W O R L D W I D E

wwPDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jul 13, 2016 – 07:59 PM EDT

PDB ID	:	5IGO
Title	:	WD40 domain of Arabidopsis thaliana E3 Ubiquitin Ligase COP1 in complex with peptide from Trib1
Authors	:	Uljon, S.; Blacklow, S.C.
Deposited on	:	2016-02-28
Resolution	:	1.60 Å(reported)

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

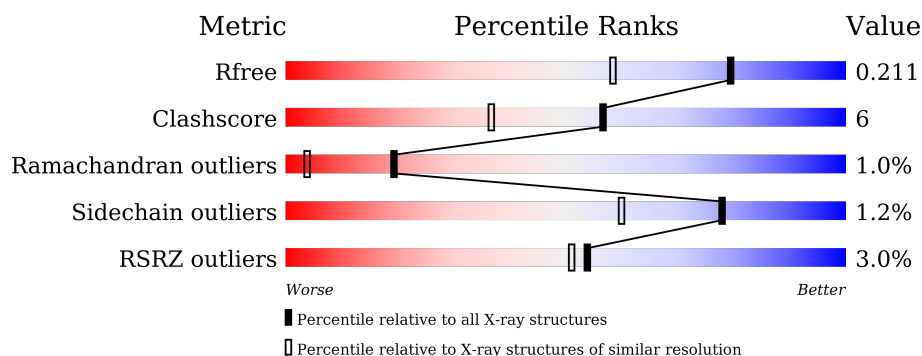|		
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027790
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

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 1.60 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	Percentile Ranks	Value
Rfree		0.211
Clashscore		6
Ramachandran outliers		1.0%
Sidechain outliers		1.2%
RSRZ outliers		3.0%

Worse — *Better*

▌ Percentile relative to all X-ray structures

❒ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

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 <=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	336	4% 85% 9% ·· ·
1	B	336	3% 86% 7% · ·
1	C	336	3% 84% 11% · ·
1	D	336	% 84% 10% · ·
2	U	8	100%
2	V	8	88% 13%

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Mol	Chain	Length	Quality of chain
2	W	8	100%
2	X	8	88% 13%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11580 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 E3 ubiquitin-protein ligase COP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total 2506	C 1568	N 434	O 488	S 16	0	1	0
1	B	321	Total 2508	C 1569	N 433	O 489	S 17	0	1	0
1	C	323	Total 2518	C 1578	N 437	O 486	S 17	0	1	0
1	D	322	Total 2524	C 1581	N 437	O 489	S 17	0	1	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	340	MET	-	expression tag	UNP P43254
A	341	HIS	-	expression tag	UNP P43254
A	342	HIS	-	expression tag	UNP P43254
A	343	HIS	-	expression tag	UNP P43254
A	344	HIS	-	expression tag	UNP P43254
A	345	HIS	-	expression tag	UNP P43254
A	346	HIS	-	expression tag	UNP P43254
A	347	HIS	-	expression tag	UNP P43254
A	348	HIS	-	expression tag	UNP P43254
B	340	MET	-	expression tag	UNP P43254
B	341	HIS	-	expression tag	UNP P43254
B	342	HIS	-	expression tag	UNP P43254
B	343	HIS	-	expression tag	UNP P43254
B	344	HIS	-	expression tag	UNP P43254
B	345	HIS	-	expression tag	UNP P43254
B	346	HIS	-	expression tag	UNP P43254
B	347	HIS	-	expression tag	UNP P43254
B	348	HIS	-	expression tag	UNP P43254
C	340	MET	-	expression tag	UNP P43254
C	341	HIS	-	expression tag	UNP P43254
C	342	HIS	-	expression tag	UNP P43254

