



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 14, 2025 – 04:04 PM EDT

PDB ID : 9O66 / pdb\_00009o66  
Title : Crystal Structure of Tryptophanyl-tRNA synthetase from *Klebsiella aerogenes*  
Authors : Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2025-04-11  
Resolution : 2.10 Å (reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

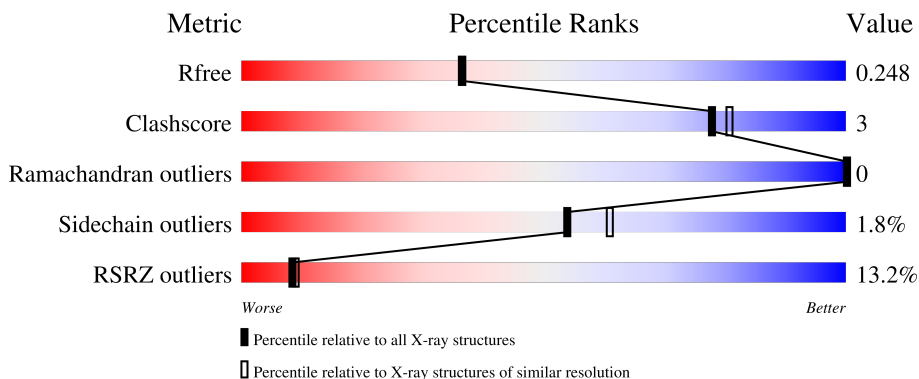
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

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  $\geq 3$ , 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	355	 10% 83% 6% 11%
1	B	355	 14% 82% 6% 12%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5009 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 Tryptophan-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	317	2458	1556	422	467	13	0	2	0
1	B	314	2371	1505	402	451	13	0	1	0

There are 42 discrepancies between the modelled and reference sequences:

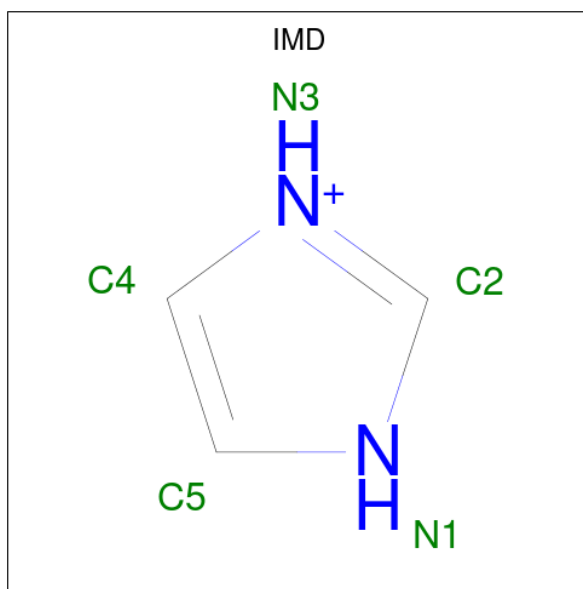
Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP A0A0H3FKK2
A	-19	ALA	-	expression tag	UNP A0A0H3FKK2
A	-18	HIS	-	expression tag	UNP A0A0H3FKK2
A	-17	HIS	-	expression tag	UNP A0A0H3FKK2
A	-16	HIS	-	expression tag	UNP A0A0H3FKK2
A	-15	HIS	-	expression tag	UNP A0A0H3FKK2
A	-14	HIS	-	expression tag	UNP A0A0H3FKK2
A	-13	HIS	-	expression tag	UNP A0A0H3FKK2
A	-12	MET	-	expression tag	UNP A0A0H3FKK2
A	-11	GLY	-	expression tag	UNP A0A0H3FKK2
A	-10	THR	-	expression tag	UNP A0A0H3FKK2
A	-9	LEU	-	expression tag	UNP A0A0H3FKK2
A	-8	GLU	-	expression tag	UNP A0A0H3FKK2
A	-7	ALA	-	expression tag	UNP A0A0H3FKK2
A	-6	GLN	-	expression tag	UNP A0A0H3FKK2
A	-5	THR	-	expression tag	UNP A0A0H3FKK2
A	-4	GLN	-	expression tag	UNP A0A0H3FKK2
A	-3	GLY	-	expression tag	UNP A0A0H3FKK2
A	-2	PRO	-	expression tag	UNP A0A0H3FKK2
A	-1	GLY	-	expression tag	UNP A0A0H3FKK2
A	0	SER	-	expression tag	UNP A0A0H3FKK2
B	-20	MET	-	initiating methionine	UNP A0A0H3FKK2
B	-19	ALA	-	expression tag	UNP A0A0H3FKK2
B	-18	HIS	-	expression tag	UNP A0A0H3FKK2
B	-17	HIS	-	expression tag	UNP A0A0H3FKK2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	expression tag	UNP A0A0H3FKK2
B	-15	HIS	-	expression tag	UNP A0A0H3FKK2
B	-14	HIS	-	expression tag	UNP A0A0H3FKK2
B	-13	HIS	-	expression tag	UNP A0A0H3FKK2
B	-12	MET	-	expression tag	UNP A0A0H3FKK2
B	-11	GLY	-	expression tag	UNP A0A0H3FKK2
B	-10	THR	-	expression tag	UNP A0A0H3FKK2
B	-9	LEU	-	expression tag	UNP A0A0H3FKK2
B	-8	GLU	-	expression tag	UNP A0A0H3FKK2
B	-7	ALA	-	expression tag	UNP A0A0H3FKK2
B	-6	GLN	-	expression tag	UNP A0A0H3FKK2
B	-5	THR	-	expression tag	UNP A0A0H3FKK2
B	-4	GLN	-	expression tag	UNP A0A0H3FKK2
B	-3	GLY	-	expression tag	UNP A0A0H3FKK2
B	-2	PRO	-	expression tag	UNP A0A0H3FKK2
B	-1	GLY	-	expression tag	UNP A0A0H3FKK2
B	0	SER	-	expression tag	UNP A0A0H3FKK2

