Full wwPDB X-ray Structure Validation Report ⓘ

Jun 2, 2025 – 04:03 pm BST

PDB ID	:	9GKH / pdb_00009gkh
Title	:	KvPepIH62A mutant,F420-dependent oxidoreductase
Authors	:	Mueller, R.; Zhao, H.; Sikandar, A.
Deposited on	:	2024-08-24
Resolution	:	1.70 Å(reported)

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

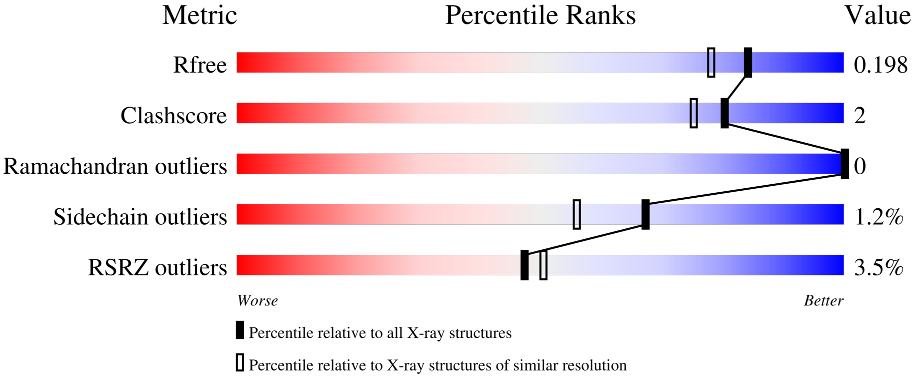
MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance ⓘ

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

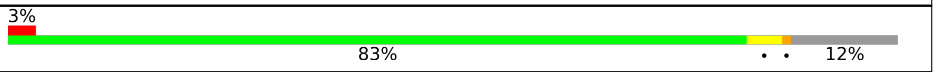
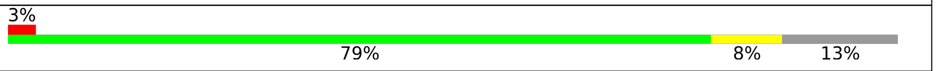
The reported resolution of this entry is 1.70 Å.

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}	164625	5161 (1.70-1.70)
Clashscore	180529	5671 (1.70-1.70)
Ramachandran outliers	177936	5594 (1.70-1.70)
Sidechain outliers	177891	5594 (1.70-1.70)
RSRZ outliers	164620	5159 (1.70-1.70)

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 <=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	308	
1	B	308	

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 4461 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 Putative F420-dependent oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total 2050	C 1292	N 365	O 383	S 10	0	0	0
1	B	268	Total 2031	C 1280	N 360	O 381	S 10	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A561UC02
A	2	GLY	-	expression tag	UNP A0A561UC02
A	3	SER	-	expression tag	UNP A0A561UC02
A	4	SER	-	expression tag	UNP A0A561UC02
A	5	HIS	-	expression tag	UNP A0A561UC02
A	6	HIS	-	expression tag	UNP A0A561UC02
A	7	HIS	-	expression tag	UNP A0A561UC02
A	8	HIS	-	expression tag	UNP A0A561UC02
A	9	HIS	-	expression tag	UNP A0A561UC02
A	10	HIS	-	expression tag	UNP A0A561UC02
A	11	SER	-	expression tag	UNP A0A561UC02
A	12	SER	-	expression tag	UNP A0A561UC02
A	13	GLY	-	expression tag	UNP A0A561UC02
A	14	LEU	-	expression tag	UNP A0A561UC02
A	15	VAL	-	expression tag	UNP A0A561UC02
A	16	PRO	-	expression tag	UNP A0A561UC02
A	17	ARG	-	expression tag	UNP A0A561UC02
A	18	GLY	-	expression tag	UNP A0A561UC02
A	19	SER	-	expression tag	UNP A0A561UC02
A	20	HIS	-	expression tag	UNP A0A561UC02
A	62	ALA	HIS	conflict	UNP A0A561UC02
B	1	MET	-	initiating methionine	UNP A0A561UC02
B	2	GLY	-	expression tag	UNP A0A561UC02
B	3	SER	-	expression tag	UNP A0A561UC02
B	4	SER	-	expression tag	UNP A0A561UC02

