



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:30 PM UTC

PDB ID : 4KP3 / pdb_00004kp3
Title : Crystal Structure of MyoVa-GTD in Complex with Two Cargos
Authors : Wei, Z.; Liu, X.; Yu, C.; Zhang, M.
Deposited on : 2013-05-13
Resolution : 2.40 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

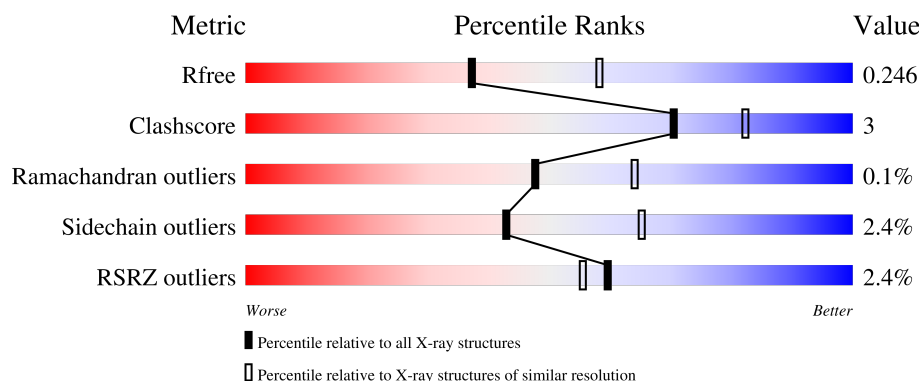
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 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	404	0% 77% 12% 11%
1	B	404	2% 80% 7% 12%
2	C	103	3% 68% 11% 21%
2	D	103	3% 72% 8% 20%
3	E	43	2% 33% 67%

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Mol	Chain	Length	Quality of chain
3	F	43	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7359 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 Unconventional myosin-Va.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	1	0
			2908	1850	501	536	21			
1	B	355	Total	C	N	O	S	0	0	0
			2847	1810	491	525	21			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1450	HIS	-	expression tag	UNP Q99104
A	1451	HIS	-	expression tag	UNP Q99104
A	1452	HIS	-	expression tag	UNP Q99104
A	1453	HIS	-	expression tag	UNP Q99104
A	1454	HIS	-	expression tag	UNP Q99104
A	1455	HIS	-	expression tag	UNP Q99104
A	1456	SER	-	expression tag	UNP Q99104
A	1457	SER	-	expression tag	UNP Q99104
A	1458	GLY	-	expression tag	UNP Q99104
A	1459	LEU	-	expression tag	UNP Q99104
A	1460	GLY	-	expression tag	UNP Q99104
A	1461	VAL	-	expression tag	UNP Q99104
A	1462	LEU	-	expression tag	UNP Q99104
A	1463	PHE	-	expression tag	UNP Q99104
A	1464	GLN	-	expression tag	UNP Q99104
A	1465	GLY	-	expression tag	UNP Q99104
A	1466	PRO	-	expression tag	UNP Q99104
A	1467	GLY	-	expression tag	UNP Q99104
A	1468	SER	-	expression tag	UNP Q99104
A	1674	SER	CYS	engineered mutation	UNP Q99104
B	1450	HIS	-	expression tag	UNP Q99104
B	1451	HIS	-	expression tag	UNP Q99104
B	1452	HIS	-	expression tag	UNP Q99104
B	1453	HIS	-	expression tag	UNP Q99104
B	1454	HIS	-	expression tag	UNP Q99104

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1455	HIS	-	expression tag	UNP Q99104
B	1456	SER	-	expression tag	UNP Q99104
B	1457	SER	-	expression tag	UNP Q99104
B	1458	GLY	-	expression tag	UNP Q99104
B	1459	LEU	-	expression tag	UNP Q99104
B	1460	GLY	-	expression tag	UNP Q99104
B	1461	VAL	-	expression tag	UNP Q99104
B	1462	LEU	-	expression tag	UNP Q99104
B	1463	PHE	-	expression tag	UNP Q99104
B	1464	GLN	-	expression tag	UNP Q99104
B	1465	GLY	-	expression tag	UNP Q99104
B	1466	PRO	-	expression tag	UNP Q99104
B	1467	GLY	-	expression tag	UNP Q99104
B	1468	SER	-	expression tag	UNP Q99104
B	1674	SER	CYS	engineered mutation	UNP Q99104

