



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 4, 2026 – 02:36 PM EDT

PDB ID : 3I04 / pdb_00003i04
Title : Cyanide-bound structure of bifunctional carbon monoxide dehydrogenase/acetate-CoA synthase from Moorella thermoacetica, cyanide-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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

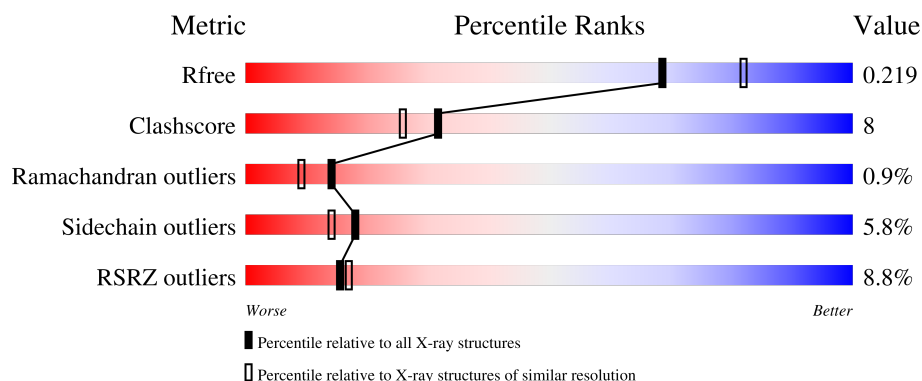
1 Overall quality at a glance

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	673	3% 88% 11%
1	B	673	3% 87% 12%
1	C	673	89% 10%
1	D	673	3% 87% 12%
2	M	728	3% 85% 12%

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Mol	Chain	Length	Quality of chain
2	N	728	
2	O	728	
2	P	728	

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	CYN	A	900	-	-	X	-
5	CYN	C	900	-	-	X	-
6	GOL	C	963	-	-	X	-
6	GOL	D	963	-	-	X	-
9	ACT	N	953	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 45801 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.

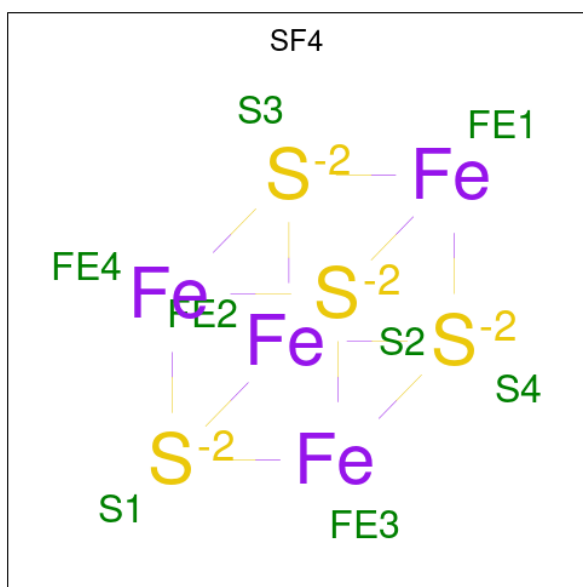
- Molecule 1 is a protein called Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	673	Total	C	N	O	S	0	5	0
			5134	3226	900	965	43			
1	B	673	Total	C	N	O	S	0	7	0
			5134	3227	895	969	43			
1	C	673	Total	C	N	O	S	0	3	0
			5103	3208	888	965	42			
1	D	673	Total	C	N	O	S	0	0	0
			5088	3199	888	959	42			

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

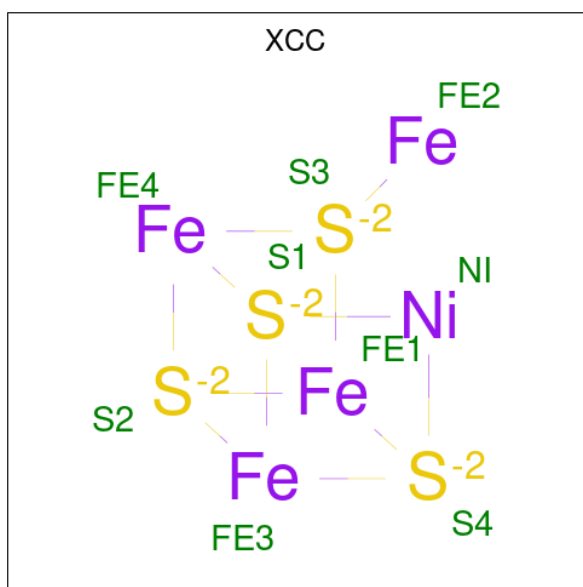
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	728	Total	C	N	O	S	0	4	0
			5766	3695	962	1074	35			
2	N	728	Total	C	N	O	S	0	1	0
			5746	3684	959	1068	35			
2	O	728	Total	C	N	O	S	0	1	0
			5746	3684	959	1068	35			
2	P	728	Total	C	N	O	S	0	2	0
			5757	3690	963	1069	35			

