



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 10, 2025 – 01:33 pm GMT

PDB ID : 9GYB
Title : Crystal structure of the recombinant CODH from Rhodospirillum rubrum produced in Escherichia coli
Authors : Cavazza, C.; Contaldo, U.
Deposited on : 2024-10-01
Resolution : 2.90 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

<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>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
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)	:	2.40

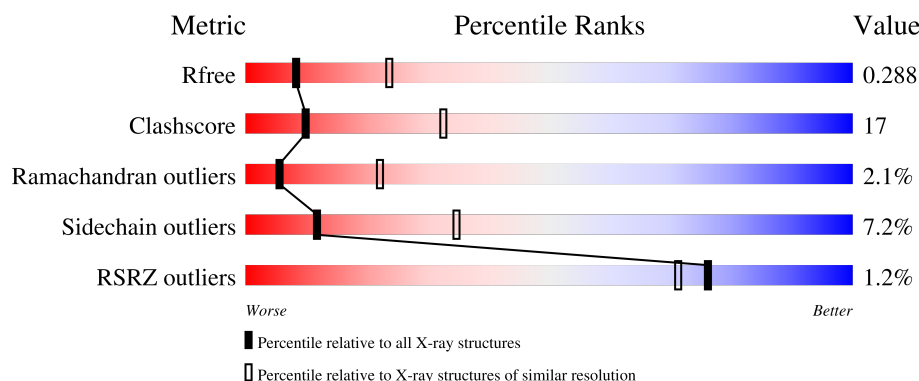
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	639	
1	B	639	
1	C	639	
1	D	639	
1	E	639	

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Mol	Chain	Length	Quality of chain
1	F	639	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	RQM	A	702	-	-	X	-
3	RQM	B	703	-	-	X	-
3	RQM	E	703	-	-	X	-
3	RQM	F	702	-	-	X	-

2 Entry composition [i](#)

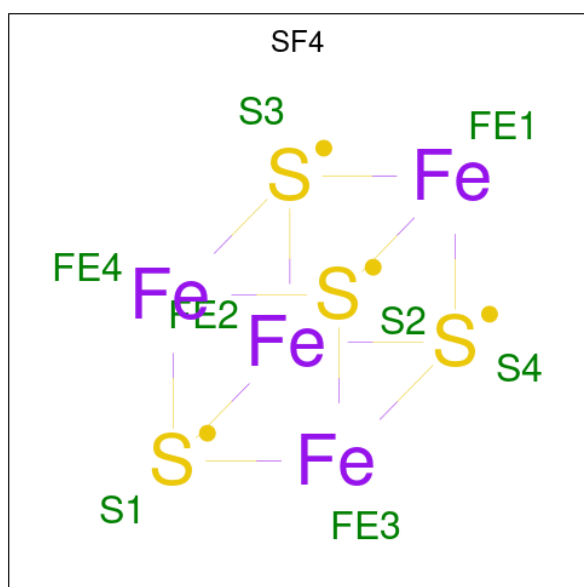
There are 4 unique types of molecules in this entry. The entry contains 27316 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

