



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:24 AM GMT

PDB ID : 3I04  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

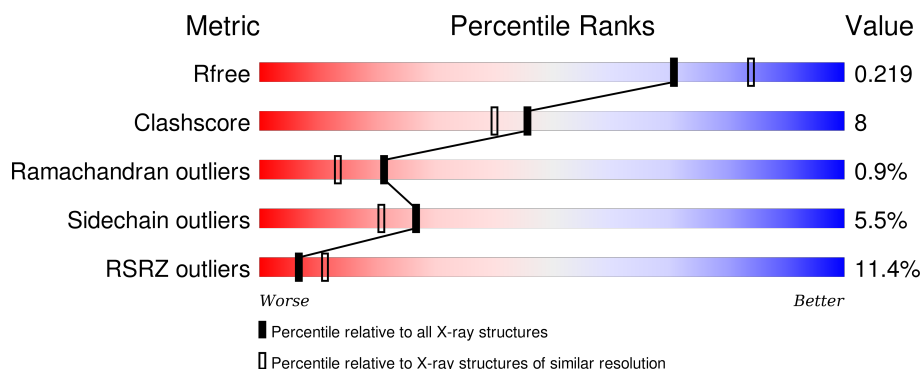
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	<div> <div>6%</div> <div>90%</div> <div>9%</div> </div>
1	B	673	<div> <div>4%</div> <div>89%</div> <div>10%</div> </div>
1	C	673	<div> <div>2%</div> <div>91%</div> <div>8%</div> </div>
1	D	673	<div> <div>4%</div> <div>88%</div> <div>11%</div> </div>
2	M	728	<div> <div>3%</div> <div>87%</div> <div>11%</div> </div>

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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	X
6	GOL	B	963	-	-	-	X
6	GOL	C	963	-	-	X	-
6	GOL	D	963	-	-	X	-
9	ACT	M	953	-	-	-	X
9	ACT	N	953	-	-	X	X
9	ACT	O	953	-	-	-	X
9	ACT	P	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.

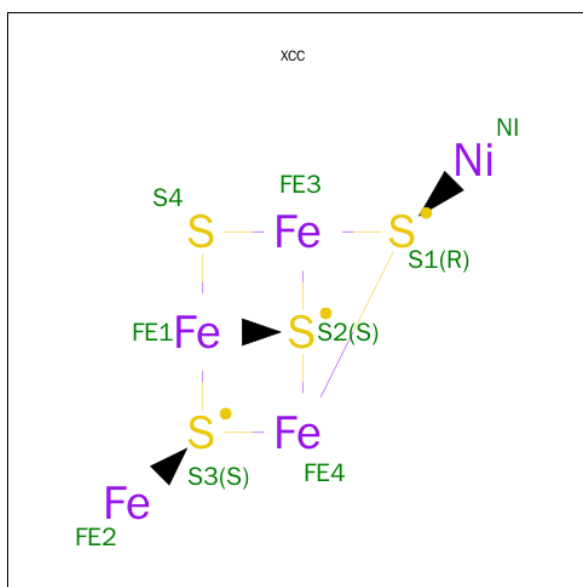
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	728	Total	C	N	O	S	0	4	0
			5766	3695	962	1074	35			
2	N	728	Total	C	N	O	S	0	1	0
			5746	3684	959	1068	35			
2	O	728	Total	C	N	O	S	0	1	0
			5746	3684	959	1068	35			
2	P	728	Total	C	N	O	S	0	2	0
			5757	3690	963	1069	35			

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



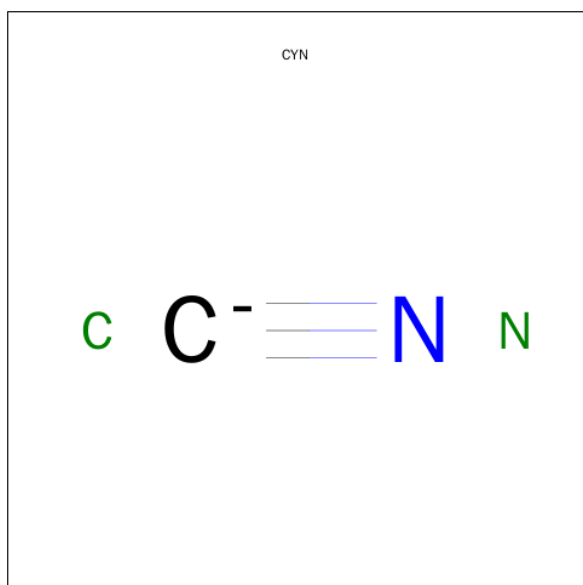
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	M	1	Total	Fe	S	0	0
			8	4	4		
3	N	1	Total	Fe	S	0	0
			8	4	4		
3	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 (three-letter code: XCC) (formula: Fe<sub>4</sub>NiS<sub>4</sub>).