- Molecule 2 is IMIDAZOLE (CCD ID: IMD) (formula: C<sub>3</sub>H<sub>5</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			5	3	2		
2	B	1	Total	C	N	0	0
			5	3	2		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Ca 1 1	0	0

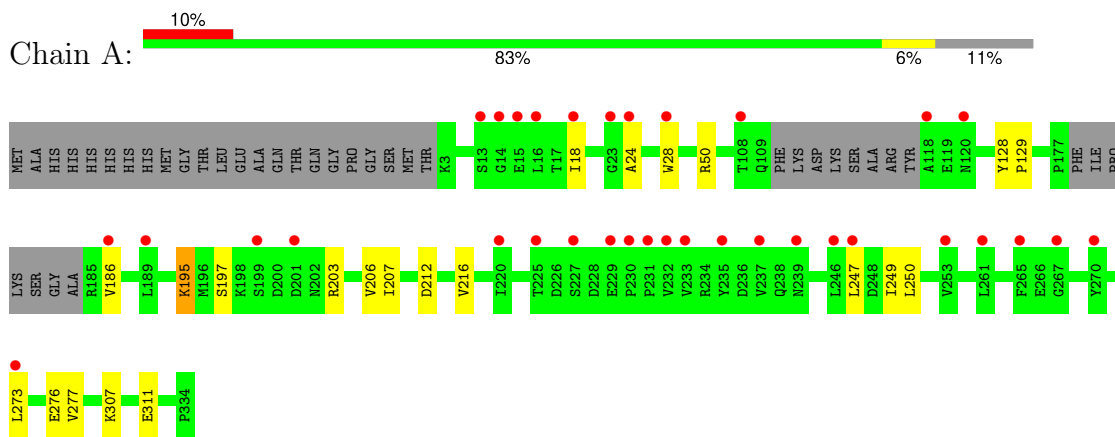
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	80	Total O 80 80	0	0
4	B	89	Total O 89 89	0	0

