



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:19 PM UTC

PDB ID : 9HV2 / pdb_00009hv2
Title : Crystal structure of tri-specific FMDV mAb-34 Fab
Authors : Ren, J.; Duyvesteyn, H.M.E.; Stuart, D.I.
Deposited on : 2024-12-24
Resolution : 1.77 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

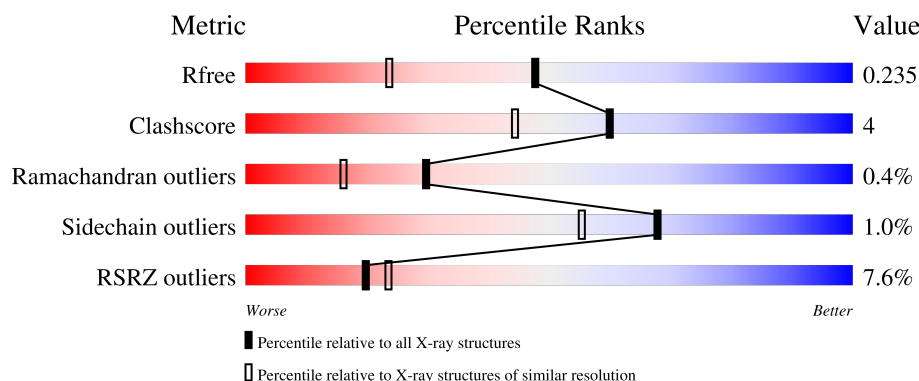
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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}	180053	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	238	<div> <div>13%</div> <div>79%</div> <div>13%</div> <div>8%</div> </div>
1	H	238	<div> <div>10%</div> <div>75%</div> <div>13%</div> <div>11%</div> </div>
2	B	213	<div> <div>%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
2	L	213	<div> <div>4%</div> <div>92%</div> <div>6%</div> <div>..</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6822 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 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1596	994	265	324	13			
1	H	211	Total	C	N	O	S	0	0	0
			1546	965	257	312	12			

- Molecule 2 is a protein called light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	211	Total	C	N	O	S	0	0	0
			1588	984	265	334	5			
2	L	210	Total	C	N	O	S	0	0	0
			1582	981	264	333	4			

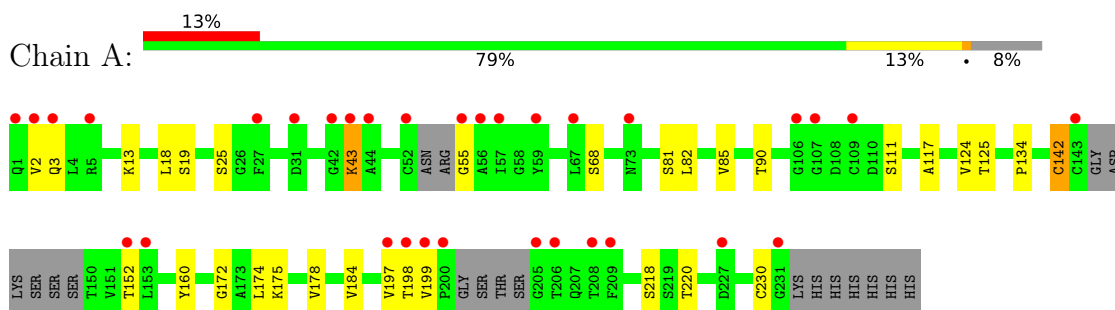
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	126	Total	O	0	0
			126	126		
3	B	123	Total	O	0	0
			123	123		
3	H	111	Total	O	0	0
			111	111		
3	L	150	Total	O	0	0
			150	150		

