



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 17, 2021 – 10:28 PM JST

PDB ID : 7DHP  
Title : Crystal structure of MazF from *Deinococcus radiodurans*  
Authors : Zhao, Y.; Dai, J.  
Deposited on : 2020-11-17  
Resolution : 1.30 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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.18
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.18

**i**

## X-RAY DIFFRACTION

A.

Metric	Percentile Banks	Value
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<b>Metric</b>	<b>Whole archive (#Entries)</b>	<b>Similar resolution (#Entries, resolution range(Å))</b>
R <sub>free</sub>	130704	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100	101	102	103	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118	119	120	121	122	123	124	125	126	127	128	129	130	131	132	133	134	135	136	137	138	139	140	141	142	143	144	145	146	147	148	149	150	151	152	153	154	155	156	157	158	159	160	161	162	163	164	165	166	167	168	169	170	171	172	173	174	175	176	177	178	179	180	181	182	183	184	185	186	187	188	189	190	191	192	193	194	195	196	197	198	199	200	201	202	203	204	205	206	207	208	209	210	211	212	213	214	215	216	217	218	219	220	221	222	223	224	225	226	227	228	229	230	231	232	233	234	235	236	237	238	239	240	241	242	243	244	245	246	247	248	249	250	251	252	253	254	255	256	257	258	259	260	261	262	263	264	265	266	267	268	269	270	271	272	273	274	275	276	277	278	279	280	281	282	283	284	285	286	287	288	289	290	291	292	293	294	295	296	297	298	299	300	301	302	303	304	305	306	307	308	309	310	311	312	313	314	315	316	317	318	319	320	321	322	323	324	325	326	327	328	329	330	331	332	333	334	335	336	337	338	339	340	341	342	343	344	345	346	347	348	349	350	351	352	353	354	355	356	357	358	359	360	361	362	363	364	365	366	367	368	369	370	371	372	373	374	375	376	377	378	379	380	381	382	383	384	385	386	387	388	389	390	391	392	393	394	395	396	397	398	399	400	401	402	403	404	405	406	407	408	409	410	411	412	413	414	415	416	417	418	419	420	421	422	423	424	425	426	427	428	429	430	431	432	433	434	435	436	437	438	439	440	441	442	443	444	445	446	447	448	449	450	451	452	453	454	455	456	457	458	459	460	461	462	463	464	465	466	467	468	469	470	471	472	473	474	475	476	477	478	479	480	481	482	483	484	485	486	487	488	489	490	491	492	493	494	495	496	497	498	499	500	501	502	503	504	505	506	507	508	509	510	511	512	513	514	515	516	517	518	519	520	521	522	523	52
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Mol	Chain	Length	Quality of chain
1	A	137	<p>2% 74% 6% 20%</p>
1	B	137	<p>5% 74% 7% 20%</p>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1935 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 Endoribonuclease MazF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	110	Total	C	N	O	S	0	3	0
			846	533	155	153	5			
1	B	110	Total	C	N	O	S	0	5	0
			874	553	161	155	5			

There are 40 discrepancies between the modelled and reference sequences:

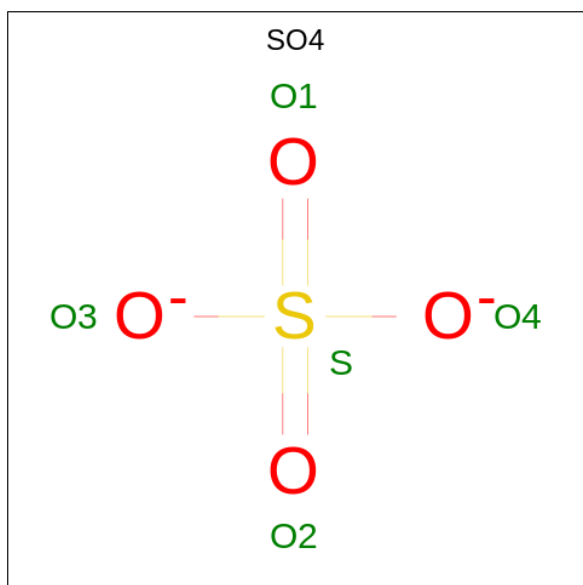
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A6G9BVQ8
A	-18	GLY	-	expression tag	UNP A0A6G9BVQ8
A	-17	SER	-	expression tag	UNP A0A6G9BVQ8
A	-16	SER	-	expression tag	UNP A0A6G9BVQ8
A	-15	HIS	-	expression tag	UNP A0A6G9BVQ8
A	-14	HIS	-	expression tag	UNP A0A6G9BVQ8
A	-13	HIS	-	expression tag	UNP A0A6G9BVQ8
A	-12	HIS	-	expression tag	UNP A0A6G9BVQ8
A	-11	HIS	-	expression tag	UNP A0A6G9BVQ8
A	-10	HIS	-	expression tag	UNP A0A6G9BVQ8
A	-9	SER	-	expression tag	UNP A0A6G9BVQ8
A	-8	SER	-	expression tag	UNP A0A6G9BVQ8
A	-7	GLY	-	expression tag	UNP A0A6G9BVQ8
A	-6	LEU	-	expression tag	UNP A0A6G9BVQ8
A	-5	VAL	-	expression tag	UNP A0A6G9BVQ8
A	-4	PRO	-	expression tag	UNP A0A6G9BVQ8
A	-3	ARG	-	expression tag	UNP A0A6G9BVQ8
A	-2	GLY	-	expression tag	UNP A0A6G9BVQ8
A	-1	SER	-	expression tag	UNP A0A6G9BVQ8
A	0	HIS	-	expression tag	UNP A0A6G9BVQ8
B	-19	MET	-	initiating methionine	UNP A0A6G9BVQ8
B	-18	GLY	-	expression tag	UNP A0A6G9BVQ8
B	-17	SER	-	expression tag	UNP A0A6G9BVQ8
B	-16	SER	-	expression tag	UNP A0A6G9BVQ8
B	-15	HIS	-	expression tag	UNP A0A6G9BVQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP A0A6G9BVQ8
B	-13	HIS	-	expression tag	UNP A0A6G9BVQ8
B	-12	HIS	-	expression tag	UNP A0A6G9BVQ8
B	-11	HIS	-	expression tag	UNP A0A6G9BVQ8
B	-10	HIS	-	expression tag	UNP A0A6G9BVQ8
B	-9	SER	-	expression tag	UNP A0A6G9BVQ8
B	-8	SER	-	expression tag	UNP A0A6G9BVQ8
B	-7	GLY	-	expression tag	UNP A0A6G9BVQ8
B	-6	LEU	-	expression tag	UNP A0A6G9BVQ8
B	-5	VAL	-	expression tag	UNP A0A6G9BVQ8
B	-4	PRO	-	expression tag	UNP A0A6G9BVQ8
B	-3	ARG	-	expression tag	UNP A0A6G9BVQ8
B	-2	GLY	-	expression tag	UNP A0A6G9BVQ8
B	-1	SER	-	expression tag	UNP A0A6G9BVQ8
B	0	HIS	-	expression tag	UNP A0A6G9BVQ8

