



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:55 AM GMT

PDB ID : 1F4F
Title : CRYSTAL STRUCTURE OF E. COLI THYMIDYLATE SYNTHASE COM-
PLEXED WITH SP-722
Authors : Erlanson, D.A.; Braisted, A.C.; Raphael, D.R.; Randal, M.; Stroud, R.M.;
Gordon, E.; Wells, J.A.
Deposited on : 2000-06-07
Resolution : 2.00 Å(reported)

This is a full wwPDB validation 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/ValidationPDFNotes.html>

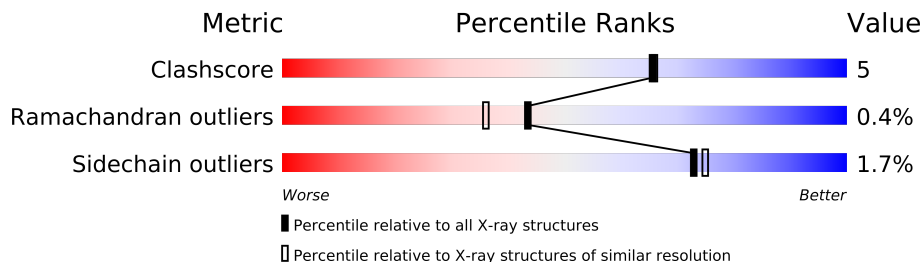
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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))
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	264	
1	B	264	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4842 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

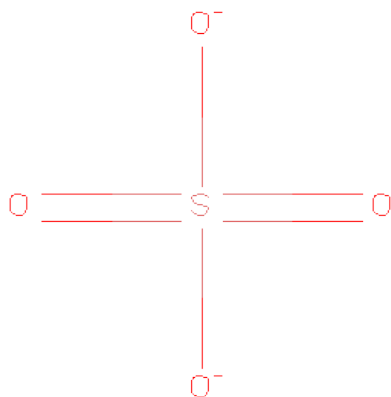
- Molecule 1 is a protein called THYMIDYLATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	1	0
			2143	1368	369	394	12			
1	B	261	Total	C	N	O	S	0	2	0
			2139	1364	369	394	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	CXM	MET	ENGINEERED	UNP P0A884
B	1	CXM	MET	ENGINEERED	UNP P0A884

- Molecule 2 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



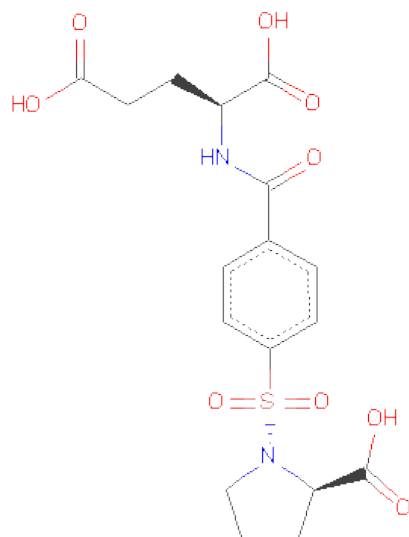
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is 4-[[GLUTAMIC ACID]-CARBONYL]-BENZENE-SULFONYL-D-PROLINE (three-letter code: TP3) (formula: C₁₇H₂₀N₂O₉S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			29	17	2	9	1		
3	B	1	Total	C	N	O	S	0	1
			33	19	2	11	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	266	Total	O	0	0
			266	266		
4	B	207	Total	O	1	0
			207	207		

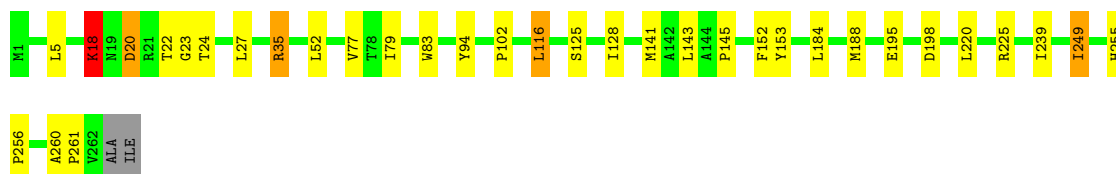
3 Residue-property plots

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

Note EDS was not executed.

