



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 02:07 pm BST

PDB ID : 3EXA
Title : Crystal structure of the full-length tRNA isopentenylpyrophosphate transferase (BH2366) from *Bacillus halodurans*, Northeast Structural Genomics Consortium target BhR41.
Authors : Forouhar, F.; Abashidze, M.; Neely, H.; Seetharaman, J.; Shastry, R.; Janjua, H.; Cunningham, K.; Ma, L.-C.; Xiao, R.; Liu, J.; Baran, M.C.; Acton, T.B.; Rost, B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2008-10-16
Resolution : 2.30 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 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)	:	1.13
EDS	:	2.11
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)	:	2.11

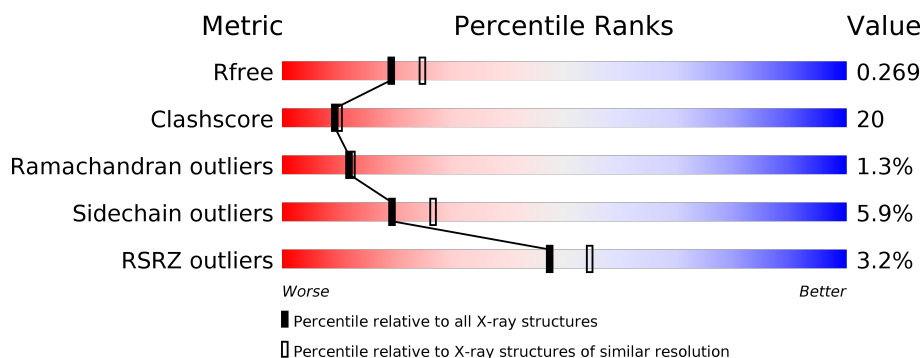
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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	322	<div> <div>3%</div> <div> <div></div> <div>54%</div> <div>36%</div> <div>6%</div> </div> </div>
1	B	322	<div> <div>2%</div> <div> <div></div> <div>59%</div> <div>30%</div> <div>6%</div> </div> </div>
1	C	322	<div> <div>2%</div> <div> <div></div> <div>54%</div> <div>37%</div> <div>6%</div> </div> </div>
1	D	322	<div> <div>4%</div> <div> <div></div> <div>61%</div> <div>30%</div> <div>6%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10249 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 tRNA delta(2)-isopentenylpyrophosphate transferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	Se	0	0	0
			2426	1530	428	457	1	10			
1	B	302	Total	C	N	O	S	Se	0	0	0
			2416	1524	425	456	1	10			
1	C	303	Total	C	N	O	S	Se	0	0	0
			2426	1530	428	457	1	10			
1	D	302	Total	C	N	O	S	Se	0	0	0
			2416	1524	425	456	1	10			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	315	LEU	-	expression tag	UNP Q9KAC3
A	316	GLU	-	expression tag	UNP Q9KAC3
A	317	HIS	-	expression tag	UNP Q9KAC3
A	318	HIS	-	expression tag	UNP Q9KAC3
A	319	HIS	-	expression tag	UNP Q9KAC3
A	320	HIS	-	expression tag	UNP Q9KAC3
A	321	HIS	-	expression tag	UNP Q9KAC3
A	322	HIS	-	expression tag	UNP Q9KAC3
B	315	LEU	-	expression tag	UNP Q9KAC3
B	316	GLU	-	expression tag	UNP Q9KAC3
B	317	HIS	-	expression tag	UNP Q9KAC3
B	318	HIS	-	expression tag	UNP Q9KAC3
B	319	HIS	-	expression tag	UNP Q9KAC3
B	320	HIS	-	expression tag	UNP Q9KAC3
B	321	HIS	-	expression tag	UNP Q9KAC3
B	322	HIS	-	expression tag	UNP Q9KAC3
C	315	LEU	-	expression tag	UNP Q9KAC3
C	316	GLU	-	expression tag	UNP Q9KAC3
C	317	HIS	-	expression tag	UNP Q9KAC3
C	318	HIS	-	expression tag	UNP Q9KAC3
C	319	HIS	-	expression tag	UNP Q9KAC3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	320	HIS	-	expression tag	UNP Q9KAC3
C	321	HIS	-	expression tag	UNP Q9KAC3
C	322	HIS	-	expression tag	UNP Q9KAC3
D	315	LEU	-	expression tag	UNP Q9KAC3
D	316	GLU	-	expression tag	UNP Q9KAC3
D	317	HIS	-	expression tag	UNP Q9KAC3
D	318	HIS	-	expression tag	UNP Q9KAC3
D	319	HIS	-	expression tag	UNP Q9KAC3
D	320	HIS	-	expression tag	UNP Q9KAC3
D	321	HIS	-	expression tag	UNP Q9KAC3
D	322	HIS	-	expression tag	UNP Q9KAC3

