



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 12:36 pm GMT

PDB ID : 3GIT  
Title : Crystal structure of a truncated acetyl-CoA synthase  
Authors : Volbeda, A.; Darnault, C.; Fontecilla-Camps, J.C.  
Deposited on : 2009-03-06  
Resolution : 3.00 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.

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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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

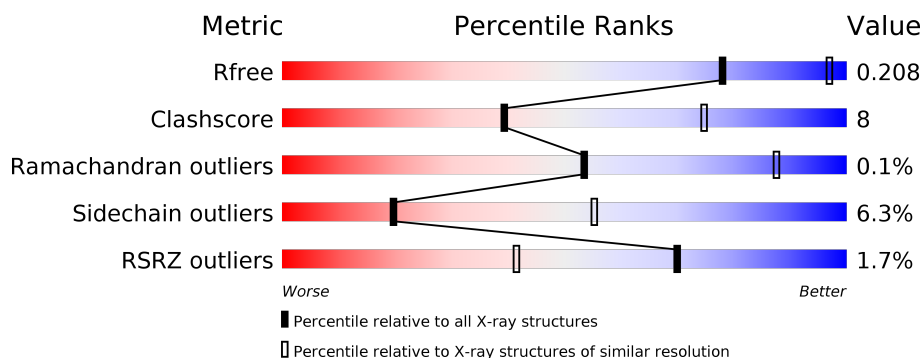
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	111664	1851 (3.00-3.00)
Clashscore	122126	2167 (3.00-3.00)
Ramachandran outliers	120053	2101 (3.00-3.00)
Sidechain outliers	120020	2104 (3.00-3.00)
RSRZ outliers	108989	1751 (3.00-3.00)

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	427	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 79%, yellow 79%, yellow 96%, green 96%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>79%</span> <span>17%</span> <span>..</span> </div> </div>
1	B	427	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, orange 3%, orange 78%, yellow 78%, yellow 97%, green 97%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>78%</span> <span>19%</span> <span>..</span> </div> </div>
1	C	427	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 2%, orange 2%, orange 77%, yellow 77%, yellow 96%, green 96%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>77%</span> <span>19%</span> <span>..</span> </div> </div>
1	D	427	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, orange 0%, orange 81%, yellow 81%, yellow 97%, green 97%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span></span> <span>81%</span> <span>16%</span> <span>..</span> </div> </div>
1	E	427	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 81%, yellow 81%, yellow 96%, green 96%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>81%</span> <span>15%</span> <span>..</span> </div> </div>
1	F	427	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 2%, orange 2%, orange 78%, yellow 78%, yellow 97%, green 97%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>78%</span> <span>19%</span> <span>..</span> </div> </div>

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
2	SF4	A	738	-	-	X	-
5	SO4	B	742	-	-	-	X
5	SO4	F	742	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20147 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 alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	0	0	0
			3297	2084	559	629	25			
1	B	421	Total	C	N	O	S	0	0	0
			3287	2078	556	628	25			
1	C	421	Total	C	N	O	S	0	0	0
			3287	2078	556	628	25			
1	D	422	Total	C	N	O	S	0	0	0
			3297	2084	559	629	25			
1	E	421	Total	C	N	O	S	0	0	0
			3287	2078	556	628	25			
1	F	421	Total	C	N	O	S	0	0	0
			3287	2078	556	628	25			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	VAL	PHE	CONFLICT	UNP P27988
A	730	ARG	-	EXPRESSION TAG	UNP P27988
A	731	SER	-	EXPRESSION TAG	UNP P27988
A	732	HIS	-	EXPRESSION TAG	UNP P27988
A	733	THR	-	EXPRESSION TAG	UNP P27988
A	734	SER	-	EXPRESSION TAG	UNP P27988
A	735	ARG	-	EXPRESSION TAG	UNP P27988
A	736	GLY	-	EXPRESSION TAG	UNP P27988
A	737	HIS	-	EXPRESSION TAG	UNP P27988
B	682	VAL	PHE	CONFLICT	UNP P27988
B	730	ARG	-	EXPRESSION TAG	UNP P27988
B	731	SER	-	EXPRESSION TAG	UNP P27988
B	732	HIS	-	EXPRESSION TAG	UNP P27988
B	733	THR	-	EXPRESSION TAG	UNP P27988
B	734	SER	-	EXPRESSION TAG	UNP P27988
B	735	ARG	-	EXPRESSION TAG	UNP P27988