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



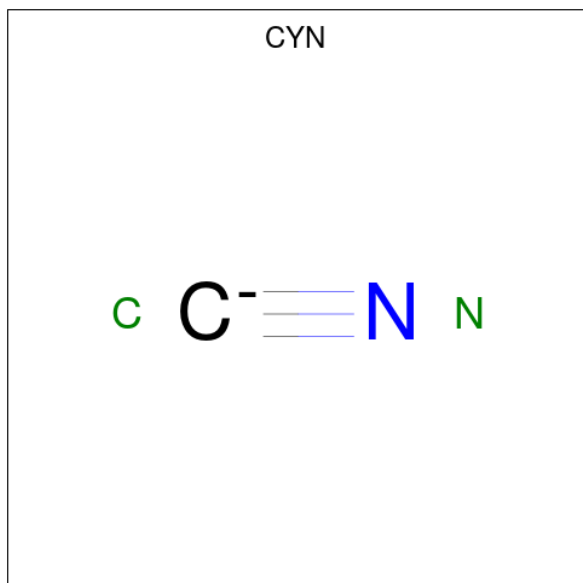
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	M	1	Total	Fe	S	0	0
			8	4	4		
3	N	1	Total	Fe	S	0	0
			8	4	4		
3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



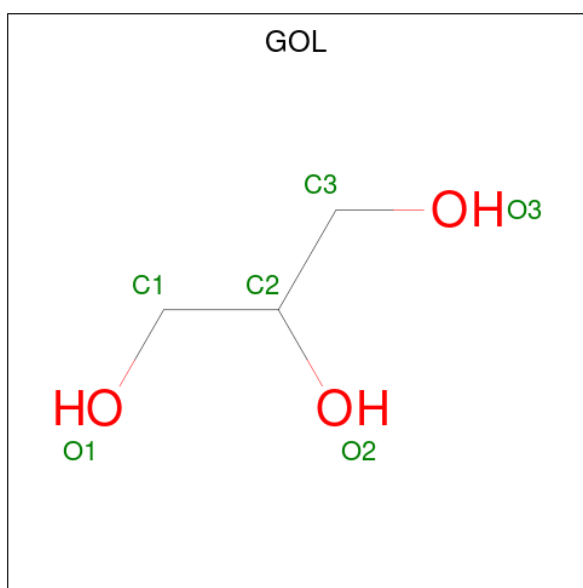
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
4	B	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
4	C	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
4	D	1	Total	Fe	Ni	S	0	0
			9	4	1	4		

- Molecule 5 is CYANIDE ION (CCD ID: CYN) (formula: CN).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			2	1	1		
5	B	1	Total	C	N	0	0
			2	1	1		
5	C	1	Total	C	N	0	0
			2	1	1		
5	D	1	Total	C	N	0	0
			2	1	1		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is COPPER (I) ION (CCD ID: CU1) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	M	1	Total	Cu	0	0
			1	1		
7	N	1	Total	Cu	0	0
			1	1		

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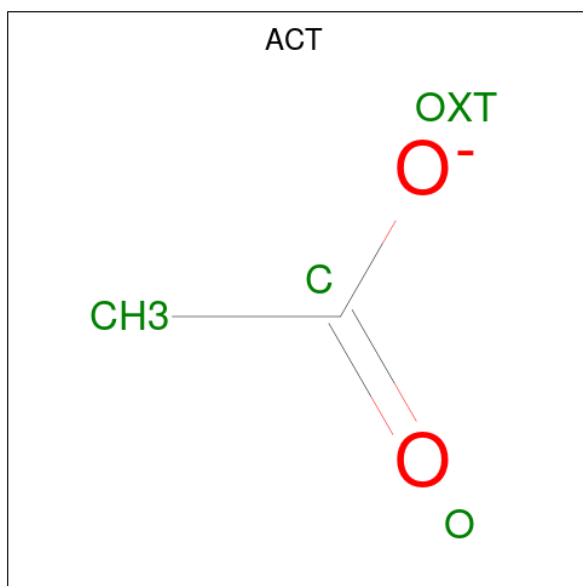
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	O	1	Total 1	Cu 1	0	0
7	P	1	Total 1	Cu 1	0	0

- Molecule 8 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

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

- Molecule 9 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

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

- Molecule 10 is SODIUM ION (CCD ID: NA) (formula: Na).

