Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 07:24 PM EDT

PDB ID	:	3ORR
Title	:	Crystal Structure of N5-Carboxyaminoimidazole synthetase from Staphylococcus aureus
Authors	:	Brugarolas, P.; Duguid, E.M.; Zhang, W.; Poor, C.B.; He, C.
Deposited on	:	2010-09-07
Resolution	:	2.23 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*
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 (i)) were used in the production of this report:

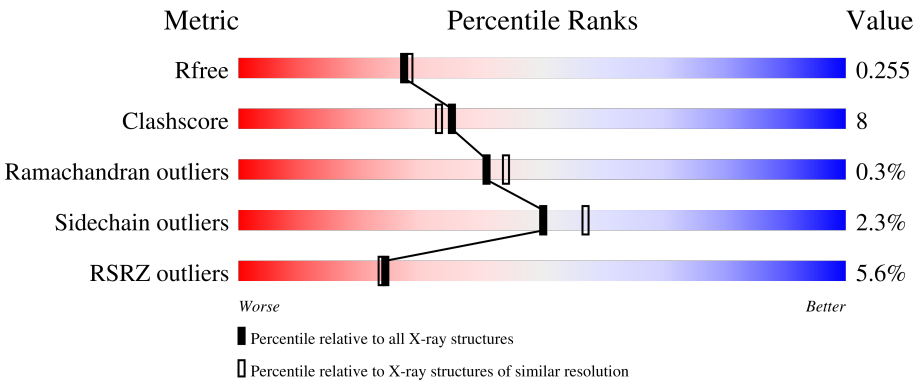
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.23 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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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	377	8% 80% 16% • •
1	B	377	3% 80% 16% • •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6105 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 N5-carboxyaminoimidazole ribonucleotide synthetase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	368	2945	1868	496	566	6	9	0	0	0
1	B	367	2945	1868	496	566	6	9	0	1	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP A6QFS4
A	-1	ASN	-	EXPRESSION TAG	UNP A6QFS4
A	0	ALA	-	EXPRESSION TAG	UNP A6QFS4
B	-2	SER	-	EXPRESSION TAG	UNP A6QFS4
B	-1	ASN	-	EXPRESSION TAG	UNP A6QFS4
B	0	ALA	-	EXPRESSION TAG	UNP A6QFS4

- Molecule 2 is water.

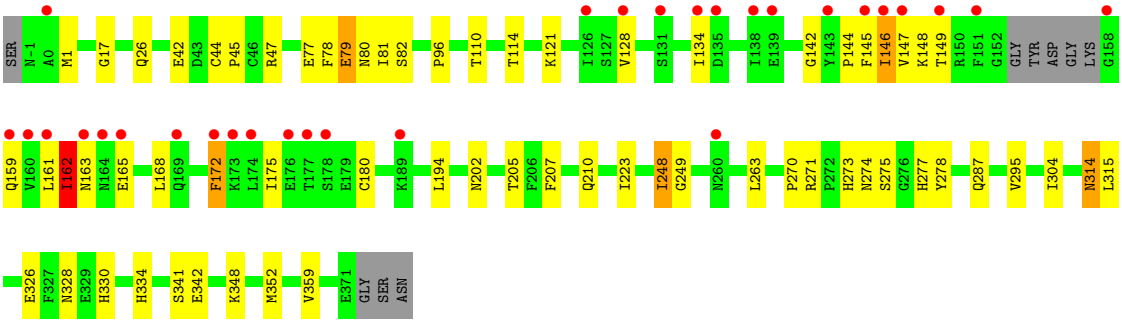
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	90	90	90	0	0
2	B	125	125	125	0	0

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.

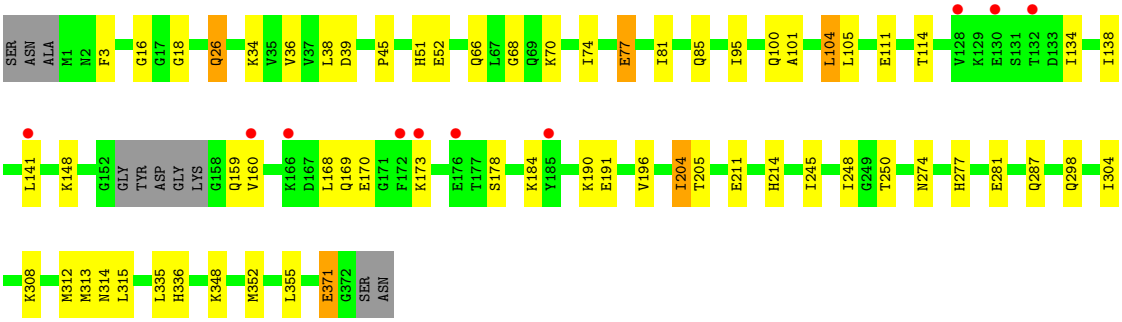
• Molecule 1: N5-carboxyaminoimidazole ribonucleotide synthetase

