wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 09:18 PM GMT

PDB ID	:	1OAO
Title	:	NIZN[FE4S4] AND NINI[FE4S4] CLUSTERS IN CLOSED AND OPEN ALPHA SUBUNITS OF ACETYL-COA SYNTHASE/CARBON MONOXIDE DEHYDROGENASE
Authors	:	Darnault, C.; Volbeda, A.; Kim, E.J.; Legrand, P.; Vernede, X.; Lindahl, P.A.; Fontecilla-Camps, J.C.
Deposited on	:	2003-01-20
Resolution	:	1.90 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

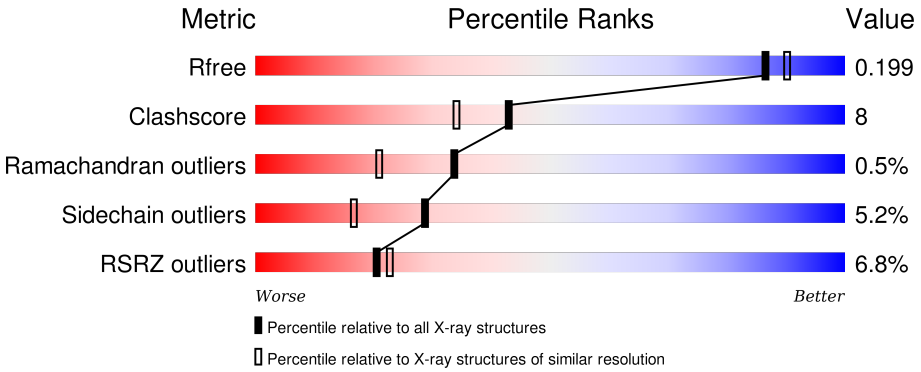
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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 >=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 <=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	3% 88% 11%
1	B	674	2% 86% 13%
2	C	729	9% 80% 17%
2	D	729	13% 73% 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
12	SX	C	1733	-	-	-	X
13	ACT	D	1733	-	-	-	X
4	XCC	A	1677	-	-	X	-
4	XCC	B	1677	-	-	X	-
5	FOR	A	1678	-	-	-	X
5	FOR	B	1678	-	-	-	X
6	SO4	A	1689	-	-	-	X
6	SO4	B	1679	-	-	-	X
6	SO4	D	1738	-	-	-	X
7	GOL	A	1687	-	-	-	X
7	GOL	B	1689	-	-	X	X
7	GOL	B	1690	-	-	-	X
7	GOL	C	1743	-	-	X	-
7	GOL	D	1736	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 23346 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.

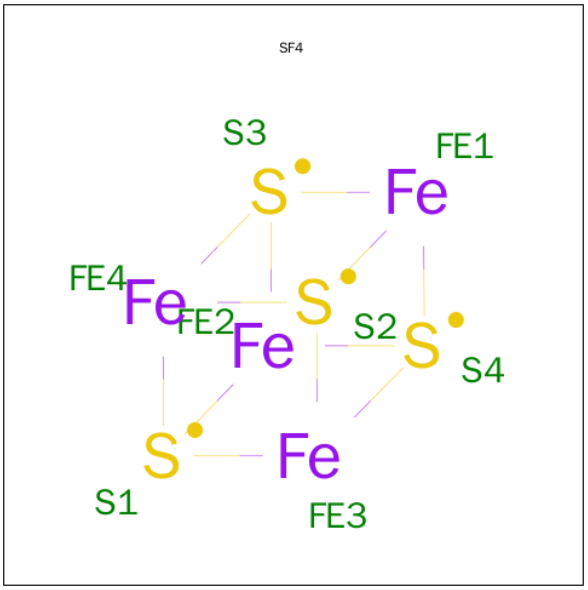
- Molecule 1 is a protein called CARBON MONOXIDE DEHYDROGENASE/ACETYL-CO A SYNTHASE SUBUNIT BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	673	Total	C	N	O	S	0	11	0
			5129	3221	894	968	46			
1	B	673	Total	C	N	O	S	0	11	0
			5131	3224	893	968	46			

- Molecule 2 is a protein called CARBON MONOXIDE DEHYDROGENASE/ACETYL-CO A SYNTHASE SUBUNIT ALPHA.

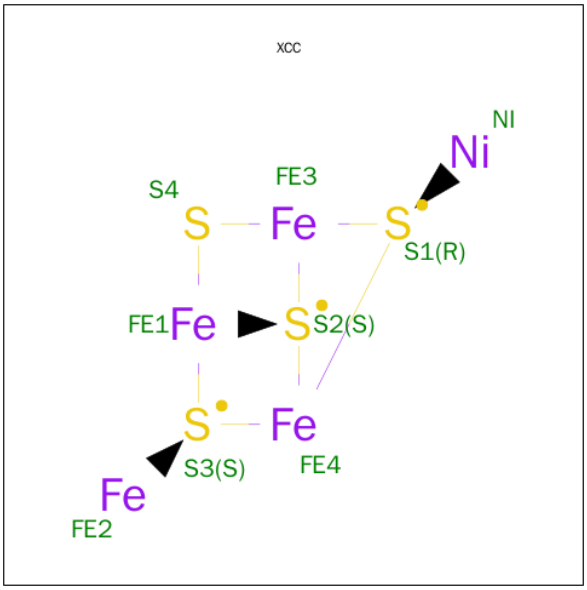
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	729	Total	C	N	O	S	0	11	0
			5788	3712	963	1076	37			
2	D	728	Total	C	N	O	S	0	2	0
			5745	3684	956	1070	35			

