Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 01:39 AM EDT

PDB ID	:	7SKS
Title	:	Crystal structure of measles virus matrix protein
Authors	:	Norris, M.J.; Saphire, E.O.
Deposited on	:	2021-10-21
Resolution	:	2.54 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

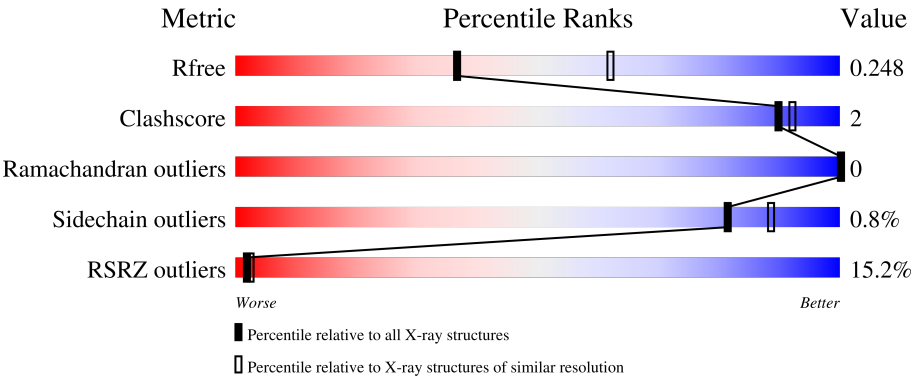
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	376	12% 68% . 28%
1	B	376	10% 71% . 25%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8924 atoms, of which 4440 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 Matrix protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	271	Total	C	H	N	O	S	2139	1	0
			4248	1351	2139	366	378	14			
1	B	282	Total	C	H	N	O	S	2301	2	0
			4536	1436	2301	388	397	14			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-40	MET	-	initiating methionine	UNP Q9W850
A	-39	ALA	-	expression tag	UNP Q9W850
A	-38	GLY	-	expression tag	UNP Q9W850
A	-37	TRP	-	expression tag	UNP Q9W850
A	-36	SER	-	expression tag	UNP Q9W850
A	-35	HIS	-	expression tag	UNP Q9W850
A	-34	PRO	-	expression tag	UNP Q9W850
A	-33	GLN	-	expression tag	UNP Q9W850
A	-32	PHE	-	expression tag	UNP Q9W850
A	-31	GLU	-	expression tag	UNP Q9W850
A	-30	LYS	-	expression tag	UNP Q9W850
A	-29	GLY	-	expression tag	UNP Q9W850
A	-28	GLY	-	expression tag	UNP Q9W850
A	-27	GLY	-	expression tag	UNP Q9W850
A	-26	SER	-	expression tag	UNP Q9W850
A	-25	GLY	-	expression tag	UNP Q9W850
A	-24	GLY	-	expression tag	UNP Q9W850
A	-23	GLY	-	expression tag	UNP Q9W850
A	-22	SER	-	expression tag	UNP Q9W850
A	-21	GLY	-	expression tag	UNP Q9W850
A	-20	GLY	-	expression tag	UNP Q9W850
A	-19	GLY	-	expression tag	UNP Q9W850
A	-18	SER	-	expression tag	UNP Q9W850
A	-17	TRP	-	expression tag	UNP Q9W850
A	-16	SER	-	expression tag	UNP Q9W850