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

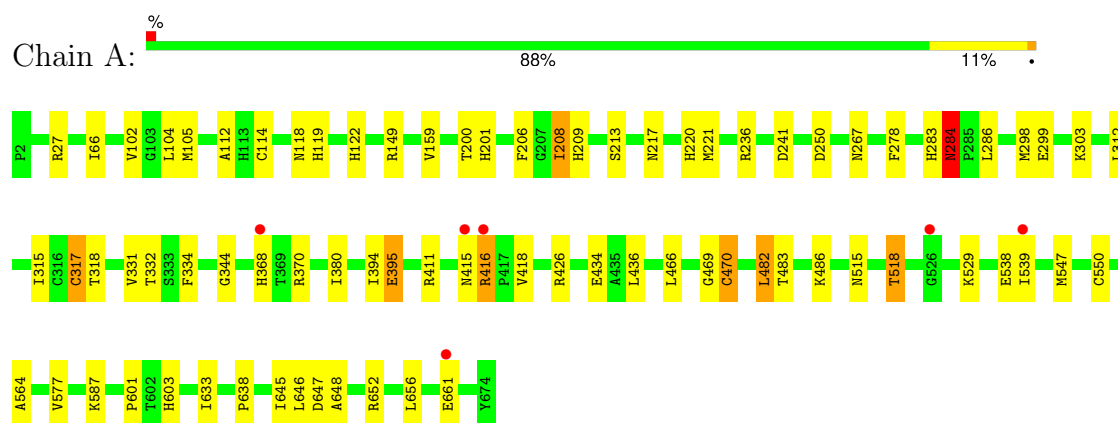
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	306	Total	O	0	0
			306	306		
11	B	375	Total	O	0	0
			375	375		
11	C	275	Total	O	0	0
			275	275		
11	D	240	Total	O	0	0
			240	240		
11	M	326	Total	O	0	0
			326	326		
11	N	337	Total	O	0	0
			337	337		
11	O	83	Total	O	0	0
			83	83		
11	P	213	Total	O	0	0
			213	213		

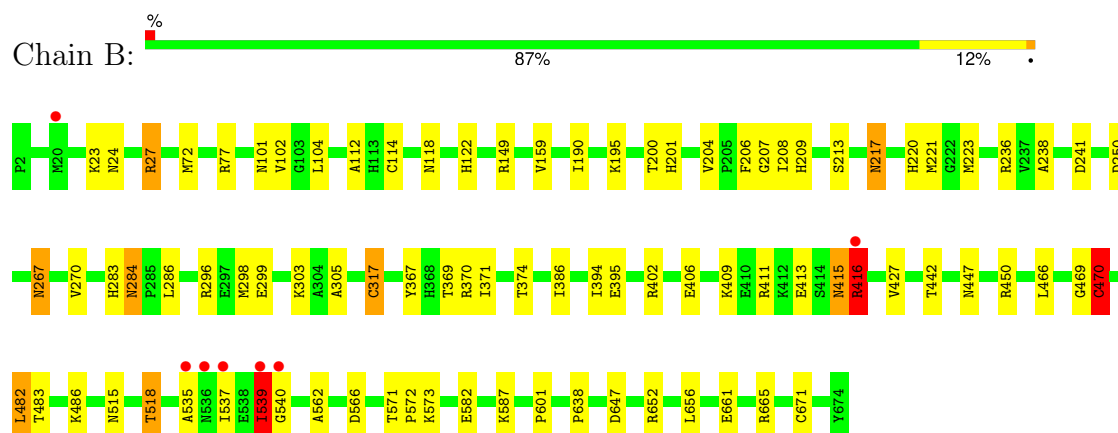
3 Residue-property plots

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.

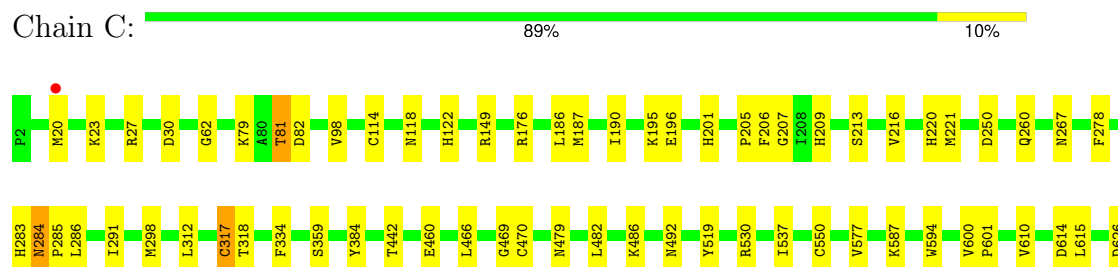
- Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta



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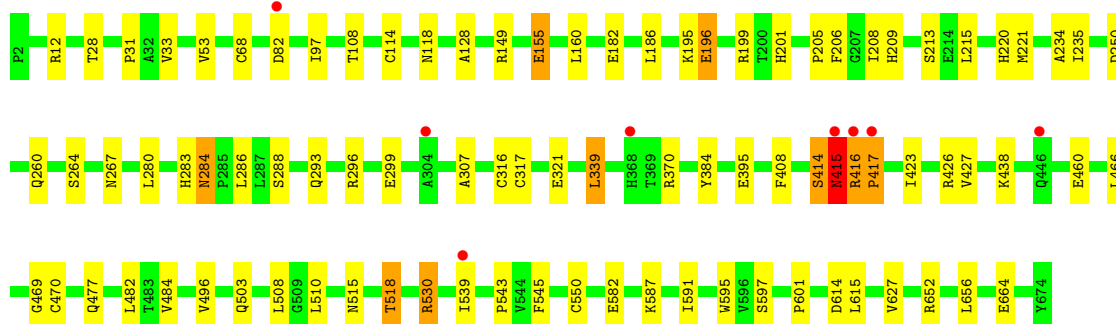
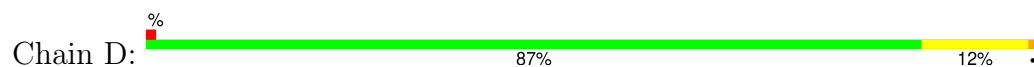


- Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta

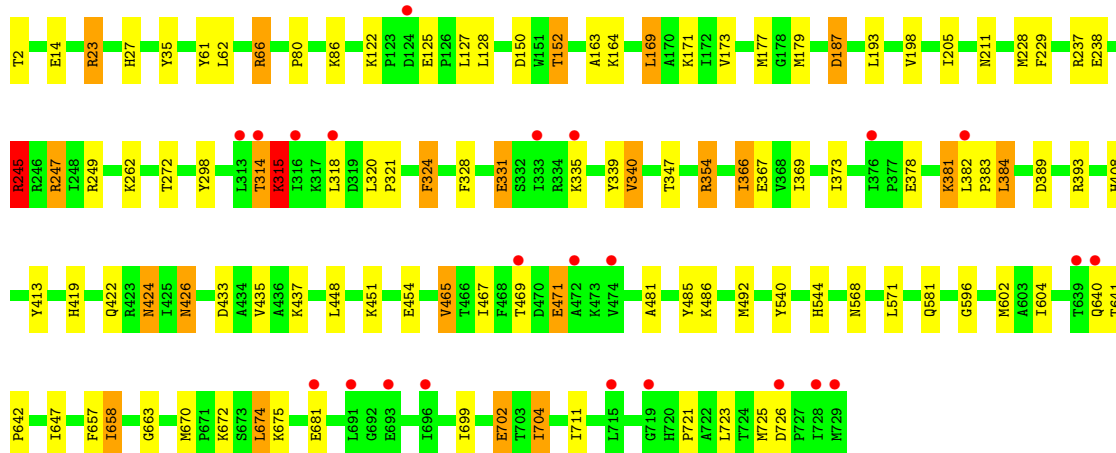
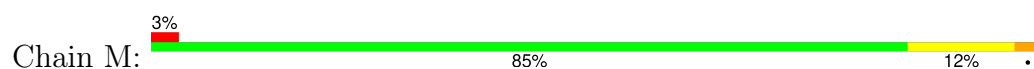




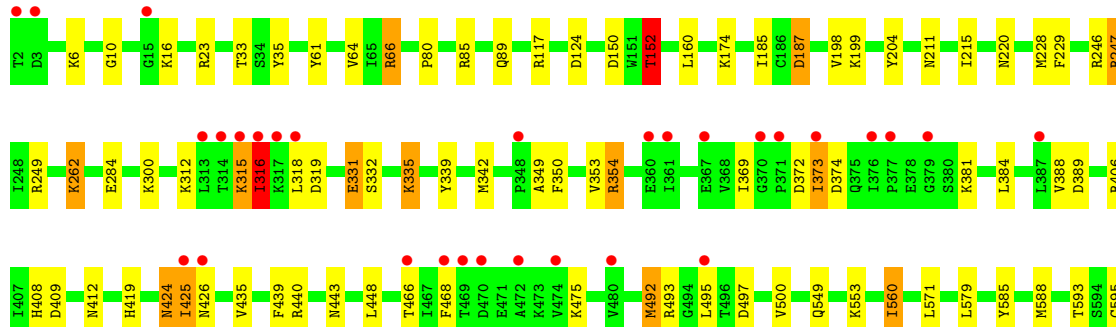
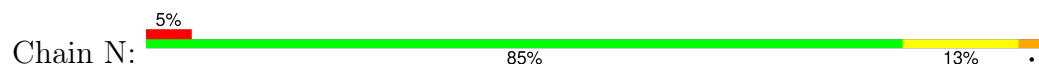
- Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta

