



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 01:09 PM UTC

PDB ID : 1NIS / pdb_00001nis
Title : CRYSTAL STRUCTURE OF ACONITASE WITH TRANS-ACONITATE
AND NITROCITRATE BOUND
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Deposited on : 1993-01-17
Resolution : 2.05 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

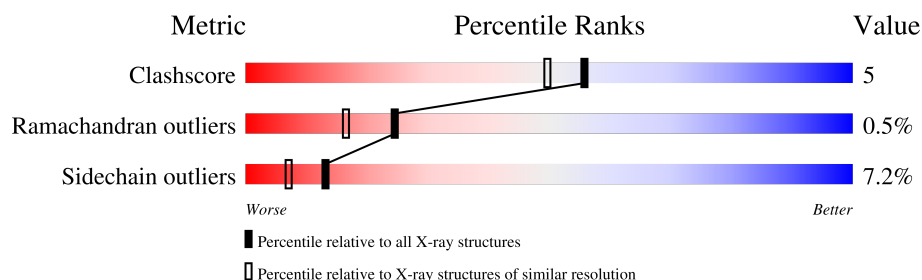
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)

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 was not executed.

Mol	Chain	Length	Quality of chain
1	A	754	 75% 19% . .

2 Entry composition [i](#)

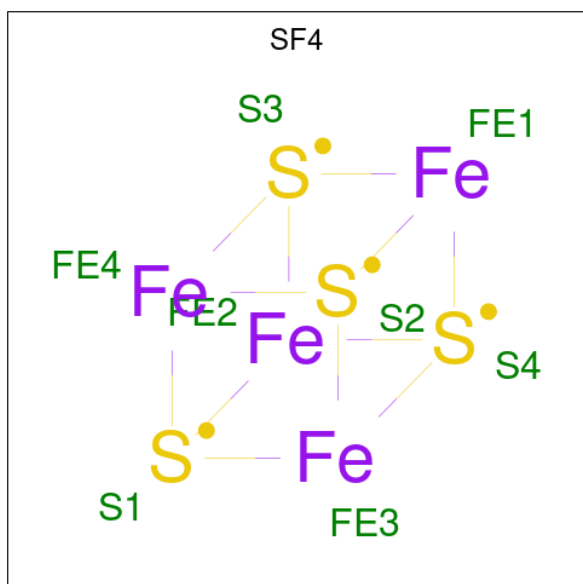
There are 4 unique types of molecules in this entry. The entry contains 6130 atoms, of which 7 are hydrogens and 0 are deuteriums.

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 ACONITASE.

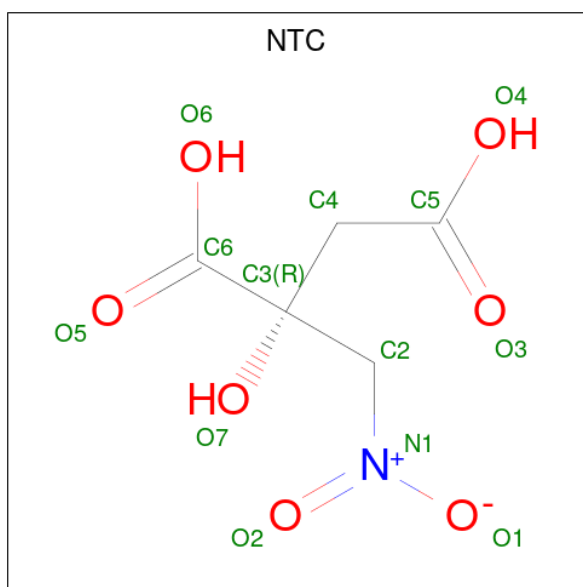
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	753	5812	3664	1031	1095	22	0	0	0

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
2	A	1	8	4	4	0	0

- Molecule 3 is 2-HYDROXY-2-NITROMETHYL SUCCINIC ACID (CCD ID: NTC) (formula: $\text{C}_5\text{H}_7\text{NO}_7$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			18	5	5	1	7		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	290	Total	H	O	0	0
			292	2	290		