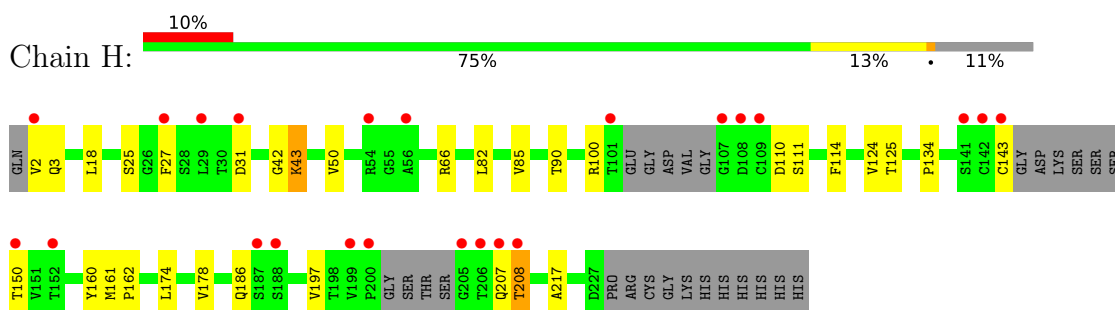
3 Residue-property plots [i](#)

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.

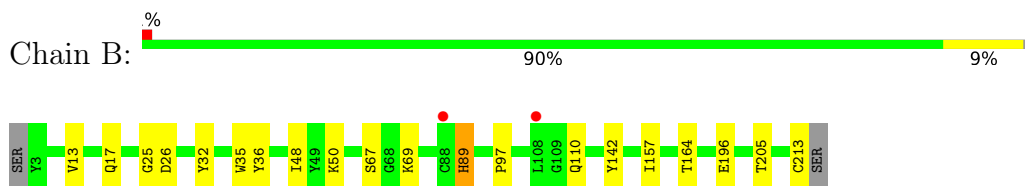
- Molecule 1: heavy chain



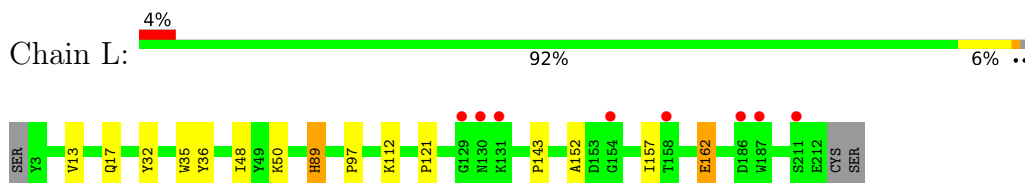
- Molecule 1: heavy chain



- Molecule 2: light chain



- Molecule 2: light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.41Å 81.47Å 74.47Å 90.00° 116.03° 90.00°	Depositor
Resolution (Å)	40.73 – 1.77 40.73 – 1.77	Depositor EDS
% Data completeness (in resolution range)	95.8 (40.73-1.77) 95.8 (40.73-1.77)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 1.77Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.208 , 0.235 0.208 , 0.235	Depositor DCC
R_{free} test set	3672 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.030 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6822	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.17	0/1627	0.44	0/2222
1	H	0.16	0/1576	0.44	0/2153
2	B	0.16	0/1623	0.40	0/2210
2	L	0.17	0/1617	0.42	0/2202
All	All	0.17	0/6443	0.42	0/8787

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 [i](#)

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	1596	0	1552	18	1
1	H	1546	0	1510	21	0
2	B	1588	0	1526	10	1
2	L	1582	0	1522	10	0
3	A	126	0	0	3	0
3	B	123	0	0	0	0
3	H	111	0	0	1	0
3	L	150	0	0	0	0
All	All	6822	0	6110	53	1