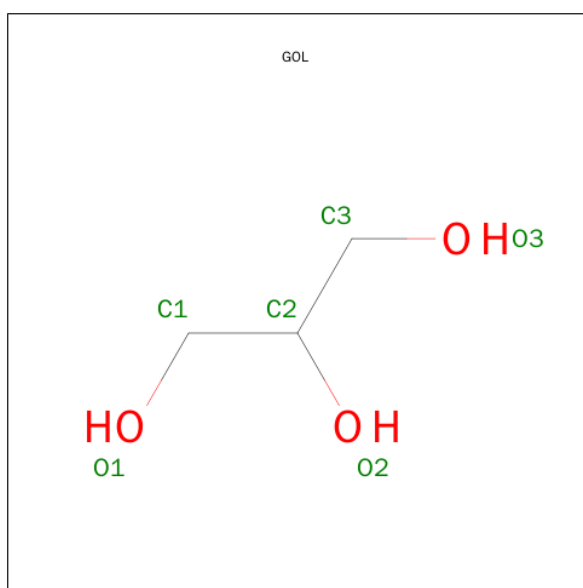
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
4	B	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
4	C	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
4	D	1	Total	Fe	Ni	S	0	0
			9	4	1	4		

- Molecule 5 is CYANIDE ION (three-letter code: CYN) (formula: CN).



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 7 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

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

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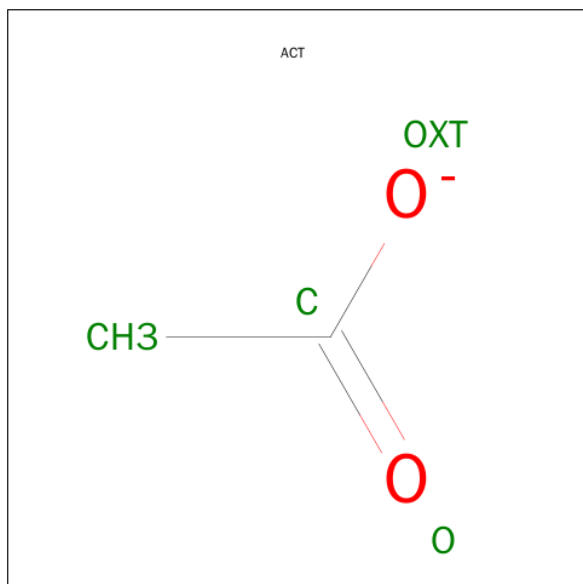
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	N	1	Total	Cu	0	0
			1	1		
7	M	1	Total	Cu	0	0
			1	1		

- Molecule 8 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

- Molecule 9 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

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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 (three-letter code: NA) (formula: Na).

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

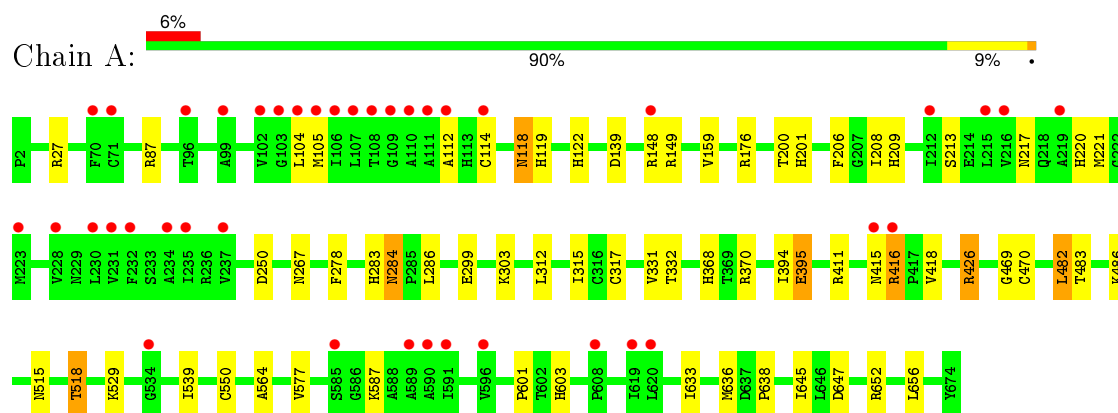
- Molecule 11 is water.

