



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:10 AM UTC

PDB ID : 2Q8A / pdb_00002q8a
Title : Structure of the malaria antigen AMA1 in complex with a growth-inhibitory antibody
Authors : Gupta, A.; Murphy, V.J.; Anders, R.F.; Batchelor, A.H.
Deposited on : 2007-06-10
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

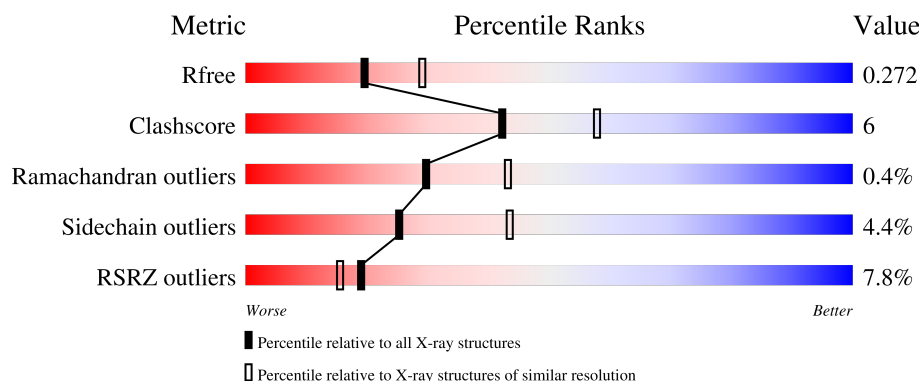
1 Overall quality at a glance

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	336	3% 81% 12% 6%
2	L	214	10% 83% 15% .
3	H	210	12% 79% 14% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5791 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 Apical membrane antigen 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2501	1580	421	483	17			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	GLY	-	expression tag	UNP Q7KQK5

- Molecule 2 is a protein called 1F9 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1591	1006	260	318	7			

- Molecule 3 is a protein called 1F9 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	199	Total	C	N	O	S	0	0	0
			1452	916	236	293	7			

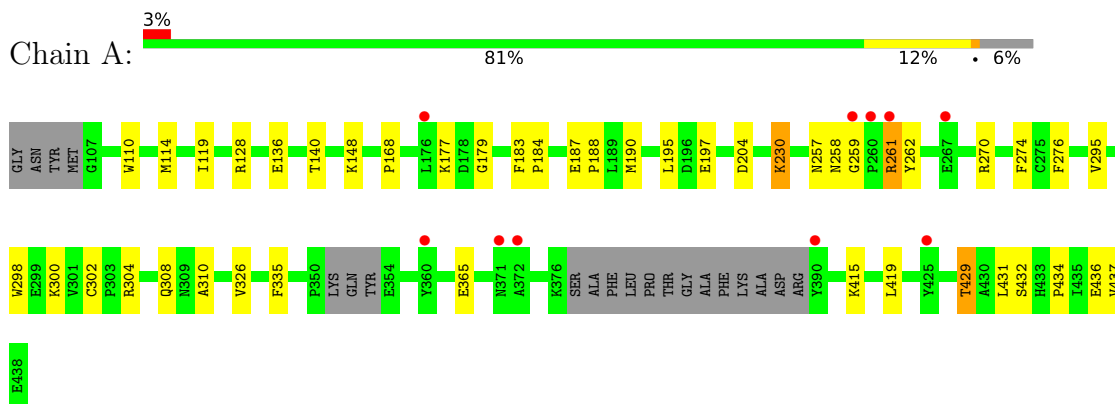
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	166	Total	O	0	0
			166	166		
4	L	43	Total	O	0	0
			43	43		
4	H	38	Total	O	0	0
			38	38		

