Full wwPDB X-ray Structure Validation Report (i)

Oct 3, 2023 – 05:14 AM EDT

PDB ID	:	6O7S
Title	:	Nitrogenase MoFeP mutant S188A from Azotobacter vinelandii in the indigo carmine oxidized state
Authors	:	Rutledge, H.L.; Tezcan, F.A.
Deposited on	:	2019-03-08
Resolution	:	2.27 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 32420 atoms, of which 15273 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 Nitrogenase molybdenum-iron protein alpha chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	476	7314	2367	3591	637	695	24	0	0	0
1	C	476	7275	2364	3566	629	692	24	0	0	0

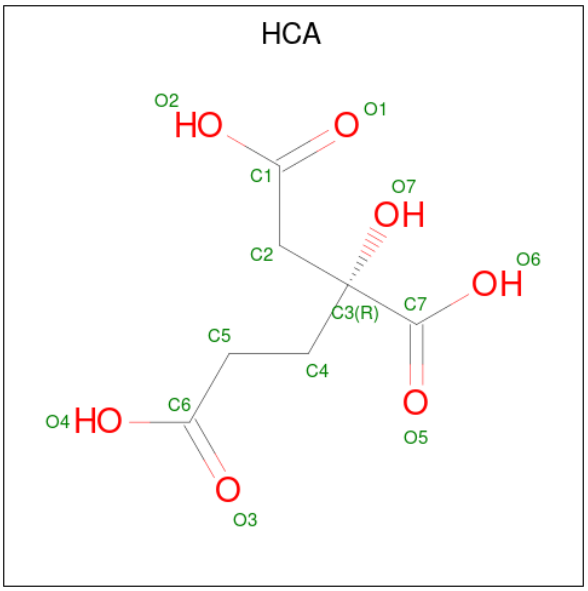
- Molecule 2 is a protein called Nitrogenase molybdenum-iron protein beta chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	522	8169	2649	4026	699	767	28	0	0	0
2	D	522	8245	2663	4078	704	772	28	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

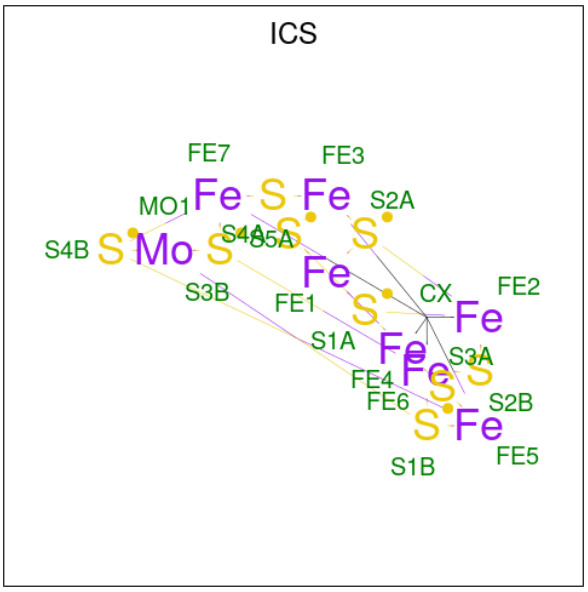
Chain	Residue	Modelled	Actual	Comment	Reference
B	188	ALA	SER	engineered mutation	UNP P07329
D	188	ALA	SER	engineered mutation	UNP P07329

- Molecule 3 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (three-letter code: HCA) (formula: $C_7H_{10}O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	A	1	20	7	6	7	0	0
			Total	C	H	O		
3	C	1	20	7	6	7	0	0

- Molecule 4 is iron-sulfur-molybdenum cluster with interstitial carbon (three-letter code: ICS) (formula: CFe_7MoS_9).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	Mo	S		
4	A	1	18	1	7	1	9	0	0