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

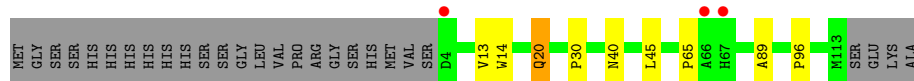
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	114	Total 114	O 114	0	0
3	B	86	Total 86	O 86	0	0

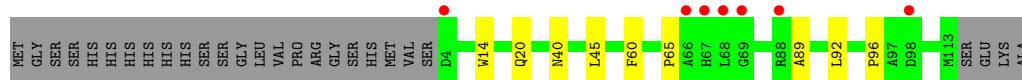
### 3 Residue-property plots [i](#)

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: Endoribonuclease MazF



- Molecule 1: Endoribonuclease MazF



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.49Å 70.49Å 111.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.83 – 1.30 27.83 – 1.30	Depositor EDS
% Data completeness (in resolution range)	96.1 (27.83-1.30) 96.1 (27.83-1.30)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.66 (at 1.30Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.172 , 0.185 0.172 , 0.185	Depositor DCC
$R_{free}$ test set	3280 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.4	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.64 , 61.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	1935	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.07% of the height of the origin peak. No significant pseudotranslation is detected.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.92	0/865	0.98	0/1176
1	B	0.86	0/896	0.92	0/1218
All	All	0.89	0/1761	0.95	0/2394

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

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	846	0	840	5	0
1	B	874	0	859	7	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
3	A	114	0	0	1	0
3	B	86	0	0	2	0
All	All	1935	0	1699	12	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 3.

The worst 5 of 12 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:20:GLN:NE2	3:A:303:HOH:O	2.34	0.60
1:B:60[A]:PHE:HB2	3:B:376:HOH:O	2.05	0.57
1:B:14[B]:TRP:NE1	1:B:92:LEU:HD13	2.25	0.52
1:B:40:ASN:HA	1:B:45:LEU:O	2.14	0.48
1:A:40:ASN:HA	1:A:45:LEU:O	2.15	0.46

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	110/137 (80%)	107 (97%)	3 (3%)	0	100	100
1	B	112/137 (82%)	110 (98%)	2 (2%)	0	100	100
All	All	222/274 (81%)	217 (98%)	5 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	87/107 (81%)	86 (99%)	1 (1%)	73	45
1	B	89/107 (83%)	88 (99%)	1 (1%)	73	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	176/214 (82%)	174 (99%)	2 (1%)	71	45

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	B	20	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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	$\# Z  > 2$
2	SO4	A	202	-	4,4,4	0.14	0	6,6,6	0.28	0
2	SO4	A	201	-	4,4,4	0.17	0	6,6,6	0.30	0
2	SO4	B	201	-	4,4,4	0.25	0	6,6,6	0.38	0

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 [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	110/137 (80%)	0.02	3 (2%) 54 52	10, 15, 28, 51	0
1	B	110/137 (80%)	0.31	7 (6%) 19 16	11, 17, 34, 48	0
All	All	220/274 (80%)	0.17	10 (4%) 33 31	10, 16, 34, 51	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	66	ALA	5.2
1	B	66	ALA	4.7
1	A	67	HIS	4.2
1	B	67	HIS	3.9
1	B	69	GLY	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 monosaccharides 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	202	5/5	0.84	0.22	80,80,81,83	0
2	SO4	A	201	5/5	0.98	0.17	24,25,31,32	0
2	SO4	B	201	5/5	0.98	0.14	24,25,33,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.