



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 06:03 AM UTC

PDB ID : 3I01 / pdb_00003i01
Title : Native structure of bifunctional carbon monoxide dehydrogenase/acetyl-CoA synthase from Moorella thermoacetica, water-bound C-cluster.
Authors : Kung, Y.; Doukov, T.I.; Drennan, C.L.
Deposited on : 2009-06-24
Resolution : 2.15 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

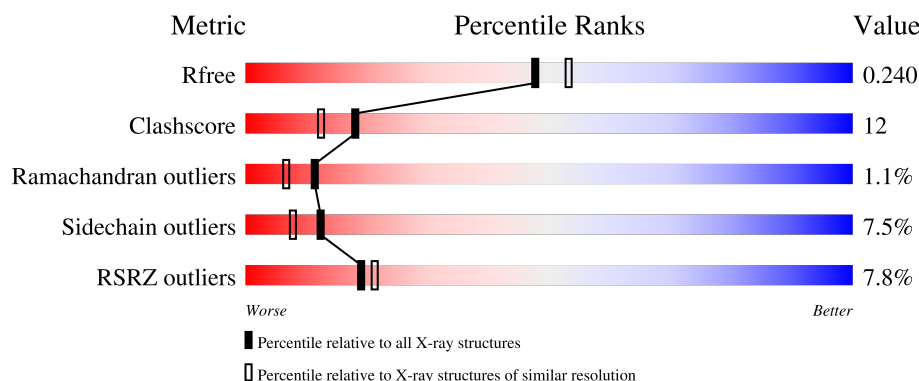
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	674	 81% 18% .
1	B	674	 80% 17% .
1	C	674	 79% 19% .
1	D	674	 77% 21% .
2	M	729	 76% 20% . .

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Mol	Chain	Length	Quality of chain
2	N	729	
2	O	729	
2	P	729	

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	SF4	O	900	-	-	X	-
4	XCC	D	800	-	-	X	-
5	GOL	C	863	-	-	X	-
5	GOL	D	863	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 45096 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.

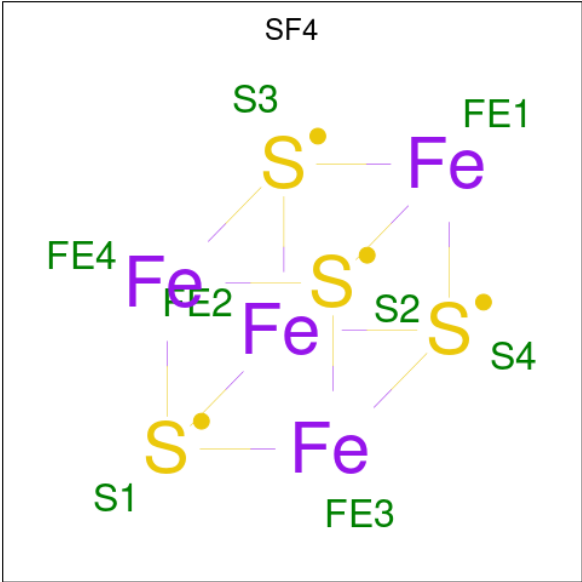
- Molecule 1 is a protein called Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	673	Total	C	N	O	S	0	7	0
			5128	3223	897	966	42			
1	B	673	Total	C	N	O	S	0	5	0
			5121	3221	895	963	42			
1	C	673	Total	C	N	O	S	0	2	0
			5094	3205	888	959	42			
1	D	673	Total	C	N	O	S	0	4	0
			5119	3218	895	964	42			

- Molecule 2 is a protein called Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha.

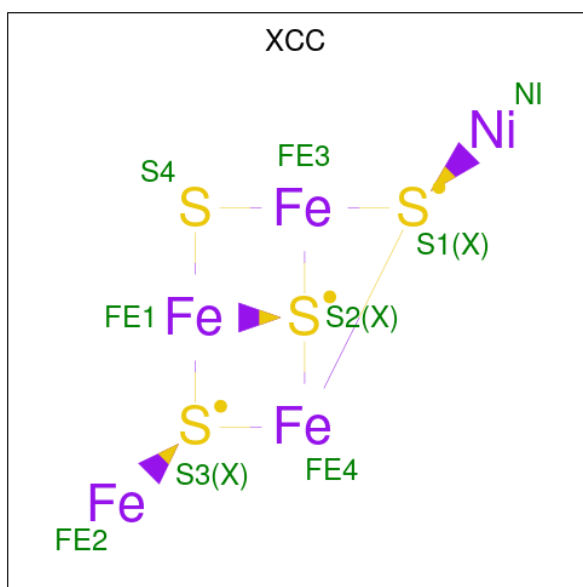
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	728	Total	C	N	O	S	0	5	0
			5778	3703	964	1076	35			
2	N	728	Total	C	N	O	S	0	6	0
			5784	3707	968	1074	35			
2	O	728	Total	C	N	O	S	0	1	0
			5749	3687	958	1069	35			
2	P	728	Total	C	N	O	S	0	1	0
			5746	3684	959	1068	35			

