



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 18, 2025 – 06:10 PM EDT

PDB ID : 8TT8 / pdb_00008tt8
Title : Joint Xray/Neutron structure of Macrophage Migration Inhibitory Factor (MIF) Bound to 4-hydroxyphenylpyruvate at room temperature
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Deposited on : 2023-08-13
Resolution : 1.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	FAILED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

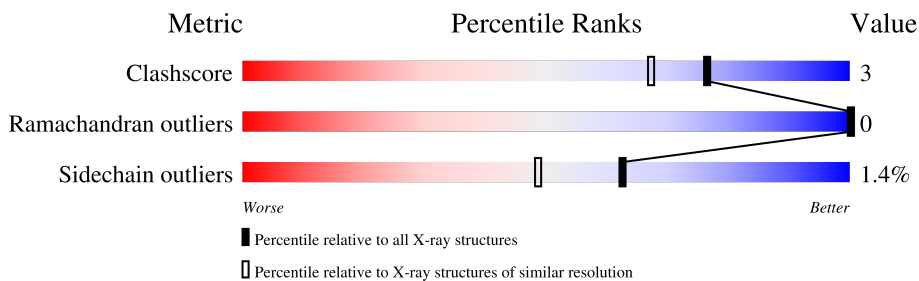
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION, NEUTRON DIFFRACTION

The reported resolution of this entry is 1.75 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))
Clashscore	180529	3097 (1.76-1.76)
Ramachandran outliers	177936	3072 (1.76-1.76)
Sidechain outliers	177891	3072 (1.76-1.76)

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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	114	
1	B	114	
1	C	114	

2 Entry composition [i](#)

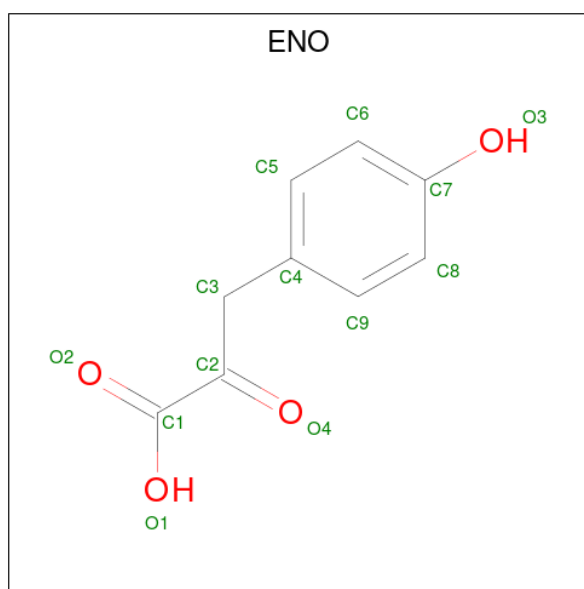
There are 5 unique types of molecules in this entry. The entry contains 6502 atoms, of which 2466 are hydrogens and 993 are deuteriums.

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 Macrophage migration inhibitory factor.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	114	Total	C	D	H	N	O	S	0	63	0
			1932	588	195	804	161	176	8			
1	B	114	Total	C	D	H	N	O	S	0	67	0
			1912	583	185	810	156	169	9			
1	C	114	Total	C	D	H	N	O	S	0	64	0
			1955	594	190	824	164	176	7			

- Molecule 2 is 3-(4-HYDROXY-PHENYL)PYRUVIC ACID (CCD ID: ENO) (formula: C₉H₈O₄) (labeled as "Ligand of Interest" by depositor).



