Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2025 – 06:15 PM EST

PDB ID	:	8VKX
Title	:	VX22 bound to GII.4 P domain
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Deposited on	:	2024-01-10
Resolution	:	3.35 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:

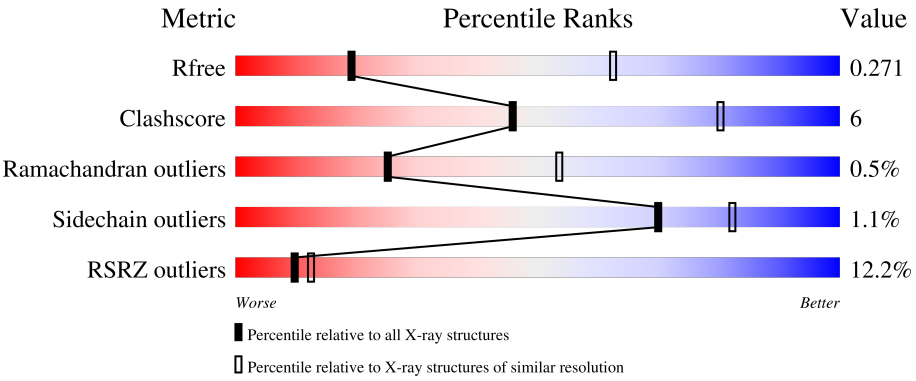
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 3.35 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	1012 (3.40-3.32)
Clashscore	180529	1035 (3.40-3.32)
Ramachandran outliers	177936	1037 (3.40-3.32)
Sidechain outliers	177891	1037 (3.40-3.32)
RSRZ outliers	164620	1012 (3.40-3.32)

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	H	235	8% 79% 18%
2	L	216	26% 81% 15%
3	A	306	5% 89% 11%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5668 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 VX22 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	230	Total	C	N	O	S	0	0	0
			1695	1064	288	336	7			

- Molecule 2 is a protein called VX22 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	211	Total	C	N	O	S	0	0	0
			1561	984	259	313	5			

- Molecule 3 is a protein called VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	306	Total	C	N	O	S	0	0	0
			2384	1513	406	455	10			

- Molecule 4 is water.

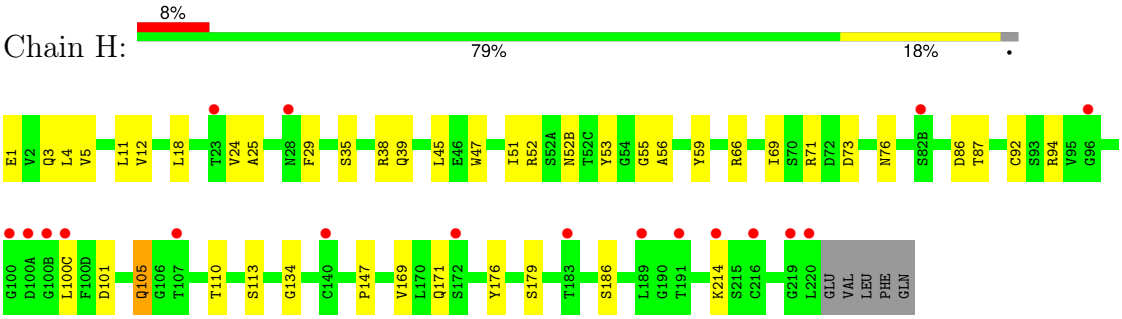
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	9	Total	O	0	0
			9	9		
4	L	6	Total	O	0	0
			6	6		
4	A	13	Total	O	0	0
			13	13		

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.

