



wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 10:25 AM GMT

PDB ID : 4DNQ
Title : Crystal Structure of DAD2 S96A mutant
Authors : Hamiaux, C.
Deposited on : 2012-02-08
Resolution : 2.80 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

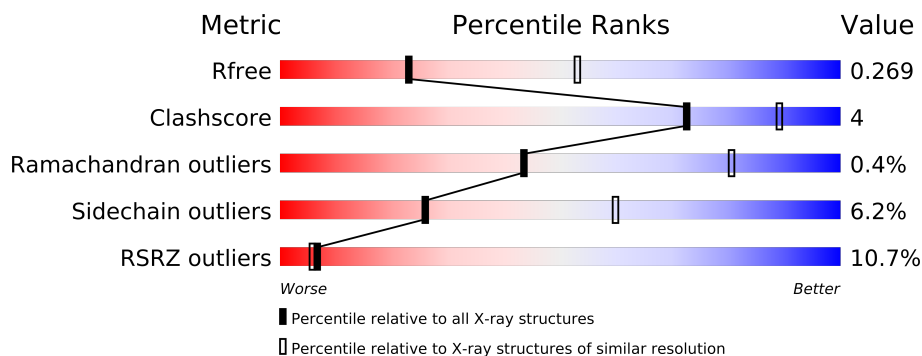
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	269	
1	B	269	
1	C	269	
1	D	269	
1	E	269	
1	F	269	
1	G	269	
1	H	269	
1	I	269	
1	J	269	
1	K	269	
1	L	269	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25042 atoms, of which 0 are hydrogen and 0 are deuterium.

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 DAD2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	0	0
			2054	1320	359	367	8			
1	B	262	Total	C	N	O	S	0	0	0
			2054	1320	359	367	8			
1	C	263	Total	C	N	O	S	0	0	0
			2063	1325	361	369	8			
1	D	263	Total	C	N	O	S	0	0	0
			2063	1325	361	369	8			
1	E	262	Total	C	N	O	S	0	0	0
			2054	1320	359	367	8			
1	F	263	Total	C	N	O	S	0	0	0
			2063	1325	361	369	8			
1	G	263	Total	C	N	O	S	0	0	0
			2063	1325	361	369	8			
1	H	262	Total	C	N	O	S	0	0	0
			2054	1320	359	367	8			
1	I	264	Total	C	N	O	S	0	0	0
			2067	1327	362	370	8			
1	J	263	Total	C	N	O	S	0	0	0
			2063	1325	361	369	8			
1	K	262	Total	C	N	O	S	0	0	0
			2054	1320	359	367	8			
1	L	264	Total	C	N	O	S	0	0	0
			2067	1327	362	370	8			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	33	Total	O	0	0
			33	33		
2	B	27	Total	O	0	0
			27	27		

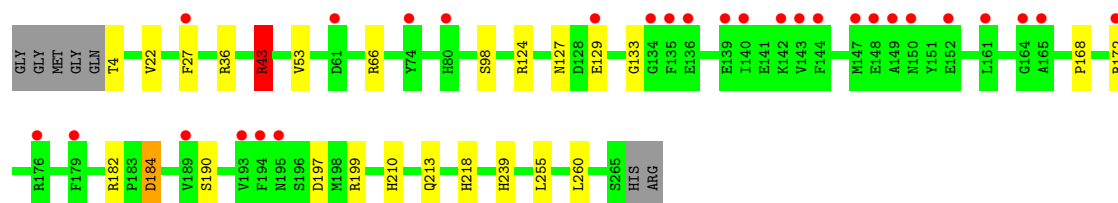
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	35	Total 35	O 35	0	0
2	D	32	Total 32	O 32	0	0
2	E	27	Total 27	O 27	0	0
2	F	27	Total 27	O 27	0	0
2	G	31	Total 31	O 31	0	0
2	H	24	Total 24	O 24	0	0
2	I	21	Total 21	O 21	0	0
2	J	12	Total 12	O 12	0	0
2	K	22	Total 22	O 22	0	0
2	L	32	Total 32	O 32	0	0

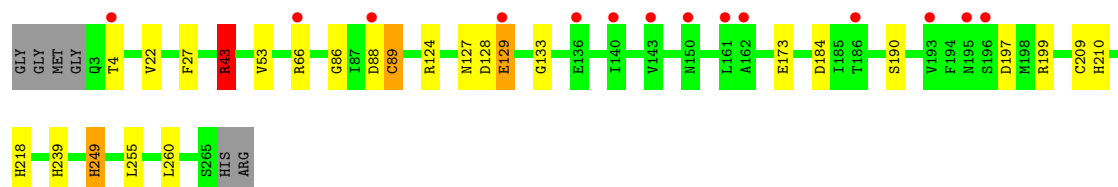
- Molecule 1: DAD2

Chain E:



