



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 30, 2024 – 08:55 PM EST

PDB ID : 1JQK  
Title : Crystal structure of carbon monoxide dehydrogenase from *Rhodospirillum rubrum*  
Authors : Drennan, C.L.; Heo, J.; Sintchak, M.D.; Schreiter, E.; Ludden, P.W.  
Deposited on : 2001-08-07  
Resolution : 2.80 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
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) : 2.36

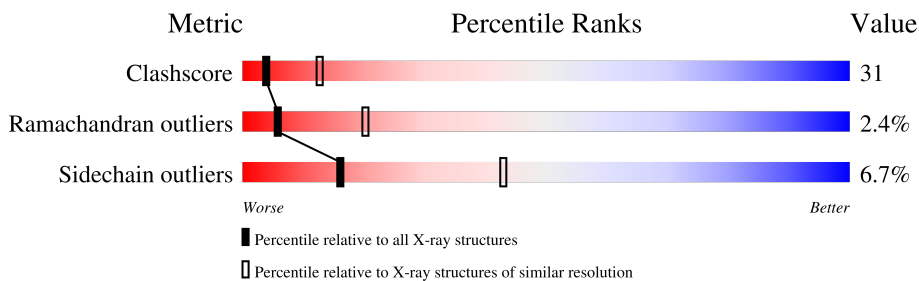
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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  $\geq 3$ , 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	639	48% (green), 43% (yellow), 5% (red), 5% (orange), 5% (grey)
1	B	639	51% (green), 38% (yellow), 5% (red), 5% (orange), 5% (grey)
1	C	639	54% (green), 36% (yellow), 5% (red), 5% (orange), 5% (grey)
1	D	639	53% (green), 38% (yellow), 5% (red), 5% (orange), 5% (grey)
1	E	639	52% (green), 38% (yellow), 5% (red), 5% (orange), 5% (grey)
1	F	639	50% (green), 41% (yellow), 5% (red), 5% (orange), 5% (grey)

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26898 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 carbon monoxide dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	610	4461	2798	792	838	33	0	0	0
1	B	610	4461	2798	792	838	33	0	0	0
1	C	610	4461	2798	792	838	33	0	0	0
1	D	610	4461	2798	792	838	33	0	0	0
1	E	610	4461	2798	792	838	33	0	0	0
1	F	610	4461	2798	792	838	33	0	0	0

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

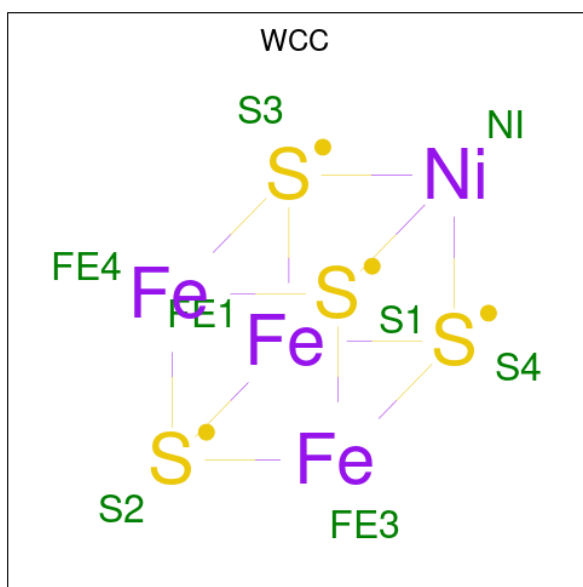
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		
2	E	1	Total	Fe	0	0
			1	1		
2	F	1	Total	Fe	0	0
			1	1		

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	E	1	Total	Fe	S	0	0
			8	4	4		
3	E	1	Total	Fe	S	0	0
			8	4	4		
3	F	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is FE(3)-NI(1)-S(4) CLUSTER (three-letter code: WCC) (formula: Fe<sub>3</sub>NiS<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Fe	Ni	S		
4	A	1	8	3	1	4	0	0
4	B	1	8	3	1	4	0	0
4	C	1	8	3	1	4	0	0
4	D	1	8	3	1	4	0	0
4	E	1	8	3	1	4	0	0
4	F	1	8	3	1	4	0	0