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	HIS	-	expression tag	UNP Q9W850
A	-14	PRO	-	expression tag	UNP Q9W850
A	-13	GLN	-	expression tag	UNP Q9W850
A	-12	PHE	-	expression tag	UNP Q9W850
A	-11	GLU	-	expression tag	UNP Q9W850
A	-10	LYS	-	expression tag	UNP Q9W850
A	-9	GLY	-	expression tag	UNP Q9W850
A	-8	GLY	-	expression tag	UNP Q9W850
A	-7	SER	-	expression tag	UNP Q9W850
A	-6	ASP	-	expression tag	UNP Q9W850
A	-5	ASP	-	expression tag	UNP Q9W850
A	-4	ASP	-	expression tag	UNP Q9W850
A	-3	ASP	-	expression tag	UNP Q9W850
A	-2	LYS	-	expression tag	UNP Q9W850
A	-1	SER	-	expression tag	UNP Q9W850
A	0	GLY	-	expression tag	UNP Q9W850
A	1	GLY	-	expression tag	UNP Q9W850
B	-40	MET	-	initiating methionine	UNP Q9W850
B	-39	ALA	-	expression tag	UNP Q9W850
B	-38	GLY	-	expression tag	UNP Q9W850
B	-37	TRP	-	expression tag	UNP Q9W850
B	-36	SER	-	expression tag	UNP Q9W850
B	-35	HIS	-	expression tag	UNP Q9W850
B	-34	PRO	-	expression tag	UNP Q9W850
B	-33	GLN	-	expression tag	UNP Q9W850
B	-32	PHE	-	expression tag	UNP Q9W850
B	-31	GLU	-	expression tag	UNP Q9W850
B	-30	LYS	-	expression tag	UNP Q9W850
B	-29	GLY	-	expression tag	UNP Q9W850
B	-28	GLY	-	expression tag	UNP Q9W850
B	-27	GLY	-	expression tag	UNP Q9W850
B	-26	SER	-	expression tag	UNP Q9W850
B	-25	GLY	-	expression tag	UNP Q9W850
B	-24	GLY	-	expression tag	UNP Q9W850
B	-23	GLY	-	expression tag	UNP Q9W850
B	-22	SER	-	expression tag	UNP Q9W850
B	-21	GLY	-	expression tag	UNP Q9W850
B	-20	GLY	-	expression tag	UNP Q9W850
B	-19	GLY	-	expression tag	UNP Q9W850
B	-18	SER	-	expression tag	UNP Q9W850
B	-17	TRP	-	expression tag	UNP Q9W850
B	-16	SER	-	expression tag	UNP Q9W850

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	expression tag	UNP Q9W850
B	-14	PRO	-	expression tag	UNP Q9W850
B	-13	GLN	-	expression tag	UNP Q9W850
B	-12	PHE	-	expression tag	UNP Q9W850
B	-11	GLU	-	expression tag	UNP Q9W850
B	-10	LYS	-	expression tag	UNP Q9W850
B	-9	GLY	-	expression tag	UNP Q9W850
B	-8	GLY	-	expression tag	UNP Q9W850
B	-7	SER	-	expression tag	UNP Q9W850
B	-6	ASP	-	expression tag	UNP Q9W850
B	-5	ASP	-	expression tag	UNP Q9W850
B	-4	ASP	-	expression tag	UNP Q9W850
B	-3	ASP	-	expression tag	UNP Q9W850
B	-2	LYS	-	expression tag	UNP Q9W850
B	-1	SER	-	expression tag	UNP Q9W850
B	0	GLY	-	expression tag	UNP Q9W850
B	1	GLY	-	expression tag	UNP Q9W850

- Molecule 2 is water.

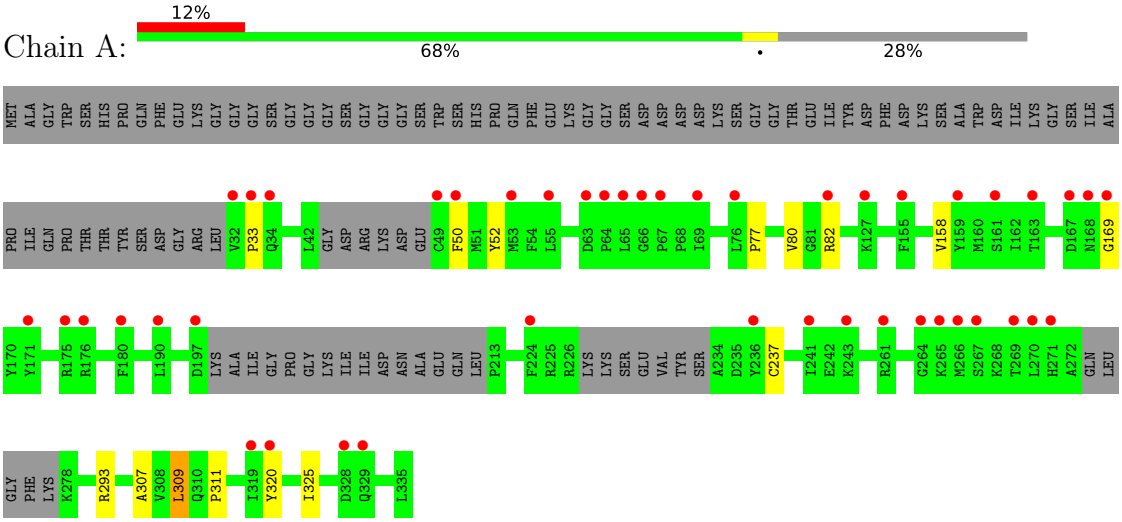
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	57	Total O 57 57	0	0
2	B	83	Total O 83 83	0	0

