



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 02:11 PM UTC

PDB ID : 1ECX / pdb\_00001ecx  
Title : NIFS-LIKE PROTEIN  
Authors : Kaiser, J.T.; Clausen, T.C.; Bourenkow, G.P.; Bartunik, H.-D.; Steinbacher, S.; Huber, R.  
Deposited on : 2000-01-26  
Resolution : 2.70 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.

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  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (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

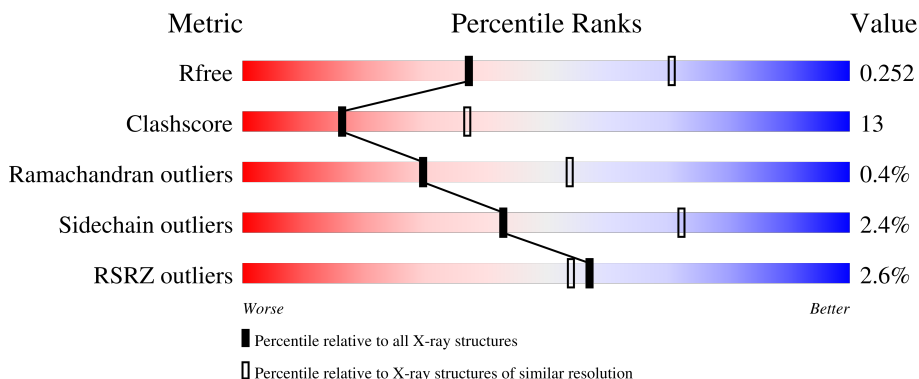
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	384	 2% 69% 24% • 5%
1	B	384	 3% 72% 20% • 5%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5938 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.

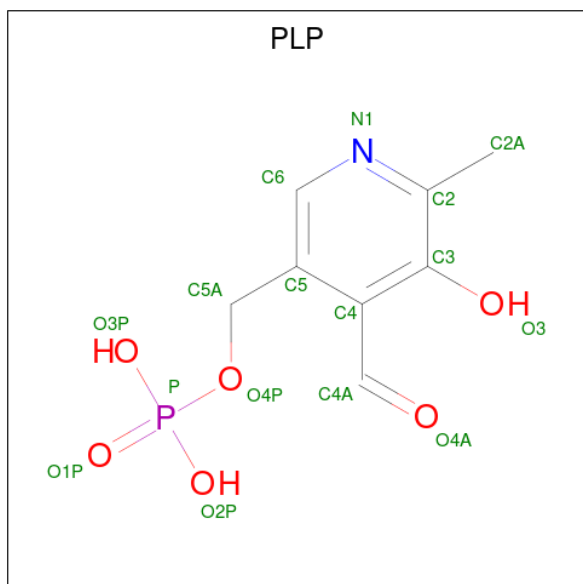
- Molecule 1 is a protein called AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	364	Total 2853	C 1817	N 492	O 531	S 13	62	0	0
1	B	365	Total 2864	C 1823	N 496	O 532	S 13	44	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	332	ARG	SER	see remark 999	UNP Q9X218
B	332	ARG	SER	see remark 999	UNP Q9X218

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



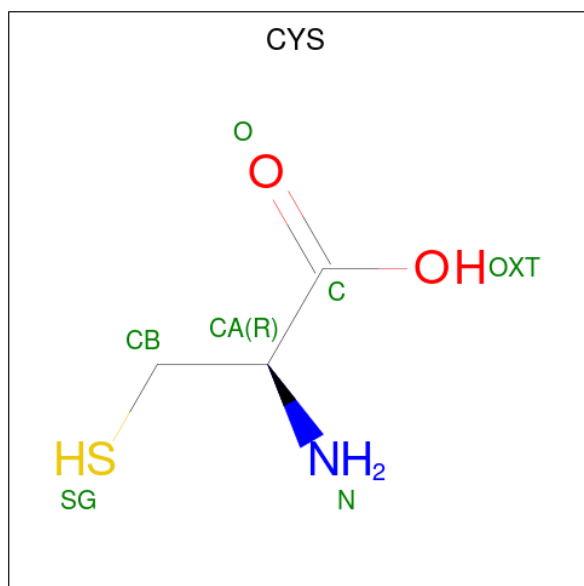
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 15	C 8	N 1	O 5	P 1	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is CYSTEINE (CCD ID: CYS) (formula: C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			6	3	1	1	1		
3	B	1	Total	C	N	O	S	0	0
			6	3	1	1	1		