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Chain	Residue	Modelled	Actual	Comment	Reference
B	736	GLY	-	EXPRESSION TAG	UNP P27988
B	737	HIS	-	EXPRESSION TAG	UNP P27988
C	682	VAL	PHE	CONFLICT	UNP P27988
C	730	ARG	-	EXPRESSION TAG	UNP P27988
C	731	SER	-	EXPRESSION TAG	UNP P27988
C	732	HIS	-	EXPRESSION TAG	UNP P27988
C	733	THR	-	EXPRESSION TAG	UNP P27988
C	734	SER	-	EXPRESSION TAG	UNP P27988
C	735	ARG	-	EXPRESSION TAG	UNP P27988
C	736	GLY	-	EXPRESSION TAG	UNP P27988
C	737	HIS	-	EXPRESSION TAG	UNP P27988
D	682	VAL	PHE	CONFLICT	UNP P27988
D	730	ARG	-	EXPRESSION TAG	UNP P27988
D	731	SER	-	EXPRESSION TAG	UNP P27988
D	732	HIS	-	EXPRESSION TAG	UNP P27988
D	733	THR	-	EXPRESSION TAG	UNP P27988
D	734	SER	-	EXPRESSION TAG	UNP P27988
D	735	ARG	-	EXPRESSION TAG	UNP P27988
D	736	GLY	-	EXPRESSION TAG	UNP P27988
D	737	HIS	-	EXPRESSION TAG	UNP P27988
E	682	VAL	PHE	CONFLICT	UNP P27988
E	730	ARG	-	EXPRESSION TAG	UNP P27988
E	731	SER	-	EXPRESSION TAG	UNP P27988
E	732	HIS	-	EXPRESSION TAG	UNP P27988
E	733	THR	-	EXPRESSION TAG	UNP P27988
E	734	SER	-	EXPRESSION TAG	UNP P27988
E	735	ARG	-	EXPRESSION TAG	UNP P27988
E	736	GLY	-	EXPRESSION TAG	UNP P27988
E	737	HIS	-	EXPRESSION TAG	UNP P27988
F	682	VAL	PHE	CONFLICT	UNP P27988
F	730	ARG	-	EXPRESSION TAG	UNP P27988
F	731	SER	-	EXPRESSION TAG	UNP P27988
F	732	HIS	-	EXPRESSION TAG	UNP P27988
F	733	THR	-	EXPRESSION TAG	UNP P27988
F	734	SER	-	EXPRESSION TAG	UNP P27988
F	735	ARG	-	EXPRESSION TAG	UNP P27988
F	736	GLY	-	EXPRESSION TAG	UNP P27988
F	737	HIS	-	EXPRESSION TAG	UNP P27988

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).

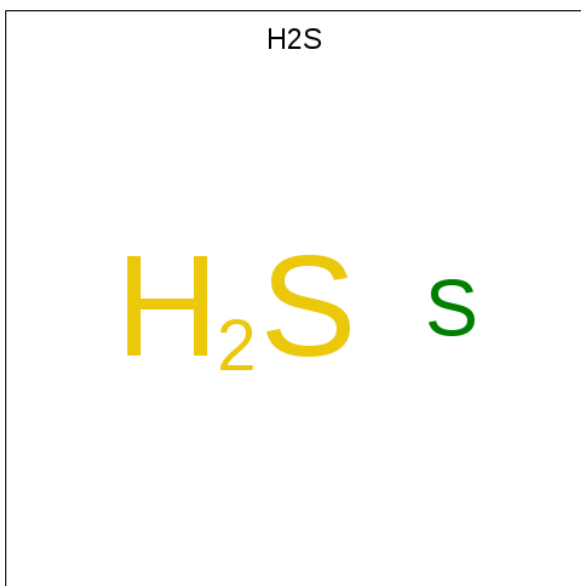


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		
2	D	1	Total	Fe	S	0	0
			8	4	4		
2	E	1	Total	Fe	S	0	0
			8	4	4		
2	F	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		

