



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 04:40 AM BST

PDB ID : 4RK1  
Title : Crystal structure of LacI family transcriptional regulator from *Enterococcus faecium*, Target EFI-512930, with bound ribose  
Authors : Patskovsky, Y.; Toro, R.; Bhosle, R.; Al Obaidi, N.; Chamala, S.; Attonito, J.D.; Scott Glenn, A.; Chowdhury, S.; Lafleur, J.; Siedel, R.D.; Hillerich, B.; Love, J.; Whalen, K.L.; Gerlt, J.A.; Almo, S.C.; Enzyme Function Initiative (EFI)  
Deposited on : 2014-10-11  
Resolution : 1.90 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](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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

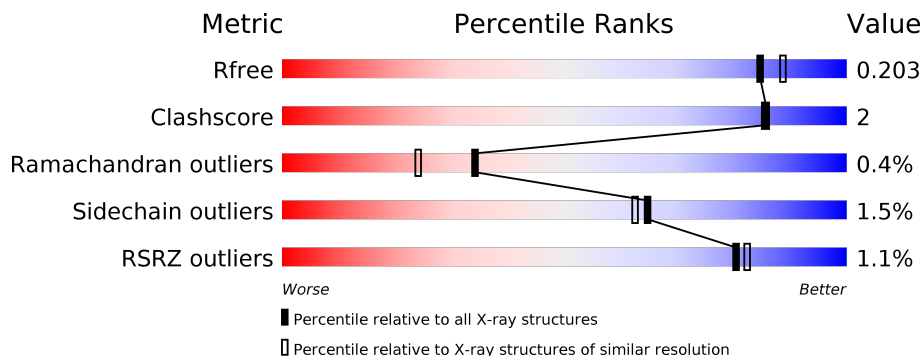
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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  $\geq 3$ , 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	280	
1	B	280	
1	C	280	
1	D	280	
1	E	280	
1	F	280	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14067 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.

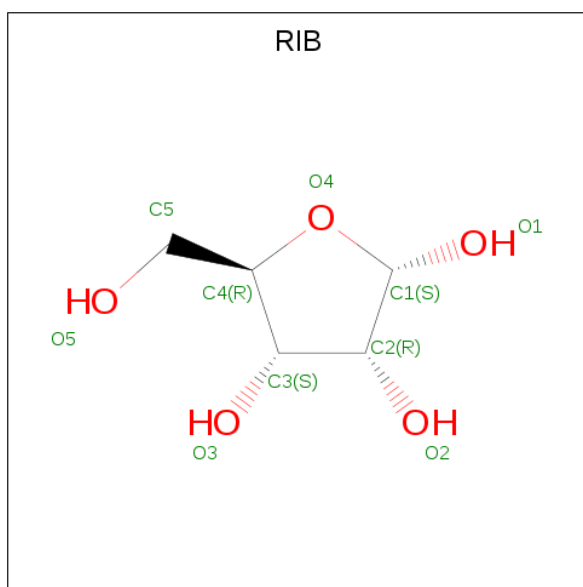
- Molecule 1 is a protein called Ribose transcriptional regulator.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	267	2119	1362	349	403	2	3	0	1	0
1	B	268	2137	1374	351	407	2	3	0	3	0
1	C	268	2150	1383	355	406	2	4	0	5	0
1	D	269	2138	1373	352	408	2	3	0	3	0
1	E	268	2130	1369	350	405	2	4	0	2	0
1	F	268	2137	1373	350	408	2	4	0	4	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	SER	-	expression tag	UNP I3TZ89
A	329	PHE	LEU	conflict	UNP I3TZ89
B	60	SER	-	expression tag	UNP I3TZ89
B	329	PHE	LEU	conflict	UNP I3TZ89
C	60	SER	-	expression tag	UNP I3TZ89
C	329	PHE	LEU	conflict	UNP I3TZ89
D	60	SER	-	expression tag	UNP I3TZ89
D	329	PHE	LEU	conflict	UNP I3TZ89
E	60	SER	-	expression tag	UNP I3TZ89
E	329	PHE	LEU	conflict	UNP I3TZ89
F	60	SER	-	expression tag	UNP I3TZ89
F	329	PHE	LEU	conflict	UNP I3TZ89