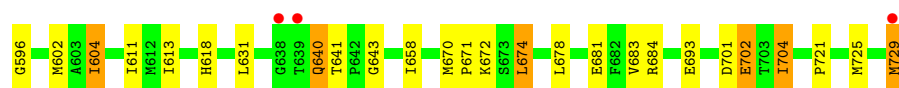


- Molecule 2: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha

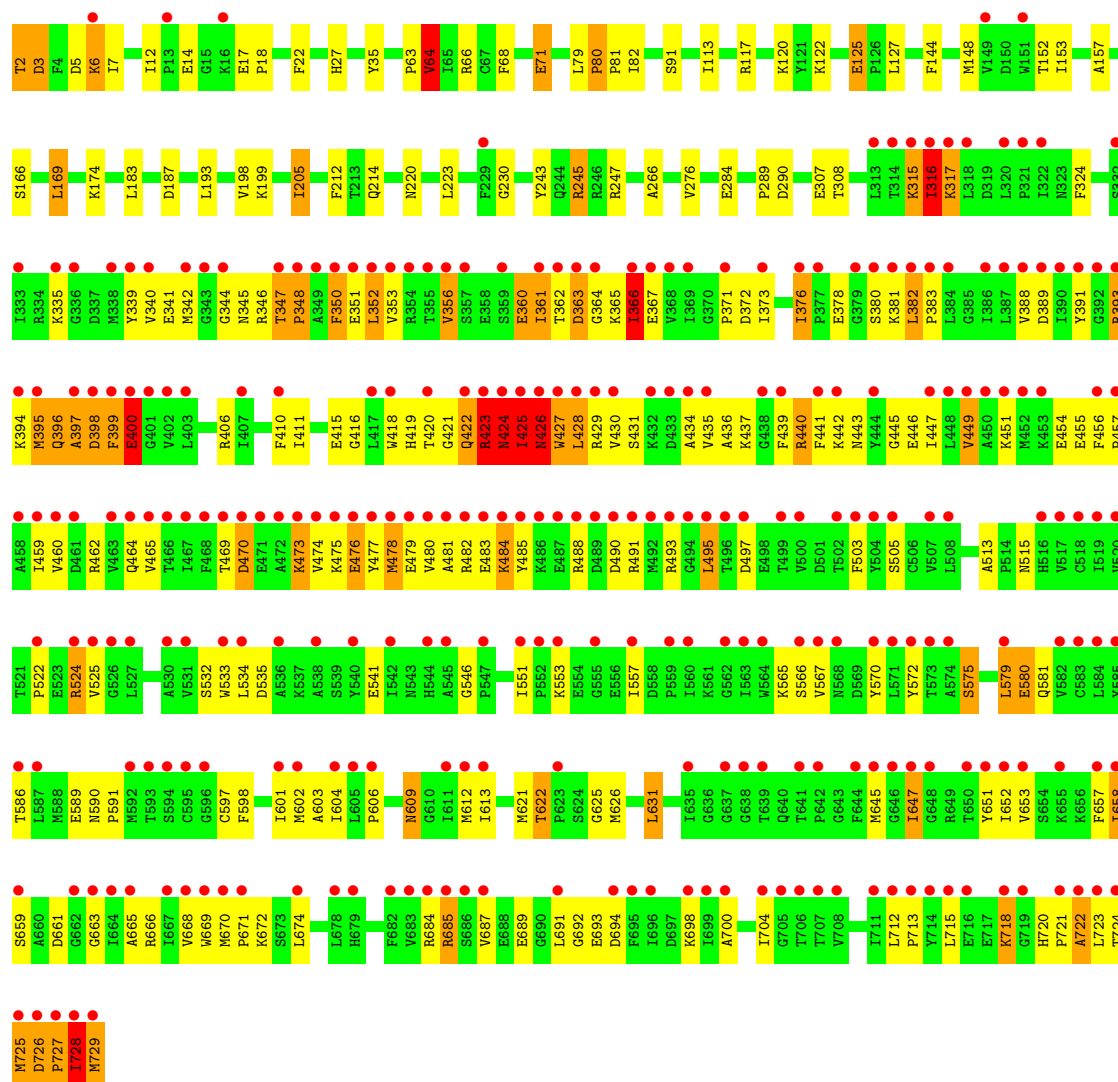


- Molecule 2: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha

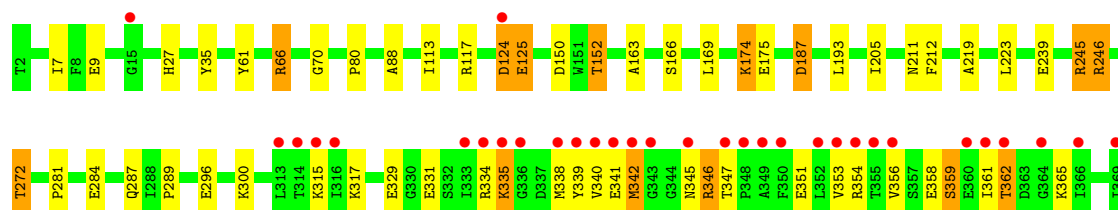
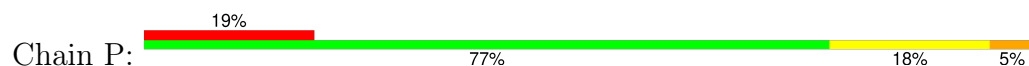


