wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 08:55 PM GMT

PDB ID	:	1MJG
Title	:	CRYSTAL STRUCTURE OF BIFUNCTIONAL CARBON MONOXIDE DEHYDROGENASE/ACETYL-COA SYNTHASE(CODH/ACS) FROM MOORELLA THERMOACETICA (F. CLOSTRIDIUM THERMOACETICUM)
Authors	:	Doukov, T.I.; Iverson, T.M.; Seravalli, J.; Ragsdale, S.W.; Drennan, C.L.
Deposited on	:	2002-08-27
Resolution	:	2.20 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 (i) symbol.

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

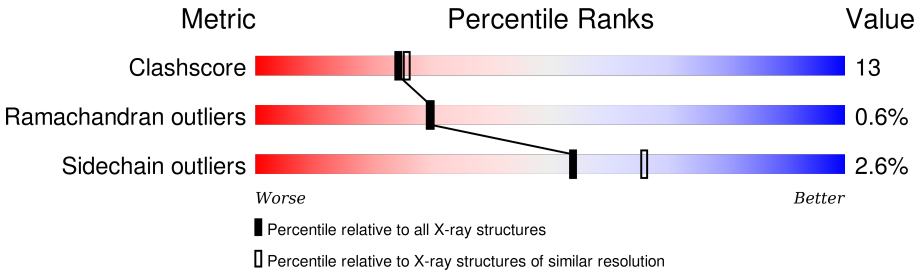
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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 <=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 was not executed.

Mol	Chain	Length	Quality of chain
1	A	674	78% 20%
1	B	674	78% 20%
1	C	674	78% 20%
1	D	674	78% 21%
2	M	729	77% 21%
2	N	729	77% 21%
2	O	729	72% 26%

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Mol	Chain	Length	Quality of chain
2	P	729	75% 24%

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
5	ACT	M	950	-	-	X	-
5	ACT	N	950	-	-	X	-
7	XCC	A	800	-	-	X	-
7	XCC	C	800	-	-	X	-
7	XCC	D	800	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 44653 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 BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	672	Total	C	N	O	S	0	0	0
			5087	3197	890	958	42			
1	B	672	Total	C	N	O	S	0	0	0
			5087	3197	890	958	42			
1	C	672	Total	C	N	O	S	0	0	0
			5087	3197	890	958	42			
1	D	672	Total	C	N	O	S	0	0	0
			5087	3197	890	958	42			

- Molecule 2 is a protein called Carbon monoxide dehydrogenase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	728	Total	C	N	O	S	0	0	0
			5735	3678	953	1069	35			
2	N	728	Total	C	N	O	S	0	0	0
			5735	3678	953	1069	35			
2	O	728	Total	C	N	O	S	0	0	0
			5735	3678	953	1069	35			
2	P	728	Total	C	N	O	S	0	0	0
			5735	3678	953	1069	35			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	685	SER	ARG	SEE REMARK 999	UNP P27988
N	685	SER	ARG	SEE REMARK 999	UNP P27988
O	685	SER	ARG	SEE REMARK 999	UNP P27988
P	685	SER	ARG	SEE REMARK 999	UNP P27988

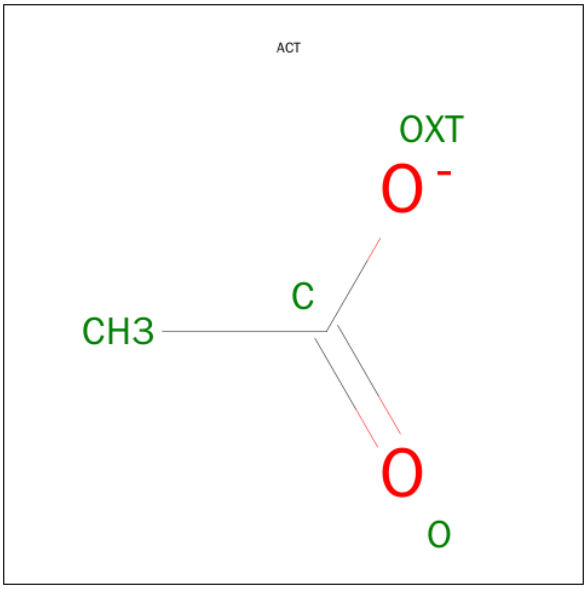
- Molecule 3 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	P	1	Total Cu 1 1	0	0
3	O	1	Total Cu 1 1	0	0
3	N	1	Total Cu 1 1	0	0
3	M	1	Total Cu 1 1	0	0