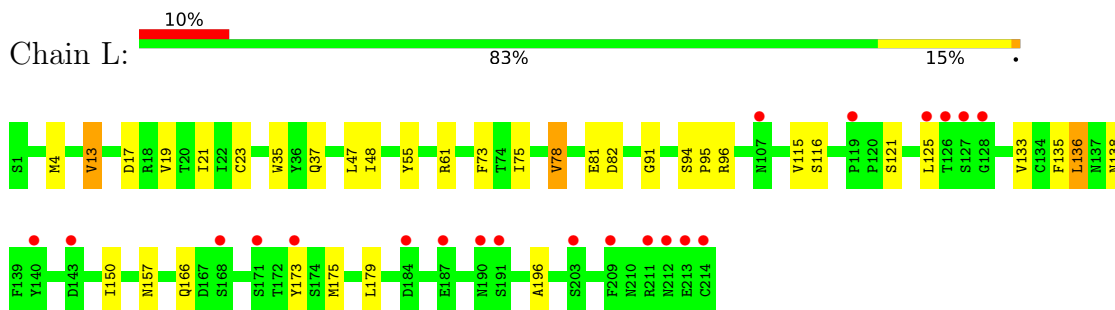
3 Residue-property plots [i](#)

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.

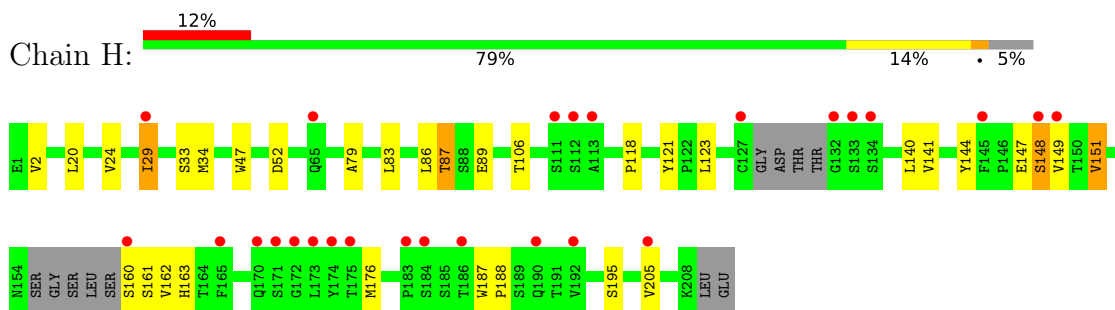
- Molecule 1: Apical membrane antigen 1



- Molecule 2: 1F9 light chain



- Molecule 3: 1F9 heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	189.76Å 51.20Å 91.52Å 90.00° 111.09° 90.00°	Depositor
Resolution (Å)	38.92 – 2.40 38.92 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (38.92-2.40) 99.9 (38.92-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.23 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.202 , 0.244 (Not available) , 0.272	Depositor DCC
R_{free} test set	1647 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5791	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% 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

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	0.54	0/2563	0.81	2/3472 (0.1%)
2	L	0.53	0/1629	0.75	0/2227
3	H	0.49	0/1488	0.76	0/2041
All	All	0.53	0/5680	0.78	2/7740 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183	PHE	CA-C-N	5.03	123.28	119.66
1	A	183	PHE	C-N-CA	5.03	123.28	119.66

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	A	2501	0	2345	32	0
2	L	1591	0	1462	23	0
3	H	1452	0	1346	21	0
4	A	166	0	0	0	0
4	H	38	0	0	0	0
4	L	43	0	0	0	0
All	All	5791	0	5153	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 6.

