W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Aug 27, 2023 – 08:20 AM EDT

PDB ID	:	3I01
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)

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

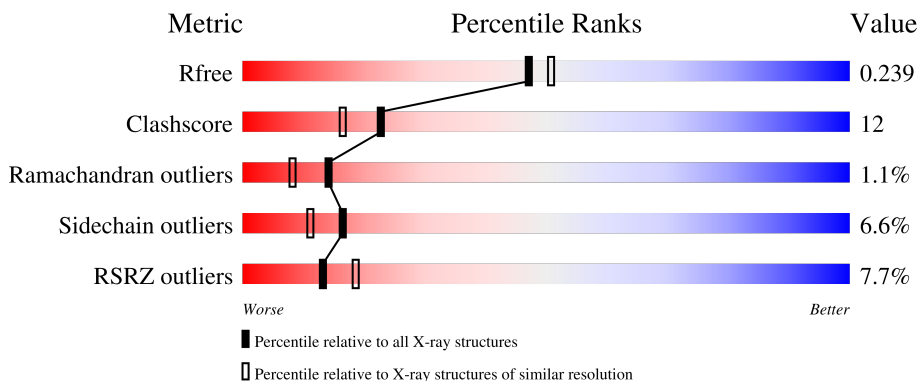|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1   Overall quality at a glance (i)

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

The reported resolution of this entry is 2.15 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	Percentile Ranks	Value
Rfree		0.239
Clashscore		12
Ramachandran outliers		1.1%
Sidechain outliers		6.6%
RSRZ outliers		7.7%

Worse ... *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (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 <=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	% — 84% / 15% ·
1	B	674	% — 84% / 15% ·
1	C	674	% — 81% / 18%
1	D	674	2% — 81% / 17% ·
2	M	729	% — 78% / 18% ·

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	N	729	2% / 78% / 19%
2	O	729	38% / 58% / 33% / 8%
2	P	729	12% / 72% / 23%

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 5128	C 3223	N 897	O 966	S 42	0	7	0
1	B	673	Total 5121	C 3221	N 895	O 963	S 42	0	5	0
1	C	673	Total 5094	C 3205	N 888	O 959	S 42	0	2	0
1	D	673	Total 5119	C 3218	N 895	O 964	S 42	0	4	0

- 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 5778	C 3703	N 964	O 1076	S 35	0	5	0
2	N	728	Total 5784	C 3707	N 968	O 1074	S 35	0	6	0
2	O	728	Total 5749	C 3687	N 958	O 1069	S 35	0	1	0
2	P	728	Total 5746	C 3684	N 959	O 1068	S 35	0	1	0

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

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

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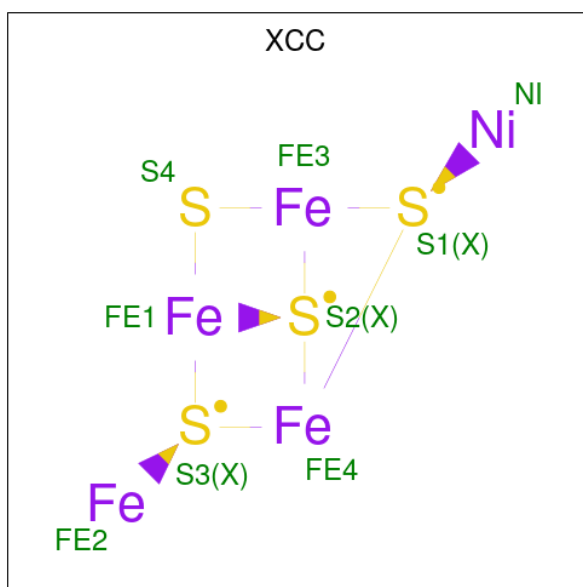
XCC

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 (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

