wwPDB X-ray Structure Validation Summary Report (i)

Aug 15, 2023 – 02:05 AM EDT

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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

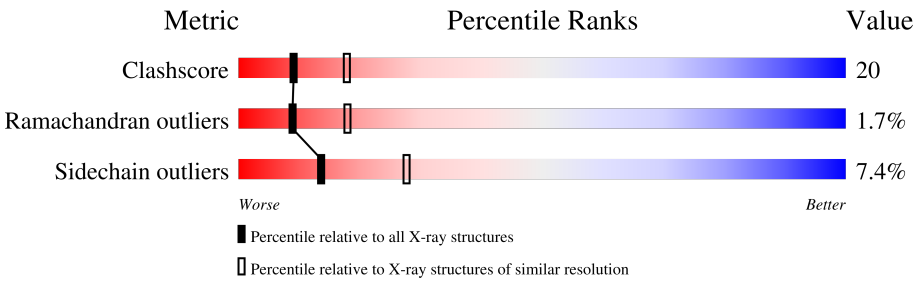
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	450	66% 27% • •
1	B	450	64% 29% • •
1	C	450	66% 27% 5% •
1	D	450	63% 31% 5%

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	-
2	DTT	B	801	X	X	X	-
3	CIT	C	800	-	X	-	-

2 Entry composition (i)

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.

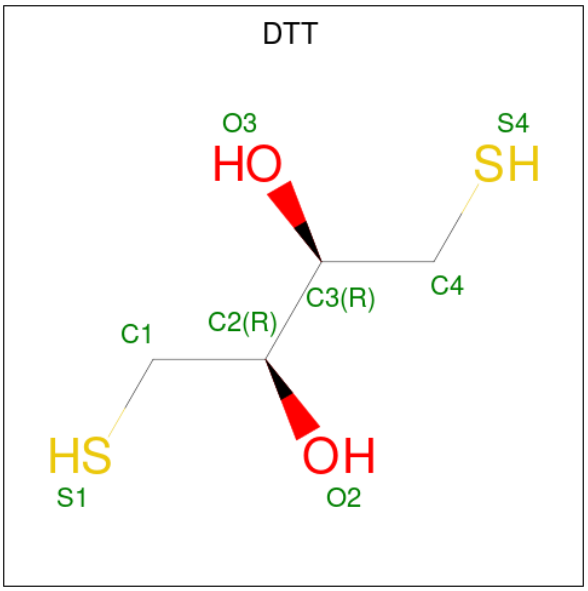
- Molecule 1 is a protein called 3-carboxy-cis,cis-muconate cycloisomerase.

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

There are 4 discrepancies between the modelled and reference sequences:

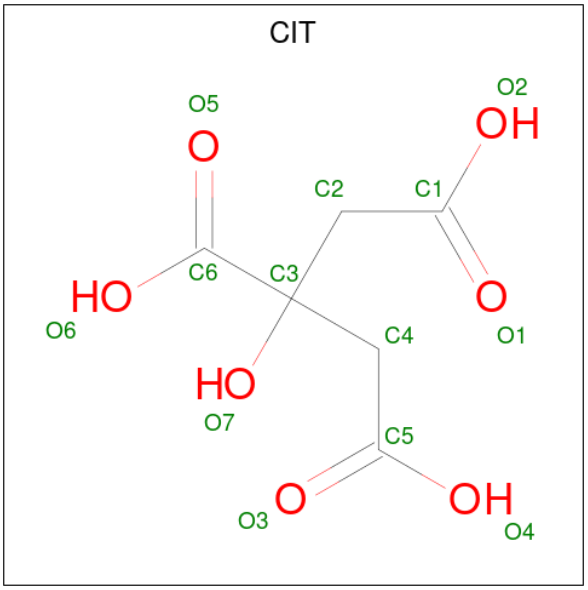
Chain	Residue	Modelled	Actual	Comment	Reference
A	64	THR	VAL	conflict	UNP Q88N37
B	64	THR	VAL	conflict	UNP Q88N37
C	64	THR	VAL	conflict	UNP Q88N37
D	64	THR	VAL	conflict	UNP Q88N37

- Molecule 2 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: $C_4H_{10}O_2S_2$).



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

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



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

- Molecule 4 is water.