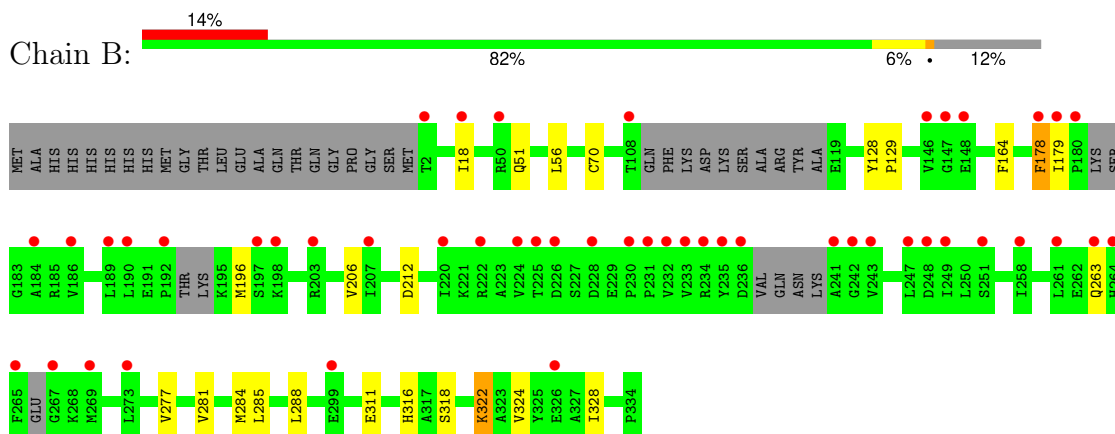
### 3 Residue-property plots [i](#)

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: Tryptophan-tRNA ligase



- Molecule 1: Tryptophan-tRNA ligase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.16Å 75.51Å 56.75Å 90.00° 95.93° 90.00°	Depositor
Resolution (Å)	43.27 – 2.10 43.27 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (43.27-2.10) 99.7 (43.27-2.10)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 2.10Å)	Xtrriage
Refinement program	PHENIX dev_5660	Depositor
R, $R_{free}$	0.201 , 0.247 0.206 , 0.248	Depositor DCC
$R_{free}$ test set	1844 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.3	Xtrriage
Anisotropy	0.386	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 50.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5009	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, IMD

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	0.25	0/2514	0.47	0/3411
1	B	0.26	0/2419	0.47	0/3283
All	All	0.26	0/4933	0.47	0/6694

There are no bond length outliers.

There are no bond angle outliers.

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	2458	0	2382	14	0
1	B	2371	0	2264	12	0
2	A	5	0	5	0	0
2	B	5	0	5	0	0
3	B	1	0	0	0	0
4	A	80	0	0	0	0
4	B	89	0	0	0	0
All	All	5009	0	4656	26	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 3.



All (26) 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:A:18:ILE:HD11	1:A:186:VAL:HG11	1.57	0.86
1:A:186:VAL:HG22	1:A:249:ILE:HG12	1.57	0.86
1:A:18:ILE:CD1	1:A:186:VAL:HG11	2.24	0.67
1:A:307:LYS:O	1:A:311:GLU:HG3	1.95	0.65
1:B:18:ILE:CD1	1:B:285:LEU:HD21	2.30	0.61
1:A:24:ALA:HB1	1:A:28[A]:TRP:CZ2	2.43	0.53
1:A:250:LEU:HD21	1:A:276:GLU:HG2	1.91	0.51
1:B:164:PHE:CE2	1:B:328:ILE:HD11	2.47	0.50
1:A:195:LYS:HZ2	1:A:197:SER:HA	1.77	0.50
1:A:212:ASP:O	1:A:216:VAL:HG23	2.15	0.47
1:B:277:VAL:O	1:B:281:VAL:HG22	2.15	0.46
1:B:318:SER:O	1:B:322:LYS:HE2	2.15	0.46
1:A:195:LYS:NZ	1:A:197:SER:HA	2.31	0.45
1:A:250:LEU:HD13	1:A:277:VAL:HA	1.98	0.45
1:A:128:TYR:N	1:A:129:PRO:CD	2.81	0.43
1:A:206:VAL:O	1:A:207:ILE:HD13	2.19	0.43
1:B:70:CYS:HA	1:B:288:LEU:HD21	2.01	0.43
1:B:18:ILE:HD11	1:B:284:MET:CE	2.49	0.43
1:B:51:GLN:HG2	1:B:56:LEU:HB2	2.00	0.42
1:A:247:LEU:CD2	1:A:273:LEU:HD21	2.49	0.42
1:B:324:VAL:O	1:B:328:ILE:HD13	2.20	0.42
1:B:178:PHE:CE1	1:B:179:ILE:O	2.72	0.42
1:B:196:MET:HG3	1:B:206:VAL:HG12	2.01	0.41
1:B:18:ILE:HD11	1:B:284:MET:HE1	2.02	0.41
1:A:195:LYS:HD2	1:A:195:LYS:C	2.41	0.41
1:B:128:TYR:N	1:B:129:PRO:CD	2.84	0.40