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

- Molecule 6 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

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

- Molecule 7 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

ACT

OXT

O⁻

C

CH3

O

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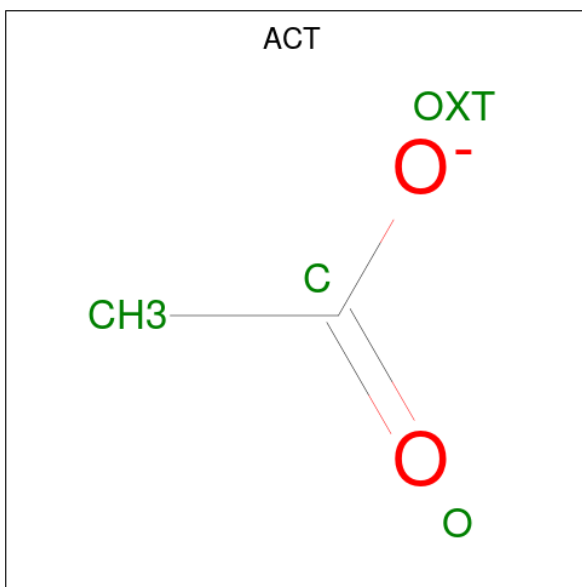
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total 3	C 2	O 1	0	0
8	N	1	Total 3	C 2	O 1	0	0
8	O	1	Total 3	C 2	O 1	0	0
8	P	1	Total 3	C 2	O 1	0	0

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 10 is water.

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

Continued on next page...

Continued from previous page...

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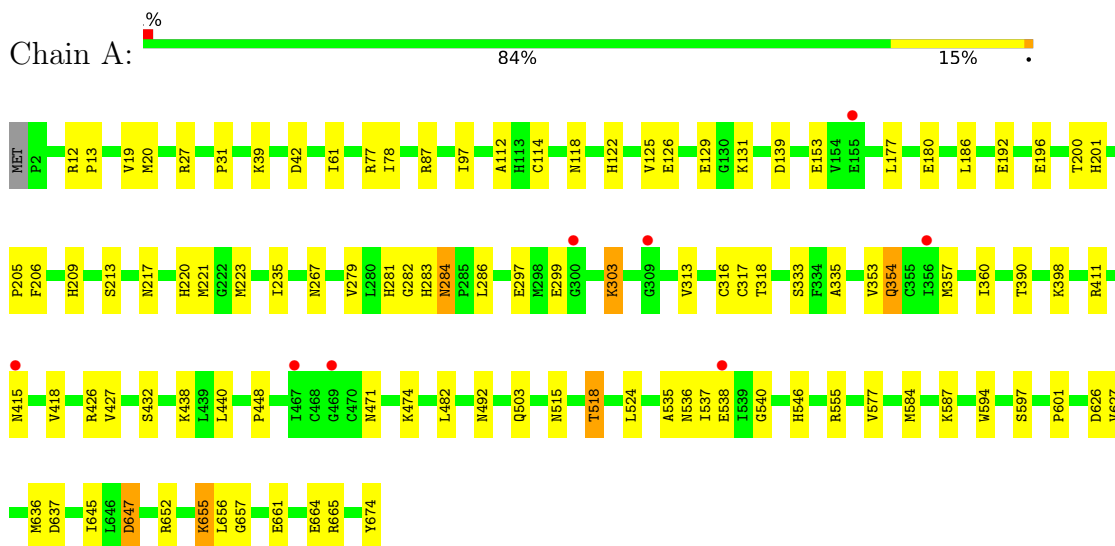
• Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta
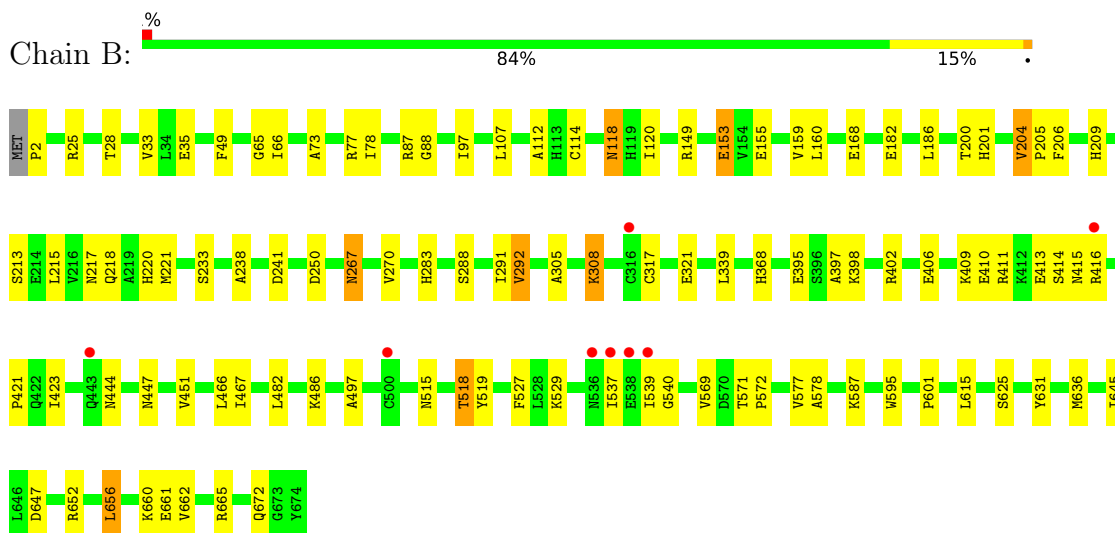
• Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta

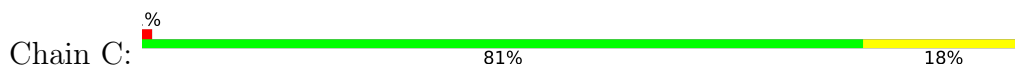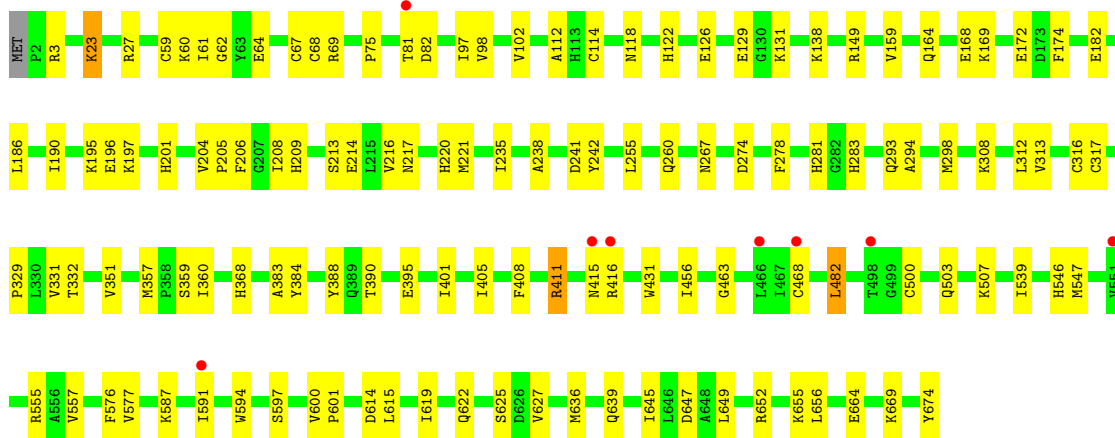• Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta