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

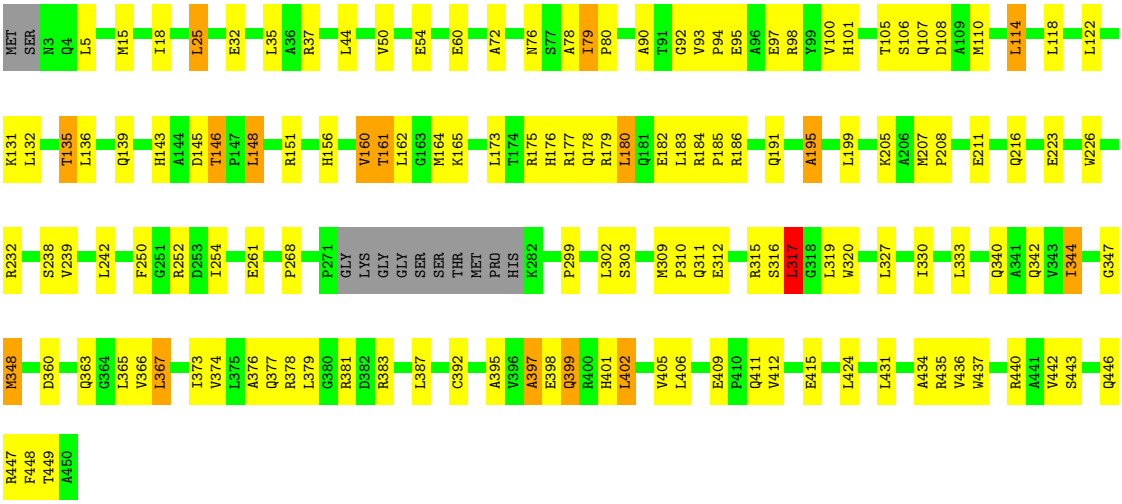
3 Residue-property plots (i)

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

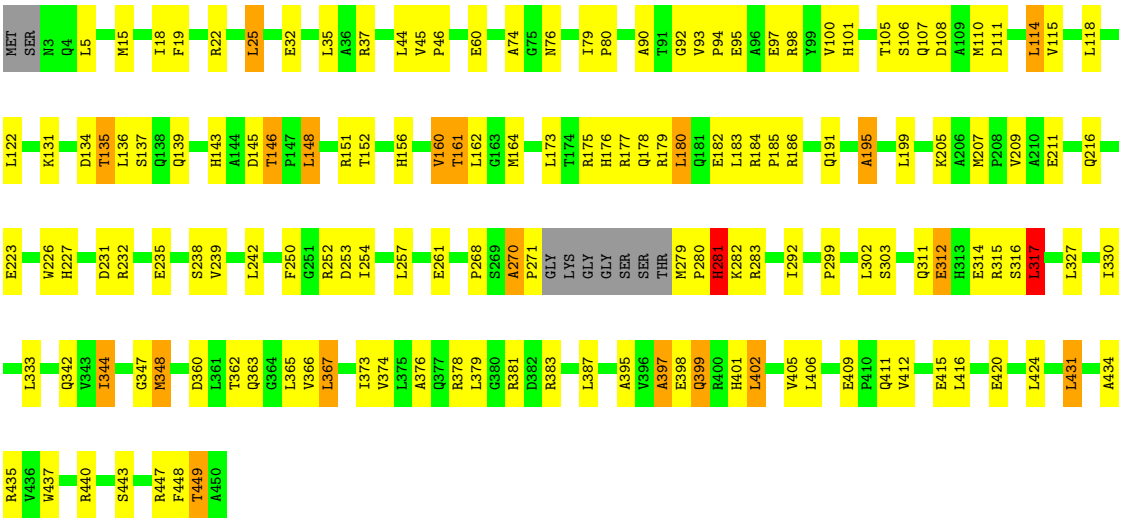
• Molecule 1: 3-carboxy-cis,cis-muconate cycloisomerase

Chain A: 66% 27%



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

Chain B: 64% 29%



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

Chain C: 66% 27% 5% •

MET SER N3 Q4 L5 M15 R16 E17 I18 R22 L25 M28 F31 E32 L35 A36 R37 L44 E60 A74 I79 P80 A90 T91 G92 V93 P94 E95 A96 E97 R98 Y99 V100 H101 T105 S106 Q107 D108 A109 M110 L114 L118 L122 K131

