



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 28, 2017 – 11:29 AM EDT

PDB ID : 5T0O
Title : Crystal Structure of a membrane protein
Authors : Su, C.-C.; Yu, E.W.
Deposited on : unknown
Resolution : 3.15 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

<http://wwpdb.org/validation/2016/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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029824

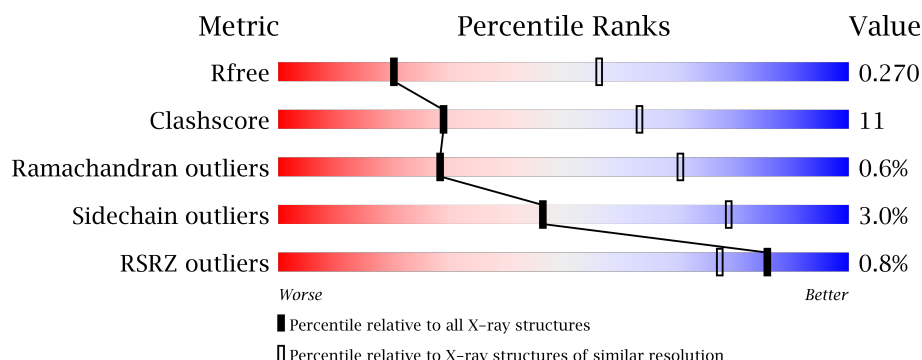
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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}	100719	1259 (3.20-3.12)
Clashscore	112137	1397 (3.20-3.12)
Ramachandran outliers	110173	1368 (3.20-3.12)
Sidechain outliers	110143	1367 (3.20-3.12)
RSRZ outliers	101464	1264 (3.20-3.12)

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. 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	1040	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 72%, green 26%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 72% 26% </div> </div>
1	B	1040	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 73%, green 24%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 73% 24% </div> </div>
1	C	1040	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 74%, green 25%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 74% 25% </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23901 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 CmeB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1033	Total	C	N	O	S	0	0	0
			7971	5154	1301	1484	32			
1	B	1026	Total	C	N	O	S	0	0	0
			7914	5119	1292	1471	32			
1	C	1035	Total	C	N	O	S	0	0	0
			7991	5166	1307	1486	32			

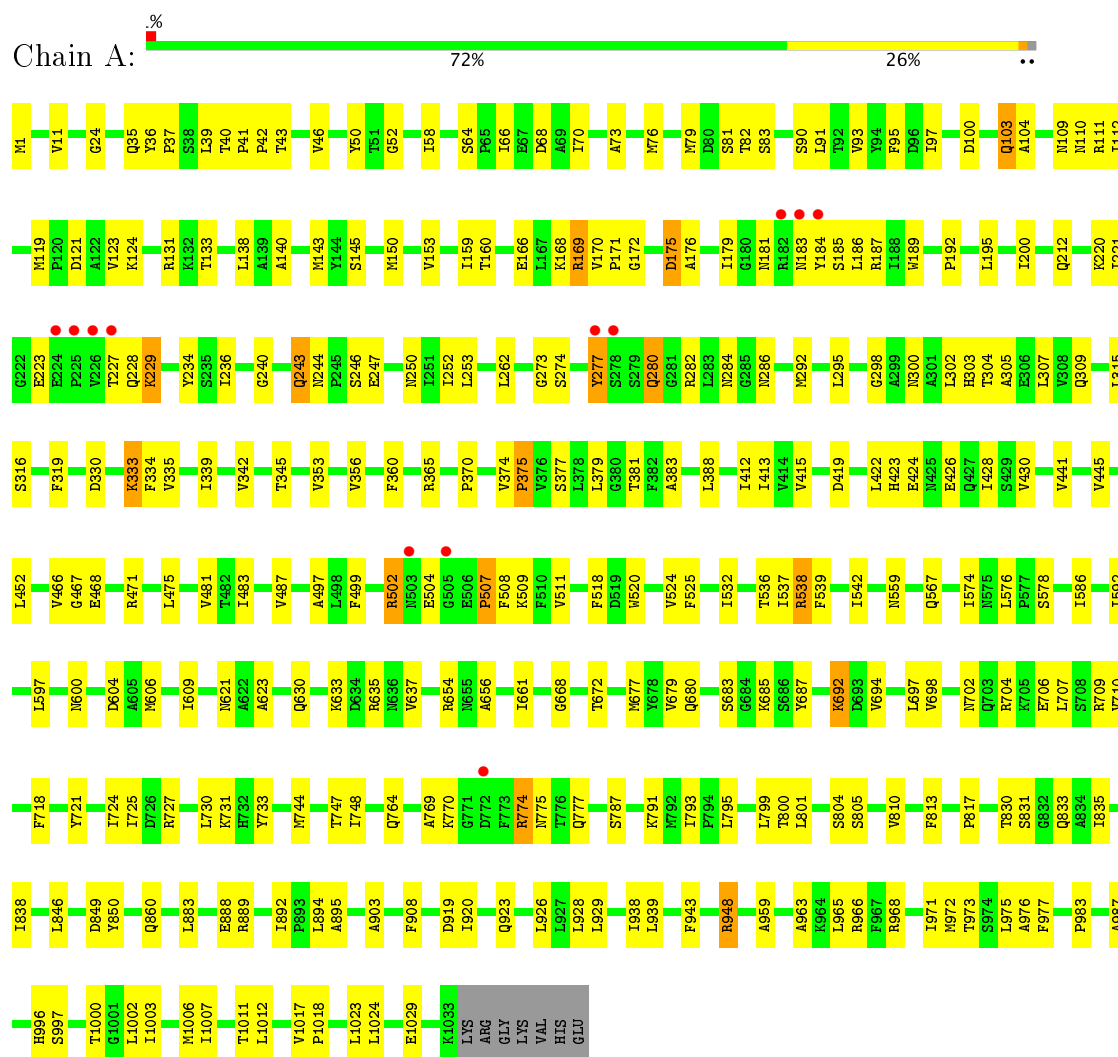
- Molecule 2 is water.