- Molecule 4 is HYDROSULFURIC ACID (three-letter code: H2S) (formula: H<sub>2</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total S 1 1	0	0
4	B	1	Total S 1 1	0	0
4	C	1	Total S 1 1	0	0
4	D	1	Total S 1 1	0	0
4	E	1	Total S 1 1	0	0
4	F	1	Total S 1 1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

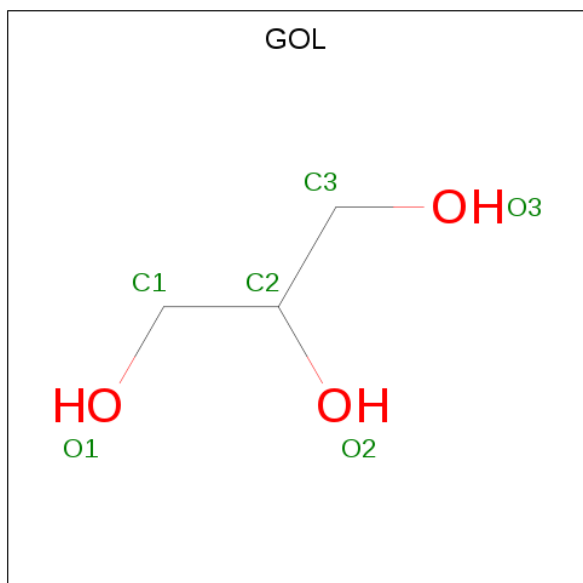
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

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

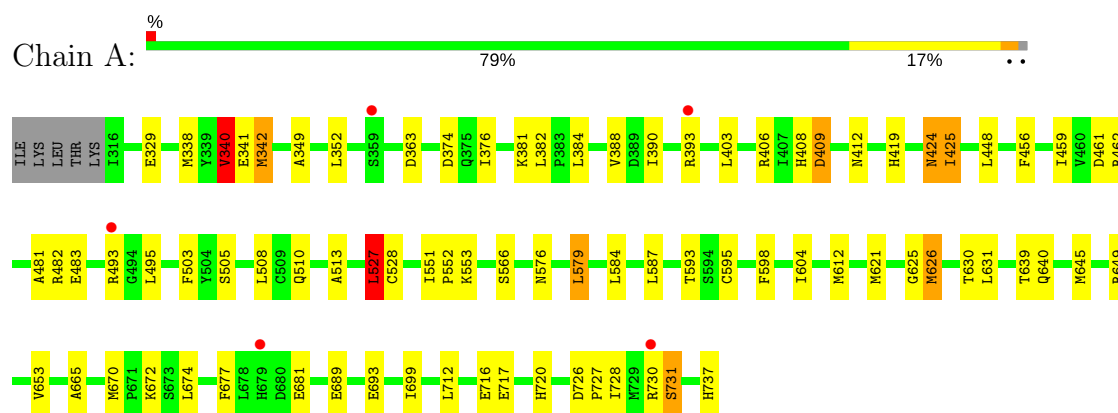
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	33	Total	O	0	0
			33	33		
7	B	27	Total	O	0	0
			27	27		
7	C	25	Total	O	0	0
			25	25		
7	D	37	Total	O	0	0
			37	37		
7	E	37	Total	O	0	0
			37	37		
7	F	30	Total	O	0	0
			30	30		

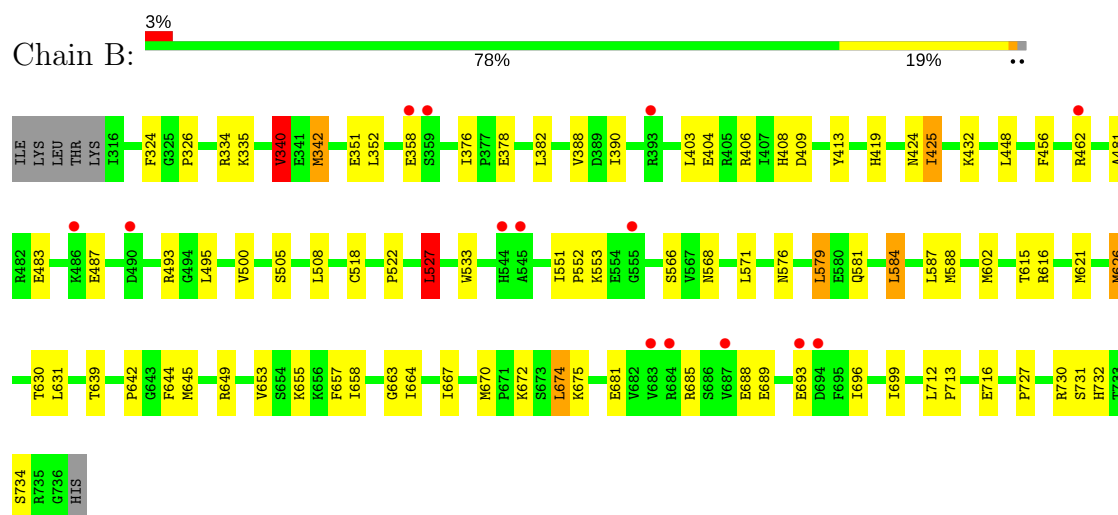
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