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Chain	Residue	Modelled	Actual	Comment	Reference
C	343	HIS	-	expression tag	UNP P43254
C	344	HIS	-	expression tag	UNP P43254
C	345	HIS	-	expression tag	UNP P43254
C	346	HIS	-	expression tag	UNP P43254
C	347	HIS	-	expression tag	UNP P43254
C	348	HIS	-	expression tag	UNP P43254
D	340	MET	-	expression tag	UNP P43254
D	341	HIS	-	expression tag	UNP P43254
D	342	HIS	-	expression tag	UNP P43254
D	343	HIS	-	expression tag	UNP P43254
D	344	HIS	-	expression tag	UNP P43254
D	345	HIS	-	expression tag	UNP P43254
D	346	HIS	-	expression tag	UNP P43254
D	347	HIS	-	expression tag	UNP P43254
D	348	HIS	-	expression tag	UNP P43254

- Molecule 2 is a protein called Tribbles homolog 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	U	8	Total 67	C 42	N 9	O 16	0	0	0
2	V	8	Total 67	C 42	N 9	O 16	0	0	0
2	W	8	Total 67	C 42	N 9	O 16	0	0	0
2	X	8	Total 67	C 42	N 9	O 16	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	283	Total 283	O 283	0	0
3	U	13	Total 13	O 13	0	0
3	B	326	Total 326	O 326	0	0
3	V	12	Total 12	O 12	0	0
3	C	300	Total 300	O 300	0	0
3	W	16	Total 16	O 16	0	0

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| Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	292	Total O 292 292	0	0
3	X	14	Total O 14 14	0	0

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 errors 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.
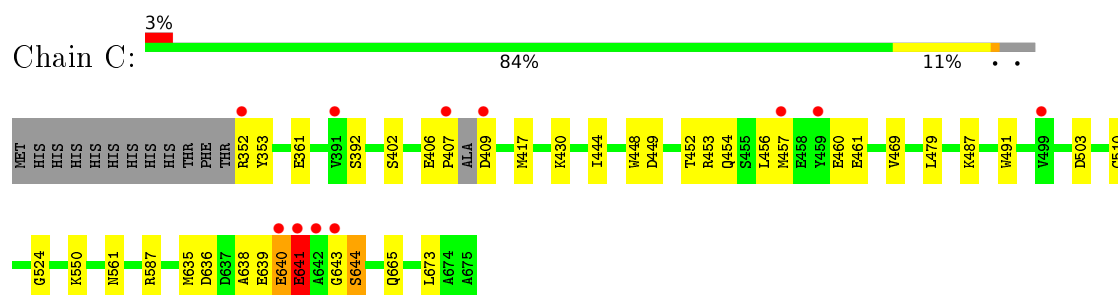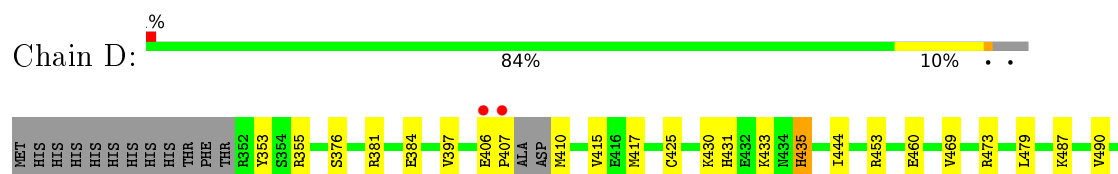
- Molecule 1: E3 ubiquitin-protein ligase COP1
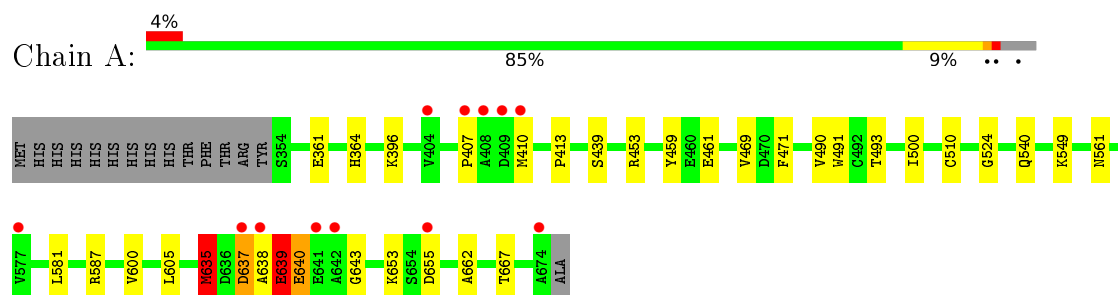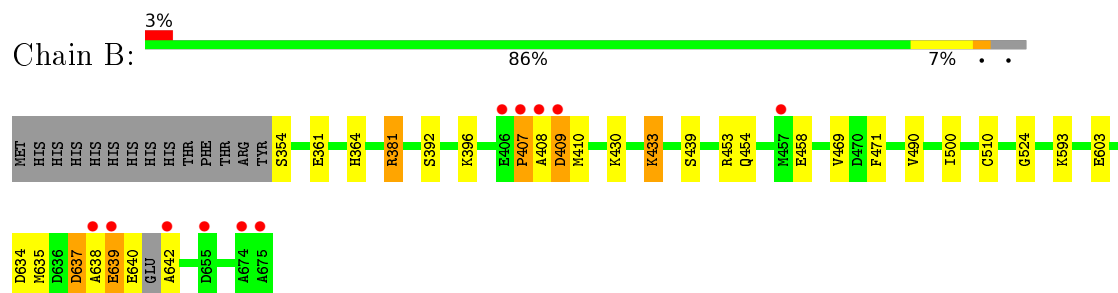
- Molecule 1: E3 ubiquitin-protein ligase COP1

