



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 04:44 PM UTC

PDB ID : 2R3V / pdb_00002r3v
Title : The Biochemical and Structural Basis for Feedback Inhibition of Mevalonate Kinase and Isoprenoid Metabolism
Authors : Fu, Z.; Voynova, N.E.; Mizioro, H.M.; Kim, J.P.
Deposited on : 2007-08-30
Resolution : 2.50 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

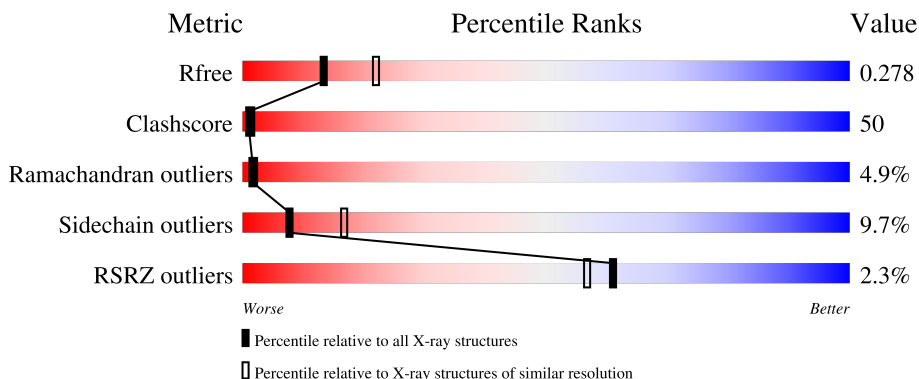
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 $\leq 5\%$. 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	396	2% 37% 52% 9% ..
1	B	396	% 36% 48% 13% ..
1	C	396	4% 35% 52% 11% .
1	D	396	2% 35% 55% 7% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11935 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 Mevalonate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			2933	1849	519	552	13			
1	B	388	Total	C	N	O	S	0	0	0
			2918	1838	517	550	13			
1	C	390	Total	C	N	O	S	0	0	0
			2933	1849	519	552	13			
1	D	389	Total	C	N	O	S	0	0	0
			2926	1844	518	551	13			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	72	Total	O	0	0
			72	72		
2	B	63	Total	O	0	0
			63	63		
2	C	45	Total	O	0	0
			45	45		
2	D	45	Total	O	0	0
			45	45		

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.

Chain A:

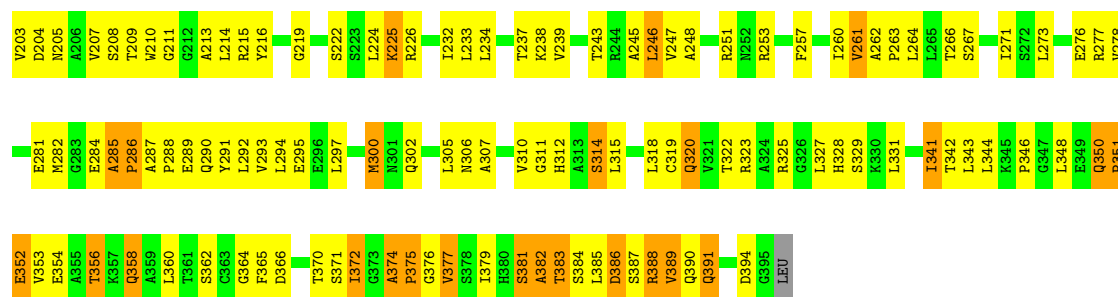
Amino Acid	Percentage
Met	2%
L2	37%
A65	37%
S3	37%
L67	37%
L6	37%
L7	37%
V8	37%
S9	37%
D71	37%
T72	37%
S73	37%
K13	37%
V14	37%
F74	37%
I15	37%
L16	37%
H17	37%
G18	37%
E19	37%
A80	37%
H20	37%
A21	37%
T22	37%
V23	37%
H24	37%
S25	37%
K26	37%
V27	37%
K28	37%
A28	37%
L29	37%
A30	37%
L91	37%
V31	37%
S32	37%
L33	37%
V34	37%
A95	37%
L35	37%
R36	37%
T37	37%
F38	37%
L39	37%
R40	37%
L41	37%
T104	37%
E105	37%
R106	37%
H44	37%
S45	37%
M46	37%
G47	37%
K48	37%
V49	37%
S118	37%
V119	37%
D50	37%
L51	37%
S52	37%
K122	37%
L123	37%
P54	37%
R124	37%
N55	37%
A126	37%
I56	37%
G57	37%
I58	37%
K59	37%
R60	37%
L129	37%
A61	37%
D130	37%
I131	37%
V62	37%
D63	37%
V133	37%
M134	37%
S135	37%
E136	37%
L137	37%
L143	37%
S146	37%
A147	37%
A148	37%
I149	37%
S156	37%
V151	37%
C152	37%
L153	37%
A154	37%
L158	37%
T159	37%
V160	37%
C161	37%
E162	37%
E163	37%
I164	37%
P165	37%
N166	37%
P167	37%
L168	37%
K169	37%
D170	37%
G171	37%
C172	37%
G173	37%
V174	37%
N175	37%
R176	37%
T177	37%
I178	37%
E180	37%
R181	37%
L182	37%
E183	37%
L184	37%
I185	37%
N186	37%
K187	37%
L188	37%
A189	37%
F190	37%
Q191	37%
G192	37%
E193	37%
R194	37%
M195	37%
L196	37%
H197	37%
D130	37%
I131	37%
V62	37%
D63	37%
V133	37%
M134	37%
S135	37%
E136	37%
L137	37%
L143	37%
S146	37%
A147	37%
A148	37%
I149	37%
S156	37%
V151	37%
C152	37%
L153	37%
A154	37%
L158	37%
T159	37%
V160	37%
C161	37%
E162	37%
E163	37%
I164	37%
P165	37%
N166	37%
P167	37%
L168	37%
K169	37%
D170	37%
G171	37%
C172	37%
G173	37%
V174	37%
N175	37%
R176	37%
T177	37%
I178	37%
E180	37%
R181	37%
L182	37%
E183	37%
L184	37%
I185	37%
N186	37%
K187	37%
L188	37%
A189	37%
F190	37%
Q191	37%
G192	37%
E193	37%
R194	37%
M195	37%
L196	37%
H197	37%
D130	37%
I131	37%
V62	37%
D63	37%
V133	37%
M134	37%
S135	37%
E136	37%
L137	37%
L143	37%
S146	37%

Chain B:

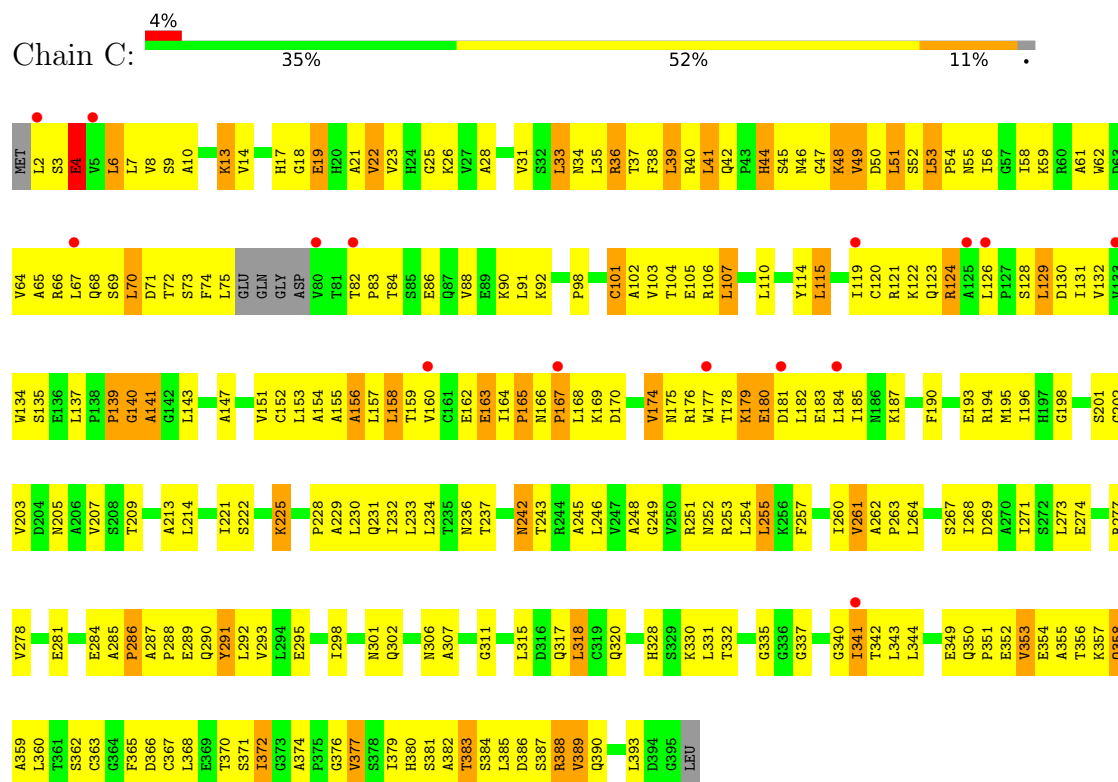
36% 48% 13%

0% 100%

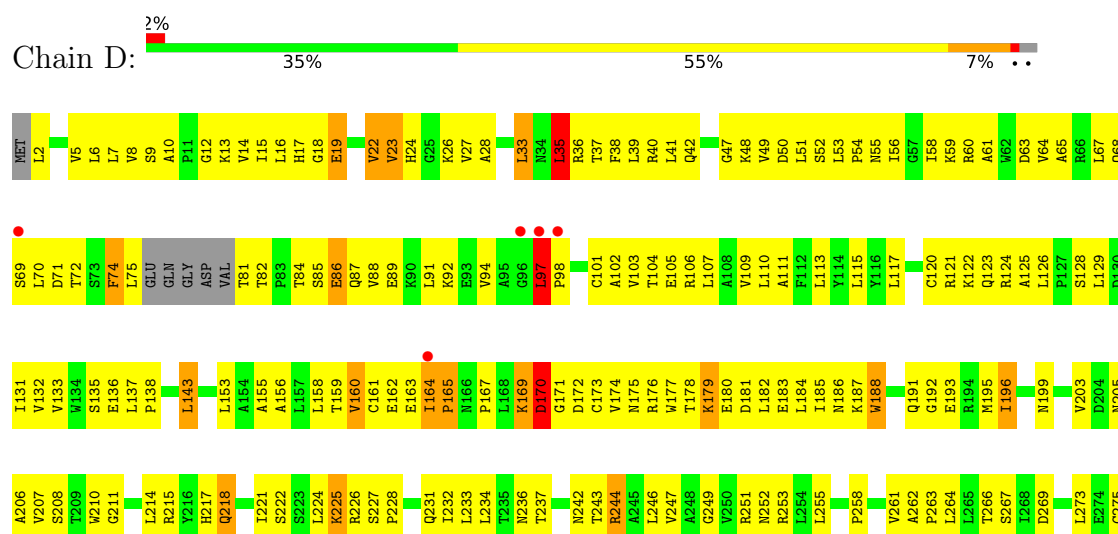
MET L2 L3 E4 V5 L6 L7 V8 S9 A10 P11 G12 K13 L16 H17 G18 E19 V22 A28 S32 L33 K34 L35 R36 T37 F38 L39 R40 L41 Q42 P43 H44 S45 N46 G47 K48 V49 D50 L51 S52 L53 P54 N55 L56 G57 R60 D63 V64 A65 R66 L67 Q68 S69 R70