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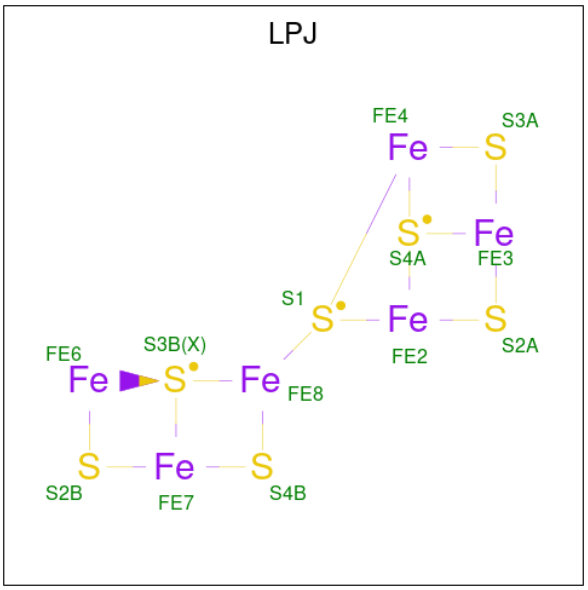
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	Mo	S		
4	C	1	18	1	7	1	9	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
5	A	1	1	1	0	0
			Total	Na		
5	C	1	1	1	0	0

- Molecule 6 is FE(6)-S(7) CLUSTER (three-letter code: LPJ) (formula: Fe_6S_7).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
6	B	1	13	6	7	0	0
			Total	Fe	S		
6	D	1	13	6	7	0	0

- Molecule 7 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
7	B	1	1	1	0	0
			Total	Fe		
7	D	1	1	1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	247	247	247	0	0
			Total	O		
8	B	417	417	417	0	0
			Total	O		
8	C	247	247	247	0	0
			Total	O		
8	D	400	400	400	0	0

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

3 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.78Å 128.05Å 107.54Å 90.00° 108.97° 90.00°	Depositor
Resolution (Å)	35.45 – 2.27	Depositor
% Data completeness (in resolution range)	91.5 (35.45-2.27)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.14 (at 2.27Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.170 , 0.208	Depositor
Wilson B-factor (Å^2)	21.9	Xtriage
Anisotropy	0.493	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
Total number of atoms	32420	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality (i)

4.1 Standard geometry (i)

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

4.2 Too-close contacts (i)

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

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

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

4.3.2 Protein sidechains (i)

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

4.3.3 RNA (i)

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

4.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

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	$\#\|Z\| > 2$
6	LPJ	D	601	1,2	0,17,17	-	-	-		
3	HCA	A	501	-	13,13,13	1.03	0	14,18,18	1.38	2 (14%)
6	LPJ	B	601	1,2	0,17,17	-	-	-		
3	HCA	C	501	-	13,13,13	1.05	0	14,18,18	1.46	2 (14%)
4	ICS	A	502	1	18,30,30	2.63	11 (61%)	-		
4	ICS	C	502	1	18,30,30	2.63	11 (61%)	-		

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	HCA	A	501	-	-	4/17/17/17	-
3	HCA	C	501	-	-	6/17/17/17	-
6	LPJ	D	601	1,2	-	-	0/6/5/5
6	LPJ	B	601	1,2	-	-	0/6/5/5

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	502	ICS	S4B-FE7	-4.38	2.21	2.32
4	A	502	ICS	S4B-FE7	-4.37	2.21	2.32
4	A	502	ICS	S3B-FE6	-4.19	2.22	2.32
4	C	502	ICS	S3B-FE6	-4.01	2.22	2.32
4	A	502	ICS	S1B-FE6	-3.83	2.22	2.32
4	C	502	ICS	S1B-FE6	-3.82	2.23	2.32
4	C	502	ICS	S2A-FE2	-3.25	2.24	2.32
4	C	502	ICS	S3B-FE7	-3.22	2.24	2.32
4	A	502	ICS	S2A-FE2	-3.19	2.24	2.32
4	A	502	ICS	S4B-FE5	-3.18	2.24	2.32
4	A	502	ICS	S3B-FE7	-3.14	2.24	2.32
4	C	502	ICS	S4B-FE5	-3.03	2.24	2.32
4	C	502	ICS	S4A-FE3	-2.91	2.25	2.32
4	A	502	ICS	S2B-FE6	-2.82	2.18	2.24
4	A	502	ICS	S4A-FE3	-2.79	2.25	2.32
4	C	502	ICS	S2B-FE6	-2.76	2.18	2.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	502	ICS	S1A-FE2	-2.58	2.26	2.32
4	A	502	ICS	S1A-FE2	-2.55	2.26	2.32
4	C	502	ICS	S1B-FE5	-2.30	2.26	2.32
4	A	502	ICS	S1B-FE5	-2.22	2.26	2.32
4	C	502	ICS	S2A-FE3	-2.14	2.27	2.32
4	A	502	ICS	S2A-FE3	-2.05	2.27	2.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	HCA	O6-C7-C3	3.29	118.76	113.05
3	C	501	HCA	O6-C7-C3	3.22	118.64	113.05
3	C	501	HCA	O5-C7-C3	-2.57	118.61	122.25
3	A	501	HCA	O5-C7-C3	-2.46	118.77	122.25

