



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 9GW5 / pdb_00009gw5
Title : type-I interferon autoantibodies pmab3, pmab19 and pmab14 in complex with Interferon alpha-2
Authors : Duquerroy, S.; Rey, F.; Mahevas, M.; Chappert, P.; Ahouzi, O.
Deposited on : 2024-09-26
Resolution : 4.00 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

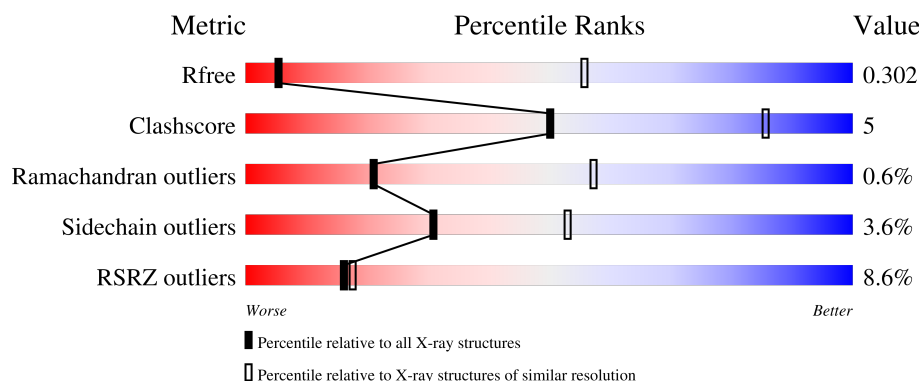
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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	188	
2	H	290	
3	U	288	
4	V	285	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6368 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 Interferon alpha-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	145	Total	C	N	O	S	0	0	0
			1198	769	201	220	8			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	166	GLY	-	expression tag	UNP P01563
A	167	GLY	-	expression tag	UNP P01563
A	168	GLY	-	expression tag	UNP P01563
A	169	GLY	-	expression tag	UNP P01563
A	170	SER	-	expression tag	UNP P01563
A	171	LEU	-	expression tag	UNP P01563
A	172	VAL	-	expression tag	UNP P01563
A	173	PRO	-	expression tag	UNP P01563
A	174	ARG	-	expression tag	UNP P01563
A	175	GLY	-	expression tag	UNP P01563
A	176	SER	-	expression tag	UNP P01563
A	177	GLY	-	expression tag	UNP P01563
A	178	GLY	-	expression tag	UNP P01563
A	179	GLY	-	expression tag	UNP P01563
A	180	SER	-	expression tag	UNP P01563
A	181	HIS	-	expression tag	UNP P01563
A	182	HIS	-	expression tag	UNP P01563
A	183	HIS	-	expression tag	UNP P01563
A	184	HIS	-	expression tag	UNP P01563
A	185	HIS	-	expression tag	UNP P01563
A	186	HIS	-	expression tag	UNP P01563
A	187	HIS	-	expression tag	UNP P01563
A	188	HIS	-	expression tag	UNP P01563

- Molecule 2 is a protein called type-I interferons autoantibody pamb14 heavy chain.

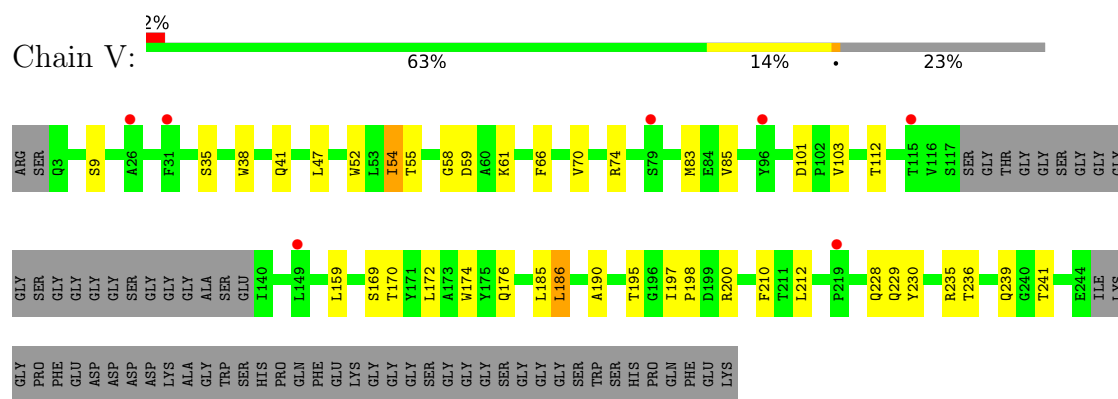
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	229	Total	C	N	O	S	0	0	0
			1724	1083	290	344	7			

