



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 25, 2023 – 12:05 PM EDT

PDB ID : 2Z8Y  
Title : Xenon-bound structure of bifunctional carbon monoxide dehydrogenase/acet  
yl-CoA synthase(CODH/ACS) from Moorella thermoacetica  
Authors : Doukov, T.I.; Blasiak, L.C.; Drennan, C.L.  
Deposited on : 2007-09-12  
Resolution : 2.51 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

<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>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

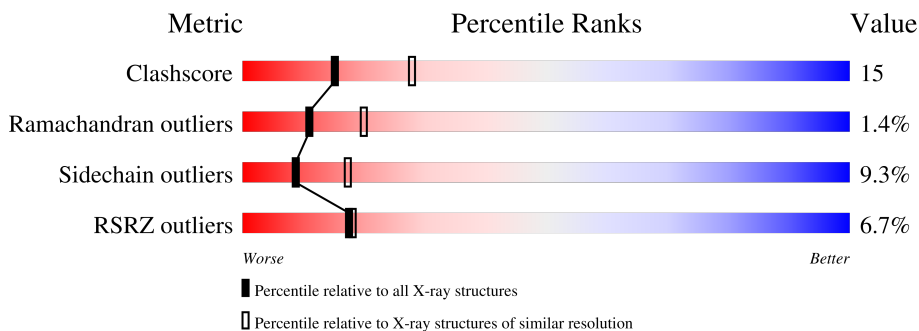
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.51 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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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  $\geq 3$ , 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	 2% 74% 23% .
1	B	674	 1% 75% 22% .
1	C	674	 1% 73% 24% .
1	D	674	 2% 70% 28% .
2	M	729	 1% 74% 22% .
2	N	729	 73% 23% .

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Mol	Chain	Length	Quality of chain
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	A	800	-	-	X	-
4	XCC	B	800	-	-	X	-
4	XCC	C	800	-	-	X	-
5	XE	A	1001	-	-	X	-
5	XE	A	1003[A]	-	-	X	-
5	XE	A	1003[B]	-	-	X	-
5	XE	A	1004	-	-	X	-
5	XE	B	1001	-	-	X	-
5	XE	B	1003[B]	-	-	X	-
5	XE	B	1004	-	-	X	-
5	XE	C	1003[B]	-	-	X	-
5	XE	C	1004	-	-	X	-
5	XE	D	1003[B]	-	-	X	-
5	XE	M	1006	-	-	X	-
5	XE	N	1006	-	-	X	-
5	XE	N	1009	-	-	X	-
5	XE	O	1006	-	-	X	-
5	XE	O	1009	-	-	X	-
5	XE	P	1008	-	-	X	-
6	GOL	D	863	-	-	X	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 44706 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
			Total	C	N	O	S			
1	A	673	5094	3202	891	959	42	0	2	0
1	B	673	5094	3202	891	959	42	0	7	0
1	C	673	5094	3202	891	959	42	0	4	0
1	D	673	5094	3202	891	959	42	0	2	0

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

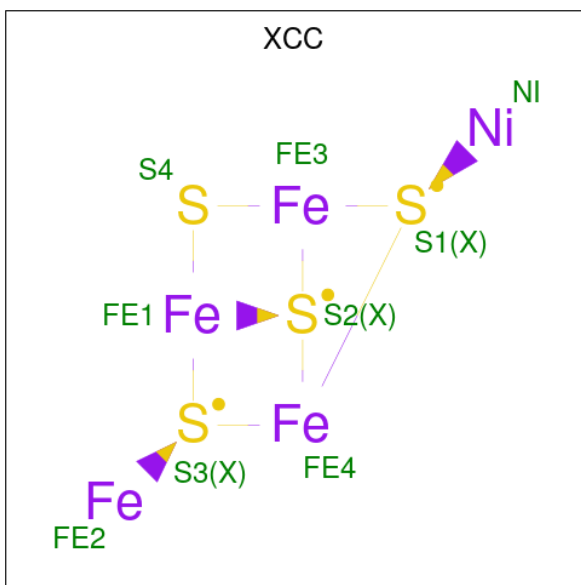
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	M	728	5740	3681	956	1068	35	0	4	0
2	N	728	5740	3681	956	1068	35	0	3	0
2	O	727	5725	3673	952	1066	34	0	1	0
2	P	728	5740	3681	956	1068	35	0	3	0

- 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>).

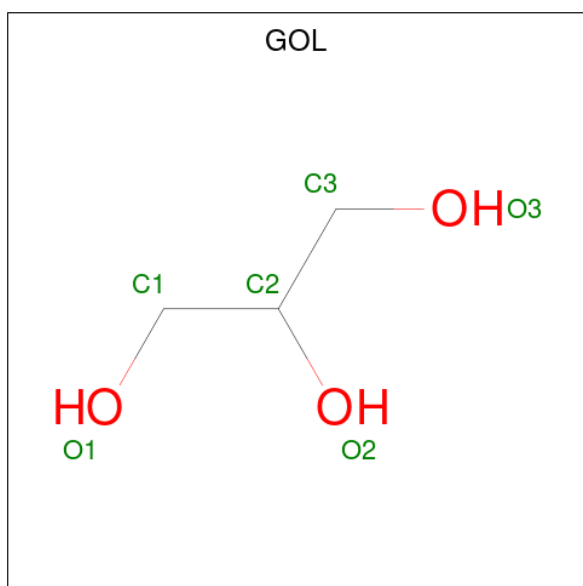


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Fe	Ni	S		
4	A	1	9	4	1	4	0	0
4	B	1	9	4	1	4	0	0
4	C	1	9	4	1	4	0	0
4	D	1	9	4	1	4	0	0

- Molecule 5 is XENON (three-letter code: XE) (formula: Xe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Xe		
5	A	6	7	7	0	1
5	B	6	7	7	0	1
5	C	6	7	7	0	1
5	D	6	7	7	0	1
5	M	3	3	3	0	0
5	N	4	4	4	0	0
5	O	3	3	3	0	0
5	P	4	4	4	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	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	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	C	1	Total C O 6 3 3	0	0
6	D	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	M	1	Total Cu 1 1	0	0
7	N	1	Total Cu 1 1	0	0
7	O	1	Total Cu 1 1	0	0
7	P	1	Total Cu 1 1	0	0

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

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

- Molecule 9 is water.

