



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 06:45 pm BST

PDB ID : 1RE5  
Title : Crystal structure of 3-carboxy-cis,cis-muconate lactonizing enzyme from *Pseudomonas putida*  
Authors : Yang, J.; Wang, Y.; Woolridge, E.M.; Petsko, G.A.; Kozarich, J.W.; Ringe, D.  
Deposited on : 2003-11-06  
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

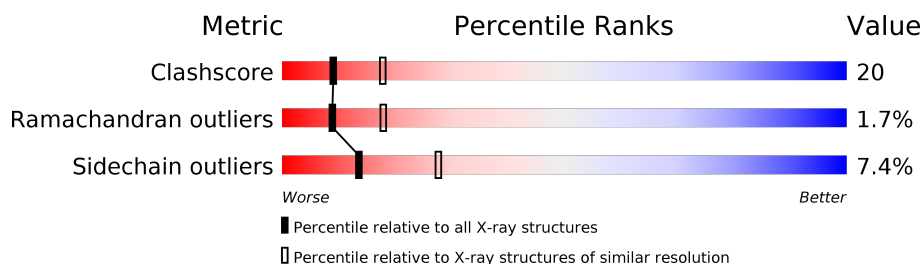
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	450	
1	B	450	
1	C	450	
1	D	450	

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	DTT	A	802	X	X	X	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DTT	B	801	X	X	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13314 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 3-carboxy-cis,cis-muconate cycloisomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	0	0
			3268	2049	595	610	14			
1	B	441	Total	C	N	O	S	0	0	0
			3297	2068	601	613	15			
1	C	440	Total	C	N	O	S	0	0	0
			3289	2062	600	613	14			
1	D	448	Total	C	N	O	S	0	0	0
			3331	2086	608	622	15			

There are 4 discrepancies between the modelled and reference sequences:

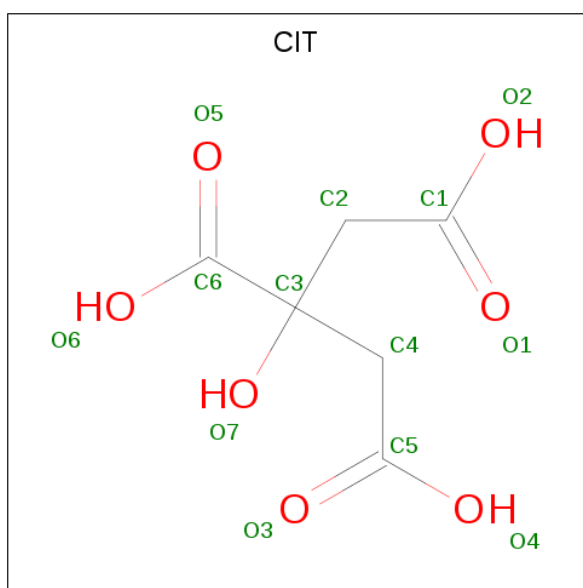
Chain	Residue	Modelled	Actual	Comment	Reference
A	64	THR	VAL	CONFLICT	UNP Q88N37
B	64	THR	VAL	CONFLICT	UNP Q88N37
C	64	THR	VAL	CONFLICT	UNP Q88N37
D	64	THR	VAL	CONFLICT	UNP Q88N37

- Molecule 2 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			8	4	2	2		
2	B	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula:  $C_6H_8O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is water.