- Molecule 3 is a protein called scFv type-I interferons autoantibody pamb03.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	U	236	Total	C	N	O	S	0	0	0
			1762	1098	302	353	9			

- Molecule 4 is a protein called scFv type-I interferons autoantibody pamb19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	V	220	Total	C	N	O	S	0	0	0
			1684	1059	295	324	6			



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	166.22Å 166.22Å 190.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 4.00 25.00 – 4.00	Depositor EDS
% Data completeness (in resolution range)	97.2 (25.00-4.00) 96.6 (25.00-4.00)	Depositor EDS
R_{merge}	0.78	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 3.97Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.294 , 0.324 (Not available) , 0.302	Depositor DCC
R_{free} test set	645 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	133.5	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 147.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	6368	wwPDB-VP
Average B, all atoms (Å ²)	151.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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	0.57	0/1221	0.99	0/1643
2	H	0.51	0/1762	0.82	1/2393 (0.0%)
3	U	0.71	1/1797 (0.1%)	0.96	5/2438 (0.2%)
4	V	0.58	0/1723	0.88	0/2336
All	All	0.60	1/6503 (0.0%)	0.91	6/8810 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	136	GLY	C-N	5.44	1.41	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	56	ASN	CA-CB-CG	5.75	118.35	112.60
3	U	136	GLY	CA-C-N	5.74	132.50	121.54
3	U	136	GLY	C-N-CA	5.74	132.50	121.54
2	H	436	ILE	N-CA-CB	5.42	118.11	111.60
3	U	29	TYR	CA-C-N	5.04	131.16	121.54
3	U	29	TYR	C-N-CA	5.04	131.16	121.54

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	1198	0	1196	16	0
2	H	1724	0	1670	2	0
3	U	1762	0	1697	27	0
4	V	1684	0	1635	32	0
All	All	6368	0	6198	67	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 5.