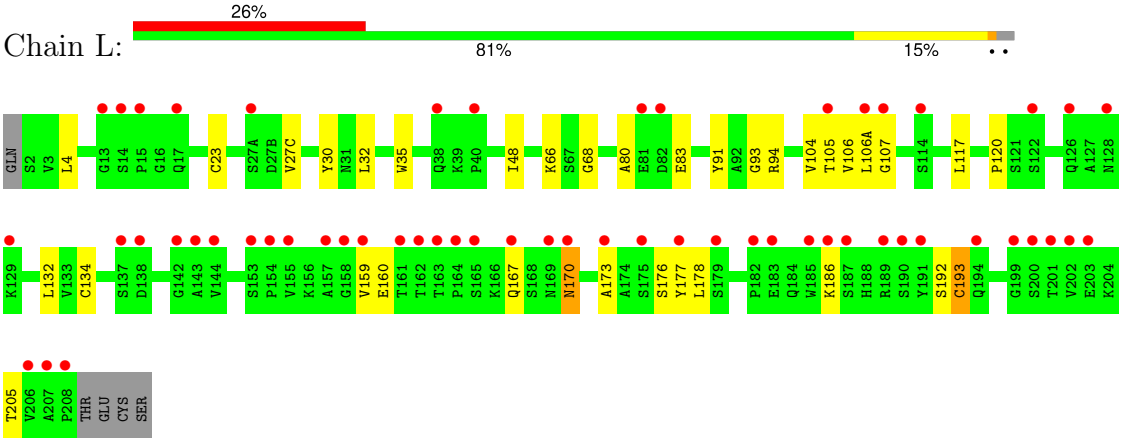
• Molecule 1: VX22 heavy chain

Chain H:



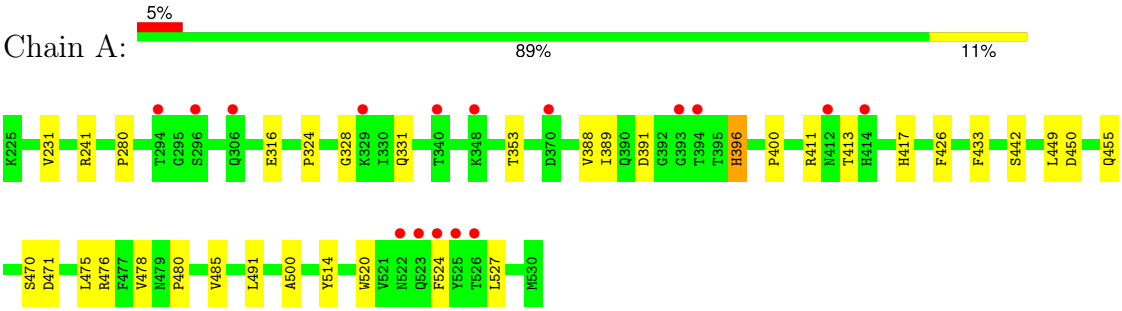
• Molecule 2: VX22 light chain

Chain L:



• Molecule 3: VP1

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	114.33Å 148.98Å 148.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.35 50.00 – 3.35	Depositor EDS
% Data completeness (in resolution range)	94.4 (50.00-3.35) 90.5 (50.00-3.35)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 3.32Å)	Xtriage
Refinement program	PHENIX 1.20.1	Depositor
R, R_{free}	0.245 , 0.272 0.243 , 0.271	Depositor DCC
R_{free} test set	15859 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å^2)	51.8	Xtriage
Anisotropy	0.563	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 32.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	5668	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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	H	0.27	0/1733	0.51	0/2356
2	L	0.27	0/1599	0.48	0/2181
3	A	0.25	0/2454	0.48	0/3358
All	All	0.26	0/5786	0.49	0/7895

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	H	1695	0	1644	25	0
2	L	1561	0	1517	22	0
3	A	2384	0	2272	19	0
4	A	13	0	0	0	0
4	H	9	0	0	0	0
4	L	6	0	0	1	0
All	All	5668	0	5433	63	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 6.