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		

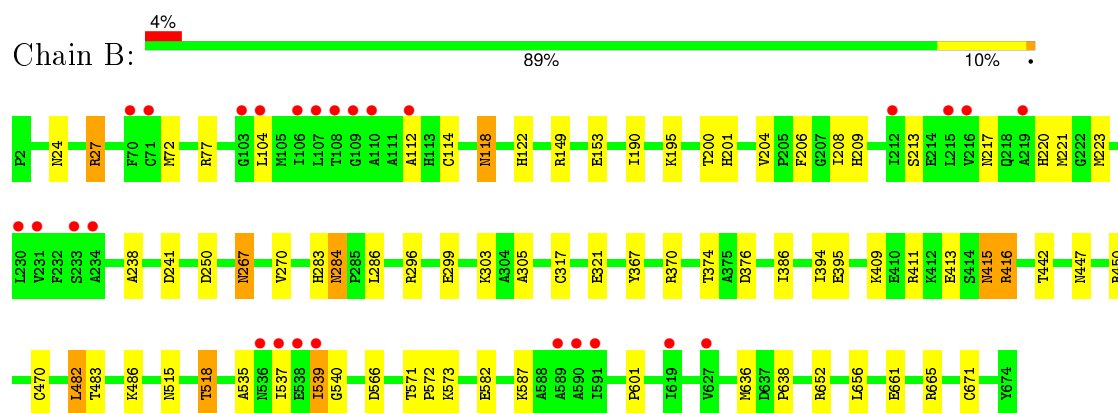
### 3 Residue-property plots

These plots are drawn for all protein, RNA 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 ( $\text{RSRZ} > 2$ ). 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.

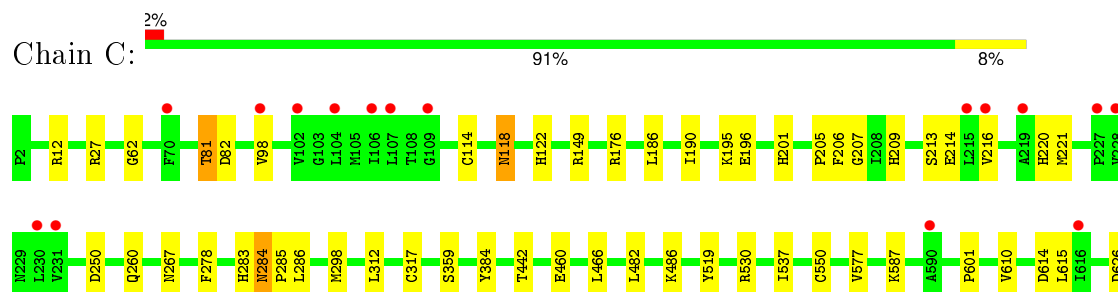
- Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta



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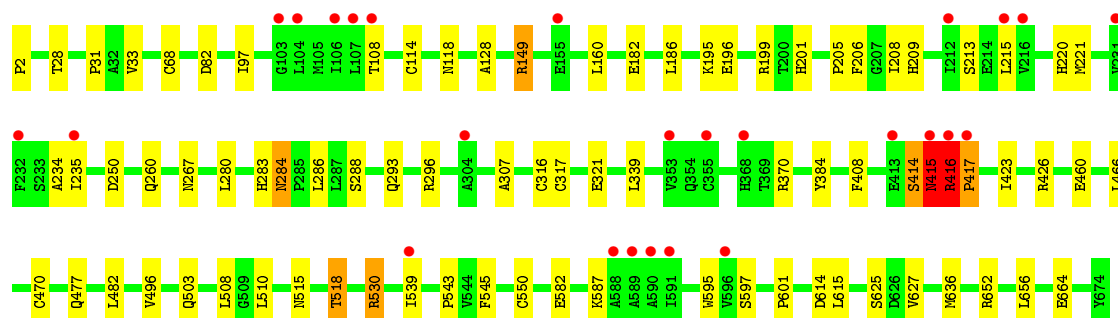
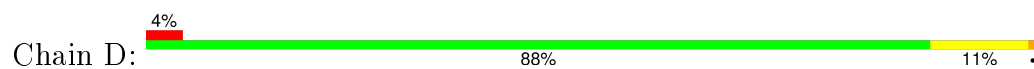


- Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta

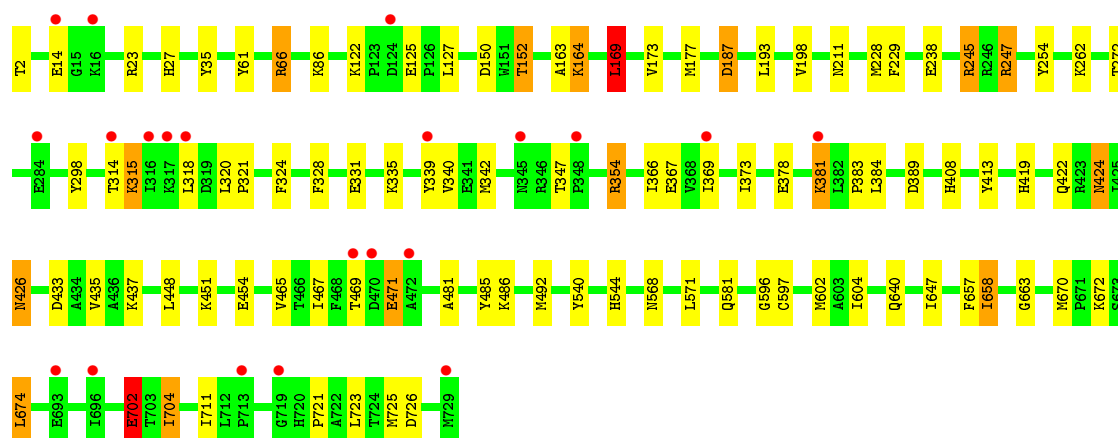
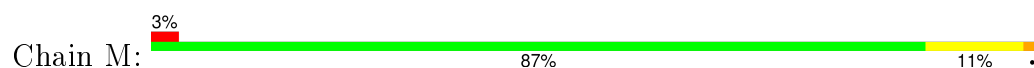




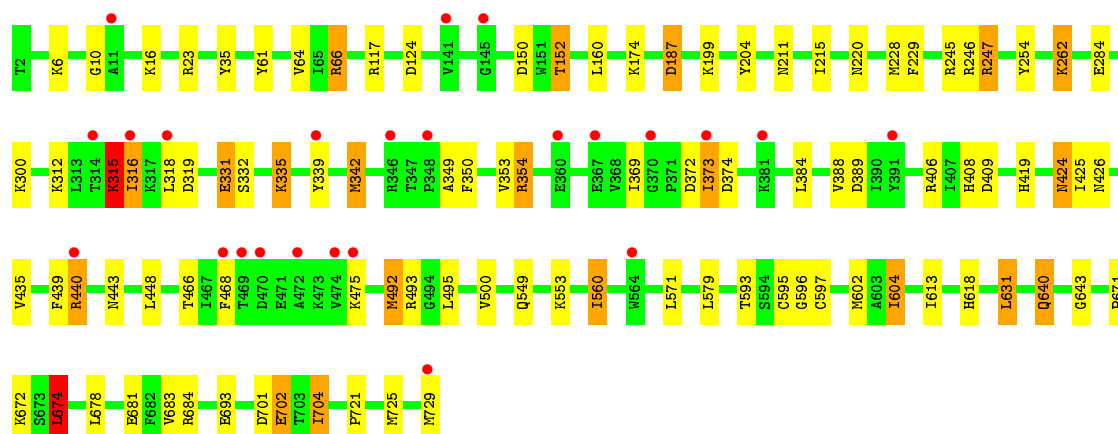
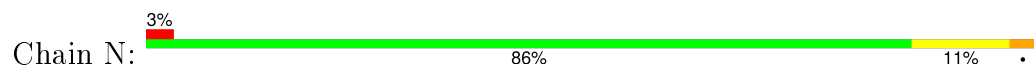
- Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta