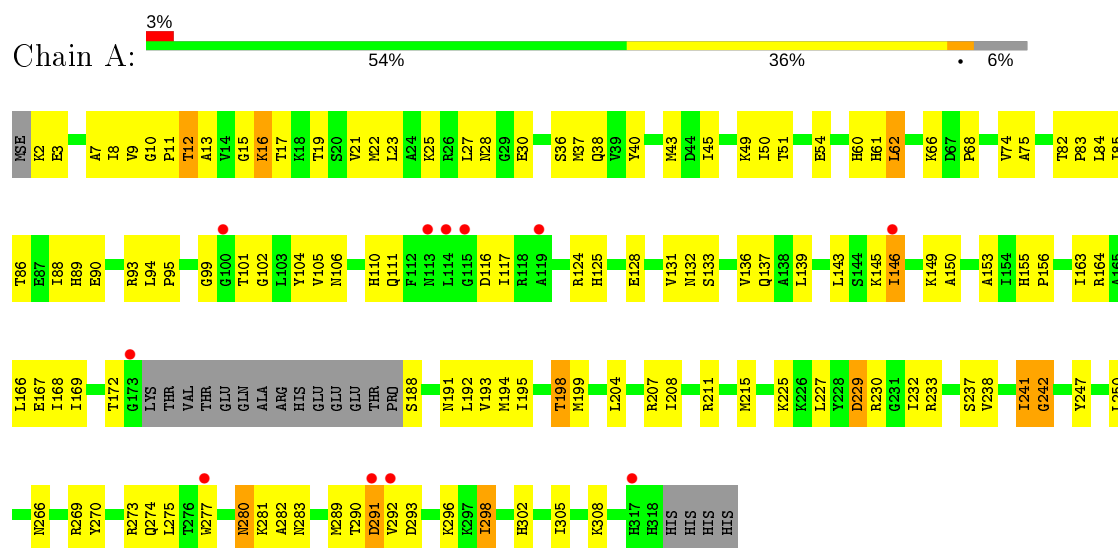
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	194	Total 194	O 194	0	0
2	B	132	Total 132	O 132	0	0
2	C	134	Total 134	O 134	0	0
2	D	105	Total 105	O 105	0	0

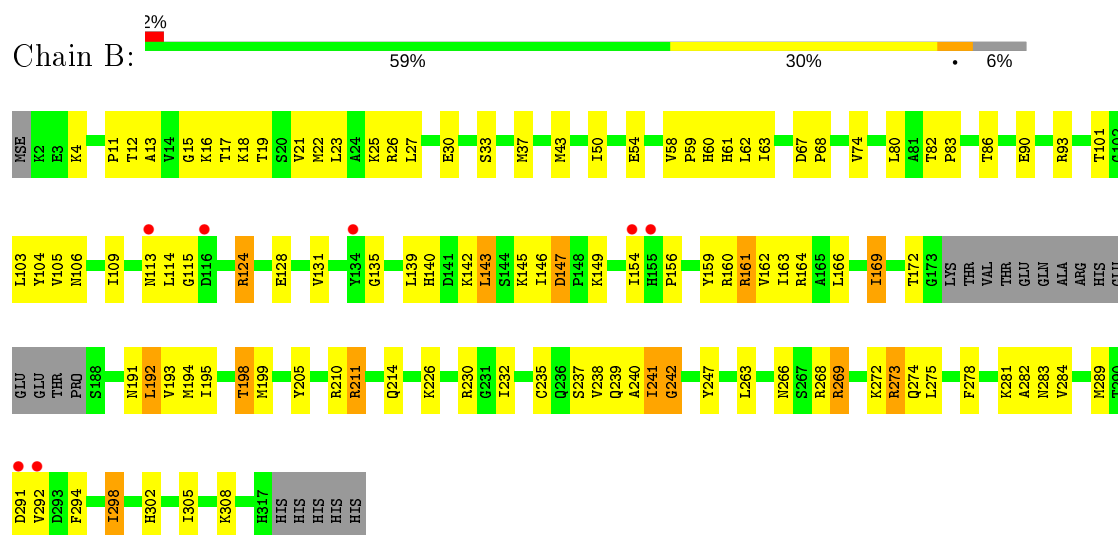
3 Residue-property plots [i](#)