All (67) 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)
3:U:49:TRP:CD1	3:U:238:LEU:HD12	2.06	0.91
2:H:435:ASP:HB2	3:U:172:ARG:HD2	1.59	0.83
1:A:16:MET:HA	3:U:29:TYR:OH	1.77	0.83
4:V:186:LEU:HA	4:V:197:ILE:HG13	1.65	0.77
3:U:55:PRO:HA	3:U:74:ARG:HD2	1.66	0.76
3:U:179:GLN:HB2	3:U:189:LEU:HD11	1.69	0.74
3:U:35:ASP:HA	3:U:55:PRO:HD3	1.70	0.71
1:A:30:LEU:CD2	1:A:33:ARG:HE	2.05	0.69
4:V:70:VAL:HG22	4:V:85:VAL:HG22	1.75	0.68
1:A:57:HIS:ND1	4:V:170:THR:CG2	2.58	0.66
3:U:49:TRP:NE1	3:U:238:LEU:HD12	2.09	0.66
1:A:33:ARG:HD3	3:U:174:TYR:CE2	2.30	0.65
3:U:175:LEU:HD11	3:U:230:CYS:HB2	1.78	0.64
1:A:93:ASN:ND2	4:V:101:ASP:HB3	2.12	0.63
4:V:176:GLN:HB2	4:V:186:LEU:HD21	1.81	0.63
1:A:30:LEU:HD23	1:A:33:ARG:HE	1.64	0.62
1:A:57:HIS:ND1	4:V:170:THR:HG22	2.18	0.58
4:V:52:TRP:NE1	4:V:61:LYS:HB2	2.18	0.58
4:V:58:GLY:HA2	4:V:74:ARG:NH1	2.19	0.57
4:V:58:GLY:CA	4:V:74:ARG:HH12	2.16	0.57
4:V:41:GLN:HB2	4:V:47:LEU:HD23	1.88	0.55
1:A:110:LEU:HD23	2:H:56:ALA:HB3	1.88	0.55
4:V:58:GLY:CA	4:V:74:ARG:NH1	2.69	0.55
3:U:154:SER:HB3	3:U:249:THR:HG23	1.88	0.55
3:U:62:TYR:CD1	3:U:70:VAL:HG13	2.42	0.54
1:A:93:ASN:HD21	4:V:101:ASP:HB3	1.71	0.53
3:U:93:THR:HG23	3:U:119:THR:HA	1.90	0.53
4:V:38:TRP:CE2	4:V:83:MET:HB2	2.42	0.53
4:V:230:TYR:HA	4:V:235:ARG:HG2	1.89	0.53
3:U:69:ARG:NH2	3:U:92:ASP:OD2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:174:TYR:HB3	3:U:233:TYR:CD2	2.45	0.52
4:V:58:GLY:HA3	4:V:74:ARG:HH12	1.74	0.52
1:A:46:GLN:HG2	1:A:49:LYS:HZ2	1.74	0.51
4:V:228:GLN:HG2	4:V:229:GLN:N	2.25	0.51
3:U:157:VAL:HG22	3:U:248:ILE:HD13	1.93	0.51
4:V:66:PHE:HB3	4:V:70:VAL:CG2	2.42	0.50
4:V:54:ILE:HD11	4:V:59:ASP:HB2	1.94	0.49
4:V:159:LEU:HD12	4:V:159:LEU:H	1.78	0.49
4:V:159:LEU:HD23	4:V:241:THR:HB	1.94	0.48
1:A:57:HIS:ND1	4:V:170:THR:HG21	2.29	0.48
3:U:177:TRP:HB2	3:U:190:ILE:HB	1.95	0.47
3:U:174:TYR:HD2	3:U:234:GLY:HA2	1.79	0.47
1:A:53:ILE:HG23	1:A:95:LEU:HD22	1.95	0.47
3:U:204:PHE:CE1	3:U:217:ILE:HG12	2.50	0.47
4:V:229:GLN:HE21	4:V:236:THR:H	1.61	0.47
1:A:22:ARG:NH2	3:U:54:ASN:OD1	2.48	0.47
1:A:110:LEU:HD13	1:A:112:LYS:H	1.80	0.46
1:A:106:THR:HG21	1:A:111:MET:HE3	1.97	0.46
4:V:83:MET:SD	4:V:85:VAL:HG23	2.56	0.45
3:U:189:LEU:HA	3:U:200:VAL:HG21	1.99	0.44
4:V:172:LEU:HD22	4:V:210:PHE:CD1	2.53	0.44
3:U:35:ASP:HA	3:U:55:PRO:CD	2.43	0.44
4:V:9:SER:O	4:V:112:THR:OG1	2.30	0.44
3:U:32:THR:O	3:U:56:ASN:HB2	2.17	0.44
4:V:66:PHE:HB3	4:V:70:VAL:HG23	2.00	0.44
4:V:103:VAL:HG21	4:V:230:TYR:CG	2.54	0.43
4:V:52:TRP:CE2	4:V:61:LYS:HB2	2.53	0.43
3:U:181:LYS:HD3	3:U:226:ALA:HB2	1.99	0.43
4:V:198:PRO:HB2	4:V:200:ARG:HG2	2.01	0.42
3:U:228:TYR:O	3:U:243:GLY:HA2	2.19	0.42
3:U:205:SER:HG	3:U:216:THR:HG1	1.63	0.42
3:U:38:TRP:CE2	3:U:83:MET:HB2	2.55	0.42
4:V:174:TRP:CE2	4:V:212:LEU:HB2	2.55	0.42
1:A:30:LEU:HD23	1:A:33:ARG:NE	2.31	0.42
4:V:55:THR:HA	4:V:74:ARG:CD	2.50	0.41
4:V:83:MET:HE3	4:V:83:MET:HB3	1.89	0.41
3:U:146:MET:HE2	3:U:232:GLN:HB3	2.03	0.41

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	141/188 (75%)	139 (99%)	2 (1%)	0	100	100
2	H	225/290 (78%)	219 (97%)	6 (3%)	0	100	100
3	U	232/288 (81%)	218 (94%)	10 (4%)	4 (2%)	7	36
4	V	216/285 (76%)	204 (94%)	11 (5%)	1 (0%)	24	60
All	All	814/1051 (78%)	780 (96%)	29 (4%)	5 (1%)	21	57