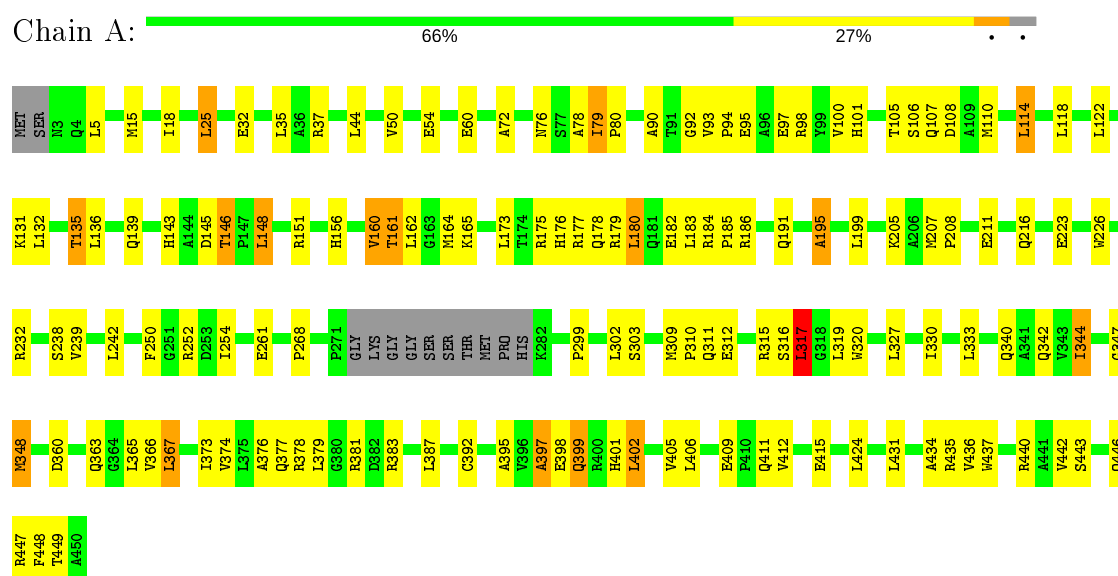
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	25	Total 25	O 25	0	0
4	B	23	Total 23	O 23	0	0
4	C	19	Total 19	O 19	0	0
4	D	33	Total 33	O 33	0	0

### 3 Residue-property plots

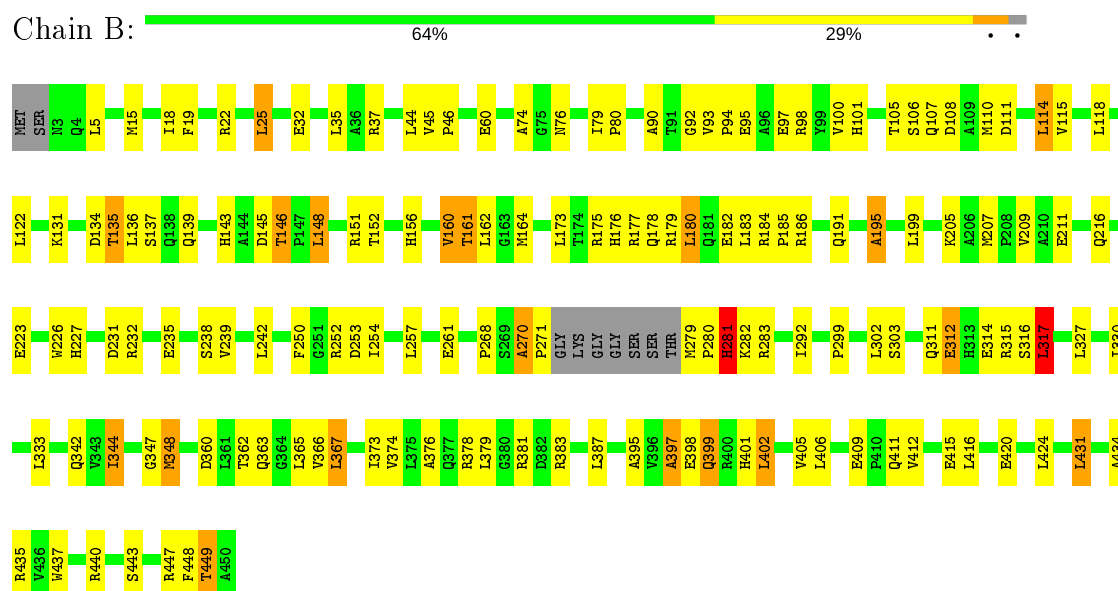
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

Note EDS was not executed.