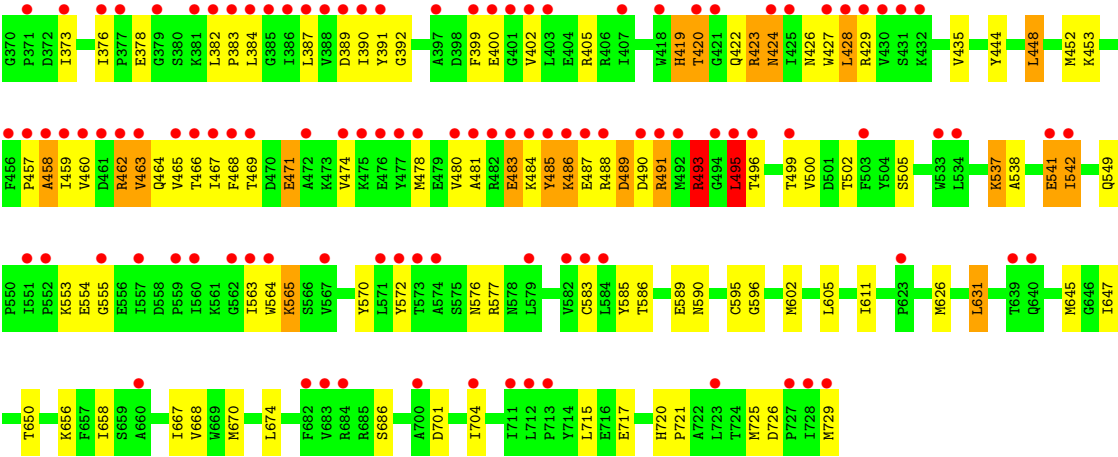


● Molecule 2: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha



● 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	99.83Å 136.77Å 141.61Å 101.23° 109.18° 103.87°	Depositor
Resolution (Å)	48.39 – 2.15 48.39 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.5 (48.39-2.15) 96.5 (48.39-2.15)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.31 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.172 , 0.221 0.172 , 0.219	Depositor DCC
R_{free} test set	17112 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	45801	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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, NI, ACT, GOL, XCC, CYN, CU1, 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	1.23	5/5230 (0.1%)	1.10	15/7086 (0.2%)
1	B	1.24	11/5244 (0.2%)	1.08	9/7105 (0.1%)
1	C	1.15	1/5200 (0.0%)	1.08	10/7048 (0.1%)
1	D	1.12	7/5181 (0.1%)	1.09	4/7021 (0.1%)
2	M	1.10	8/5909 (0.1%)	1.06	7/8000 (0.1%)
2	N	1.09	4/5885 (0.1%)	1.05	6/7968 (0.1%)
2	O	0.98	11/5885 (0.2%)	1.09	20/7968 (0.3%)
2	P	0.95	3/5896 (0.1%)	1.03	14/7982 (0.2%)
All	All	1.11	50/44430 (0.1%)	1.07	85/60178 (0.1%)

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	425	ILE	CA-CB	-9.76	1.45	1.55
2	O	400	GLU	CA-C	-8.92	1.40	1.52
1	D	414	SER	CA-C	-8.74	1.41	1.52
1	D	414	SER	C-O	-8.12	1.12	1.24
2	O	425	ILE	CG1-CD1	-7.75	1.21	1.51

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	398	ASP	CA-C-N	-9.29	110.77	122.84
2	O	398	ASP	C-N-CA	-9.29	110.77	122.84
1	B	470	CYS	N-CA-C	8.90	121.22	110.19
2	O	477	TYR	N-CA-C	-8.69	102.69	113.20
1	A	470	CYS	N-CA-C	8.63	122.26	110.35

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	5134	0	5139	60	0
1	B	5134	0	5133	66	0
1	C	5103	0	5090	50	0
1	D	5088	0	5086	61	0
2	M	5766	0	5723	63	0
2	N	5746	0	5710	66	0
2	O	5746	0	5711	242	0
2	P	5757	0	5722	129	0
3	A	16	0	0	0	0
3	B	8	0	0	0	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	0	0
3	O	8	0	0	0	0
3	P	8	0	0	0	0
4	A	9	0	0	0	0
4	B	9	0	0	0	0
4	C	9	0	0	0	0
4	D	9	0	0	0	0
5	A	2	0	0	2	0
5	B	2	0	0	0	0
5	C	2	0	0	3	0
5	D	2	0	0	1	0
6	A	6	0	8	1	0
6	B	6	0	8	0	0
6	C	6	0	8	4	0
6	D	6	0	8	6	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	1	0	0	0	0
8	N	1	0	0	0	0
8	O	1	0	0	0	0
8	P	1	0	0	0	0
9	M	3	0	3	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	N	3	0	3	3	0
9	O	3	0	3	1	0
9	P	3	0	3	1	0
10	M	1	0	0	0	0
10	N	1	0	0	0	0
10	O	1	0	0	0	0
10	P	1	0	0	0	0
11	A	306	0	0	5	0
11	B	375	0	0	5	0
11	C	275	0	0	6	0
11	D	240	0	0	5	0
11	M	326	0	0	5	0
11	N	337	0	0	9	0
11	O	83	0	0	1	0
11	P	213	0	0	3	0
All	All	45801	0	43358	707	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 8.

