



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:38 AM GMT

PDB ID : 3BNJ
Title : W. succinogenes NrfA Y218F Sulfite Complex
Authors : Lukat, P.; Einsle, O.
Deposited on : 2007-12-14
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
A user guide is available at
<http://wwpdb.org/validation/2016/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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : **FAILED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

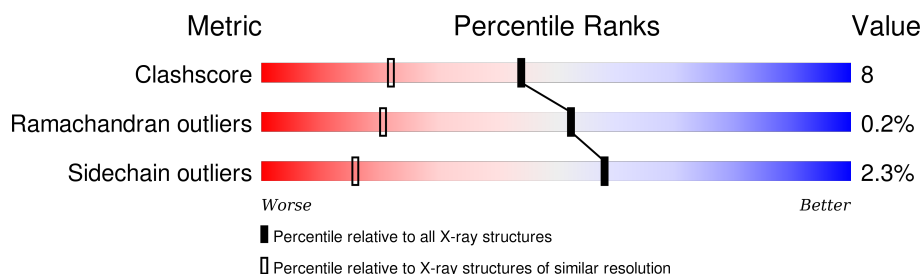
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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	102246	1031 (1.32-1.28)
Ramachandran outliers	100387	1504 (1.34-1.26)
Sidechain outliers	100360	1503 (1.34-1.26)

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.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	485	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 4756 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 Cytochrome c-552.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	471	Total	C	N	O	S	14	6	0
			3802	2410	651	720	21			

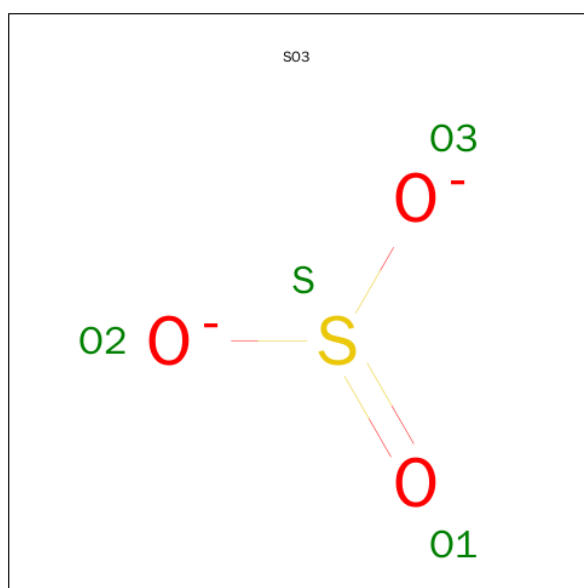
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	218	PHE	TYR	ENGINEERED	UNP Q9S1E5

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is SULFITE ION (three-letter code: SO3) (formula: O₃S).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 5 is YTTRIUM ION (three-letter code: Y1) (formula: Y).

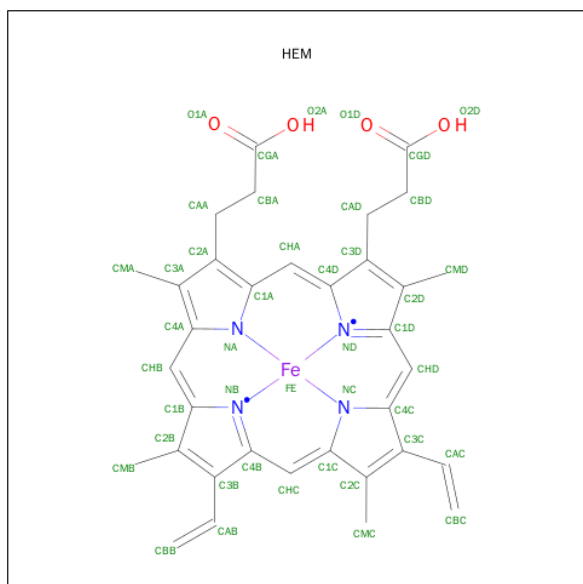
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Y	0	0
			3	3		

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 8 is water.

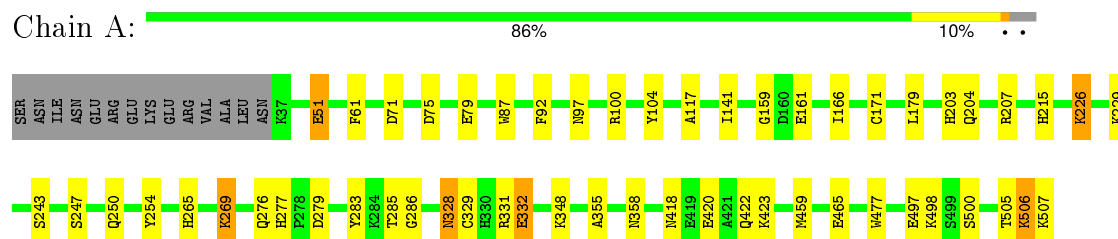
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	714	Total	O	0	0
			714	714		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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.