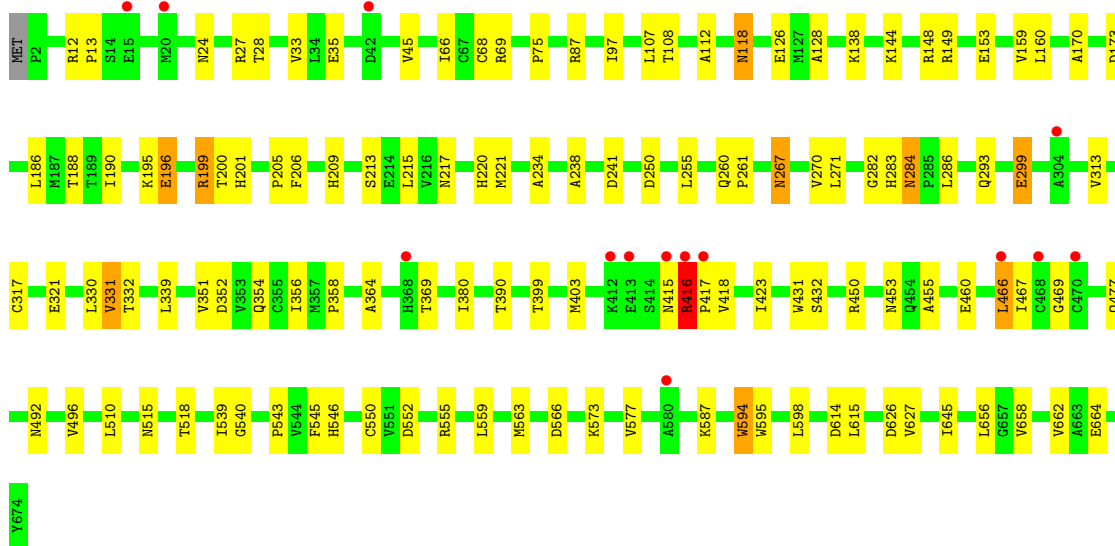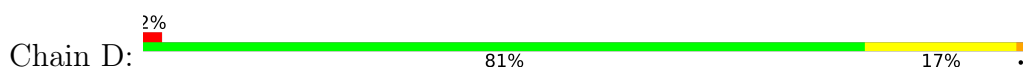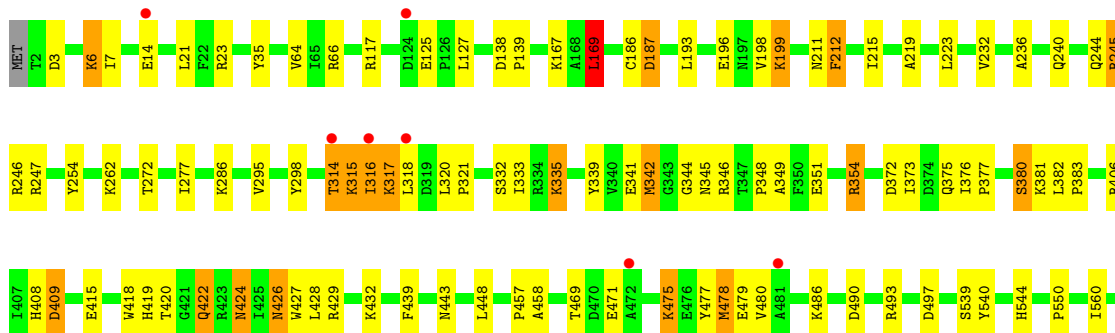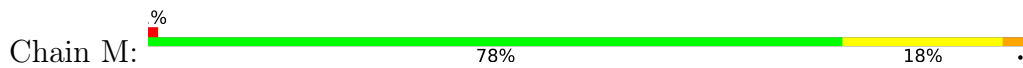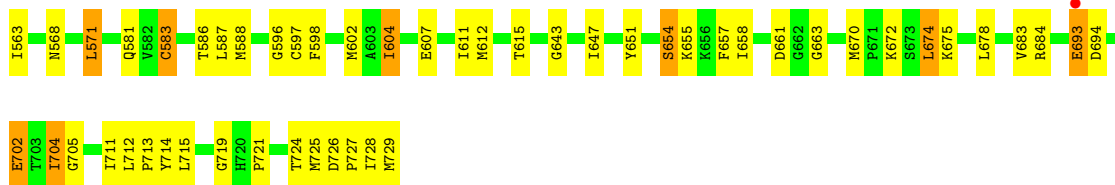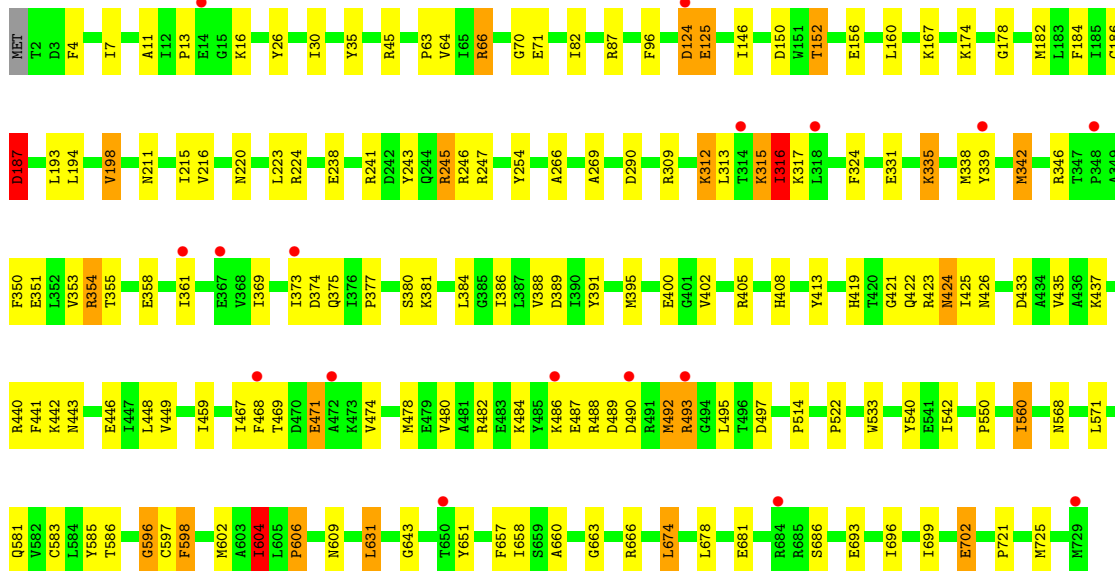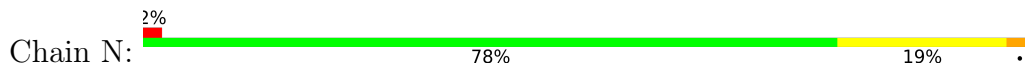• Molecule 2: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha
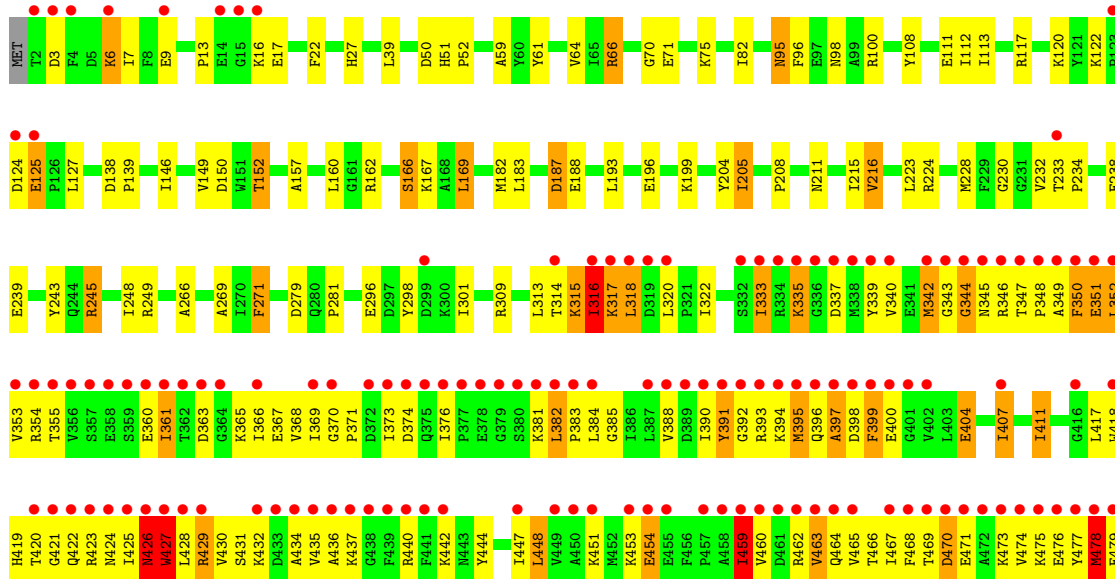
• Molecule 2: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha

Chain N:

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

Chain O:

V480 A481 R482 E483 K484 Y485 K486 E487 R488 D489 D490 R491 M492 R493 G494 L495 T496 D497 E498 T499 V500 D501 T502 F503 Y504 S505 C506 V507 L508 C509 Q510 N515 H516 V517 C518 I519 V520 T521 P522 E523 R524 L527 W533 L534 A538 S539 Y540 E541 I542 H544 A545 I551 P552 K553

E554 G555 E556 I557 D558 P559 I560 I563 W564 K565 S566 V567 N568 D569 Y570 L571 Y572 T573 A574 S575 N576 R577 N578 L579 E580 Q581 V582 C583 L584 Y585 T586 L587 N590 P591 M592 T593 S594 F598 I601 M602 A603 I604 L605 P606 E607 C608 N609 G610 I611 M612 I613 T614 G620 M621 T622

P623 S624 G625 M626 T630 L631 A632 G633 M634 I635 G636 G637 G638 T639 Q640 T641 P642 I647 G648 R649 T650 Y651 I652 V653 S654 K655 K656 F657 I658 S659 A660 D661 G662 G663 I664 A665 R666 I667 V668 W669 M670 P671 K672 D676 F677 L678 H679 D680 E681 F682 R684 V683 R685 S686 V687 E688 E689

G690 L691 G692 E693 D694 F695 I696 D697 K698 I699 A700 D701 E702 T703 I704 G705 T706 T707 V708 D709 E710 I711 L712 P713 Y714 L715 E716 E717 K718 G719 H720 P721 A722 L723 T724 M725 D726 P727 I728 M729

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

Chain P:

12% ▬▬▬▬▬▬▬ 72% ▬▬▬▬▬▬▬▬▬▬▬▬▬▬▬▬▬▬▬▬▬▬▬▬▬▬▬ 23% ▬▬▬▬▬▬ •

MET T2 D3 F4 D5 K6 P13 E14 G15 K16 E17 P18 L21 H27 Y35 L39 Y61 V64 I65 R66 G70 L79 P80 P81 R85 K86 R87 A88 F96 E111 I112 R117 D124 E125 P126 L127 D138 P139 V149 D150 W151 T152 S166

K174 E175 D187 L194 E195 E196 N197 V198 K199 N211 F212 I215 V216 H217 A218 G226 M227 M228 E238 R245 Y254 A266 A269 P275 T278 E284 D285 K286 Q287 I288 P289 D290 K300 R309 K312 L313 T314 K315 I316 K317 L318 D319 L320

E331 S332 I333 R334 K335 G336 D337 M338 Y339 V340 E341 M342 G343 C344 N345 R346 T347 F350 E351 L352 V353 R354 T355 V356 S357 E358 S359 E360 I361 T362 D363 G364 I369 D372 T373 D374 Q375 I376 P383 L384 G385 D389 I390 Y391 G392 R393 D398 V402 L403 E404 H408

D409 E415 G416 L417 W418 H419 T420 G421 Q422 R423 N424 I425 N426 W427 L428 R429 V430 S431 K432 V435 F439 R440 F441 K442 N443 Y444 L448 P457 A458 I459 V460 D461 R462 V463 Q464 I467 F468 T469 D470 E471 A472 K473 V474 K475 E476 Y477 M478 E479 V480 A481 R482 E483 K484 Y485

K486 E487 R488 D489 D490 R491 M492 R493 G494 E498 T499 V500 D501 T502 F503 Y504 S505 H516 P522 W533 K537 A538 E541 I542 N543 Q549 P550 I551 P552 K553 E554 G555 E556 I557 D558 P559 W564 K565 S566 V567 N568 D569 Y570 L571 Y572 T573 A574 S575 N576 R577 N578 L579

E580 Q581 V582 C583 L584 Y585 T586 L587 M588 E589 N590 T593 S594 G595 C596 C597 F598 I601 M602 A603 I604 L605 G610 P623 L631 G638 I647 K655 K656 F657 G663 R666 I667 L674 H679 F682 V683 R684 R685 S686 V687 E688 G692 E693 D694 F695

I696 A700 I704 T707 I711 L712 P713 Y714 E717 D726 P727 I728 M729

4 Data and refinement statistics (i)

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 36.54 – 2.15	Depositor EDS
% Data completeness (in resolution range)	92.3 (36.96-2.15) 92.3 (36.54-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$<I/\sigma(I)>$ [1]	2.33 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.186 , 0.242 0.187 , 0.239	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)	0.37 , 53.4	EDS
L-test for twinning[2]	$<|L|> = 0.50$, $<L^2> = 0.33$	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.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ 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: CU1, ACT, NA, XCC, NI, SF4, GOL

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	1.06	0/5244	0.91	6/7106 (0.1%)
1	B	1.11	6/5231 (0.1%)	0.92	3/7086 (0.0%)
1	C	1.06	6/5193 (0.1%)	0.90	2/7038 (0.0%)
1	D	0.95	1/5212 (0.0%)	0.90	3/7062 (0.0%)
2	M	1.00	5/5921 (0.1%)	0.89	7/8015 (0.1%)
2	N	0.99	3/5928 (0.1%)	0.91	8/8023 (0.1%)
2	O	0.89	1/5883 (0.0%)	0.89	7/7965 (0.1%)
2	P	0.86	0/5885	0.83	2/7968 (0.0%)
All	All	0.99	22/44497 (0.0%)	0.89	38/60263 (0.1%)

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	388	TYR	CD1-CE1	5.96	1.48	1.39
2	O	725	MET	C-O	-5.83	1.12	1.23
1	B	292	VAL	CB-CG1	5.82	1.65	1.52
2	N	184	PHE	CE2-CZ	5.80	1.48	1.37
2	M	186	CYS	CB-SG	5.76	1.92	1.82

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	597	CYS	CA-CB-SG	-5.99	103.21	114.00
2	O	685	ARG	N-CA-CB	-5.98	99.83	110.60
2	M	597	CYS	CA-CB-SG	-5.93	103.32	114.00
1	B	339	LEU	CA-CB-CG	-5.89	101.75	115.30
1	B	87	ARG	NE-CZ-NH2	-5.76	117.42	120.30

There are no chirality outliers.

