



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 16, 2017 – 09:36 AM EDT

PDB ID : 3CF4  
Title : Structure of the CODH component of the M. barkeri ACDS complex  
Authors : Gong, W.; Hao, B.; Wei, Z.; Ferguson Jr., D.J.; Tallant, T.; Krzycki, J.A.;  
Chan, M.K.  
Deposited on : unknown  
Resolution : 2.00 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030345

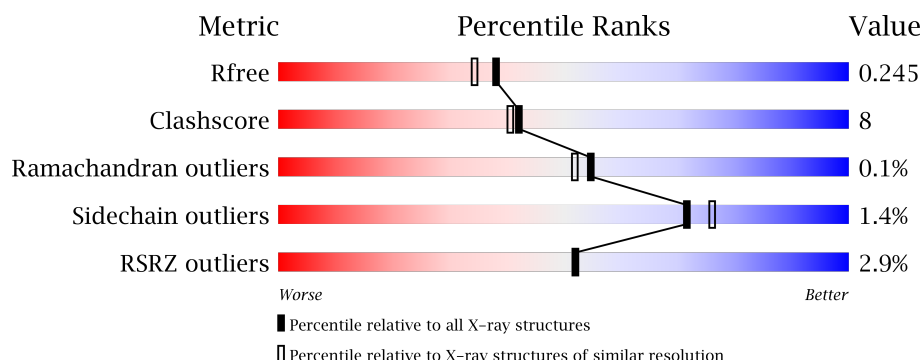
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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	807	<div> <div>3%</div> <div>79%</div> <div>16%</div> <div>5%</div> </div>
2	G	170	<div> <div>2%</div> <div>82%</div> <div>16%</div> <div>..</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
7	ACY	A	818	-	-	-	X
7	ACY	A	819	-	-	-	X
7	ACY	A	821	-	-	-	X
7	ACY	A	822	-	-	-	X
7	ACY	A	823	-	-	-	X
7	ACY	A	824	-	-	-	X
8	GOL	A	825	-	-	-	X
8	GOL	G	172	-	-	-	X
9	PEG	G	173	-	-	-	X

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 7813 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.

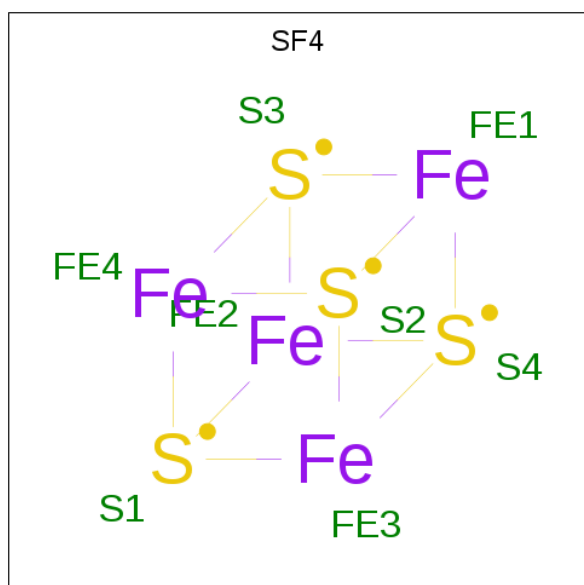
- Molecule 1 is a protein called Acetyl-CoA decarboxylase/synthase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	766	Total	C	N	O	S	0	4	0
			5878	3712	995	1114	57			

- Molecule 2 is a protein called Acetyl-CoA decarboxylase/synthase epsilon subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	169	Total	C	N	O	S	0	0	0
			1285	825	212	243	5			

- 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
			4	2	2		
3	A	1	Total	Fe	S	0	0
			8	4	4		