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



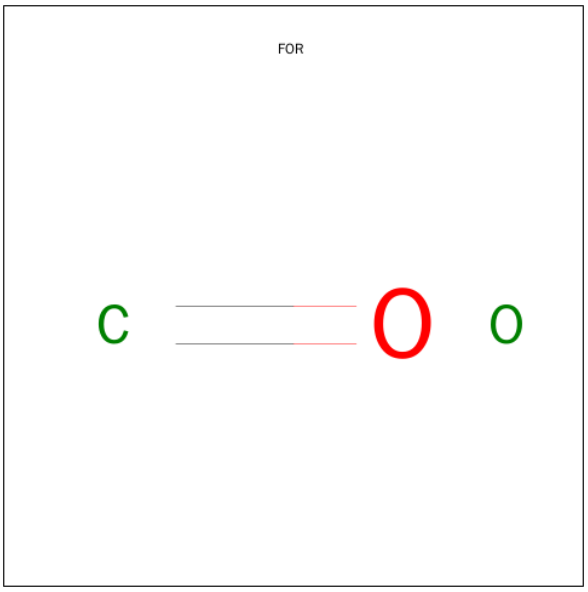
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 8 4 4	0	0
3	B	1	Total Fe S 8 4 4	0	0
3	B	1	Total Fe S 8 4 4	0	0
3	C	1	Total Fe S 8 4 4	0	0
3	D	1	Total Fe S 8 4 4	0	0

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



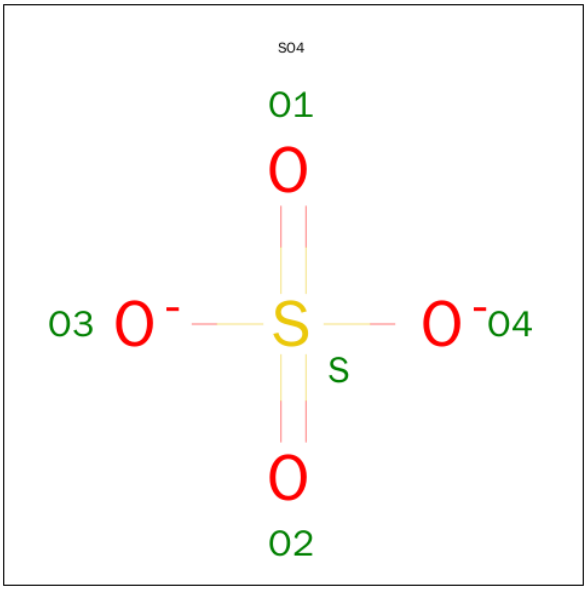
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Fe Ni S 9 4 1 4	0	0
4	B	1	Total Fe Ni S 9 4 1 4	0	0

- Molecule 5 is FORMYL GROUP (three-letter code: FOR) (formula: CH_2O).



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0

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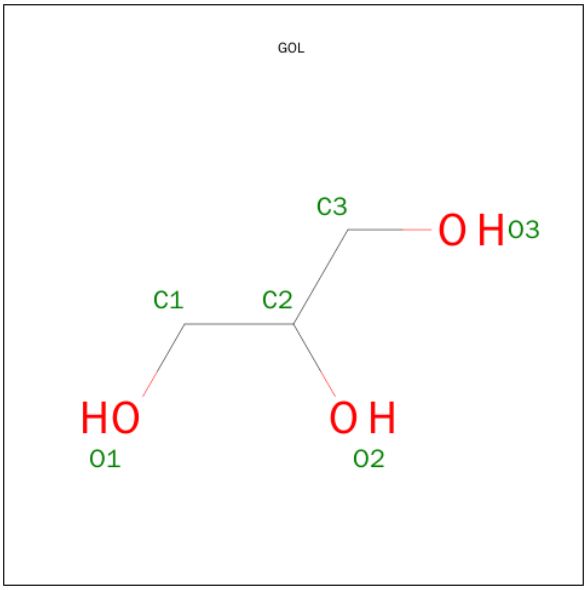
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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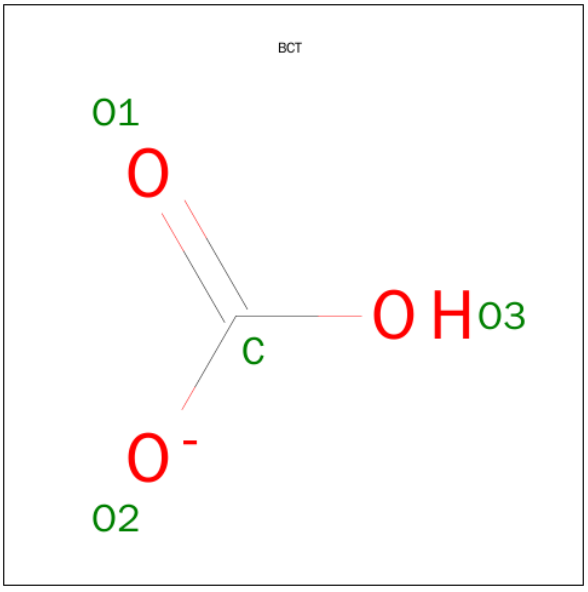
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 6 3 3	0	0
7	C	1	Total C O 6 3 3	0	0
7	C	1	Total C O 6 3 3	0	0
7	C	1	Total C O 6 3 3	0	0
7	D	1	Total C O 6 3 3	0	0

