



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 09:05 am GMT

PDB ID : 1DD7
Title : MURINE INDUCIBLE NITRIC OXIDE SYNTHASE OXYGENASE DOMAIN (DELTA 114) (N-[(1,3-BENZODIOXOL-5-YL)METHYL]-1-[2-(1 H-IMIDAZOL-1-YL)PYRIMIDIN-4-YL]-4-(METHOXYCARBONYL)-PIPERAZINE-2-ACETAMIDE COMPLEX
Authors : Adler, M.; Whitlow, M.
Deposited on : 1999-11-08
Resolution : 2.25 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

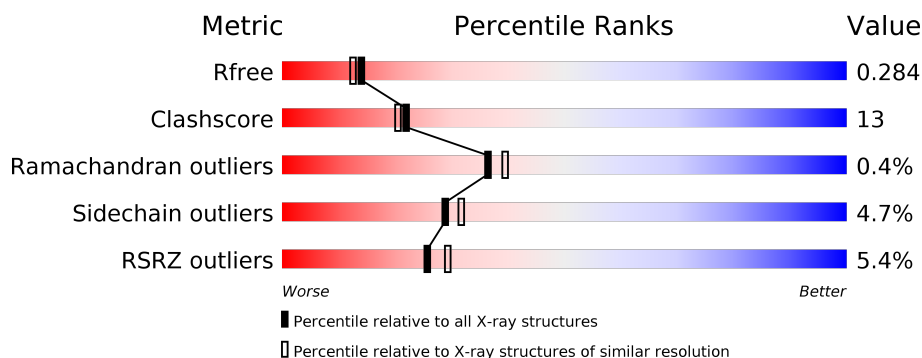
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	111664	1178 (2.26-2.26)
Clashscore	122126	1286 (2.26-2.26)
Ramachandran outliers	120053	1253 (2.26-2.26)
Sidechain outliers	120020	1254 (2.26-2.26)
RSRZ outliers	108989	1158 (2.26-2.26)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	389	<div> <div>4%</div> <div>54%</div> <div>20%</div> <div>•</div> <div>24%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3588 atoms, of which 907 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.

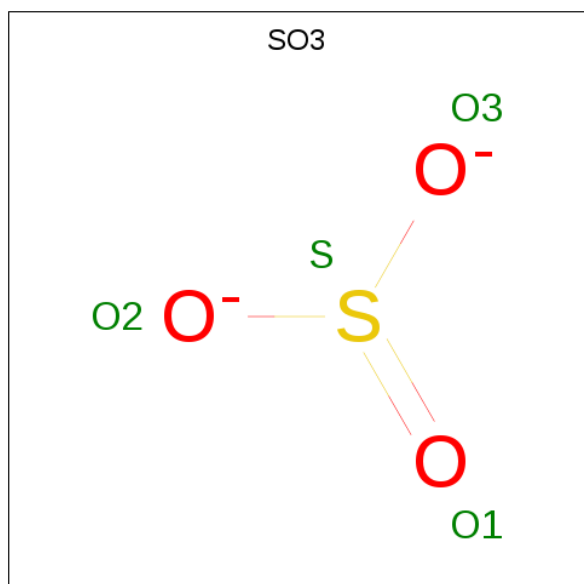
- Molecule 1 is a protein called INDUCIBLE NITRIC OXIDE SYNTHASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	295	2931	1549	522	412	434	14	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	499	HIS	-	C-TERMINAL HIS TAG	UNP P29477
A	500	HIS	-	C-TERMINAL HIS TAG	UNP P29477
A	501	HIS	-	C-TERMINAL HIS TAG	UNP P29477
A	502	HIS	-	C-TERMINAL HIS TAG	UNP P29477

- Molecule 2 is SULFITE ION (three-letter code: SO3) (formula: O₃S).



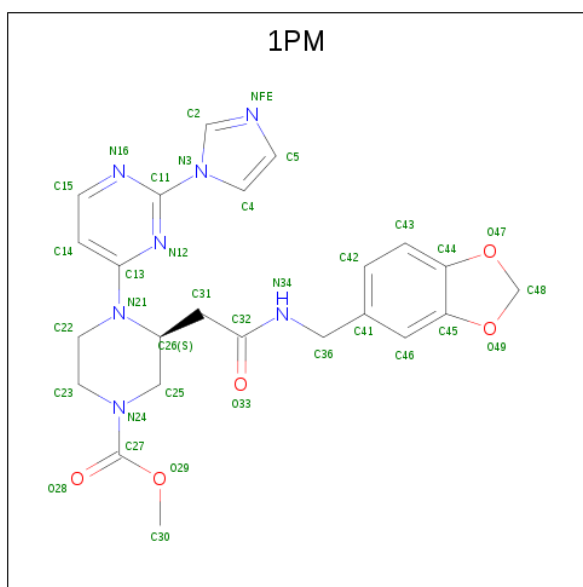
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	4	3	1	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Fe	H	N	O	0	0
			47	34	1	4	4	4		

