wwPDB X-ray Structure Validation Summary Report (i)

Oct 25, 2023 – 08:44 PM EDT

PDB ID	:	3G7K
Title	:	Crystal Structure of Methylitaconate-delta-isomerase
Authors	:	Messerschmidt, A.; Macieira, S.; Velarde, M.
Deposited on	:	2009-02-10
Resolution	:	2.70 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 (1)) were used in the production of this report:

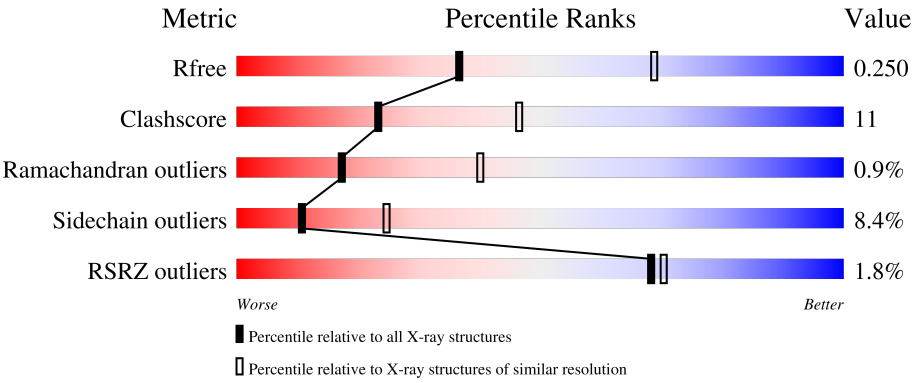
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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% 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	391	80% 13%
1	B	391	76% 20%
1	C	391	4% 41% 13% 43%
1	D	391	75% 19%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10592 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-methylitaconate isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	0	0
			2807	1757	474	558	18			
1	B	387	Total	C	N	O	S	0	0	0
			2868	1795	486	569	18			
1	C	224	Total	C	N	O	S	0	0	0
			1645	1033	284	319	9			
1	D	379	Total	C	N	O	S	0	0	0
			2807	1757	474	558	18			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	381	GLY	-	expression tag	UNP Q0QLE6
A	382	SER	-	expression tag	UNP Q0QLE6
A	383	ALA	-	expression tag	UNP Q0QLE6
A	384	TRP	-	expression tag	UNP Q0QLE6
A	385	SER	-	expression tag	UNP Q0QLE6
A	386	HIS	-	expression tag	UNP Q0QLE6
A	387	PRO	-	expression tag	UNP Q0QLE6
A	388	GLN	-	expression tag	UNP Q0QLE6
A	389	PHE	-	expression tag	UNP Q0QLE6
A	390	GLU	-	expression tag	UNP Q0QLE6
A	391	LYS	-	expression tag	UNP Q0QLE6
B	381	GLY	-	expression tag	UNP Q0QLE6
B	382	SER	-	expression tag	UNP Q0QLE6
B	383	ALA	-	expression tag	UNP Q0QLE6
B	384	TRP	-	expression tag	UNP Q0QLE6
B	385	SER	-	expression tag	UNP Q0QLE6
B	386	HIS	-	expression tag	UNP Q0QLE6
B	387	PRO	-	expression tag	UNP Q0QLE6
B	388	GLN	-	expression tag	UNP Q0QLE6
B	389	PHE	-	expression tag	UNP Q0QLE6
B	390	GLU	-	expression tag	UNP Q0QLE6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	391	LYS	-	expression tag	UNP Q0QLE6
C	381	GLY	-	expression tag	UNP Q0QLE6
C	382	SER	-	expression tag	UNP Q0QLE6
C	383	ALA	-	expression tag	UNP Q0QLE6
C	384	TRP	-	expression tag	UNP Q0QLE6
C	385	SER	-	expression tag	UNP Q0QLE6
C	386	HIS	-	expression tag	UNP Q0QLE6
C	387	PRO	-	expression tag	UNP Q0QLE6
C	388	GLN	-	expression tag	UNP Q0QLE6
C	389	PHE	-	expression tag	UNP Q0QLE6
C	390	GLU	-	expression tag	UNP Q0QLE6
C	391	LYS	-	expression tag	UNP Q0QLE6
D	381	GLY	-	expression tag	UNP Q0QLE6
D	382	SER	-	expression tag	UNP Q0QLE6
D	383	ALA	-	expression tag	UNP Q0QLE6
D	384	TRP	-	expression tag	UNP Q0QLE6
D	385	SER	-	expression tag	UNP Q0QLE6
D	386	HIS	-	expression tag	UNP Q0QLE6
D	387	PRO	-	expression tag	UNP Q0QLE6
D	388	GLN	-	expression tag	UNP Q0QLE6
D	389	PHE	-	expression tag	UNP Q0QLE6
D	390	GLU	-	expression tag	UNP Q0QLE6
D	391	LYS	-	expression tag	UNP Q0QLE6