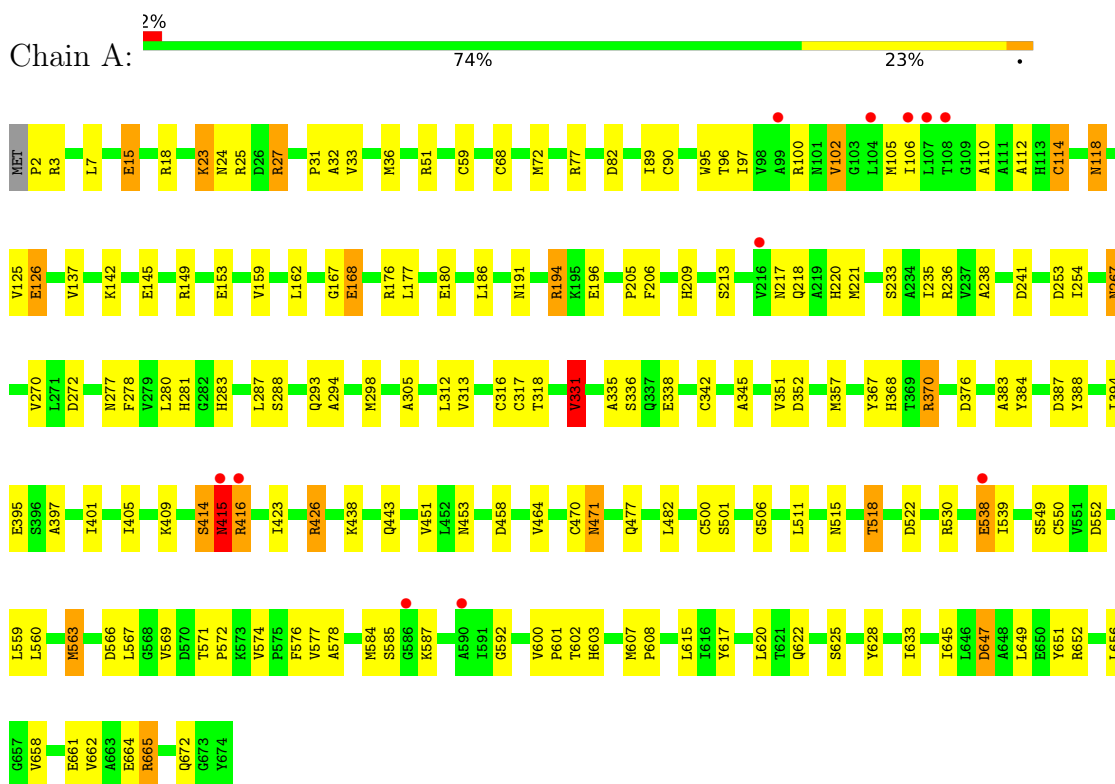
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	168	Total O 168 168	0	0
9	B	220	Total O 220 220	0	0
9	C	130	Total O 130 130	0	0
9	D	105	Total O 105 105	0	0
9	M	201	Total O 201 201	0	0
9	N	222	Total O 222 222	0	0
9	O	27	Total O 27 27	0	0
9	P	80	Total O 80 80	0	0



### 3 Residue-property plots i

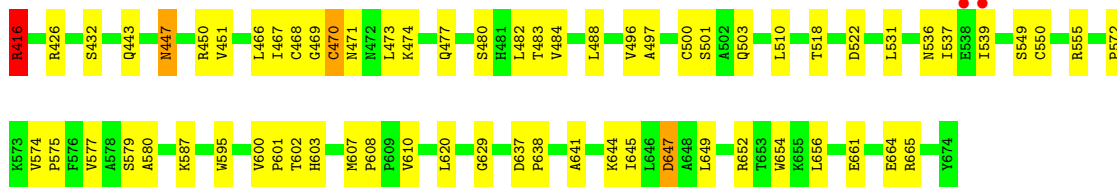
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