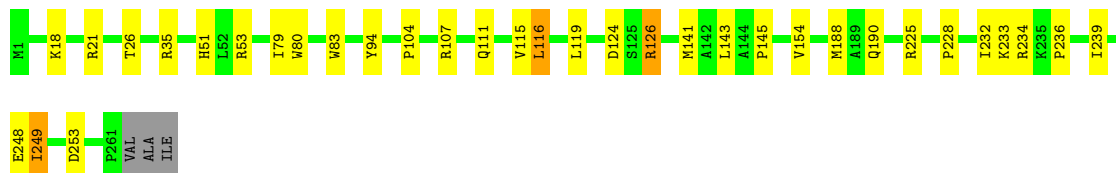
• Molecule 1: THYMIDYLATE SYNTHASE

Chain A: 



• Molecule 1: THYMIDYLATE SYNTHASE

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	126.14Å 126.14Å 66.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.00	Depositor
% Data completeness (in resolution range)	99.4 (10.00-2.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.194 , 0.251	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4842	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: TP3, SO4, CXM

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	0.42	0/2197	1.06	5/2984 (0.2%)
1	B	0.39	0/2198	1.10	8/2985 (0.3%)
All	All	0.41	0/4395	1.08	13/5969 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	35	ARG	NE-CZ-NH1	10.49	125.55	120.30
1	A	225	ARG	CD-NE-CZ	8.85	135.99	123.60
1	B	126	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	B	35	ARG	NE-CZ-NH2	-8.47	116.06	120.30
1	A	18	LYS	CA-CB-CG	6.93	128.65	113.40
1	B	35	ARG	CD-NE-CZ	6.68	132.95	123.60
1	A	225	ARG	CG-CD-NE	6.21	124.83	111.80
1	B	107	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	B	107	ARG	CD-NE-CZ	5.67	131.54	123.60
1	A	35	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	195	GLU	OE1-CD-OE2	-5.15	117.12	123.30
1	B	26	THR	N-CA-CB	5.13	120.05	110.30
1	B	53	ARG	NE-CZ-NH1	-5.10	117.75	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2143	0	2066	28	0
1	B	2139	0	2059	25	0
2	A	15	0	0	0	0
2	B	10	0	0	0	0
3	A	29	0	17	1	0
3	B	33	0	8	1	0
4	A	266	0	0	3	0
4	B	207	0	0	2	0
All	All	4842	0	4150	44	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (44) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:20:ASP:HB2	1:B:126:ARG:HH12	1.41	0.83
1:A:83:TRP:CZ3	1:A:143:LEU:HD21	2.33	0.63
1:A:52:LEU:HD22	1:A:249:ILE:HG13	1.82	0.61
1:A:79:ILE:HG22	3:A:701:TP3:H222	1.83	0.58
1:B:79:ILE:HG22	3:B:702[B]:TP3:H222	1.86	0.57
1:B:141:MET:SD	1:B:145:PRO:HD3	2.48	0.54
1:A:116:LEU:HD22	1:A:188:MET:CE	2.38	0.53
1:A:20:ASP:HB2	1:B:126:ARG:NH1	2.18	0.53
1:A:125:SER:HB2	1:B:21:ARG:HH21	1.74	0.53
1:B:83:TRP:CE2	1:B:143:LEU:HD11	2.44	0.53
1:A:141:MET:SD	1:A:145:PRO:HD3	2.50	0.51
1:B:228:PRO:HB2	1:B:249:ILE:HD12	1.93	0.51
1:A:35:ARG:HD3	1:A:198:ASP:OD2	2.10	0.51
