



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 08:37 PM GMT

PDB ID : 1KSU
Title : Crystal Structure of His505Tyr Mutant Flavocytochrome c3 from *Shewanella frigidimarina*
Authors : Pankhurst, K.L.; Mowat, C.G.; Miles, C.S.; Leys, D.; Walkinshaw, M.D.; Reid, G.A.; Chapman, S.K.
Deposited on : 2002-01-14
Resolution : 2.00 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

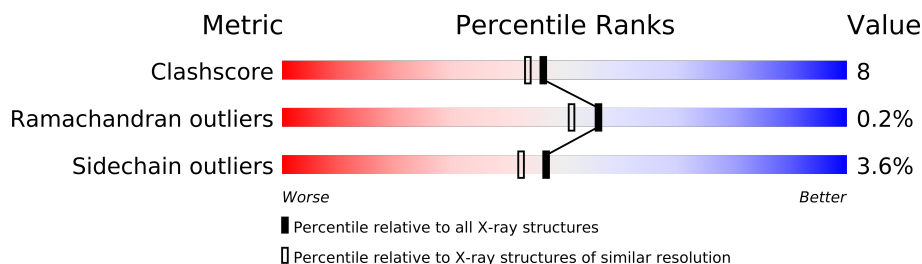
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : NOT EXECUTED
EDS : NOT EXECUTED
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.00 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	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	571	
1	B	571	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	FUM	B	3806	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10753 atoms, of which 0 are hydrogen and 0 are deuterium.

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 flavocytochrome c.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	568	Total	C	N	O	S	0	0	0
			4202	2608	738	831	25			
1	B	568	Total	C	N	O	S	0	0	0
			4216	2617	742	832	25			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	505	TYR	HIS	ENGINEERED	UNP Q02469
B	505	TYR	HIS	ENGINEERED	UNP Q02469

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Na	0	0
			1	1		
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



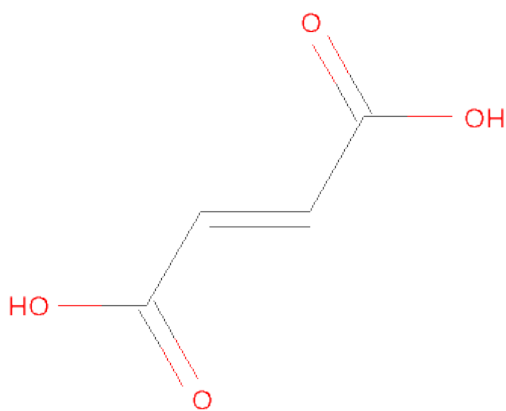
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B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

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is FUMARIC ACID (three-letter code: FUM) (formula: $C_4H_4O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	4	4		
5	B	1	Total	C	O	0	0
			8	4	4		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	932	Total 932	O 932	0	0
6	B	935	Total 935	O 935	0	0

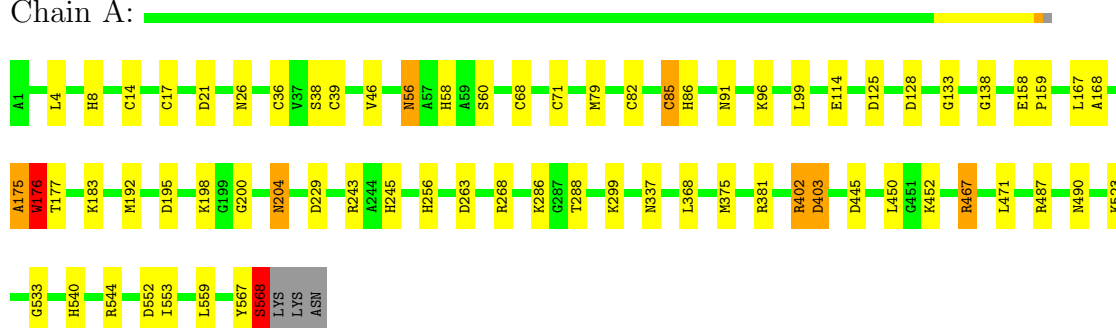
3 Residue-property plots

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 ($RSRZ > 2$). 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 was not executed.

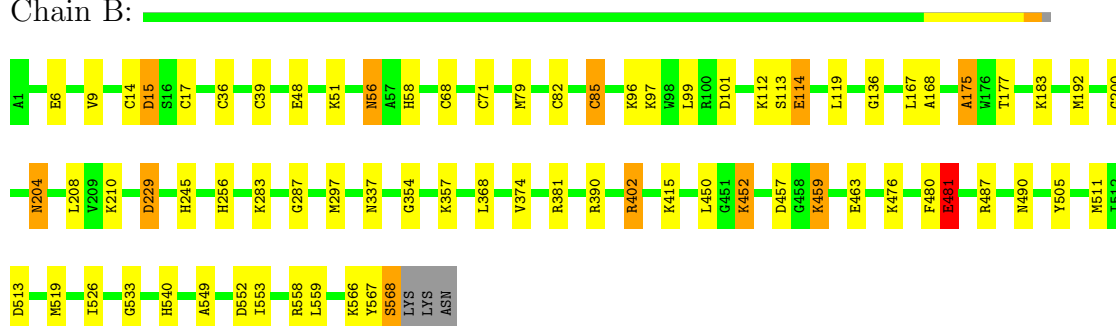
- Molecule 1: flavocytochrome c

Chain A:



- Molecule 1: flavocytochrome c

Chain B:



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.99Å 87.27Å 89.37Å 90.00° 104.43° 90.00°	Depositor
Resolution (Å)	15.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-2.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.167 , 0.239	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10753	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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: HEM, FUM, FAD, NA