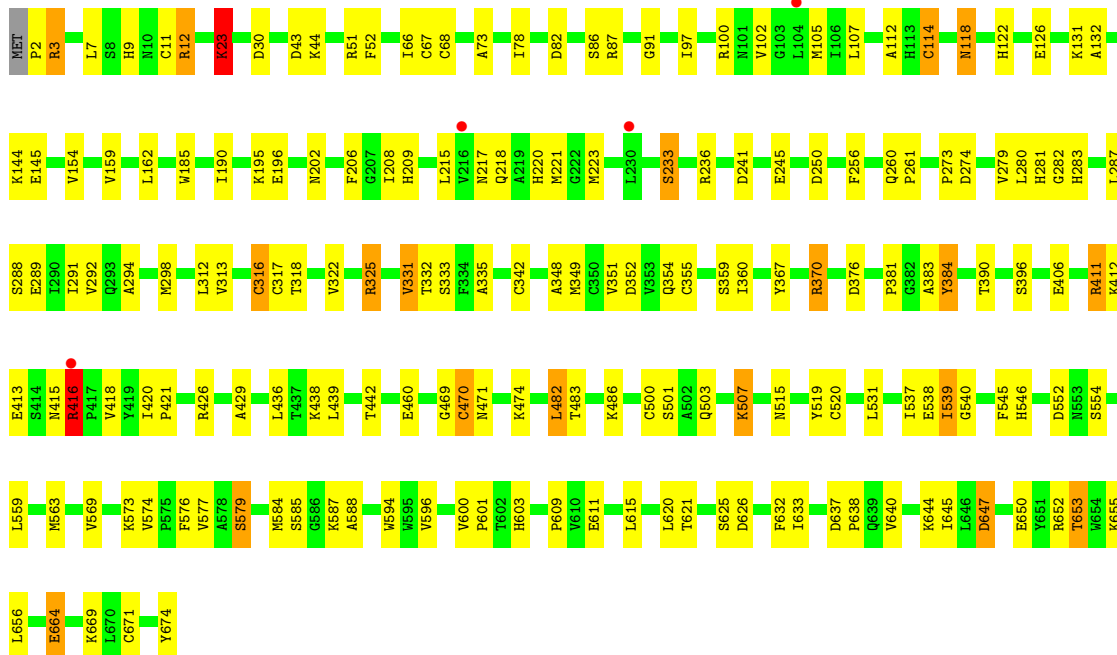


- Molecule 1: Carbon monoxide dehydrogenase/acetyl CoA synthase subunit beta

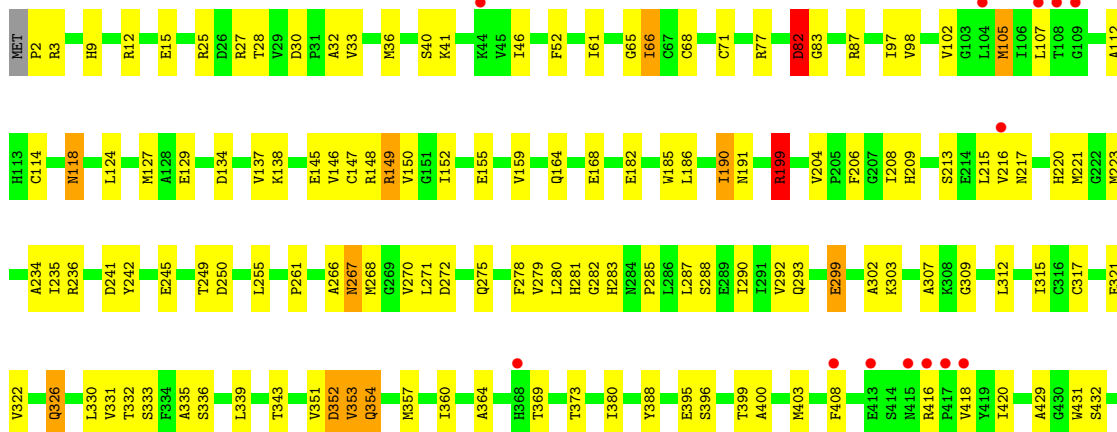


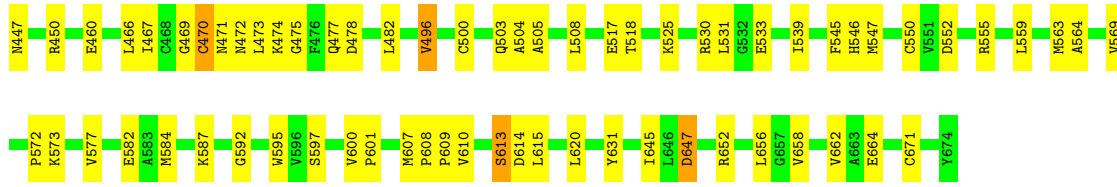


• Molecule 1: Carbon monoxide dehydrogenase/acetyl CoA synthase subunit beta

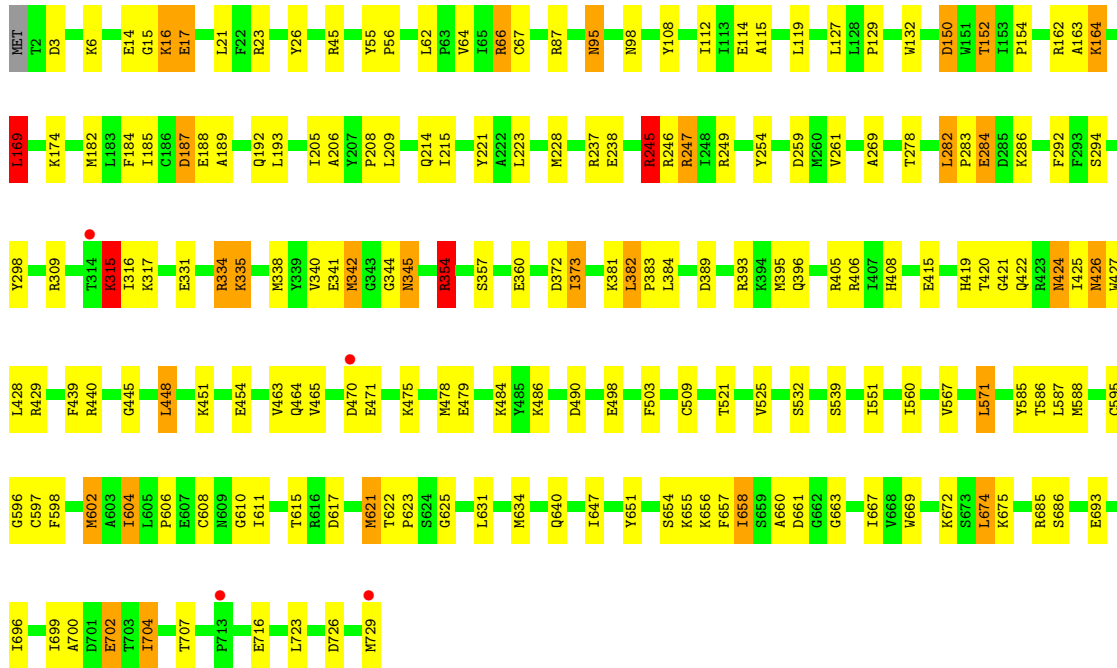
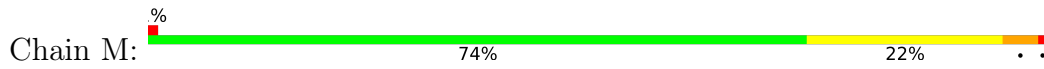