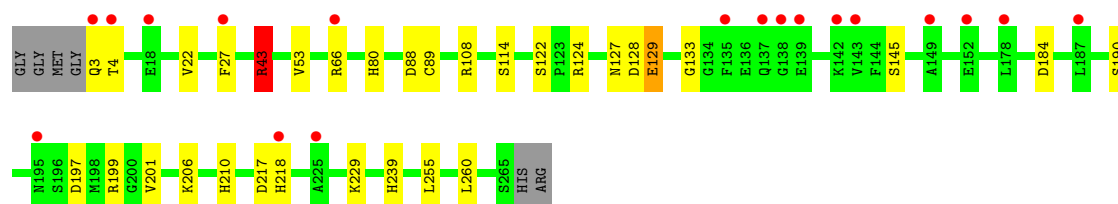
- Molecule 1: DAD2

Chain F:



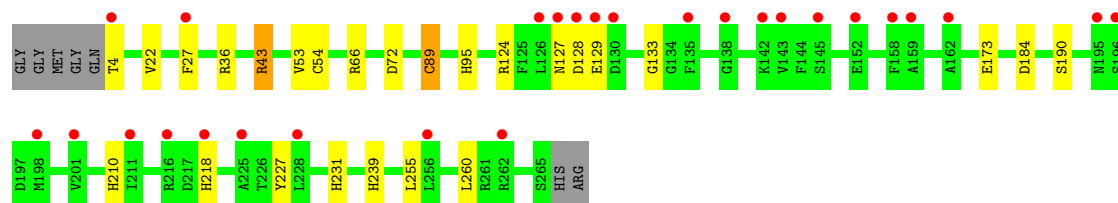
- Molecule 1: DAD2

Chain G:



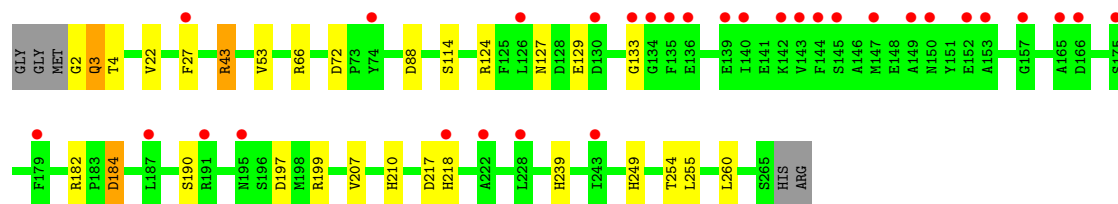
- Molecule 1: DAD2

Chain H:



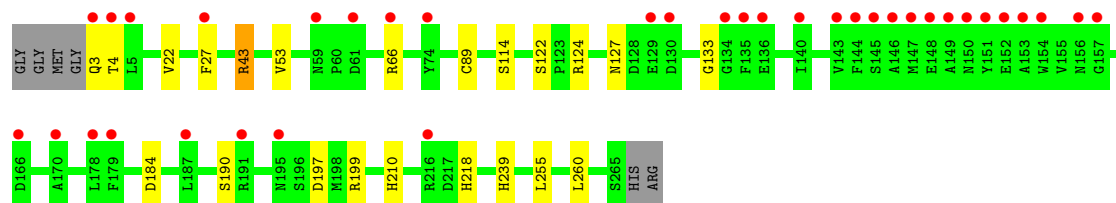
- Molecule 1: DAD2

Chain I:



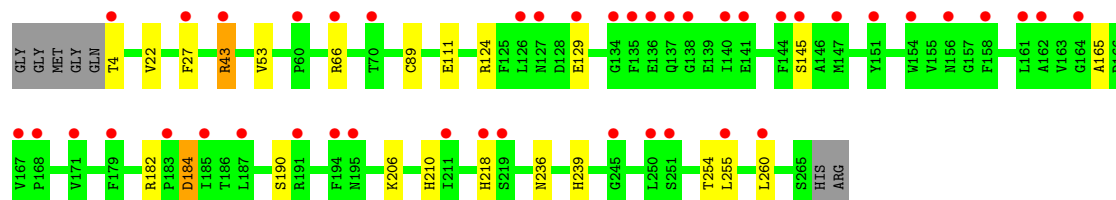
- Molecule 1: DAD2

Chain J:



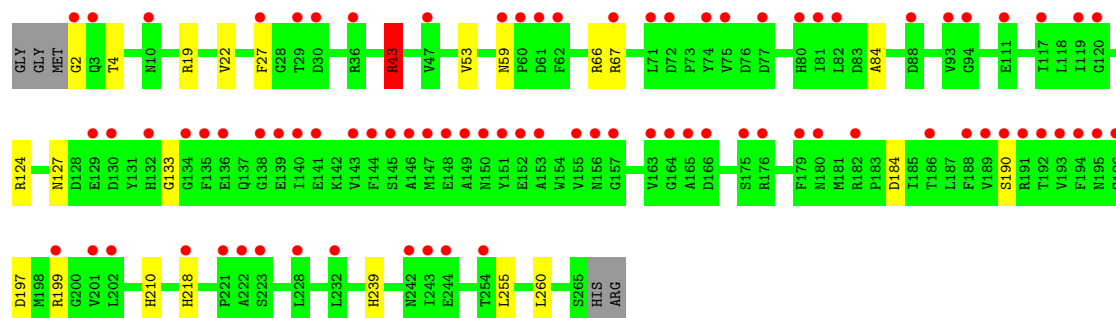
- Molecule 1: DAD2

Chain K:



- Molecule 1: DAD2

Chain L:



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	176.66Å 176.66Å 107.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	62.36 – 2.80 62.36 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (62.36-2.80) 100.0 (62.36-2.80)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.86 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.242 , 0.272 0.245 , 0.269	Depositor DCC
R_{free} test set	4632 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 26.7	EDS
Estimated twinning fraction	0.015 for -h,-k,l 0.046 for h,-h-k,-l 0.017 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 92536 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	25042	wwPDB-VP
Average B, all atoms (Å ²)	52.0	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 39.05 % 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 3.3633e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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	0.82	2/2105 (0.1%)	0.77	1/2865 (0.0%)
1	B	0.69	0/2105	0.75	1/2865 (0.0%)
1	C	0.70	0/2114	0.75	2/2877 (0.1%)
1	D	0.75	1/2114 (0.0%)	0.77	1/2877 (0.0%)
1	E	0.74	0/2105	0.71	1/2865 (0.0%)
1	F	0.76	2/2114 (0.1%)	0.75	2/2877 (0.1%)
1	G	0.72	1/2114 (0.0%)	0.74	1/2877 (0.0%)
1	H	0.75	2/2105 (0.1%)	0.75	1/2865 (0.0%)
1	I	0.70	0/2118	0.73	0/2882
1	J	0.64	0/2114	0.70	1/2877 (0.0%)
1	K	0.70	1/2105 (0.0%)	0.74	2/2865 (0.1%)
1	L	0.68	0/2118	0.70	1/2882 (0.0%)
All	All	0.72	9/25331 (0.0%)	0.74	14/34474 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	89	CYS	CB-SG	-12.59	1.60	1.82
1	A	89	CYS	CB-SG	-11.16	1.63	1.82
1	A	54	CYS	CB-SG	-7.76	1.69	1.82
1	G	89	CYS	CB-SG	-6.99	1.70	1.82
1	H	89	CYS	CB-SG	-6.10	1.71	1.82

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	89	CYS	CA-CB-SG	12.01	135.62	114.00
1	B	89	CYS	CA-CB-SG	10.46	132.83	114.00
1	D	89	CYS	CA-CB-SG	8.35	129.03	114.00
1	K	89	CYS	CB-CA-C	-8.08	94.23	110.40
1	H	89	CYS	CA-CB-SG	7.47	127.45	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2054	0	0	11	0
1	B	2054	0	0	8	0
1	C	2063	0	7	18	0
1	D	2063	0	7	7	0
1	E	2054	0	0	15	0
1	F	2063	0	7	14	0
1	G	2063	0	7	13	0
1	H	2054	0	0	9	0
1	I	2067	0	10	8	1
1	J	2063	0	7	6	0
1	K	2054	0	0	8	0
1	L	2067	0	10	16	0
2	A	33	0	0	1	0
2	B	27	0	0	1	0
2	C	35	0	0	2	0
2	D	32	0	0	1	0
2	E	27	0	0	3	0
2	F	27	0	0	0	0
2	G	31	0	0	2	0
2	H	24	0	0	3	0
2	I	21	0	0	0	0
2	J	12	0	0	1	0
2	K	22	0	0	2	0
2	L	32	0	0	3	0
All	All	25042	0	55	106	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

The worst 5 of 106 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:88:ASP:OD2	1:L:19:ARG:CD	2.06	1.03