3 Residue-property plots (i)

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.

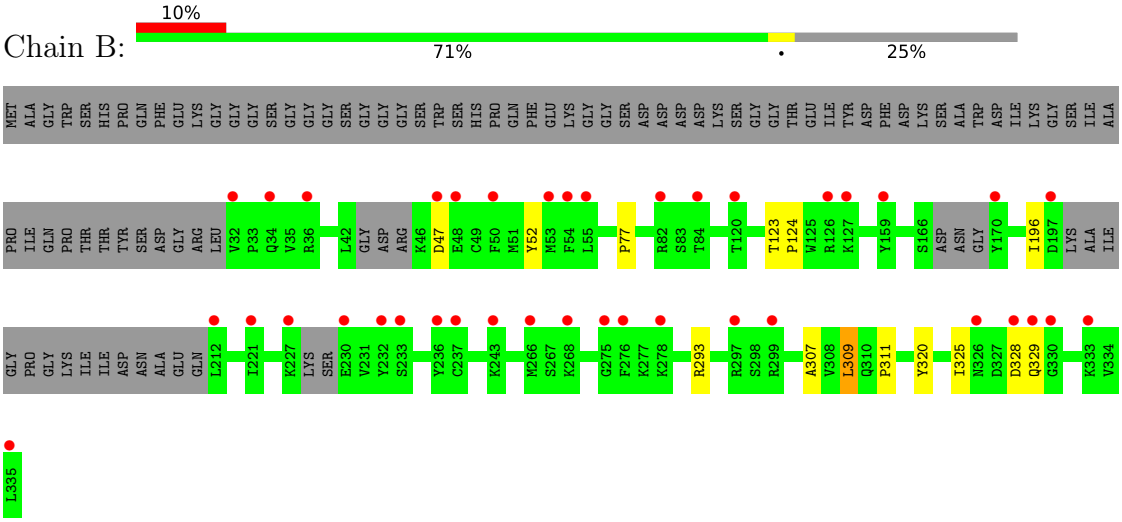
• Molecule 1: Matrix protein

Chain A:



• Molecule 1: Matrix protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	85.95Å 85.95Å 402.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.54 20.00 – 2.54	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.54) 99.9 (20.00-2.54)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 2.53Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.231 , 0.257 0.215 , 0.248	Depositor DCC
R_{free} test set	1517 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	85.6	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 74.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8924	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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

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	0.37	0/2155	0.57	0/2922
1	B	0.37	0/2286	0.57	0/3092
All	All	0.37	0/4441	0.57	0/6014

There are no bond length outliers.

There are no bond angle outliers.

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	2109	2139	2133	8	0
1	B	2235	2301	2296	8	0
2	A	57	0	0	0	0
2	B	83	0	0	0	0
All	All	4484	4440	4429	16	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 2.