1:B:234:ARG:O	1:B:236:PRO:HD3	2.11	0.51
1:A:18:LYS:HE3	1:B:154:VAL:O	2.11	0.50
1:A:116:LEU:HD23	1:A:239:ILE:HG21	1.94	0.49
4:A:1015:HOH:O	1:B:104:PRO:HG2	2.12	0.49
1:A:83:TRP:CE2	1:A:143:LEU:HD11	2.49	0.47
1:B:233:LYS:HD2	1:B:248:GLU:HG2	1.97	0.47
1:B:190:GLN:HE22	1:B:232:ILE:HG21	1.79	0.47
1:A:52:LEU:HD22	1:A:249:ILE:CG1	2.44	0.47
1:A:5:LEU:HD22	1:A:220:LEU:HD23	1.97	0.47
1:A:116:LEU:HD22	1:A:188:MET:HE1	1.97	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:116:LEU:HD22	4:B:859:HOH:O	2.16	0.45
1:B:225:ARG:HD3	1:B:253:ASP:O	2.17	0.45
1:A:255:HIS:HB3	1:A:256:PRO:CD	2.46	0.45
1:A:77:VAL:HA	4:A:885:HOH:O	2.16	0.45
1:A:125:SER:CB	1:B:21:ARG:HH21	2.30	0.45
1:A:20:ASP:CB	1:B:126:ARG:HH12	2.20	0.45
1:B:233:LYS:HD2	1:B:248:GLU:CG	2.47	0.45
1:A:23:GLY:O	1:A:24:THR:C	2.56	0.44
1:A:153:TYR:CE2	1:B:18:LYS:HE3	2.53	0.44
1:A:116:LEU:HD22	1:A:188:MET:HE3	2.01	0.43
1:B:119:LEU:HD12	1:B:188:MET:HE2	2.00	0.43
1:B:51:HIS:HB3	4:B:994:HOH:O	2.18	0.42
1:A:18:LYS:HE2	1:B:124:ASP:OD1	2.19	0.42
1:A:153:TYR:CZ	1:B:18:LYS:HE3	2.55	0.41
1:A:184:LEU:O	1:A:188:MET:HG3	2.21	0.41
1:A:260:ALA:HB1	1:A:261:PRO:HD2	2.01	0.41
1:A:102:PRO:HG2	4:A:1008:HOH:O	2.20	0.41
1:B:111:GLN:O	1:B:115:VAL:HG23	2.20	0.41
1:B:116:LEU:HD13	1:B:239:ILE:HG21	2.03	0.41
1:A:128:ILE:CG2	1:A:152:PHE:HB2	2.51	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	261/264 (99%)	252 (97%)	8 (3%)	1 (0%)	43	36
1	B	261/264 (99%)	255 (98%)	5 (2%)	1 (0%)	43	36
All	All	522/528 (99%)	507 (97%)	13 (2%)	2 (0%)	43	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	TYR
1	B	94	TYR

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	232/232 (100%)	226 (97%)	6 (3%)	59	58
1	B	232/232 (100%)	230 (99%)	2 (1%)	87	90
All	All	464/464 (100%)	456 (98%)	8 (2%)	73	75

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	20	ASP
1	A	22	THR
1	A	27	LEU
1	A	116	LEU
1	A	249	ILE
1	B	116	LEU
1	B	249	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	190	GLN
1	A	219	GLN
1	B	87	ASN
1	B	190	GLN
1	B	219	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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$
1	CXM	A	1	1	10,10,11	7.66	5 (50%)	8,11,13	11.20	4 (50%)
1	CXM	B	1	1	10,10,11	7.75	5 (50%)	8,11,13	14.18	4 (50%)