- Molecule 8 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Fe 1 1	0	0
8	A	1	Total Fe 1 1	0	0

- Molecule 9 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O 4 1 3	0	0

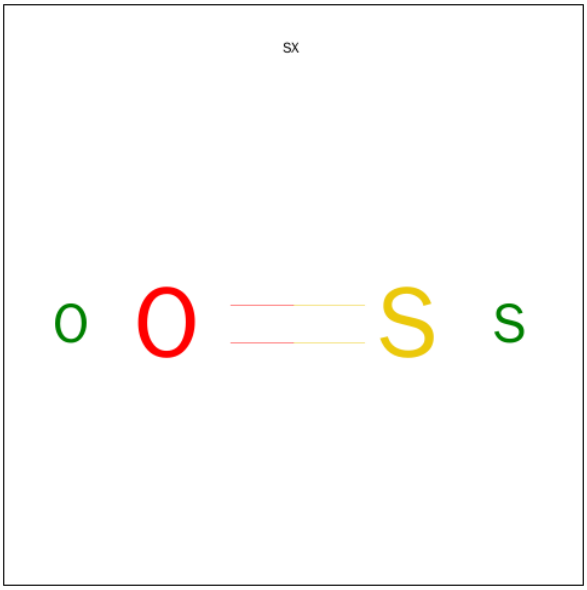
- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	1	Total Zn 1 1	0	0

- Molecule 11 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

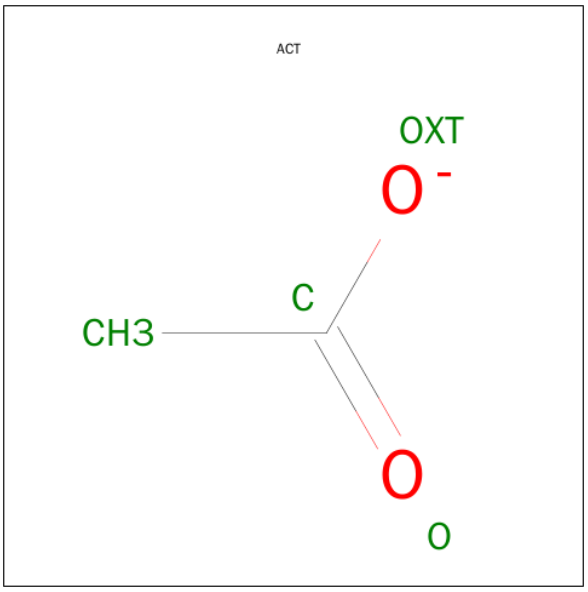
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	D	2	Total Ni 3 3	0	1
11	C	1	Total Ni 1 1	0	0

- Molecule 12 is SULFUR OXIDE (three-letter code: SX) (formula: OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	1	Total O S 2 1 1	0	0

- Molecule 13 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	D	1	Total C O 4 2 2	0	0

- Molecule 14 is water.

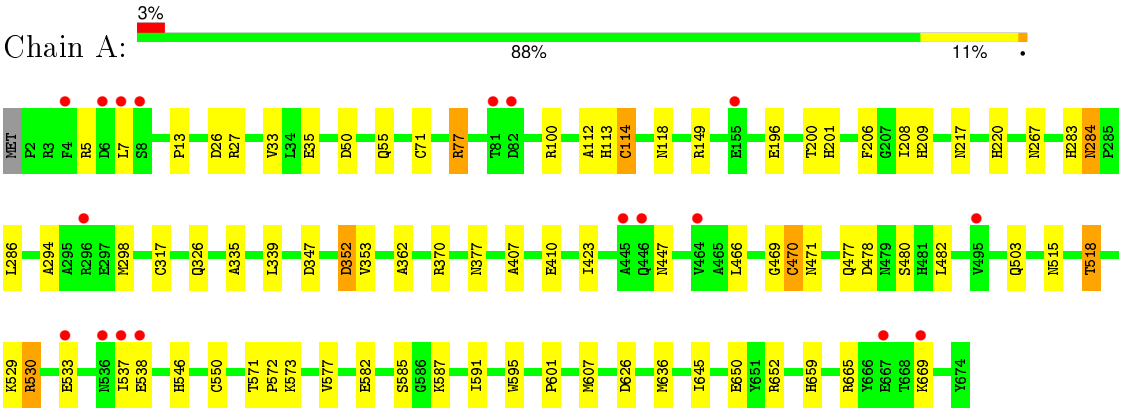
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	331	Total O 331 331	0	0
14	B	357	Total O 357 357	0	0
14	C	341	Total O 341 341	0	0
14	D	242	Total O 242 242	0	0

3 Residue-property plots (i)

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 (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.