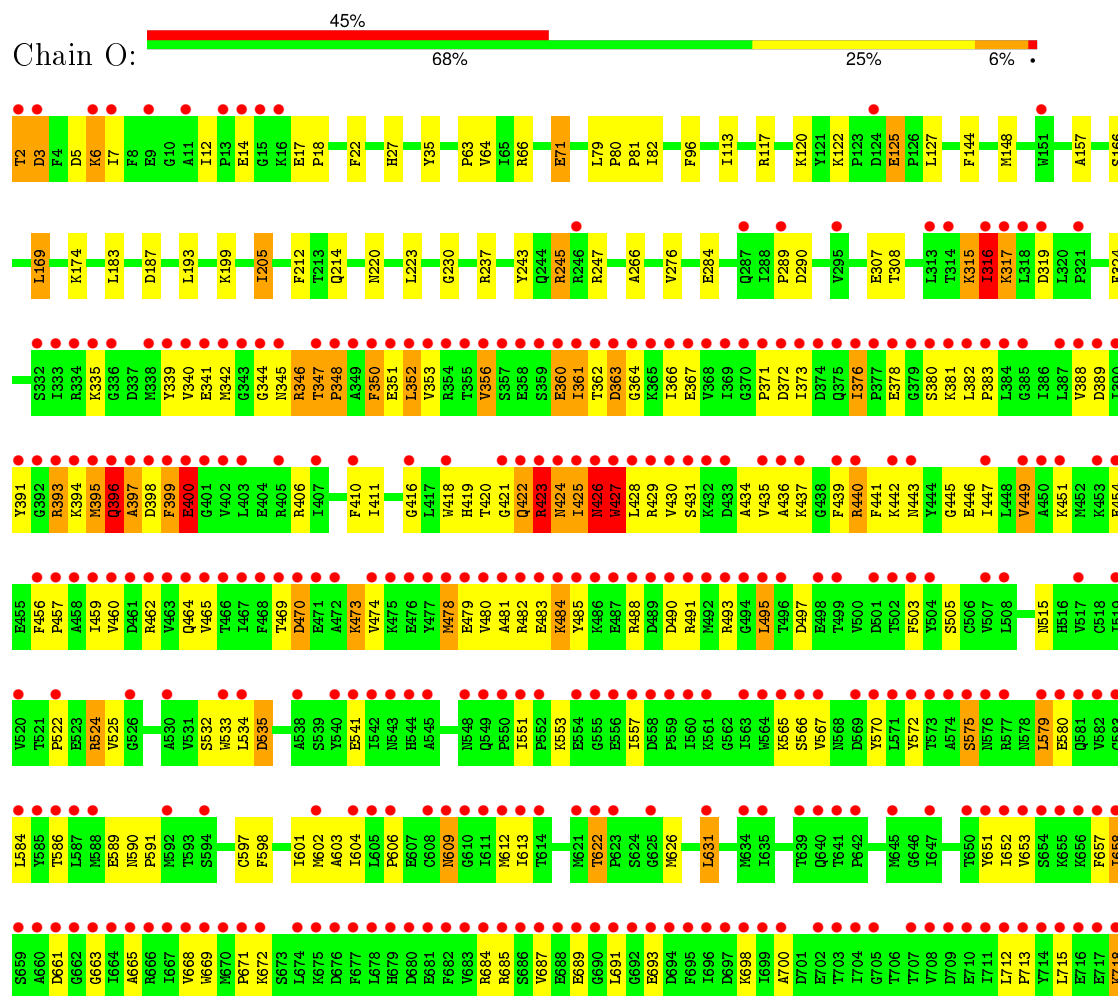
- Molecule 2: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha



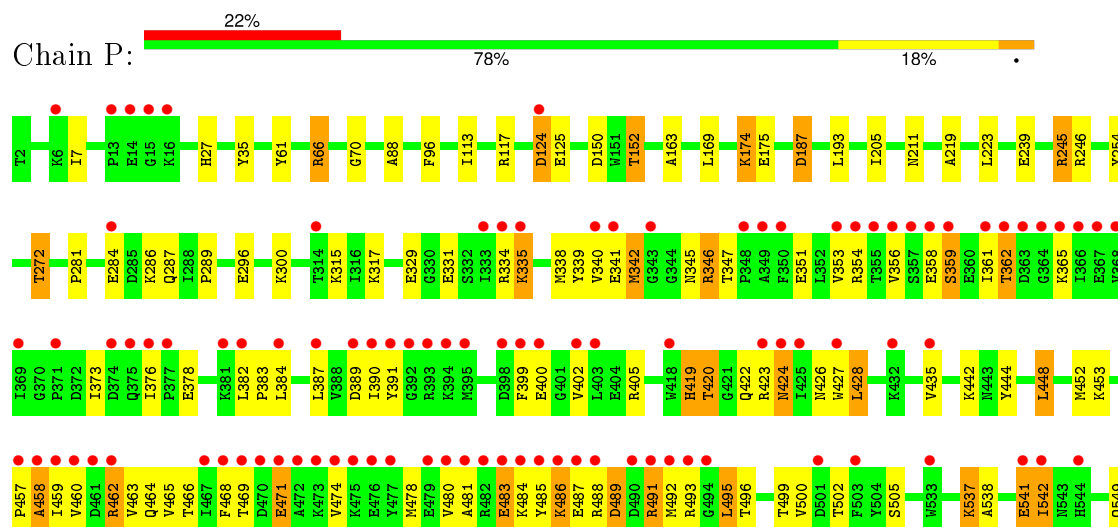
- Molecule 2: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha

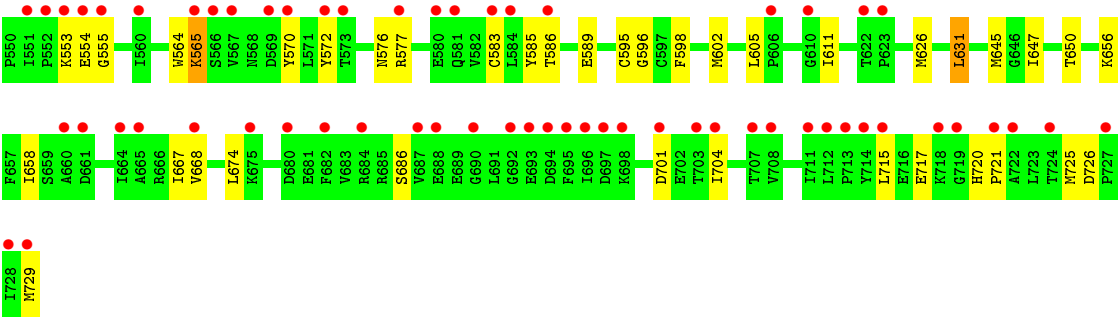


## Chain O:



Chain P:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.83Å 136.77Å 141.61Å 101.23° 109.18° 103.87°	Depositor
Resolution (Å)	48.39 – 2.15 48.40 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.5 (48.39-2.15) 86.8 (48.40-2.15)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.7	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 57.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 344234 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	45801	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, CU1, NI, NA, SF4, ACT, XCC, CYN

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	0.97	2/5230 (0.0%)	0.82	3/7086 (0.0%)
1	B	0.99	2/5244 (0.0%)	0.82	1/7105 (0.0%)
1	C	0.92	1/5200 (0.0%)	0.81	1/7048 (0.0%)
1	D	0.88	1/5181 (0.0%)	0.80	3/7021 (0.0%)
2	M	0.89	1/5909 (0.0%)	0.81	3/8000 (0.0%)
2	N	0.88	0/5885	0.80	3/7968 (0.0%)
2	O	0.76	0/5885	0.79	3/7968 (0.0%)
2	P	0.76	0/5896	0.75	2/7982 (0.0%)
All	All	0.88	7/44430 (0.0%)	0.80	19/60178 (0.0%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	469	GLY	CA-C	-5.65	1.42	1.51
1	D	414	SER	C-O	-5.59	1.12	1.23
1	C	214	GLU	CG-CD	5.53	1.60	1.51
1	B	204	VAL	CB-CG1	5.34	1.64	1.52
1	A	564	ALA	CA-CB	5.25	1.63	1.52

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	428	LEU	CA-CB-CG	5.72	128.46	115.30
2	M	198	VAL	CG1-CB-CG2	5.67	119.98	110.90
2	O	237	ARG	NE-CZ-NH2	5.65	123.12	120.30
2	N	631	LEU	CA-CB-CG	5.62	128.22	115.30
1	D	149	ARG	NE-CZ-NH1	5.56	123.08	120.30

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	59	0
1	B	5134	0	5133	64	0
1	C	5103	0	5090	47	0
1	D	5088	0	5086	61	0
2	M	5766	0	5723	59	0
2	N	5746	0	5710	61	0
2	O	5746	0	5711	228	0
2	P	5757	0	5722	124	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	5	0
11	D	240	0	0	5	0
11	M	326	0	0	4	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	673	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 673 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: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
2:O:425:ILE:HD12	2:O:425:ILE:C	1.47	1.27
1:A:105:MET:CE	1:B:72:MET:HG3	1.69	1.23

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%)	46	42
1	B	678/673 (101%)	653 (96%)	23 (3%)	2 (0%)	46	42
1	C	674/673 (100%)	648 (96%)	25 (4%)	1 (0%)	56	57
1	D	671/673 (100%)	645 (96%)	22 (3%)	4 (1%)	30	21
2	M	730/728 (100%)	697 (96%)	28 (4%)	5 (1%)	26	18
2	N	727/728 (100%)	700 (96%)	22 (3%)	5 (1%)	26	18
2	O	727/728 (100%)	650 (89%)	51 (7%)	26 (4%)	4	1
2	P	728/728 (100%)	684 (94%)	37 (5%)	7 (1%)	19	11
All	All	5611/5604 (100%)	5328 (95%)	231 (4%)	52 (1%)	21	13

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%)	530 (97%)	17 (3%)	47	47
1	B	549/542 (101%)	534 (97%)	15 (3%)	52	53
1	C	543/542 (100%)	530 (98%)	13 (2%)	57	60
1	D	541/542 (100%)	529 (98%)	12 (2%)	60	63
2	M	614/610 (101%)	581 (95%)	33 (5%)	27	22
2	N	611/610 (100%)	571 (94%)	40 (6%)	21	15
2	O	611/610 (100%)	540 (88%)	71 (12%)	7	3
2	P	612/610 (100%)	557 (91%)	55 (9%)	12	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4628/4608 (100%)	4372 (94%)	256 (6%)	27 21