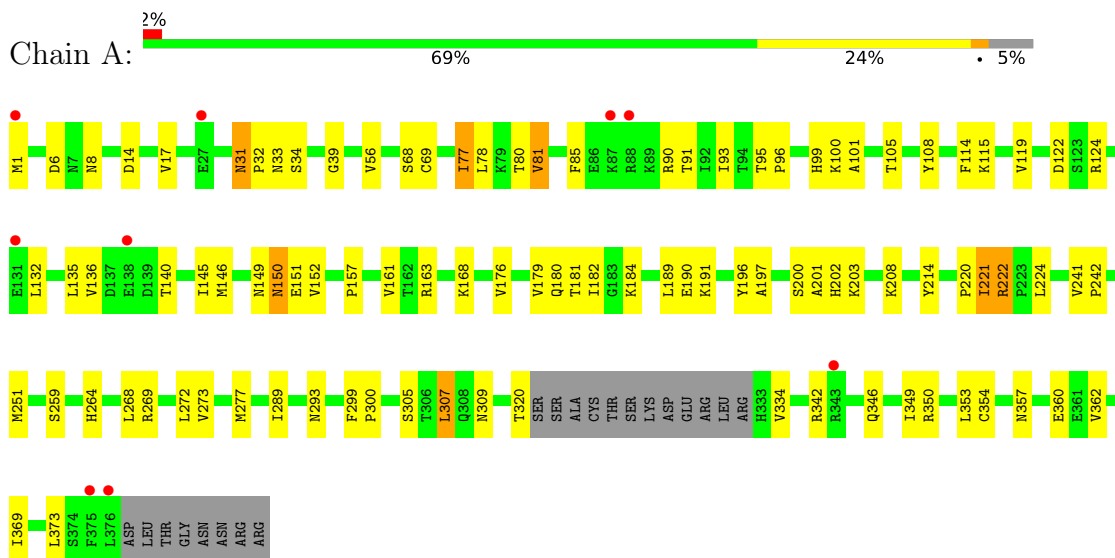
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	75	Total	O	0	0
			75	75		
4	B	104	Total	O	0	0
			104	104		

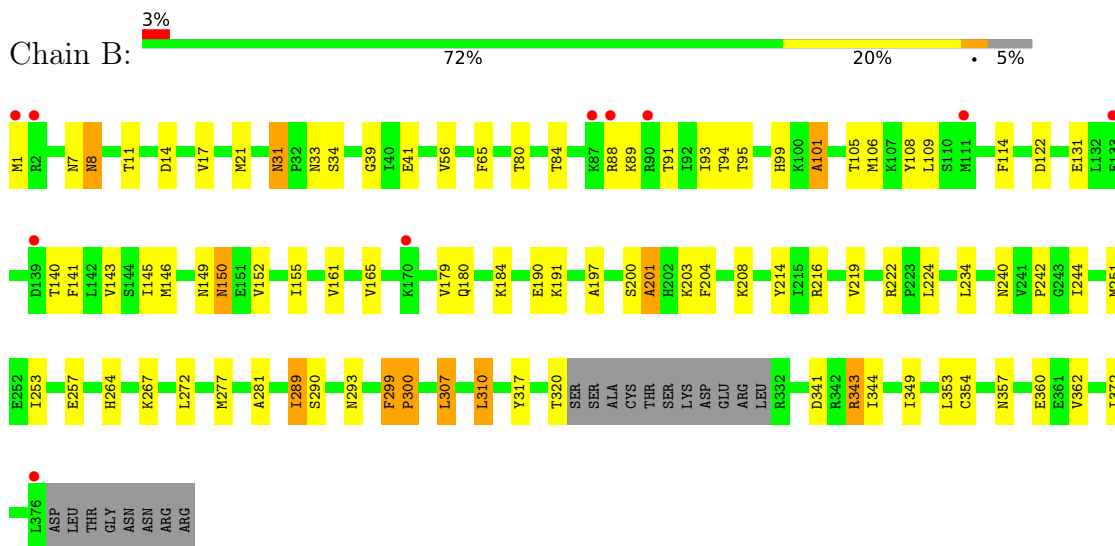
### 3 Residue-property plots

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: AMINOTRANSFERASE



- Molecule 1: AMINOTRANSFERASE



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.41Å 115.41Å 156.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.04 – 2.70 34.04 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (34.04-2.70) 99.2 (34.04-2.70)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 2.68Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.207 , 0.256 0.206 , 0.252	Depositor DCC
$R_{free}$ test set	1661 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.5	Xtrriage
Anisotropy	0.071	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 56.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5938	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.43% 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: PLP

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	0.42	0/2899	0.92	6/3907 (0.2%)
1	B	0.43	0/2910	0.94	8/3921 (0.2%)
All	All	0.42	0/5809	0.93	14/7828 (0.2%)

