



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 29, 2024 – 10:23 AM EDT

PDB ID : 3KEA
Title : Structure function studies of vaccinia virus host-range protein K1 reveal a novel ankyrin repeat interaction surface for K1s function
Authors : Li, Y.
Deposited on : 2009-10-25
Resolution : 2.30 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

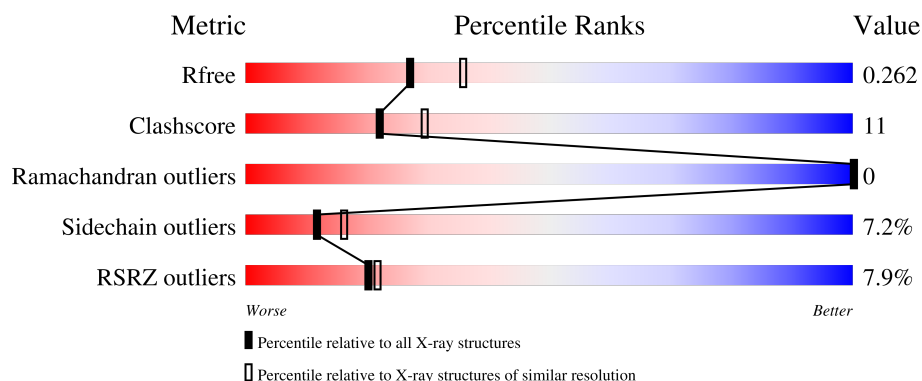
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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 $\leq 5\%$. 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	285	<div> <div>4%</div> <div>79%</div> <div>18%</div> <div>..</div> </div>
1	B	285	<div> <div>11%</div> <div>79%</div> <div>18%</div> <div>..</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4762 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 K1L.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	Se	72	0	0
			2268	1459	366	430	3	10			
1	B	283	Total	C	N	O	S	Se	68	0	0
			2268	1459	366	430	3	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q6IV60
B	0	GLY	-	expression tag	UNP Q6IV60

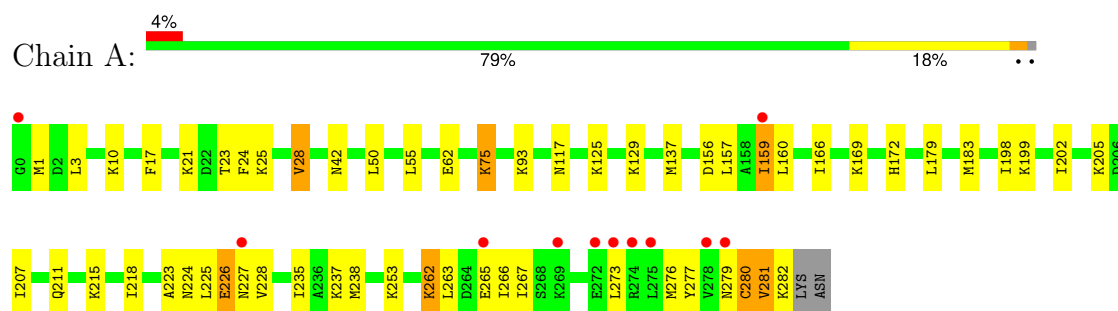
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	132	Total	O	0	0
			132	132		
2	B	94	Total	O	0	0
			94	94		

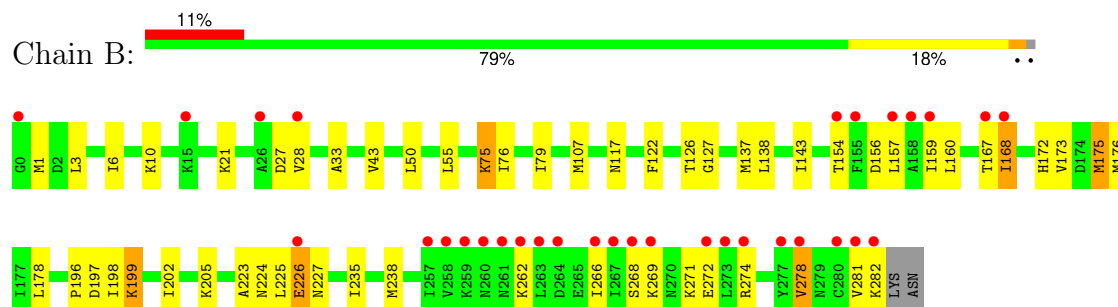
3 Residue-property plots [i](#)