- Molecule 5 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	X		
5	A	1	1	1	0	0
5	B	1	1	1	0	0
5	C	1	1	1	0	0
5	D	1	1	1	0	0
5	E	1	1	1	0	0
5	F	1	1	1	0	0

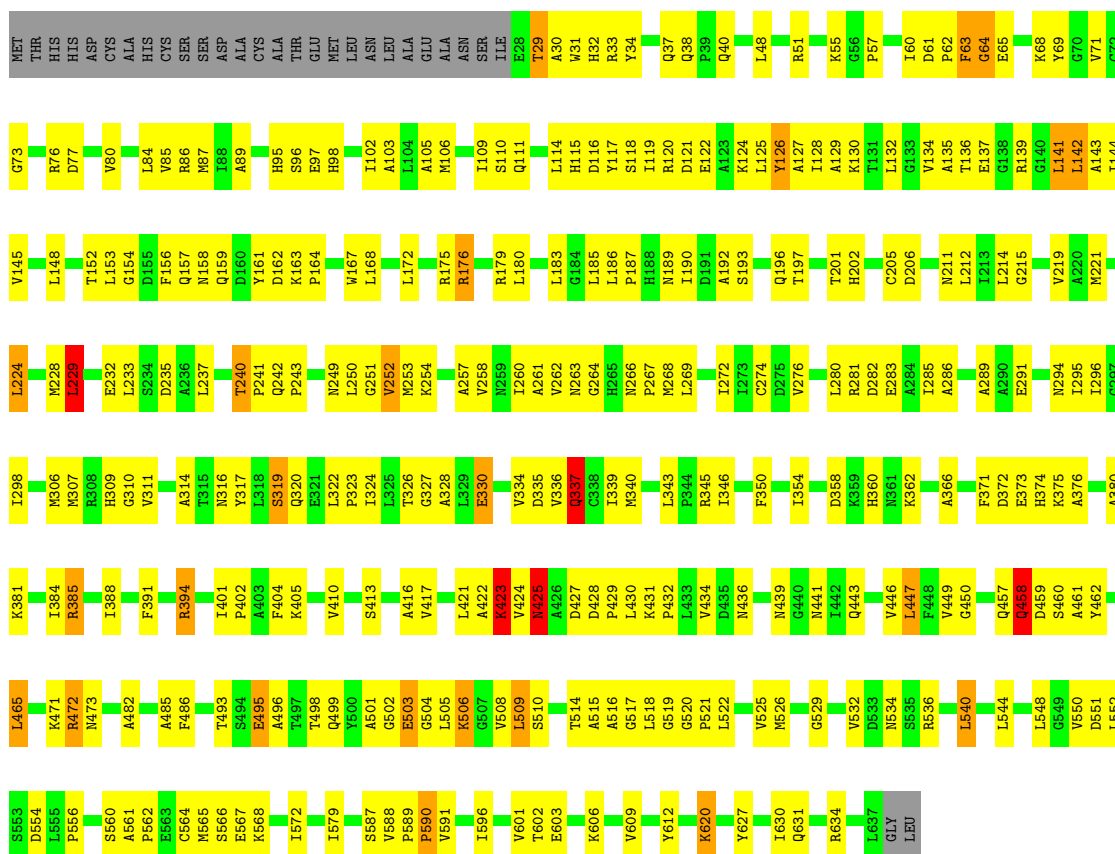
### 3 Residue-property plots

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. 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: carbon monoxide dehydrogenase