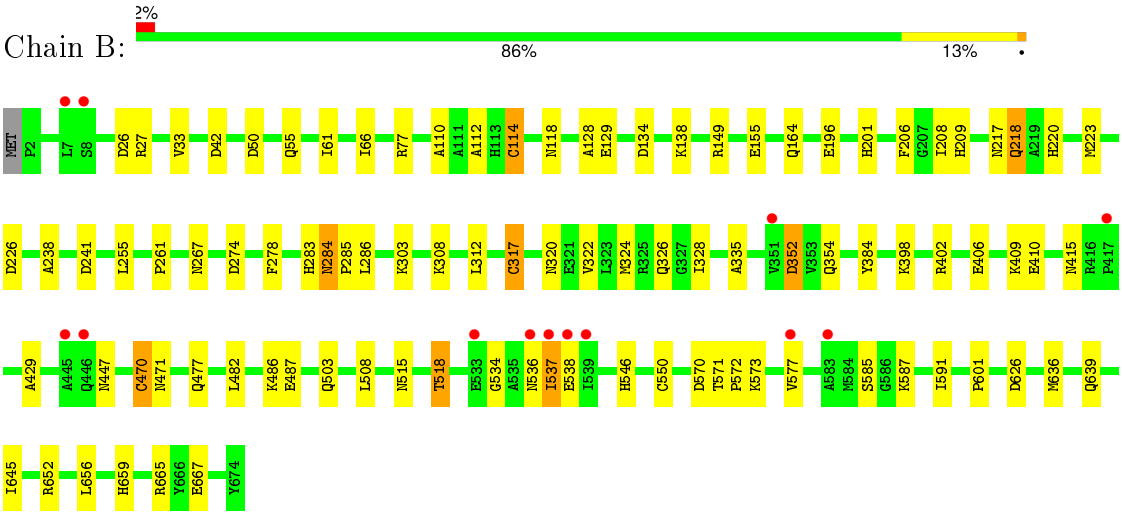
• Molecule 1: CARBON MONOXIDE DEHYDROGENASE/ACETYL-COA SYNTHASE SUBUNIT BETA

Chain A:



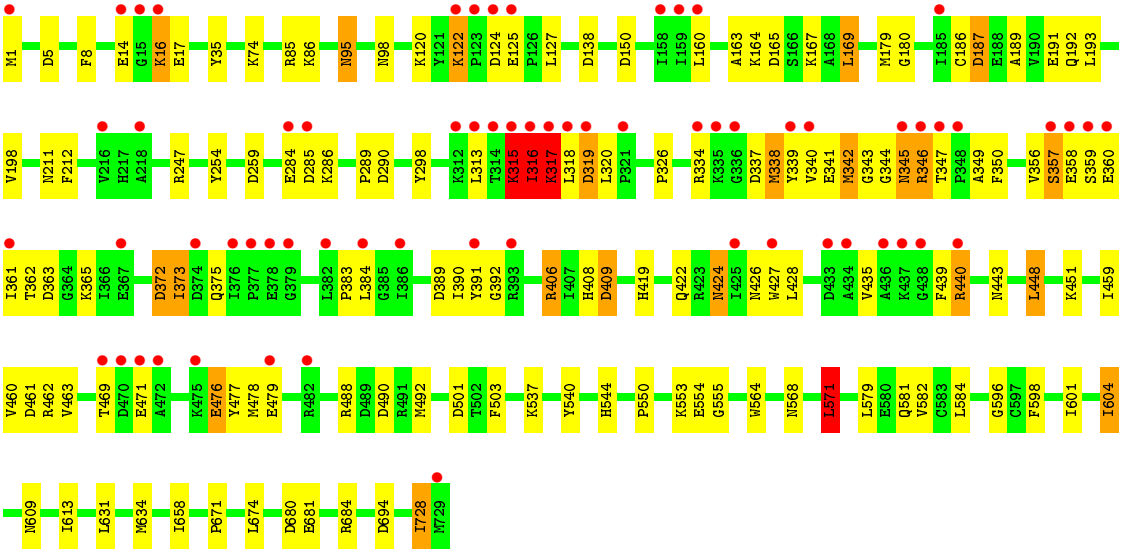
• Molecule 1: CARBON MONOXIDE DEHYDROGENASE/ACETYL-COA SYNTHASE SUBUNIT BETA

Chain B:



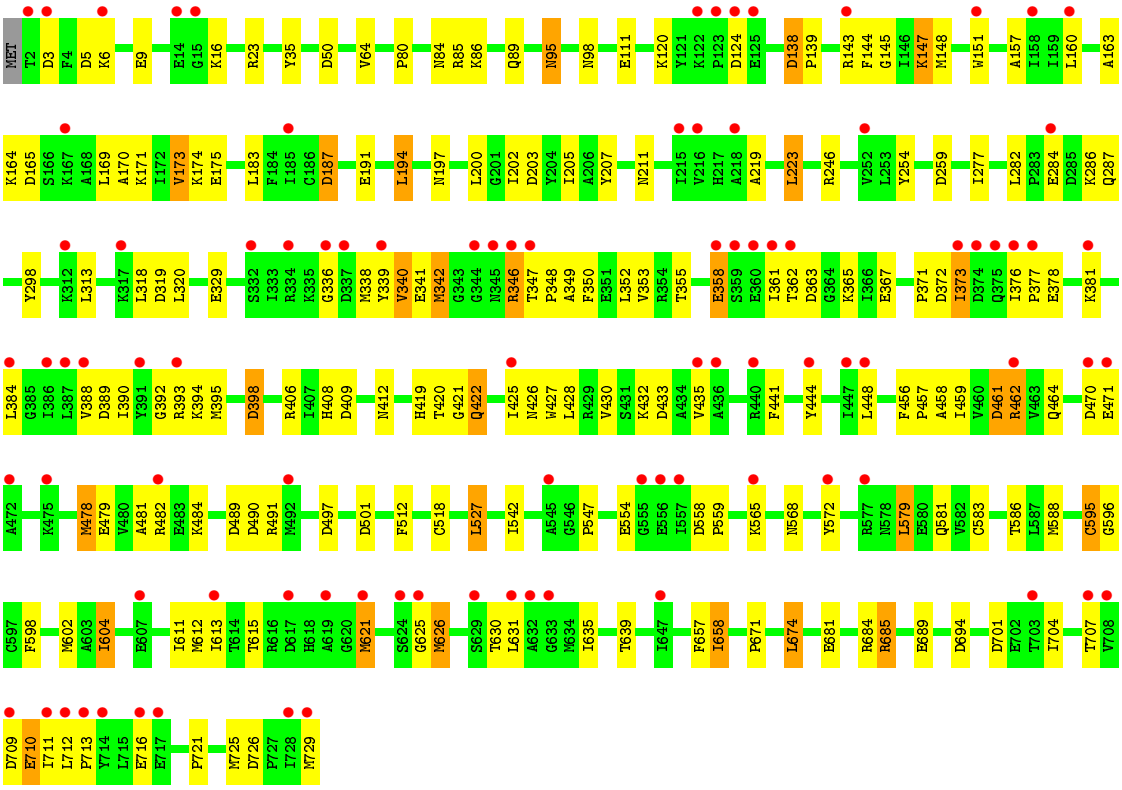
• Molecule 2: CARBON MONOXIDE DEHYDROGENASE/ACETYL-COA SYNTHASE SUBUNIT ALPHA

Chain C:



• Molecule 2: CARBON MONOXIDE DEHYDROGENASE/ACETYL-COA SYNTHASE SUBUNIT ALPHA

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	244.57Å 81.89Å 167.22Å 90.00° 96.19° 90.00°	Depositor
Resolution (Å)	25.00 – 1.90 29.17 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.9 (25.00-1.90) 97.8 (29.17-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.52 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.1.27	Depositor
R, R_{free}	0.147 , 0.179 0.172 , 0.199	Depositor DCC
R_{free} test set	12688 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	21.8	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 55.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 252670 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	23346	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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, 0.375 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: NI, ZN, SX, FOR, GOL, SF4, FE2, SO4, ACT, BCT, XCC

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	0.62	0/5275	0.78	12/7148 (0.2%)
1	B	0.65	0/5278	0.79	12/7152 (0.2%)
2	C	0.60	1/5973 (0.0%)	0.79	18/8087 (0.2%)
2	D	0.47	1/5888 (0.0%)	0.74	21/7974 (0.3%)
All	All	0.59	2/22414 (0.0%)	0.78	63/30361 (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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	357	SER	C-O	6.54	1.35	1.23
2	D	710	GLU	CD-OE2	6.19	1.32	1.25

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	85	ARG	NE-CZ-NH2	-8.76	115.92	120.30
1	B	114[A]	CYS	CA-CB-SG	-8.33	99.01	114.00
1	B	114[B]	CYS	CA-CB-SG	-8.33	99.01	114.00
1	A	339	LEU	CA-CB-CG	-6.73	99.82	115.30
1	A	352	ASP	CB-CG-OD2	6.66	124.30	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	469	GLY	Peptide

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	5129	0	5124	69	0
1	B	5131	0	5123	81	1
2	C	5788	0	5763	102	0
2	D	5745	0	5704	128	0
3	A	8	0	0	0	0
3	B	16	0	0	0	0
3	C	8	0	0	0	0
3	D	8	0	0	0	0
4	A	9	0	0	2	0
4	B	9	0	0	3	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	55	0	0	0	0
6	B	50	0	0	3	0
6	C	30	0	0	0	0
6	D	20	0	0	0	0
7	A	6	0	8	2	0
7	B	12	0	16	10	0
7	C	24	0	32	7	0
7	D	6	0	8	1	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	B	4	0	0	1	0
10	C	1	0	0	0	0
11	C	1	0	0	0	0
11	D	3	0	0	0	0
12	C	2	0	0	0	0
13	D	4	0	3	0	0
14	A	331	0	0	4	0
14	B	357	0	0	9	0
14	C	341	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	D	242	0	0	3	0
All	All	23346	0	21781	361	1

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 361 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:C:571:LEU:HD11	2:C:582[A]:VAL:HG23	1.34	1.05
2:D:362:THR:H	2:D:464:GLN:NE2	1.62	0.98
2:D:707:THR:OG1	2:D:710:GLU:HG3	1.65	0.97
6:B:1688:SO4:O2	14:B:2354:HOH:O	1.85	0.92
1:B:550[C]:CYS:SG	1:B:591:ILE:HD11	2.13	0.89

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:LYS:NZ	1:B:667:GLU:OE2[4_656]	2.17	0.03