- Molecule 2 is water.

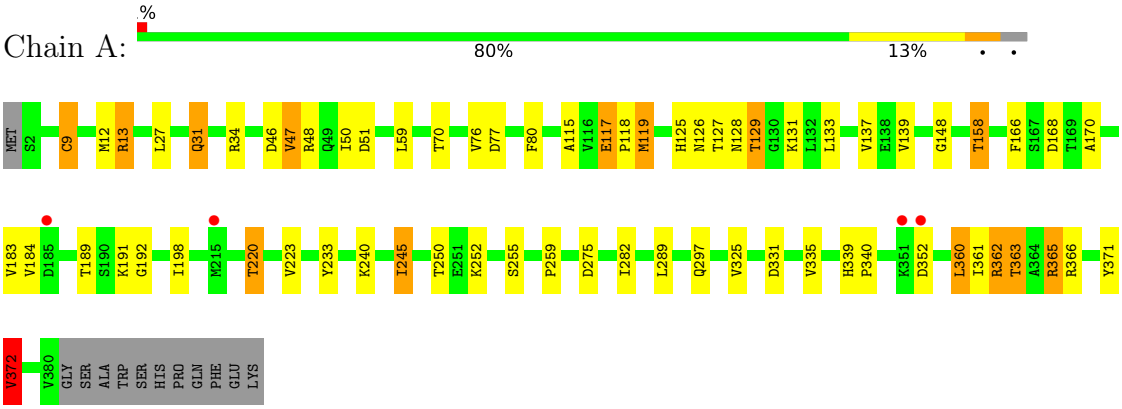
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	129	Total O 129 129	0	0
2	B	107	Total O 107 107	0	0
2	C	77	Total O 77 77	0	0
2	D	152	Total O 152 152	0	0

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 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.

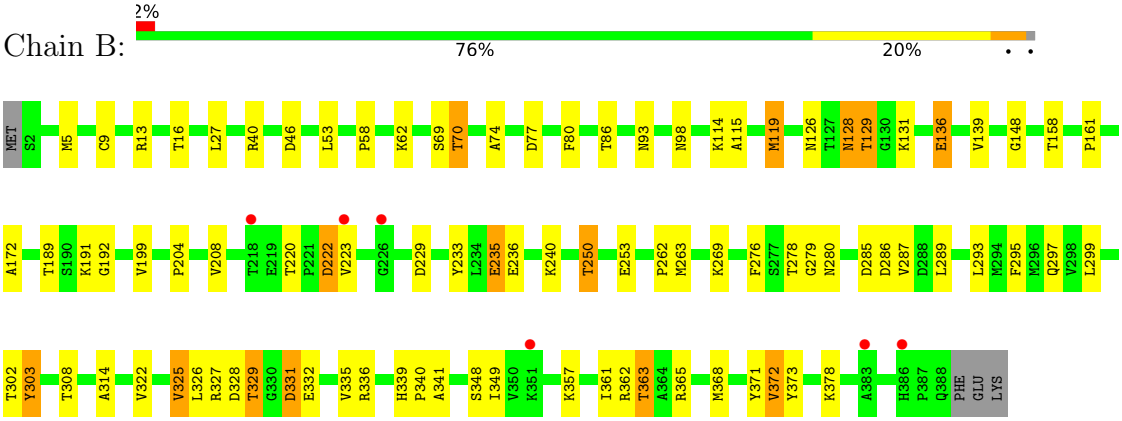
• Molecule 1: 3-methylitaconate isomerase