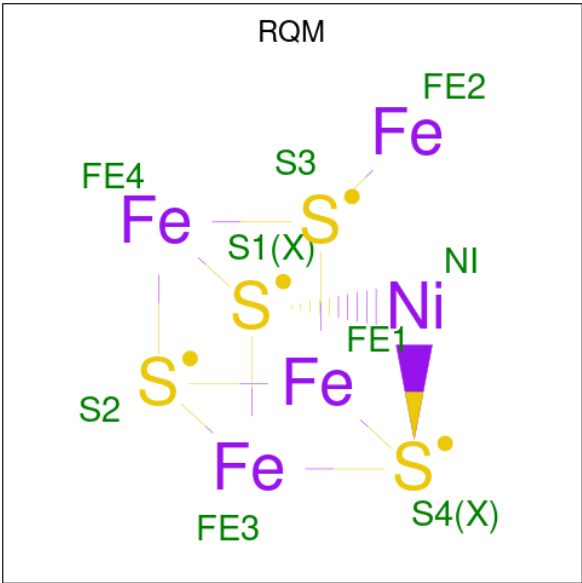
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	620	Total	C	N	O	S	0	0	0
			4538	2845	804	855	34			
1	B	620	Total	C	N	O	S	0	0	0
			4538	2845	804	855	34			
1	C	620	Total	C	N	O	S	0	0	0
			4538	2845	804	855	34			
1	D	621	Total	C	N	O	S	0	0	0
			4547	2850	805	858	34			
1	E	617	Total	C	N	O	S	0	0	0
			4514	2830	800	851	33			
1	F	617	Total	C	N	O	S	0	0	0
			4514	2830	800	851	33			

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 3 is Fe(3)-Ni(1)-S(4) cluster (three-letter code: RQM) (formula: Fe₄NiS₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe Ni S 9 4 1 4	0	0
3	B	1	Total Fe Ni S 9 4 1 4	0	0
3	C	1	Total Fe Ni S 9 4 1 4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
3	E	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
3	F	1	Total	Fe	Ni	S	0	0
			9	4	1	4		

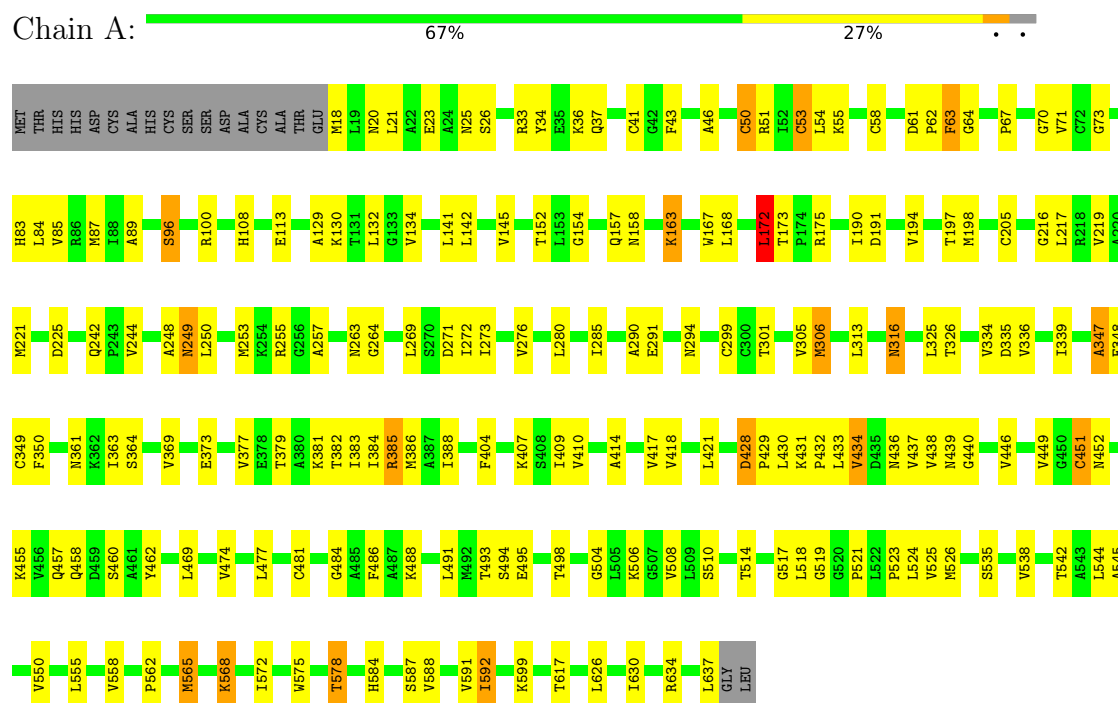
- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Na	0	0
			1	1		