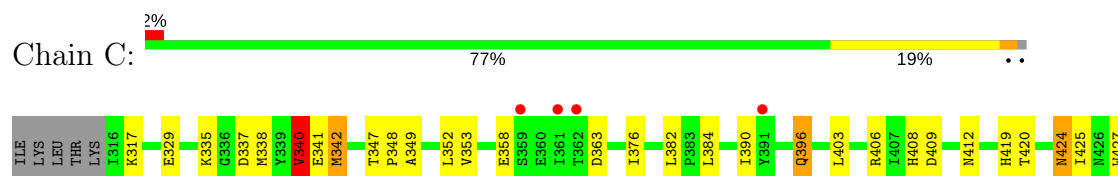
- Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha

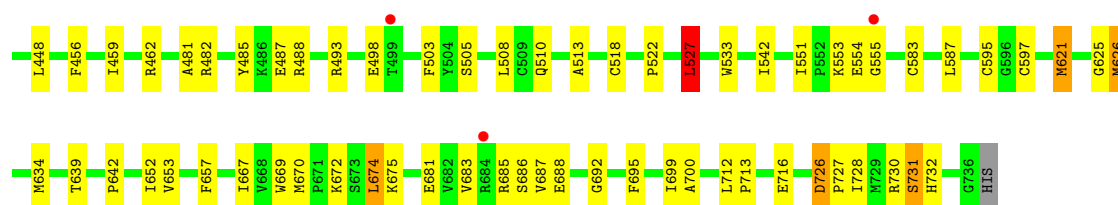


- Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha



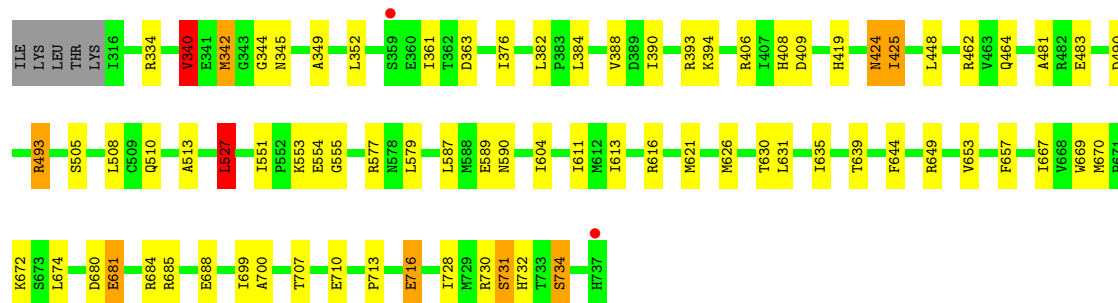
- Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha





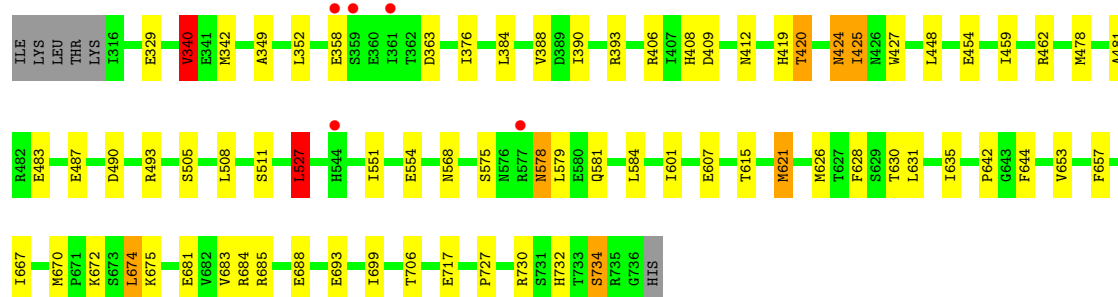
• Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha

Chain D: 81% 16% ..