Chain A:



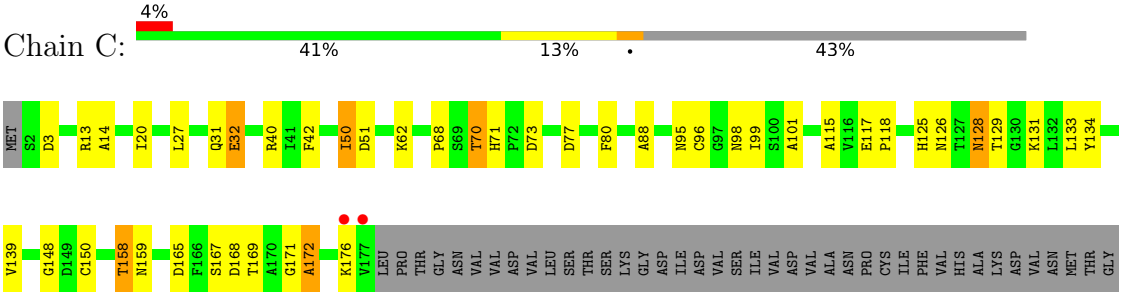
• Molecule 1: 3-methylitaconate isomerase

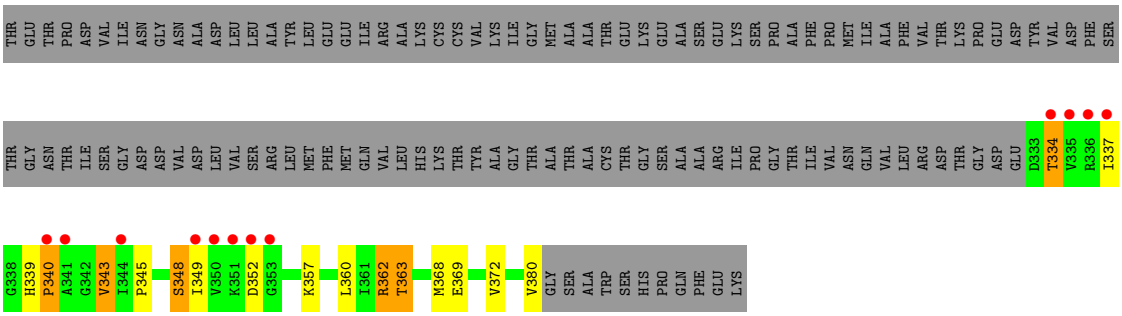
Chain B:



• Molecule 1: 3-methylitaconate isomerase

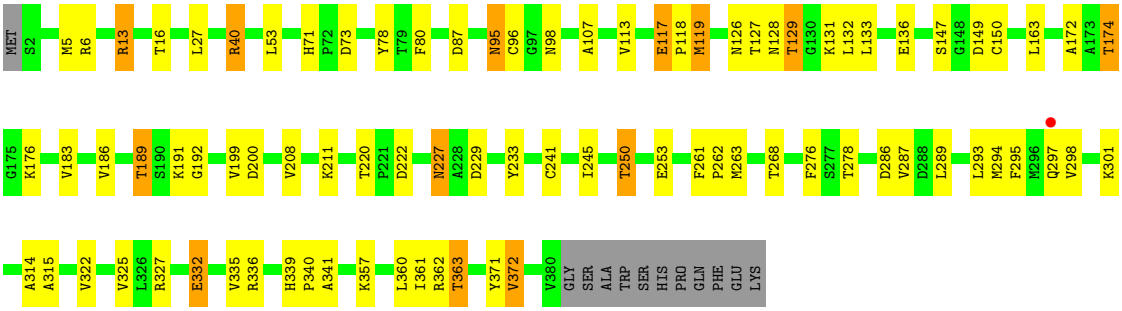
Chain C:





• Molecule 1: 3-methylitaconate isomerase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	53.08Å 142.08Å 228.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 49.72 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.8 (50.00-2.70) 97.7 (49.72-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.65 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.200 , 0.256 0.199 , 0.250	Depositor DCC
R_{free} test set	2402 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	50.3	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 53.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10592	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.63	1/2849 (0.0%)	0.74	3/3871 (0.1%)
1	B	0.58	0/2914	0.70	1/3961 (0.0%)
1	C	0.60	0/1669	0.70	0/2265
1	D	0.65	1/2849 (0.0%)	0.73	2/3871 (0.1%)
All	All	0.62	2/10281 (0.0%)	0.72	6/13968 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	332	GLU	CG-CD	6.73	1.62	1.51
1	A	9	CYS	CB-SG	-6.25	1.71	1.82

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	13	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	B	365	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	D	13	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	A	372	VAL	CB-CA-C	-5.33	101.28	111.40
1	A	117	GLU	C-N-CD	-5.27	109.00	120.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	GLU	Peptide
1	C	117	GLU	Peptide
1	D	117	GLU	Peptide

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	2807	0	2819	53	0
1	B	2868	0	2869	77	0
1	C	1645	0	1652	44	0
1	D	2807	0	2819	66	0
2	A	129	0	0	5	0
2	B	107	0	0	5	0
2	C	77	0	0	5	0
2	D	152	0	0	8	0
All	All	10592	0	10159	229	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 11.

The worst 5 of 229 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:D:13:ARG:NH2	1:D:363:THR:HG22	1.45	1.31
1:D:297:GLN:HG3	2:D:434:HOH:O	1.34	1.28
1:A:13:ARG:NH2	1:A:363:THR:HG22	1.51	1.25
1:B:13:ARG:NH2	1:B:363:THR:HG22	1.53	1.21
1:D:13:ARG:HH22	1:D:363:THR:CG2	1.56	1.18

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	377/391 (96%)	361 (96%)	14 (4%)	2 (0%)	29 54
1	B	385/391 (98%)	360 (94%)	22 (6%)	3 (1%)	19 43
1	C	220/391 (56%)	200 (91%)	15 (7%)	5 (2%)	6 16
1	D	377/391 (96%)	356 (94%)	19 (5%)	2 (0%)	29 54
All	All	1359/1564 (87%)	1277 (94%)	70 (5%)	12 (1%)	17 40

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	PRO
1	B	93	ASN
1	B	279	GLY
1	C	118	PRO
1	C	172	ALA

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	308/319 (97%)	285 (92%)	23 (8%)	13 31
1	B	314/319 (98%)	291 (93%)	23 (7%)	14 33
1	C	175/319 (55%)	157 (90%)	18 (10%)	7 16
1	D	308/319 (97%)	279 (91%)	29 (9%)	8 20
All	All	1105/1276 (87%)	1012 (92%)	93 (8%)	11 25

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	343	VAL
1	D	129	THR
1	C	360	LEU
1	D	40	ARG
1	D	183	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	95	ASN
1	D	128	ASN
1	D	280	ASN
1	D	227	ASN
1	B	126	ASN

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)

There are no ligands in this entry.

5.7 Other polymers (i)

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

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^{th} 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^2)	Q<0.9
1	A	379/391 (96%)	-0.11	4 (1%)	80	82	26, 43, 59, 68	0
1	B	387/391 (98%)	0.06	6 (1%)	72	74	28, 48, 71, 84	0
1	C	224/391 (57%)	0.17	14 (6%)	20	19	32, 51, 100, 108	0
1	D	379/391 (96%)	-0.21	1 (0%)	94	95	24, 39, 55, 61	0
All	All	1369/1564 (87%)	-0.04	25 (1%)	68	70	24, 44, 69, 108	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	341	ALA	5.3
1	C	337	ILE	5.2
1	C	344	ILE	5.1
1	C	340	PRO	4.9
1	C	352	ASP	4.4

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.