L132 A133 D134 T135 L136 S137 Q138 Q139 H143 A144 D145 T146 P147 L148 V149 G150 R151 H156 V160 T161 L162 G163 M164 L173 T174 R175 H176 R177 Q178 R179 L180 Q181 E182 L183 R184 P185 R186 Q191 F192 G193 G194 A195 L199 K205 A206 M207 E211 Q216 E223

W226 D231 R232 V239 L242 R252 D253 I254 E261 E264 P268 S269 ALA PRO GLY LYS GLY GLY SER SER T278 M279 P280 H281 K282 P299 L302 L305 F306 A307 Q311 E312 H313 E314 R315 S316 L317 L327 I330 L333 Q340 A341 Q342 V343 I344

G347 M348 D351 M355 Q363 V366 L367 I373 V374 L375 A376 Q377 R378 L379 G380 R381 D382 R383 L387 A395 V396 A397 E398 Q399 R400 H401 L402 V405 L406 E409 P410 Q411 V412 E415 L416 S417 E420 L424 L425 D426 P427 L431 R435 V436 W437

R440 A441 V442 S443 Q446 R447 F448 T449 A450

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

Chain D: 63% 31% 5%

MET SER N3 Q4 L5 F6 D7 A8 Y9 F10 M15 R16 E17 I18 F19 R22 L25 E32 L35 A36 R37 L44 V45 E60 A74 G75 N76 S77 A78 I79 P80 A90 T91 G92 V93 P94 E95 A96 E97 R98 Y99 V100 H101 T105 S106 Q107 D108 A109 M110

L114 L118 L122 K131 L132 A133 D134 T135 L136 S137 Q138 Q139 H143 T146 P147 L148 R151 T152 W153 H156 V160 T161 M164 K165 L173 T174 R175 H176 R177 Q178 R179 L180 Q181 E182 L183 R184 P185 R186 L190 Q191 A195 L199 K205 A206 M207 P208

V209 A210 E211 Q216 L217 K218 E223 Q224 P225 W226 H227 D231 R232 S238 V239 L242 R252 D253 I254 E261 P268 S269 A270 P271 G272 S276 S277 T278 M279 P280 H281 K282 R283 N284 I292 P299 G300 L301 L302 S303 Q311 E312 H313 E314 R315 S316 L317 G318

L319 E325 T326 L327 P328 D329 I330 L333 G336 Q340 A341 Q342 V343 I344 G347 M348 D351 M355 D360 Q363 V366 L367 I373 V374 L375 A376 Q377 R378 L379 G380 R381 D382 R383 L387 C391 A395 V396 A397 E398 Q399 R400 H401 L402 V405 L406

E409 P410 Q411 V412 E415 L424 L431 R435 R440 F448 T449 A450

4 Data and refinement statistics (i)

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, α, β, γ	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^2)	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(^{o})	Ideal(^{o})
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

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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

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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 (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	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	C	146	THR
1	C	402	LEU
1	C	161	THR
1	C	327	LEU
1	D	114	LEU

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

Mol	Chain	Res	Type
1	D	156	HIS
1	D	178	GLN
1	D	399	GLN
1	B	156	HIS
1	B	143	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 monosaccharides 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	B	801	-	7,7,7	6.40	4 (57%)	4,8,8	5.30	4 (100%)
2	DTT	A	802	-	7,7,7	6.37	4 (57%)	4,8,8	5.61	4 (100%)
3	CIT	C	800	-	12,12,12	4.68	4 (33%)	17,17,17	8.04	9 (52%)

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	DTT	B	801	-	2/2/2/2	6/8/8/8	-
2	DTT	A	802	-	2/2/2/2	5/8/8/8	-
3	CIT	C	800	-	-	11/16/16/16	-

The worst 5 of 12 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	C3-C6	14.91	1.68	1.53
2	A	802	DTT	C4-S4	-4.04	1.73	1.81
3	C	800	CIT	O7-C3	3.58	1.50	1.43

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	800	CIT	O7-C3-C6	-27.31	70.53	108.86
3	C	800	CIT	C4-C3-C6	-12.38	83.51	110.11
3	C	800	CIT	O7-C3-C4	8.84	130.08	109.40
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

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 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	802	DTT	S1-C1-C2-O2
2	A	802	DTT	S1-C1-C2-C3
2	A	802	DTT	C1-C2-C3-C4
2	B	801	DTT	S1-C1-C2-C3
2	B	801	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	B	801	DTT	5	0
2	A	802	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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.