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: K1L



• Molecule 1: K1L



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	95.11Å 110.26Å 86.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.28 – 2.30 39.28 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.5 (39.28-2.30) 90.4 (39.28-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.210 , 0.254 0.223 , 0.262	Depositor DCC
R_{free} test set	1884 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4762	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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 45.11 % 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 1.3862e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.80	2/2298 (0.1%)	0.72	1/3088 (0.0%)
1	B	0.67	0/2298	0.70	0/3088
All	All	0.74	2/4596 (0.0%)	0.71	1/6176 (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	1
1	B	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	25	LYS	CD-CE	5.68	1.65	1.51
1	A	280	CYS	CB-SG	-5.29	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	157	LEU	CA-CB-CG	5.32	127.54	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	280	CYS	Peptide
1	B	281	VAL	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	2268	0	2300	44	0
1	B	2268	0	2300	49	0
2	A	132	0	0	5	0
2	B	94	0	0	5	0
All	All	4762	0	4600	92	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 11.

All (92) 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:226:GLU:OE1	1:A:262:LYS:HB2	1.44	1.18
1:B:175:MSE:CE	1:B:178:LEU:HD12	1.77	1.15
1:B:168:ILE:HG12	1:B:176:MSE:HE3	1.34	1.08
1:B:175:MSE:SE	2:B:352:HOH:O	2.21	1.08
1:B:168:ILE:HG12	1:B:176:MSE:CE	1.89	1.01
1:B:226:GLU:OE1	1:B:262:LYS:HB2	1.70	0.90
1:A:1:MSE:CE	1:A:17:PHE:HE1	1.86	0.89
1:B:157:LEU:HD21	1:B:159:ILE:HG12	1.58	0.86
1:B:175:MSE:HE1	1:B:178:LEU:HD12	1.58	0.84
1:A:273:LEU:HA	1:A:276:MSE:HE3	1.61	0.82
1:B:175:MSE:HE3	1:B:178:LEU:HD12	1.63	0.80
1:B:175:MSE:HE3	1:B:175:MSE:HA	1.64	0.78
1:B:157:LEU:CD2	1:B:159:ILE:HG12	2.14	0.77
1:A:172:HIS:HD2	2:B:288:HOH:O	1.67	0.76
1:B:157:LEU:HD21	1:B:159:ILE:CG1	2.17	0.73
1:A:1:MSE:HE2	1:A:3:LEU:HD21	1.69	0.73
1:A:226:GLU:OE1	1:A:262:LYS:CB	2.33	0.72
1:B:167:THR:HG22	1:B:176:MSE:HE2	1.73	0.71
1:B:168:ILE:CG1	1:B:176:MSE:HE3	2.18	0.71
1:A:1:MSE:CE	1:A:17:PHE:CE1	2.73	0.71
1:B:167:THR:CG2	1:B:176:MSE:HE2	2.23	0.68
1:A:159:ILE:O	1:A:159:ILE:CG2	2.42	0.67
1:A:1:MSE:HE3	1:A:17:PHE:HE1	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:MSE:CE	1:B:175:MSE:HA	2.27	0.64
2:A:288:HOH:O	1:B:172:HIS:HD2	1.82	0.63
1:B:137:MSE:HE3	2:B:365:HOH:O	1.98	0.63
1:B:235:ILE:HA	1:B:238:MSE:HE3	1.81	0.63
1:A:273:LEU:HA	1:A:276:MSE:CE	2.30	0.62
1:B:205:LYS:HG3	1:B:235:ILE:HD11	1.80	0.62
1:B:268:SER:O	1:B:274:ARG:NH1	2.34	0.60
1:A:223:ALA:HB3	1:A:225:LEU:HG	1.83	0.60
1:B:168:ILE:HG12	1:B:176:MSE:HE1	1.76	0.60
1:B:137:MSE:CE	2:B:365:HOH:O	2.50	0.59