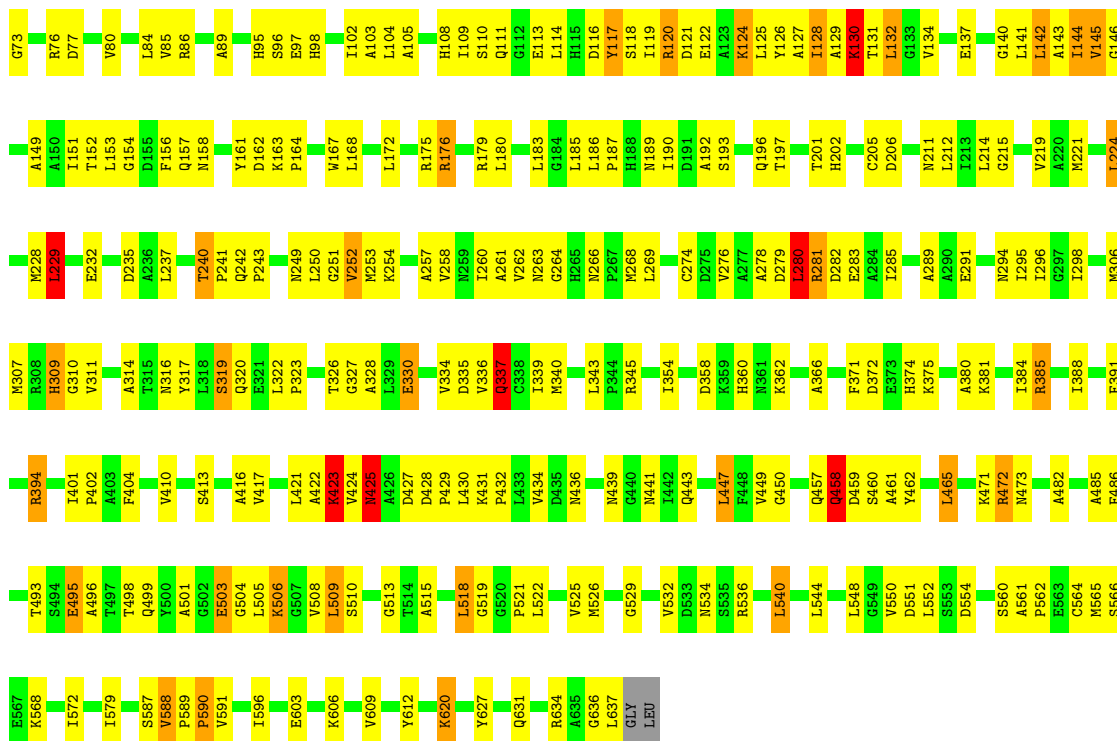
Chain A: 



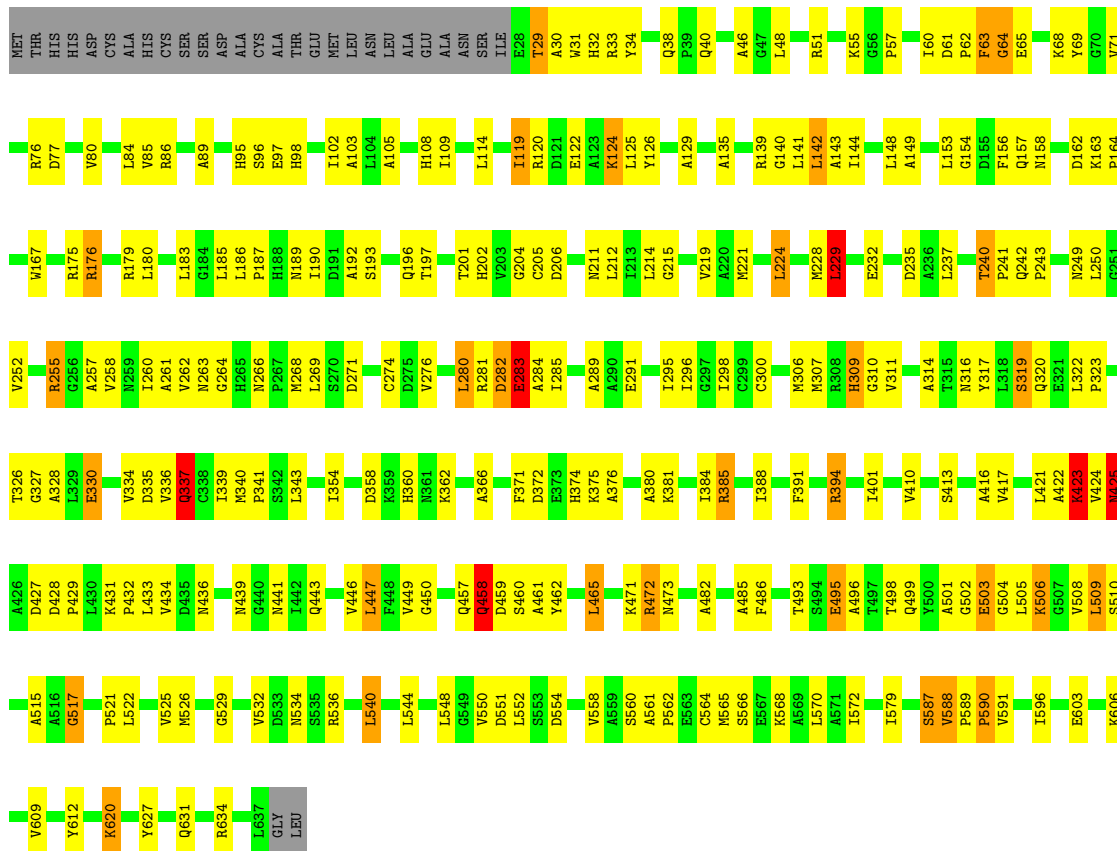
- Molecule 1: carbon monoxide dehydrogenase