- Molecule 2 is alpha-D-ribofuranose (three-letter code: RIB) (formula: C<sub>5</sub>H<sub>10</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 5 5	0	0
2	B	1	Total C O 10 5 5	0	0
2	C	1	Total C O 10 5 5	0	0
2	D	1	Total C O 10 5 5	0	0
2	E	1	Total C O 10 5 5	0	0
2	F	1	Total C O 10 5 5	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	4	Total Cl 4 4	0	0
3	E	1	Total Cl 1 1	0	0
3	B	5	Total Cl 5 5	0	0
3	C	5	Total Cl 5 5	0	0
3	A	3	Total Cl 3 3	0	0
3	F	3	Total Cl 3 3	0	0

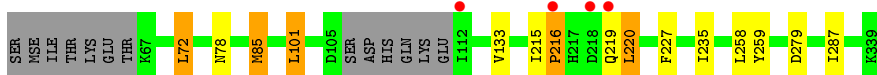
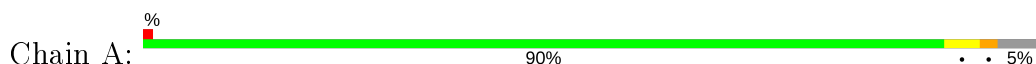
- Molecule 4 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	A	208	Total 208	O 208	0	0
4	B	197	Total 197	O 197	0	0
4	C	195	Total 195	O 195	0	0
4	D	205	Total 205	O 205	0	0
4	E	175	Total 175	O 175	0	0
4	F	195	Total 195	O 195	0	0

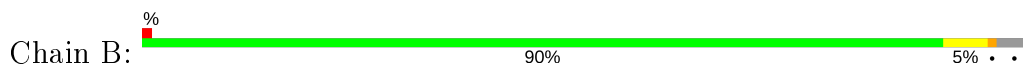
### 3 Residue-property plots [i](#)

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.

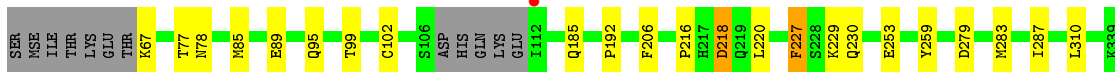
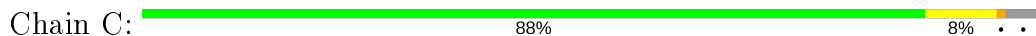
- Molecule 1: Ribose transcriptional regulator



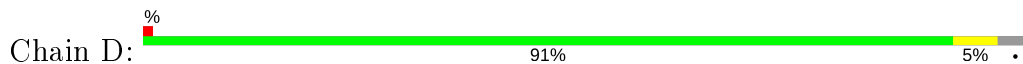
- Molecule 1: Ribose transcriptional regulator



- Molecule 1: Ribose transcriptional regulator




- Molecule 1: Ribose transcriptional regulator



- Molecule 1: Ribose transcriptional regulator



- Molecule 1: Ribose transcriptional regulator

Chain F:  %  
91%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.37Å 95.24Å 123.60Å 90.00° 119.47° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 40.74 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-1.90) 99.4 (40.74-1.89)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.159 , 0.192 0.174 , 0.203	Depositor DCC
$R_{free}$ test set	5744 reflections (2.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.0	Xtriage
Anisotropy	0.558	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.115 for -h-l,k,h 0.115 for l,k,-h-l 0.309 for h,-k,-h-l 0.125 for -h-l,-k,l 0.138 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14067	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.88% 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: RIB, CL

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	0.38	0/2162	0.61	1/2922 (0.0%)
1	B	0.37	0/2186	0.58	0/2953
1	C	0.39	0/2205	0.59	0/2977
1	D	0.36	0/2187	0.57	0/2956
1	E	0.37	0/2176	0.58	0/2940
1	F	0.36	0/2189	0.57	0/2959
All	All	0.37	0/13105	0.58	1/17707 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	MSE	CG-SE-CE	-5.27	87.31	98.90