1:A:1:MSE:O	1:A:28:VAL:HG22	2.03	0.59
1:B:274:ARG:O	1:B:278:VAL:HG12	2.02	0.58
1:A:1:MSE:HE1	1:A:17:PHE:HE1	1.67	0.58
1:A:172:HIS:HE1	2:A:332:HOH:O	1.88	0.56
1:A:205:LYS:HG3	1:A:235:ILE:HD11	1.87	0.56
1:A:160:LEU:HD21	1:A:183:MSE:HG2	1.87	0.55
1:A:159:ILE:O	1:A:159:ILE:HG23	2.06	0.55
1:A:226:GLU:HG2	1:A:227:ASN:H	1.72	0.55
1:B:224:ASN:HB3	1:B:227:ASN:ND2	2.23	0.54
1:A:62:GLU:HG2	2:A:374:HOH:O	2.06	0.54
1:B:50:LEU:HD22	1:B:55:LEU:HG	1.88	0.54
1:A:207:ILE:HD13	1:B:138:LEU:HB3	1.90	0.54
1:B:75:LYS:O	1:B:79:ILE:HG12	2.08	0.54
1:B:175:MSE:CE	1:B:178:LEU:CD1	2.69	0.53
1:B:197:ASP:HA	1:B:199:LYS:HE2	1.90	0.53
1:B:175:MSE:HE1	1:B:178:LEU:CD1	2.32	0.53
1:A:23:THR:HG23	1:A:24:PHE:CD2	2.44	0.52
1:A:226:GLU:HG2	1:A:227:ASN:N	2.23	0.52
1:A:238:MSE:HE3	2:A:378:HOH:O	2.09	0.52
1:B:223:ALA:HB3	1:B:225:LEU:HG	1.91	0.52
1:A:50:LEU:HD22	1:A:55:LEU:HG	1.92	0.52
1:B:156:ASP:O	1:B:156:ASP:OD1	2.29	0.51
1:B:122:PHE:CE2	1:B:159:ILE:HD11	2.46	0.50
1:A:156:ASP:OD1	1:A:156:ASP:O	2.29	0.50
1:A:281:VAL:O	1:A:281:VAL:CG1	2.58	0.49
1:A:277:TYR:C	1:A:277:TYR:CD2	2.86	0.48
1:B:224:ASN:HA	1:B:226:GLU:OE2	2.14	0.48
1:A:159:ILE:HA	2:A:331:HOH:O	2.14	0.48
1:B:1:MSE:O	1:B:28:VAL:HG22	2.14	0.48
1:A:1:MSE:HE1	1:A:17:PHE:CE1	2.47	0.47
1:A:93:LYS:O	1:A:129:LYS:HE2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ILE:HG21	1:A:277:TYR:CD1	2.51	0.45
1:A:156:ASP:OD1	1:A:156:ASP:N	2.44	0.45
1:A:1:MSE:HE3	1:A:17:PHE:CE1	2.48	0.45
1:A:179:LEU:O	1:A:183:MSE:HG3	2.17	0.45
1:B:196:PRO:O	1:B:199:LYS:HD3	2.17	0.45
1:B:117:ASN:HA	2:B:300:HOH:O	2.17	0.44
1:B:235:ILE:HA	1:B:238:MSE:CE	2.46	0.44
1:B:43:VAL:HG22	1:B:76:ILE:HD11	2.00	0.44
1:B:197:ASP:HA	1:B:199:LYS:HD3	1.99	0.44
1:B:198:ILE:O	1:B:202:ILE:HG12	2.17	0.44
1:B:235:ILE:HG12	1:B:238:MSE:CE	2.48	0.44
1:B:126:THR:HG22	1:B:127:GLY:N	2.32	0.44
1:A:237:LYS:O	1:A:237:LYS:HG3	2.18	0.43
1:B:157:LEU:HD22	1:B:160:LEU:N	2.33	0.43
1:A:224:ASN:O	1:A:227:ASN:HB2	2.19	0.43
1:B:157:LEU:HD21	1:B:159:ILE:HG13	1.99	0.43
1:B:122:PHE:CD2	1:B:159:ILE:HD11	2.54	0.42
1:A:263:LEU:O	1:A:267:ILE:HG12	2.20	0.42
1:B:107:MSE:HE1	1:B:143:ILE:HA	2.02	0.42
1:A:226:GLU:HB2	1:A:266:ILE:HG13	2.02	0.42
1:A:202:ILE:HD12	1:A:235:ILE:HG21	2.02	0.41
1:B:3:LEU:HG	1:B:27:ASP:HB3	2.02	0.41
1:A:159:ILE:O	1:A:159:ILE:HG22	2.19	0.41
1:A:75:LYS:NZ	1:A:75:LYS:HB2	2.36	0.41
1:A:281:VAL:O	1:A:281:VAL:HG13	2.20	0.41
1:A:211:GLN:O	1:A:215:LYS:HG3	2.21	0.40
1:A:277:TYR:CE2	1:A:281:VAL:HG21	2.56	0.40
1:B:6:ILE:HD13	1:B:33:ALA:HB1	2.02	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	281/285 (99%)	268 (95%)	13 (5%)	0	100	100
1	B	281/285 (99%)	271 (96%)	10 (4%)	0	100	100
All	All	562/570 (99%)	539 (96%)	23 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	257/249 (103%)	235 (91%)	22 (9%)	8	11
1	B	257/249 (103%)	242 (94%)	15 (6%)	17	24
All	All	514/498 (103%)	477 (93%)	37 (7%)	12	16