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



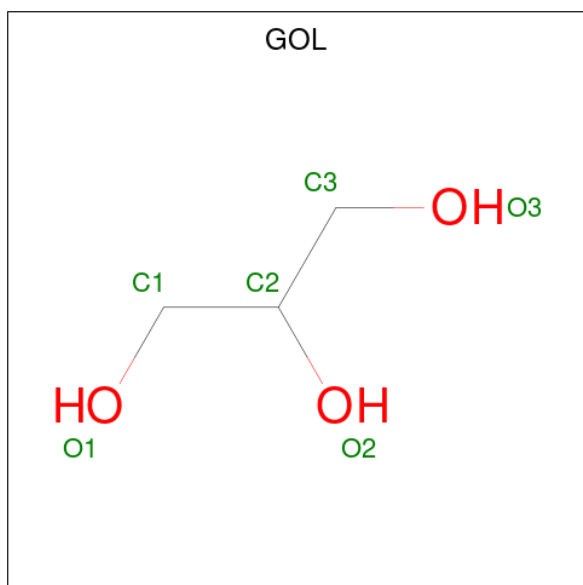
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	M	1	Total	Fe	S	0	0
			8	4	4		
3	N	1	Total	Fe	S	0	0
			8	4	4		
3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

- Molecule 4 is FE(4)-NI(1)-S(4) CLUSTER (CCD ID: XCC) (formula: Fe₄NiS₄).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0

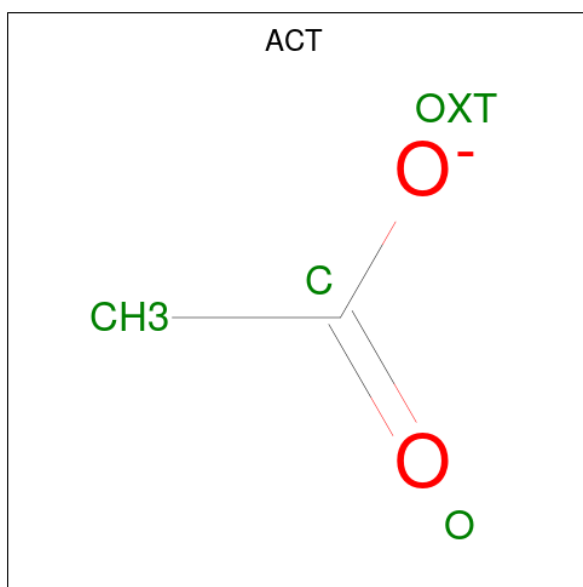
- Molecule 6 is COPPER (I) ION (CCD ID: CU1) (formula: Cu).

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

- Molecule 7 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

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

- Molecule 8 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	M	1	Total	Na	0	0
			1	1		
9	N	1	Total	Na	0	0
			1	1		
9	O	1	Total	Na	0	0
			1	1		
9	P	1	Total	Na	0	0
			1	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	215	Total	O	0	0
			215	215		

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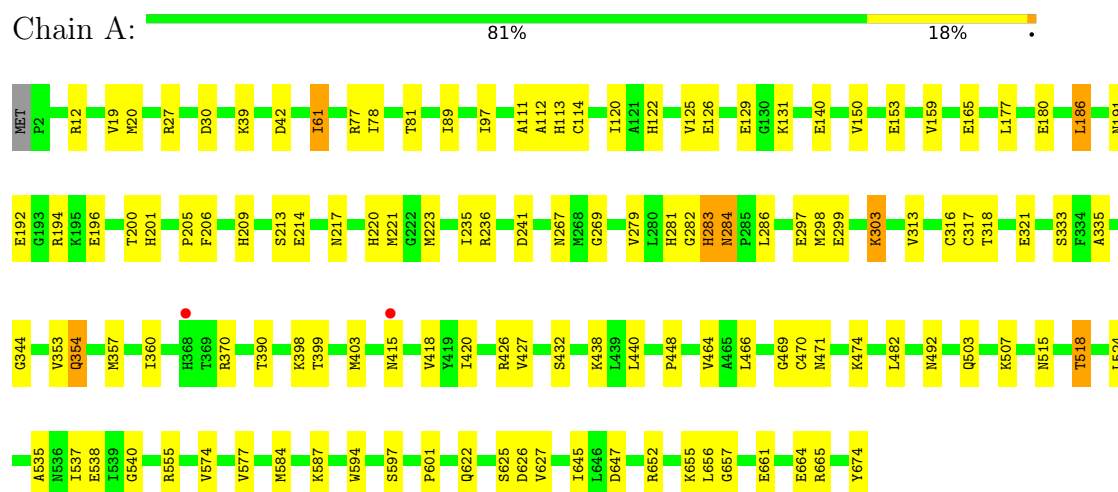
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	288	Total 288	O 288	0	0
10	C	169	Total 169	O 169	0	0
10	D	151	Total 151	O 151	0	0
10	M	218	Total 218	O 218	0	0
10	N	227	Total 227	O 227	0	0
10	O	27	Total 27	O 27	0	0
10	P	118	Total 118	O 118	0	0