All (63) 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:H:11:LEU:HD12	1:H:147:PRO:HD3	1.66	0.77
3:A:470:SER:HB3	3:A:520:TRP:HB3	1.68	0.76
2:L:83:GLU:HG3	2:L:105:THR:HA	1.70	0.72
1:H:4:LEU:HD23	1:H:24:VAL:HG12	1.70	0.72
2:L:117:LEU:HD11	2:L:193:CYS:H	1.53	0.72
2:L:159:VAL:HG22	2:L:178:LEU:HD13	1.71	0.71
1:H:171:GLN:HA	2:L:160:GLU:OE1	1.95	0.67
2:L:167:GLN:HE21	2:L:173:ALA:HB2	1.60	0.66
1:H:94:ARG:NH2	1:H:101:ASP:OD2	2.27	0.65
3:A:331:GLN:HB2	3:A:389:ILE:HD11	1.78	0.65
3:A:280:PRO:HB3	3:A:455:GLN:HG2	1.79	0.64
3:A:389:ILE:HG23	3:A:442:SER:HB3	1.78	0.64
1:H:87:THR:HG23	1:H:110:THR:HA	1.78	0.63
1:H:52(B):ASN:ND2	1:H:73:ASP:OD2	2.32	0.63
3:A:433:PHE:HB3	3:A:450:ASP:HB3	1.82	0.61
2:L:35:TRP:HB2	2:L:48:ILE:HB	1.84	0.59
1:H:35:SER:OG	1:H:47:TRP:NE1	2.36	0.59
1:H:59:TYR:HE1	1:H:69:ILE:HG22	1.68	0.58
1:H:51:ILE:HD13	1:H:71:ARG:HG2	1.86	0.57
2:L:167:GLN:NE2	2:L:173:ALA:HB2	2.21	0.54
2:L:66:LYS:HE2	2:L:68:GLY:H	1.72	0.54
2:L:120:PRO:HD3	2:L:132:LEU:HD23	1.90	0.54
2:L:170:ASN:O	2:L:170:ASN:ND2	2.40	0.52
1:H:29:PHE:HE2	1:H:71:ARG:HB2	1.73	0.52
2:L:27(C):VAL:HG11	2:L:94:ARG:HE	1.75	0.50
1:H:12:VAL:HG11	1:H:18:LEU:HB2	1.93	0.50
2:L:30:TYR:CZ	2:L:32:LEU:HD11	2.47	0.49
2:L:4:LEU:HD12	2:L:23:CYS:SG	2.53	0.49
2:L:106(A):LEU:HD23	2:L:107:GLY:N	2.27	0.48
3:A:476:ARG:HG3	3:A:485:VAL:HG11	1.95	0.48
3:A:470:SER:OG	3:A:471:ASP:N	2.48	0.47
1:H:134:GLY:O	1:H:186:SER:N	2.40	0.46
3:A:500:ALA:HB2	3:A:527:LEU:HB2	1.97	0.46
3:A:231:VAL:HG13	3:A:514:TYR:CE2	2.51	0.46
1:H:39:GLN:HB2	1:H:45:LEU:HD23	1.98	0.46
3:A:411:ARG:O	3:A:413:THR:N	2.44	0.46
1:H:5:VAL:HG13	1:H:105:GLN:HE22	1.79	0.46
2:L:134:CYS:HB3	2:L:176:SER:HB3	1.98	0.46
3:A:480:PRO:HG3	3:A:514:TYR:HE1	1.81	0.46
1:H:179:SER:HG	2:L:177:TYR:HE2	1.64	0.46
1:H:29:PHE:CE2	1:H:71:ARG:HB2	2.50	0.45
2:L:83:GLU:HA	2:L:104:VAL:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:3:GLN:HG3	1:H:25:ALA:HB3	1.99	0.45
3:A:475:LEU:HD11	3:A:491:LEU:HD22	1.99	0.44
1:H:214:LYS:HD3	1:H:214:LYS:HA	1.78	0.44
1:H:38:ARG:NH1	1:H:86:ASP:OD1	2.47	0.44
2:L:91:TYR:CZ	2:L:93:GLY:HA2	2.52	0.44
2:L:80:ALA:HA	2:L:106:VAL:HG21	1.99	0.43
1:H:53:TYR:CE1	3:A:478:VAL:HG11	2.54	0.43
3:A:316:GLU:HG2	3:A:417:HIS:CG	2.53	0.43
3:A:426:PHE:CE1	3:A:524:PHE:HB3	2.53	0.43
1:H:66:ARG:NH2	1:H:86:ASP:OD2	2.51	0.42
3:A:241:ARG:HB2	3:A:449:LEU:HD21	2.01	0.42
1:H:169:VAL:O	1:H:176:TYR:HA	2.18	0.42
3:A:328:GLY:HA3	3:A:400:PRO:HB3	2.00	0.42
1:H:52:ARG:HB2	1:H:55:GLY:O	2.19	0.42
1:H:24:VAL:O	1:H:76:ASN:ND2	2.53	0.41
2:L:186:LYS:HE2	4:L:306:HOH:O	2.20	0.41
2:L:192:SER:HB3	2:L:205:THR:HG22	2.01	0.41
1:H:59:TYR:CE1	1:H:69:ILE:HG22	2.52	0.41
2:L:66:LYS:HE2	2:L:68:GLY:N	2.34	0.41
3:A:324:PRO:HB2	3:A:353:THR:HG21	2.02	0.41
3:A:388:VAL:HG11	3:A:400:PRO:HG3	2.03	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	H	228/235 (97%)	208 (91%)	18 (8%)	2 (1%)	14 41
2	L	209/216 (97%)	197 (94%)	12 (6%)	0	100 100
3	A	304/306 (99%)	283 (93%)	19 (6%)	2 (1%)	19 47
All	All	741/757 (98%)	688 (93%)	49 (7%)	4 (0%)	25 53