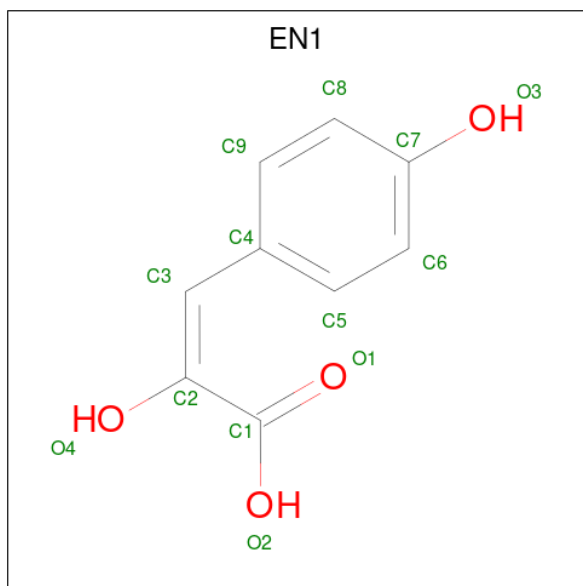
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	D	H	O	0	1
			21	9	1	7	4		
2	B	1	Total	C	D	H	O	0	1
			21	9	1	7	4		

- Molecule 3 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C₃H₈O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	D	H	O	0	1
			13	3	1	8	1		

- Molecule 4 is (2E)-2-hydroxy-3-(4-hydroxyphenyl)prop-2-enoic acid (CCD ID: EN1) (formula: $C_9H_8O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	D	H	O	0	1
			21	9	2	6	4		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	80	Total 240	D 160	O 80	0	0
5	B	58	Total 174	D 116	O 58	0	0
5	C	71	Total 213	D 142	O 71	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. 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. 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.

Note EDS failed to run properly.

- Molecule 1: Macrophage migration inhibitory factor

Chain A:  96% .



- Molecule 1: Macrophage migration inhibitory factor

Chain B:  98% .



- Molecule 1: Macrophage migration inhibitory factor

Chain C:  95% 5% .



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.61Å 69.23Å 89.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.69 – 1.75	Depositor
% Data completeness (in resolution range)	100.0 (54.69-1.75)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.154 , 0.180	Depositor
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.059	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
Total number of atoms	6502	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% 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: ENO, EN1, IPA

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	0.84	1/1370 (0.1%)	0.72	0/1860
1	B	0.73	0/1446	0.74	0/1960
1	C	0.77	0/1374	0.77	0/1859
All	All	0.78	1/4190 (0.0%)	0.74	0/5679

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	47	MET	SD-CE	-9.16	1.56	1.79

There are no bond angle outliers.

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	1128	804	528	3	0
1	B	1102	810	473	1	0
1	C	1131	824	547	4	0
2	A	14	7	0	0	0
2	B	14	7	0	0	0
3	B	5	8	0	0	0
4	C	15	6	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	240	0	0	1	0
5	B	174	0	0	2	0
5	C	213	0	0	1	0
All	All	4036	2466	1548	9	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.

All (9) 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:25[A]:GLN:OE1	1:A:78:LEU:HD11	2.04	0.52
1:C:2[B]:MET:HE3	1:C:4:ILE:HD11	1.84	0.47
1:A:25[A]:GLN:NE2	5:A:301:HOH:O	2.29	0.46
1:B:71:GLN:HG3	5:B:348:HOH:O	2.15	0.41
1:C:73[B]:ARG:NH1	5:C:302:HOH:O	2.46	0.41

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	173/114 (152%)	170 (98%)	3 (2%)	0	100	100
1	B	182/114 (160%)	180 (99%)	2 (1%)	0	100	100
1	C	175/114 (154%)	173 (99%)	2 (1%)	0	100	100
All	All	530/342 (155%)	523 (99%)	7 (1%)	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	147/94 (156%)	146 (99%)	1 (1%)	81	74
1	B	155/94 (165%)	153 (99%)	2 (1%)	65	51
1	C	147/94 (156%)	145 (99%)	2 (1%)	62	49
All	All	449/282 (159%)	444 (99%)	5 (1%)	62	58

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	LEU
1	B	66[A]	LYS
1	B	66[B]	LYS
1	C	52	SER
1	C	88	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	62	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

8 ligands are modelled in this entry.

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

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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.