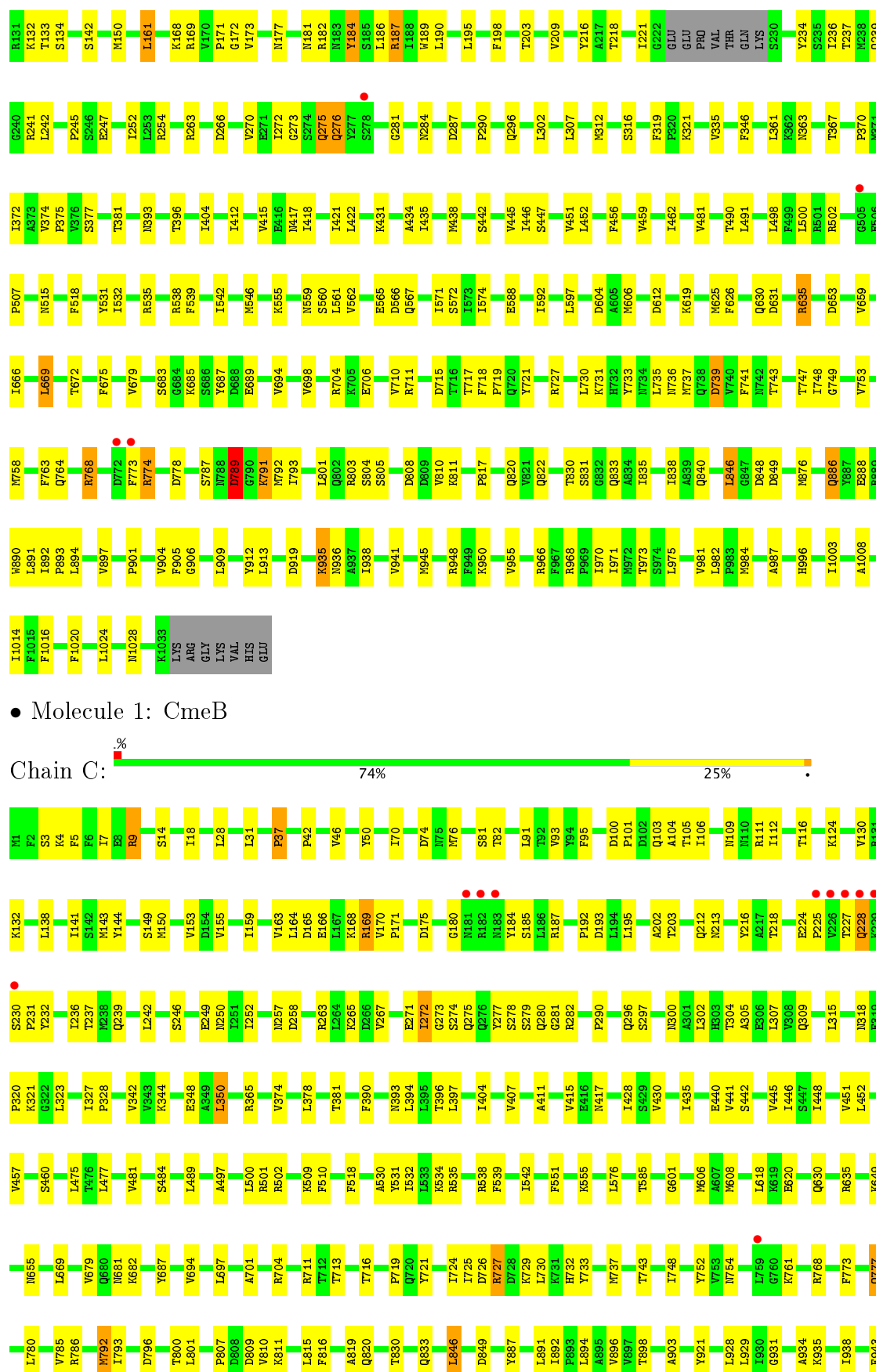
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	O	0	0
			5	5		
2	B	11	Total	O	0	0
			11	11		
2	C	9	Total	O	0	0
			9	9		