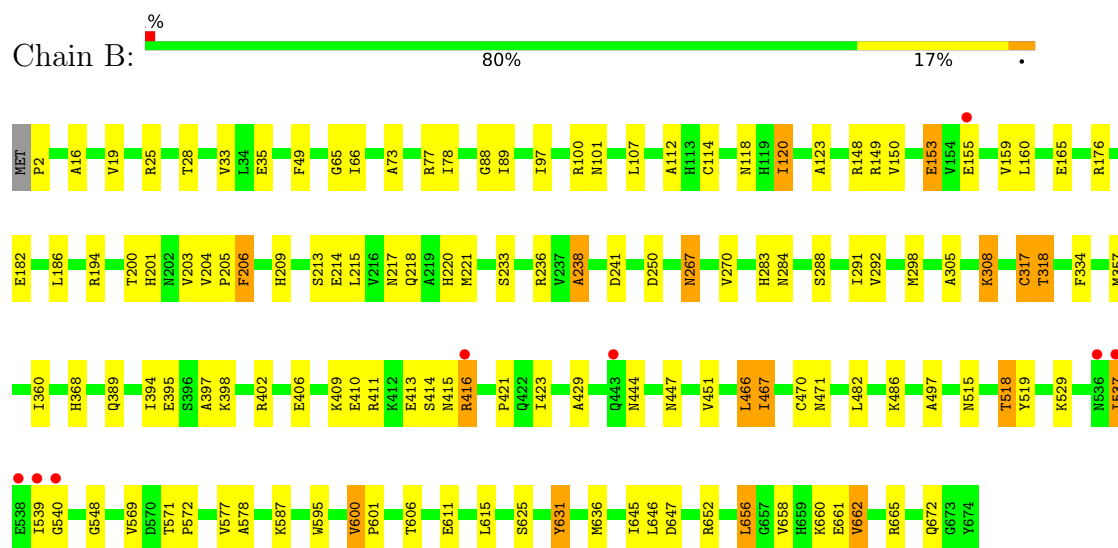
3 Residue-property plots

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.

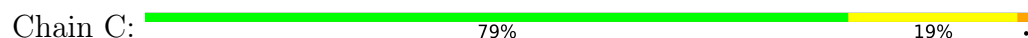
- Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta

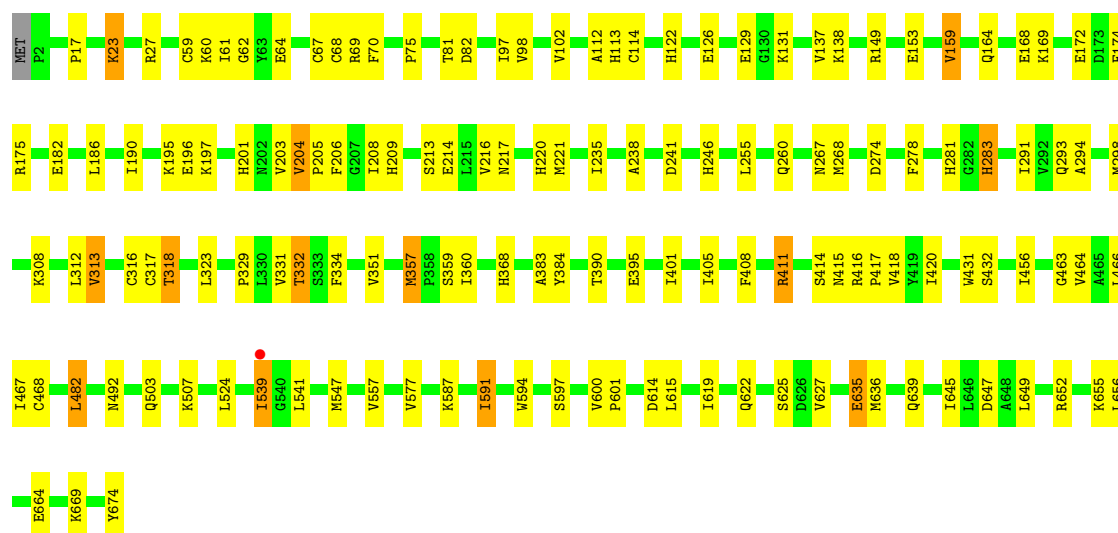


- Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta

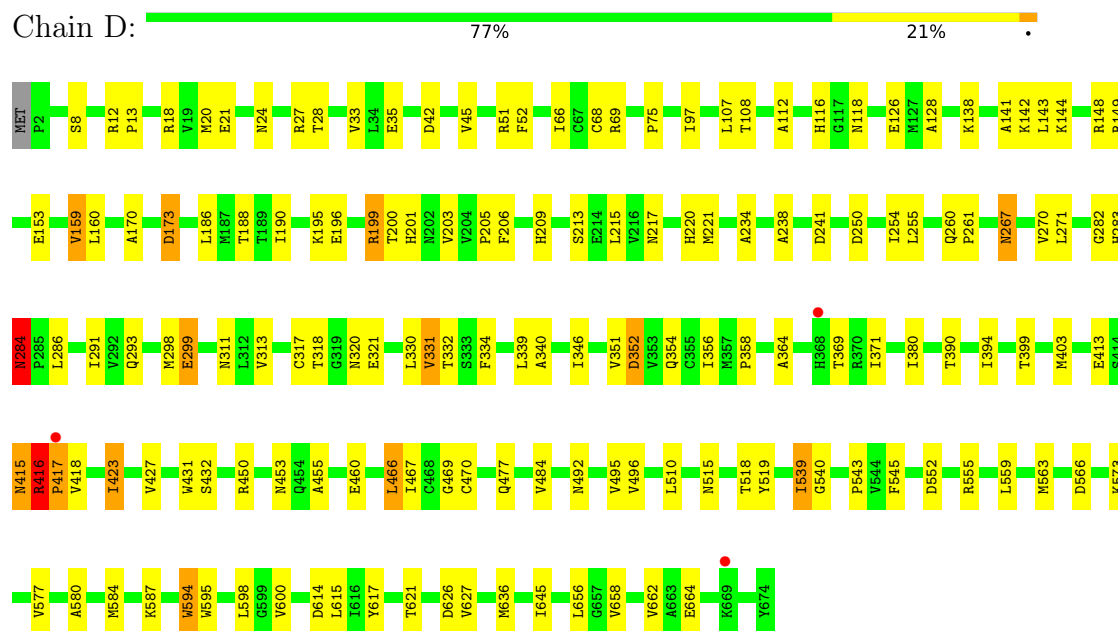


- Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta

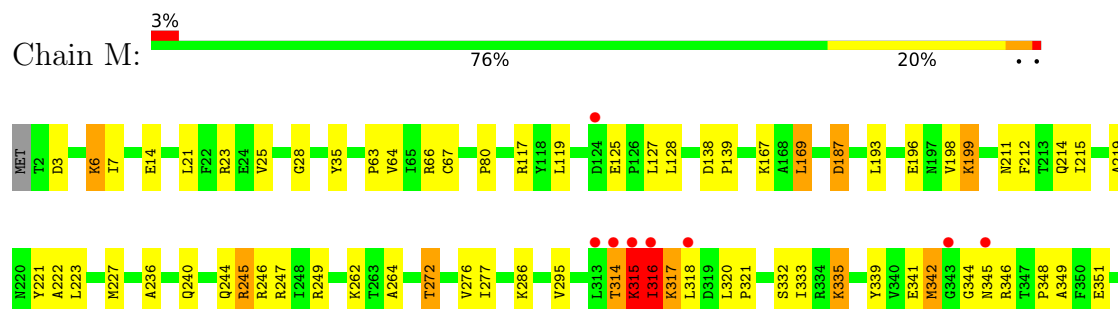


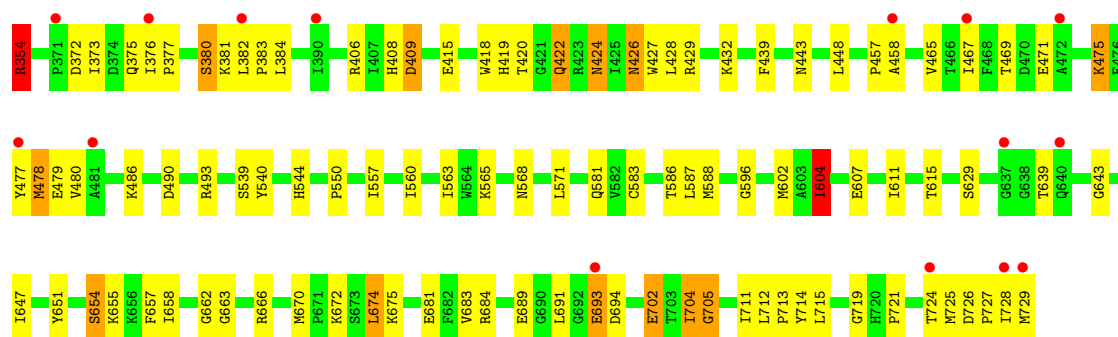


- Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta

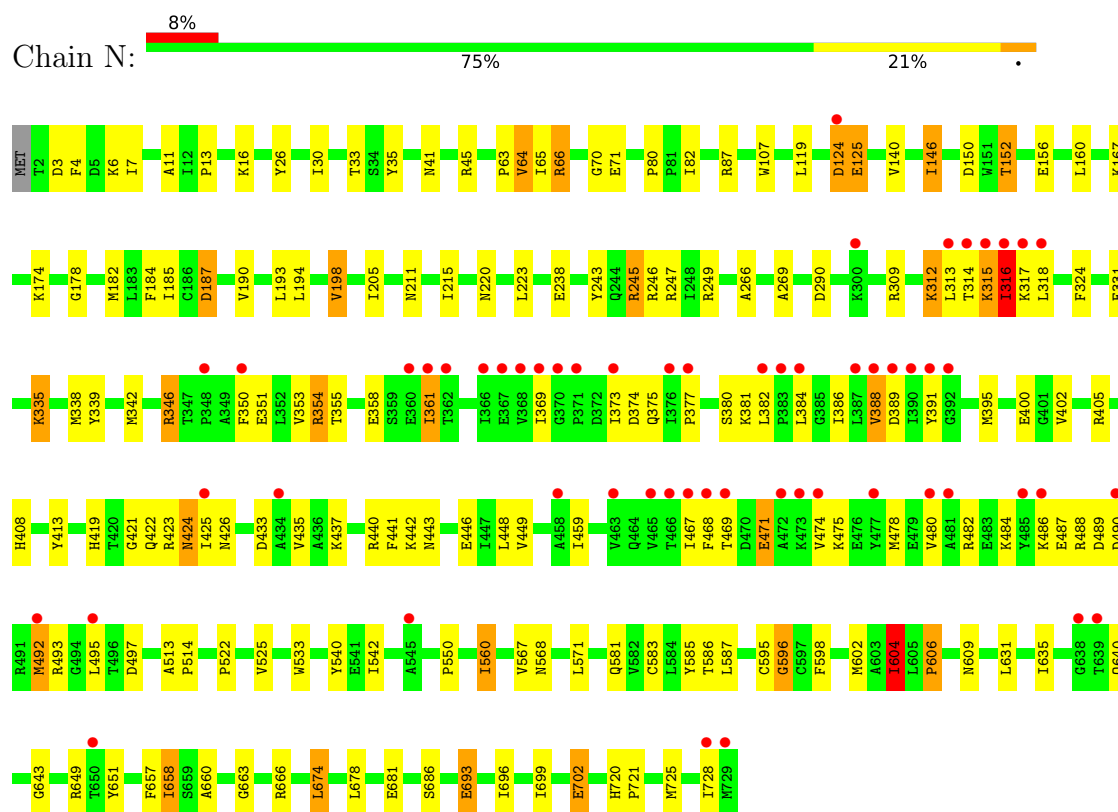


- Molecule 2: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha

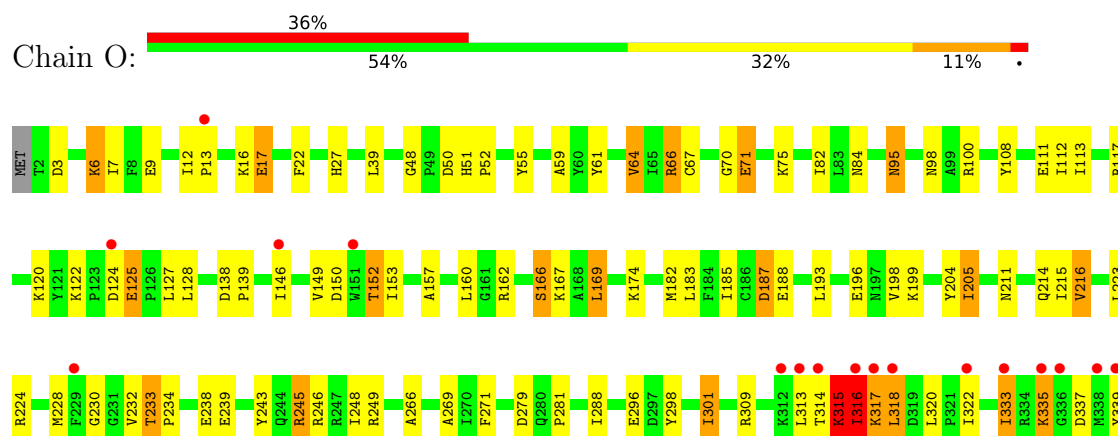




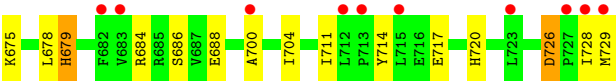
- Molecule 2: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha



- Molecule 2: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha







4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	99.65Å 136.87Å 140.86Å 101.26° 109.11° 104.08°	Depositor
Resolution (Å)	36.96 – 2.15 36.96 – 2.15	Depositor EDS
% Data completeness (in resolution range)	92.3 (36.96-2.15) 92.3 (36.96-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.186 , 0.242 0.187 , 0.240	Depositor DCC
R_{free} test set	16243 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	29.4	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	45096	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CU1, XCC, SF4, ACT, NI, GOL, 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	1.35	9/5244 (0.2%)	1.24	13/7106 (0.2%)
1	B	1.41	18/5231 (0.3%)	1.27	28/7086 (0.4%)
1	C	1.35	21/5193 (0.4%)	1.24	16/7038 (0.2%)
1	D	1.22	8/5212 (0.2%)	1.22	17/7062 (0.2%)
2	M	1.22	10/5921 (0.2%)	1.19	19/8015 (0.2%)
2	N	1.24	11/5928 (0.2%)	1.22	23/8023 (0.3%)
2	O	1.14	13/5883 (0.2%)	1.29	49/7965 (0.6%)
2	P	1.07	6/5885 (0.1%)	1.15	13/7968 (0.2%)
All	All	1.25	96/44497 (0.2%)	1.23	178/60263 (0.3%)

The worst 5 of 96 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	725	MET	C-O	-9.29	1.12	1.24
2	O	478	MET	CA-C	8.62	1.64	1.52
2	P	316	ILE	C-N	-7.73	1.23	1.33
1	C	415	ASN	C-O	-7.57	1.12	1.23
2	N	107	TRP	C-O	-7.50	1.15	1.24

The worst 5 of 178 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	480	VAL	N-CA-C	-12.86	99.04	110.74
2	O	476	GLU	N-CA-C	-11.60	98.64	111.28
2	O	479	GLU	N-CA-C	-10.78	99.23	112.38
2	O	473	LYS	N-CA-C	10.26	122.54	111.36
2	O	723	LEU	N-CA-C	9.77	121.53	111.07

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	5128	0	5128	68	0
1	B	5121	0	5134	75	0
1	C	5094	0	5097	93	0
1	D	5119	0	5115	112	0
2	M	5778	0	5736	104	0
2	N	5784	0	5749	108	0
2	O	5749	0	5716	394	0
2	P	5746	0	5710	151	0
3	A	16	0	0	0	0
3	B	8	0	0	1	0
3	C	16	0	0	1	0
3	D	8	0	0	0	0
3	M	8	0	0	0	0
3	N	8	0	0	1	0
3	O	8	0	0	2	0
3	P	8	0	0	0	0
4	A	9	0	0	1	0
4	B	9	0	0	0	0
4	C	9	0	0	0	0
4	D	9	0	0	2	0
5	A	6	0	8	0	0
5	B	6	0	7	0	0
5	C	6	0	8	5	0
5	D	6	0	8	6	0
6	M	1	0	0	0	0
6	N	1	0	0	0	0
6	O	1	0	0	0	0
6	P	1	0	0	0	0
7	M	1	0	0	0	0
7	N	1	0	0	0	0
7	O	1	0	0	0	0
7	P	1	0	0	0	0
8	M	3	0	3	0	0
8	N	3	0	3	0	0
8	O	3	0	3	1	0
8	P	3	0	3	1	0
9	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	N	1	0	0	0	0
9	O	1	0	0	0	0
9	P	1	0	0	0	0
10	A	215	0	0	5	0
10	B	288	0	0	4	0
10	C	169	0	0	6	0
10	D	151	0	0	4	0
10	M	218	0	0	5	0
10	N	227	0	0	6	0
10	O	27	0	0	2	0
10	P	118	0	0	6	0
All	All	45096	0	43428	1063	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 12.