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Chain	Residue	Modelled	Actual	Comment	Reference
B	5	HIS	-	expression tag	UNP A0A561UC02
B	6	HIS	-	expression tag	UNP A0A561UC02
B	7	HIS	-	expression tag	UNP A0A561UC02
B	8	HIS	-	expression tag	UNP A0A561UC02
B	9	HIS	-	expression tag	UNP A0A561UC02
B	10	HIS	-	expression tag	UNP A0A561UC02
B	11	SER	-	expression tag	UNP A0A561UC02
B	12	SER	-	expression tag	UNP A0A561UC02
B	13	GLY	-	expression tag	UNP A0A561UC02
B	14	LEU	-	expression tag	UNP A0A561UC02
B	15	VAL	-	expression tag	UNP A0A561UC02
B	16	PRO	-	expression tag	UNP A0A561UC02
B	17	ARG	-	expression tag	UNP A0A561UC02
B	18	GLY	-	expression tag	UNP A0A561UC02
B	19	SER	-	expression tag	UNP A0A561UC02
B	20	HIS	-	expression tag	UNP A0A561UC02
B	62	ALA	HIS	conflict	UNP A0A561UC02

- Molecule 2 is water.

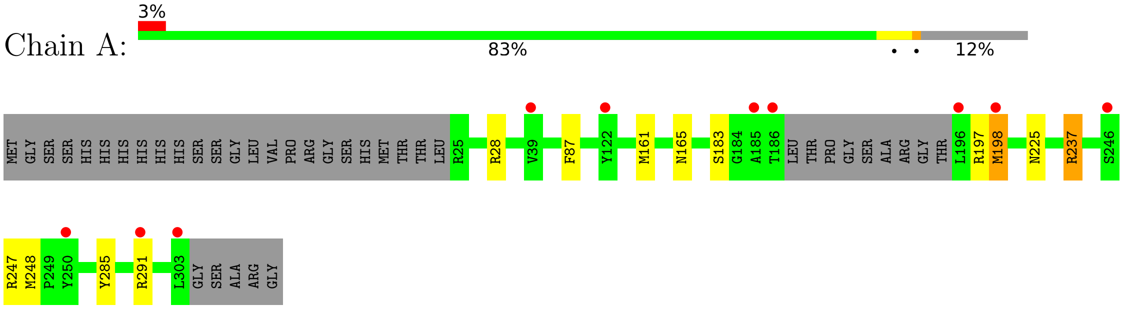
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	205	Total O 205 205	0	0
2	B	175	Total O 175 175	0	0

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 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.

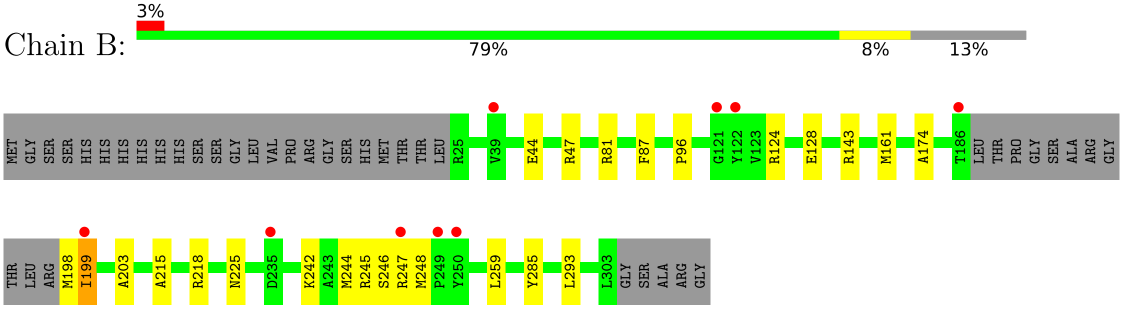
- Molecule 1: Putative F420-dependent oxidoreductase

Chain A:



- Molecule 1: Putative F420-dependent oxidoreductase

Chain B:



4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	56.21Å 94.28Å 110.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.28 – 1.70 48.28 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.28-1.70) 100.0 (48.28-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 1.70Å)	Xtriage
Refinement program	PHENIX (1.19.1_4122: ???)	Depositor
R, R_{free}	0.173 , 0.194 0.184 , 0.198	Depositor DCC
R_{free} test set	3297 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	24.6	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 30.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4461	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 6.15% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.51	0/2086	0.73	0/2838
1	B	0.54	0/2067	0.71	0/2813
All	All	0.52	0/4153	0.72	0/5651

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	4
1	B	0	3
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	**Chain**	**Res**	**Type**	**Group**
1	A	197	ARG	Sidechain
1	A	237	ARG	Sidechain
1	A	247	ARG	Sidechain
1	A	291	ARG	Sidechain
1	B	218	ARG	Sidechain
1	B	245	ARG	Sidechain
1	B	247	ARG	Sidechain

5.2 Too-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 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	2050	0	2057	6	0
1	B	2031	0	2033	14	0
2	A	205	0	0	0	0
2	B	175	0	0	1	0
All	All	4461	0	4090	20	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 2.

All (20) 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:B:198:MET:HE3	1:B:259:LEU:HD13	1.76	0.66
1:B:87:PHE:HD1	1:B:161:MET:HE1	1.64	0.63
1:B:244:MET:HE2	1:B:248:MET:HE1	1.84	0.59
1:B:87:PHE:CD1	1:B:161:MET:HE1	2.40	0.56
1:B:44:GLU:OE1	1:B:47:ARG:NH1	2.44	0.51
1:B:81:ARG:NH1	2:B:403:HOH:O	2.44	0.48
1:A:165:ASN:ND2	1:A:183:SER:O	2.39	0.48
1:B:124:ARG:O	1:B:128:GLU:HG3	2.16	0.46
1:A:225:ASN:HA	1:A:285:TYR:O	2.16	0.46
1:A:87:PHE:CD1	1:A:161:MET:HE1	2.52	0.45
1:B:199:ILE:HG23	1:B:203:ALA:HB3	1.99	0.45
1:A:198:MET:HE2	1:A:198:MET:HA	1.99	0.44
1:B:96:PRO:HG3	1:B:143:ARG:NH2	2.32	0.44
1:B:225:ASN:HA	1:B:285:TYR:O	2.17	0.44
1:A:198:MET:HG3	1:A:248:MET:SD	2.59	0.42
1:B:293:LEU:HD23	1:B:293:LEU:C	2.44	0.42
1:B:96:PRO:CG	1:B:143:ARG:NH2	2.83	0.42
1:B:174:ALA:HB1	1:B:215:ALA:HA	2.02	0.41
1:A:28:ARG:HH11	1:A:28:ARG:HD2	1.74	0.40
1:B:244:MET:HE2	1:B:248:MET:CE	2.52	0.40

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	266/308 (86%)	263 (99%)	3 (1%)	0	100	100
1	B	264/308 (86%)	261 (99%)	3 (1%)	0	100	100
All	All	530/616 (86%)	524 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	210/239 (88%)	208 (99%)	2 (1%)	73	64
1	B	208/239 (87%)	205 (99%)	3 (1%)	62	49
All	All	418/478 (87%)	413 (99%)	5 (1%)	67	56

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	MET
1	A	237	ARG
1	B	199	ILE
1	B	242	LYS
1	B	246	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	221	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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

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	270/308 (87%)	0.12	10 (3%) 45 48	19, 25, 42, 50	0
1	B	268/308 (87%)	0.13	9 (3%) 48 51	19, 25, 47, 89	0
All	All	538/616 (87%)	0.12	19 (3%) 47 50	19, 25, 43, 89	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	122	TYR	5.7
1	B	122	TYR	5.4
1	B	186	THR	4.3
1	A	186	THR	3.9
1	B	250	TYR	3.2
1	A	185	ALA	3.2
1	A	196	LEU	3.2
1	A	291	ARG	3.0
1	B	247	ARG	2.9
1	B	249	PRO	2.8
1	B	235	ASP	2.7
1	B	39	VAL	2.7
1	A	303	LEU	2.7
1	B	199	ILE	2.6
1	A	250	TYR	2.3
1	A	198	MET	2.1
1	A	246	SER	2.1
1	A	39	VAL	2.1
1	B	121	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.