5 of 256 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	N	448	LEU
2	O	214	GLN
2	P	486	LYS
2	N	495	LEU
2	O	2	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	477	GLN
2	M	424	ASN
2	P	408	HIS
1	D	503	GLN
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 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
3	SF4	A	700	1	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	A	750	1	0,12,12	0.00	-	0,24,24	0.00	-
4	XCC	A	800	1,11	0,11,11	0.00	-	0,19,19	0.00	-
5	CYN	A	900	-	0,1,1	0.00	-	0,0,0	0.00	-
6	GOL	A	963	-	5,5,5	0.66	0	5,5,5	1.69	1 (20%)
3	SF4	B	750	1	0,12,12	0.00	-	0,24,24	0.00	-
4	XCC	B	800	1,11	0,11,11	0.00	-	0,19,19	0.00	-
5	CYN	B	900	-	0,1,1	0.00	-	0,0,0	0.00	-
6	GOL	B	963	-	5,5,5	0.80	0	5,5,5	1.59	1 (20%)
3	SF4	C	700	1	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	C	750	1	0,12,12	0.00	-	0,24,24	0.00	-
4	XCC	C	800	1,11	0,11,11	0.00	-	0,19,19	0.00	-
5	CYN	C	900	-	0,1,1	0.00	-	0,0,0	0.00	-
6	GOL	C	963	-	5,5,5	0.55	0	5,5,5	0.89	0
3	SF4	D	750	1	0,12,12	0.00	-	0,24,24	0.00	-
4	XCC	D	800	1,11	0,11,11	0.00	-	0,19,19	0.00	-
5	CYN	D	900	-	0,1,1	0.00	-	0,0,0	0.00	-
6	GOL	D	963	-	5,5,5	0.71	0	5,5,5	1.31	1 (20%)
3	SF4	M	900	2	0,12,12	0.00	-	0,24,24	0.00	-
9	ACT	M	953	-	2,2,3	0.77	0	0,1,3	0.00	-
3	SF4	N	900	2	0,12,12	0.00	-	0,24,24	0.00	-
9	ACT	N	953	-	2,2,3	0.83	0	0,1,3	0.00	-
3	SF4	O	900	2	0,12,12	0.00	-	0,24,24	0.00	-
9	ACT	O	953	-	2,2,3	0.83	0	0,1,3	0.00	-
3	SF4	P	900	2	0,12,12	0.00	-	0,24,24	0.00	-
9	ACT	P	953	-	2,2,3	0.86	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
3	SF4	A	700	1	-	0/0/48/48	0/6/5/5
3	SF4	A	750	1	-	0/0/48/48	0/6/5/5
4	XCC	A	800	1,11	-	0/0/32/32	0/0/3/3
5	CYN	A	900	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	963	-	-	0/4/4/4	0/0/0/0
3	SF4	B	750	1	-	0/0/48/48	0/6/5/5
4	XCC	B	800	1,11	-	0/0/32/32	0/0/3/3
5	CYN	B	900	-	-	0/0/0/0	0/0/0/0
6	GOL	B	963	-	-	0/4/4/4	0/0/0/0
3	SF4	C	700	1	-	0/0/48/48	0/6/5/5
3	SF4	C	750	1	-	0/0/48/48	0/6/5/5
4	XCC	C	800	1,11	-	0/0/32/32	0/0/3/3
5	CYN	C	900	-	-	0/0/0/0	0/0/0/0
6	GOL	C	963	-	-	0/4/4/4	0/0/0/0
3	SF4	D	750	1	-	0/0/48/48	0/6/5/5
4	XCC	D	800	1,11	-	0/0/32/32	0/0/3/3
5	CYN	D	900	-	-	0/0/0/0	0/0/0/0
6	GOL	D	963	-	-	0/4/4/4	0/0/0/0
3	SF4	M	900	2	-	0/0/48/48	0/6/5/5
9	ACT	M	953	-	-	0/0/0/0	0/0/0/0
3	SF4	N	900	2	-	0/0/48/48	0/6/5/5
9	ACT	N	953	-	-	0/0/0/0	0/0/0/0
3	SF4	O	900	2	-	0/0/48/48	0/6/5/5
9	ACT	O	953	-	-	0/0/0/0	0/0/0/0
3	SF4	P	900	2	-	0/0/48/48	0/6/5/5
9	ACT	P	953	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	963	GOL	O1-C1-C2	-2.29	99.10	110.18
6	A	963	GOL	O1-C1-C2	-2.26	99.24	110.18
6	B	963	GOL	O2-C2-C3	-2.21	98.50	108.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	900	CYN	2	0
6	A	963	GOL	1	0
3	C	700	SF4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	900	CYN	3	0
6	C	963	GOL	4	0
5	D	900	CYN	1	0
6	D	963	GOL	6	0
9	M	953	ACT	1	0
9	N	953	ACT	3	0
9	O	953	ACT	1	0
9	P	953	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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	673/673 (100%)	0.03	40 (5%)	26	36	14, 24, 42, 62	0
1	B	673/673 (100%)	-0.01	27 (4%)	42	52	14, 22, 39, 66	0
1	C	673/673 (100%)	-0.17	16 (2%)	62	71	18, 26, 41, 57	0
1	D	673/673 (100%)	0.01	26 (3%)	43	54	19, 28, 43, 62	0
2	M	728/728 (100%)	-0.02	21 (2%)	55	65	16, 31, 58, 76	0
2	N	728/728 (100%)	0.04	24 (3%)	50	60	16, 30, 57, 71	0
2	O	728/728 (100%)	2.11	326 (44%)	0	1	25, 62, 88, 123	0
2	P	728/728 (100%)	0.86	159 (21%)	1	2	19, 45, 79, 107	0
All	All	5604/5604 (100%)	0.37	639 (11%)	7	11	14, 29, 74, 123	0