Chain B: 



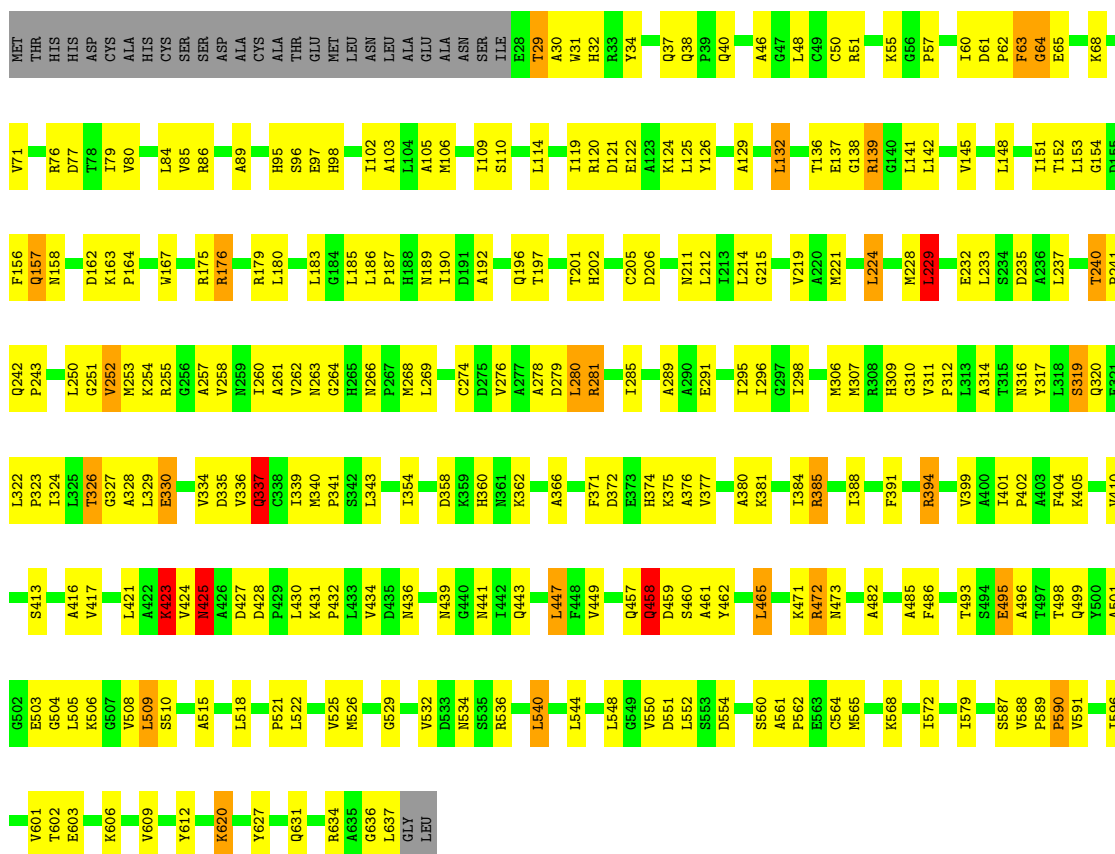


• Molecule 1: carbon monoxide dehydrogenase



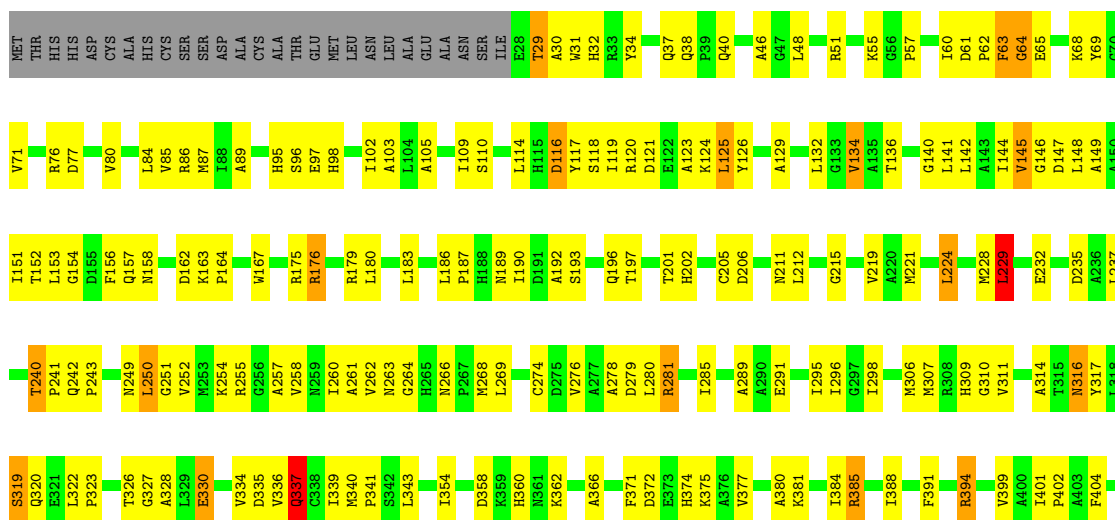
- Molecule 1: carbon monoxide dehydrogenase