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)
1:A:304:ARG:NH1	1:A:436:GLU:OE2	2.06	0.88
1:A:335:PHE:HD1	1:A:434:PRO:HB2	1.56	0.70
3:H:87:THR:HG22	3:H:89:GLU:H	1.60	0.67
1:A:190:MET:HG3	3:H:2:VAL:HG21	1.76	0.67
1:A:429:THR:HG22	1:A:431:LEU:H	1.59	0.66
3:H:147:GLU:O	3:H:148:SER:HB2	1.95	0.66
1:A:274:PHE:HB3	1:A:276:PHE:HD2	1.60	0.66
1:A:230:LYS:H	1:A:230:LYS:HD2	1.61	0.65
3:H:118:PRO:HB3	3:H:144:TYR:HB3	1.79	0.63
2:L:133:VAL:HG11	3:H:123:LEU:HD13	1.79	0.63
1:A:259:GLY:C	1:A:261:ARG:H	2.08	0.60
1:A:197:GLU:HG2	2:L:55:TYR:CE1	2.37	0.59
1:A:230:LYS:H	1:A:230:LYS:CD	2.13	0.59
2:L:166:GLN:HG3	2:L:173:TYR:CZ	2.39	0.57
1:A:335:PHE:CD1	1:A:434:PRO:HB2	2.39	0.57
1:A:230:LYS:HD2	1:A:230:LYS:N	2.19	0.57
2:L:61:ARG:NH1	2:L:82:ASP:OD1	2.39	0.56
2:L:21:ILE:HD12	2:L:73:PHE:HD2	1.71	0.56
1:A:168:PRO:HB3	1:A:184:PRO:HA	1.89	0.54
1:A:429:THR:HG22	1:A:431:LEU:N	2.23	0.53
1:A:110:TRP:HB3	1:A:114:MET:HG2	1.91	0.52
3:H:121:TYR:HB2	3:H:140:LEU:HB3	1.90	0.52
2:L:35:TRP:CE2	2:L:73:PHE:HB2	2.46	0.51
2:L:35:TRP:CD2	2:L:73:PHE:HB2	2.46	0.50
2:L:115:VAL:HA	2:L:135:PHE:O	2.11	0.50
2:L:136:LEU:HD12	2:L:196:ALA:HB2	1.93	0.50
2:L:138:ASN:HD21	3:H:163:HIS:HE1	1.59	0.50
2:L:21:ILE:HD12	2:L:73:PHE:CD2	2.47	0.49
3:H:123:LEU:HD21	3:H:140:LEU:HB2	1.94	0.49
1:A:190:MET:HG3	3:H:2:VAL:CG2	2.43	0.48
3:H:160:SER:C	3:H:162:VAL:H	2.21	0.48
2:L:121:SER:O	2:L:125:LEU:HB2	2.14	0.47
1:A:429:THR:CG2	1:A:431:LEU:H	2.26	0.47
3:H:24:VAL:HG21	3:H:29:ILE:HD11	1.97	0.47
2:L:4:MET:HE3	2:L:23:CYS:SG	2.54	0.46
2:L:150:ILE:HD11	2:L:179:LEU:HD21	1.96	0.46
1:A:190:MET:CG	3:H:2:VAL:HG21	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:ARG:HH11	1:A:304:ARG:HG2	1.81	0.46
2:L:91:GLY:HA2	2:L:96:ARG:HG2	1.98	0.46
1:A:257:ASN:ND2	1:A:365:GLU:OE1	2.48	0.45
3:H:187:TRP:CG	3:H:188:PRO:HA	2.52	0.45
2:L:17:ASP:O	2:L:78:VAL:HG22	2.17	0.45
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.99	0.45
2:L:61:ARG:HG3	2:L:75:ILE:HG23	1.98	0.45
1:A:119:ILE:HD11	1:A:429:THR:HG23	1.99	0.44
3:H:151:VAL:HA	3:H:195:SER:O	2.17	0.44
3:H:20:LEU:HD22	3:H:106:THR:HG21	1.99	0.44
1:A:259:GLY:HA3	1:A:262:TYR:HB2	1.99	0.44
3:H:34:MET:HG3	3:H:79:ALA:HB2	1.99	0.44
3:H:141:VAL:HB	3:H:176:MET:HG3	2.00	0.44
2:L:94:SER:HA	2:L:95:PRO:C	2.43	0.43
1:A:298:TRP:O	1:A:302:CYS:HB2	2.18	0.43
1:A:308:GLN:HG3	1:A:437:VAL:HB	1.99	0.43
1:A:179:GLY:O	1:A:274:PHE:HZ	2.01	0.43
1:A:136:GLU:HA	1:A:140:THR:O	2.18	0.43
2:L:13:VAL:HG11	2:L:19:VAL:HG22	2.01	0.42
1:A:429:THR:HB	1:A:432:SER:OG	2.19	0.42
3:H:24:VAL:CB	3:H:29:ILE:HD11	2.48	0.42
1:A:187:GLU:HA	1:A:188:PRO:C	2.44	0.42
2:L:138:ASN:ND2	3:H:163:HIS:HE1	2.18	0.42
3:H:24:VAL:HG11	3:H:29:ILE:HD11	2.00	0.42
1:A:310:ALA:HB1	1:A:419:LEU:HD22	2.02	0.41
1:A:177:LYS:HA	1:A:274:PHE:CE2	2.55	0.41
1:A:204:ASP:CG	2:L:96:ARG:HH12	2.27	0.41
2:L:95:PRO:HA	3:H:47:TRP:CZ3	2.56	0.41
1:A:148:LYS:O	1:A:295:VAL:HG22	2.21	0.41
1:A:274:PHE:CB	1:A:276:PHE:HD2	2.31	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	310/336 (92%)	296 (96%)	13 (4%)	1 (0%)	36	50
2	L	212/214 (99%)	202 (95%)	10 (5%)	0	100	100
3	H	193/210 (92%)	184 (95%)	7 (4%)	2 (1%)	12	20
All	All	715/760 (94%)	682 (95%)	30 (4%)	3 (0%)	30	43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	148	SER
1	A	261	ARG
3	H	161	SER