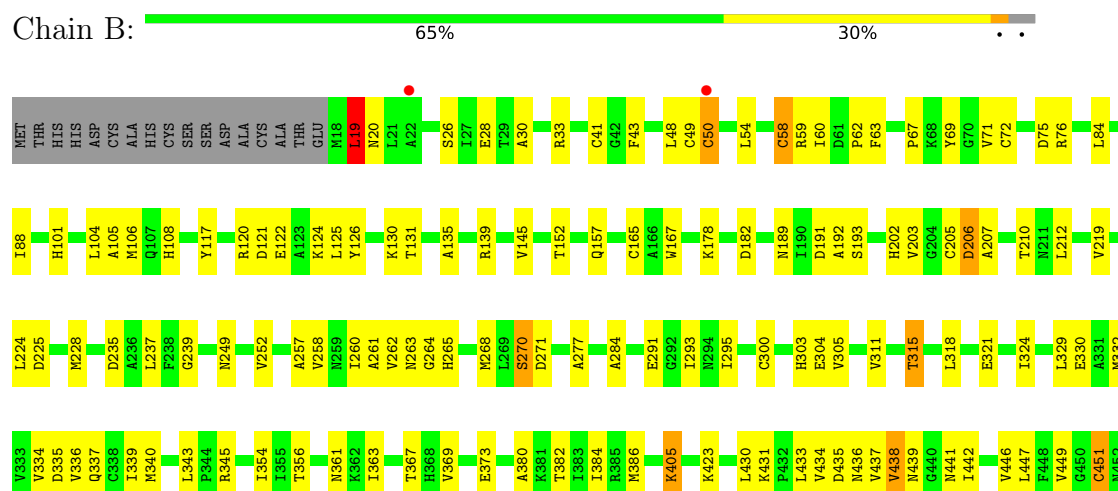
3 Residue-property plots

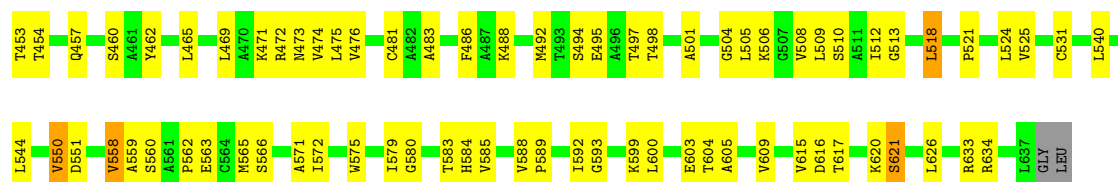
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Carbon monoxide dehydrogenase



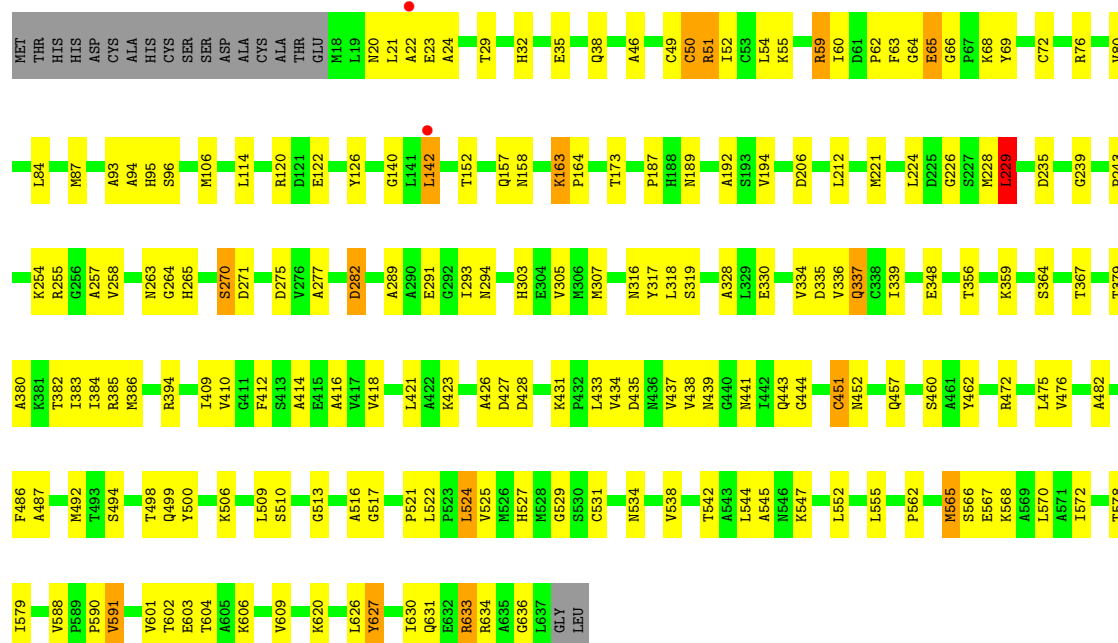
• Molecule 1: Carbon monoxide dehydrogenase