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	LEU	N-CA-C	-9.46	101.87	113.41
1	B	224	LEU	N-CA-C	-7.66	102.86	112.90
1	B	179	VAL	N-CA-C	5.87	117.31	110.62
1	A	77	ILE	N-CA-C	5.57	115.77	110.53
1	A	179	VAL	N-CA-C	5.54	116.18	110.36

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	2853	0	2941	78	0
1	B	2864	0	2954	73	0
2	A	15	0	6	2	0
2	B	15	0	7	2	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	6	0	4	2	0
3	B	6	0	4	1	0
4	A	75	0	0	4	0
4	B	104	0	0	5	0
All	All	5938	0	5916	148	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 13.

The worst 5 of 148 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:203:LYS:HZ1	2:A:500:PLP:C4A	1.59	1.15
1:A:353:LEU:C	1:A:354:CYS:N	2.24	0.95
1:B:150:ASN:HD22	1:B:150:ASN:H	1.14	0.94
1:A:119:VAL:HG22	1:A:135:LEU:HD12	1.49	0.94
1:A:150:ASN:H	1:A:150:ASN:HD22	1.14	0.91

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	358/384 (93%)	336 (94%)	21 (6%)	1 (0%)	36	60
1	B	359/384 (94%)	340 (95%)	17 (5%)	2 (1%)	21	44
All	All	717/768 (93%)	676 (94%)	38 (5%)	3 (0%)	30	54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	ILE
1	B	300	PRO
1	B	289	ILE

### 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	315/333 (95%)	308 (98%)	7 (2%)	45 74
1	B	316/333 (95%)	309 (98%)	7 (2%)	45 74
All	All	631/666 (95%)	617 (98%)	14 (2%)	43 74

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	31	ASN
1	B	131	GLU
1	B	343	ARG
1	B	307	LEU
1	B	310	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	7	ASN
1	B	33	ASN
1	B	264	HIS
1	B	31	ASN
1	B	75	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](#)

4 ligands are modelled in this entry.

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	PLP	B	501	-	15,15,16	1.69	4 (26%)	21,22,23	2.03	5 (23%)
3	CYS	A	502	-	4,5,6	1.20	0	1,5,7	0.00	0
3	CYS	B	503	-	4,5,6	0.53	0	1,5,7	0.08	0
2	PLP	A	500	-	15,15,16	1.77	4 (26%)	21,22,23	2.07	4 (19%)

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	PLP	B	501	-	-	0/6/6/8	0/1/1/1
3	CYS	A	502	-	-	1/1/4/6	-
3	CYS	B	503	-	-	0/1/4/6	-
2	PLP	A	500	-	-	0/6/6/8	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	PLP	C3-C2	-3.40	1.37	1.41
2	B	501	PLP	C3-C2	-2.94	1.37	1.41

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	PLP	C5-C4	2.84	1.43	1.40
2	A	500	PLP	C5-C4	2.82	1.43	1.40
2	A	500	PLP	C2-N1	2.76	1.38	1.33

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	PLP	O4P-C5A-C5	6.21	121.00	109.36
2	B	501	PLP	O4P-C5A-C5	5.65	119.94	109.36
2	B	501	PLP	O2P-P-O4P	-4.29	95.48	106.67
2	A	500	PLP	O2P-P-O4P	-4.18	95.76	106.67
2	B	501	PLP	O3P-P-O1P	2.66	121.19	110.83

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	CYS	N-CA-CB-SG

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	PLP	2	0
3	A	502	CYS	2	0
3	B	503	CYS	1	0
2	A	500	PLP	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	353:LEU	C	354:CYS	N	2.38
1	A	353:LEU	C	354:CYS	N	2.24

## 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	364/384 (94%)	-0.17	9 (2%) 58 55	19, 33, 54, 65	25 (6%)
1	B	365/384 (95%)	-0.30	10 (2%) 56 53	18, 31, 50, 70	21 (5%)
All	All	729/768 (94%)	-0.24	19 (2%) 57 54	18, 32, 53, 70	46 (6%)

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	376	LEU	4.6
1	B	376	LEU	3.6
1	B	1	MET	2.9
1	B	133	GLU	2.7
1	B	88	ARG	2.6

### 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 oligosaccharides 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( $\text{\AA}^2$ )	Q<0.9
3	CYS	A	502	6/7	0.87	0.23	58,61,62,63	0
3	CYS	B	503	6/7	0.91	0.16	46,49,51,52	0
2	PLP	A	500	15/16	0.97	0.07	32,34,40,41	0
2	PLP	B	501	15/16	0.97	0.08	24,28,30,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.