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	391	ASP
1	H	100(C)	LEU
1	H	56	ALA
3	A	396	HIS

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	H	186/194 (96%)	182 (98%)	4 (2%)	47	68
2	L	173/182 (95%)	171 (99%)	2 (1%)	67	80
3	A	263/266 (99%)	262 (100%)	1 (0%)	89	94
All	All	622/642 (97%)	615 (99%)	7 (1%)	70	82

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	1	GLU
1	H	92	CYS
1	H	105	GLN
1	H	113	SER
2	L	170	ASN
2	L	193	CYS
3	A	396	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	167	GLN
3	A	282	ASN

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 oligosaccharides 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, 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	H	230/235 (97%)	0.82	18 (7%) 20 20	42, 60, 81, 98	0
2	L	211/216 (97%)	1.42	57 (27%) 2 4	42, 77, 105, 115	0
3	A	306/306 (100%)	0.49	16 (5%) 34 30	35, 50, 80, 100	0
All	All	747/757 (98%)	0.85	91 (12%) 10 12	35, 58, 92, 115	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	524	PHE	4.3
3	A	522	ASN	4.0
3	A	348	LYS	3.8
2	L	165	SER	3.7
1	H	100(A)	ASP	3.7
2	L	189	ARG	3.6
2	L	154	PRO	3.6
2	L	201	THR	3.6
1	H	100(C)	LEU	3.6
1	H	100(B)	GLY	3.6
2	L	153	SER	3.6
2	L	190	SER	3.5
2	L	203	GLU	3.4
2	L	159	VAL	3.4
2	L	143	ALA	3.4
2	L	158	GLY	3.4
1	H	172	SER	3.3
2	L	206	VAL	3.3
1	H	23	THR	3.3
1	H	189	LEU	3.3
1	H	96	GLY	3.2
2	L	169	ASN	3.2
2	L	105	THR	3.2

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Mol	Chain	Res	Type	RSRZ
2	L	194	GLN	3.1
2	L	207	ALA	3.1
2	L	161	THR	3.1
3	A	393	GLY	3.1
3	A	414	HIS	3.1
3	A	523	GLN	3.0
2	L	186	LYS	3.0
1	H	140	CYS	3.0
2	L	38	GLN	2.9
3	A	525	TYR	2.9
2	L	107	GLY	2.9
3	A	306	GLN	2.9
3	A	370	ASP	2.9
1	H	216	CYS	2.8
2	L	106(A)	LEU	2.8
1	H	28	ASN	2.8
2	L	191	TYR	2.8
2	L	40	PRO	2.8
2	L	126	GLN	2.8
2	L	114	SER	2.8
2	L	162	THR	2.8
3	A	394	THR	2.8
2	L	157	ALA	2.7
2	L	164	PRO	2.7
2	L	179	SER	2.7
1	H	219	GLY	2.6
2	L	163	THR	2.6
2	L	137	SER	2.6
2	L	200	SER	2.5
1	H	214	LYS	2.5
2	L	185	TRP	2.5
3	A	329	LYS	2.5
2	L	182	PRO	2.5
2	L	81	GLU	2.5
2	L	175	SER	2.5
2	L	142	GLY	2.4
2	L	14	SER	2.4
2	L	128	ASN	2.4
3	A	340	THR	2.4
2	L	138	ASP	2.4
2	L	177	TYR	2.4
2	L	82	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	191	THR	2.4
2	L	208	PRO	2.4
2	L	129	LYS	2.3
1	H	100	GLY	2.3
2	L	173	ALA	2.3
2	L	15	PRO	2.3
3	A	294	THR	2.3
2	L	183	GLU	2.3
2	L	17	GLN	2.2
2	L	199	GLY	2.2
3	A	412	ASN	2.2
2	L	27(A)	SER	2.2
2	L	13	GLY	2.1
2	L	155	VAL	2.1
2	L	187	SER	2.1
2	L	122	SER	2.1
3	A	526	THR	2.1
2	L	202	VAL	2.1
1	H	107	THR	2.1
1	H	183	THR	2.1
3	A	296	SER	2.1
2	L	170	ASN	2.1
1	H	82(B)	SER	2.0
2	L	167	GLN	2.0
1	H	220	LEU	2.0
2	L	144	VAL	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.