- Molecule 4 is methyl (3S)-3-{2-[(1,3-benzodioxol-5-ylmethyl)amino]-2-oxoethyl}-4-[2-(1H-imidazol-1-yl)pyrimidin-4-yl]piperazine-1-carboxylate (three-letter code: 1PM) (formula: $C_{23}H_{25}N_7O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			36	23	1	7	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	190	Total	H	O	0	0
			570	380	190		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.42Å 73.93Å 93.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.25 8.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	1.0 (8.00-2.25) 98.0 (8.00-2.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.25Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.197 , 0.284 0.213 , 0.284	Depositor DCC
R_{free} test set	835 reflections (4.07%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.14 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3588	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% 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: HEM, SO3, 1PM

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	0.60	0/2474	0.77	1/3358 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	292	ARG	N-CA-C	-5.38	96.47	111.00

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	2409	522	2339	61	2
2	A	4	0	0	0	0
3	A	43	4	30	2	0
4	A	35	1	25	2	0
5	A	190	380	0	6	2
All	All	2681	907	2394	62	2

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 13.

The worst 5 of 62 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:305:ALA:O	1:A:308:GLN:HG2	1.81	0.80
1:A:152:LYS:HB2	1:A:155:GLU:HB2	1.65	0.79
1:A:414:VAL:HA	1:A:417:LEU:HG	1.66	0.77
1:A:264:TYR:HE1	1:A:291:PRO:HB2	1.62	0.64
1:A:336:LEU:HD12	1:A:336:LEU:H	1.62	0.64

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:SER:OG	5:A:1157:HOH:H1[3_756]	1.49	0.11
1:A:314:GLU:O	5:A:1186:HOH:H1[4_446]	1.58	0.02

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	285/389 (73%)	273 (96%)	11 (4%)	1 (0%)	36 39

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	149	LYS

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	258/341 (76%)	246 (95%)	12 (5%)	29	32

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	308	GLN
1	A	325	MET
1	A	418	HIS
1	A	292	ARG
1	A	413	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	230	ASN
1	A	442	GLN
1	A	257	GLN
1	A	156	HIS
1	A	421	GLN

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 carbohydrates 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	$\# Z > 2$
3	HEM	A	600	1,4	27,50,50	2.20	7 (25%)	17,82,82	2.15	5 (29%)
4	1PM	A	601	3	38,39,39	1.78	10 (26%)	46,54,54	3.04	16 (34%)
2	SO3	A	602	-	1,3,3	3.69	1 (100%)	0,3,3	0.00	-

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	HEM	A	600	1,4	-	0/6/54/54	0/0/8/8
4	1PM	A	601	3	-	0/19/42/42	0/5/5/5
2	SO3	A	602	-	-	0/0/0/0	0/0/0/0

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	HEM	C3B-CAB	-4.65	1.38	1.47
3	A	600	HEM	C3C-CAC	-3.86	1.40	1.47
4	A	601	1PM	C2-N3	-3.02	1.33	1.36
4	A	601	1PM	O49-C45	-3.00	1.34	1.38
4	A	601	1PM	O47-C44	-2.71	1.34	1.38

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	1PM	N16-C11-N12	-7.80	116.92	126.08
3	A	600	HEM	CMD-C2D-C1D	-5.67	119.75	128.46
4	A	601	1PM	C14-C13-N12	-4.28	116.77	123.53
4	A	601	1PM	C14-C15-N16	-3.61	119.54	123.92
4	A	601	1PM	O29-C27-O28	-3.47	117.96	124.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	HEM	2	0
4	A	601	1PM	2	0

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	295/389 (75%)	-0.19	16 (5%) 26 29	23, 42, 97, 133	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	416	VAL	4.6
1	A	415	ALA	4.4
1	A	265	GLN	4.1
1	A	336	LEU	3.4
1	A	414	VAL	3.1

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 carbohydrates 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	SO3	A	602	4/4	0.73	0.28	114,115,118,121	0
4	1PM	A	601	35/35	0.95	0.10	12,41,60,67	0
3	HEM	A	600	43/43	0.96	0.10	12,32,51,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.