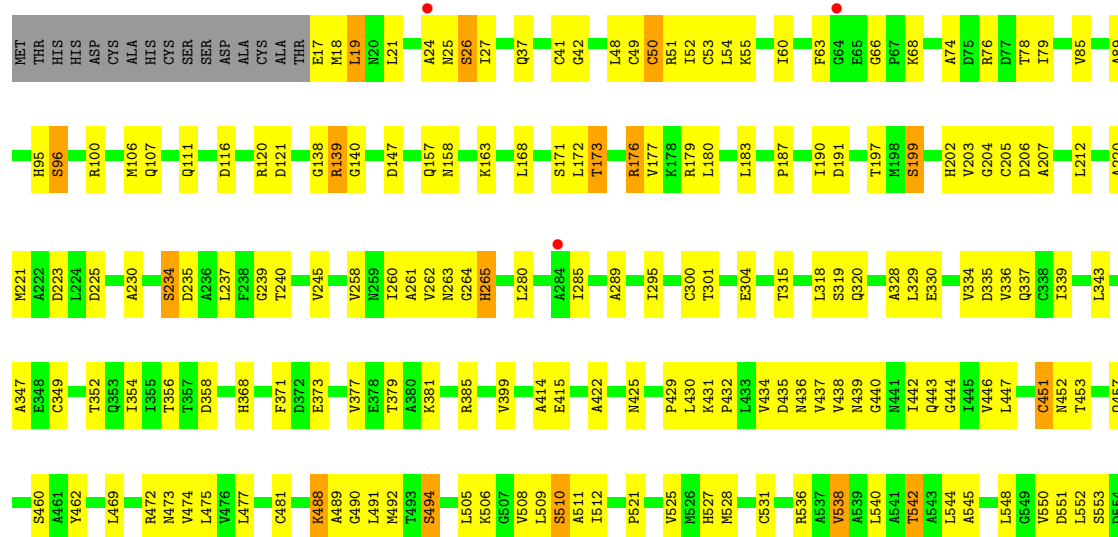
• Molecule 1: Carbon monoxide dehydrogenase

