



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:57 PM GMT

PDB ID : 3SAQ
Title : Structure of D13, the scaffolding protein of vaccinia virus
Authors : Coulibaly, F.
Deposited on : 2011-06-03
Resolution : 3.51 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

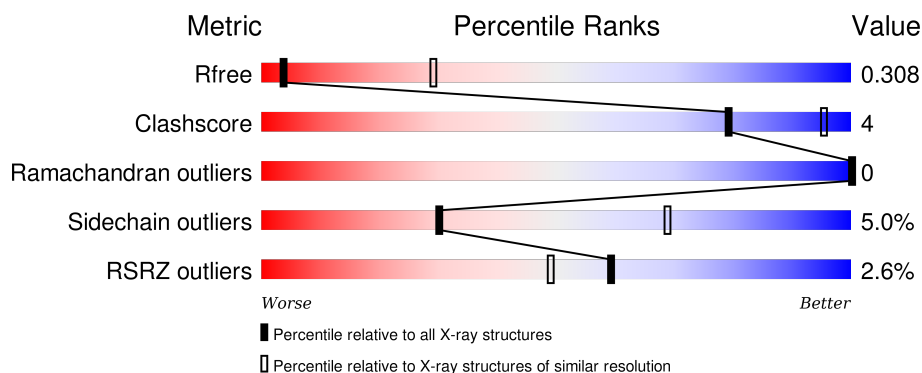
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

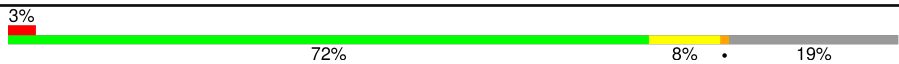

The reported resolution of this entry is 3.51 Å.

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}	91344	1089 (3.64-3.40)
Clashscore	102246	1197 (3.64-3.40)
Ramachandran outliers	100387	1159 (3.64-3.40)
Sidechain outliers	100360	1160 (3.64-3.40)
RSRZ outliers	91569	1096 (3.64-3.40)

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	576	 3% 72% 8% • 19%
1	B	576	 % 76% 8% • 15%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7428 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 Rifampicin resistance protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	0	0
			3612	2321	571	709	11			
1	B	492	Total	C	N	O	S	0	0	0
			3816	2446	608	751	11			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	EXPRESSION TAG	UNP P68440
A	-23	SER	-	EXPRESSION TAG	UNP P68440
A	-22	TYR	-	EXPRESSION TAG	UNP P68440
A	-21	TYR	-	EXPRESSION TAG	UNP P68440
A	-20	HIS	-	EXPRESSION TAG	UNP P68440
A	-19	HIS	-	EXPRESSION TAG	UNP P68440
A	-18	HIS	-	EXPRESSION TAG	UNP P68440
A	-17	HIS	-	EXPRESSION TAG	UNP P68440
A	-16	HIS	-	EXPRESSION TAG	UNP P68440
A	-15	HIS	-	EXPRESSION TAG	UNP P68440
A	-14	ASP	-	EXPRESSION TAG	UNP P68440
A	-13	TYR	-	EXPRESSION TAG	UNP P68440
A	-12	ASP	-	EXPRESSION TAG	UNP P68440
A	-11	ILE	-	EXPRESSION TAG	UNP P68440
A	-10	PRO	-	EXPRESSION TAG	UNP P68440
A	-9	THR	-	EXPRESSION TAG	UNP P68440
A	-8	THR	-	EXPRESSION TAG	UNP P68440
A	-7	GLU	-	EXPRESSION TAG	UNP P68440
A	-6	ASN	-	EXPRESSION TAG	UNP P68440
A	-5	LEU	-	EXPRESSION TAG	UNP P68440
A	-4	TYR	-	EXPRESSION TAG	UNP P68440
A	-3	PHE	-	EXPRESSION TAG	UNP P68440
A	-2	GLN	-	EXPRESSION TAG	UNP P68440
A	-1	GLY	-	EXPRESSION TAG	UNP P68440
A	0	ALA	-	EXPRESSION TAG	UNP P68440

Continued on next page...