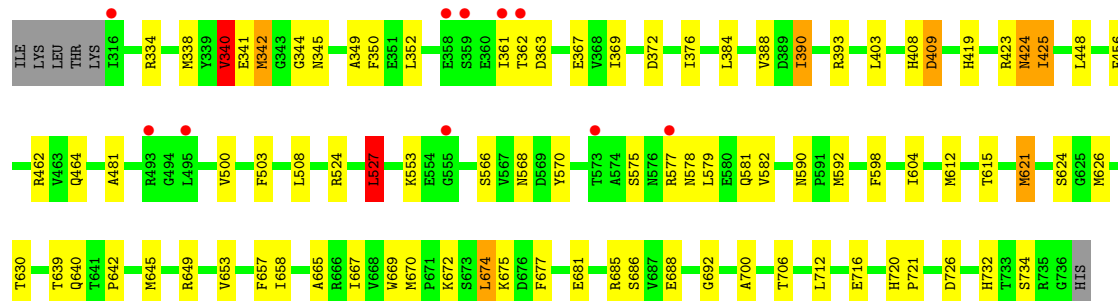
• Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha

Chain E: 81% 15% ..



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

Chain F: 78% 19% ..



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	166.40Å 166.40Å 245.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.98 – 3.00 28.82 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.98-3.00) 99.8 (28.82-2.90)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.84 (at 2.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.171 , 0.208 0.178 , 0.208	Depositor DCC
$R_{free}$ test set	4339 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.6	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 69.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	20147	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, SF4, H2S, SO4

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	0.67	0/3366	0.78	4/4549 (0.1%)
1	B	0.63	0/3355	0.75	3/4534 (0.1%)
1	C	0.61	2/3355 (0.1%)	0.73	3/4534 (0.1%)
1	D	0.74	0/3366	0.81	4/4549 (0.1%)
1	E	0.73	1/3355 (0.0%)	0.80	3/4534 (0.1%)
1	F	0.64	0/3355	0.76	4/4534 (0.1%)
All	All	0.67	3/20152 (0.0%)	0.77	21/27234 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	597	CYS	CB-SG	-5.86	1.72	1.81
1	E	734	SER	CB-OG	5.54	1.49	1.42
1	C	583	CYS	CB-SG	-5.18	1.73	1.81

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	527	LEU	CA-CB-CG	7.63	132.86	115.30
1	F	409	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	E	527	LEU	CA-CB-CG	7.48	132.50	115.30
1	D	527	LEU	CA-CB-CG	7.27	132.02	115.30
1	A	374	ASP	CB-CG-OD1	7.25	124.82	118.30

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	3297	0	3242	50	0
1	B	3287	0	3235	56	0
1	C	3287	0	3235	69	0
1	D	3297	0	3242	47	0
1	E	3287	0	3235	44	0
1	F	3287	0	3235	57	0
2	A	8	0	0	2	0
2	B	8	0	0	1	0
2	C	8	0	0	1	0
2	D	8	0	0	1	0
2	E	8	0	0	1	0
2	F	8	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	25	0	0	0	0
5	B	20	0	0	1	0
5	C	20	0	0	1	0
5	D	20	0	0	2	0
5	E	15	0	0	0	0
5	F	20	0	0	0	0
6	A	6	0	8	0	0
6	B	6	0	8	0	0
6	C	6	0	8	0	0
6	D	6	0	8	1	0
6	E	6	0	8	0	0
6	F	6	0	8	0	0
7	A	33	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	27	0	0	2	0
7	C	25	0	0	2	0
7	D	37	0	0	1	0
7	E	37	0	0	1	0
7	F	30	0	0	1	0
All	All	20147	0	19472	316	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 316 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:E:653:VAL:HG11	1:E:681:GLU:HB2	1.46	0.94
1:F:670:MET:HE3	1:F:675:LYS:HG3	1.49	0.92
1:B:657:PHE:HE2	1:B:667:ILE:HD11	1.36	0.90
1:A:625:GLY:HA3	1:C:634:MET:CE	2.04	0.88
1:C:527:LEU:HD22	2:C:738:SF4:S1	2.13	0.88