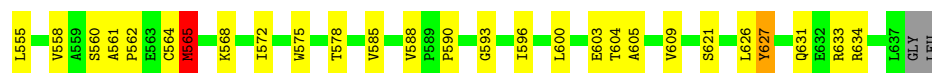
Chain C: 68% 27%



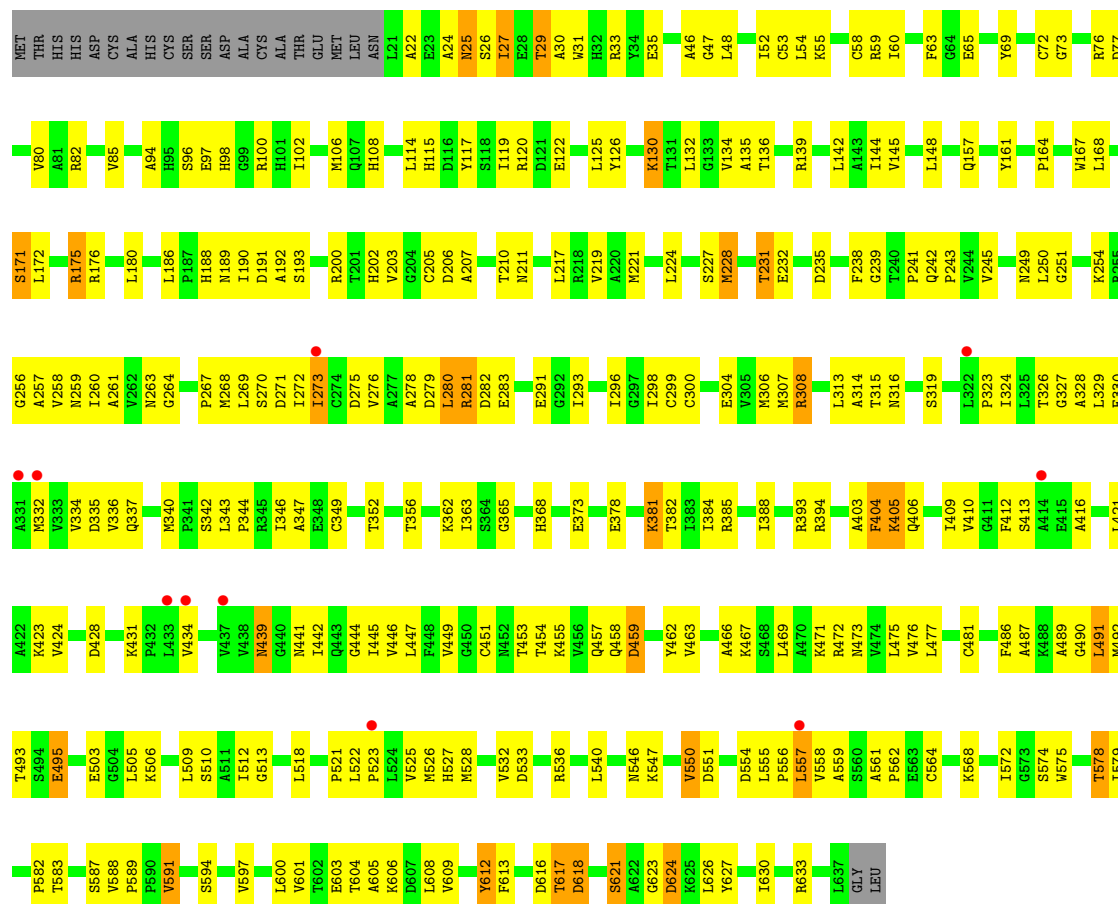
• Molecule 1: Carbon monoxide dehydrogenase

