wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 4, 2024 – 08:48 am GMT

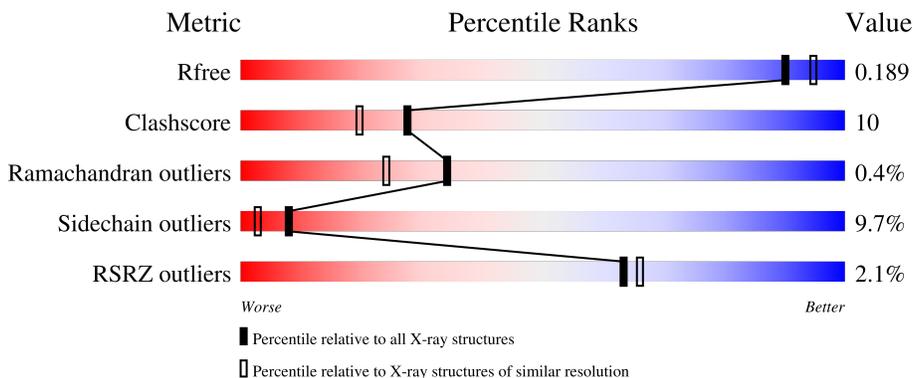|		
PDB ID	:	5FJZ
Title	:	Yeast delta-COP-I mu-homology domain complexed with Dsl1 WxWxV peptide
Authors	:	Suckling, R.J.; Evans, P.R.; Owen, D.J.
Deposited on	:	2015-10-14
Resolution	:	1.90 Å(reported)

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	Percentile Ranks	Value
Rfree		0.189
Clashscore		10
Ramachandran outliers		0.4%
Sidechain outliers		9.7%
RSRZ outliers		2.1%

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$_{free}$	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 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	270	% 76% 15% 6% ·
1	B	270	% 76% 18% · ·
1	C	270	77% 14% 6% ·
1	D	270	3% 73% 20% · ·
2	P	9	11% 22% 22% 22% 33%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	Q	9	22% · 33% / 33% / 33%
2	R	9	33% · 22% / 44% / 33%
2	S	9	22% · 22% / 33% / 11% / 33%
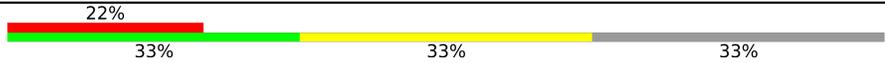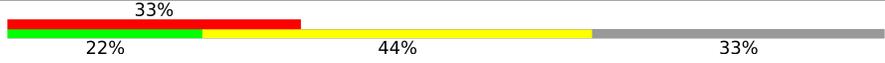
2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 9030 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 COATOMER SUBUNIT DELTA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	6	0
			2068	1301	336	425	6			
1	B	260	Total	C	N	O	S	0	7	0
			2055	1298	332	420	5			
1	C	262	Total	C	N	O	S	0	8	0
			2074	1306	334	428	6			
1	D	262	Total	C	N	O	S	0	4	0
			2053	1293	331	423	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	277	GLY	-	expression tag	UNP P43621
A	278	PRO	-	expression tag	UNP P43621
A	279	LEU	-	expression tag	UNP P43621
A	280	GLY	-	expression tag	UNP P43621
A	281	SER	-	expression tag	UNP P43621
A	404	ALA	TRP	engineered mutation	UNP P43621
B	277	GLY	-	expression tag	UNP P43621
B	278	PRO	-	expression tag	UNP P43621
B	279	LEU	-	expression tag	UNP P43621
B	280	GLY	-	expression tag	UNP P43621
B	281	SER	-	expression tag	UNP P43621
B	404	ALA	TRP	engineered mutation	UNP P43621
C	277	GLY	-	expression tag	UNP P43621
C	278	PRO	-	expression tag	UNP P43621
C	279	LEU	-	expression tag	UNP P43621
C	280	GLY	-	expression tag	UNP P43621
C	281	SER	-	expression tag	UNP P43621
C	404	ALA	TRP	engineered mutation	UNP P43621
D	277	GLY	-	expression tag	UNP P43621
D	278	PRO	-	expression tag	UNP P43621
D	279	LEU	-	expression tag	UNP P43621

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	280	GLY	-	expression tag	UNP P43621
D	281	SER	-	expression tag	UNP P43621
D	404	ALA	TRP	conflict	UNP P43621