• Molecule 1: Carbon monoxide dehydrogenase/acetyl CoA synthase subunit beta

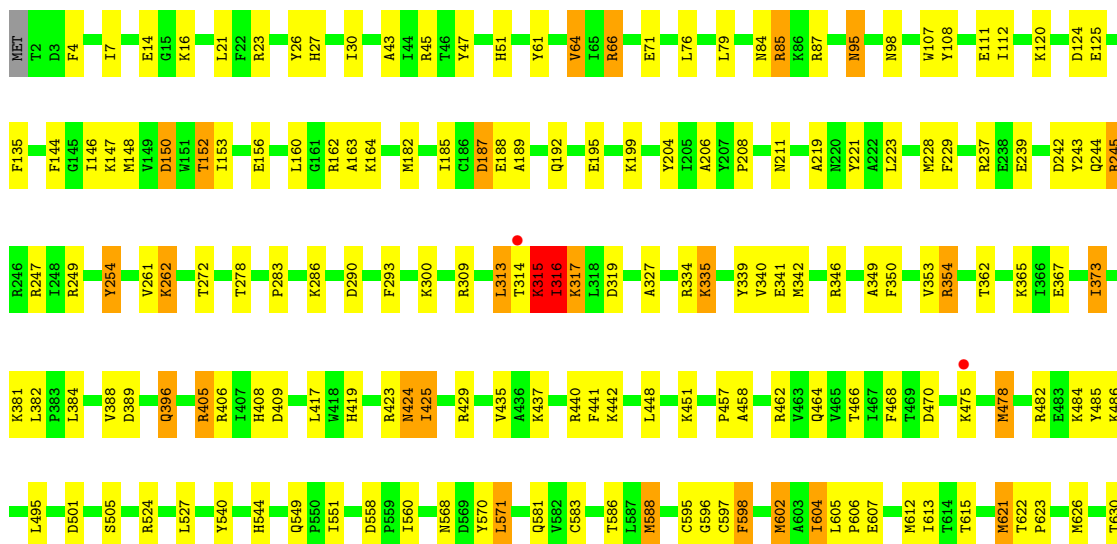


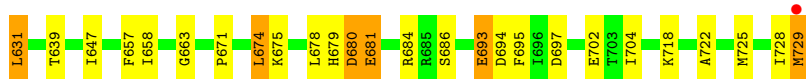


● Molecule 2: Carbon monoxide dehydrogenase/acetyl CoA synthase subunit alpha

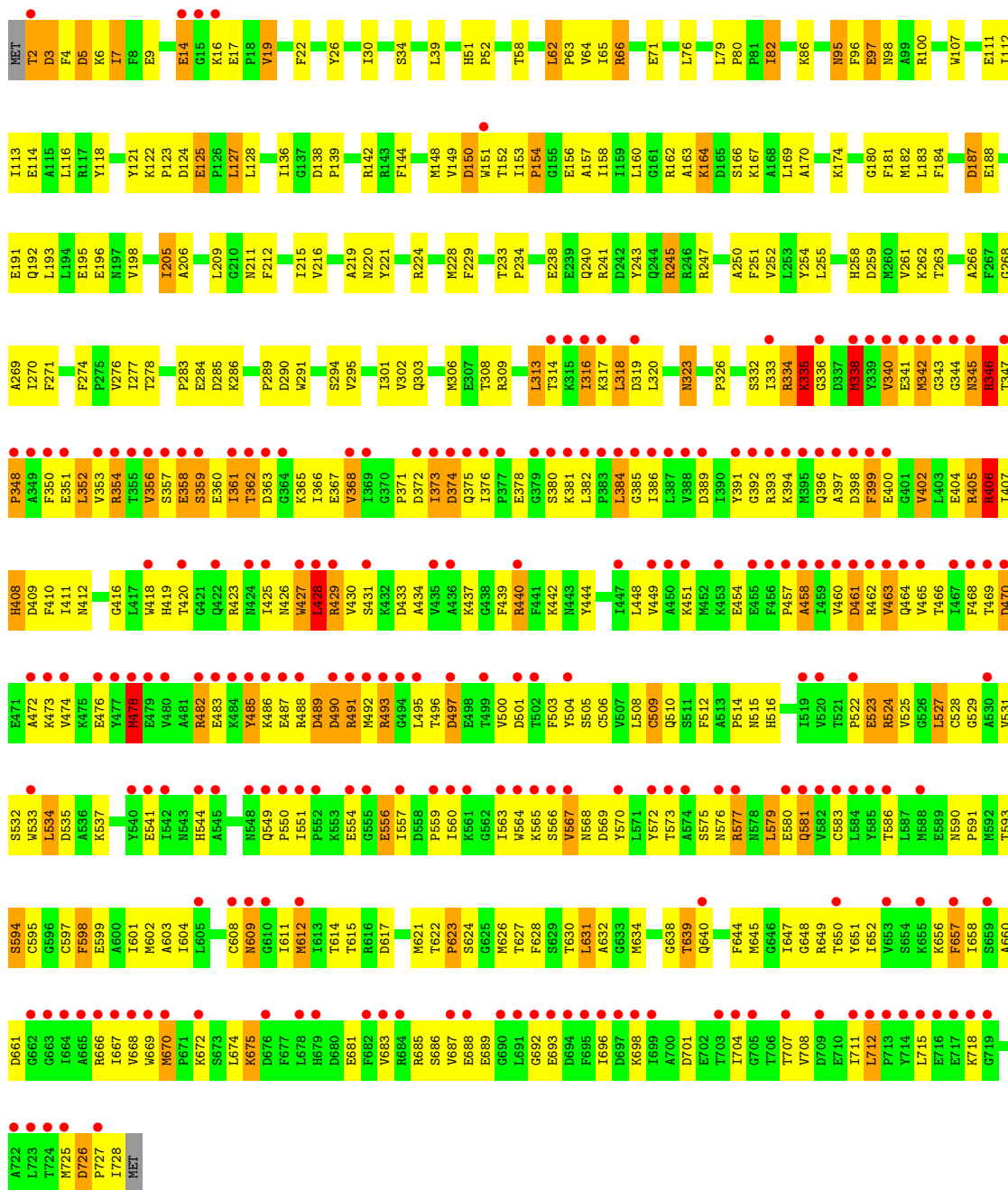


● Molecule 2: Carbon monoxide dehydrogenase/acetyl CoA synthase subunit alpha



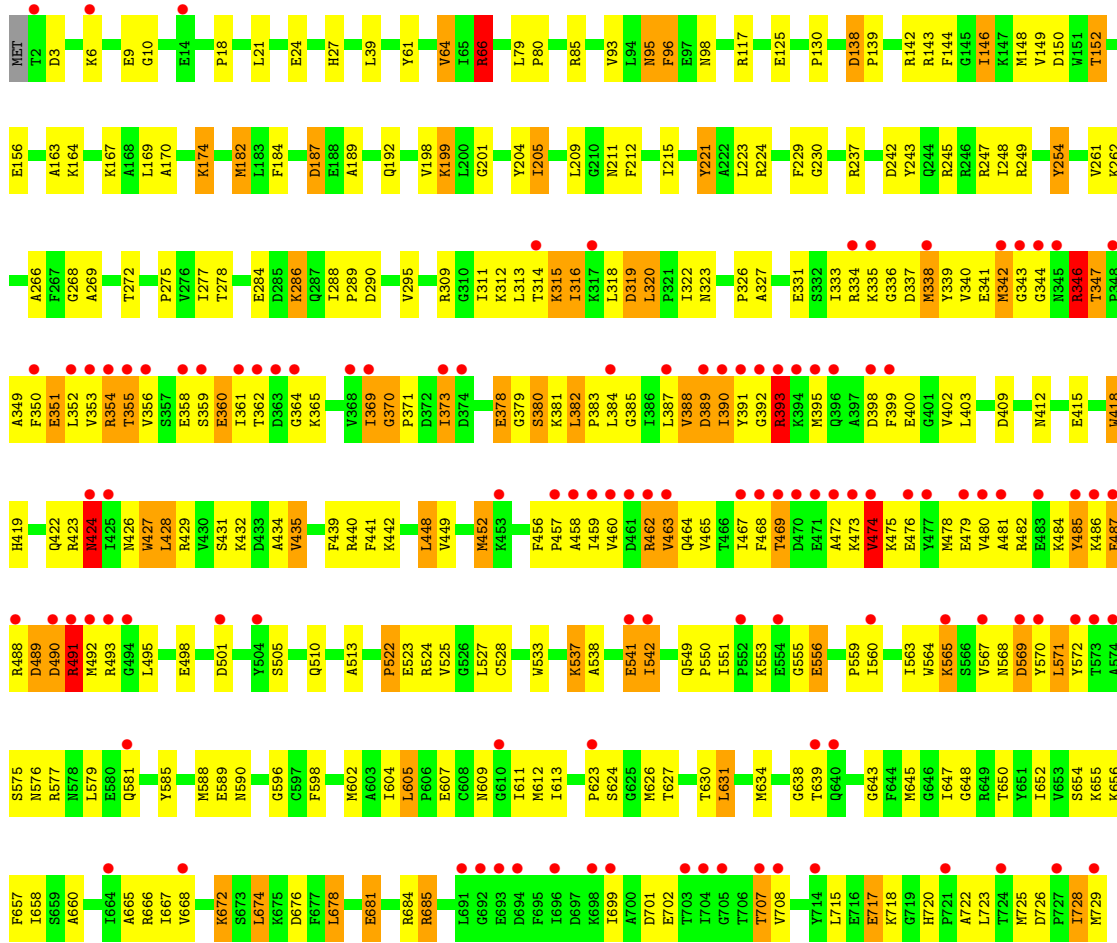


• Molecule 2: Carbon monoxide dehydrogenase/acetyl CoA synthase subunit alpha



• 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, $\alpha$ , $\beta$ , $\gamma$	99.54Å 136.60Å 141.75Å 101.29° 109.22° 103.91°	Depositor
Resolution (Å)	49.00 – 2.51 48.25 – 2.49	Depositor EDS
% Data completeness (in resolution range)	96.1 (49.00-2.51) 95.0 (48.25-2.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 2.48Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.178 , 0.250 0.179 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.5	Xtrriage
Anisotropy	0.322	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 43.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	44706	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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, 0.333 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: XCC, CU1, SF4, GOL, XE, 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	1.29	19/5187 (0.4%)	1.13	26/7028 (0.4%)
1	B	1.29	15/5187 (0.3%)	1.10	13/7028 (0.2%)
1	C	1.25	12/5187 (0.2%)	1.08	17/7028 (0.2%)
1	D	1.18	7/5187 (0.1%)	1.07	12/7028 (0.2%)
2	M	1.21	13/5874 (0.2%)	1.09	20/7954 (0.3%)
2	N	1.27	14/5874 (0.2%)	1.12	26/7954 (0.3%)
2	O	1.17	1/5859 (0.0%)	0.99	8/7937 (0.1%)
2	P	1.15	2/5874 (0.0%)	1.03	14/7954 (0.2%)
All	All	1.23	83/44229 (0.2%)	1.08	136/59911 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	2
1	D	0	1
2	N	0	1
2	P	0	2
All	All	0	8