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 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: tRNA delta(2)-isopentenylpyrophosphate transferase

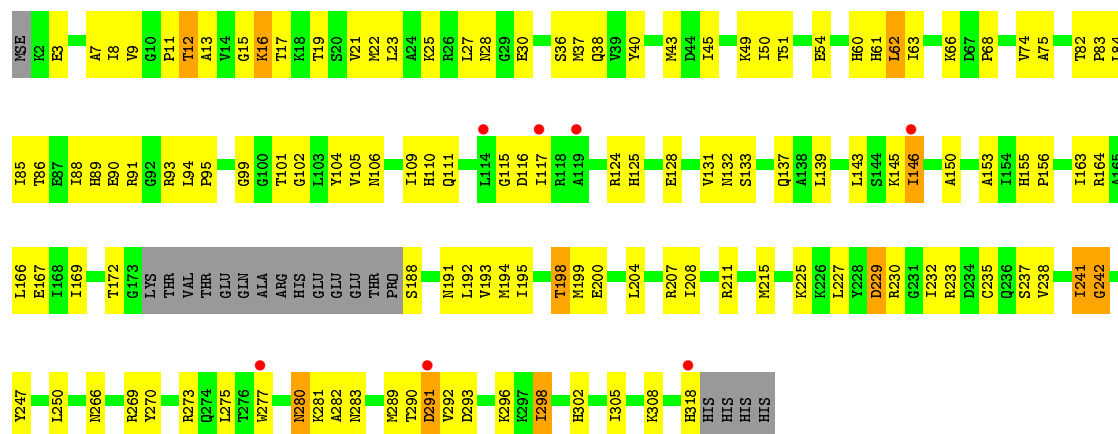


- Molecule 1: tRNA delta(2)-isopentenylpyrophosphate transferase

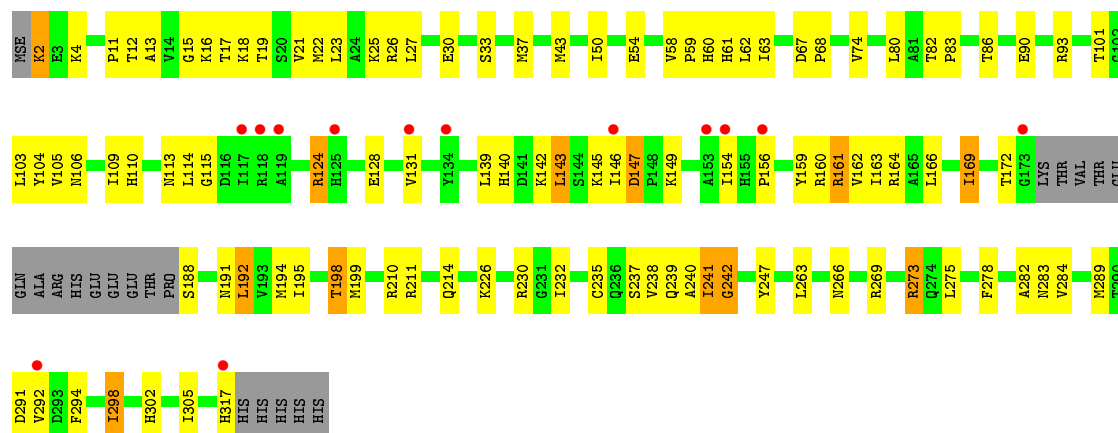


- Molecule 1: tRNA delta(2)-isopentenylpyrophosphate transferase





• Molecule 1: tRNA delta(2)-isopentenylpyrophosphate transferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.80Å 73.82Å 95.56Å 89.99° 93.73° 90.02°	Depositor
Resolution (Å)	19.96 – 2.30 28.97 – 2.29	Depositor EDS
% Data completeness (in resolution range)	68.4 (19.96-2.30) 80.9 (28.97-2.29)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.90 (at 2.29Å)	Xtriage
Refinement program	CNS 1.2, XTALVIEW	Depositor
R, R_{free}	0.220 , 0.263 0.232 , 0.269	Depositor DCC
R_{free} test set	4065 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å ²)	20.2	Xtriage
Anisotropy	0.805	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 23.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.458 for -h,k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10249	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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 38.05 % 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 3.9084e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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

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	0.36	0/2457	0.57	1/3294 (0.0%)
1	B	0.37	0/2446	0.83	9/3279 (0.3%)
1	C	0.36	0/2457	0.56	1/3294 (0.0%)
1	D	0.36	0/2446	0.84	9/3279 (0.3%)
All	All	0.36	0/9806	0.71	20/13146 (0.2%)

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	164	ARG	NE-CZ-NH1	-14.60	113.00	120.30
1	D	164	ARG	NE-CZ-NH2	-13.97	113.31	120.30
1	D	164	ARG	NE-CZ-NH1	13.61	127.11	120.30
1	D	161	ARG	NE-CZ-NH1	13.61	127.10	120.30
1	D	161	ARG	NE-CZ-NH2	-13.46	113.57	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	2426	0	2431	105	0
1	B	2416	0	2424	94	0