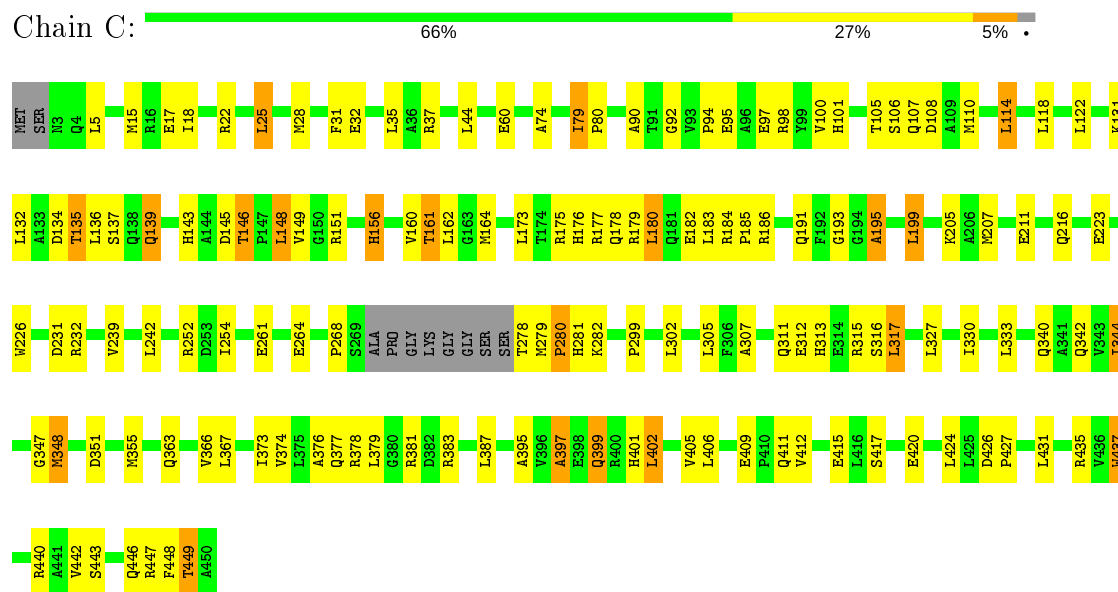
- Molecule 1: 3-carboxy-cis,cis-muconate cycloisomerase



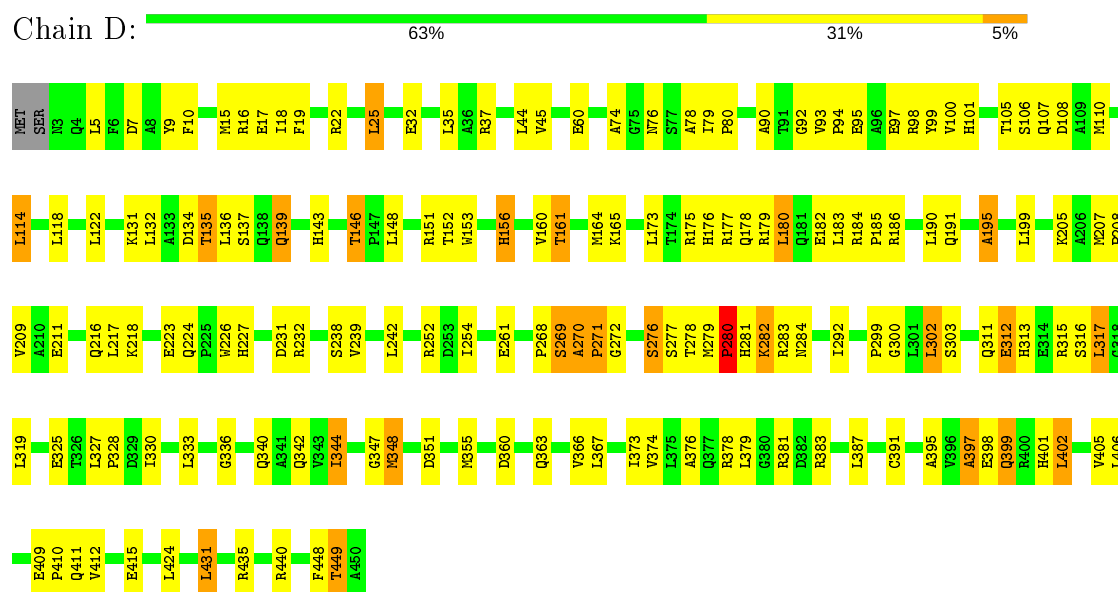
- Molecule 1: 3-carboxy-cis,cis-muconate cycloisomerase



• Molecule 1: 3-carboxy-cis,cis-muconate cycloisomerase



• Molecule 1: 3-carboxy-cis,cis-muconate cycloisomerase





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	231.52Å 231.52Å 78.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.60	Depositor
% Data completeness (in resolution range)	86.4 (20.00-2.60)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.212 , 0.242	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13314	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