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	2119	0	2122	10	0
1	B	2137	0	2146	10	0
1	C	2150	0	2170	13	0
1	D	2138	0	2140	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2130	0	2136	9	0
1	F	2137	0	2137	7	0
2	A	10	0	0	2	0
2	B	10	0	0	3	0
2	C	10	0	0	2	0
2	D	10	0	0	3	0
2	E	10	0	0	3	0
2	F	10	0	0	3	0
3	A	3	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	4	0	0	0	0
3	E	1	0	0	0	0
3	F	3	0	0	0	0
4	A	208	0	0	0	0
4	B	197	0	0	0	0
4	C	195	0	0	1	0
4	D	205	0	0	0	0
4	E	175	0	0	0	0
4	F	195	0	0	0	0
All	All	14067	0	12851	56	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 2.

The worst 5 of 56 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:78:ASN:HD21	2:A:401:RIB:C5	2.00	0.74
1:A:85:MSE:HG3	1:A:101:LEU:HD13	1.70	0.73
1:A:78:ASN:ND2	2:A:401:RIB:C5	2.53	0.72
1:F:78:ASN:HD21	2:F:401:RIB:C5	2.03	0.71
1:D:78:ASN:HD21	2:D:401:RIB:C5	2.09	0.66

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	264/280 (94%)	255 (97%)	7 (3%)	2 (1%)	19	9
1	B	267/280 (95%)	260 (97%)	6 (2%)	1 (0%)	34	24
1	C	269/280 (96%)	261 (97%)	7 (3%)	1 (0%)	34	24
1	D	268/280 (96%)	261 (97%)	6 (2%)	1 (0%)	34	24
1	E	266/280 (95%)	259 (97%)	6 (2%)	1 (0%)	34	24
1	F	268/280 (96%)	261 (97%)	6 (2%)	1 (0%)	34	24
All	All	1602/1680 (95%)	1557 (97%)	38 (2%)	7 (0%)	34	24

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	279	ASP
1	B	279	ASP
1	C	279	ASP
1	D	279	ASP
1	E	279	ASP

### 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	230/238 (97%)	226 (98%)	4 (2%)	60	57
1	B	233/238 (98%)	231 (99%)	2 (1%)	78	79
1	C	235/238 (99%)	229 (97%)	6 (3%)	46	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	233/238 (98%)	231 (99%)	2 (1%)	78	79
1	E	232/238 (98%)	228 (98%)	4 (2%)	60	57
1	F	233/238 (98%)	229 (98%)	4 (2%)	60	57
All	All	1396/1428 (98%)	1374 (98%)	22 (2%)	65	60

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	185[B]	GLN
1	D	105	ASP
1	F	227	PHE
1	C	218	ASP
1	C	227	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	226	GLN
1	C	296	GLN
1	E	296	GLN
1	C	217	HIS
1	E	226	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 monosaccharides in this entry.

## 5.6 Ligand geometry

Of 27 ligands modelled in this entry, 21 are monoatomic - leaving 6 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	RIB	C	401	-	10,10,10	1.13	2 (20%)	13,14,14	3.12	7 (53%)
2	RIB	D	401	-	10,10,10	0.84	0	13,14,14	3.19	6 (46%)
2	RIB	E	401	-	10,10,10	0.90	0	13,14,14	3.12	7 (53%)
2	RIB	F	401	-	10,10,10	1.12	0	13,14,14	3.46	8 (61%)
2	RIB	A	401	-	10,10,10	0.91	0	13,14,14	2.79	6 (46%)
2	RIB	B	401	-	10,10,10	0.86	0	13,14,14	2.85	4 (30%)