The worst 5 of 1063 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:482:ARG:HA	2:O:482:ARG:CZ	1.72	1.19
2:P:588:MET:HE1	2:P:604:ILE:HD13	1.17	1.17
2:O:490:ASP:HB2	2:O:491:ARG:NH1	1.61	1.16
2:O:685:ARG:O	2:O:688:GLU:HB3	1.44	1.15
2:O:482:ARG:HA	2:O:482:ARG:NH1	1.62	1.13

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	678/674 (101%)	652 (96%)	24 (4%)	2 (0%)	36 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	676/674 (100%)	652 (96%)	23 (3%)	1 (0%)	48	50
1	C	673/674 (100%)	648 (96%)	24 (4%)	1 (0%)	48	50
1	D	675/674 (100%)	640 (95%)	30 (4%)	5 (1%)	18	13
2	M	731/729 (100%)	687 (94%)	36 (5%)	8 (1%)	11	7
2	N	732/729 (100%)	689 (94%)	34 (5%)	9 (1%)	10	5
2	O	727/729 (100%)	641 (88%)	60 (8%)	26 (4%)	2	0
2	P	727/729 (100%)	679 (93%)	41 (6%)	7 (1%)	12	8
All	All	5619/5612 (100%)	5288 (94%)	272 (5%)	59 (1%)	11	7

5 of 59 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	267	ASN
1	D	267	ASN
2	M	316	ILE
2	M	693	GLU
2	O	315	LYS

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	548/543 (101%)	525 (96%)	23 (4%)	26	25
1	B	547/543 (101%)	524 (96%)	23 (4%)	26	25
1	C	542/543 (100%)	519 (96%)	23 (4%)	26	25
1	D	544/543 (100%)	520 (96%)	24 (4%)	25	23
2	M	615/611 (101%)	566 (92%)	49 (8%)	11	7
2	N	615/611 (101%)	571 (93%)	44 (7%)	13	8
2	O	611/611 (100%)	510 (84%)	101 (16%)	2	1
2	P	611/611 (100%)	547 (90%)	64 (10%)	6	3
All	All	4633/4616 (100%)	4282 (92%)	351 (8%)	12	8

5 of 351 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	411	ILE
2	O	729	MET
2	O	449	VAL
2	O	541	GLU
2	P	238	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 96 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	426	ASN
2	O	95	ASN
2	M	581	GLN
2	N	424	ASN
2	O	515	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 12 are monoatomic - leaving 22 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	XCC	C	800	10,1	0,11,11	-	-	-		
3	SF4	P	900	2	0,12,12	-	-	-		
3	SF4	C	700	1	0,12,12	-	-	-		
4	XCC	A	800	10,1	0,11,11	-	-	-		
5	GOL	A	863	-	5,5,5	0.45	0	5,5,5	1.82	2 (40%)
5	GOL	B	863	-	5,5,5	1.10	1 (20%)	5,5,5	1.85	1 (20%)
8	ACT	P	953	-	1,2,3	1.54	0	0,1,3	-	-
8	ACT	N	953	-	1,2,3	1.45	0	0,1,3	-	-
3	SF4	M	900	2	0,12,12	-	-	-		
3	SF4	N	900	2	0,12,12	-	-	-		
4	XCC	B	800	10,1	0,11,11	-	-	-		
8	ACT	M	953	-	1,2,3	1.35	0	0,1,3	-	-
3	SF4	A	700	1	0,12,12	-	-	-		
3	SF4	D	750	1	0,12,12	-	-	-		
8	ACT	O	953	-	1,2,3	1.23	0	0,1,3	-	-
3	SF4	O	900	2	0,12,12	-	-	-		
3	SF4	A	750	1	0,12,12	-	-	-		
4	XCC	D	800	10,1	0,11,11	-	-	-		
3	SF4	B	750	1	0,12,12	-	-	-		
5	GOL	C	863	-	5,5,5	0.31	0	5,5,5	0.65	0
3	SF4	C	750	1	0,12,12	-	-	-		
5	GOL	D	863	-	5,5,5	0.54	0	5,5,5	1.72	2 (40%)

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	SF4	N	900	2	-	-	0/6/5/5
5	GOL	C	863	-	-	2/4/4/4	-
5	GOL	A	863	-	-	2/4/4/4	-
3	SF4	B	750	1	-	-	0/6/5/5
3	SF4	O	900	2	-	-	0/6/5/5
3	SF4	P	900	2	-	-	0/6/5/5
3	SF4	C	700	1	-	-	0/6/5/5
4	XCC	C	800	10,1	-	-	0/3/3/3
3	SF4	A	750	1	-	-	0/6/5/5
3	SF4	C	750	1	-	-	0/6/5/5
4	XCC	B	800	10,1	-	-	0/3/3/3
5	GOL	B	863	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	XCC	A	800	10,1	-	-	0/3/3/3
3	SF4	A	700	1	-	-	0/6/5/5
4	XCC	D	800	10,1	-	-	0/3/3/3
3	SF4	D	750	1	-	-	0/6/5/5
5	GOL	D	863	-	-	3/4/4/4	-
3	SF4	M	900	2	-	-	0/6/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	863	GOL	O2-C2	-2.41	1.36	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	863	GOL	O2-C2-C3	-3.29	95.57	109.18
5	D	863	GOL	O1-C1-C2	-2.87	97.45	110.38
5	A	863	GOL	O1-C1-C2	-2.49	99.16	110.38
5	A	863	GOL	O3-C3-C2	-2.06	101.10	110.38
5	D	863	GOL	O2-C2-C1	-2.01	100.86	109.18

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	863	GOL	O1-C1-C2-C3
5	C	863	GOL	O1-C1-C2-C3
5	D	863	GOL	O1-C1-C2-C3
5	C	863	GOL	O1-C1-C2-O2
5	D	863	GOL	O1-C1-C2-O2

There are no ring outliers.