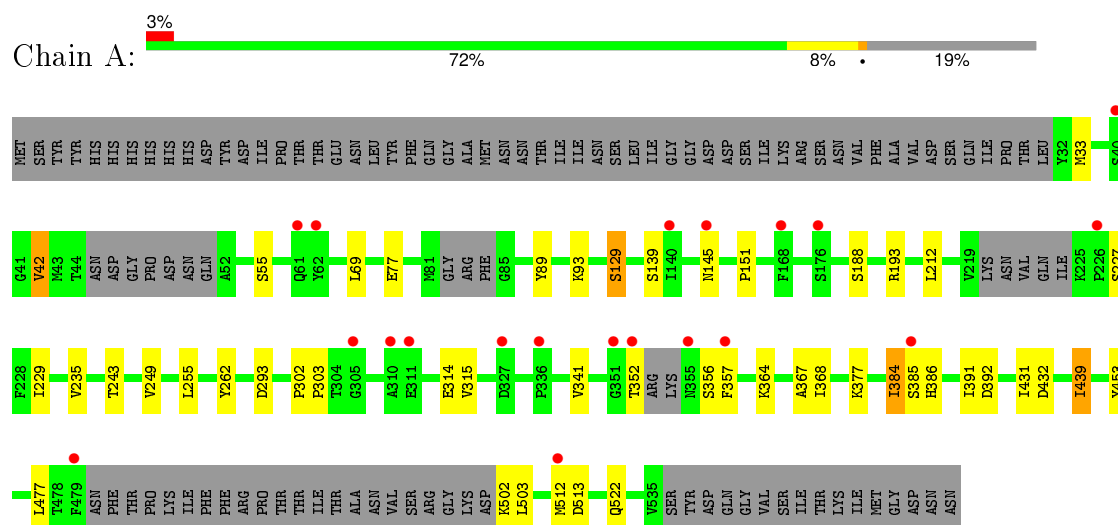
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-24	MET	-	EXPRESSION TAG	UNP P68440
B	-23	SER	-	EXPRESSION TAG	UNP P68440
B	-22	TYR	-	EXPRESSION TAG	UNP P68440
B	-21	TYR	-	EXPRESSION TAG	UNP P68440
B	-20	HIS	-	EXPRESSION TAG	UNP P68440
B	-19	HIS	-	EXPRESSION TAG	UNP P68440
B	-18	HIS	-	EXPRESSION TAG	UNP P68440
B	-17	HIS	-	EXPRESSION TAG	UNP P68440
B	-16	HIS	-	EXPRESSION TAG	UNP P68440
B	-15	HIS	-	EXPRESSION TAG	UNP P68440
B	-14	ASP	-	EXPRESSION TAG	UNP P68440
B	-13	TYR	-	EXPRESSION TAG	UNP P68440
B	-12	ASP	-	EXPRESSION TAG	UNP P68440
B	-11	ILE	-	EXPRESSION TAG	UNP P68440
B	-10	PRO	-	EXPRESSION TAG	UNP P68440
B	-9	THR	-	EXPRESSION TAG	UNP P68440
B	-8	THR	-	EXPRESSION TAG	UNP P68440
B	-7	GLU	-	EXPRESSION TAG	UNP P68440
B	-6	ASN	-	EXPRESSION TAG	UNP P68440
B	-5	LEU	-	EXPRESSION TAG	UNP P68440
B	-4	TYR	-	EXPRESSION TAG	UNP P68440
B	-3	PHE	-	EXPRESSION TAG	UNP P68440
B	-2	GLN	-	EXPRESSION TAG	UNP P68440
B	-1	GLY	-	EXPRESSION TAG	UNP P68440
B	0	ALA	-	EXPRESSION TAG	UNP P68440

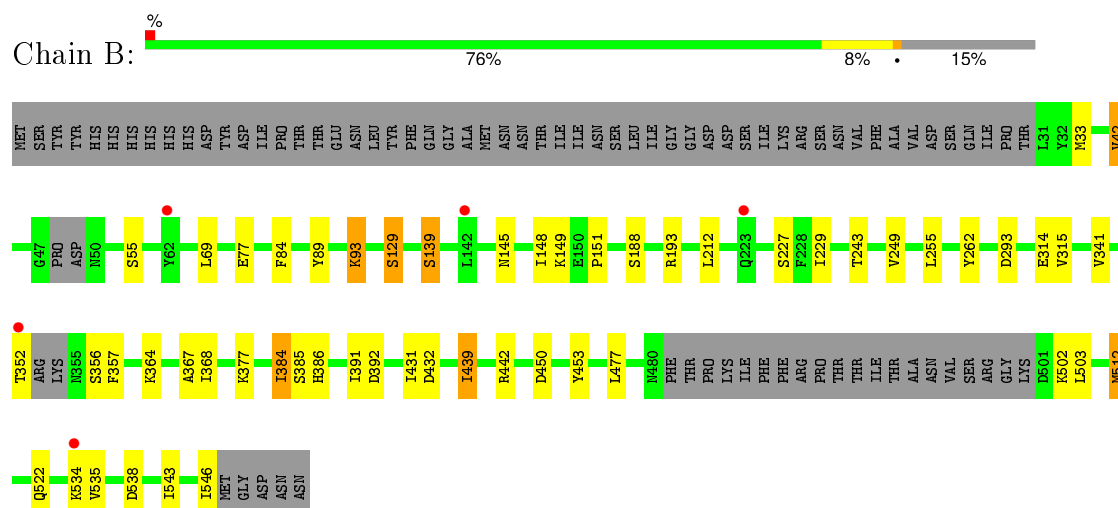
3 Residue-property plots [i](#)