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	683/674 (101%)	664 (97%)	18 (3%)	1 (0%)	56	46
1	B	683/674 (101%)	659 (96%)	21 (3%)	3 (0%)	39	27
2	C	738/729 (101%)	710 (96%)	22 (3%)	6 (1%)	24	11
2	D	728/729 (100%)	705 (97%)	20 (3%)	3 (0%)	39	27
All	All	2832/2806 (101%)	2738 (97%)	81 (3%)	13 (0%)	34	21

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	537	ILE
2	C	316	ILE
2	C	317	LYS
2	D	658	ILE
1	A	267	ASN

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	554/543 (102%)	535 (97%)	19 (3%)	44 33
1	B	554/543 (102%)	534 (96%)	20 (4%)	42 30
2	C	622/611 (102%)	582 (94%)	40 (6%)	22 10
2	D	612/611 (100%)	570 (93%)	42 (7%)	19 8
All	All	2342/2308 (102%)	2221 (95%)	121 (5%)	29 17

5 of 121 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	338	MET
2	C	426	ASN
2	D	595	CYS
2	C	342	MET
2	C	375	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	447	ASN
1	B	622	GLN
2	D	510	GLN
1	B	477	GLN
2	C	95	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 58 ligands modelled in this entry, 7 are monoatomic - leaving 51 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	1676	1	0,12,12	0.00	-	0,24,24	0.00	-
4	XCC	A	1677	1,8,5	0,11,11	0.00	-	0,19,19	0.00	-
5	FOR	A	1678	4	0,1,1	0.00	-	0,0,0	0.00	-
6	SO4	A	1679	-	4,4,4	0.45	0	6,6,6	0.41	0
6	SO4	A	1680	-	4,4,4	0.44	0	6,6,6	0.40	0
6	SO4	A	1681	-	4,4,4	0.14	0	6,6,6	0.18	0
6	SO4	A	1682	-	4,4,4	0.39	0	6,6,6	0.33	0
6	SO4	A	1683	-	4,4,4	0.20	0	6,6,6	0.17	0
6	SO4	A	1684	-	4,4,4	0.30	0	6,6,6	0.68	0
6	SO4	A	1685	-	4,4,4	0.12	0	6,6,6	0.22	0
6	SO4	A	1686	-	4,4,4	0.16	0	6,6,6	0.11	0
7	GOL	A	1687	-	5,5,5	0.48	0	5,5,5	0.97	0
6	SO4	A	1688	-	4,4,4	0.18	0	6,6,6	0.21	0
6	SO4	A	1689	-	4,4,4	0.12	0	6,6,6	0.23	0
6	SO4	A	1690	-	4,4,4	0.22	0	6,6,6	0.22	0
3	SF4	B	1675	1	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	B	1676	1	0,12,12	0.00	-	0,24,24	0.00	-
4	XCC	B	1677	1,8,5	0,11,11	0.00	-	0,19,19	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	FOR	B	1678	4	0,1,1	0.00	-	0,0,0	0.00	-
6	SO4	B	1679	-	4,4,4	0.69	0	6,6,6	0.23	0
6	SO4	B	1680	-	4,4,4	0.14	0	6,6,6	0.46	0
6	SO4	B	1681	-	4,4,4	0.24	0	6,6,6	0.14	0
6	SO4	B	1682	-	4,4,4	0.12	0	6,6,6	0.24	0
6	SO4	B	1683	-	4,4,4	0.28	0	6,6,6	0.36	0
6	SO4	B	1684	-	4,4,4	0.20	0	6,6,6	0.23	0
6	SO4	B	1685	-	4,4,4	0.27	0	6,6,6	0.32	0
6	SO4	B	1686	-	4,4,4	0.15	0	6,6,6	0.20	0
6	SO4	B	1687	-	4,4,4	0.22	0	6,6,6	0.20	0
6	SO4	B	1688	-	4,4,4	0.31	0	6,6,6	0.10	0
7	GOL	B	1689	-	5,5,5	0.37	0	5,5,5	0.20	0
7	GOL	B	1690	-	5,5,5	0.43	0	5,5,5	0.27	0
9	BCT	B	1691	-	0,3,3	0.00	-	0,3,3	0.00	-
3	SF4	C	1730	2	0,12,12	0.00	-	0,24,24	0.00	-
12	SX	C	1733	10	0,1,1	0.00	-	0,0,0	0.00	-
6	SO4	C	1734	-	4,4,4	0.22	0	6,6,6	0.35	0
6	SO4	C	1735	-	4,4,4	0.20	0	6,6,6	0.91	0
6	SO4	C	1736	-	4,4,4	0.17	0	6,6,6	0.25	0
7	GOL	C	1737	-	5,5,5	0.27	0	5,5,5	0.30	0
6	SO4	C	1738	-	4,4,4	0.86	0	6,6,6	0.26	0
7	GOL	C	1739	-	5,5,5	0.32	0	5,5,5	0.40	0
6	SO4	C	1740	-	4,4,4	0.35	0	6,6,6	0.33	0
7	GOL	C	1741	-	5,5,5	0.33	0	5,5,5	0.51	0
6	SO4	C	1742	-	4,4,4	0.22	0	6,6,6	0.10	0
7	GOL	C	1743	-	5,5,5	0.51	0	5,5,5	0.68	0
3	SF4	D	1730	11,2	0,12,12	0.00	-	0,24,24	0.00	-
13	ACT	D	1733	-	1,3,3	0.89	0	0,3,3	0.00	-
6	SO4	D	1734	-	4,4,4	0.14	0	6,6,6	0.20	0
6	SO4	D	1735	-	4,4,4	0.32	0	6,6,6	0.16	0
7	GOL	D	1736	-	5,5,5	0.48	0	5,5,5	0.61	0
6	SO4	D	1737	-	4,4,4	0.21	0	6,6,6	0.10	0
6	SO4	D	1738	-	4,4,4	0.23	0	6,6,6	0.22	0