- Molecule 2 is a protein called PROTEIN TRANSPORT PROTEIN DSL1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	6	Total 60	C 40	N 9	O 11	0	0	0
2	Q	6	Total 60	C 40	N 9	O 11	0	0	0
2	R	6	Total 60	C 40	N 9	O 11	0	0	0
2	S	6	Total 60	C 40	N 9	O 11	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	159	Total 159	O 159	0	0
3	B	124	Total 124	O 124	0	0
3	C	139	Total 139	O 139	0	0
3	D	115	Total 115	O 115	0	0
3	P	2	Total 2	O 2	0	0
3	R	1	Total 1	O 1	0	0

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: COATOMER SUBUNIT DELTA
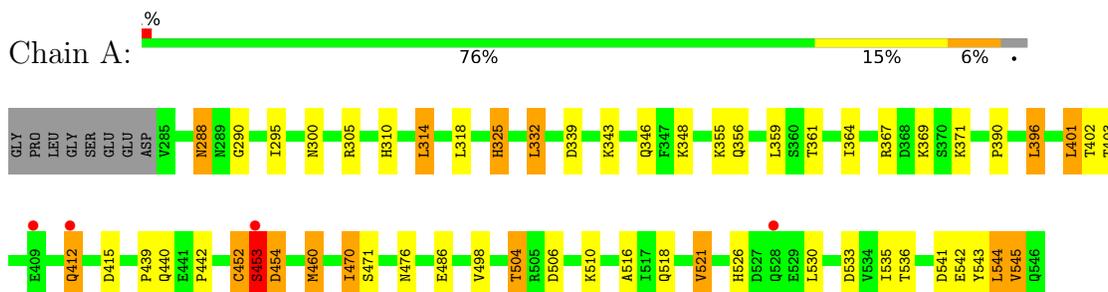
Chain A:

- Molecule 1: COATOMER SUBUNIT DELTA
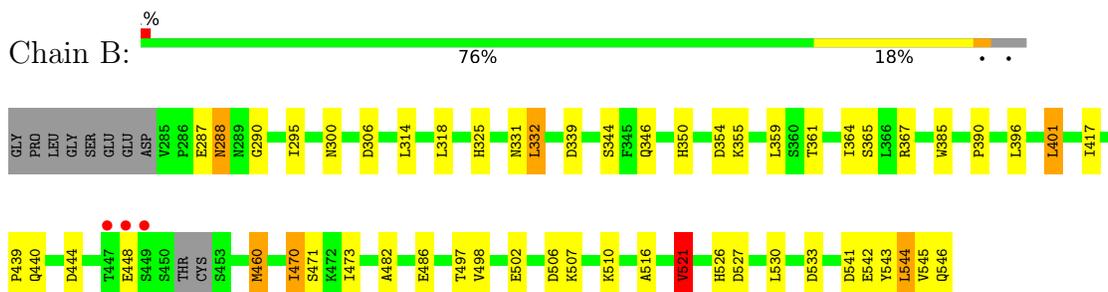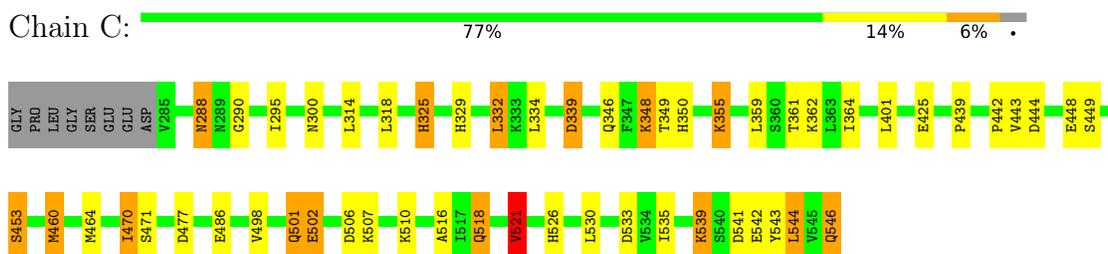
Chain B:

- Molecule 1: COATOMER SUBUNIT DELTA

Chain C:

- Molecule 1: COATOMER SUBUNIT DELTA

Chain D:

S410 Q411 Q412 D415 V423 P439 T447 E448 S449 S450 T451 C452 M460 I470 S471 A480 L481 A482 E486 V498 E502 S503 T504 R505 D506 K507 L508 A509 K510 M515 A516 I517 Q518 V521 N524 D525 H526 D527 L530 D533 D541 E542 Y543 L544

V545 Q546

• Molecule 2: PROTEIN TRANSPORT PROTEIN DSL1

Chain P:

11%
22% 22% 22% 33%

ASP D2 W3 N4 W5 E6 V7 GLU ASP

• Molecule 2: PROTEIN TRANSPORT PROTEIN DSL1

Chain Q:

22%
33% 33% 33%

ASP D2 W3 N4 V7 GLU ASP

• Molecule 2: PROTEIN TRANSPORT PROTEIN DSL1

Chain R:

33%
22% 44% 33%

ASP D2 W3 N4 W5 E6 V7 GLU ASP

• Molecule 2: PROTEIN TRANSPORT PROTEIN DSL1

Chain S:

22%
22% 33% 11% 33%

ASP D2 W3 N4 W5 E6 V7 GLU ASP
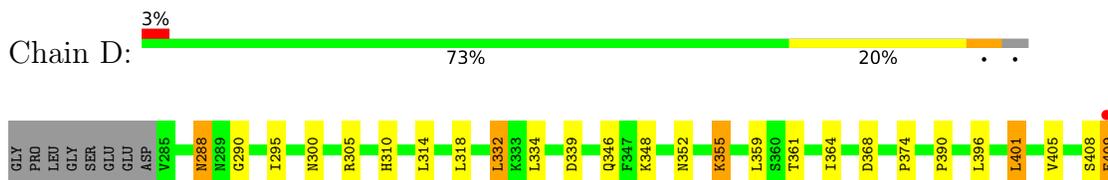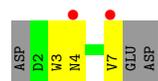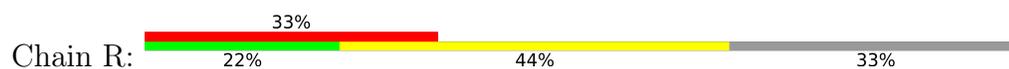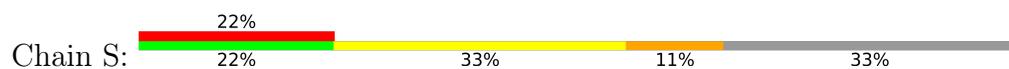
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	72.81Å 72.81Å 343.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.40 – 1.90 36.41 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.0 (36.40-1.90) 98.0 (36.41-1.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.87 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.145 , 0.186 0.148 , 0.189	Depositor DCC
R_{free} test set	4186 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	23.1	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 24.2	EDS
L-test for twinning[2]	$< |L| > = 0.36, < L^2 > = 0.18$	Xtriage
Estimated twinning fraction	0.397 for -h,-k,l	Xtriage
Reported twinning fraction	0.589 for H, K, L 0.411 for -h,-k,l	Depositor
Outliers	0 of 83159 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9030	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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	0.98	0/2121	1.06	11/2878 (0.4%)
1	B	1.01	1/2110 (0.0%)	1.06	8/2860 (0.3%)
1	C	0.98	1/2133 (0.0%)	1.08	12/2894 (0.4%)
1	D	0.93	0/2099	1.06	5/2849 (0.2%)
2	P	1.42	0/63	1.10	0/87
2	Q	0.73	0/63	0.74	0/87
2	R	0.90	0/63	0.77	0/87
2	S	1.12	1/63 (1.6%)	0.85	0/87
All	All	0.98	3/8715 (0.0%)	1.06	36/11829 (0.3%)

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	1
1	D	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	385	TRP	CE3-CZ3	-7.03	1.26	1.38
1	C	502	GLU	CD-OE1	6.80	1.33	1.25
2	S	3	TRP	CB-CG	5.02	1.59	1.50

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	325[A]	HIS	N-CA-CB	-7.44	97.21	110.60
1	C	325[B]	HIS	N-CA-CB	-7.44	97.21	110.60
1	A	453	SER	N-CA-CB	6.83	120.75	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	444	ASP	CB-CG-OD1	6.79	124.41	118.30
1	C	521	VAL	N-CA-CB	-6.42	97.37	111.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	453	SER	Peptide
1	D	452	CYS	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	2068	0	2050	48	0
1	B	2055	0	2049	34	0
1	C	2074	0	2059	45	1
1	D	2053	0	2037	45	1
2	P	60	0	44	5	0
2	Q	60	0	44	1	0
2	R	60	0	44	4	0
2	S	60	0	44	6	0
3	A	159	0	0	18	3
3	B	124	0	0	8	1
3	C	139	0	0	15	2
3	D	115	0	0	11	0
3	P	2	0	0	3	0
3	R	1	0	0	0	0
All	All	9030	0	8371	169	5

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 10.