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	P	1	Total Ni 1 1	0	0
4	O	1	Total Ni 1 1	0	0
4	N	1	Total Ni 1 1	0	0
4	M	1	Total Ni 1 1	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	M	1	Total C O 3 2 1	0	0
5	N	1	Total C O 3 2 1	0	0

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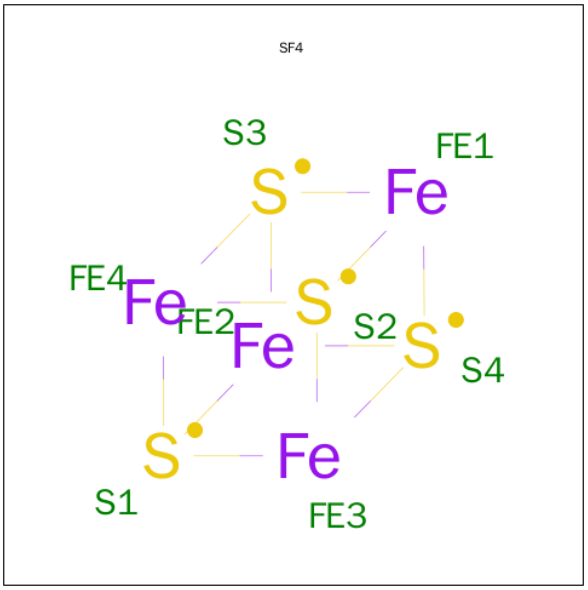
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	O	1	Total C O 3 2 1	0	0
5	P	1	Total C O 3 2 1	0	0

- Molecule 6 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Fe S 8 4 4	0	0
6	A	1	Total Fe S 8 4 4	0	0
6	B	1	Total Fe S 8 4 4	0	0
6	C	1	Total Fe S 8 4 4	0	0
6	C	1	Total Fe S 8 4 4	0	0
6	D	1	Total Fe S 8 4 4	0	0
6	M	1	Total Fe S 8 4 4	0	0
6	N	1	Total Fe S 8 4 4	0	0
6	O	1	Total Fe S 8 4 4	0	0

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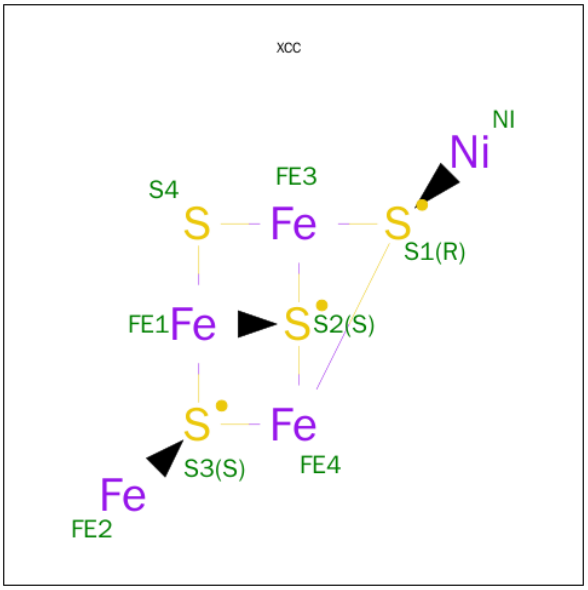
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	P	1	Total Fe S 8 4 4	0	0

- Molecule 7 is FE(4)-NI(1)-S(4) CLUSTER (three-letter code: XCC) (formula: Fe_4NiS_4).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	179	Total O 179 179	0	0
8	B	217	Total O 217 217	0	0
8	C	148	Total O 148 148	0	0
8	D	131	Total O 131 131	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	M	206	Total O 206 206	0	0
8	N	221	Total O 221 221	0	0
8	O	26	Total O 26 26	0	0
8	P	101	Total O 101 101	0	0