Chain D: 65% 30%

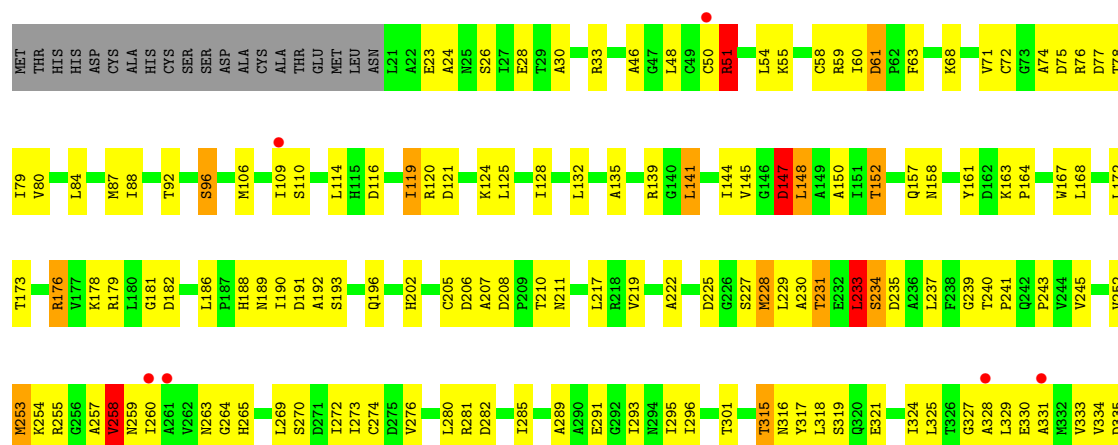


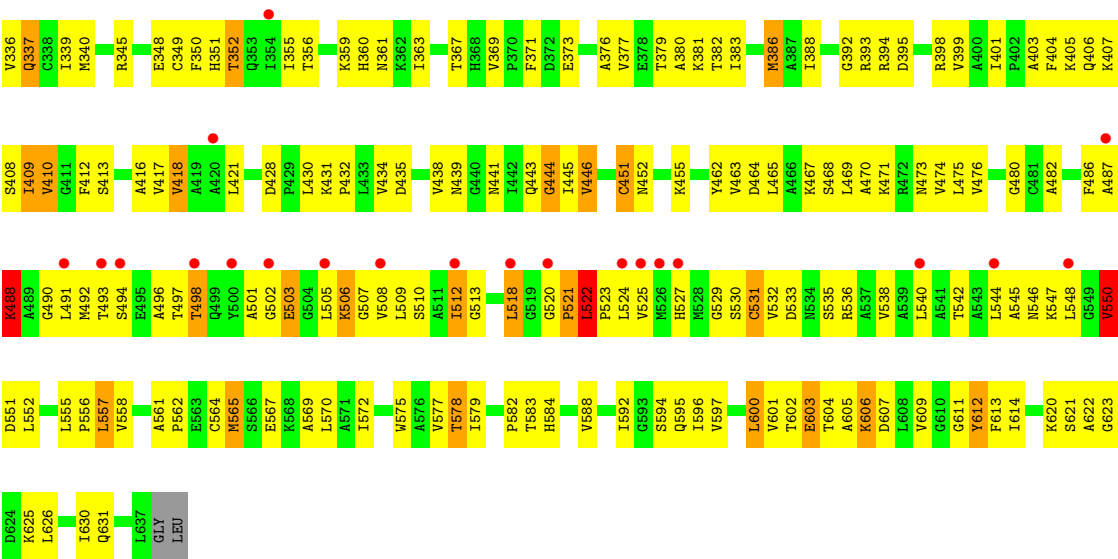


• Molecule 1: Carbon monoxide dehydrogenase



• Molecule 1: Carbon monoxide dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.45Å 200.57Å 116.37Å 90.00° 111.21° 90.00°	Depositor
Resolution (Å)	47.71 – 2.90 47.71 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.1 (47.71-2.90) 99.1 (47.71-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.227 , 0.288 0.227 , 0.288	Depositor DCC
R_{free} test set	1100 reflections (1.27%)	wwPDB-VP
Wilson B-factor (Å ²)	81.6	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 61.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.044 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	27316	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, NA, RQM

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	0.26	0/4611	0.52	1/6265 (0.0%)
1	B	0.25	0/4611	0.51	0/6265
1	C	0.25	0/4611	0.51	1/6265 (0.0%)
1	D	0.26	0/4620	0.52	0/6277
1	E	0.28	0/4587	0.57	0/6233
1	F	0.29	0/4587	0.61	4/6233 (0.1%)
All	All	0.27	0/27627	0.54	6/37538 (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	3
1	F	0	1
All	All	0	4