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	420/427 (98%)	398 (95%)	22 (5%)	0	100	100
1	B	419/427 (98%)	403 (96%)	15 (4%)	1 (0%)	49	85
1	C	419/427 (98%)	396 (94%)	22 (5%)	1 (0%)	49	85
1	D	420/427 (98%)	402 (96%)	18 (4%)	0	100	100
1	E	419/427 (98%)	405 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	F	419/427 (98%)	403 (96%)	15 (4%)	1 (0%)	49 85
All	All	2516/2562 (98%)	2407 (96%)	106 (4%)	3 (0%)	53 87

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	317	LYS
1	F	658	ILE
1	B	658	ILE

### 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	357/364 (98%)	329 (92%)	28 (8%)	14 45
1	B	356/364 (98%)	335 (94%)	21 (6%)	21 58
1	C	356/364 (98%)	337 (95%)	19 (5%)	25 62
1	D	357/364 (98%)	334 (94%)	23 (6%)	19 55
1	E	356/364 (98%)	330 (93%)	26 (7%)	15 48
1	F	356/364 (98%)	339 (95%)	17 (5%)	28 66
All	All	2138/2184 (98%)	2004 (94%)	134 (6%)	20 55

5 of 134 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	587	LEU
1	D	483	GLU
1	F	425	ILE
1	C	626	MET
1	D	340	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	581	GLN
1	D	464	GLN
1	F	578	ASN
1	C	590	ASN
1	D	408	HIS