- Molecule 2 is a protein called RILP-like protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	81	Total	C	N	O	S	0	0	0
			642	398	110	130	4			
2	D	82	Total	C	N	O	S	0	1	0
			659	409	115	131	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	GLY	-	expression tag	UNP Q99LE1
C	-4	PRO	-	expression tag	UNP Q99LE1
C	-3	GLY	-	expression tag	UNP Q99LE1
C	-2	SER	-	expression tag	UNP Q99LE1
C	-1	GLU	-	expression tag	UNP Q99LE1
C	0	PHE	-	expression tag	UNP Q99LE1
D	-5	GLY	-	expression tag	UNP Q99LE1
D	-4	PRO	-	expression tag	UNP Q99LE1
D	-3	GLY	-	expression tag	UNP Q99LE1
D	-2	SER	-	expression tag	UNP Q99LE1
D	-1	GLU	-	expression tag	UNP Q99LE1
D	0	PHE	-	expression tag	UNP Q99LE1

- Molecule 3 is a protein called Melanophilin.

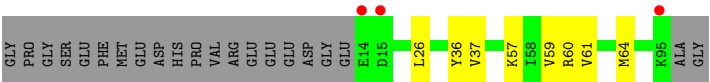
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	14	Total	C	N	O	0	0	0
			121	78	22	21			
3	F	14	Total	C	N	O	0	0	0
			125	81	23	21			

There are 8 discrepancies between the modelled and reference sequences:

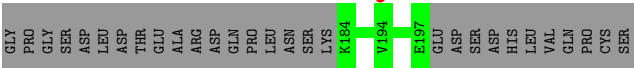
Chain	Residue	Modelled	Actual	Comment	Reference
E	166	GLY	-	expression tag	UNP Q91V27
E	167	PRO	-	expression tag	UNP Q91V27
E	168	GLY	-	expression tag	UNP Q91V27
E	169	SER	-	expression tag	UNP Q91V27
F	166	GLY	-	expression tag	UNP Q91V27
F	167	PRO	-	expression tag	UNP Q91V27
F	168	GLY	-	expression tag	UNP Q91V27
F	169	SER	-	expression tag	UNP Q91V27

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	33	Total	O	0	0
			33	33		
4	C	6	Total	O	0	0
			6	6		
4	E	1	Total	O	0	0
			1	1		
4	B	13	Total	O	0	0
			13	13		
4	D	3	Total	O	0	0
			3	3		
4	F	1	Total	O	0	0
			1	1		



• Molecule 3: Melanophilin



• Molecule 3: Melanophilin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.85Å 107.93Å 83.51Å 90.00° 96.14° 90.00°	Depositor
Resolution (Å)	38.69 – 2.40 38.69 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.8 (38.69-2.40) 97.9 (38.69-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.8.1 _1168	Depositor
R, R_{free}	0.192 , 0.241 0.195 , 0.246	Depositor DCC
R_{free} test set	2798 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	48.2	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7359	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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	0.34	0/2960	0.73	0/3995
1	B	0.31	0/2894	0.72	0/3906
2	C	0.33	0/646	0.75	0/869
2	D	0.34	0/666	0.70	0/894
3	E	0.26	0/122	0.55	0/160
3	F	0.23	0/126	0.56	0/164
All	All	0.32	0/7414	0.72	0/9988

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	2908	0	2960	27	0
1	B	2847	0	2890	15	0
2	C	642	0	650	7	0
2	D	659	0	676	6	0
3	E	121	0	121	0	0
3	F	125	0	132	1	0
4	A	33	0	0	0	0
4	B	13	0	0	0	0
4	C	6	0	0	0	0
4	D	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	1	0	0	0	0
4	F	1	0	0	0	0
All	All	7359	0	7429	50	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 3.