- Molecule 1: E3 ubiquitin-protein ligase COP1

- Molecule 1: E3 ubiquitin-protein ligase COP1

I500 D503 C510 G524 S525 A526 M635 D636 D637 A638 E639 E640 E641 A642 G643 S644 D655 Q665 L673 A674 A675
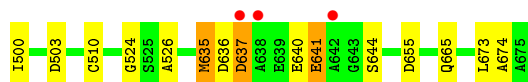
- Molecule 2: Tribbles homolog 1

Chain U:

100%

There are no outlier residues recorded for this chain.

- Molecule 2: Tribbles homolog 1

Chain V:

88%   13%

S354 Y361

- Molecule 2: Tribbles homolog 1

Chain W:

100%

There are no outlier residues recorded for this chain.

- Molecule 2: Tribbles homolog 1

Chain X:

88%   13%

S354 Y361

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.52Å 87.47Å 94.61Å 90.00° 92.55° 90.00°	Depositor
Resolution (Å)	64.20 – 1.60 94.52 – 1.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (64.20-1.60) 90.2 (94.52-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	0.86 (at 1.59Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.189 , 0.213 0.185 , 0.211	Depositor DCC
R_{free} test set	7975 reflections (5.24%)	DCC
Wilson B-factor (Å^2)	16.8	Xtriage
Anisotropy	0.633	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 56.3	EDS
L-test for twinning [2]	$<|L|> = 0.48, <L^2> = 0.31$	Xtriage
Estimated twinning fraction	0.115 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11580	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 79.94 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.0002e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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	0.43	0/2562	0.63	1/3480 (0.0%)
1	B	0.42	0/2563	0.66	0/3479
1	C	0.41	0/2574	0.65	1/3495 (0.0%)
1	D	0.42	0/2580	0.64	0/3501
2	U	0.37	0/68	0.46	0/91
2	V	0.34	0/68	0.48	0/91
2	W	0.46	0/68	0.50	0/91
2	X	0.49	0/68	0.50	0/91
All	All	0.42	0/10551	0.64	2/14319 (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	A	0	2
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	640	GLU	C-N-CA	5.47	135.37	121.70
1	A	635	MET	CG-SD-CE	5.22	108.55	100.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	637	ASP	Peptide
1	A	639	GLU	Peptide
1	C	641	GLU	Peptide
1	D	635	MET	Peptide

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	2506	0	2389	31	0
1	B	2508	0	2394	27	0
1	C	2518	0	2396	35	0
1	D	2524	0	2411	28	0
2	U	67	0	58	0	0
2	V	67	0	58	1	0
2	W	67	0	58	0	0
2	X	67	0	58	1	0
3	A	283	0	0	6	3
3	B	326	0	0	10	3
3	C	300	0	0	13	2
3	D	292	0	0	5	3
3	U	13	0	0	0	0
3	V	12	0	0	1	0
3	W	16	0	0	0	1
3	X	14	0	0	0	0
All	All	11580	0	9822	122	9

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 6.