Chain A:



• Molecule 1: N5-carboxyaminoimidazole ribonucleotide synthetase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	66.11Å 53.33Å 107.41Å 90.00° 95.34° 90.00°	Depositor
Resolution (Å)	40.00 – 2.23 39.73 – 2.23	Depositor EDS
% Data completeness (in resolution range)	99.3 (40.00-2.23) 99.3 (39.73-2.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.27 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.194 , 0.251 0.204 , 0.255	Depositor DCC
R_{free} test set	1869 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	30.2	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 22.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6105	wwPDB-VP
Average B, all atoms (Å^2)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% 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 (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	0.75	0/2989	0.70	0/4016
1	B	0.80	1/2990 (0.0%)	0.70	0/4018
All	All	0.77	1/5979 (0.0%)	0.70	0/8034

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	371	GLU	CG-CD	5.12	1.59	1.51

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	2945	0	2930	52	0
1	B	2945	0	2929	47	0
2	A	90	0	0	3	0
2	B	125	0	0	5	0
All	All	6105	0	5859	96	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 8.

All (96) 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:B:315:LEU:HD21	1:B:352:MSE:HE3	1.27	1.13
1:A:26:GLN:HE21	1:B:26:GLN:NE2	1.73	0.86
1:A:26:GLN:HE21	1:B:26:GLN:HE21	1.29	0.81
1:A:78:PHE:HB3	1:A:80:ASN:ND2	2.02	0.74
1:A:146:ILE:HD11	1:A:159:GLN:HB3	1.74	0.70
1:B:101:ALA:O	1:B:105:LEU:HG	1.92	0.69
1:A:334:HIS:HD2	2:B:494:HOH:O	1.74	0.68
1:B:68:GLY:HA2	1:B:74:ILE:HD11	1.75	0.68
1:A:165:GLU:HA	1:A:168:LEU:HG	1.77	0.67
1:A:17:GLY:O	1:A:45:PRO:HD2	1.95	0.67
1:B:100:GLN:NE2	1:B:245:ILE:HA	2.12	0.64
1:B:336:HIS:HD2	2:B:453:HOH:O	1.78	0.64
1:B:308:LYS:HD3	1:B:355:LEU:HB3	1.80	0.64
1:B:315:LEU:HD21	1:B:352:MSE:CE	2.18	0.63
1:B:138:ILE:HD11	1:B:168:LEU:HD21	1.79	0.63
1:B:274:ASN:HD22	1:B:348:LYS:NZ	1.94	0.63
1:B:214:HIS:HE1	2:B:474:HOH:O	1.82	0.62
1:A:273:HIS:HD2	1:A:275:SER:OG	1.85	0.60
1:B:104:LEU:HD22	1:B:111:GLU:HA	1.84	0.60
1:A:148:LYS:HD3	1:A:159:GLN:HE21	1.66	0.59
1:A:271:ARG:HB2	2:A:451:HOH:O	2.01	0.59
1:B:134:ILE:O	1:B:138:ILE:HG12	2.01	0.59
1:A:274:ASN:HD22	1:A:348:LYS:NZ	2.02	0.58
1:B:315:LEU:CD2	1:B:352:MSE:HE3	2.18	0.58
1:A:78:PHE:HB3	1:A:80:ASN:HD21	1.68	0.57
1:A:271:ARG:HG3	1:A:271:ARG:HH11	1.70	0.56
1:B:205:THR:HG22	1:B:304:ILE:HD12	1.87	0.56
1:B:277:HIS:HE1	2:B:454:HOH:O	1.88	0.56
1:A:96:PRO:HB2	1:A:248:ILE:HG12	1.87	0.55
1:B:281:GLU:OE2	1:B:336:HIS:HE1	1.89	0.55
1:B:274:ASN:HD21	1:B:314:ASN:HD21	1.53	0.55
1:A:248:ILE:HD12	1:A:249:GLY:N	2.21	0.55
1:A:334:HIS:CD2	2:B:494:HOH:O	2.53	0.54