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 (53) 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:111:SER:HB2	2:B:97:PRO:HG3	1.63	0.80
2:L:152:ALA:HB2	2:L:157:ILE:HD11	1.72	0.70
1:H:31:ASP:HB3	1:H:100:ARG:HD2	1.74	0.68
1:A:178:VAL:HG22	1:A:197:VAL:HG22	1.75	0.68
2:B:13:VAL:HG22	2:B:17:GLN:HB2	1.76	0.67
1:A:55:GLY:N	3:A:302:HOH:O	2.27	0.67
1:H:186:GLN:NE2	2:L:162:GLU:OE1	2.28	0.66
1:H:143:CYS:SG	2:L:121:PRO:HG3	2.36	0.65
1:A:13:LYS:NZ	3:A:301:HOH:O	2.26	0.63
1:A:152:THR:HG22	1:A:198:THR:HG22	1.81	0.63
1:H:150:THR:N	3:H:304:HOH:O	2.32	0.62
1:H:111:SER:HB2	2:L:97:PRO:HG3	1.84	0.59
1:H:178:VAL:HG22	1:H:197:VAL:HG22	1.85	0.58
2:L:13:VAL:HG22	2:L:17:GLN:HB2	1.85	0.58
2:B:36:TYR:HE1	2:B:89:HIS:HB3	1.69	0.57
1:A:82:LEU:HD22	1:A:85:VAL:HG12	1.87	0.56
2:B:110:GLN:HB2	2:B:142:TYR:CE1	2.43	0.54
1:H:82:LEU:HD22	1:H:85:VAL:HG12	1.89	0.54
1:A:18:LEU:HD13	1:A:124:VAL:HG11	1.90	0.53
1:H:3:GLN:HB3	1:H:25:SER:HB3	1.90	0.52
1:H:2:VAL:HG22	1:H:27:PHE:HD2	1.76	0.51
1:H:18:LEU:HD13	1:H:124:VAL:HG11	1.92	0.50
1:A:134:PRO:HB3	1:A:160:TYR:HB3	1.97	0.47
2:B:26:ASP:HA	2:B:69:LYS:HD3	1.96	0.47
2:B:196:GLU:HG2	2:B:205:THR:HG23	1.97	0.46
1:H:66:ARG:NH1	1:H:82:LEU:HD21	2.31	0.46
1:A:174:LEU:HD21	1:A:197:VAL:HG11	1.97	0.45
1:H:2:VAL:HG22	1:H:27:PHE:CD2	2.51	0.45
1:A:184:VAL:HG12	2:B:164:THR:HG23	1.99	0.45
2:B:35:TRP:HB2	2:B:48:ILE:HB	1.98	0.45
2:L:35:TRP:HB2	2:L:48:ILE:HB	1.99	0.44
1:A:2:VAL:H	1:A:117:ALA:HB2	1.82	0.44
1:A:3:GLN:HB3	1:A:25:SER:HB3	2.00	0.44
1:H:110:ASP:OD2	2:L:50:LYS:NZ	2.47	0.44
1:H:207:GLN:OE1	1:H:208:THR:N	2.49	0.44
2:L:32:TYR:HB3	2:L:50:LYS:HA	2.00	0.43
2:L:36:TYR:HE1	2:L:89:HIS:HB3	1.83	0.43
1:A:218:SER:O	1:A:220:THR:HG23	2.18	0.43
1:A:172:GLY:O	1:A:175:LYS:HE3	2.18	0.42
2:B:32:TYR:HB3	2:B:50:LYS:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:134:PRO:HB3	1:H:160:TYR:HB3	2.02	0.42
1:H:174:LEU:HD21	1:H:197:VAL:HG11	2.01	0.42
1:H:162:PRO:HD2	1:H:217:ALA:CB	2.49	0.41
1:H:50:VAL:HG11	1:H:114:PHE:CE2	2.56	0.41
1:H:90:THR:HG23	1:H:125:THR:HA	2.02	0.41
1:A:90:THR:HG23	1:A:125:THR:HA	2.02	0.41
2:B:25:GLY:O	2:B:69:LYS:HB3	2.21	0.41
1:A:142:CYS:SG	1:A:230:CYS:N	2.94	0.41
1:A:68:SER:HB3	1:A:81:SER:HB2	2.02	0.41
2:L:112:LYS:HD3	2:L:143:PRO:HD3	2.03	0.40
1:A:43:LYS:HG2	3:A:405:HOH:O	2.20	0.40
1:H:42:GLY:O	1:H:43:LYS:HB2	2.21	0.40
1:H:161:MET:HE2	1:H:161:MET:HB2	1.93	0.40

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	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:SER:OG	2:B:67:SER:OG[2_545]	2.17	0.03