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	501	HCA	C2-C3-C4-C5
3	C	501	HCA	O7-C3-C4-C5
3	C	501	HCA	C7-C3-C4-C5
3	A	501	HCA	C4-C5-C6-O4
3	A	501	HCA	C1-C2-C3-C4
3	A	501	HCA	C4-C5-C6-O3
3	A	501	HCA	C1-C2-C3-C7
3	C	501	HCA	O1-C1-C2-C3
3	C	501	HCA	O2-C1-C2-C3
3	C	501	HCA	C4-C5-C6-O4

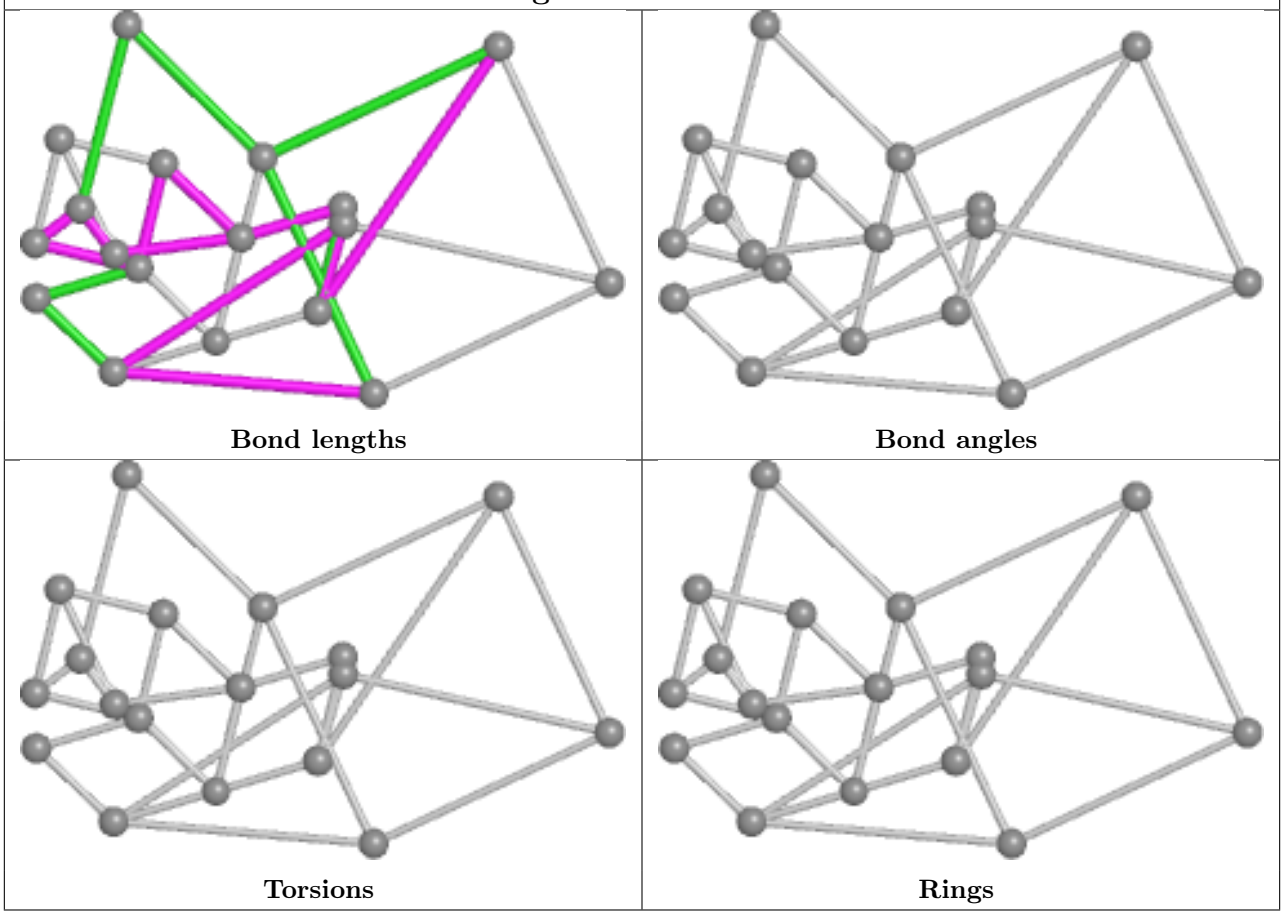
There are no ring outliers.