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	F	522	LEU	CB-CG-CD1	-6.78	99.48	111.00
1	F	233	LEU	CB-CG-CD2	-6.74	99.55	111.00
1	F	233	LEU	CB-CG-CD1	6.60	122.22	111.00
1	A	172	LEU	CA-CB-CG	6.33	129.86	115.30
1	C	229	LEU	CA-CB-CG	5.71	128.44	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	25	ASN	Peptide
1	E	423	LYS	Peptide
1	E	616	ASP	Peptide
1	F	348	GLU	Peptide

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	4538	0	4609	125	0
1	B	4538	0	4608	135	0
1	C	4538	0	4609	127	0
1	D	4547	0	4614	138	0
1	E	4514	0	4582	224	1
1	F	4514	0	4582	269	1
2	A	8	0	0	1	0
2	B	16	0	0	0	0
2	C	16	0	0	0	0
2	D	8	0	0	0	0
2	E	16	0	0	1	0
2	F	8	0	0	0	0
3	A	9	0	0	2	0
3	B	9	0	0	3	0
3	C	9	0	0	1	0
3	D	9	0	0	0	0
3	E	9	0	0	2	0
3	F	9	0	0	2	0
4	D	1	0	0	0	0
All	All	27316	0	27604	947	1

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 17.

The worst 5 of 947 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:F:503:GLU:HA	1:F:506:LYS:HD2	1.46	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:106:MET:HA	1:F:109:ILE:HG12	1.47	0.93
1:F:318:LEU:HD13	1:F:452:ASN:HB3	1.52	0.89
1:F:230:ALA:O	1:F:234:SER:OG	1.93	0.85
1:F:497:THR:OG1	1:F:522:LEU:O	1.94	0.85

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:254:LYS:NZ	1:F:291:GLU:OE2[1_655]	2.15	0.05

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	618/639 (97%)	558 (90%)	53 (9%)	7 (1%)	12	37
1	B	618/639 (97%)	553 (90%)	58 (9%)	7 (1%)	12	37
1	C	618/639 (97%)	561 (91%)	49 (8%)	8 (1%)	10	33
1	D	619/639 (97%)	556 (90%)	51 (8%)	12 (2%)	6	24
1	E	615/639 (96%)	527 (86%)	73 (12%)	15 (2%)	5	19
1	F	615/639 (96%)	523 (85%)	64 (10%)	28 (5%)	2	8
All	All	3703/3834 (97%)	3278 (88%)	348 (9%)	77 (2%)	5	22

5 of 77 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	26	SER
1	C	65	GLU
1	D	265	HIS
1	D	490	GLY

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Mol	Chain	Res	Type
1	E	27	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	475/490 (97%)	443 (93%)	32 (7%)	13	39
1	B	475/490 (97%)	441 (93%)	34 (7%)	12	35
1	C	475/490 (97%)	447 (94%)	28 (6%)	16	45
1	D	476/490 (97%)	447 (94%)	29 (6%)	15	43
1	E	472/490 (96%)	438 (93%)	34 (7%)	12	35
1	F	472/490 (96%)	423 (90%)	49 (10%)	5	18
All	All	2845/2940 (97%)	2639 (93%)	206 (7%)	12	35