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	1676	1	-	0/0/48/48	0/6/5/5
4	XCC	A	1677	1,8,5	-	0/0/32/32	0/0/3/3
5	FOR	A	1678	4	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SO4	A	1679	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1680	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1681	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1682	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1683	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1684	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1685	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1686	-	-	0/0/0/0	0/0/0/0
7	GOL	A	1687	-	-	0/4/4/4	0/0/0/0
6	SO4	A	1688	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1689	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1690	-	-	0/0/0/0	0/0/0/0
3	SF4	B	1675	1	-	0/0/48/48	0/6/5/5
3	SF4	B	1676	1	-	0/0/48/48	0/6/5/5
4	XCC	B	1677	1,8,5	-	0/0/32/32	0/0/3/3
5	FOR	B	1678	4	-	0/0/0/0	0/0/0/0
6	SO4	B	1679	-	-	0/0/0/0	0/0/0/0
6	SO4	B	1680	-	-	0/0/0/0	0/0/0/0
6	SO4	B	1681	-	-	0/0/0/0	0/0/0/0
6	SO4	B	1682	-	-	0/0/0/0	0/0/0/0
6	SO4	B	1683	-	-	0/0/0/0	0/0/0/0
6	SO4	B	1684	-	-	0/0/0/0	0/0/0/0
6	SO4	B	1685	-	-	0/0/0/0	0/0/0/0
6	SO4	B	1686	-	-	0/0/0/0	0/0/0/0
6	SO4	B	1687	-	-	0/0/0/0	0/0/0/0
6	SO4	B	1688	-	-	0/0/0/0	0/0/0/0
7	GOL	B	1689	-	-	0/4/4/4	0/0/0/0
7	GOL	B	1690	-	-	0/4/4/4	0/0/0/0
9	BCT	B	1691	-	-	0/0/0/0	0/0/0/0
3	SF4	C	1730	2	-	0/0/48/48	0/6/5/5
12	SX	C	1733	10	-	0/0/0/0	0/0/0/0
6	SO4	C	1734	-	-	0/0/0/0	0/0/0/0
6	SO4	C	1735	-	-	0/0/0/0	0/0/0/0
6	SO4	C	1736	-	-	0/0/0/0	0/0/0/0
7	GOL	C	1737	-	-	0/4/4/4	0/0/0/0
6	SO4	C	1738	-	-	0/0/0/0	0/0/0/0
7	GOL	C	1739	-	-	0/4/4/4	0/0/0/0
6	SO4	C	1740	-	-	0/0/0/0	0/0/0/0
7	GOL	C	1741	-	-	0/4/4/4	0/0/0/0
6	SO4	C	1742	-	-	0/0/0/0	0/0/0/0
7	GOL	C	1743	-	-	0/4/4/4	0/0/0/0
3	SF4	D	1730	11,2	-	0/0/48/48	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	ACT	D	1733	-	-	0/0/0/0	0/0/0/0
6	SO4	D	1734	-	-	0/0/0/0	0/0/0/0
6	SO4	D	1735	-	-	0/0/0/0	0/0/0/0
7	GOL	D	1736	-	-	0/4/4/4	0/0/0/0
6	SO4	D	1737	-	-	0/0/0/0	0/0/0/0
6	SO4	D	1738	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1677	XCC	2	0
7	A	1687	GOL	2	0
4	B	1677	XCC	3	0
6	B	1679	SO4	1	0
6	B	1683	SO4	1	0
6	B	1688	SO4	1	0
7	B	1689	GOL	10	0
9	B	1691	BCT	1	0
7	C	1737	GOL	2	0
7	C	1741	GOL	1	0
7	C	1743	GOL	4	0
7	D	1736	GOL	1	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	673/674 (99%)	-0.00	18 (2%)	58	61	5, 10, 20, 32	15 (2%)
1	B	673/674 (99%)	-0.04	13 (1%)	70	73	5, 10, 19, 39	18 (2%)
2	C	729/729 (100%)	0.34	66 (9%)	11	13	3, 11, 22, 35	7 (0%)
2	D	728/729 (99%)	0.60	93 (12%)	5	5	4, 11, 21, 39	7 (0%)
All	All	2803/2806 (99%)	0.23	190 (6%)	20	23	3, 10, 21, 39	47 (1%)

The worst 5 of 190 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	345	ASN	8.0
1	B	536	ASN	7.7
2	C	317	LYS	7.6
1	B	537	ILE	6.5
2	C	472	ALA	6.2