All (50) 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:1726:GLU:OE2	1:A:1729:ARG:NH1	2.28	0.66
1:B:1630:HIS:O	1:B:1716:GLN:NE2	2.30	0.64
1:B:1539:LYS:HE3	1:B:1603:LEU:HD13	1.82	0.62
1:A:1623:ILE:HD12	1:A:1697:ILE:HD12	1.85	0.59
1:A:1763:GLU:OE1	1:A:1805:ARG:NH2	2.36	0.59
1:A:1623:ILE:HD13	1:A:1694:VAL:HA	1.87	0.56
1:A:1660:ASP:HB3	1:A:1664:ARG:NH2	2.21	0.55
1:B:1502:LEU:HD13	2:D:59:VAL:HG22	1.89	0.54
1:B:1610:GLN:OE1	1:B:1613:ARG:NH1	2.41	0.53
1:A:1502:LEU:HD13	2:C:59:VAL:HG22	1.90	0.53
2:C:42:LEU:HD11	2:C:58:ILE:HD12	1.91	0.52
1:A:1615:LEU:HD21	1:A:1690:MET:HG2	1.91	0.52
1:A:1615:LEU:HD11	1:A:1690:MET:SD	2.49	0.52
1:A:1531:LEU:HB3	1:A:1596:TYR:CE1	2.44	0.52
1:B:1590:ASN:OD1	3:F:184:LYS:NZ	2.33	0.51
1:A:1630:HIS:O	1:A:1716:GLN:NE2	2.34	0.50
1:A:1512:PHE:CZ	1:A:1569:TYR:HB2	2.48	0.49
1:B:1531:LEU:HB3	1:B:1596:TYR:CE1	2.47	0.48
1:B:1535:ILE:HG23	1:B:1603:LEU:HD22	1.96	0.47
2:C:48:ASP:OD1	2:C:50:ARG:HG2	2.15	0.47
2:D:61:VAL:HA	2:D:64:MET:HE2	1.97	0.47
2:C:15:ASP:HB3	2:C:37:VAL:HG21	1.97	0.47
1:A:1475:LEU:HG	1:A:1513:MET:HE2	1.97	0.46
1:A:1656:THR:OG1	1:A:1657:TYR:N	2.48	0.45
1:A:1807:ARG:C	1:A:1809:ARG:H	2.23	0.45
1:A:1713:LYS:HD3	1:A:1713:LYS:HA	1.72	0.45
2:C:61:VAL:HA	2:C:64:MET:HE2	1.97	0.45
1:B:1512:PHE:CZ	1:B:1569:TYR:HB2	2.52	0.45
1:B:1603:LEU:O	1:B:1607:ILE:HG13	2.17	0.45
1:B:1620:GLN:HA	1:B:1623:ILE:HD12	1.98	0.44
1:B:1675:GLN:HA	2:D:36:TYR:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1615:LEU:HD21	1:A:1690:MET:CG	2.48	0.43
1:A:1692:TYR:OH	1:A:1818:ASP:O	2.35	0.43
1:B:1726:GLU:OE1	1:B:1729:ARG:NH1	2.51	0.43
1:A:1718:ARG:HD2	1:A:1718:ARG:HA	1.86	0.43
2:C:64:MET:SD	2:D:26:LEU:HD11	2.59	0.43
1:A:1740:GLU:OE1	1:A:1740:GLU:N	2.49	0.43
1:B:1620:GLN:HG2	1:B:1697:ILE:HD13	2.01	0.43
1:A:1502:LEU:HD23	2:C:39:GLY:HA2	2.01	0.43
1:B:1484:LYS:HD2	1:B:1849:PHE:CE1	2.54	0.42
2:D:60[A]:ARG:HA	2:D:60[A]:ARG:HD2	1.84	0.42
1:A:1619:LEU:HD23	1:A:1622:MET:HE2	2.02	0.42
1:A:1789:GLU:H	1:A:1789:GLU:HG3	1.68	0.42
1:B:1660:ASP:HB3	1:B:1664:ARG:NH2	2.36	0.41
1:A:1811:ASP:N	1:A:1811:ASP:OD1	2.54	0.41
1:A:1837:GLU:HG2	1:A:1838:THR:HG23	2.03	0.40
1:A:1566:LEU:O	1:A:1570:SER:HB3	2.21	0.40
1:A:1787:VAL:HG12	1:A:1791:GLU:OE1	2.20	0.40
1:A:1847:LEU:O	1:A:1850:ILE:HG12	2.21	0.40
2:D:57:LYS:HE3	2:D:57:LYS:HB2	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	358/404 (89%)	351 (98%)	7 (2%)	0	100	100
1	B	349/404 (86%)	341 (98%)	7 (2%)	1 (0%)	36	50
2	C	79/103 (77%)	79 (100%)	0	0	100	100
2	D	81/103 (79%)	81 (100%)	0	0	100	100
3	E	12/43 (28%)	12 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	12/43 (28%)	11 (92%)	1 (8%)	0	100	100
All	All	891/1100 (81%)	875 (98%)	15 (2%)	1 (0%)	48	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1629	GLU