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	U	137	SER
3	U	235	ASP
3	U	29	TYR
4	V	190	ALA
3	U	172	ARG

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	133/167 (80%)	128 (96%)	5 (4%)	29	51
2	H	189/225 (84%)	185 (98%)	4 (2%)	47	65
3	U	187/221 (85%)	178 (95%)	9 (5%)	23	46
4	V	180/218 (83%)	173 (96%)	7 (4%)	28	51
All	All	689/831 (83%)	664 (96%)	25 (4%)	31	53

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	27	PHE
1	A	49	LYS
1	A	106	THR
1	A	110	LEU
2	H	13	LEU
2	H	91	GLU
2	H	116	GLN
2	H	445	LEU
3	U	26	THR
3	U	109	ASP
3	U	156	SER
3	U	160	ARG
3	U	164	THR
3	U	196	LEU
3	U	207	SER
3	U	216	THR
3	U	239	THR
4	V	35	SER
4	V	54	ILE
4	V	169	SER
4	V	185	LEU
4	V	186	LEU
4	V	195	THR
4	V	239	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	61	GLN
1	A	124	GLN
2	H	116	GLN
3	U	169	GLN
4	V	41	GLN
4	V	229	GLN

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	145/188 (77%)	0.50	11 (7%) 20 20	117, 142, 294, 300	0
2	H	229/290 (78%)	1.30	50 (21%) 2 4	53, 65, 81, 124	229 (100%)
3	U	236/288 (81%)	0.16	3 (1%) 75 57	62, 113, 135, 144	0
4	V	220/285 (77%)	0.57	7 (3%) 50 37	136, 175, 300, 300	0
All	All	830/1051 (78%)	0.64	71 (8%) 16 17	53, 122, 300, 300	229 (27%)

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	12	GLY	9.5
2	H	530	LEU	8.8
2	H	11	GLY	5.2
2	H	461	GLN	4.7
2	H	90	ALA	4.6
1	A	113	GLU	4.6
2	H	115	GLY	4.4
2	H	21	ARG	4.3
2	H	24	CYS	3.9
2	H	59	SER	3.8
2	H	26	ALA	3.8
2	H	107	THR	3.7
2	H	54	SER	3.6
2	H	87	SER	3.1
4	V	79	SER	3.1
2	H	69	ARG	3.1
2	H	53	ILE	3.1
2	H	122	VAL	3.1
2	H	521	TYR	3.0
2	H	106	THR	3.0
1	A	100	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
2	H	116	GLN	2.9
2	H	542	GLY	2.9
2	H	458	ARG	2.9
2	H	35	ALA	2.9
4	V	149	LEU	2.8
2	H	462	SER	2.8
1	A	97	ALA	2.8
2	H	10	GLY	2.8
2	H	529	PRO	2.7
2	H	470	TYR	2.7
2	H	523	GLN	2.7
2	H	460	SER	2.7
4	V	26	ALA	2.7
2	H	23	SER	2.7
2	H	89	ARG	2.6
1	A	116	ILE	2.6
2	H	25	ALA	2.6
2	H	20	LEU	2.6
2	H	67	LYS	2.4
2	H	6	LEU	2.4
3	U	56	ASN	2.4
4	V	96	TYR	2.4
2	H	55	ALA	2.3
2	H	433	ALA	2.3
1	A	111	MET	2.3
2	H	477	ALA	2.3
2	H	68	GLY	2.3
2	H	464	SER	2.3
2	H	56	ALA	2.3
1	A	94	ASP	2.3
4	V	219	PRO	2.2
3	U	107	GLY	2.2
2	H	27	SER	2.2
2	H	447	ALA	2.2
1	A	24	ILE	2.2
2	H	111	PHE	2.2
1	A	95	LEU	2.2
3	U	35	ASP	2.1
2	H	509	ILE	2.1
4	V	115	THR	2.1
2	H	98	CYS	2.1
4	V	31	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	442	PRO	2.1
1	A	110	LEU	2.1
2	H	121	THR	2.1
2	H	105	VAL	2.1
1	A	23	ARG	2.0
2	H	445	LEU	2.0
1	A	47	PHE	2.0
2	H	101	GLU	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.