The worst 5 of 639 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	481	ALA	14.6
2	O	486	LYS	10.0
2	O	490	ASP	9.9
2	O	474	VAL	9.9
2	O	485	TYR	9.9

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
9	ACT	P	953	3/4	0.87	0.51	22.18	75,75,76,76	0
9	ACT	O	953	3/4	0.85	0.41	7.42	109,109,109,109	0
5	CYN	C	900	2/2	0.93	0.28	3.37	31,31,31,33	0
6	GOL	B	963	6/6	0.90	0.18	3.07	27,37,38,44	0
9	ACT	M	953	3/4	0.95	0.23	2.62	55,55,56,56	0
9	ACT	N	953	3/4	0.92	0.23	2.04	71,71,71,71	0
6	GOL	C	963	6/6	0.91	0.20	1.91	50,53,54,55	0
6	GOL	A	963	6/6	0.90	0.18	1.58	26,30,37,38	0
10	NA	P	730	1/1	0.88	0.14	0.59	35,35,35,35	0
6	GOL	D	963	6/6	0.93	0.13	0.52	38,43,45,45	0
3	SF4	D	750	8/8	0.99	0.13	-0.29	24,24,26,26	0
3	SF4	M	900	8/8	0.99	0.11	-0.53	20,22,23,23	0
4	XCC	D	800	9/9	0.99	0.12	-0.65	27,30,36,36	0
4	XCC	C	800	9/9	0.99	0.11	-0.65	19,25,28,31	0
3	SF4	C	750	8/8	0.99	0.10	-0.69	26,27,28,29	0
3	SF4	A	750	8/8	1.00	0.13	-0.71	17,17,18,19	0
3	SF4	N	900	8/8	0.99	0.11	-0.78	20,23,24,25	0
3	SF4	C	700	8/8	0.99	0.09	-0.80	24,29,31,31	0
3	SF4	B	750	8/8	0.99	0.12	-0.88	16,16,18,18	0
4	XCC	A	800	9/9	0.99	0.13	-0.89	21,22,25,26	0
10	NA	N	730	1/1	0.94	0.08	-0.93	26,26,26,26	0
3	SF4	A	700	8/8	0.99	0.09	-1.04	16,17,19,20	0
5	CYN	A	900	2/2	0.94	0.17	-1.13	31,31,31,32	0
4	XCC	B	800	9/9	0.99	0.12	-1.15	18,19,24,26	0
7	CU1	M	950	1/1	0.99	0.09	-1.15	35,35,35,35	0
10	NA	O	730	1/1	0.76	0.07	-1.37	64,64,64,64	0
3	SF4	P	900	8/8	0.99	0.05	-1.49	38,41,42,42	0
8	NI	N	951	1/1	1.00	0.10	-1.49	24,24,24,24	0
5	CYN	B	900	2/2	0.94	0.13	-1.57	25,25,25,25	0
8	NI	M	951	1/1	1.00	0.10	-1.70	24,24,24,24	0
5	CYN	D	900	2/2	0.98	0.13	-2.10	42,42,42,43	0
3	SF4	O	900	8/8	0.93	0.06	-2.13	57,60,62,64	0
7	CU1	N	950	1/1	0.99	0.09	-2.32	34,34,34,34	0
8	NI	P	951	1/1	0.99	0.04	-2.55	41,41,41,41	0
7	CU1	P	950	1/1	0.98	0.03	-2.56	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	CU1	O	950	1/1	0.98	0.03	-3.31	73,73,73,73	0
10	NA	M	1	1/1	0.97	0.07	-3.38	28,28,28,28	0
8	NI	O	951	1/1	0.97	0.04	-3.78	66,66,66,66	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.