No monomer is involved in short contacts.

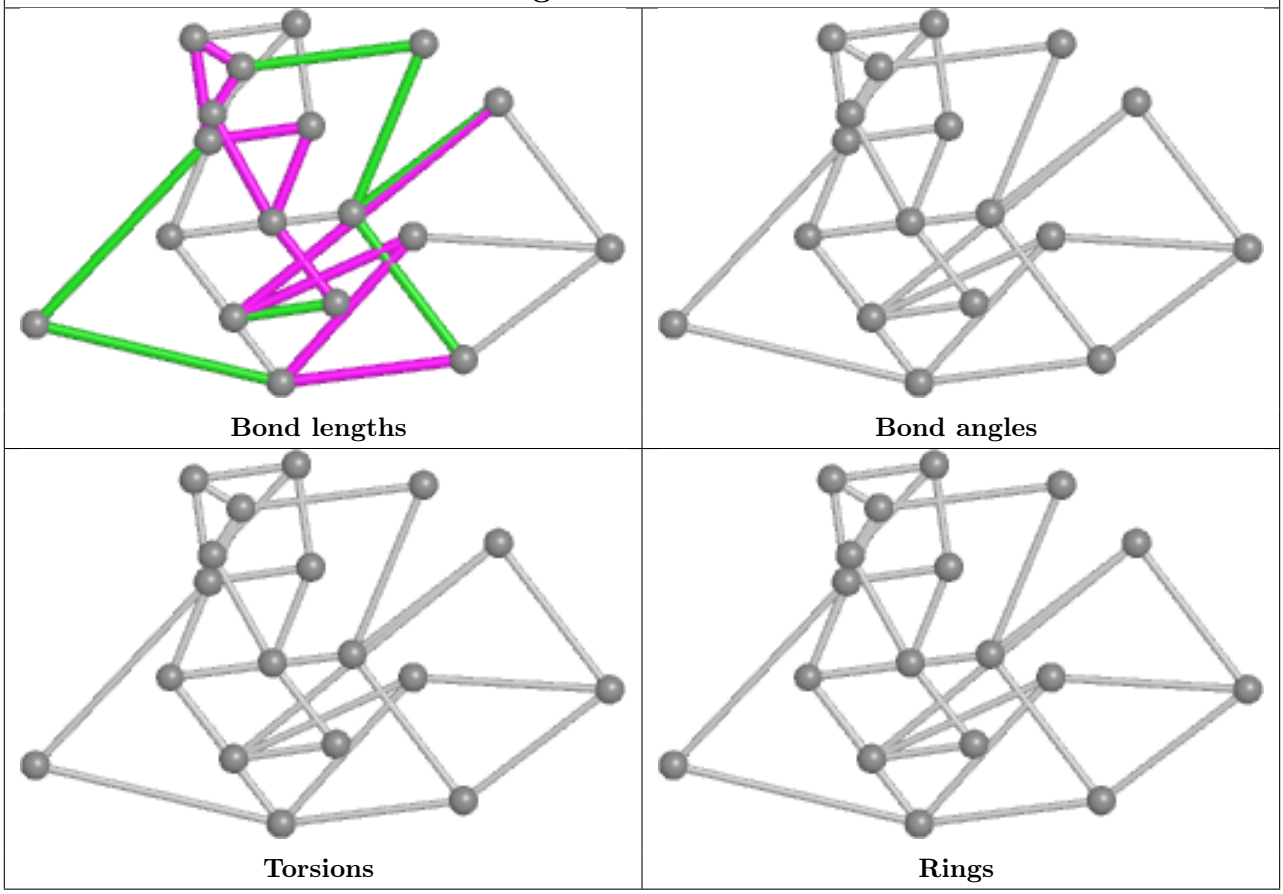
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ICS A 502



Ligand ICS C 502



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

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

5.2 Non-standard residues in protein, DNA, RNA chains (i)

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

5.3 Carbohydrates (i)

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

5.4 Ligands (i)

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

5.5 Other polymers (i)

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