1:A:134:ILE:HG21	1:A:172:PHE:HE1	1.72	0.54
1:B:196:VAL:HG11	1:B:204:ILE:HD11	1.89	0.54
1:B:16:GLY:O	1:B:77:GLU:HG2	2.07	0.53
1:B:81:ILE:HD11	1:B:85:GLN:HG3	1.90	0.53
1:B:274:ASN:ND2	1:B:314:ASN:HD21	2.07	0.53
1:B:52:GLU:OE2	1:B:70:LYS:HE2	2.11	0.51
1:A:147:VAL:HG11	1:A:175:ILE:HD11	1.93	0.51
1:B:66:GLN:O	1:B:70:LYS:HG3	2.11	0.51
1:A:207:PHE:CD1	1:A:304:ILE:HD13	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:HIS:H	1:A:287:GLN:HE22	1.59	0.50
1:A:121:LYS:HD2	1:A:263:LEU:O	2.11	0.50
1:B:141:LEU:O	1:B:184:LYS:HE2	2.12	0.50
1:A:273:HIS:CD2	1:A:275:SER:H	2.31	0.49
1:B:335:LEU:CD1	1:B:352:MSE:HE2	2.42	0.49
1:A:274:ASN:HD22	1:A:348:LYS:HZ2	1.61	0.49
1:A:110:THR:O	1:A:114:THR:HG23	2.12	0.49
1:B:3:PHE:CE2	1:B:248:ILE:HG13	2.47	0.48
1:B:308:LYS:CD	1:B:355:LEU:HB3	2.43	0.48
1:B:190:LYS:HE3	1:B:211:GLU:OE2	2.14	0.48
1:A:144:PRO:HB3	1:A:163:ASN:HD22	1.79	0.48
1:A:326:GLU:O	1:A:330:HIS:HD2	1.97	0.48
1:B:18:GLY:HA2	1:B:45:PRO:HG2	1.96	0.48
1:A:194:LEU:HD12	2:A:427:HOH:O	2.14	0.47
1:A:277:HIS:HE1	2:A:411:HOH:O	1.97	0.47
1:A:145:PHE:CE1	1:A:162:ILE:HD12	2.51	0.46
1:A:128:VAL:HG11	1:A:134:ILE:HD12	1.98	0.46
1:B:274:ASN:HD22	1:B:348:LYS:HZ3	1.60	0.45
1:A:1:MSE:HE1	1:A:202:ASN:HB2	1.98	0.45
1:A:314:ASN:HD22	1:A:314:ASN:HA	1.63	0.45
1:B:36:VAL:HG22	1:B:52:GLU:HB3	1.97	0.45
1:A:148:LYS:HG2	1:A:159:GLN:HG2	1.99	0.45
1:A:81:ILE:HG12	1:A:82:SER:O	2.17	0.45
1:B:148:LYS:HD3	1:B:159:GLN:HE21	1.82	0.45
1:A:128:VAL:HG12	1:A:175:ILE:HG12	1.99	0.44
1:A:223:ILE:HG21	1:A:359:VAL:HG11	1.99	0.44
1:A:248:ILE:HD11	1:A:295:VAL:HA	1.98	0.44
1:A:315:LEU:HD11	1:A:352:MSE:HE3	2.00	0.44
1:B:74:ILE:HB	1:B:95:ILE:HG12	2.00	0.44
1:B:191:GLU:OE1	1:B:214:HIS:HD2	1.99	0.44
1:B:104:LEU:HD11	1:B:114:THR:HG21	1.99	0.44
1:A:142:GLY:HA3	1:A:145:PHE:HD2	1.83	0.44
1:B:38:LEU:C	1:B:38:LEU:HD23	2.38	0.44
1:B:312:MSE:HG2	1:B:313:MSE:N	2.32	0.44
1:A:147:VAL:HG12	1:A:180:CYS:HB3	1.99	0.43
1:B:160:VAL:HG21	1:B:170:GLU:HG2	2.00	0.43
1:B:169:GLN:HG2	1:B:173:LYS:HE3	2.00	0.43
1:A:205:THR:HG22	1:A:304:ILE:HD12	2.01	0.43
1:B:250:THR:HG21	1:B:287:GLN:HB2	2.01	0.43
1:B:52:GLU:CD	1:B:70:LYS:HE2	2.39	0.42
1:A:44:CYS:HA	1:A:45:PRO:HD3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MSE:SE	1:A:202:ASN:HB2	2.69	0.42
1:B:196:VAL:CG1	1:B:204:ILE:HD11	2.50	0.42
1:A:79:GLU:OE2	1:A:270:PRO:HD2	2.19	0.42
1:A:223:ILE:CG2	1:A:359:VAL:HG11	2.49	0.41
1:A:145:PHE:O	1:A:162:ILE:HB	2.21	0.41
1:A:17:GLY:O	1:A:44:CYS:HB2	2.20	0.41
1:A:328:ASN:HA	1:B:298:GLN:NE2	2.36	0.41
1:B:38:LEU:HD23	1:B:39:ASP:N	2.34	0.41
1:A:1:MSE:CE	1:A:202:ASN:HB2	2.50	0.41
1:B:34:LYS:HA	1:B:51:HIS:CE1	2.55	0.41
1:A:42:GLU:HG2	1:A:47:ARG:HH12	1.86	0.40
1:A:146:ILE:HD12	1:A:161:LEU:HA	2.02	0.40
1:A:210:GLN:HG2	1:A:278:TYR:CE1	2.57	0.40

