	0
2	D	206	Total 206	O 206	0	0





I373	I374	E375	A376	L377	S378	V379	D380	G381	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS																																												
M813	L314	D315	Q316	S317	S318	P319	V320	Q321	V322	R323	F324	P325	D326	D327	Q328	K329	V330	V331	Q332	V333	S334	C335	G336	M337	R338	H339	T340	L341	A342	V343	T344	E345	R346	N347	N348	V349	F350	A351	W352	G353	R354	G355	T356	M357	G358	Q359	L360	G361	I362	G363	E364	S365	V366	D367	R368	N369	F370	P371	K372	
Y253	G254	Q255	L256	G257	H258	G259	D260	L261	E262	D263	H264	L265	I266	P267	H268	K269	L270	E271	A272	L273	S274	N275	S276	F277	I278	S279	Q280	L281	S282	G283	G284	W285	R286	H287	T288	M289	A290	L291	T292	S293	D294	G295	K296	L297	Y298	G299	W300	G301	W302	N303	K304	F305	G306	Q307	V308	G309	V310	S311	N312	
L193	Y194	G195	M196	G197	W198	G199	R200	Y201	G202	N203	L204	G205	L206	G207	D208	R209	T210	D211	R212	L213	V214	P215	E216	R217	V218	T219	S220	T221	G222	G223	E224	R225	M226	S227	W228	W229	A230	C231	G232	W233	R234	H235	T236	L237	S238	V239	S240	Y241	S242	G243	L244	L245	Y246	T247	Y248	G249	W250	S251	H252	
L193	A194	V195	T196	M197	E198	G199	E140	V141	Q142	Y82	S83	Q84	S85	G86	M87	Q148	E88	A29	Y90	S91	W92	W94	G95	D156	T157	E158	D159	S160	L161	V162	P163	Q164	A165	I166	Q167	A168	F169	E170	G171	I172	R173	I174	K175	M176	V177	A178	G179	G180	A181	E182	H183	T184	A185	A186	T187	T188	E189	D190	G191	D192
P80	P14	R15	K16	G17	V17	L18	I19	L20	S21	A22	G23	A24	S25	H26	S27	V28	A29	L30	L31	S32	G33	D34	I35	V36	C37	S38	W39	G40	R41	G42	F43	D44	G45	Q46	L47	G48	H49	G50	D51	A52	E53	D54	R55	P56	S57	P58	T59	Q60	L61	S62	A63	L64	D65	G66	H67	Q68	I69	V70	S71	V72
T73	C74	G75	A76	D77	H78	T79	V80	A81	Y82	S83	Q84	S85	G86	M87	Q148	E88	A29	Y90	S91	W92	W94	G95	D156	T157	E158	D159	S160	L161	V162	P163	Q164	A165	I166	Q167	A168	F169	E170	G171	I172	R173	I174	K175	M176	V177	A178	G179	G180	A181	E182	H183	T184	A185	A186	T187	T188	E189	D190	G191	D192	

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.20Å 80.30Å 190.00Å 90.00° 94.80° 90.00°	Depositor
Resolution (Å)	47.33 – 2.00 47.33 – 2.00	Depositor EDS
% Data completeness (in resolution range)	86.6 (47.33-2.00) 87.2 (47.33-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.68 (at 1.94Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.254 , 0.328 0.254 , 0.329	Depositor DCC
$R_{free}$ test set	5010 reflections (3.25%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.9	Xtrriage
Anisotropy	0.063	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 106.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.42	EDS
Total number of atoms	12160	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.98 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5245e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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	0.37	0/2860	0.62	2/3877 (0.1%)
1	B	0.46	0/2860	0.66	0/3877
1	C	0.44	0/2860	0.68	0/3877
1	D	0.35	0/2860	0.56	0/3877
All	All	0.41	0/11440	0.63	2/15508 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	SER	CA-C-N	5.34	131.31	121.70
1	A	365	SER	C-N-CA	5.34	131.31	121.70

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	2793	0	2670	99	0
1	B	2793	0	2670	85	0
1	C	2793	0	2670	74	0
1	D	2793	0	2670	79	0
2	A	200	0	0	15	0
2	B	306	0	0	40	0
2	C	276	0	0	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	206	0	0	24	0
All	All	12160	0	10680	332	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 15.

The worst 5 of 332 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:348:ASN:HD22	1:A:378:SER:HB2	1.29	0.95
1:D:200:ARG:NH2	2:D:404:HOH:O	2.05	0.89
1:C:145:GLY:O	2:C:401:HOH:O	1.90	0.89
1:D:76:ALA:O	2:D:401:HOH:O	1.93	0.87
1:B:98:GLY:O	2:B:401:HOH:O	1.96	0.84

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	366/377 (97%)	336 (92%)	23 (6%)	7 (2%)	<b>6</b> <b>3</b>
1	B	366/377 (97%)	337 (92%)	26 (7%)	3 (1%)	<b>16</b> <b>11</b>
1	C	366/377 (97%)	343 (94%)	19 (5%)	4 (1%)	<b>11</b> <b>7</b>
1	D	366/377 (97%)	335 (92%)	29 (8%)	2 (0%)	<b>24</b> <b>21</b>
All	All	1464/1508 (97%)	1351 (92%)	97 (7%)	16 (1%)	<b>11</b> <b>7</b>

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	ARG

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Mol	Chain	Res	Type
1	A	364	GLU
1	B	365	SER
1	C	364	GLU
1	C	365	SER

### 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	291/300 (97%)	246 (84%)	45 (16%)	2	1
1	B	291/300 (97%)	264 (91%)	27 (9%)	8	5
1	C	291/300 (97%)	262 (90%)	29 (10%)	7	4
1	D	291/300 (97%)	260 (89%)	31 (11%)	6	4
All	All	1164/1200 (97%)	1032 (89%)	132 (11%)	5	3

5 of 132 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	214	VAL
1	D	270	LEU
1	D	374	ILE
1	B	57	SER
1	B	53	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	164	GLN
1	C	203	ASN
1	D	268	HIS
1	D	235	HIS
1	D	264	HIS

### 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, 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	368/377 (97%)	12.23	368 (100%) 0 0	40, 53, 84, 106	0
1	B	368/377 (97%)	9.20	368 (100%) 0 0	17, 33, 58, 81	0
1	C	368/377 (97%)	8.46	368 (100%) 0 0	16, 30, 52, 76	0
1	D	368/377 (97%)	11.60	368 (100%) 0 0	38, 50, 68, 89	0
All	All	1472/1508 (97%)	10.37	1472 (100%) 0 0	16, 44, 69, 106	0

The worst 5 of 1472 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	172	ILE	34.5
1	A	360	LEU	27.0
1	D	174	ILE	25.0
1	D	362	ILE	24.9
1	A	145	GLY	24.9

### 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.