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	329/365 (90%)	318 (97%)	11 (3%)	33	55
1	B	321/365 (88%)	314 (98%)	7 (2%)	45	67
2	C	72/89 (81%)	71 (99%)	1 (1%)	59	79
2	D	74/89 (83%)	73 (99%)	1 (1%)	59	79
3	E	13/40 (32%)	13 (100%)	0	100	100
3	F	14/40 (35%)	14 (100%)	0	100	100
All	All	823/988 (83%)	803 (98%)	20 (2%)	43	65

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1476	GLU
1	A	1502	LEU
1	A	1631	GLU
1	A	1658	THR
1	A	1701	ASN
1	A	1706	LYS
1	A	1732	ASN
1	A	1760	ASP
1	A	1796	VAL
1	A	1809	ARG

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Mol	Chain	Res	Type
1	A	1834	LEU
2	C	43	MET
1	B	1479	ARG
1	B	1502	LEU
1	B	1543	LYS
1	B	1616	GLU
1	B	1660	ASP
1	B	1701	ASN
1	B	1734	MET
2	D	37	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1590	ASN
1	A	1665	GLN
1	A	1770	ASN
2	C	55	GLN
2	C	88	GLN
1	B	1586	HIS
1	B	1670	HIS
1	B	1723	GLN
1	B	1782	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 [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	361/404 (89%)	-0.23	6 (1%) 69 65	23, 44, 83, 118	1 (0%)
1	B	355/404 (87%)	0.00	7 (1%) 65 60	27, 55, 85, 119	1 (0%)
2	C	81/103 (78%)	-0.26	3 (3%) 45 41	28, 44, 73, 95	2 (2%)
2	D	82/103 (79%)	-0.22	3 (3%) 45 41	17, 43, 71, 96	1 (1%)
3	E	14/43 (32%)	0.18	1 (7%) 22 18	41, 57, 84, 104	0
3	F	14/43 (32%)	1.14	2 (14%) 6 5	66, 86, 114, 124	0
All	All	907/1100 (82%)	-0.11	22 (2%) 59 55	17, 50, 87, 124	5 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1632	THR	5.2
1	B	1786	PRO	4.2
1	B	1656	THR	3.8
1	B	1812	SER	3.5
1	A	1630	HIS	3.3
1	A	1656	THR	3.1
3	E	194	VAL	3.0
2	D	95	LYS	2.9
1	B	1476	GLU	2.5
1	B	1715	MET	2.5
1	A	1792	GLU	2.4
2	C	15	ASP	2.3
1	A	1706	LYS	2.3
1	B	1810	LYS	2.3
2	D	15	ASP	2.3
3	F	197	GLU	2.3
2	C	43	MET	2.2
2	C	94	ARG	2.2
3	F	194	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	14	GLU	2.1
1	A	1755	LYS	2.1
1	B	1706	LYS	2.1

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.