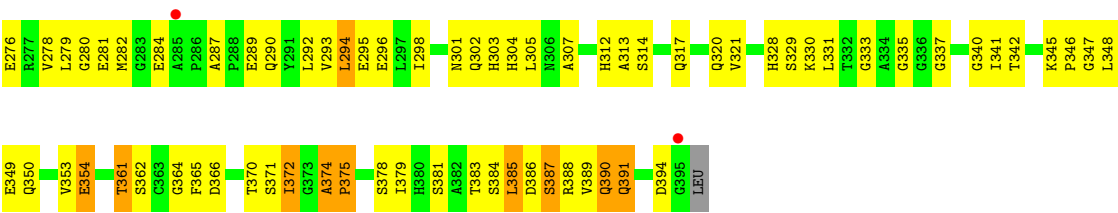


• Molecule 1: Mevalonate kinase



• Molecule 1: Mevalonate kinase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.03Å 78.20Å 109.45Å 90.00° 113.33° 90.00°	Depositor
Resolution (Å)	29.37 – 2.50 29.37 – 2.50	Depositor EDS
% Data completeness (in resolution range)	84.1 (29.37-2.50) 84.1 (29.37-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.239 , 0.282 0.236 , 0.278	Depositor DCC
R_{free} test set	3916 reflections (8.45%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.733	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11935	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.75 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6120e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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](#)

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	0.51	0/2983	1.05	15/4055 (0.4%)
1	B	0.50	0/2968	1.01	16/4034 (0.4%)
1	C	0.44	0/2983	0.97	13/4055 (0.3%)
1	D	0.45	0/2976	0.99	11/4045 (0.3%)
All	All	0.48	0/11910	1.00	55/16189 (0.3%)

There are no bond length outliers.

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	387	SER	N-CA-C	-10.19	101.52	112.93
1	D	97	LEU	N-CA-C	9.72	123.14	110.40
1	D	35	LEU	N-CA-C	-9.41	95.75	109.11
1	A	35	LEU	N-CA-C	-8.08	97.63	109.11
1	A	148	ALA	N-CA-C	-8.03	102.61	111.36

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	2933	0	3003	294	0
1	B	2918	0	2983	292	0
1	C	2933	0	3003	315	0
1	D	2926	0	2994	289	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	72	0	0	7	0
2	B	63	0	0	5	0
2	C	45	0	0	4	0
2	D	45	0	0	5	0
All	All	11935	0	11983	1173	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 50.

The worst 5 of 1173 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:119:ILE:HD11	1:C:158:LEU:HD13	1.27	1.08
1:C:50:ASP:HB2	1:C:130:ASP:HA	1.33	1.06
1:C:52:SER:HB3	1:C:132:VAL:HG22	1.35	1.06
1:B:232:ILE:HG12	1:B:372:ILE:HD13	1.36	1.04
1:A:52:SER:HB3	1:A:132:VAL:HG22	1.40	1.03

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	386/396 (98%)	327 (85%)	44 (11%)	15 (4%)	2	3
1	B	384/396 (97%)	304 (79%)	58 (15%)	22 (6%)	1	1
1	C	386/396 (98%)	292 (76%)	73 (19%)	21 (5%)	1	1
1	D	385/396 (97%)	310 (80%)	58 (15%)	17 (4%)	2	2
All	All	1541/1584 (97%)	1233 (80%)	233 (15%)	75 (5%)	1	2

5 of 75 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	95	ALA
1	A	99	ASP
1	A	169	LYS
1	A	284	GLU

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	321/326 (98%)	284 (88%)	37 (12%)	5	11
1	B	319/326 (98%)	281 (88%)	38 (12%)	5	11
1	C	321/326 (98%)	294 (92%)	27 (8%)	10	22
1	D	320/326 (98%)	298 (93%)	22 (7%)	14	30
All	All	1281/1304 (98%)	1157 (90%)	124 (10%)	8	17

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	178	THR
1	D	160	VAL
1	B	372	ILE
1	D	159	THR
1	D	320	GLN

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	217	HIS
1	D	231	GLN
1	D	350	GLN
1	B	302	GLN
1	B	301	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 oligosaccharides 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 [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, 95th 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	390/396 (98%)	-0.07	9 (2%) 61 57	10, 37, 71, 90	0
1	B	388/396 (97%)	0.05	5 (1%) 75 71	9, 41, 74, 94	0
1	C	390/396 (98%)	0.48	15 (3%) 44 39	27, 56, 76, 86	0
1	D	389/396 (98%)	0.40	7 (1%) 67 64	27, 53, 77, 82	0
All	All	1557/1584 (98%)	0.21	36 (2%) 61 57	9, 49, 75, 94	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	81	THR	3.9
1	A	395	GLY	3.8
1	C	2	LEU	3.6
1	A	82	THR	3.4
1	B	74	PHE	3.4

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.