Chain D: 53% 38% 5%

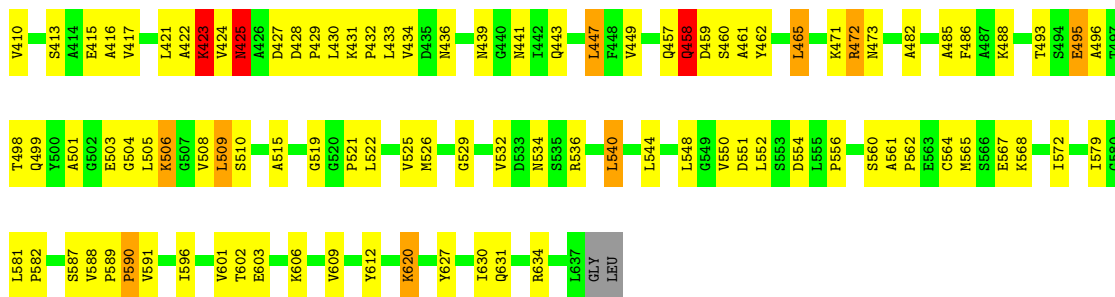


- Molecule 1: carbon monoxide dehydrogenase

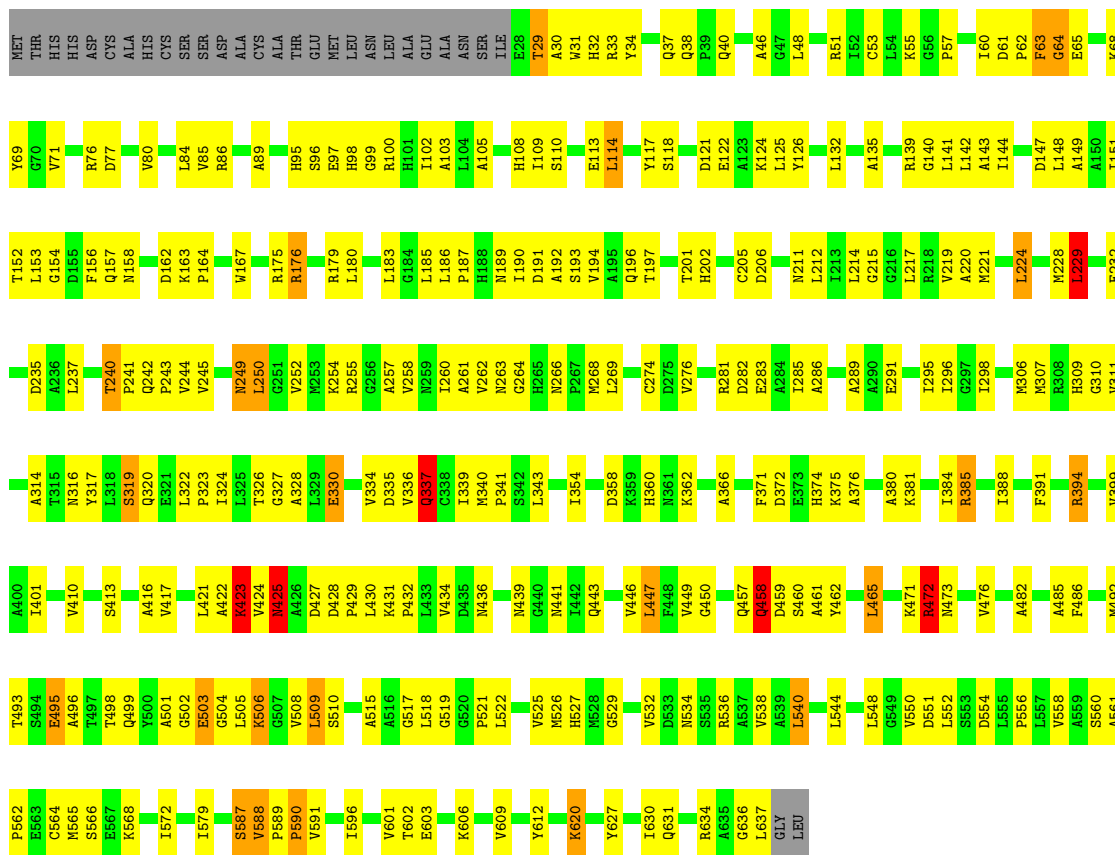
Chain E: 52% 38% 5%







● Molecule 1: carbon monoxide dehydrogenase



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.60Å 200.10Å 116.80Å 90.00° 111.50° 90.00°	Depositor
Resolution (Å)	100.00 – 2.80	Depositor
% Data completeness (in resolution range)	76.9 (100.00-2.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.257 , 0.287	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	26898	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

## 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: SF4, FE2, UNX, WCC

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	0.35	0/4534	0.62	1/6161 (0.0%)
1	B	0.36	0/4534	0.63	1/6161 (0.0%)
1	C	0.40	0/4534	0.64	1/6161 (0.0%)
1	D	0.41	0/4534	0.64	1/6161 (0.0%)
1	E	0.41	0/4534	0.65	1/6161 (0.0%)
1	F	0.42	0/4534	0.65	1/6161 (0.0%)
All	All	0.39	0/27204	0.64	6/36966 (0.0%)

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	E	0	1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	229	LEU	CA-CB-CG	6.07	129.27	115.30
1	A	229	LEU	CA-CB-CG	5.67	128.35	115.30
1	D	229	LEU	CA-CB-CG	5.59	128.16	115.30
1	C	229	LEU	CA-CB-CG	5.47	127.89	115.30
1	F	229	LEU	CA-CB-CG	5.45	127.84	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	126	TYR	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	4461	0	4529	311	0
1	B	4461	0	4529	341	0
1	C	4461	0	4529	262	0
1	D	4461	0	4528	267	0
1	E	4461	0	4528	273	0
1	F	4461	0	4528	280	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	1	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	16	0	0	0	0
3	B	8	0	0	0	0
3	C	16	0	0	0	0
3	D	8	0	0	0	0
3	E	16	0	0	0	0
3	F	8	0	0	0	0
4	A	8	0	0	1	0
4	B	8	0	0	1	0
4	C	8	0	0	1	0
4	D	8	0	0	0	0
4	E	8	0	0	0	0
4	F	8	0	0	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
All	All	26898	0	27171	1652	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 31.