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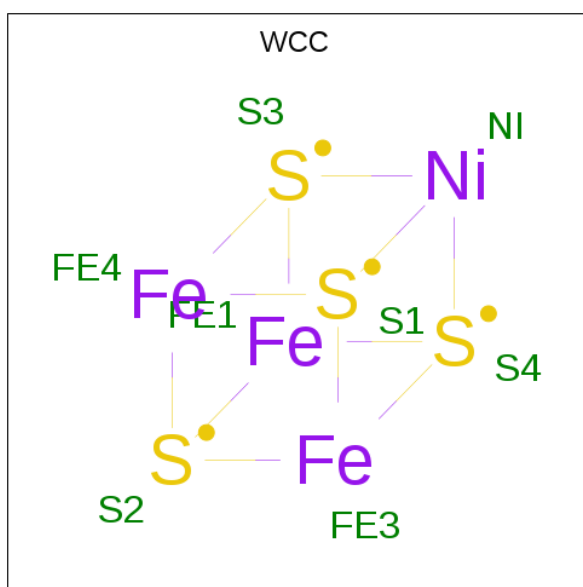
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

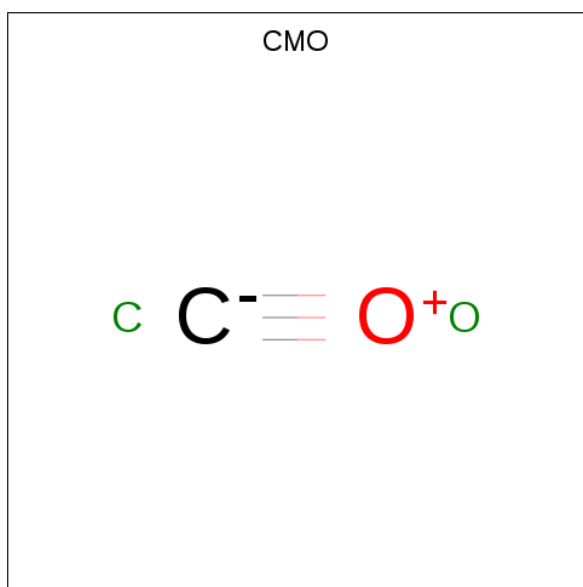
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe		0	0
			1	1			

- Molecule 5 is FE(3)-NI(1)-S(4) CLUSTER (three-letter code: WCC) (formula: Fe<sub>3</sub>NiS<sub>4</sub>).



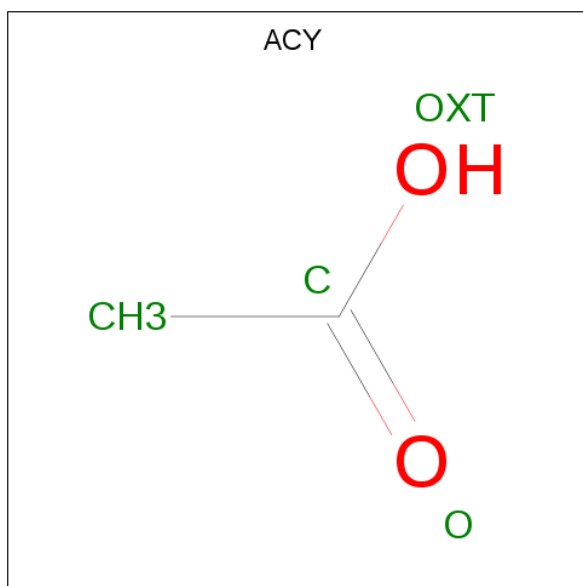
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	Fe	Ni	S	0	0
			8	3	1	4		

- Molecule 6 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



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

- Molecule 7 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		

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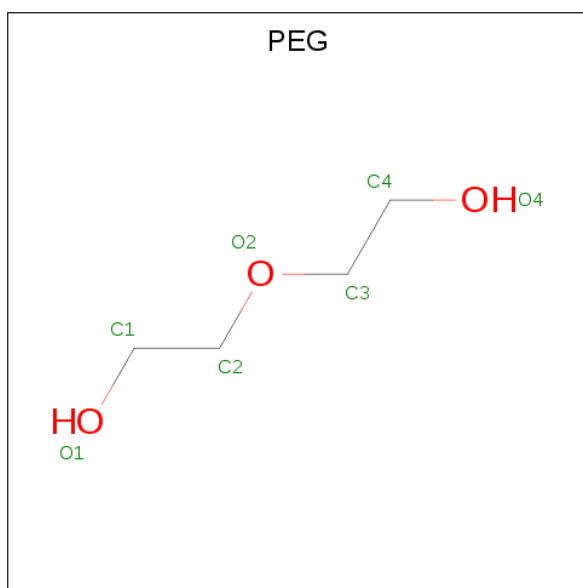
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	G	1	Total	C	O	0	0
			7	4	3		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	439	Total	O	0	0
			439	439		
10	G	103	Total	O	0	0
			103	103		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.29 Å   81.68 Å   101.12 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (20.00-2.00) 97.5 (20.00-2.00)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.08 (at 2.01 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.209   ,   0.248 0.207   ,   0.245	Depositor DCC
$R_{free}$ test set	3697 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.3	Xtriage
Anisotropy	0.721	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 63.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7813	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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: CMO, GOL, SF4, WCC, FE, ACY, PEG