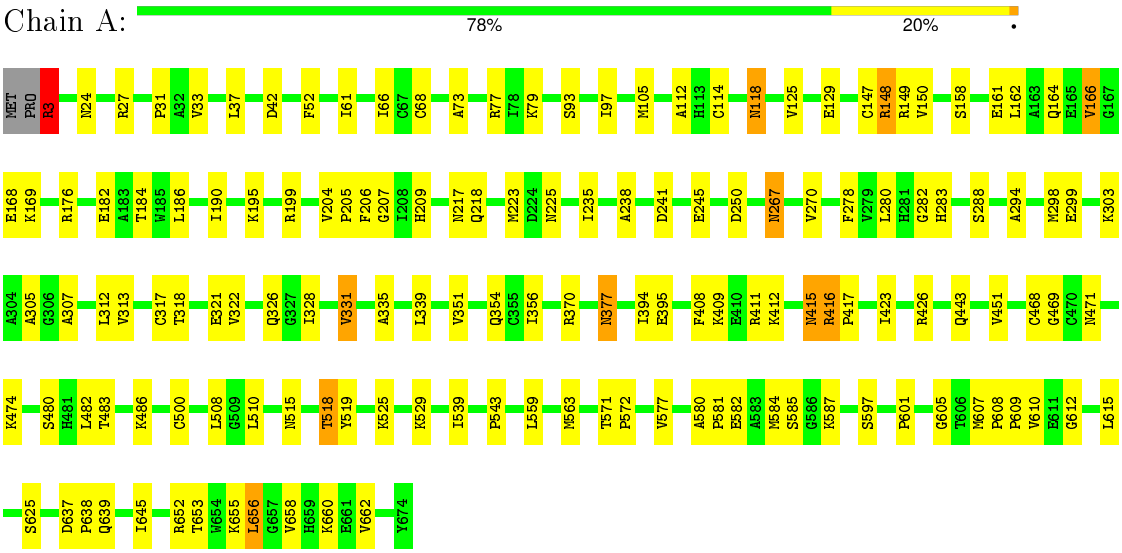
3 Residue-property plots (i)

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.

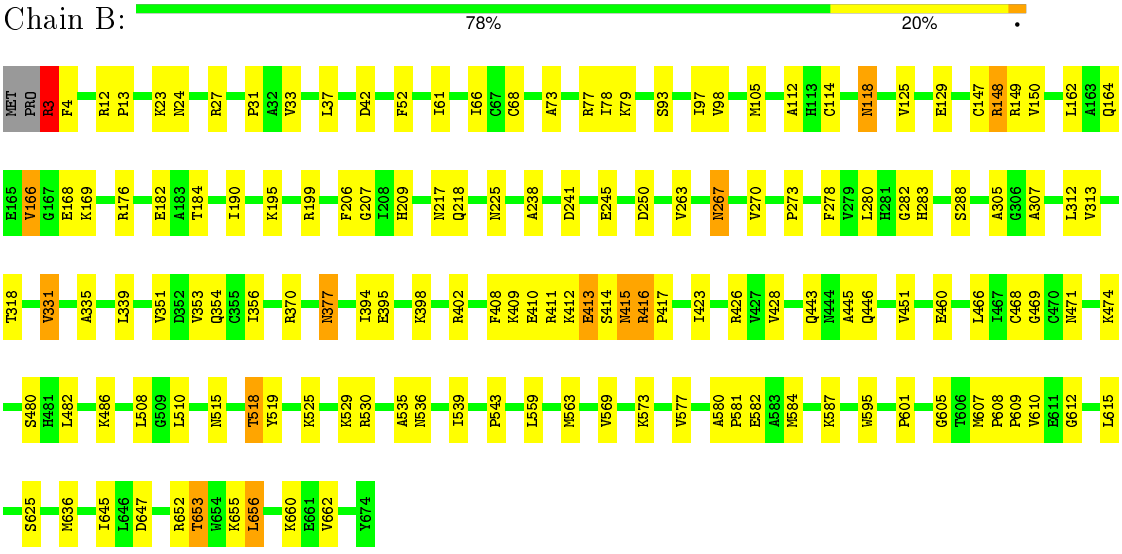
• Molecule 1: CARBON MONOXIDE DEHYDROGENASE BETA SUBUNIT

Chain A:



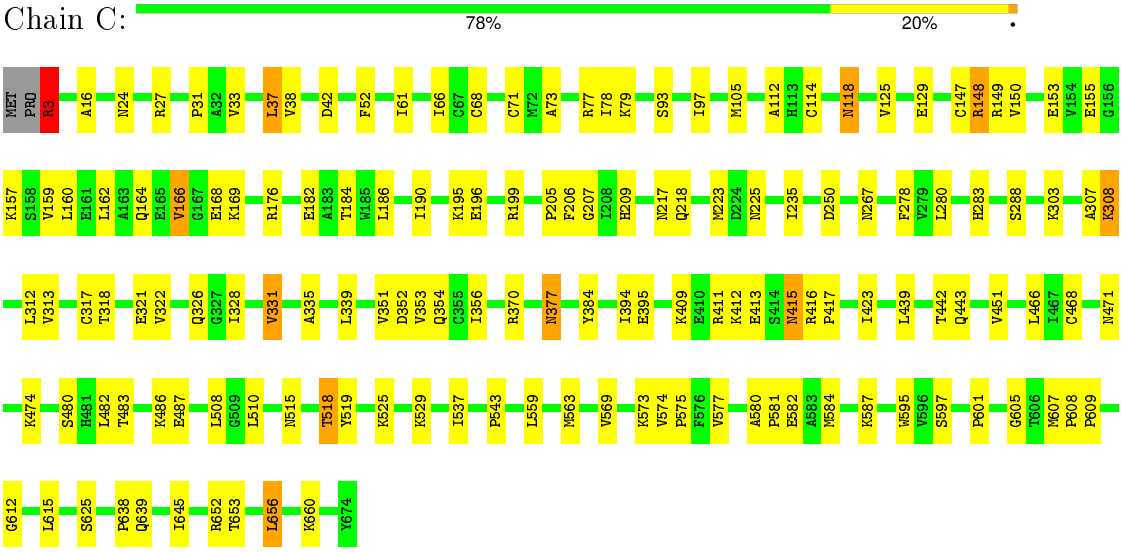
• Molecule 1: CARBON MONOXIDE DEHYDROGENASE BETA SUBUNIT

Chain B:



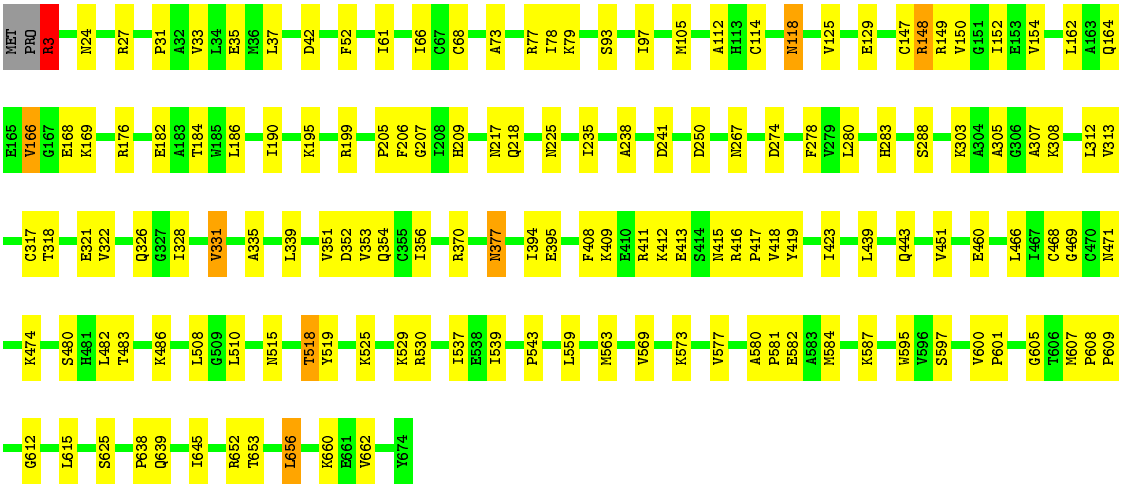
• Molecule 1: CARBON MONOXIDE DEHYDROGENASE BETA SUBUNIT

Chain C:



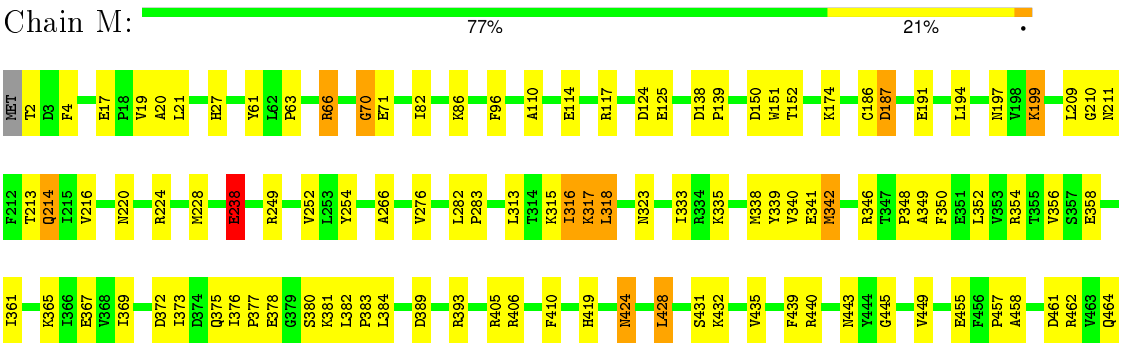
• Molecule 1: CARBON MONOXIDE DEHYDROGENASE BETA SUBUNIT