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^{th} 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^2)	Q<0.9
5	FOR	B	1678	2/2	0.91	0.45	17.83	23,23,23,24	2
6	SO4	A	1689	5/5	0.83	0.26	14.01	48,49,50,50	5
7	GOL	A	1687	6/6	0.81	0.23	9.67	29,31,33,34	0
5	FOR	A	1678	2/2	0.96	0.23	6.17	23,23,23,23	2
7	GOL	B	1689	6/6	0.93	0.20	6.00	54,55,56,57	0
13	ACT	D	1733	4/4	0.74	0.26	5.04	18,18,19,19	4
6	SO4	B	1679	5/5	0.99	0.12	4.87	24,24,26,28	0
12	SX	C	1733	2/2	0.99	0.15	3.89	15,15,15,18	0
7	GOL	D	1736	6/6	0.85	0.20	3.35	41,45,47,48	0
6	SO4	D	1738	5/5	0.93	0.22	2.34	58,59,59,60	0
7	GOL	B	1690	6/6	0.74	0.21	2.20	58,60,61,61	0
7	GOL	C	1743	6/6	0.91	0.15	2.00	50,52,53,53	0
6	SO4	B	1688	5/5	0.96	0.16	1.23	42,45,46,46	5
6	SO4	C	1740	5/5	0.88	0.15	1.23	19,25,26,27	5
6	SO4	A	1680	5/5	0.98	0.10	1.03	23,23,24,26	0
6	SO4	A	1679	5/5	0.97	0.11	0.78	18,18,21,25	0
7	GOL	C	1741	6/6	0.91	0.20	0.72	21,30,33,38	0
6	SO4	C	1742	5/5	0.92	0.23	0.71	31,31,31,32	0
6	SO4	B	1685	5/5	0.96	0.12	0.65	59,59,60,60	0
11	NI	D	1731[A]	1/1	0.98	0.12	0.38	17,17,17,17	1
6	SO4	B	1683	5/5	0.90	0.14	0.34	33,33,35,36	5
6	SO4	A	1683	5/5	0.97	0.17	0.14	33,33,34,35	0
7	GOL	C	1739	6/6	0.96	0.09	-0.02	10,16,17,19	0
9	BCT	B	1691	4/4	0.93	0.12	-0.08	36,37,37,38	0
6	SO4	D	1737	5/5	0.93	0.13	-0.27	61,61,61,62	5
6	SO4	C	1738	5/5	0.99	0.09	-0.27	21,23,25,27	0
6	SO4	D	1735	5/5	0.98	0.10	-0.43	33,33,35,35	0
11	NI	C	1732	1/1	1.00	0.08	-0.84	9,9,9,9	0
3	SF4	B	1675	8/8	0.99	0.07	-0.99	9,11,11,12	0
8	FE2	A	1700	1/1	0.97	0.10	-1.09	22,22,22,22	1
6	SO4	A	1690	5/5	0.98	0.07	-1.37	49,50,51,52	0
3	SF4	C	1730	8/8	1.00	0.07	-1.39	5,7,8,8	0
11	NI	D	1732	1/1	1.00	0.07	-1.51	9,9,9,9	0
10	ZN	C	1731	1/1	0.99	0.06	-1.63	12,12,12,12	0
3	SF4	D	1730	8/8	0.99	0.06	-1.65	9,9,10,11	0
4	XCC	A	1677	9/9	0.96	0.09	-1.68	17,17,23,24	9
4	XCC	B	1677	9/9	0.97	0.08	-2.39	17,17,22,23	9
8	FE2	B	1700	1/1	0.99	0.06	-2.84	20,20,20,20	1
3	SF4	A	1676	8/8	0.99	0.04	-3.33	7,8,8,9	0
3	SF4	B	1676	8/8	0.99	0.04	-4.20	7,8,8,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	SO4	D	1734	5/5	0.92	0.17	-	30,30,30,31	5
6	SO4	B	1682	5/5	0.98	0.21	-	29,31,31,31	0
6	SO4	A	1684	5/5	0.98	0.14	-	38,38,39,39	0
6	SO4	B	1680	5/5	0.97	0.13	-	29,31,32,33	0
11	NI	D	1731[B]	1/1	0.98	0.12	-	16,16,16,16	1
6	SO4	B	1686	5/5	0.94	0.26	-	58,58,59,60	0
6	SO4	B	1681	5/5	0.97	0.18	-	31,34,35,36	0
6	SO4	C	1734	5/5	0.94	0.17	-	15,16,23,23	5
6	SO4	A	1681	5/5	0.97	0.18	-	33,34,36,36	0
7	GOL	C	1737	6/6	0.86	0.19	-	36,37,38,38	0
6	SO4	A	1685	5/5	0.98	0.17	-	28,30,32,32	0
6	SO4	A	1682	5/5	0.98	0.14	-	26,28,28,29	0
6	SO4	C	1736	5/5	0.96	0.21	-	27,30,31,31	0
6	SO4	A	1686	5/5	0.92	0.17	-	36,36,37,39	5
6	SO4	B	1684	5/5	0.93	0.28	-	59,59,61,61	0
6	SO4	A	1688	5/5	0.92	0.24	-	59,60,60,61	0
6	SO4	B	1687	5/5	0.83	0.16	-	51,51,51,52	5
6	SO4	C	1735	5/5	0.96	0.17	-	33,35,35,36	0

6.5 Other polymers (i)

There are no such residues in this entry.