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	364/377 (97%)	352 (97%)	10 (3%)	2 (0%)	29 28
1	B	364/377 (97%)	350 (96%)	14 (4%)	0	100 100
All	All	728/754 (97%)	702 (96%)	24 (3%)	2 (0%)	41 44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	ILE
1	A	79	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	327/324 (101%)	318 (97%)	9 (3%)	43	49
1	B	327/324 (101%)	321 (98%)	6 (2%)	59	66
All	All	654/648 (101%)	639 (98%)	15 (2%)	50	57

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	GLU
1	A	146	ILE
1	A	149	THR
1	A	162	ILE
1	A	172	PHE
1	A	248	ILE
1	A	314	ASN
1	A	341	SER
1	A	342	GLU
1	B	26	GLN
1	B	77	GLU
1	B	104	LEU
1	B	178	SER
1	B	204	ILE
1	B	371	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	80	ASN
1	A	84	GLN
1	A	159	GLN
1	A	210	GLN
1	A	273	HIS
1	A	274	ASN

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Mol	Chain	Res	Type
1	A	277	HIS
1	A	287	GLN
1	A	302	ASN
1	A	314	ASN
1	A	330	HIS
1	A	334	HIS
1	B	26	GLN
1	B	29	GLN
1	B	100	GLN
1	B	106	GLN
1	B	159	GLN
1	B	210	GLN
1	B	214	HIS
1	B	274	ASN
1	B	277	HIS
1	B	298	GLN
1	B	334	HIS
1	B	336	HIS

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 (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	359/377 (95%)	0.23	30 (8%)	11	11	2, 6, 45, 54	0
1	B	358/377 (94%)	0.05	10 (2%)	53	53	2, 3, 40, 49	0
All	All	717/754 (95%)	0.14	40 (5%)	24	23	2, 4, 43, 54	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	160	VAL	4.9
1	A	135	ASP	4.7
1	A	145	PHE	4.5
1	A	172	PHE	4.2
1	A	169	GLN	4.2
1	A	174	LEU	3.9
1	A	158	GLY	3.6
1	A	138	ILE	3.5
1	A	147	VAL	3.4
1	A	134	ILE	3.3
1	B	130	GLU	3.3
1	A	177	THR	3.3
1	A	189	LYS	3.1
1	A	163	ASN	3.0
1	A	131	SER	3.0
1	A	146	ILE	3.0
1	B	185	TYR	2.9
1	A	173	LYS	2.9
1	A	128	VAL	2.9
1	B	128	VAL	2.9
1	A	143	TYR	2.9
1	A	178	SER	2.8
1	A	0	ALA	2.8
1	A	176	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	149	THR	2.7
1	A	126	ILE	2.6
1	A	151	PHE	2.6
1	A	159	GLN	2.6
1	A	161	LEU	2.6
1	A	260	ASN	2.4
1	B	176	GLU	2.4
1	A	165	GLU	2.3
1	B	160	VAL	2.2
1	B	172	PHE	2.1
1	A	139	GLU	2.1
1	A	164	ASN	2.1
1	B	132	THR	2.1
1	B	166	LYS	2.1
1	B	141	LEU	2.0
1	B	173	LYS	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.