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	21	LYS
1	A	28	VAL
1	A	42	ASN
1	A	75	LYS
1	A	117	ASN
1	A	125	LYS
1	A	137	MSE
1	A	159	ILE
1	A	166	ILE
1	A	169	LYS
1	A	198	ILE
1	A	199	LYS
1	A	218	ILE
1	A	226	GLU
1	A	228	VAL
1	A	253	LYS
1	A	262	LYS

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Mol	Chain	Res	Type
1	A	265	GLU
1	A	279	ASN
1	A	281	VAL
1	A	282	LYS
1	B	10	LYS
1	B	21	LYS
1	B	75	LYS
1	B	154	THR
1	B	168	ILE
1	B	173	VAL
1	B	175	MSE
1	B	199	LYS
1	B	226	GLU
1	B	266	ILE
1	B	269	LYS
1	B	271	LYS
1	B	272	GLU
1	B	278	VAL
1	B	282	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	117	ASN
1	A	170	ASN
1	A	172	HIS
1	A	189	ASN
1	A	270	ASN
1	B	13	GLN
1	B	89	GLN
1	B	106	ASN
1	B	165	HIS
1	B	170	ASN
1	B	172	HIS
1	B	227	ASN

5.3.3 RNA ⓘ

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 oligosaccharides 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	273/285 (95%)	0.13	11 (4%)	43	44	11, 30, 47, 61	29 (10%)
1	B	273/285 (95%)	0.57	32 (11%)	10	12	15, 30, 47, 57	27 (9%)
All	All	546/570 (95%)	0.35	43 (7%)	20	22	11, 30, 47, 61	56 (10%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	0	GLY	6.9
1	B	257	ILE	5.0
1	B	267	ILE	4.8
1	B	282	LYS	4.8
1	B	28	VAL	4.7
1	B	266	ILE	4.5
1	B	277	TYR	4.4
1	A	0	GLY	4.2
1	B	262	LYS	4.1
1	A	278	VAL	4.1
1	B	155	PHE	3.8
1	B	274	ARG	3.6
1	B	281	VAL	3.5
1	B	269	LYS	3.5
1	B	158	ALA	3.3
1	B	159	ILE	3.3
1	B	260	ASN	3.3
1	B	261	ASN	3.3
1	B	259	LYS	3.3
1	B	263	LEU	3.3
1	B	264	ASP	3.1
1	B	157	LEU	3.0
1	B	26	ALA	3.0
1	B	280	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	275	LEU	2.8
1	A	159	ILE	2.7
1	B	258	VAL	2.7
1	B	278	VAL	2.7
1	B	167	THR	2.6
1	B	168	ILE	2.6
1	B	226	GLU	2.5
1	B	273	LEU	2.5
1	A	265	GLU	2.5
1	B	15	LYS	2.5
1	A	272	GLU	2.4
1	A	274	ARG	2.4
1	A	273	LEU	2.4
1	A	227	ASN	2.4
1	B	154	THR	2.2
1	A	279	ASN	2.2
1	B	268	SER	2.1
1	B	272	GLU	2.1
1	A	269	LYS	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.