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
1	CXM	A	1	1	-	0/8/10/12	0/0/0/0
1	CXM	B	1	1	-	0/8/10/12	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	CXM	O-C	23.46	1.27	1.11
1	A	1	CXM	O-C	22.78	1.27	1.11
1	A	1	CXM	CA-N	-5.33	1.39	1.46
1	A	1	CXM	CN-N	4.26	1.37	1.33
1	B	1	CXM	CA-N	-3.95	1.41	1.46
1	A	1	CXM	CA-C	3.68	1.55	1.48
1	B	1	CXM	CA-C	3.63	1.55	1.48
1	B	1	CXM	CN-N	3.52	1.37	1.33
1	B	1	CXM	ON1-CN	2.87	1.27	1.21
1	A	1	CXM	ON1-CN	2.22	1.25	1.21

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1	CXM	ON2-CN-ON1	-38.36	74.29	122.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	CXM	ON2-CN-ON1	-27.42	87.95	122.17
1	A	1	CXM	ON2-CN-N	-10.97	102.68	116.33
1	A	1	CXM	CA-N-CN	-10.04	106.33	121.67
1	B	1	CXM	ON2-CN-N	-7.77	106.66	116.33
1	B	1	CXM	CA-N-CN	-7.05	110.90	121.67
1	A	1	CXM	CB-CA-N	5.06	117.47	110.48
1	B	1	CXM	CB-CA-N	4.93	117.30	110.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 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	$\# Z > 2$
3	TP3	A	701	-	30,30,30	3.27	3 (10%)	43,43,43	2.11	13 (30%)
2	SO4	A	801	-	4,4,4	0.77	0	6,6,6	0.29	0
2	SO4	A	811	-	4,4,4	0.98	0	6,6,6	0.17	0
2	SO4	A	812	-	4,4,4	0.93	0	6,6,6	0.17	0
3	TP3	B	702[A]	-	2,3,30	1.56	0	1,3,43	0.60	0
3	TP3	B	702[B]	-	2,3,30	1.61	0	1,3,43	0.09	0
2	SO4	B	802	-	4,4,4	0.89	0	6,6,6	0.40	0
2	SO4	B	814	-	4,4,4	0.92	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
3	TP3	A	701	-	-	0/33/43/43	0/2/2/2
2	SO4	A	801	-	-	0/0/0/0	0/0/0/0
2	SO4	A	811	-	-	0/0/0/0	0/0/0/0
2	SO4	A	812	-	-	0/0/0/0	0/0/0/0
3	TP3	B	702[A]	-	-	0/0/0/43	0/0/0/2
3	TP3	B	702[B]	-	-	0/0/0/43	0/0/0/2
2	SO4	B	802	-	-	0/0/0/0	0/0/0/0
2	SO4	B	814	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	TP3	O12-S9	12.64	1.59	1.43
3	A	701	TP3	O11-S9	10.16	1.56	1.43
3	A	701	TP3	S9-N3	6.02	1.72	1.63

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	TP3	C6-C4-N3	6.69	123.13	111.65
3	A	701	TP3	C25-C20-N19	-4.20	99.72	110.53
3	A	701	TP3	O12-S9-O11	-4.08	112.10	119.38
3	A	701	TP3	C21-C20-N19	3.57	117.63	110.83
3	A	701	TP3	C4-N3-S9	3.07	124.65	119.67
3	A	701	TP3	C17-C10-C13	2.90	124.99	120.39
3	A	701	TP3	O11-S9-N3	2.87	113.45	106.96
3	A	701	TP3	O24-C18-N19	-2.59	117.76	122.44
3	A	701	TP3	O8-C6-O7	-2.29	118.89	124.07
3	A	701	TP3	C17-C10-S9	-2.20	117.35	119.80
3	A	701	TP3	C16-C17-C10	-2.19	117.00	119.50
3	A	701	TP3	C2-N3-C4	2.11	114.18	111.41
3	A	701	TP3	C1-C2-N3	-2.03	99.06	103.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.