There are no planarity outliers.

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	5128	0	5128	62	0
1	B	5121	0	5134	71	0
1	C	5094	0	5097	89	0
1	D	5119	0	5115	99	0
2	M	5778	0	5736	96	0
2	N	5784	0	5749	106	0
2	O	5749	0	5716	377	0
2	P	5746	0	5710	142	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	0	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

Continued on next page...

Continued from previous page...

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	3	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	1002	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 1002 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: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
2:M:335:LYS:HD2	2:M:335:LYS:H	1.07	1.12

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%)	41	37

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	676/674 (100%)	652 (96%)	23 (3%)	1 (0%)	51	53
1	C	673/674 (100%)	648 (96%)	24 (4%)	1 (0%)	51	53
1	D	675/674 (100%)	640 (95%)	30 (4%)	5 (1%)	22	15
2	M	731/729 (100%)	687 (94%)	36 (5%)	8 (1%)	14	8
2	N	732/729 (100%)	689 (94%)	34 (5%)	9 (1%)	13	7
2	O	727/729 (100%)	641 (88%)	60 (8%)	26 (4%)	3	0
2	P	727/729 (100%)	679 (93%)	41 (6%)	7 (1%)	15	9
All	All	5619/5612 (100%)	5288 (94%)	272 (5%)	59 (1%)	14	8

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%)	524 (96%)	24 (4%)	28	25
1	B	547/543 (101%)	529 (97%)	18 (3%)	38	37
1	C	542/543 (100%)	521 (96%)	21 (4%)	32	30
1	D	544/543 (100%)	525 (96%)	19 (4%)	36	34
2	M	615/611 (101%)	570 (93%)	45 (7%)	14	9
2	N	615/611 (101%)	574 (93%)	41 (7%)	16	11
2	O	611/611 (100%)	532 (87%)	79 (13%)	4	1
2	P	611/611 (100%)	550 (90%)	61 (10%)	7	4
All	All	4633/4616 (100%)	4325 (93%)	308 (7%)	16	11

5 of 308 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	579	LEU
2	P	469	THR
2	O	647	ILE
2	P	300	LYS
2	P	605	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
2	N	581	GLN
2	P	408	HIS
2	N	640	GLN
2	O	549	GLN
2	P	516	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	A	800	1,10	0,11,11	-	-	-		
3	SF4	B	750	1	0,12,12	-	-	-		
3	SF4	C	700	1	0,12,12	-	-	-		
3	SF4	A	700	1	0,12,12	-	-	-		
3	SF4	A	750	1	0,12,12	-	-	-		
3	SF4	N	900	2	0,12,12	-	-	-		
5	GOL	C	863	-	5,5,5	0.30	0	5,5,5	0.62	0
8	ACT	N	953	-	1,2,3	1.38	0	1,1,3	0.10	0
5	GOL	A	863	-	5,5,5	0.44	0	5,5,5	1.69	1 (20%)
4	XCC	D	800	1,10	0,11,11	-	-	-		
8	ACT	M	953	-	1,2,3	1.29	0	1,1,3	0.75	0
5	GOL	B	863	-	5,5,5	1.08	1 (20%)	5,5,5	1.73	1 (20%)
3	SF4	D	750	1	0,12,12	-	-	-		
3	SF4	M	900	2	0,12,12	-	-	-		
4	XCC	C	800	1,10	0,11,11	-	-	-		
8	ACT	O	953	-	1,2,3	1.17	0	1,1,3	0.47	0
8	ACT	P	953	-	1,2,3	1.47	0	1,1,3	0.23	0
3	SF4	O	900	2	0,12,12	-	-	-		
5	GOL	D	863	-	5,5,5	0.51	0	5,5,5	1.60	1 (20%)
3	SF4	C	750	1	0,12,12	-	-	-		
3	SF4	P	900	2	0,12,12	-	-	-		
4	XCC	B	800	1,10	0,11,11	-	-	-		

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SF4	O	900	2	-	-	0/6/5/5
5	GOL	D	863	-	-	3/4/4/4	-
5	GOL	A	863	-	-	2/4/4/4	-
3	SF4	C	750	1	-	-	0/6/5/5
5	GOL	B	863	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	863	GOL	O2-C2	-2.36	1.36	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	863	GOL	O2-C2-C3	-3.08	95.57	109.12
5	D	863	GOL	O1-C1-C2	-2.66	97.45	110.20
5	A	863	GOL	O1-C1-C2	-2.30	99.16	110.20

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.