The worst 5 of 707 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:A:105:MET:HE1	1:B:72:MET:CG	1.54	1.37
2:O:425:ILE:HD12	2:O:425:ILE:C	1.47	1.32
1:B:370:ARG:HD2	11:B:1495:HOH:O	1.33	1.28
2:O:425:ILE:HD12	2:O:426:ASN:N	1.48	1.28
2:O:395:MET:SD	2:O:399:PHE:HE2	1.57	1.27

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	676/673 (100%)	651 (96%)	23 (3%)	2 (0%)	36	34
1	B	678/673 (101%)	653 (96%)	23 (3%)	2 (0%)	36	34
1	C	674/673 (100%)	648 (96%)	25 (4%)	1 (0%)	48	50
1	D	671/673 (100%)	645 (96%)	22 (3%)	4 (1%)	21	15
2	M	730/728 (100%)	697 (96%)	28 (4%)	5 (1%)	18	13
2	N	727/728 (100%)	700 (96%)	22 (3%)	5 (1%)	18	13
2	O	727/728 (100%)	650 (89%)	51 (7%)	26 (4%)	2	0
2	P	728/728 (100%)	684 (94%)	37 (5%)	7 (1%)	12	8
All	All	5611/5604 (100%)	5328 (95%)	231 (4%)	52 (1%)	14	9

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	ASN
1	B	267	ASN
1	B	415	ASN
1	D	415	ASN
1	D	416	ARG

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	547/542 (101%)	529 (97%)	18 (3%)	33	34
1	B	549/542 (101%)	533 (97%)	16 (3%)	37	39
1	C	543/542 (100%)	530 (98%)	13 (2%)	43	47
1	D	541/542 (100%)	524 (97%)	17 (3%)	35	37
2	M	614/610 (101%)	576 (94%)	38 (6%)	16	12
2	N	611/610 (100%)	571 (94%)	40 (6%)	15	11
2	O	611/610 (100%)	537 (88%)	74 (12%)	5	2
2	P	612/610 (100%)	558 (91%)	54 (9%)	9	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	4628/4608 (100%)	4358 (94%)	270 (6%)	18	14

5 of 270 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	P	342	MET
2	P	419	HIS
2	P	563	ILE
2	M	681	GLU
2	M	604	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
2	N	581	GLN
2	P	211	ASN
2	N	679	HIS
2	O	578	ASN
2	P	424	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 38 ligands modelled in this entry, 12 are monoatomic - leaving 26 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	A	800	5,11,1	0,12,12	-	-	-		
9	ACT	M	953	-	1,2,3	1.24	0	0,1,3	-	-
3	SF4	P	900	2	0,12,12	-	-	-		
6	GOL	A	963	-	5,5,5	0.68	0	5,5,5	1.88	3 (60%)
5	CYN	B	900	4	1,1,1	0.58	0	-		
3	SF4	O	900	2	0,12,12	-	-	-		
4	XCC	C	800	5,11,1	0,12,12	-	-	-		
3	SF4	B	750	1	0,12,12	-	-	-		
3	SF4	N	900	2	0,12,12	-	-	-		
6	GOL	B	963	-	5,5,5	0.81	0	5,5,5	1.79	1 (20%)
3	SF4	C	750	1	0,12,12	-	-	-		
9	ACT	N	953	-	1,2,3	1.30	0	0,1,3	-	-
9	ACT	O	953	-	1,2,3	1.33	0	0,1,3	-	-
5	CYN	C	900	4	1,1,1	0.08	0	-		
3	SF4	C	700	1	0,12,12	-	-	-		
5	CYN	A	900	4	1,1,1	0.28	0	-		
9	ACT	P	953	-	1,2,3	1.37	0	0,1,3	-	-
6	GOL	C	963	-	5,5,5	0.54	0	5,5,5	1.00	0
3	SF4	A	700	1	0,12,12	-	-	-		
3	SF4	A	750	1	0,12,12	-	-	-		
4	XCC	B	800	5,11,1	0,12,12	-	-	-		
4	XCC	D	800	11,1	0,12,12	-	-	-		
3	SF4	M	900	2	0,12,12	-	-	-		
5	CYN	D	900	-	1,1,1	0.16	0	-		
6	GOL	D	963	-	5,5,5	0.69	0	5,5,5	1.43	1 (20%)
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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SF4	C	750	1	-	-	0/6/5/5
3	SF4	A	700	1	-	-	0/6/5/5
3	SF4	O	900	2	-	-	0/6/5/5
4	XCC	D	800	11,1	-	-	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	XCC	A	800	5,11,1	-	-	0/4/4/4
3	SF4	M	900	2	-	-	0/6/5/5
3	SF4	C	700	1	-	-	0/6/5/5
4	XCC	C	800	5,11,1	-	-	0/4/4/4
3	SF4	B	750	1	-	-	0/6/5/5
3	SF4	A	750	1	-	-	0/6/5/5
3	SF4	P	900	2	-	-	0/6/5/5
3	SF4	N	900	2	-	-	0/6/5/5
6	GOL	C	963	-	-	3/4/4/4	-
6	GOL	A	963	-	-	2/4/4/4	-
6	GOL	B	963	-	-	1/4/4/4	-
3	SF4	D	750	1	-	-	0/6/5/5
4	XCC	B	800	5,11,1	-	-	0/4/4/4
6	GOL	D	963	-	-	4/4/4/4	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	963	GOL	O2-C2-C3	-2.58	98.50	109.18
6	D	963	GOL	O1-C1-C2	-2.50	99.10	110.38
6	A	963	GOL	O1-C1-C2	-2.47	99.24	110.38
6	A	963	GOL	O2-C2-C3	-2.28	99.73	109.18
6	A	963	GOL	O3-C3-C2	-2.17	100.62	110.38

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	963	GOL	O1-C1-C2-C3
6	C	963	GOL	O1-C1-C2-C3
6	D	963	GOL	C1-C2-C3-O3
6	B	963	GOL	C1-C2-C3-O3
6	D	963	GOL	O1-C1-C2-C3

There are no ring outliers.