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	211/238 (89%)	203 (96%)	6 (3%)	2 (1%)	14	4
1	H	203/238 (85%)	197 (97%)	5 (2%)	1 (0%)	24	11
2	B	209/213 (98%)	203 (97%)	6 (3%)	0	100	100
2	L	208/213 (98%)	202 (97%)	6 (3%)	0	100	100
All	All	831/902 (92%)	805 (97%)	23 (3%)	3 (0%)	30	16

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	142	CYS
1	A	43	LYS
1	H	43	LYS

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	187/204 (92%)	186 (100%)	1 (0%)	81	73
1	H	182/204 (89%)	181 (100%)	1 (0%)	81	73
2	B	183/185 (99%)	180 (98%)	3 (2%)	55	38
2	L	182/185 (98%)	180 (99%)	2 (1%)	65	51
All	All	734/778 (94%)	727 (99%)	7 (1%)	68	55

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

Mol	Chain	Res	Type
1	A	199	VAL
2	B	89	HIS
2	B	157	ILE
2	B	213	CYS
1	H	208	THR
2	L	89	HIS
2	L	162	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	207	GLN
2	B	130	ASN
1	H	39	GLN
2	L	31	GLN
2	L	38	GLN
2	L	130	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 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	219/238 (92%)	0.83	32 (14%) 6 6	28, 42, 82, 108	0
1	H	211/238 (88%)	0.68	23 (10%) 10 12	26, 40, 78, 126	0
2	B	211/213 (99%)	0.45	2 (0%) 81 86	25, 42, 62, 88	0
2	L	210/213 (98%)	0.36	8 (3%) 44 50	25, 37, 66, 110	0
All	All	851/902 (94%)	0.58	65 (7%) 20 23	25, 40, 72, 126	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	56	ALA	5.9
1	A	2	VAL	5.3
1	H	2	VAL	4.7
1	H	200	PRO	4.6
1	H	141	SER	4.3
1	A	55	GLY	3.9
1	H	109	CYS	3.7
1	H	101	THR	3.7
1	H	206	THR	3.5
2	B	88	CYS	3.5
1	H	108	ASP	3.3
1	H	150	THR	3.3
1	H	143	CYS	3.2
1	H	27	PHE	3.2
1	A	205	GLY	3.2
1	A	200	PRO	3.2
1	H	29	LEU	3.1
1	A	106	GLY	3.1
1	A	1	GLN	3.1
1	H	107	GLY	3.1
1	A	73	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
2	L	130	ASN	3.0
1	H	208	THR	2.9
1	A	107	GLY	2.9
1	A	199	VAL	2.9
1	H	207	GLN	2.8
1	H	142	CYS	2.8
2	L	129	GLY	2.8
2	L	211	SER	2.8
1	A	143	CYS	2.7
1	H	205	GLY	2.6
2	L	187	TRP	2.6
1	A	109	CYS	2.6
1	A	52	CYS	2.5
2	L	158	THR	2.5
1	A	44	ALA	2.5
1	A	27	PHE	2.4
1	A	206	THR	2.4
1	A	208	THR	2.4
1	A	227	ASP	2.3
1	A	59	TYR	2.3
1	H	187	SER	2.3
2	L	186	ASP	2.3
1	H	188	SER	2.3
1	A	153	LEU	2.3
1	A	57	ILE	2.3
1	A	67	LEU	2.2
1	H	54	ARG	2.2
1	A	231	GLY	2.2
2	L	154	GLY	2.2
1	A	198	THR	2.2
1	H	199	VAL	2.2
1	A	3	GLN	2.2
1	A	5	ARG	2.2
1	H	31	ASP	2.1
2	B	108	LEU	2.1
2	L	131	LYS	2.1
1	H	152	THR	2.1
1	H	56	ALA	2.1
1	A	197	VAL	2.1
1	A	31	ASP	2.1
1	A	152	THR	2.1
1	A	209	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	43	LYS	2.0
1	A	42	GLY	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 oligosaccharides 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.