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: Rifampicin resistance protein



- Molecule 1: Rifampicin resistance protein



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	125.13Å 125.13Å 370.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.81 – 3.51 26.81 – 3.51	Depositor EDS
% Data completeness (in resolution range)	97.8 (26.81-3.51) 97.3 (26.81-3.51)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.73 (at 3.55Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.245 , 0.257 0.283 , 0.308	Depositor DCC
R_{free} test set	699 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	83.3	Xtriage
Anisotropy	0.600	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 57.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 13943 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	7428	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.47	0/3691	0.67	1/5038 (0.0%)
1	B	0.48	0/3899	0.67	1/5322 (0.0%)
All	All	0.47	0/7590	0.67	2/10360 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	SER	C-N-CA	5.48	133.80	122.30
1	B	129	SER	C-N-CA	5.21	133.24	122.30

There are no chirality outliers.

There are no planarity outliers.

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	3612	0	3479	27	0
1	B	3816	0	3674	32	0
All	All	7428	0	7153	51	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 4.

All (51) 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:262:TYR:HE1	1:B:450:ASP:HB3	1.20	1.05
1:A:262:TYR:CE1	1:B:450:ASP:HB3	1.98	0.98
1:A:262:TYR:HE1	1:B:450:ASP:CB	1.84	0.91
1:B:535:VAL:HG12	1:B:543:ILE:HG22	1.66	0.77
1:A:89:TYR:HA	1:A:129:SER:OG	1.92	0.69
1:B:89:TYR:HA	1:B:129:SER:OG	1.93	0.68
1:B:391:ILE:HD13	1:B:432:ASP:HB3	1.76	0.68
1:A:391:ILE:HD13	1:A:432:ASP:HB3	1.75	0.67
1:A:262:TYR:HE1	1:B:450:ASP:CG	1.98	0.66
1:B:249:VAL:HG11	1:B:503:LEU:HD13	1.80	0.63
1:B:384:ILE:HG22	1:B:386:HIS:HD2	1.65	0.62
1:A:384:ILE:HG22	1:A:386:HIS:HD2	1.65	0.61
1:A:249:VAL:HG11	1:A:503:LEU:HD13	1.82	0.60
1:A:262:TYR:CE1	1:B:450:ASP:CB	2.72	0.57
1:A:262:TYR:CE1	1:B:450:ASP:CG	2.78	0.55
1:B:255:LEU:HD22	1:B:503:LEU:HD23	1.90	0.53
1:A:255:LEU:HD22	1:A:503:LEU:HD23	1.90	0.53
1:A:391:ILE:CD1	1:A:431:ILE:HD12	2.39	0.52
1:B:384:ILE:CG2	1:B:386:HIS:HD2	2.23	0.52
1:A:384:ILE:CG2	1:A:386:HIS:HD2	2.22	0.52
1:B:391:ILE:CD1	1:B:431:ILE:HD12	2.40	0.51
1:A:391:ILE:HD12	1:A:431:ILE:HD12	1.91	0.51
1:B:84:PHE:HB3	1:B:148:ILE:HG21	1.92	0.51
1:B:391:ILE:HD12	1:B:431:ILE:HD12	1.93	0.49
1:B:315:VAL:HG22	1:B:341:VAL:HB	1.95	0.48
1:B:439:ILE:H	1:B:439:ILE:HD13	1.78	0.48
1:A:315:VAL:HG22	1:A:341:VAL:HB	1.96	0.48
1:A:439:ILE:H	1:A:439:ILE:HD13	1.78	0.47
1:B:367:ALA:HB3	1:B:385:SER:HB2	1.98	0.45
1:B:77:GLU:HB2	1:B:151:PRO:HD3	1.98	0.45
1:A:262:TYR:HB3	1:A:522:GLN:HB2	1.98	0.45
1:B:368:ILE:HG23	1:B:384:ILE:HD11	1.97	0.45
1:A:77:GLU:HB2	1:A:151:PRO:HD3	1.97	0.45
1:A:367:ALA:HB3	1:A:385:SER:HB2	1.98	0.45
1:A:368:ILE:HG23	1:A:384:ILE:HD11	1.97	0.44
1:B:364:LYS:HE3	1:B:392:ASP:OD1	2.18	0.44
1:B:512:MET:HG2	1:B:512:MET:H	1.57	0.44
1:A:364:LYS:HE3	1:A:392:ASP:OD1	2.18	0.43
1:B:453:TYR:CD2	1:B:477:LEU:HD21	2.53	0.43
1:B:139:SER:OG	1:B:149:LYS:HE2	2.18	0.43
1:B:262:TYR:HB3	1:B:522:GLN:HB2	2.00	0.43
1:A:42:VAL:HG23	1:A:55:SER:HB2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:LEU:CD2	1:A:212:LEU:HD11	2.50	0.42
1:B:42:VAL:HG23	1:B:55:SER:HB2	2.02	0.42
1:A:235:VAL:HG13	1:B:442:ARG:CZ	2.50	0.41
1:B:89:TYR:O	1:B:93:LYS:HD2	2.20	0.41
1:A:453:TYR:CD2	1:A:477:LEU:HD21	2.56	0.40
1:B:69:LEU:CD2	1:B:212:LEU:HD11	2.51	0.40
1:A:262:TYR:CE1	1:B:450:ASP:OD1	2.74	0.40
1:B:534:LYS:HB2	1:B:546:ILE:HD11	2.03	0.40
1:A:302:PRO:HA	1:A:303:PRO:HD3	2.01	0.40