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	270/296 (91%)	261 (97%)	9 (3%)	33	55
2	L	168/191 (88%)	160 (95%)	8 (5%)	23	40
3	H	157/183 (86%)	148 (94%)	9 (6%)	18	33
All	All	595/670 (89%)	569 (96%)	26 (4%)	25	43

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	ARG
1	A	195	LEU
1	A	230	LYS
1	A	258	ASN
1	A	270	ARG
1	A	300	LYS
1	A	326	VAL

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Mol	Chain	Res	Type
1	A	415	LYS
1	A	429	THR
2	L	13	VAL
2	L	48	ILE
2	L	78	VAL
2	L	81	GLU
2	L	116	SER
2	L	136	LEU
2	L	157	ASN
2	L	175	MET
3	H	29	ILE
3	H	33	SER
3	H	52	ASP
3	H	83	LEU
3	H	86	LEU
3	H	87	THR
3	H	149	VAL
3	H	151	VAL
3	H	205	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	258	ASN
1	A	319	ASN
1	A	393	HIS
1	A	421	ASN
2	L	79	GLN
2	L	107	ASN
2	L	138	ASN
2	L	161	ASN
3	H	3	GLN
3	H	43	GLN
3	H	154	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	316/336 (94%)	0.45	10 (3%)	50 46	27, 35, 45, 54	0
2	L	214/214 (100%)	0.70	21 (9%)	13 10	32, 35, 39, 41	0
3	H	199/210 (94%)	0.94	26 (13%)	7 5	31, 36, 41, 44	0
All	All	729/760 (95%)	0.66	57 (7%)	19 15	27, 35, 42, 54	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	212	ASN	5.0
3	H	172	GLY	4.4
1	A	390	TYR	4.0
2	L	213	GLU	3.8
2	L	214	CYS	3.7
3	H	134	SER	3.5
2	L	126	THR	3.4
1	A	372	ALA	3.3
1	A	260	PRO	3.3
3	H	184	SER	3.2
2	L	143	ASP	3.2
3	H	186	THR	3.2
1	A	267	GLU	3.1
3	H	127	CYS	3.0
3	H	113	ALA	3.0
2	L	171	SER	2.9
3	H	145	PHE	2.9
3	H	192	VAL	2.9
2	L	173	TYR	2.8
3	H	112	SER	2.7
1	A	371	ASN	2.6
2	L	190	ASN	2.6
3	H	133	SER	2.6

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Mol	Chain	Res	Type	RSRZ
2	L	209	PHE	2.6
3	H	171	SER	2.5
2	L	140	TYR	2.4
3	H	65	GLN	2.4
2	L	119	PRO	2.4
2	L	125	LEU	2.4
2	L	184	ASP	2.3
2	L	168	SER	2.3
2	L	107	ASN	2.3
3	H	132	GLY	2.3
3	H	111	SER	2.3
1	A	261	ARG	2.3
3	H	174	TYR	2.3
1	A	360	TYR	2.2
3	H	190	GLN	2.2
2	L	127	SER	2.2
1	A	425	TYR	2.2
3	H	149	VAL	2.1
2	L	187	GLU	2.1
3	H	205	VAL	2.1
1	A	259	GLY	2.1
1	A	176	LEU	2.1
3	H	173	LEU	2.1
3	H	165	PHE	2.1
2	L	211	ARG	2.1
2	L	203	SER	2.1
3	H	148	SER	2.1
3	H	160	SER	2.1
2	L	128	GLY	2.0
3	H	29	ILE	2.0
2	L	191	SER	2.0
3	H	170	GLN	2.0
3	H	175	THR	2.0
3	H	183	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.