### 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 48 ligands modelled in this entry, 6 are modelled with single atom and 6 are monoatomic - leaving 36 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	$\# Z  > 2$
2	SF4	A	738	1	0,12,12	0.00	-	0,24,24	0.00	-
5	SO4	A	741	-	4,4,4	0.37	0	6,6,6	0.32	0
5	SO4	A	742	-	4,4,4	0.23	0	6,6,6	0.18	0
6	GOL	A	743	-	5,5,5	0.28	0	5,5,5	0.53	0
5	SO4	A	744	-	4,4,4	0.32	0	6,6,6	0.68	0
5	SO4	A	745	-	4,4,4	0.23	0	6,6,6	0.26	0
5	SO4	A	746	-	4,4,4	0.27	0	6,6,6	0.34	0
2	SF4	B	738	1	0,12,12	0.00	-	0,24,24	0.00	-
5	SO4	B	741	-	4,4,4	0.19	0	6,6,6	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SO4	B	742	-	4,4,4	0.81	0	6,6,6	0.27	0
6	GOL	B	743	-	5,5,5	0.35	0	5,5,5	0.44	0
5	SO4	B	744	-	4,4,4	0.31	0	6,6,6	0.83	0
5	SO4	B	745	-	4,4,4	0.22	0	6,6,6	0.29	0
2	SF4	C	738	1	0,12,12	0.00	-	0,24,24	0.00	-
5	SO4	C	741	-	4,4,4	0.28	0	6,6,6	0.22	0
5	SO4	C	742	-	4,4,4	0.25	0	6,6,6	0.39	0
6	GOL	C	743	-	5,5,5	0.34	0	5,5,5	0.37	0
5	SO4	C	744	-	4,4,4	0.28	0	6,6,6	0.64	0
5	SO4	C	745	-	4,4,4	0.16	0	6,6,6	0.22	0
2	SF4	D	738	1	0,12,12	0.00	-	0,24,24	0.00	-
5	SO4	D	741	-	4,4,4	0.38	0	6,6,6	0.32	0
5	SO4	D	742	-	4,4,4	0.22	0	6,6,6	0.46	0
6	GOL	D	743	-	5,5,5	0.49	0	5,5,5	0.64	0
5	SO4	D	744	-	4,4,4	0.30	0	6,6,6	0.80	0
5	SO4	D	745	-	4,4,4	0.31	0	6,6,6	0.23	0
2	SF4	E	738	1	0,12,12	0.00	-	0,24,24	0.00	-
5	SO4	E	742	-	4,4,4	0.25	0	6,6,6	0.21	0
6	GOL	E	743	-	5,5,5	0.51	0	5,5,5	0.52	0
5	SO4	E	744	-	4,4,4	0.49	0	6,6,6	0.83	0
5	SO4	E	745	-	4,4,4	0.26	0	6,6,6	0.31	0
2	SF4	F	738	1	0,12,12	0.00	-	0,24,24	0.00	-
5	SO4	F	741	-	4,4,4	0.33	0	6,6,6	0.47	0
5	SO4	F	742	-	4,4,4	0.26	0	6,6,6	0.25	0
6	GOL	F	743	-	5,5,5	0.41	0	5,5,5	0.27	0
5	SO4	F	744	-	4,4,4	0.22	0	6,6,6	0.66	0
5	SO4	F	745	-	4,4,4	0.31	0	6,6,6	0.27	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
2	SF4	A	738	1	-	0/0/48/48	0/6/5/5
5	SO4	A	741	-	-	0/0/0/0	0/0/0/0
5	SO4	A	742	-	-	0/0/0/0	0/0/0/0
6	GOL	A	743	-	-	0/4/4/4	0/0/0/0
5	SO4	A	744	-	-	0/0/0/0	0/0/0/0
5	SO4	A	745	-	-	0/0/0/0	0/0/0/0
5	SO4	A	746	-	-	0/0/0/0	0/0/0/0
2	SF4	B	738	1	-	0/0/48/48	0/6/5/5
5	SO4	B	741	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	B	742	-	-	0/0/0/0	0/0/0/0
6	GOL	B	743	-	-	0/4/4/4	0/0/0/0
5	SO4	B	744	-	-	0/0/0/0	0/0/0/0
5	SO4	B	745	-	-	0/0/0/0	0/0/0/0
2	SF4	C	738	1	-	0/0/48/48	0/6/5/5
5	SO4	C	741	-	-	0/0/0/0	0/0/0/0
5	SO4	C	742	-	-	0/0/0/0	0/0/0/0
6	GOL	C	743	-	-	0/4/4/4	0/0/0/0
5	SO4	C	744	-	-	0/0/0/0	0/0/0/0
5	SO4	C	745	-	-	0/0/0/0	0/0/0/0
2	SF4	D	738	1	-	0/0/48/48	0/6/5/5
5	SO4	D	741	-	-	0/0/0/0	0/0/0/0
5	SO4	D	742	-	-	0/0/0/0	0/0/0/0
6	GOL	D	743	-	-	0/4/4/4	0/0/0/0
5	SO4	D	744	-	-	0/0/0/0	0/0/0/0
5	SO4	D	745	-	-	0/0/0/0	0/0/0/0
2	SF4	E	738	1	-	0/0/48/48	0/6/5/5
5	SO4	E	742	-	-	0/0/0/0	0/0/0/0
6	GOL	E	743	-	-	0/4/4/4	0/0/0/0
5	SO4	E	744	-	-	0/0/0/0	0/0/0/0
5	SO4	E	745	-	-	0/0/0/0	0/0/0/0
2	SF4	F	738	1	-	0/0/48/48	0/6/5/5
5	SO4	F	741	-	-	0/0/0/0	0/0/0/0
5	SO4	F	742	-	-	0/0/0/0	0/0/0/0
6	GOL	F	743	-	-	0/4/4/4	0/0/0/0
5	SO4	F	744	-	-	0/0/0/0	0/0/0/0
5	SO4	F	745	-	-	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.

11 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	738	SF4	2	0
2	B	738	SF4	1	0
5	B	744	SO4	1	0
2	C	738	SF4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	742	SO4	1	0
2	D	738	SF4	1	0
5	D	742	SO4	1	0
6	D	743	GOL	1	0
5	D	744	SO4	1	0
2	E	738	SF4	1	0
2	F	738	SF4	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 [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	422/427 (98%)	-0.18	5 (1%) 79 53	53, 57, 60, 64	11 (2%)
1	B	421/427 (98%)	-0.08	14 (3%) 46 20	53, 57, 60, 65	11 (2%)
1	C	421/427 (98%)	-0.13	7 (1%) 70 41	54, 57, 60, 64	11 (2%)
1	D	422/427 (98%)	-0.24	2 (0%) 90 74	53, 57, 61, 77	12 (2%)
1	E	421/427 (98%)	-0.23	5 (1%) 79 53	53, 57, 61, 67	11 (2%)
1	F	421/427 (98%)	-0.15	10 (2%) 59 30	54, 57, 60, 64	11 (2%)
All	All	2528/2562 (98%)	-0.17	43 (1%) 70 41	53, 57, 60, 77	67 (2%)