## 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: CIT, DTT

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	0.37	0/3321	0.62	2/4512 (0.0%)
1	B	0.38	0/3352	0.63	2/4553 (0.0%)
1	C	0.38	0/3343	0.62	1/4541 (0.0%)
1	D	0.39	0/3387	0.62	1/4601 (0.0%)
All	All	0.38	0/13403	0.62	6/18207 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	148	LEU	CA-CB-CG	6.97	131.33	115.30
1	B	148	LEU	CA-CB-CG	6.85	131.06	115.30
1	C	148	LEU	CA-CB-CG	6.85	131.05	115.30
1	A	148	LEU	CA-CB-CG	6.59	130.45	115.30
1	A	317	LEU	CA-CB-CG	5.59	128.15	115.30

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	3268	0	3277	134	0
1	B	3297	0	3311	150	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3289	0	3299	138	0
1	D	3331	0	3335	169	0
2	A	8	0	9	5	0
2	B	8	0	8	5	0
3	C	13	0	5	4	0
4	A	25	0	0	3	0
4	B	23	0	0	4	0
4	C	19	0	0	2	0
4	D	33	0	0	6	0
All	All	13314	0	13244	531	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 20.

The worst 5 of 531 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:C:279:MET:HA	1:C:282:LYS:HE3	1.32	1.11
1:B:362:THR:HB	1:D:280:PRO:HG3	1.34	1.10
1:C:161:THR:HG22	1:C:164:MET:HB2	1.40	1.04
1:C:135:THR:HG21	1:C:342:GLN:HE22	1.23	1.01
1:B:107:GLN:HE21	1:B:315:ARG:HH11	1.05	1.00

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	434/450 (96%)	411 (95%)	19 (4%)	4 (1%)	17	35
1	B	437/450 (97%)	408 (93%)	21 (5%)	8 (2%)	8	16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	436/450 (97%)	412 (94%)	19 (4%)	5 (1%)	14	30
1	D	446/450 (99%)	411 (92%)	23 (5%)	12 (3%)	5	8
All	All	1753/1800 (97%)	1642 (94%)	82 (5%)	29 (2%)	9	18

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	399	GLN
1	B	281	HIS
1	B	282	LYS
1	B	399	GLN
1	C	280	PRO

### 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	326/343 (95%)	302 (93%)	24 (7%)	13	28
1	B	330/343 (96%)	304 (92%)	26 (8%)	12	24
1	C	329/343 (96%)	306 (93%)	23 (7%)	15	30
1	D	332/343 (97%)	308 (93%)	24 (7%)	14	29
All	All	1317/1372 (96%)	1220 (93%)	97 (7%)	13	28

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	344	ILE
1	C	122	LEU
1	D	333	LEU
1	B	360	ASP
1	B	431	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	284	ASN
1	C	117	GLN
1	D	216	GLN
1	B	342	GLN
1	C	4	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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	DTT	A	802	-	7,7,7	6.37	4 (57%)	4,8,8	5.61	4 (100%)
2	DTT	B	801	-	7,7,7	6.40	4 (57%)	4,8,8	5.30	4 (100%)
3	CIT	C	800	-	3,12,12	2.93	2 (66%)	3,17,17	5.56	2 (66%)

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	CIT	C	800	-	-	3/6/16/16	-
2	DTT	A	802	-	2/2/2/2	5/8/8/8	-
2	DTT	B	801	-	2/2/2/2	6/8/8/8	-

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	DTT	O2-C2	-16.01	1.09	1.43
2	A	802	DTT	O2-C2	-15.72	1.10	1.43
3	C	800	CIT	O7-C3	4.54	1.50	1.43
2	A	802	DTT	C4-S4	-4.04	1.73	1.81
2	B	801	DTT	C4-S4	-3.23	1.74	1.81

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	800	CIT	C3-C2-C1	8.14	128.01	114.98
2	A	802	DTT	C3-C4-S4	-7.96	91.33	114.47
2	B	801	DTT	C3-C4-S4	-7.51	92.62	114.47
2	A	802	DTT	C2-C1-S1	-6.36	95.98	114.47
2	B	801	DTT	C2-C1-S1	-5.95	97.17	114.47

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	802	DTT	C2
2	A	802	DTT	C3
2	B	801	DTT	C2
2	B	801	DTT	C3

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	800	CIT	C1-C2-C3-C6
3	C	800	CIT	O7-C3-C4-C5
2	A	802	DTT	S1-C1-C2-O2
2	A	802	DTT	S1-C1-C2-C3
2	A	802	DTT	C1-C2-C3-C4

There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	802	DTT	5	0
2	B	801	DTT	5	0
3	C	800	CIT	4	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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.