The worst 5 of 83 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	168	GLU	CG-CD	12.53	1.70	1.51
1	B	196	GLU	CG-CD	9.77	1.66	1.51
2	N	681	GLU	CG-CD	8.11	1.64	1.51
2	N	702	GLU	CB-CG	-7.98	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	114[A]	CYS	CB-SG	-7.91	1.68	1.82

The worst 5 of 136 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	236	ARG	NE-CZ-NH2	-13.82	113.39	120.30
1	C	236	ARG	NE-CZ-NH2	-11.53	114.53	120.30
1	A	176	ARG	NE-CZ-NH1	10.58	125.59	120.30
2	N	237	ARG	NE-CZ-NH2	-9.94	115.33	120.30
2	N	621	MET	CG-SD-CE	-9.91	84.33	100.20

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	414	SER	Peptide
1	B	469	GLY	Peptide
1	C	415	ASN	Peptide
1	C	469	GLY	Peptide
1	D	469	GLY	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5094	0	5088	114	0
1	B	5094	0	5082	133	0
1	C	5094	0	5086	140	0
1	D	5094	0	5093	154	0
2	M	5740	0	5693	116	0
2	N	5740	0	5695	127	0
2	O	5725	0	5680	308	0
2	P	5740	0	5693	243	0
3	A	16	0	0	0	0
3	B	8	0	0	1	0
3	C	16	0	0	0	0
3	D	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	M	8	0	0	0	0
3	N	8	0	0	0	0
3	O	8	0	0	5	0
3	P	8	0	0	1	0
4	A	9	0	0	2	0
4	B	9	0	0	3	0
4	C	9	0	0	3	0
4	D	9	0	0	1	0
5	A	7	0	0	11	0
5	B	7	0	0	12	0
5	C	7	0	0	7	0
5	D	7	0	0	6	0
5	M	3	0	0	2	0
5	N	4	0	0	5	0
5	O	3	0	0	4	0
5	P	4	0	0	4	0
6	A	24	0	32	4	0
6	B	18	0	24	5	0
6	C	12	0	16	1	0
6	D	12	0	16	7	0
7	M	1	0	0	0	0
7	N	1	0	0	0	0
7	O	1	0	0	1	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	A	168	0	0	5	0
9	B	220	0	0	12	0
9	C	130	0	0	14	0
9	D	105	0	0	11	0
9	M	201	0	0	9	0
9	N	222	0	0	20	0
9	O	27	0	0	5	0
9	P	80	0	0	8	0
All	All	44706	0	43198	1297	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 15.

The worst 5 of 1297 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:114[A]:CYS:HB2	9:B:1217:HOH:O	1.29	1.28
2:O:373:ILE:HG22	2:O:440:ARG:HG3	1.28	1.09
1:B:148[A]:ARG:NH1	9:B:1185:HOH:O	1.78	1.08
1:D:114:CYS:HB2	9:D:1050:HOH:O	1.50	1.08
1:D:279:VAL:HG11	1:D:315:ILE:HD12	1.34	1.07

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	671/674 (100%)	637 (95%)	31 (5%)	3 (0%)	34	54
1	B	671/674 (100%)	638 (95%)	31 (5%)	2 (0%)	41	61
1	C	671/674 (100%)	636 (95%)	33 (5%)	2 (0%)	41	61
1	D	671/674 (100%)	632 (94%)	36 (5%)	3 (0%)	34	54
2	M	726/729 (100%)	678 (93%)	41 (6%)	7 (1%)	15	28
2	N	726/729 (100%)	692 (95%)	27 (4%)	7 (1%)	15	28
2	O	725/729 (100%)	592 (82%)	104 (14%)	29 (4%)	3	3
2	P	726/729 (100%)	622 (86%)	78 (11%)	26 (4%)	3	4
All	All	5587/5612 (100%)	5127 (92%)	381 (7%)	79 (1%)	11	20

5 of 79 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	O	316	ILE
2	O	335	LYS
2	O	348	PRO
2	O	372	ASP
2	O	408	HIS

### 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	542/543 (100%)	513 (95%)	29 (5%)	22	42
1	B	542/543 (100%)	519 (96%)	23 (4%)	30	54
1	C	542/543 (100%)	504 (93%)	38 (7%)	15	29
1	D	542/543 (100%)	510 (94%)	32 (6%)	19	37
2	M	610/611 (100%)	556 (91%)	54 (9%)	9	19
2	N	610/611 (100%)	567 (93%)	43 (7%)	15	29
2	O	608/611 (100%)	489 (80%)	119 (20%)	1	2
2	P	610/611 (100%)	519 (85%)	91 (15%)	3	5
All	All	4606/4616 (100%)	4177 (91%)	429 (9%)	9	17