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	313/355 (88%)	304 (97%)	9 (3%)	0	100	100
1	B	303/355 (85%)	299 (99%)	4 (1%)	0	100	100
All	All	616/710 (87%)	603 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	259/301 (86%)	256 (99%)	3 (1%)	67	74
1	B	243/301 (81%)	237 (98%)	6 (2%)	42	47
All	All	502/602 (83%)	493 (98%)	9 (2%)	54	61

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ARG
1	A	195	LYS
1	A	203	ARG
1	B	178	PHE
1	B	212	ASP
1	B	263	GLN
1	B	311	GLU
1	B	316	HIS
1	B	322	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN

### 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](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	IMD	A	401	-	3,5,5	0.14	0	4,5,5	0.98	0
2	IMD	B	402	-	3,5,5	0.15	0	4,5,5	0.99	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
2	IMD	A	401	-	-	-	0/1/1/1
2	IMD	B	402	-	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	317/355 (89%)	0.68	34 (10%) <b>12</b> <b>13</b>	16, 41, 89, 116	2 (0%)
1	B	314/355 (88%)	0.72	49 (15%) <b>6</b> <b>6</b>	17, 38, 94, 114	1 (0%)
All	All	631/710 (88%)	0.70	83 (13%) <b>8</b> <b>9</b>	16, 40, 93, 116	3 (0%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	261	LEU	4.9
1	A	14	GLY	4.9
1	B	267	GLY	4.6
1	A	186	VAL	4.5
1	B	241	ALA	4.5
1	A	28[A]	TRP	4.5
1	B	233	VAL	4.3
1	B	235	TYR	4.3
1	A	13	SER	4.2
1	B	265	PHE	4.1
1	B	179	ILE	4.1
1	B	232	VAL	3.9
1	A	231	PRO	3.8
1	B	243	VAL	3.8
1	A	24	ALA	3.8
1	A	118	ALA	3.7
1	B	247	LEU	3.7
1	B	299	GLU	3.7
1	B	225	THR	3.6
1	B	147	GLY	3.5
1	A	16	LEU	3.3
1	A	237	VAL	3.2
1	B	146	VAL	3.2
1	A	201	ASP	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	261	LEU	3.1
1	A	18	ILE	3.0
1	B	180	PRO	3.0
1	A	233	VAL	3.0
1	B	178	PHE	2.9
1	B	269	MET	2.9
1	B	226	ASP	2.9
1	B	236	ASP	2.8
1	B	18	ILE	2.8
1	A	253	VAL	2.8
1	B	230	PRO	2.8
1	B	222	ARG	2.8
1	B	258	ILE	2.7
1	A	232	VAL	2.7
1	A	270	TYR	2.7
1	A	23	GLY	2.6
1	A	199	SER	2.6
1	B	189	LEU	2.6
1	A	247	LEU	2.5
1	B	190	LEU	2.5
1	B	228	ASP	2.5
1	B	2	THR	2.5
1	B	234	ARG	2.5
1	A	225	THR	2.5
1	A	265	PHE	2.5
1	B	326	GLU	2.5
1	B	198	LYS	2.5
1	A	229	GLU	2.4
1	B	184	ALA	2.4
1	B	186	VAL	2.4
1	B	242	GLY	2.4
1	A	273	LEU	2.4
1	B	148	GLU	2.4
1	B	108	THR	2.4
1	B	224	VAL	2.4
1	B	248	ASP	2.4
1	B	264	HIS	2.3
1	B	273	LEU	2.3
1	B	220	ILE	2.3
1	B	50	ARG	2.3
1	B	197	SER	2.3
1	B	263	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	227	SER	2.3
1	A	120	ASN	2.2
1	B	207	ILE	2.2
1	A	220	ILE	2.2
1	A	235	TYR	2.2
1	B	251	SER	2.2
1	A	267	GLY	2.2
1	B	231	PRO	2.1
1	A	239	ASN	2.1
1	B	249	ILE	2.1
1	B	203	ARG	2.1
1	A	230	PRO	2.1
1	B	192	PRO	2.0
1	A	108	THR	2.0
1	A	189	LEU	2.0
1	A	246	LEU	2.0
1	A	15	GLU	2.0

## 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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	IMD	B	402	5/5	0.76	0.15	44,45,52,58	0
2	IMD	A	401	5/5	0.91	0.15	30,31,35,38	0
3	CA	B	401	1/1	1.00	0.04	22,22,22,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.