All (16) 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:307:ALA:HB3	1:A:325:ILE:HB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:PRO:HA	1:A:158:VAL:O	2.06	0.56
1:B:328:ASP:O	1:B:329:GLN:HB2	2.10	0.52
1:B:196:ILE:HD12	1:B:196:ILE:N	2.29	0.48
1:B:307:ALA:HB3	1:B:325:ILE:HB	1.97	0.47
1:A:80:VAL:HG21	1:A:169:GLY:HA2	1.98	0.46
1:B:311:PRO:HG3	1:B:320:TYR:HB2	1.99	0.45
1:A:311:PRO:HG3	1:A:320:TYR:HB2	1.98	0.43
1:B:309:LEU:CD2	1:B:309:LEU:N	2.84	0.41
1:A:50:PHE:CD2	1:A:82:ARG:HG2	2.56	0.41
1:A:52:TYR:OH	1:A:77:PRO:HB3	2.21	0.40
1:A:309:LEU:N	1:A:309:LEU:CD2	2.84	0.40
1:B:123:THR:N	1:B:124:PRO:CD	2.85	0.40
1:B:52:TYR:OH	1:B:77:PRO:HB3	2.22	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	262/376 (70%)	252 (96%)	10 (4%)	0	100	100
1	B	274/376 (73%)	266 (97%)	8 (3%)	0	100	100
All	All	536/752 (71%)	518 (97%)	18 (3%)	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	233/320 (73%)	231 (99%)	2 (1%)	78 86
1	B	250/320 (78%)	248 (99%)	2 (1%)	81 88
All	All	483/640 (76%)	479 (99%)	4 (1%)	81 88

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	237	CYS
1	A	309	LEU
1	B	47	ASP
1	B	309	LEU

Sometimes 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 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 (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, 95^{th} 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	271/376 (72%)	0.66	45 (16%)	1	1	65, 91, 144, 171	0
1	B	282/376 (75%)	0.68	39 (13%)	2	3	69, 88, 126, 157	0
All	All	553/752 (73%)	0.67	84 (15%)	2	2	65, 90, 133, 171	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	276	PHE	7.2
1	A	65	LEU	6.1
1	A	64	PRO	6.0
1	A	270	LEU	5.9
1	B	212	LEU	5.4
1	A	271	HIS	5.3
1	B	32	VAL	5.2
1	B	47	ASP	5.1
1	B	236	TYR	5.0
1	A	168	ASN	4.7
1	B	328	ASP	4.4
1	A	167	ASP	4.3
1	B	50	PHE	4.3
1	B	329	GLN	4.3
1	A	267	SER	4.3
1	A	32	VAL	4.3
1	B	127	LYS	4.0
1	A	171	TYR	3.9
1	A	180	PHE	3.9
1	A	82	ARG	3.9
1	A	197	ASP	3.8
1	A	329	GLN	3.8
1	B	55	LEU	3.8
1	B	232	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	53	MET	3.6
1	B	299	ARG	3.6
1	B	170	TYR	3.6
1	A	241	ILE	3.5
1	B	159	TYR	3.5
1	A	67	PRO	3.4
1	A	224	PHE	3.4
1	B	82	ARG	3.4
1	A	63	ASP	3.3
1	A	66	GLY	3.3
1	A	55	LEU	3.2
1	A	269	THR	3.1
1	B	221	ILE	3.1
1	A	161	SER	3.0
1	B	197	ASP	3.0
1	B	297	ARG	2.9
1	B	275	GLY	2.9
1	A	127	LYS	2.9
1	A	319	ILE	2.8
1	A	176	ARG	2.8
1	A	264	GLY	2.8
1	B	230	GLU	2.8
1	A	50	PHE	2.7
1	B	335	LEU	2.6
1	A	49	CYS	2.6
1	A	175	ARG	2.5
1	B	233	SER	2.5
1	A	265	LYS	2.5
1	B	36	ARG	2.5
1	B	237	CYS	2.5
1	A	320	TYR	2.4
1	A	53	MET	2.4
1	A	266	MET	2.4
1	A	261	ARG	2.4
1	A	190	LEU	2.4
1	A	236	TYR	2.4
1	A	69	ILE	2.4
1	B	34	GLN	2.4
1	B	126	ARG	2.3
1	B	266	MET	2.3
1	A	243	LYS	2.3
1	A	163	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	326	ASN	2.3
1	B	330	GLY	2.2
1	B	268	LYS	2.2
1	A	159	TYR	2.2
1	B	243	LYS	2.2
1	A	169	GLY	2.1
1	A	155	PHE	2.1
1	B	333	LYS	2.1
1	B	54	PHE	2.1
1	B	48	GLU	2.1
1	A	33	PRO	2.1
1	B	84	THR	2.1
1	A	328	ASP	2.1
1	B	227	LYS	2.1
1	A	76	LEU	2.1
1	A	34	GLN	2.1
1	B	278	LYS	2.1
1	B	120	THR	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 monosaccharides 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.