5 of 206 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	542	THR
1	E	439	ASN
1	F	550	VAL
1	D	578	THR
1	E	134	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	98	HIS
1	E	38	GLN
1	F	361	ASN
1	D	441	ASN
1	E	196	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 1 is monoatomic - 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	$\# Z > 2$
3	RQM	C	703	1	0,12,12	-	-	-		
3	RQM	F	702	1	0,12,12	-	-	-		
2	SF4	C	701	1	0,12,12	-	-	-		
2	SF4	A	701	1	0,12,12	-	-	-		
3	RQM	D	702	1	0,12,12	-	-	-		
3	RQM	E	703	1	0,12,12	-	-	-		
2	SF4	C	702	1	0,12,12	-	-	-		
2	SF4	B	701	1	0,12,12	-	-	-		
2	SF4	E	702	1	0,12,12	-	-	-		
2	SF4	F	701	1	0,12,12	-	-	-		
2	SF4	B	702	1	0,12,12	-	-	-		
2	SF4	D	701	1	0,12,12	-	-	-		
2	SF4	E	701	1	0,12,12	-	-	-		
3	RQM	A	702	1	0,12,12	-	-	-		
3	RQM	B	703	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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	RQM	C	703	1	-	-	0/4/4/4
3	RQM	F	702	1	-	-	0/4/4/4
2	SF4	C	701	1	-	-	0/6/5/5
2	SF4	A	701	1	-	-	0/6/5/5
3	RQM	D	702	1	-	-	0/4/4/4
3	RQM	E	703	1	-	-	0/4/4/4
2	SF4	C	702	1	-	-	0/6/5/5
2	SF4	B	701	1	-	-	0/6/5/5
2	SF4	E	702	1	-	-	0/6/5/5
2	SF4	F	701	1	-	-	0/6/5/5
2	SF4	B	702	1	-	-	0/6/5/5
2	SF4	D	701	1	-	-	0/6/5/5
2	SF4	E	701	1	-	-	0/6/5/5
3	RQM	A	702	1	-	-	0/4/4/4
3	RQM	B	703	1	-	-	0/4/4/4

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.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	703	RQM	1	0
3	F	702	RQM	2	0
2	A	701	SF4	1	0
3	E	703	RQM	2	0
2	E	701	SF4	1	0
3	A	702	RQM	2	0
3	B	703	RQM	3	0

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 [i](#)

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

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	620/639 (97%)	-0.25	0 100 100	43, 69, 90, 110	0
1	B	620/639 (97%)	-0.34	2 (0%) 90 88	44, 67, 87, 107	0
1	C	620/639 (97%)	-0.33	2 (0%) 90 88	47, 68, 90, 116	0
1	D	621/639 (97%)	-0.37	3 (0%) 87 84	43, 67, 88, 108	0
1	E	617/639 (96%)	0.16	10 (1%) 70 64	72, 103, 129, 146	0
1	F	617/639 (96%)	0.34	27 (4%) 39 33	76, 109, 135, 149	0
All	All	3715/3834 (96%)	-0.13	44 (1%) 76 71	43, 75, 123, 149	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	50	CYS	4.5
1	F	520	GLY	4.1
1	F	512	ILE	3.9
1	F	544	LEU	3.8
1	E	414	ALA	3.6

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	RQM	A	702	9/9	0.82	0.13	72,80,95,97	9
3	RQM	F	702	9/9	0.85	0.09	92,104,115,118	9
3	RQM	D	702	9/9	0.87	0.09	61,79,94,107	9
3	RQM	C	703	9/9	0.91	0.09	71,88,98,108	9
2	SF4	C	701	8/8	0.91	0.16	89,110,130,132	0
3	RQM	B	703	9/9	0.91	0.08	62,74,84,97	9
3	RQM	E	703	9/9	0.93	0.07	84,105,115,125	9
2	SF4	F	701	8/8	0.93	0.12	93,116,127,132	0
2	SF4	A	701	8/8	0.95	0.11	64,87,94,96	0
2	SF4	B	701	8/8	0.96	0.10	79,93,111,115	0
2	SF4	C	702	8/8	0.96	0.10	73,91,107,109	0
2	SF4	D	701	8/8	0.96	0.11	62,86,95,101	0
2	SF4	E	701	8/8	0.96	0.10	76,83,90,102	8
2	SF4	E	702	8/8	0.96	0.10	75,114,125,129	0
2	SF4	B	702	8/8	0.96	0.10	64,84,97,98	0
4	NA	D	703	1/1	0.96	0.13	42,42,42,42	0

6.5 Other polymers

There are no such residues in this entry.