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	RIB	C	401	-	-	0/2/18/18	0/1/1/1
2	RIB	D	401	-	-	0/2/18/18	0/1/1/1
2	RIB	E	401	-	-	0/2/18/18	0/1/1/1
2	RIB	F	401	-	-	0/2/18/18	0/1/1/1
2	RIB	A	401	-	-	0/2/18/18	0/1/1/1
2	RIB	B	401	-	-	0/2/18/18	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	RIB	C1-C2	2.32	1.55	1.52
2	C	401	RIB	C5-C4	-2.20	1.44	1.51

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	RIB	C5-C4-C3	-6.95	98.33	115.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	RIB	C5-C4-C3	-6.49	99.44	115.09
2	D	401	RIB	C5-C4-C3	-6.23	100.08	115.09
2	C	401	RIB	O4-C1-C2	6.00	111.84	104.46
2	D	401	RIB	O4-C1-C2	5.98	111.82	104.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	RIB	2	0
2	D	401	RIB	3	0
2	E	401	RIB	3	0
2	F	401	RIB	3	0
2	A	401	RIB	2	0
2	B	401	RIB	3	0

## 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, 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	264/280 (94%)	-0.40	4 (1%) 73 76	22, 30, 63, 110	0
1	B	265/280 (94%)	-0.38	3 (1%) 80 82	22, 32, 64, 107	0
1	C	265/280 (94%)	-0.43	1 (0%) 92 93	21, 31, 61, 113	0
1	D	266/280 (95%)	-0.38	4 (1%) 73 76	22, 32, 67, 104	0
1	E	265/280 (94%)	-0.45	3 (1%) 80 82	23, 33, 63, 109	0
1	F	265/280 (94%)	-0.45	2 (0%) 86 87	24, 33, 62, 126	0
All	All	1590/1680 (94%)	-0.42	17 (1%) 80 82	21, 32, 64, 126	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	218	ASP	5.0
1	E	112	ILE	4.9
1	A	219	GLN	4.1
1	A	112	ILE	3.6
1	C	112	ILE	3.6

### 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	RIB	D	401	10/10	0.86	0.14	23,29,42,52	0
2	RIB	C	401	10/10	0.88	0.17	20,26,36,46	0
2	RIB	F	401	10/10	0.89	0.16	23,30,36,52	0
2	RIB	E	401	10/10	0.89	0.17	21,28,36,52	0
2	RIB	B	401	10/10	0.92	0.14	25,27,40,47	0
2	RIB	A	401	10/10	0.92	0.15	21,26,40,42	0
3	CL	F	403	1/1	0.94	0.07	48,48,48,48	0
3	CL	D	402	1/1	0.96	0.06	46,46,46,46	0
3	CL	D	404	1/1	0.96	0.04	62,62,62,62	0
3	CL	A	403	1/1	0.97	0.09	48,48,48,48	0
3	CL	B	405	1/1	0.97	0.05	56,56,56,56	0
3	CL	B	406	1/1	0.97	0.11	46,46,46,46	0
3	CL	F	402	1/1	0.97	0.09	47,47,47,47	0
3	CL	B	403	1/1	0.98	0.07	43,43,43,43	0
3	CL	C	406	1/1	0.98	0.08	50,50,50,50	0
3	CL	B	402	1/1	0.98	0.07	46,46,46,46	0
3	CL	F	404	1/1	0.98	0.07	45,45,45,45	0
3	CL	C	403	1/1	0.99	0.26	63,63,63,63	0
3	CL	C	402	1/1	0.99	0.09	51,51,51,51	0
3	CL	D	403	1/1	0.99	0.09	43,43,43,43	0
3	CL	B	404	1/1	0.99	0.12	45,45,45,45	0
3	CL	A	402	1/1	0.99	0.05	28,28,28,28	0
3	CL	A	404	1/1	0.99	0.07	39,39,39,39	0
3	CL	D	405	1/1	0.99	0.08	39,39,39,39	0
3	CL	C	404	1/1	1.00	0.05	28,28,28,28	0
3	CL	C	405	1/1	1.00	0.03	38,38,38,38	0
3	CL	E	402	1/1	1.00	0.06	32,32,32,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.