1	C	2426	0	2431	106	0
1	D	2416	0	2424	88	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	194	0	0	19	0
2	B	132	0	0	11	0
2	C	134	0	0	20	0
2	D	105	0	0	10	0
All	All	10249	0	9710	384	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 384 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:273:ARG:HH21	1:D:273:ARG:HB2	1.32	0.95
1:B:273:ARG:HH21	1:B:273:ARG:HB2	1.32	0.94
1:C:102:GLY:HA3	1:C:277:TRP:CD1	2.17	0.80
1:A:102:GLY:HA3	1:A:277:TRP:CD1	2.17	0.79
1:C:51:THR:OG1	1:C:54:GLU:HG3	1.85	0.76

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	299/322 (93%)	280 (94%)	16 (5%)	3 (1%)	15	17
1	B	298/322 (92%)	279 (94%)	14 (5%)	5 (2%)	9	8
1	C	299/322 (93%)	279 (93%)	17 (6%)	3 (1%)	15	17
1	D	298/322 (92%)	280 (94%)	13 (4%)	5 (2%)	9	8
All	All	1194/1288 (93%)	1118 (94%)	60 (5%)	16 (1%)	12	12

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	241	ILE
1	B	241	ILE
1	C	241	ILE
1	D	241	ILE
1	A	291	ASP

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	261/268 (97%)	244 (94%)	17 (6%)	17	23
1	B	260/268 (97%)	248 (95%)	12 (5%)	27	38
1	C	261/268 (97%)	244 (94%)	17 (6%)	17	23
1	D	260/268 (97%)	245 (94%)	15 (6%)	20	27
All	All	1042/1072 (97%)	981 (94%)	61 (6%)	19	27

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	291	ASP
1	C	133	SER
1	D	269	ARG
1	B	298	ILE
1	C	16	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	157	ASN
1	C	110	HIS
1	D	157	ASN
1	B	253	ASN
1	B	283	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 carbohydrates 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	293/322 (90%)	0.05	11 (3%) 40 47	9, 27, 52, 80	0
1	B	292/322 (90%)	0.09	7 (2%) 59 66	8, 26, 62, 75	0
1	C	293/322 (90%)	0.00	7 (2%) 59 66	10, 27, 53, 74	0
1	D	292/322 (90%)	0.16	13 (4%) 33 40	10, 27, 61, 74	0
All	All	1170/1288 (90%)	0.08	38 (3%) 47 54	8, 27, 58, 80	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	292	VAL	6.3
1	D	173	GLY	4.5
1	A	173	GLY	4.5
1	D	154	ILE	4.3
1	B	134	TYR	4.1

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 carbohydrates 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.