9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	750	SF4	1	0
3	C	700	SF4	1	0
3	N	900	SF4	1	0
5	C	863	GOL	5	0
4	D	800	XCC	2	0
8	O	953	ACT	1	0
8	P	953	ACT	1	0
3	O	900	SF4	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	863	GOL	6	0

5.7 Other polymers ⓘ

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 ⓘ

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, 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(Å²)	Q<0.9
1	A	673/674 (99%)	-0.19	8 (1%)	79	83	14, 25, 43, 60	0
1	B	673/674 (99%)	-0.18	8 (1%)	79	83	13, 22, 39, 68	0
1	C	673/674 (99%)	-0.27	8 (1%)	79	83	19, 28, 42, 58	0
1	D	673/674 (99%)	-0.16	14 (2%)	63	71	21, 31, 45, 59	0
2	M	728/729 (99%)	-0.13	8 (1%)	80	85	16, 33, 62, 74	0
2	N	728/729 (99%)	-0.07	17 (2%)	60	68	15, 32, 66, 76	0
2	O	728/729 (99%)	1.77	278 (38%)	0	0	26, 64, 92, 126	0
2	P	728/729 (99%)	0.43	90 (12%)	4	5	22, 45, 76, 92	0
All	All	5604/5612 (99%)	0.16	431 (7%)	13	18	13, 31, 74, 126	0

The worst 5 of 431 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	458	ALA	11.9
2	O	474	VAL	10.9
2	O	471	GLU	9.8
2	O	485	TYR	9.5
2	O	457	PRO	9.3

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 monosaccharides in this entry.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

6.4 Ligands (i)

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	0.66	0.32	47,56,56,58	0
9	NA	P	730	1/1	0.84	0.10	35,35,35,35	0
9	NA	O	730	1/1	0.86	0.06	70,70,70,70	0
5	GOL	D	863	6/6	0.89	0.14	43,46,48,48	0
5	GOL	A	863	6/6	0.92	0.13	26,30,33,37	0
8	ACT	P	953	3/4	0.92	0.26	53,53,54,54	0
8	ACT	O	953	3/4	0.93	0.30	100,100,100,100	0
8	ACT	N	953	3/4	0.93	0.17	59,59,59,59	0
3	SF4	O	900	8/8	0.94	0.07	61,63,67,67	0
8	ACT	M	953	3/4	0.96	0.13	44,44,44,45	0
5	GOL	B	863	6/6	0.96	0.09	26,30,34,37	0
7	NI	O	951	1/1	0.96	0.04	76,76,76,76	0
6	CU1	O	950	1/1	0.97	0.06	82,82,82,82	0
6	CU1	P	950	1/1	0.98	0.05	55,55,55,55	0
4	XCC	C	800	9/9	0.98	0.13	25,27,34,35	0
9	NA	M	730	1/1	0.98	0.09	29,29,29,29	0
9	NA	N	730	1/1	0.98	0.07	28,28,28,28	0
3	SF4	C	700	8/8	0.98	0.09	28,32,35,35	0
3	SF4	P	900	8/8	0.98	0.07	40,40,41,46	0
6	CU1	N	950	1/1	0.99	0.05	38,38,38,38	0
3	SF4	A	750	8/8	0.99	0.11	14,17,17,18	0
3	SF4	B	750	8/8	0.99	0.11	17,18,18,19	0
4	XCC	A	800	9/9	0.99	0.12	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	0.12	16,20,25,27	0
3	SF4	A	700	8/8	0.99	0.08	17,19,20,22	0
4	XCC	D	800	9/9	0.99	0.13	33,35,41,45	0
3	SF4	C	750	8/8	0.99	0.09	28,30,31,32	0
3	SF4	D	750	8/8	0.99	0.12	26,28,29,29	0
3	SF4	M	900	8/8	0.99	0.09	22,25,26,28	0
3	SF4	N	900	8/8	0.99	0.09	25,26,27,28	0
6	CU1	M	950	1/1	0.99	0.07	43,43,43,43	0
7	NI	M	951	1/1	1.00	0.07	28,28,28,28	0
7	NI	N	951	1/1	1.00	0.08	29,29,29,29	0

6.5 Other polymers ⓘ

There are no such residues in this entry.