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	1/4272 (0.0%)	1.29	24/5779 (0.4%)
1	B	0.58	0/4286	1.26	21/5794 (0.4%)
All	All	0.59	1/8558 (0.0%)	1.28	45/11573 (0.4%)

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	2
1	B	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	176	TRP	N-CA	-5.74	1.34	1.46

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ALA	C-N-CA	18.36	167.60	121.70
1	A	467	ARG	NE-CZ-NH2	12.80	126.70	120.30
1	B	175	ALA	O-C-N	-11.50	104.30	122.70
1	A	487	ARG	NE-CZ-NH2	11.50	126.05	120.30
1	A	381	ARG	NE-CZ-NH1	10.86	125.73	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	ASP	Mainchain
1	A	175	ALA	Peptide
1	B	175	ALA	Mainchain,Peptide

5.2 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4202	0	4124	61	0
1	B	4216	0	4160	80	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	172	0	120	28	0
3	B	172	0	120	32	0
4	A	53	0	30	5	0
4	B	53	0	30	6	0
5	A	8	0	2	3	0
5	B	8	0	2	1	0
6	A	932	0	0	8	0
6	B	935	0	0	18	0
All	All	10753	0	8588	143	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

The worst 5 of 143 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:36:CYS:SG	3:A:802:HEM:CAB	2.44	1.04
1:B:36:CYS:SG	3:B:802:HEM:CAB	2.44	1.04
1:B:82:CYS:SG	3:B:804:HEM:CAB	2.48	1.02
1:B:68:CYS:SG	3:B:803:HEM:CAB	2.51	0.99
1:B:82:CYS:HG	3:B:804:HEM:CAB	1.77	0.97

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	566/571 (99%)	546 (96%)	19 (3%)	1 (0%)	56	51
1	B	566/571 (99%)	548 (97%)	17 (3%)	1 (0%)	56	51
All	All	1132/1142 (99%)	1094 (97%)	36 (3%)	2 (0%)	56	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	TRP
1	B	114	GLU

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	437/445 (98%)	422 (97%)	15 (3%)	49	45
1	B	441/445 (99%)	424 (96%)	17 (4%)	43	38
All	All	878/890 (99%)	846 (96%)	32 (4%)	47	42

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	568	SER
1	B	56	ASN
1	B	481	GLU
1	B	51	LYS
1	B	99	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such

sidechains are listed below:

Mol	Chain	Res	Type
1	B	35	GLN
1	B	54	HIS
1	B	245	HIS
1	A	540	HIS
1	B	256	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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, 2 are monoatomic - leaving 12 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	$\# Z > 2$
4	FAD	A	2805	-	58,58,58	1.67	11 (18%)	85,89,89	2.28	26 (30%)
5	FUM	A	2806	-	7,7,7	2.34	4 (57%)	8,8,8	2.11	4 (50%)
3	HEM	A	801	1	49,50,50	2.51	12 (24%)	46,82,82	1.94	7 (15%)
3	HEM	A	802	1	49,50,50	2.69	14 (28%)	46,82,82	2.02	8 (17%)
3	HEM	A	803	1	49,50,50	2.32	12 (24%)	46,82,82	1.86	9 (19%)
3	HEM	A	804	1	49,50,50	2.53	12 (24%)	46,82,82	1.70	5 (10%)
4	FAD	B	3805	-	58,58,58	1.80	11 (18%)	85,89,89	2.14	21 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FUM	B	3806	-	7,7,7	2.33	4 (57%)	8,8,8	2.26	6 (75%)
3	HEM	B	801	1	49,50,50	2.95	12 (24%)	46,82,82	1.94	9 (19%)
3	HEM	B	802	1	49,50,50	2.76	11 (22%)	46,82,82	2.31	12 (26%)
3	HEM	B	803	1	49,50,50	2.17	12 (24%)	46,82,82	1.90	10 (21%)
3	HEM	B	804	1	49,50,50	2.79	16 (32%)	46,82,82	1.82	11 (23%)

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
4	FAD	A	2805	-	1/1/9/9	0/34/50/50	0/1/6/6
5	FUM	A	2806	-	-	0/5/5/5	0/0/0/0
3	HEM	A	801	1	-	0/14/114/114	0/0/8/8
3	HEM	A	802	1	-	0/14/114/114	0/0/8/8
3	HEM	A	803	1	-	0/14/114/114	0/0/8/8
3	HEM	A	804	1	-	0/14/114/114	0/0/8/8
4	FAD	B	3805	-	1/1/9/9	0/34/50/50	0/1/6/6
5	FUM	B	3806	-	-	0/5/5/5	0/0/0/0
3	HEM	B	801	1	-	0/14/114/114	0/0/8/8
3	HEM	B	802	1	-	0/14/114/114	0/0/8/8
3	HEM	B	803	1	-	0/14/114/114	0/0/8/8
3	HEM	B	804	1	-	0/14/114/114	0/0/8/8

The worst 5 of 131 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	HEM	C2B-C1B	10.59	1.47	1.44
3	B	804	HEM	C2D-C1D	9.83	1.47	1.44
3	B	801	HEM	C2D-C1D	9.29	1.46	1.44
3	B	802	HEM	C2D-C1D	8.56	1.46	1.44
3	A	804	HEM	C2D-C1D	8.23	1.46	1.44

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	HEM	C3B-C4B-NB	-10.25	106.67	114.00
3	A	802	HEM	C3B-C4B-NB	-9.53	107.18	114.00
3	A	801	HEM	C3B-C4B-NB	-9.03	107.54	114.00
4	B	3805	FAD	C4X-C10-N10	-8.06	116.49	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2805	FAD	C4X-C10-N10	-7.83	116.60	120.51

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	3805	FAD	C4'
4	A	2805	FAD	C4'

There are no torsion outliers.

There are no ring outliers.

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 was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.