11 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	M	953	ACT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	963	GOL	1	0
9	N	953	ACT	3	0
9	O	953	ACT	1	0
5	C	900	CYN	3	0
3	C	700	SF4	1	0
5	A	900	CYN	2	0
9	P	953	ACT	1	0
6	C	963	GOL	4	0
5	D	900	CYN	1	0
6	D	963	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	673/673 (100%)	-0.34	6 (0%) 81 83	8, 24, 42, 62	5 (0%)
1	B	673/673 (100%)	-0.50	7 (1%) 79 82	7, 22, 39, 66	7 (1%)
1	C	673/673 (100%)	-0.30	1 (0%) 92 93	15, 26, 41, 57	3 (0%)
1	D	673/673 (100%)	-0.17	8 (1%) 76 79	19, 28, 43, 62	0
2	M	728/728 (100%)	0.09	23 (3%) 50 54	13, 31, 58, 76	4 (0%)
2	N	728/728 (100%)	0.02	33 (4%) 38 43	11, 30, 57, 71	1 (0%)
2	O	728/728 (100%)	1.65	277 (38%) 1 1	17, 62, 88, 123	1 (0%)
2	P	728/728 (100%)	0.81	140 (19%) 3 4	13, 45, 79, 107	2 (0%)
All	All	5604/5604 (100%)	0.18	495 (8%) 15 17	7, 29, 74, 123	23 (0%)

The worst 5 of 495 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	728	ILE	7.6
2	O	450	ALA	7.2
2	O	366	ILE	6.2
2	O	481	ALA	6.0
2	O	427	TRP	6.0

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
9	ACT	P	953	3/4	0.86	0.41	75,75,76,76	0
10	NA	P	730	1/1	0.86	0.10	35,35,35,35	0
6	GOL	A	963	6/6	0.88	0.12	26,30,37,38	0
6	GOL	B	963	6/6	0.88	0.15	27,37,38,44	0
9	ACT	N	953	3/4	0.89	0.33	71,71,71,71	0
10	NA	O	730	1/1	0.89	0.08	64,64,64,64	0
9	ACT	O	953	3/4	0.89	0.34	109,109,109,109	0
6	GOL	D	963	6/6	0.90	0.12	38,43,45,45	0
6	GOL	C	963	6/6	0.90	0.14	50,53,54,55	0
9	ACT	M	953	3/4	0.91	0.29	55,55,56,56	0
5	CYN	C	900	2/2	0.91	0.32	31,31,31,33	0
3	SF4	O	900	8/8	0.94	0.07	57,60,62,64	0
5	CYN	D	900	2/2	0.94	0.24	42,42,42,43	0
5	CYN	A	900	2/2	0.94	0.23	31,31,31,32	0
5	CYN	B	900	2/2	0.96	0.15	25,25,25,25	0
10	NA	N	730	1/1	0.96	0.04	26,26,26,26	0
10	NA	M	1	1/1	0.97	0.04	28,28,28,28	0
8	NI	O	951	1/1	0.97	0.08	66,66,66,66	0
4	XCC	D	800	9/9	0.98	0.04	27,30,36,36	0
7	CU1	O	950	1/1	0.98	0.07	73,73,73,73	0
7	CU1	P	950	1/1	0.98	0.06	49,49,49,49	0
3	SF4	P	900	8/8	0.99	0.04	38,41,42,42	0
7	CU1	M	950	1/1	0.99	0.03	35,35,35,35	0
7	CU1	N	950	1/1	0.99	0.03	34,34,34,34	0
4	XCC	A	800	9/9	0.99	0.03	21,22,25,26	0
4	XCC	B	800	9/9	0.99	0.03	18,19,24,26	0
4	XCC	C	800	9/9	0.99	0.03	19,25,28,31	0
8	NI	P	951	1/1	0.99	0.05	41,41,41,41	0
3	SF4	A	750	8/8	0.99	0.03	17,17,18,19	0
3	SF4	B	750	8/8	0.99	0.02	16,16,18,18	0
3	SF4	C	700	8/8	0.99	0.04	24,29,31,31	0
3	SF4	C	750	8/8	0.99	0.03	26,27,28,29	0
3	SF4	D	750	8/8	0.99	0.04	24,24,26,26	0
3	SF4	M	900	8/8	0.99	0.03	20,22,23,23	0
3	SF4	N	900	8/8	0.99	0.02	20,23,24,25	0
3	SF4	A	700	8/8	0.99	0.03	16,17,19,20	0
8	NI	M	951	1/1	1.00	0.01	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	NI	N	951	1/1	1.00	0.01	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.