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	0.38	0/6017	0.64	1/8137 (0.0%)
2	G	0.38	0/1307	0.63	0/1770
All	All	0.38	0/7324	0.64	1/9907 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	514	THR	N-CA-C	-6.62	93.13	111.00

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	5878	0	5836	94	0
2	G	1285	0	1319	20	0
3	A	28	0	0	0	0
4	A	1	0	0	0	0
5	A	8	0	0	0	0
6	A	2	0	0	0	0
7	A	40	0	30	0	0
7	G	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	12	0	16	2	0
8	G	6	0	8	1	0
9	G	7	0	10	1	0
10	A	439	0	0	7	1
10	G	103	0	0	3	0
All	All	7813	0	7222	114	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 114 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:A:134:GLU:HG3	1:A:162:GLY:HA3	1.40	1.03
1:A:142:GLN:H	1:A:142:GLN:CD	1.76	0.89
1:A:347:MET:HE2	1:A:374:VAL:HG21	1.62	0.82
2:G:96:ASP:OD2	2:G:98:LYS:HG2	1.79	0.81
1:A:134:GLU:HG3	1:A:162:GLY:CA	2.15	0.76

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)
10:A:1173:HOH:O	10:A:1173:HOH:O[2_655]	2.10	0.10

## 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	768/807 (95%)	739 (96%)	28 (4%)	1 (0%)	55	52
2	G	167/170 (98%)	163 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	935/977 (96%)	902 (96%)	32 (3%)	1 (0%)	55 52

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	322	GLN

### 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	629/663 (95%)	620 (99%)	9 (1%)	71 76
2	G	137/139 (99%)	135 (98%)	2 (2%)	70 74
All	All	766/802 (96%)	755 (99%)	11 (1%)	71 76