The worst 5 of 122 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:510[B]:CYS:SG	3:B:849:HOH:O	1.96	1.24
1:C:510[B]:CYS:SG	3:C:755:HOH:O	2.01	1.17
1:A:510[B]:CYS:SG	3:A:834:HOH:O	2.08	1.08
1:C:352:ARG:NH2	3:C:701:HOH:O	1.91	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:GLU:OE1	3:B:701:HOH:O	1.81	0.96

The worst 5 of 9 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:854:HOH:O	3:D:961:HOH:O[2_656]	1.38	0.82
3:B:981:HOH:O	3:D:943:HOH:O[1_556]	1.84	0.36
3:A:742:HOH:O	3:A:756:HOH:O[2_556]	1.86	0.34
3:A:921:HOH:O	3:A:958:HOH:O[2_546]	1.97	0.23
3:D:989:HOH:O	3:D:992:HOH:O[2_646]	2.06	0.14

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	320/336 (95%)	304 (95%)	13 (4%)	3 (1%)	21	5
1	B	318/336 (95%)	304 (96%)	10 (3%)	4 (1%)	15	2
1	C	320/336 (95%)	302 (94%)	14 (4%)	4 (1%)	15	2
1	D	319/336 (95%)	304 (95%)	13 (4%)	2 (1%)	30	9
2	U	6/8 (75%)	6 (100%)	0	0	100	100
2	V	6/8 (75%)	6 (100%)	0	0	100	100
2	W	6/8 (75%)	6 (100%)	0	0	100	100
2	X	6/8 (75%)	6 (100%)	0	0	100	100
All	All	1301/1376 (94%)	1238 (95%)	50 (4%)	13 (1%)	19	4

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	639	GLU
1	A	640	GLU
1	B	410	MET
1	D	637	ASP
1	D	641	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	280/302 (93%)	275 (98%)	5 (2%)	66	41
1	B	281/302 (93%)	275 (98%)	6 (2%)	61	33
1	C	279/302 (92%)	279 (100%)	0	100	100
1	D	282/302 (93%)	279 (99%)	3 (1%)	80	63
2	U	8/8 (100%)	8 (100%)	0	100	100
2	V	8/8 (100%)	8 (100%)	0	100	100
2	W	8/8 (100%)	8 (100%)	0	100	100
2	X	8/8 (100%)	8 (100%)	0	100	100
All	All	1154/1240 (93%)	1140 (99%)	14 (1%)	78	60

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

Mol	Chain	Res	Type
1	B	381	ARG
1	B	409	ASP
1	D	435	HIS
1	B	354	SER
1	B	635	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	519	ASN

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Mol	Chain	Res	Type
1	D	665	GLN
1	D	435	HIS
1	B	364	HIS
1	C	665	GLN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

5.4   Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5   Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6   Ligand geometry ⓘ

There are no ligands in this entry.

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 (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	321/336 (95%)	0.17	12 (3%)	45	43	14, 23, 44, 72	0
1	B	321/336 (95%)	0.07	11 (3%)	49	45	14, 21, 42, 68	0
1	C	323/336 (96%)	0.09	11 (3%)	49	45	14, 22, 42, 64	0
1	D	322/336 (95%)	0.03	5 (1%)	74	74	15, 23, 44, 66	0
2	U	8/8 (100%)	0.05	0	100	100	20, 24, 36, 38	0
2	V	8/8 (100%)	-0.33	0	100	100	17, 22, 33, 33	0
2	W	8/8 (100%)	0.11	0	100	100	18, 22, 33, 34	0
2	X	8/8 (100%)	0.16	0	100	100	20, 25, 35, 41	0
All	All	1319/1376 (95%)	0.09	39 (2%)	54	51	14, 22, 44, 72	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	638	ALA	12.7
1	C	643	GLY	10.8
1	B	407	PRO	7.6
1	B	408	ALA	7.6
1	A	408	ALA	7.4

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.