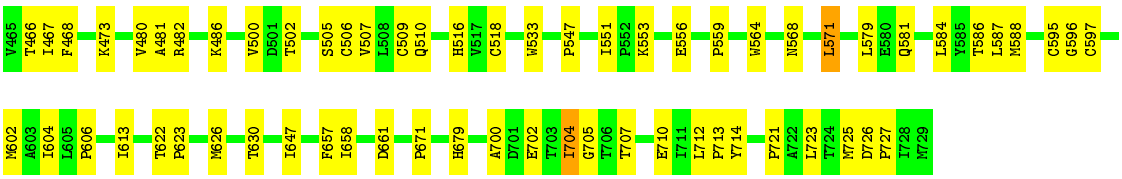
Chain D:



• Molecule 2: Carbon monoxide dehydrogenase alpha subunit

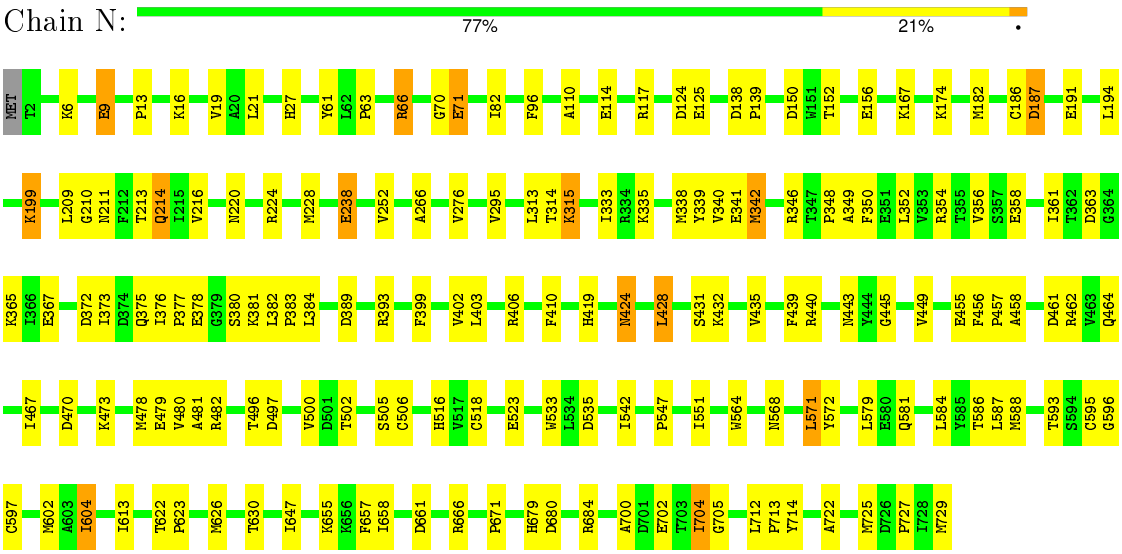
Chain M:





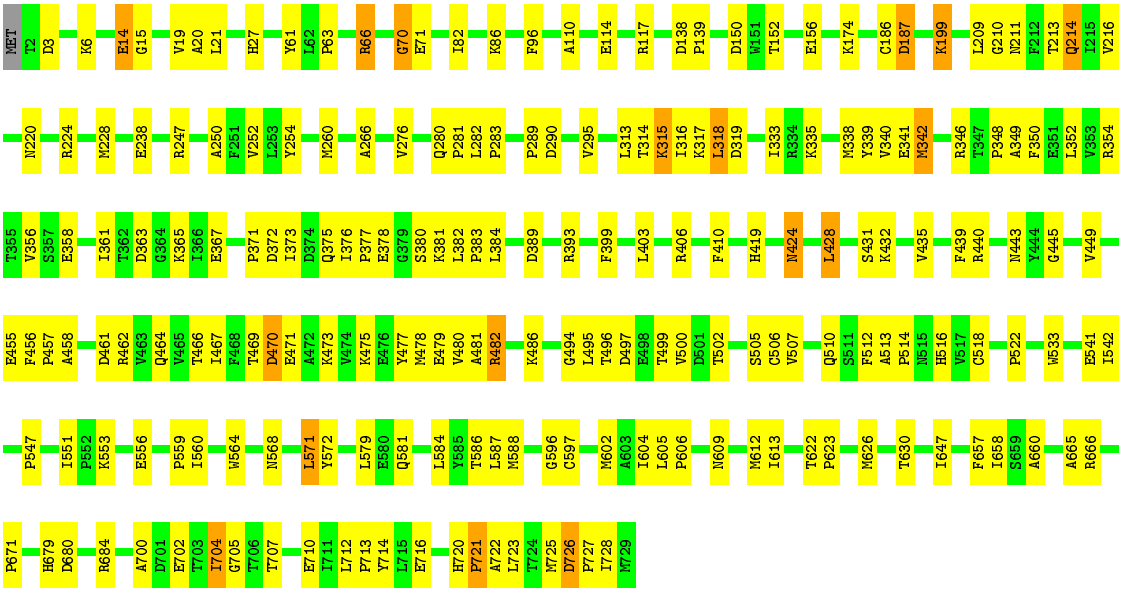
• Molecule 2: Carbon monoxide dehydrogenase alpha subunit