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:12:ARG:NH1	2:C:311:HOH:O	2.08	0.84
1:E:36:ARG:CG	2:E:306:HOH:O	2.26	0.82
1:B:95:HIS:CD2	2:B:322:HOH:O	2.38	0.76
1:A:216:ARG:NH2	2:A:312:HOH:O	2.21	0.72

All (1) 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	Distance(Å)	Clash(Å)
1:I:72:ASP:OD2	1:I:254:THR:OG1[2_545]	1.83	0.37

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	260/269 (97%)	251 (96%)	8 (3%)	1 (0%)	43	80
1	B	260/269 (97%)	247 (95%)	12 (5%)	1 (0%)	43	80
1	C	261/269 (97%)	252 (97%)	7 (3%)	2 (1%)	27	65
1	D	261/269 (97%)	250 (96%)	10 (4%)	1 (0%)	43	80
1	E	260/269 (97%)	249 (96%)	10 (4%)	1 (0%)	43	80
1	F	261/269 (97%)	251 (96%)	9 (3%)	1 (0%)	43	80
1	G	261/269 (97%)	251 (96%)	9 (3%)	1 (0%)	43	80
1	H	260/269 (97%)	252 (97%)	7 (3%)	1 (0%)	43	80
1	I	262/269 (97%)	252 (96%)	8 (3%)	2 (1%)	27	65
1	J	261/269 (97%)	253 (97%)	7 (3%)	1 (0%)	43	80
1	K	260/269 (97%)	250 (96%)	9 (4%)	1 (0%)	43	80
1	L	262/269 (97%)	250 (95%)	11 (4%)	1 (0%)	43	80
All	All	3129/3228 (97%)	3008 (96%)	107 (3%)	14 (0%)	43	80

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	3	GLN
1	I	184	ASP
1	A	184	ASP
1	B	184	ASP
1	C	184	ASP

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	219/223 (98%)	206 (94%)	13 (6%)	28	62
1	B	219/223 (98%)	204 (93%)	15 (7%)	22	54
1	C	220/223 (99%)	206 (94%)	14 (6%)	25	58
1	D	220/223 (99%)	206 (94%)	14 (6%)	25	58
1	E	219/223 (98%)	206 (94%)	13 (6%)	28	62
1	F	220/223 (99%)	206 (94%)	14 (6%)	25	58
1	G	220/223 (99%)	203 (92%)	17 (8%)	18	45
1	H	219/223 (98%)	207 (94%)	12 (6%)	30	65
1	I	220/223 (99%)	205 (93%)	15 (7%)	22	54
1	J	220/223 (99%)	208 (94%)	12 (6%)	30	65
1	K	219/223 (98%)	205 (94%)	14 (6%)	25	58
1	L	220/223 (99%)	209 (95%)	11 (5%)	34	70
All	All	2635/2676 (98%)	2471 (94%)	164 (6%)	26	60

5 of 164 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	66	ARG
1	G	129	GLU
1	K	255	LEU
1	F	124	ARG
1	G	3	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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	262/269 (97%)	0.11	11 (4%) 35 35	21, 38, 63, 76	0
1	B	262/269 (97%)	0.26	13 (4%) 28 28	29, 47, 72, 89	0
1	C	263/269 (97%)	0.29	17 (6%) 18 17	24, 45, 75, 93	0
1	D	263/269 (97%)	0.24	13 (4%) 28 29	25, 43, 70, 85	0
1	E	262/269 (97%)	0.43	28 (10%) 6 6	27, 47, 80, 105	0
1	F	263/269 (97%)	0.38	14 (5%) 25 26	29, 43, 68, 80	0
1	G	263/269 (97%)	0.38	18 (6%) 17 15	27, 45, 69, 87	0
1	H	262/269 (97%)	0.52	27 (10%) 7 6	27, 46, 72, 97	0
1	I	264/269 (98%)	0.50	31 (11%) 5 4	26, 53, 119, 145	0
1	J	263/269 (97%)	0.73	36 (13%) 4 3	32, 60, 132, 168	0
1	K	262/269 (97%)	0.82	44 (16%) 2 2	35, 59, 102, 124	0
1	L	264/269 (98%)	1.52	84 (31%) 1 1	42, 58, 86, 100	0
All	All	3153/3228 (97%)	0.51	336 (10%) 6 6	21, 49, 90, 168	0

The worst 5 of 336 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	138	GLY	11.5
1	J	147	MET	9.4
1	L	189	VAL	8.2
1	J	179	PHE	7.2
1	J	144	PHE	7.2

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 carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.