Note EDS failed to run properly.

- Molecule 1: Cytochrome c-552



4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	119.35Å 119.47Å 184.79Å 89.76° 89.90° 90.22°	Depositor
Resolution (Å)	40.39 – 1.30	Depositor
% Data completeness (in resolution range)	98.4 (40.39-1.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 1.30Å)	Xtriage
Refinement program	REFMAC 5.3.0008	Depositor
R, R_{free}	0.181 , 0.208	Depositor
Wilson B-factor (Å ²)	18.2	Xtriage
Anisotropy	0.329	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 160805 reflections	Xtriage
Total number of atoms	4756	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CA, SO3, SO4, ACT, Y1, HEM

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	0.50	1/3911 (0.0%)	0.64	2/5265 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	229	LYS	CG-CD	-9.51	1.20	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	LYS	N-CA-CB	-5.70	100.33	110.60
1	A	229	LYS	CB-CG-CD	5.31	125.40	111.60

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	3802	0	3732	62	0
2	A	1	0	0	0	0
3	A	4	0	0	0	0
4	A	5	0	0	1	0
5	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	12	0	9	0	0
7	A	215	0	150	15	0
8	A	714	0	0	8	0
All	All	4756	0	3891	63	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 8.

The worst 5 of 63 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:171:CYS:SG	7:A:514:HEM:CAC	2.04	1.43
1:A:171:CYS:SG	7:A:514:HEM:HAC	1.69	1.22
1:A:329:CYS:SG	7:A:517:HEM:CAC	2.38	1.11
1:A:329:CYS:HG	7:A:517:HEM:CAC	1.71	1.01
1:A:100:ARG:HH12	1:A:507:LYS:HD3	1.26	1.00

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	475/485 (98%)	466 (98%)	8 (2%)	1 (0%)	52 20

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	ILE

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	403/410 (98%)	394 (98%)	9 (2%)	60 17

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	328	ASN
1	A	506	LYS
1	A	348	LYS
1	A	269	LYS
1	A	332	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	GLN
1	A	452	GLN
1	A	418	ASN
1	A	204	GLN
1	A	352	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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	ACT	A	4	-	1,3,3	1.30	0	0,3,3	0.00	-
3	SO3	A	508	7	1,3,3	0.56	0	0,3,3	0.00	-
4	SO4	A	509	-	4,4,4	0.24	0	6,6,6	0.28	0
6	ACT	A	511	-	1,3,3	1.25	0	0,3,3	0.00	-
6	ACT	A	512	-	1,3,3	1.45	0	0,3,3	0.00	-
7	HEM	A	513	1,3	30,50,50	2.17	6 (20%)	24,82,82	2.67	9 (37%)
7	HEM	A	514	1	30,50,50	2.33	5 (16%)	24,82,82	2.46	11 (45%)
7	HEM	A	515	1	30,50,50	2.23	5 (16%)	24,82,82	2.77	12 (50%)
7	HEM	A	516	1	30,50,50	2.46	6 (20%)	24,82,82	2.87	9 (37%)
7	HEM	A	517	1	30,50,50	2.26	7 (23%)	24,82,82	2.57	10 (41%)

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
6	ACT	A	4	-	-	0/0/0/0	0/0/0/0
3	SO3	A	508	7	-	0/0/0/0	0/0/0/0
4	SO4	A	509	-	-	0/0/0/0	0/0/0/0
6	ACT	A	511	-	-	0/0/0/0	0/0/0/0
6	ACT	A	512	-	-	0/0/0/0	0/0/0/0
7	HEM	A	513	1,3	-	0/10/54/54	0/0/8/8
7	HEM	A	514	1	-	0/10/54/54	0/0/8/8
7	HEM	A	515	1	-	0/10/54/54	0/0/8/8
7	HEM	A	516	1	-	0/10/54/54	0/0/8/8
7	HEM	A	517	1	-	0/10/54/54	0/0/8/8

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	516	HEM	C3B-C4B	-10.20	1.42	1.51
7	A	517	HEM	C3B-C4B	-8.39	1.44	1.51
7	A	514	HEM	C3B-C4B	-8.12	1.44	1.51
7	A	515	HEM	C3B-C4B	-7.41	1.45	1.51
7	A	513	HEM	C3B-C4B	-7.23	1.45	1.51

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	516	HEM	C3B-CAB-CBB	-7.73	112.60	124.46
7	A	513	HEM	C3B-CAB-CBB	-6.57	114.38	124.46
7	A	515	HEM	C3B-CAB-CBB	-4.97	116.84	124.46
7	A	517	HEM	CBA-CAA-C2A	-4.04	105.29	112.53
7	A	514	HEM	C3B-CAB-CBB	-3.84	118.57	124.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	509	SO4	1	0
7	A	514	HEM	9	0
7	A	515	HEM	1	0
7	A	517	HEM	6	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 failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.