Chain N:



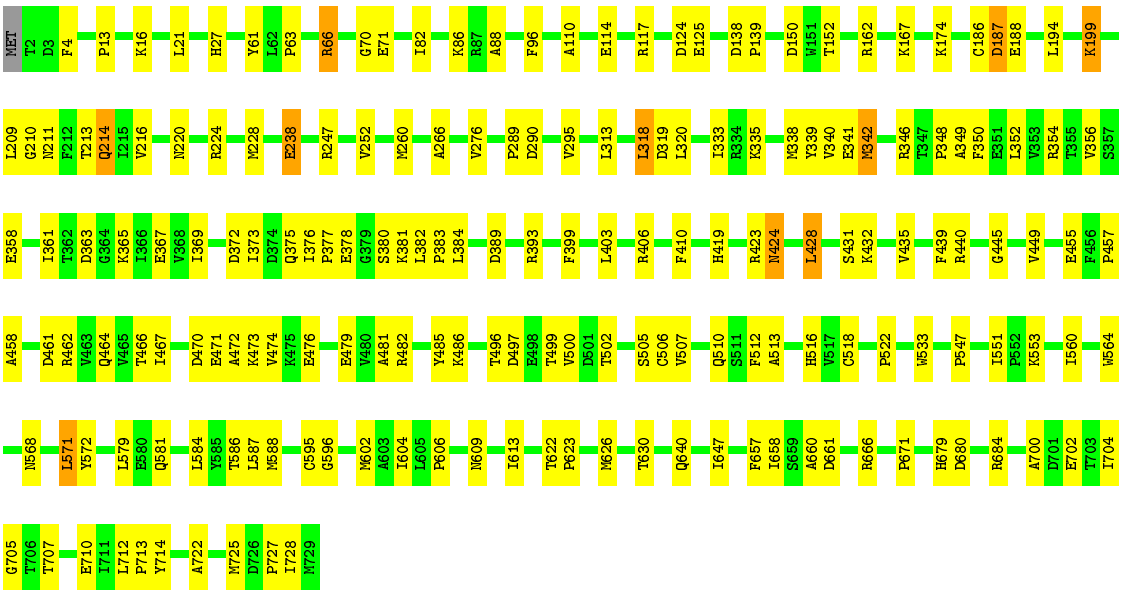
• Molecule 2: Carbon monoxide dehydrogenase alpha subunit

Chain O:



• Molecule 2: Carbon monoxide dehydrogenase alpha subunit

Chain P:


MET T2 D3 F4 P13 K16 L21 H27 Y61 L62 P63 R66 G70 E71 I82 K86 R87 A88 F96 A110 E114 R117 D124 E125 D138 P139 D150 W151 T152 R162 K167 K174 C186 D187 E188 L194 K199
L209 G210 N211 F212 T213 Q214 I215 V216 N220 R224 M228 E238 R247 V252 M260 A266 V276 P289 D290 V295 L313 L318 D319 L320 I333 R334 K335 M338 Y339 V340 E341 M342 R346 T347 P348 A349 F350 E351 L352 V353 R354 T355 V356 S357
E358 I361 T362 D363 G364 K365 I366 E367 V368 I369 D372 I373 D374 Q375 I376 P377 E378 G379 S380 K381 L382 P383 L384 D389 R393 F399 L403 R406 F410 H419 R423 N424 L428 S431 K432 V435 F439 R440 G445 V449 E455 F456 P457
A458 D461 R462 V463 Q464 V465 T466 I467 D470 E471 A472 K473 V474 K475 E476 E479 V480 A481 R482 Y485 K486 T496 D497 E498 T499 V500 D501 T502 S505 C506 V507 Q510 S511 F512 A513 H516 W517 C518 P522 W533 P547 I551 P552 K553 I560 W564
N568 L571 Y572 L579 E580 Q581 L584 Y585 T586 L587 M588 C595 G596 M602 A603 I604 L605 P606 M609 I613 T622 P623 M626 T630 Q640 I647 F657 I658 S659 A660 D661 R666 P671 H679 D680 R684 A700 D701 E702 T703 I704
G705 T706 T707 E710 T711 L712 P713 Y714 A722 M725 D726 P727 I728 M729