10 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	700	SF4	1	0
4	A	800	XCC	1	0
8	P	953	ACT	1	0
3	N	900	SF4	1	0
8	O	953	ACT	1	0
3	O	900	SF4	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	800	XCC	2	0
3	B	750	SF4	1	0
5	C	863	GOL	5	0
5	D	863	GOL	6	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](#)

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	673/674 (99%)	-0.26	2 (0%)	90 91	14, 25, 43, 60	7 (1%)
1	B	673/674 (99%)	-0.39	8 (1%)	76 79	11, 22, 39, 68	5 (0%)
1	C	673/674 (99%)	-0.17	1 (0%)	92 93	15, 28, 42, 58	2 (0%)
1	D	673/674 (99%)	-0.01	3 (0%)	88 90	13, 31, 45, 59	4 (0%)
2	M	728/729 (99%)	0.18	23 (3%)	50 54	12, 33, 62, 74	5 (0%)
2	N	728/729 (99%)	0.22	57 (7%)	19 21	10, 32, 66, 76	6 (0%)
2	O	728/729 (99%)	1.61	261 (35%)	1 1	26, 64, 92, 126	1 (0%)
2	P	728/729 (99%)	0.66	84 (11%)	9 10	15, 45, 76, 92	1 (0%)
All	All	5604/5612 (99%)	0.25	439 (7%)	19 21	10, 31, 74, 126	31 (0%)

The worst 5 of 439 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	312[A]	LYS	6.6
2	O	728	ILE	6.4
2	O	458	ALA	5.9
2	O	428	LEU	5.9
2	O	495	LEU	5.8

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 oligosaccharides 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
5	GOL	C	863	6/6	0.77	0.17	47,56,56,58	0
9	NA	O	730	1/1	0.86	0.10	70,70,70,70	0
5	GOL	D	863	6/6	0.87	0.13	43,46,48,48	0
9	NA	P	730	1/1	0.87	0.08	35,35,35,35	0
8	ACT	N	953	3/4	0.89	0.21	59,59,59,59	0
8	ACT	P	953	3/4	0.90	0.21	53,53,54,54	0
8	ACT	M	953	3/4	0.93	0.15	44,44,44,45	0
5	GOL	A	863	6/6	0.93	0.10	26,30,33,37	0
8	ACT	O	953	3/4	0.93	0.23	100,100,100,100	0
3	SF4	O	900	8/8	0.94	0.07	61,63,67,67	0
5	GOL	B	863	6/6	0.96	0.08	26,30,34,37	0
6	CU1	P	950	1/1	0.96	0.05	55,55,55,55	0
9	NA	M	730	1/1	0.97	0.05	29,29,29,29	0
9	NA	N	730	1/1	0.97	0.03	28,28,28,28	0
6	CU1	O	950	1/1	0.97	0.04	82,82,82,82	0
7	NI	O	951	1/1	0.97	0.06	76,76,76,76	0
3	SF4	C	700	8/8	0.98	0.04	28,32,35,35	0
3	SF4	P	900	8/8	0.98	0.04	40,40,41,46	0
4	XCC	C	800	9/9	0.98	0.04	25,27,34,35	0
6	CU1	N	950	1/1	0.99	0.04	38,38,38,38	0
3	SF4	A	750	8/8	0.99	0.03	14,17,17,18	0
3	SF4	B	750	8/8	0.99	0.03	17,18,18,19	0
7	NI	M	951	1/1	0.99	0.02	28,28,28,28	0
4	XCC	A	800	9/9	0.99	0.03	20,24,29,30	0
7	NI	P	951	1/1	0.99	0.04	39,39,39,39	0
4	XCC	B	800	9/9	0.99	0.03	16,20,25,27	0
3	SF4	A	700	8/8	0.99	0.03	17,19,20,22	0
4	XCC	D	800	9/9	0.99	0.03	33,35,41,45	0
3	SF4	C	750	8/8	0.99	0.03	28,30,31,32	0
3	SF4	D	750	8/8	0.99	0.05	26,28,29,29	0
3	SF4	M	900	8/8	0.99	0.03	22,25,26,28	0
3	SF4	N	900	8/8	0.99	0.03	25,26,27,28	0
6	CU1	M	950	1/1	0.99	0.03	43,43,43,43	0
7	NI	N	951	1/1	1.00	0.01	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.