5 of 429 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	66	ARG
2	O	461	ASP
2	P	490	ASP
2	O	205	ILE
2	O	357	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	510	GLN
2	O	192	GLN
2	M	590	ASN
2	N	510	GLN
2	O	396	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 75 ligands modelled in this entry, 50 are monoatomic - leaving 25 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	D	700	1	0,12,12	-	-	-		
4	XCC	A	800	1	0,11,11	-	-	-		
3	SF4	B	700	1	0,12,12	-	-	-		
6	GOL	B	861	-	5,5,5	0.69	0	5,5,5	0.97	0
4	XCC	C	800	1	0,11,11	-	-	-		
3	SF4	C	750	1	0,12,12	-	-	-		
4	XCC	B	800	1	0,11,11	-	-	-		
4	XCC	D	800	1	0,11,11	-	-	-		
3	SF4	O	900	2	0,12,12	-	-	-		
6	GOL	A	862	-	5,5,5	1.00	0	5,5,5	1.12	0
6	GOL	B	860	-	5,5,5	0.81	0	5,5,5	1.17	0
3	SF4	C	700	1	0,12,12	-	-	-		
6	GOL	C	860	-	5,5,5	0.52	0	5,5,5	0.65	0
3	SF4	A	750	1	0,12,12	-	-	-		
3	SF4	P	900	2	0,12,12	-	-	-		
6	GOL	C	861	-	5,5,5	0.59	0	5,5,5	0.78	0
6	GOL	A	860	-	5,5,5	0.97	0	5,5,5	1.68	1 (20%)
3	SF4	M	900	2	0,12,12	-	-	-		
6	GOL	D	863	-	5,5,5	0.84	0	5,5,5	1.33	1 (20%)
3	SF4	A	700	1	0,12,12	-	-	-		
6	GOL	B	863	-	5,5,5	0.77	0	5,5,5	1.63	2 (40%)
6	GOL	A	861	-	5,5,5	0.70	0	5,5,5	1.30	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	GOL	A	863	-	5,5,5	0.61	0	5,5,5	1.97	2 (40%)
6	GOL	D	860	-	5,5,5	0.52	0	5,5,5	0.37	0
3	SF4	N	900	2	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	D	700	1	-	-	0/6/5/5
4	XCC	A	800	1	-	-	0/3/3/3
3	SF4	B	700	1	-	-	0/6/5/5
6	GOL	B	861	-	-	4/4/4/4	-
4	XCC	C	800	1	-	-	0/3/3/3
3	SF4	C	750	1	-	-	0/6/5/5
4	XCC	B	800	1	-	-	0/3/3/3
4	XCC	D	800	1	-	-	0/3/3/3
6	GOL	B	860	-	-	4/4/4/4	-
6	GOL	A	862	-	-	4/4/4/4	-
3	SF4	O	900	2	-	-	0/6/5/5
3	SF4	C	700	1	-	-	0/6/5/5
6	GOL	C	860	-	-	2/4/4/4	-
3	SF4	A	750	1	-	-	0/6/5/5
3	SF4	P	900	2	-	-	0/6/5/5
6	GOL	C	861	-	-	2/4/4/4	-
6	GOL	A	860	-	-	2/4/4/4	-
3	SF4	M	900	2	-	-	0/6/5/5
6	GOL	D	863	-	-	4/4/4/4	-
3	SF4	A	700	1	-	-	0/6/5/5
6	GOL	B	863	-	-	0/4/4/4	-
6	GOL	A	861	-	-	2/4/4/4	-
6	GOL	A	863	-	-	0/4/4/4	-
6	GOL	D	860	-	-	2/4/4/4	-
3	SF4	N	900	2	-	-	0/6/5/5

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	863	GOL	O3-C3-C2	-3.68	92.56	110.20
6	A	860	GOL	O1-C1-C2	2.84	123.80	110.20
6	D	863	GOL	O2-C2-C3	2.69	120.95	109.12
6	B	863	GOL	O2-C2-C1	-2.67	97.36	109.12
6	A	861	GOL	O3-C3-C2	2.56	122.46	110.20

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	861	GOL	C1-C2-C3-O3
6	A	861	GOL	O2-C2-C3-O3
6	A	862	GOL	O1-C1-C2-O2
6	A	862	GOL	O1-C1-C2-C3
6	A	862	GOL	C1-C2-C3-O3

There are no ring outliers.

14 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	800	XCC	2	0
3	B	700	SF4	1	0
6	B	861	GOL	3	0
4	C	800	XCC	3	0
4	B	800	XCC	3	0
4	D	800	XCC	1	0
3	O	900	SF4	5	0
6	A	862	GOL	3	0
3	P	900	SF4	1	0
6	C	861	GOL	1	0
6	D	863	GOL	6	0
6	B	863	GOL	2	0
6	A	861	GOL	1	0
6	D	860	GOL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	673/674 (99%)	-0.39	11 (1%) 72 74	9, 18, 36, 61	2 (0%)
1	B	673/674 (99%)	-0.46	6 (0%) 84 86	8, 18, 35, 67	7 (1%)
1	C	673/674 (99%)	-0.44	4 (0%) 89 90	10, 23, 40, 61	3 (0%)
1	D	673/674 (99%)	-0.29	13 (1%) 66 69	11, 25, 46, 70	2 (0%)
2	M	728/729 (99%)	-0.43	4 (0%) 91 91	9, 25, 49, 70	4 (0%)
2	N	728/729 (99%)	-0.47	3 (0%) 92 93	7, 23, 48, 64	3 (0%)
2	O	727/729 (99%)	1.19	221 (30%) 0 0	24, 58, 90, 130	1 (0%)
2	P	728/729 (99%)	0.41	112 (15%) 2 1	12, 40, 84, 112	3 (0%)
All	All	5603/5612 (99%)	-0.10	374 (6%) 17 18	7, 25, 71, 130	25 (0%)

The worst 5 of 374 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	399	PHE	7.9
2	P	461	ASP	7.2
2	P	481	ALA	7.0
2	P	472	ALA	7.0
2	O	545	ALA	6.9

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.



## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å <sup>2</sup> )	Q<0.9
6	GOL	C	861	6/6	0.73	0.18	53,59,59,60	0
6	GOL	B	861	6/6	0.78	0.30	45,51,52,54	0
6	GOL	A	861	6/6	0.81	0.28	34,47,51,53	0
6	GOL	D	860	6/6	0.87	0.17	47,51,52,52	0
6	GOL	D	863	6/6	0.87	0.23	28,36,42,42	0
6	GOL	C	860	6/6	0.90	0.15	39,48,50,51	0
7	CU1	O	950	1/1	0.90	0.04	88,88,88,88	0
4	XCC	D	800	9/9	0.91	0.13	52,61,69,69	0
5	XE	B	1001	1/1	0.92	0.41	32,32,32,32	1
6	GOL	B	860	6/6	0.93	0.12	27,27,30,30	0
5	XE	C	1001	1/1	0.94	0.27	13,13,13,13	1
4	XCC	B	800	9/9	0.94	0.12	37,52,54,57	0
4	XCC	C	800	9/9	0.94	0.11	40,54,66,66	0
4	XCC	A	800	9/9	0.95	0.11	37,48,56,57	0
6	GOL	A	863	6/6	0.95	0.17	22,26,32,35	0
5	XE	P	1008	1/1	0.95	0.29	19,19,19,19	1
5	XE	O	1007	1/1	0.96	0.15	33,33,33,33	1
6	GOL	A	862	6/6	0.96	0.17	27,30,35,35	0
6	GOL	B	863	6/6	0.96	0.17	30,34,37,37	0
3	SF4	O	900	8/8	0.96	0.05	59,60,62,62	0
7	CU1	P	950	1/1	0.96	0.05	52,52,52,52	0
5	XE	N	1008	1/1	0.97	0.20	25,25,25,25	1
5	XE	D	1001	1/1	0.97	0.11	34,34,34,34	1
5	XE	M	1006	1/1	0.97	0.15	29,29,29,29	1
5	XE	D	1010	1/1	0.98	0.13	25,25,25,25	1
5	XE	A	1003[B]	1/1	0.98	0.20	14,14,14,14	1
6	GOL	A	860	6/6	0.98	0.10	17,20,23,27	0
7	CU1	M	950	1/1	0.98	0.10	30,30,30,30	0
5	XE	N	1006	1/1	0.98	0.13	27,27,27,27	1
5	XE	A	1003[A]	1/1	0.98	0.20	30,30,30,30	1
8	NI	O	951	1/1	0.98	0.04	75,75,75,75	0
5	XE	D	1003[B]	1/1	0.99	0.22	30,30,30,30	1
5	XE	D	1004	1/1	0.99	0.14	28,28,28,28	1
3	SF4	A	750	8/8	0.99	0.08	12,15,16,17	0
3	SF4	B	700	8/8	0.99	0.12	7,9,11,15	0
5	XE	M	1008	1/1	0.99	0.14	30,30,30,30	1
3	SF4	C	700	8/8	0.99	0.10	21,23,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	SF4	C	750	8/8	0.99	0.07	22,26,28,28	0
5	XE	O	1006	1/1	0.99	0.30	30,30,30,30	1
5	XE	A	1001	1/1	0.99	0.18	23,23,23,23	1
5	XE	O	1009	1/1	0.99	0.09	42,42,42,42	1
5	XE	P	1006	1/1	0.99	0.20	29,29,29,29	1
5	XE	A	1002	1/1	0.99	0.12	27,27,27,27	0
3	SF4	D	700	8/8	0.99	0.11	18,19,20,22	0
3	SF4	M	900	8/8	0.99	0.08	13,14,17,20	0
5	XE	A	1010	1/1	0.99	0.03	31,31,31,31	1
3	SF4	N	900	8/8	0.99	0.09	12,14,16,17	0
5	XE	B	1003[A]	1/1	0.99	0.14	26,26,26,26	1
5	XE	B	1003[B]	1/1	0.99	0.14	25,25,25,25	1
5	XE	B	1010	1/1	0.99	0.07	24,24,24,24	1
3	SF4	A	700	8/8	0.99	0.12	10,12,14,14	0
5	XE	C	1002	1/1	0.99	0.10	33,33,33,33	0
5	XE	C	1003[A]	1/1	0.99	0.15	29,29,29,29	1
5	XE	C	1003[B]	1/1	0.99	0.15	33,33,33,33	1
5	XE	C	1005	1/1	0.99	0.13	31,31,31,31	1
7	CU1	N	950	1/1	0.99	0.12	28,28,28,28	0
5	XE	C	1010	1/1	0.99	0.07	35,35,35,35	1
3	SF4	P	900	8/8	0.99	0.05	31,34,36,37	0
8	NI	M	951	1/1	0.99	0.08	18,18,18,18	0
5	XE	D	1003[A]	1/1	0.99	0.22	28,28,28,28	1
8	NI	P	951	1/1	0.99	0.06	44,44,44,44	0
5	XE	N	1009	1/1	1.00	0.13	34,34,34,34	1
5	XE	B	1005	1/1	1.00	0.10	21,21,21,21	0
5	XE	C	1004	1/1	1.00	0.14	30,30,30,30	1
5	XE	D	1005	1/1	1.00	0.10	27,27,27,27	0
5	XE	B	1002	1/1	1.00	0.12	25,25,25,25	0
5	XE	P	1007	1/1	1.00	0.11	29,29,29,29	0
5	XE	A	1004	1/1	1.00	0.10	30,30,30,30	1
5	XE	P	1009	1/1	1.00	0.15	31,31,31,31	1
5	XE	M	1007	1/1	1.00	0.12	27,27,27,27	0
5	XE	A	1005	1/1	1.00	0.10	24,24,24,24	0
5	XE	D	1002	1/1	1.00	0.15	29,29,29,29	1
8	NI	N	951	1/1	1.00	0.09	17,17,17,17	0
5	XE	N	1007	1/1	1.00	0.11	21,21,21,21	0
5	XE	B	1004	1/1	1.00	0.11	29,29,29,29	1

## 6.5 Other polymers

There are no such residues in this entry.