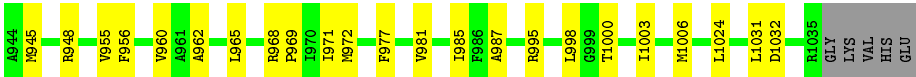
3 Residue-property plots

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: CmeB







4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	300.71Å 147.54Å 120.03Å 90.00° 99.87° 90.00°	Depositor
Resolution (Å)	84.93 – 3.15 84.93 – 3.15	Depositor EDS
% Data completeness (in resolution range)	89.1 (84.93-3.15) 89.2 (84.93-3.15)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 3.13Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.211 , 0.268 0.213 , 0.270	Depositor DCC
R_{free} test set	4021 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	57.2	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	23901	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.30	2/8127 (0.0%)	0.48	0/11029
1	B	0.27	0/8068	0.48	4/10947 (0.0%)
1	C	0.29	0/8147	0.48	0/11054
All	All	0.29	2/24342 (0.0%)	0.48	4/33030 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	C	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	103	GLN	CD-OE1	-6.53	1.09	1.24
1	A	103	GLN	CD-NE2	-5.57	1.19	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	39	LEU	CA-CB-CG	7.16	131.76	115.30
1	B	789	ASP	CB-CG-OD2	5.60	123.34	118.30
1	B	161	LEU	CA-CB-CG	5.56	128.08	115.30
1	B	498	LEU	CA-CB-CG	5.49	127.93	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	275	GLN	Peptide
1	B	886	GLN	Peptide
1	C	185	SER	Peptide

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	7971	0	8114	196	0
1	B	7914	0	8057	180	0
1	C	7991	0	8140	187	0
2	A	5	0	0	0	0
2	B	11	0	0	0	0
2	C	9	0	0	0	0
All	All	23901	0	24311	525	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 11.

The worst 5 of 525 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:789:ASP:OD2	1:B:791:LYS:NZ	1.91	1.01
1:A:333:LYS:NZ	1:A:567:GLN:O	2.06	0.89
1:C:687:TYR:CZ	1:C:810:VAL:HG13	2.10	0.86
1:C:82:THR:HB	1:C:811:LYS:HE3	1.59	0.84
1:C:46:VAL:HG13	1:C:130:VAL:HG12	1.60	0.84

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	1031/1040 (99%)	959 (93%)	67 (6%)	5 (0%)	32	73
1	B	1022/1040 (98%)	956 (94%)	62 (6%)	4 (0%)	38	76
1	C	1033/1040 (99%)	956 (92%)	67 (6%)	10 (1%)	18	60
All	All	3086/3120 (99%)	2871 (93%)	196 (6%)	19 (1%)	28	70

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	507	PRO
1	C	394	LEU
1	B	150	MET
1	B	276	GLN
1	C	37	PRO

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	868/875 (99%)	844 (97%)	24 (3%)	49	80
1	B	861/875 (98%)	829 (96%)	32 (4%)	39	75
1	C	870/875 (99%)	849 (98%)	21 (2%)	54	83
All	All	2599/2625 (99%)	2522 (97%)	77 (3%)	46	79

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	266	ASP
1	B	635	ARG
1	C	773	PHE
1	B	287	ASP
1	B	546	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	239	GLN
1	A	243	GLN
1	B	923	GLN
1	C	775	ASN
1	C	777	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 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	1033/1040 (99%)	-0.16	12 (1%) 79 66	17, 41, 87, 160	0
1	B	1026/1040 (98%)	-0.23	4 (0%) 92 89	13, 39, 78, 139	0
1	C	1035/1040 (99%)	-0.32	10 (0%) 82 71	9, 30, 72, 126	0
All	All	3094/3120 (99%)	-0.24	26 (0%) 86 77	9, 38, 80, 160	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	183	ASN	6.0
1	A	225	PRO	5.5
1	A	277	TYR	4.5
1	C	229	LYS	4.3
1	C	228	GLN	3.9

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.