The worst 5 of 1652 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:C:65:GLU:HA	1:C:68:LYS:HE2	1.34	1.09
1:D:65:GLU:HA	1:D:68:LYS:HE2	1.35	1.08
1:E:65:GLU:HA	1:E:68:LYS:HE2	1.34	1.08
1:A:65:GLU:HA	1:A:68:LYS:HE2	1.33	1.07
1:F:65:GLU:HA	1:F:68:LYS:HE2	1.34	1.06

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	608/639 (95%)	523 (86%)	69 (11%)	16 (3%)	5	18
1	B	608/639 (95%)	510 (84%)	79 (13%)	19 (3%)	4	14
1	C	608/639 (95%)	535 (88%)	58 (10%)	15 (2%)	5	19
1	D	608/639 (95%)	535 (88%)	64 (10%)	9 (2%)	10	33
1	E	608/639 (95%)	530 (87%)	66 (11%)	12 (2%)	7	24
1	F	608/639 (95%)	537 (88%)	56 (9%)	15 (2%)	5	19
All	All	3648/3834 (95%)	3170 (87%)	392 (11%)	86 (2%)	6	20

5 of 86 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	GLY
1	A	141	LEU
1	A	337	GLN
1	A	425	ASN
1	A	458	GLN

### 5.3.2 Protein sidechains [i](#)

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	466/490 (95%)	438 (94%)	28 (6%)	19	48
1	B	466/490 (95%)	433 (93%)	33 (7%)	14	39
1	C	466/490 (95%)	436 (94%)	30 (6%)	17	45
1	D	466/490 (95%)	432 (93%)	34 (7%)	14	38
1	E	466/490 (95%)	433 (93%)	33 (7%)	14	39
1	F	466/490 (95%)	437 (94%)	29 (6%)	18	47
All	All	2796/2940 (95%)	2609 (93%)	187 (7%)	16	43

5 of 187 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	458	GLN
1	E	337	GLN
1	D	508	VAL
1	E	125	LEU
1	E	465	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	202	HIS
1	F	202	HIS
1	E	266	ASN
1	E	441	ASN
1	F	361	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 6 are monoatomic and 6 are unknown - leaving 15 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	WCC	E	800	2,5,1	0,12,12	-	-	-		
4	WCC	B	800	2,5,1	0,12,12	-	-	-		
3	SF4	B	750	1	0,12,12	-	-	-		
3	SF4	A	700	1	0,12,12	-	-	-		
3	SF4	E	750	1	0,12,12	-	-	-		
3	SF4	A	750	1	0,12,12	-	-	-		
3	SF4	E	702	1	0,12,12	-	-	-		
4	WCC	D	800	2,5,1	0,12,12	-	-	-		
3	SF4	C	701	1	0,12,12	-	-	-		
3	SF4	F	750	1	0,12,12	-	-	-		
3	SF4	C	750	1	0,12,12	-	-	-		
4	WCC	A	800	2,5,1	0,12,12	-	-	-		
4	WCC	F	800	2,5,1	0,12,12	-	-	-		
4	WCC	C	800	2,5,1	0,12,12	-	-	-		
3	SF4	D	750	1	0,12,12	-	-	-		

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	WCC	E	800	2,5,1	-	-	0/6/5/5
4	WCC	B	800	2,5,1	-	-	0/6/5/5
3	SF4	B	750	1	-	-	0/6/5/5
3	SF4	A	700	1	-	-	0/6/5/5
3	SF4	E	750	1	-	-	0/6/5/5
3	SF4	A	750	1	-	-	0/6/5/5
3	SF4	E	702	1	-	-	0/6/5/5
4	WCC	D	800	2,5,1	-	-	0/6/5/5
3	SF4	C	701	1	-	-	0/6/5/5
3	SF4	F	750	1	-	-	0/6/5/5
3	SF4	C	750	1	-	-	0/6/5/5
4	WCC	A	800	2,5,1	-	-	0/6/5/5
4	WCC	F	800	2,5,1	-	-	0/6/5/5
4	WCC	C	800	2,5,1	-	-	0/6/5/5
3	SF4	D	750	1	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	800	WCC	1	0
4	A	800	WCC	1	0
4	F	800	WCC	1	0
4	C	800	WCC	1	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.