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	453/576 (79%)	437 (96%)	16 (4%)	0	100	100
1	B	484/576 (84%)	466 (96%)	18 (4%)	0	100	100
All	All	937/1152 (81%)	903 (96%)	34 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	407/528 (77%)	386 (95%)	21 (5%)	29	68
1	B	429/528 (81%)	408 (95%)	21 (5%)	31	70
All	All	836/1056 (79%)	794 (95%)	42 (5%)	30	69

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	MET
1	A	42	VAL
1	A	93	LYS
1	A	139	SER
1	A	145	ASN
1	A	188	SER
1	A	193	ARG
1	A	227	SER
1	A	229	ILE
1	A	243	THR
1	A	293	ASP
1	A	314	GLU
1	A	352	THR
1	A	356	SER
1	A	357	PHE
1	A	377	LYS
1	A	384	ILE
1	A	439	ILE
1	A	502	LYS
1	A	512	MET
1	A	513	ASP
1	B	33	MET
1	B	42	VAL
1	B	93	LYS
1	B	139	SER
1	B	145	ASN
1	B	188	SER
1	B	193	ARG
1	B	227	SER
1	B	229	ILE
1	B	243	THR
1	B	293	ASP
1	B	314	GLU
1	B	352	THR
1	B	356	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	357	PHE
1	B	377	LYS
1	B	384	ILE
1	B	439	ILE
1	B	502	LYS
1	B	512	MET
1	B	538	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	45	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 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

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	465/576 (80%)	0.28	20 (4%) 39 30	64, 110, 162, 201	0
1	B	492/576 (85%)	-0.18	5 (1%) 84 76	34, 84, 145, 192	0
All	All	957/1152 (83%)	0.04	25 (2%) 59 49	34, 99, 154, 201	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	355	ASN	4.6
1	A	310	ALA	3.6
1	B	223	GLN	3.3
1	A	352	THR	3.2
1	A	62	TYR	3.2
1	A	512	MET	3.1
1	A	351	GLY	2.7
1	A	327	ASP	2.7
1	A	145	ASN	2.6
1	A	226	PRO	2.5
1	A	305	GLY	2.5
1	B	534	LYS	2.4
1	A	40	SER	2.4
1	A	140	ILE	2.3
1	B	62	TYR	2.3
1	A	385	SER	2.2
1	A	168	PHE	2.2
1	B	352	THR	2.2
1	B	142	LEU	2.2
1	A	479	PHE	2.1
1	A	336	PRO	2.1
1	A	311	GLU	2.1
1	A	357	PHE	2.0
1	A	61	GLN	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	176	SER	2.0

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.