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	99.75Å 136.97Å 141.53Å 101.45° 109.05° 103.94°	Depositor
Resolution (Å)	20.00 – 2.20	Depositor
% Data completeness (in resolution range)	90.6 (20.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.215 , 0.241	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	44653	wwPDB-VP
Average B, all atoms (Å^2)	42.0	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: XCC, SF4, ACT, CU1, NI

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	0.38	0/5179	0.61	1/7017 (0.0%)
1	B	0.39	0/5179	0.62	1/7017 (0.0%)
1	C	0.36	0/5179	0.61	2/7017 (0.0%)
1	D	0.34	0/5179	0.60	1/7017 (0.0%)
2	M	0.36	0/5869	0.61	3/7948 (0.0%)
2	N	0.37	0/5869	0.61	0/7948
2	O	0.30	0/5869	0.58	1/7948 (0.0%)
2	P	0.32	0/5869	0.59	0/7948
All	All	0.35	0/44192	0.60	9/59860 (0.0%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	3	ARG	NE-CZ-NH2	7.28	123.94	120.30
1	A	3	ARG	NE-CZ-NH1	7.19	123.90	120.30
1	D	3	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	C	3	ARG	NE-CZ-NH2	6.54	123.57	120.30
2	M	238	GLU	CA-CB-CG	6.13	126.88	113.40

There are no chirality outliers.

There are no planarity outliers.

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	5087	0	5089	126	0
1	B	5087	0	5089	139	0
1	C	5087	0	5089	128	0
1	D	5087	0	5089	118	0
2	M	5735	0	5693	155	0
2	N	5735	0	5693	148	0
2	O	5735	0	5693	190	0
2	P	5735	0	5693	166	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
4	O	1	0	0	0	0
4	P	1	0	0	0	0
5	M	3	0	3	2	0
5	N	3	0	3	2	0
5	O	3	0	3	1	0
5	P	3	0	3	1	0
6	A	16	0	0	0	0
6	B	8	0	0	0	0
6	C	16	0	0	0	0
6	D	8	0	0	0	0
6	M	8	0	0	0	0
6	N	8	0	0	0	0
6	O	8	0	0	0	0
6	P	8	0	0	0	0
7	A	9	0	0	3	0
7	B	9	0	0	1	0
7	C	9	0	0	2	0
7	D	9	0	0	2	0
8	A	179	0	0	3	0
8	B	217	0	0	6	0
8	C	148	0	0	3	0
8	D	131	0	0	0	0
8	M	206	0	0	2	0
8	N	221	0	0	7	0
8	O	26	0	0	0	0
8	P	101	0	0	1	0
All	All	44653	0	43140	1127	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 13.

The worst 5 of 1127 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)
2:O:335:LYS:HD2	2:O:335:LYS:H	1.21	1.06
2:M:335:LYS:H	2:M:335:LYS:HD2	1.20	1.03
2:P:335:LYS:HD2	2:P:335:LYS:H	1.21	1.03
1:B:446:GLN:HE22	1:C:38:VAL:HG11	1.22	1.02
2:N:335:LYS:HD2	2:N:335:LYS:H	1.20	1.02

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	670/674 (99%)	646 (96%)	21 (3%)	3 (0%)	39	42
1	B	670/674 (99%)	644 (96%)	22 (3%)	4 (1%)	30	29
1	C	670/674 (99%)	647 (97%)	21 (3%)	2 (0%)	46	50
1	D	670/674 (99%)	646 (96%)	22 (3%)	2 (0%)	46	50
2	M	726/729 (100%)	696 (96%)	26 (4%)	4 (1%)	30	29
2	N	726/729 (100%)	696 (96%)	26 (4%)	4 (1%)	30	29
2	O	726/729 (100%)	682 (94%)	34 (5%)	10 (1%)	14	10
2	P	726/729 (100%)	691 (95%)	29 (4%)	6 (1%)	24	22
All	All	5584/5612 (100%)	5348 (96%)	201 (4%)	35 (1%)	30	29