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	358	GLU	4.5
1	B	687	VAL	3.8
1	C	362	THR	3.6
1	A	730	ARG	3.4
1	F	493	ARG	3.3

### 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 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. 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
5	SO4	B	742	5/5	0.71	0.55	52,52,53,53	5
5	SO4	F	742	5/5	0.75	0.42	64,65,66,66	5
5	SO4	C	745	5/5	0.78	0.37	62,62,63,63	5
5	SO4	F	741	5/5	0.79	0.23	79,79,81,81	5
6	GOL	D	743	6/6	0.80	0.29	79,84,85,87	0
5	SO4	A	742	5/5	0.80	0.25	56,57,57,57	5
5	SO4	E	745	5/5	0.81	0.25	65,66,67,67	5
6	GOL	E	743	6/6	0.82	0.32	84,87,87,87	0
5	SO4	B	745	5/5	0.82	0.33	62,62,64,64	5
5	SO4	C	742	5/5	0.83	0.41	58,58,59,59	5
5	SO4	F	745	5/5	0.85	0.25	65,66,67,67	5
5	SO4	D	745	5/5	0.86	0.24	70,71,72,72	5
4	H2S	F	740	1/1	0.87	0.23	59,59,59,59	1
6	GOL	A	743	6/6	0.88	0.22	80,81,81,82	0
6	GOL	F	743	6/6	0.88	0.34	81,83,83,84	0
5	SO4	A	745	5/5	0.88	0.19	63,63,64,65	5
6	GOL	C	743	6/6	0.89	0.29	87,90,91,92	0
5	SO4	B	744	5/5	0.89	0.25	77,79,82,83	5
4	H2S	C	740	1/1	0.89	0.24	58,58,58,58	1
6	GOL	B	743	6/6	0.90	0.30	81,83,84,85	0
5	SO4	D	741	5/5	0.90	0.32	71,71,73,74	5
5	SO4	A	746	5/5	0.90	0.28	69,70,71,71	5
5	SO4	A	744	5/5	0.90	0.19	72,72,75,76	5
4	H2S	E	740	1/1	0.90	0.22	59,59,59,59	1
5	SO4	A	741	5/5	0.91	0.15	78,79,80,81	5
5	SO4	D	742	5/5	0.91	0.26	57,57,58,58	5
5	SO4	E	744	5/5	0.91	0.18	72,75,77,77	5
4	H2S	D	740	1/1	0.91	0.22	58,58,58,58	1
5	SO4	E	742	5/5	0.92	0.40	59,59,60,61	5
5	SO4	D	744	5/5	0.92	0.18	71,73,75,77	5
5	SO4	C	741	5/5	0.92	0.25	68,69,70,70	5
5	SO4	B	741	5/5	0.92	0.23	70,71,71,71	5
5	SO4	F	744	5/5	0.93	0.13	65,66,68,70	5
5	SO4	C	744	5/5	0.93	0.20	66,66,67,70	5
4	H2S	B	740	1/1	0.95	0.21	57,57,57,57	1
4	H2S	A	740	1/1	0.95	0.13	60,60,60,60	1
3	ZN	D	739	1/1	0.96	0.11	57,57,57,57	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	E	739	1/1	0.97	0.11	59,59,59,59	1
3	ZN	F	739	1/1	0.97	0.12	57,57,57,57	1
3	ZN	B	739	1/1	0.97	0.07	57,57,57,57	1
3	ZN	C	739	1/1	0.97	0.10	57,57,57,57	1
3	ZN	A	739	1/1	0.98	0.09	57,57,57,57	1
2	SF4	C	738	8/8	0.99	0.09	54,55,57,57	0
2	SF4	E	738	8/8	0.99	0.11	54,55,57,57	0
2	SF4	F	738	8/8	0.99	0.11	54,56,56,57	0
2	SF4	D	738	8/8	0.99	0.10	52,54,56,58	0
2	SF4	B	738	8/8	0.99	0.10	54,55,57,57	0
2	SF4	A	738	8/8	0.99	0.10	56,56,57,58	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.