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	333	GLN
1	A	494	ARG
1	A	805	LYS
1	A	194	ASP
1	A	663	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	463	GLN
2	G	17	ASN
1	A	525	ASN
1	A	144	ASN
1	A	772	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 1 is monoatomic - leaving 21 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	809	1	0,4,12	0.00	-	0,4,24	0.00	-
3	SF4	A	810	1	0,12,12	0.00	-	0,24,24	0.00	-
5	WCC	A	811	1,4,6	0,12,12	0.00	-	0,24,24	0.00	-
6	CMO	A	812	5	0,1,1	0.00	-	0,0,0	0.00	-
3	SF4	A	813	1	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	A	814	1	0,12,12	0.00	-	0,24,24	0.00	-
7	ACY	A	815	-	1,3,3	1.13	0	0,3,3	0.00	-
7	ACY	A	816	-	1,3,3	1.20	0	0,3,3	0.00	-
7	ACY	A	817	-	1,3,3	1.32	0	0,3,3	0.00	-
7	ACY	A	818	-	1,3,3	1.14	0	0,3,3	0.00	-
7	ACY	A	819	-	1,3,3	0.79	0	0,3,3	0.00	-
7	ACY	A	820	-	1,3,3	1.35	0	0,3,3	0.00	-
7	ACY	A	821	-	1,3,3	1.01	0	0,3,3	0.00	-
7	ACY	A	822	-	1,3,3	0.64	0	0,3,3	0.00	-
7	ACY	A	823	-	1,3,3	1.98	0	0,3,3	0.00	-
7	ACY	A	824	-	1,3,3	1.70	0	0,3,3	0.00	-
8	GOL	A	825	-	5,5,5	0.48	0	5,5,5	0.20	0
8	GOL	A	826	-	5,5,5	0.87	0	5,5,5	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	ACY	G	171	-	1,3,3	1.18	0	0,3,3	0.00	-
8	GOL	G	172	-	5,5,5	0.37	0	5,5,5	0.34	0
9	PEG	G	173	-	6,6,6	0.71	0	5,5,5	1.00	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	809	1	-	0/0/4/48	0/1/1/5
3	SF4	A	810	1	-	0/0/48/48	0/6/5/5
5	WCC	A	811	1,4,6	-	0/0/48/48	0/6/5/5
6	CMO	A	812	5	-	0/0/0/0	0/0/0/0
3	SF4	A	813	1	-	0/0/48/48	0/6/5/5
3	SF4	A	814	1	-	0/0/48/48	0/6/5/5
7	ACY	A	815	-	-	0/0/0/0	0/0/0/0
7	ACY	A	816	-	-	0/0/0/0	0/0/0/0
7	ACY	A	817	-	-	0/0/0/0	0/0/0/0
7	ACY	A	818	-	-	0/0/0/0	0/0/0/0
7	ACY	A	819	-	-	0/0/0/0	0/0/0/0
7	ACY	A	820	-	-	0/0/0/0	0/0/0/0
7	ACY	A	821	-	-	0/0/0/0	0/0/0/0
7	ACY	A	822	-	-	0/0/0/0	0/0/0/0
7	ACY	A	823	-	-	0/0/0/0	0/0/0/0
7	ACY	A	824	-	-	0/0/0/0	0/0/0/0
8	GOL	A	825	-	-	0/4/4/4	0/0/0/0
8	GOL	A	826	-	-	0/4/4/4	0/0/0/0
7	ACY	G	171	-	-	0/0/0/0	0/0/0/0
8	GOL	G	172	-	-	0/4/4/4	0/0/0/0
9	PEG	G	173	-	-	0/4/4/4	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.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	826	GOL	2	0
8	G	172	GOL	1	0
9	G	173	PEG	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	766/807 (94%)	0.04	23 (3%) 51 51	8, 18, 31, 38	0
2	G	169/170 (99%)	-0.03	4 (2%) 59 59	11, 19, 27, 31	0
All	All	935/977 (95%)	0.03	27 (2%) 52 52	8, 18, 30, 38	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	400	GLY	3.7
1	A	399	ALA	3.2
1	A	142	GLN	3.2
1	A	778	TRP	3.1
1	A	759	ALA	3.0

### 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 [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	ACY	A	823	4/4	0.93	0.17	8.48	20,22,23,24	0
7	ACY	A	824	4/4	0.81	0.23	7.20	38,38,39,39	0
9	PEG	G	173	7/7	0.93	0.22	6.43	27,29,34,39	0
7	ACY	A	818	4/4	0.89	0.20	4.60	38,38,38,39	0
7	ACY	A	822	4/4	0.81	0.28	4.58	62,62,63,63	0
7	ACY	A	819	4/4	0.84	0.18	4.25	37,38,39,39	0
7	ACY	A	821	4/4	0.84	0.15	3.58	31,32,33,33	0
8	GOL	A	825	6/6	0.89	0.17	2.49	33,33,34,35	0
8	GOL	G	172	6/6	0.94	0.15	2.05	24,27,28,29	0
7	ACY	G	171	4/4	0.88	0.19	2.00	54,54,54,54	0
8	GOL	A	826	6/6	0.92	0.13	0.41	28,30,32,33	0
6	CMO	A	812	2/2	0.97	0.11	0.14	19,19,19,24	0
7	ACY	A	815	4/4	0.96	0.09	-1.01	22,24,24,24	0
3	SF4	A	814	8/8	0.99	0.04	-2.08	16,17,20,20	0
3	SF4	A	809	4/8	0.99	0.05	-2.26	14,15,17,18	0
3	SF4	A	813	8/8	0.98	0.06	-2.38	14,14,17,19	0
3	SF4	A	810	8/8	0.99	0.06	-2.55	11,12,14,14	0
5	WCC	A	811	8/8	0.98	0.06	-2.98	19,21,22,26	0
4	FE	A	808	1/1	0.98	0.04	-	25,25,25,25	0
7	ACY	A	816	4/4	0.83	0.13	-	52,52,52,53	0
7	ACY	A	820	4/4	0.86	0.14	-	50,51,52,52	0
7	ACY	A	817	4/4	0.90	0.19	-	39,40,40,41	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.