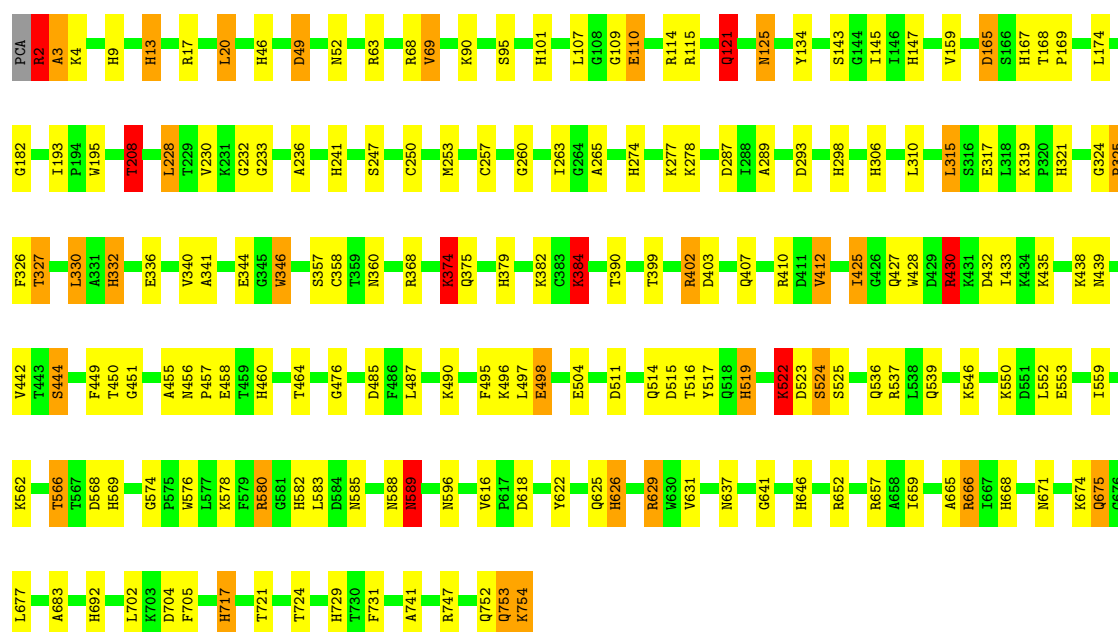
3 Residue-property plots

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 was not executed.

• Molecule 1: ACONITASE

Chain A: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	B 1 1 2	Depositor
Cell constants a, b, c, α , β , γ	185.50Å 72.00Å 73.00Å 90.00° 90.00° 77.70°	Depositor
Resolution (Å)	8.00 – 2.05	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.05)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.172 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6130	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, NTC

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	1.08	29/5938 (0.5%)	1.78	128/8044 (1.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	626	HIS	CD2-NE2	-7.29	1.29	1.37
1	A	13	HIS	CD2-NE2	-7.15	1.29	1.37
1	A	519	HIS	CD2-NE2	-7.07	1.30	1.37
1	A	321	HIS	CD2-NE2	-7.01	1.30	1.37
1	A	717	HIS	CD2-NE2	-6.76	1.30	1.37

The worst 5 of 128 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	580	ARG	NE-CZ-NH2	-10.47	109.78	119.20
1	A	402	ARG	NE-CZ-NH2	-9.84	110.34	119.20
1	A	63	ARG	NE-CZ-NH2	-7.79	112.18	119.20
1	A	498	GLU	CA-CB-CG	7.74	129.58	114.10
1	A	3	ALA	N-CA-C	-7.50	100.42	110.55

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	324	GLY	Peptide
1	A	580	ARG	Sidechain
1	A	666	ARG	Sidechain

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	5812	0	5793	54	0
2	A	8	0	0	0	0
3	A	13	5	5	2	0
4	A	290	2	0	1	0
All	All	6123	7	5798	55	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 5.

The worst 5 of 55 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:430:ARG:HH22	1:A:439:ASN:HD21	1.24	0.84
1:A:13:HIS:HB3	4:A:1193:HOH:O	1.85	0.77
1:A:228:LEU:HD23	1:A:263:ILE:HD12	1.69	0.74
1:A:430:ARG:HH22	1:A:439:ASN:ND2	1.86	0.73
1:A:250:CYS:HA	1:A:253:MET:HE3	1.74	0.69

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	751/754 (100%)	716 (95%)	31 (4%)	4 (0%)	24 16

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	524	SER
1	A	525	SER
1	A	109	GLY
1	A	753	GLN

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	621/622 (100%)	576 (93%)	45 (7%)	13 7

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	490	LYS
1	A	553	GLU
1	A	496	LYS
1	A	514	GLN
1	A	578	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	589	ASN
1	A	585	ASN
1	A	439	ASN
1	A	536	GLN
1	A	419	ASN

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 ⓘ

2 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	SF4	A	999	4,1	0,12,12	-	-	-		
3	NTC	A	755	-	9,12,12	2.19	3 (33%)	14,17,17	3.29	4 (28%)

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
2	SF4	A	999	4,1	-	-	0/6/5/5
3	NTC	A	755	-	-	8/15/16/16	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	755	NTC	C3-C6	3.80	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	755	NTC	C4-C3	3.80	1.58	1.54
3	A	755	NTC	O4-C5	-2.93	1.21	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	755	NTC	C2-C3-C4	-8.25	92.31	109.08
3	A	755	NTC	O7-C3-C4	6.19	123.50	109.38
3	A	755	NTC	C3-C4-C5	4.31	125.72	113.92
3	A	755	NTC	O6-C6-C3	2.88	118.67	113.14

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	755	NTC	N1-C2-C3-C4
3	A	755	NTC	N1-C2-C3-C6
3	A	755	NTC	C4-C3-C6-O5
3	A	755	NTC	C4-C3-C6-O6
3	A	755	NTC	C2-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	755	NTC	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.