The worst 5 of 169 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:D:415:ASP:O	3:D:2063:HOH:O	1.72	1.07
1:C:325[B]:HIS:NE2	3:C:2037:HOH:O	1.87	1.06
1:C:535:ILE:O	3:C:2006:HOH:O	1.73	1.06
1:A:439:PRO:O	3:A:2106:HOH:O	1.79	1.00
1:A:452:CYS:SG	1:A:454:ASP:HB3	2.06	0.96

All (5) 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:A:2078:HOH:O	3:B:2014:HOH:O[5_554]	1.80	0.40
3:A:2035:HOH:O	3:A:2043:HOH:O[5_554]	1.87	0.33
3:A:2078:HOH:O	3:A:2079:HOH:O[5_554]	1.98	0.22
1:C:518:GLN:NE2	3:C:2071:HOH:O[4_555]	2.02	0.18
1:D:518:GLN:NE2	3:C:2114:HOH:O[4_655]	2.08	0.12

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	266/270 (98%)	257 (97%)	8 (3%)	1 (0%)	34	24
1	B	263/270 (97%)	256 (97%)	7 (3%)	0	100	100
1	C	268/270 (99%)	258 (96%)	10 (4%)	0	100	100
1	D	264/270 (98%)	254 (96%)	7 (3%)	3 (1%)	14	5
2	P	4/9 (44%)	3 (75%)	1 (25%)	0	100	100
2	Q	4/9 (44%)	3 (75%)	1 (25%)	0	100	100
2	R	4/9 (44%)	4 (100%)	0	0	100	100
2	S	4/9 (44%)	3 (75%)	1 (25%)	0	100	100
All	All	1077/1116 (96%)	1038 (96%)	35 (3%)	4 (0%)	34	24

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	454	ASP
1	D	410	SER
1	D	411	GLN
1	D	390	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	241/241 (100%)	215 (89%)	26 (11%)	6	2
1	B	240/241 (100%)	218 (91%)	22 (9%)	9	3
1	C	243/241 (101%)	216 (89%)	27 (11%)	6	2
1	D	239/241 (99%)	217 (91%)	22 (9%)	9	3
2	P	6/9 (67%)	4 (67%)	2 (33%)	0	0
2	Q	6/9 (67%)	4 (67%)	2 (33%)	0	0
2	R	6/9 (67%)	6 (100%)	0	100	100
2	S	6/9 (67%)	5 (83%)	1 (17%)	2	0
All	All	987/1000 (99%)	885 (90%)	102 (10%)	8	2

5 of 102 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	425	GLU
1	C	530	LEU
2	Q	4	ASN
1	C	448	GLU
1	C	471	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	300	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	S	4	ASN
1	C	501	GLN
1	D	501	GLN
1	C	411	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 monosaccharides 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	262/270 (97%)	-0.31	4 (1%)	73	76	14, 24, 44, 69	0
1	B	260/270 (96%)	-0.27	3 (1%)	79	81	13, 25, 45, 93	0
1	C	262/270 (97%)	-0.37	0	100	100	12, 25, 40, 53	0
1	D	262/270 (97%)	-0.18	8 (3%)	49	51	13, 27, 54, 82	0
2	P	6/9 (66%)	1.43	1 (16%)	1	1	34, 51, 56, 58	0
2	Q	6/9 (66%)	1.64	2 (33%)	0	0	38, 51, 67, 75	0
2	R	6/9 (66%)	1.92	3 (50%)	0	0	34, 60, 67, 71	0
2	S	6/9 (66%)	2.32	2 (33%)	0	0	38, 63, 64, 65	0
All	All	1070/1116 (95%)	-0.23	23 (2%)	63	66	12, 26, 51, 93	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	S	7	VAL	5.9
1	D	452	CYS	4.5
2	Q	7	VAL	4.5
2	S	4	ASN	4.4
1	D	412	GLN	4.3

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.