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	316	ILE
2	O	315	LYS
1	B	415	ASN

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Mol	Chain	Res	Type
1	A	267	ASN
1	B	267	ASN

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	541/543 (100%)	528 (98%)	13 (2%)	57	69
1	B	541/543 (100%)	528 (98%)	13 (2%)	57	69
1	C	541/543 (100%)	526 (97%)	15 (3%)	51	63
1	D	541/543 (100%)	528 (98%)	13 (2%)	57	69
2	M	610/611 (100%)	593 (97%)	17 (3%)	51	63
2	N	610/611 (100%)	593 (97%)	17 (3%)	51	63
2	O	610/611 (100%)	593 (97%)	17 (3%)	51	63
2	P	610/611 (100%)	597 (98%)	13 (2%)	61	74
All	All	4604/4616 (100%)	4486 (97%)	118 (3%)	54	66

5 of 118 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	656	LEU
2	M	424	ASN
2	P	209	LEU
2	M	17	GLU
2	M	209	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	217	ASN
2	M	323	ASN
2	P	240	GLN

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Mol	Chain	Res	Type
1	D	225	ASN
1	D	639	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 26 ligands modelled in this entry, 8 are monoatomic - leaving 18 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	SF4	A	700	1	0,12,12	0.00	-	0,24,24	0.00	-
6	SF4	A	750	1	0,12,12	0.00	-	0,24,24	0.00	-
7	XCC	A	800	1	0,11,11	0.00	-	0,19,19	0.00	-
6	SF4	B	750	1	0,12,12	0.00	-	0,24,24	0.00	-
7	XCC	B	800	1	0,11,11	0.00	-	0,19,19	0.00	-
6	SF4	C	700	1	0,12,12	0.00	-	0,24,24	0.00	-
6	SF4	C	750	1	0,12,12	0.00	-	0,24,24	0.00	-
7	XCC	C	800	1	0,11,11	0.00	-	0,19,19	0.00	-
6	SF4	D	750	1	0,12,12	0.00	-	0,24,24	0.00	-
7	XCC	D	800	1	0,11,11	0.00	-	0,19,19	0.00	-
6	SF4	M	900	2	0,12,12	0.00	-	0,24,24	0.00	-
5	ACT	M	950	3	2,2,3	1.18	0	0,1,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	SF4	N	900	2	0,12,12	0.00	-	0,24,24	0.00	-
5	ACT	N	950	3	2,2,3	1.42	0	0,1,3	0.00	-
6	SF4	O	900	2	0,12,12	0.00	-	0,24,24	0.00	-
5	ACT	O	950	3	2,2,3	1.15	0	0,1,3	0.00	-
6	SF4	P	900	2	0,12,12	0.00	-	0,24,24	0.00	-
5	ACT	P	950	3	2,2,3	1.24	0	0,1,3	0.00	-

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	SF4	A	700	1	-	0/0/48/48	0/6/5/5
6	SF4	A	750	1	-	0/0/48/48	0/6/5/5
7	XCC	A	800	1	-	0/0/32/32	0/0/3/3
6	SF4	B	750	1	-	0/0/48/48	0/6/5/5
7	XCC	B	800	1	-	0/0/32/32	0/0/3/3
6	SF4	C	700	1	-	0/0/48/48	0/6/5/5
6	SF4	C	750	1	-	0/0/48/48	0/6/5/5
7	XCC	C	800	1	-	0/0/32/32	0/0/3/3
6	SF4	D	750	1	-	0/0/48/48	0/6/5/5
7	XCC	D	800	1	-	0/0/32/32	0/0/3/3
6	SF4	M	900	2	-	0/0/48/48	0/6/5/5
5	ACT	M	950	3	-	0/0/0/0	0/0/0/0
6	SF4	N	900	2	-	0/0/48/48	0/6/5/5
5	ACT	N	950	3	-	0/0/0/0	0/0/0/0
6	SF4	O	900	2	-	0/0/48/48	0/6/5/5
5	ACT	O	950	3	-	0/0/0/0	0/0/0/0
6	SF4	P	900	2	-	0/0/48/48	0/6/5/5
5	ACT	P	950	3	-	0/0/0/0	0/0/0/0

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.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	800	XCC	3	0
7	B	800	XCC	1	0
7	C	800	XCC	2	0
7	D	800	XCC	2	0
5	M	950	ACT	2	0
5	N	950	ACT	2	0
5	O	950	ACT	1	0
5	P	950	ACT	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

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.