



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:19 AM GMT

PDB ID : 2Q8B
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 : 2.30 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

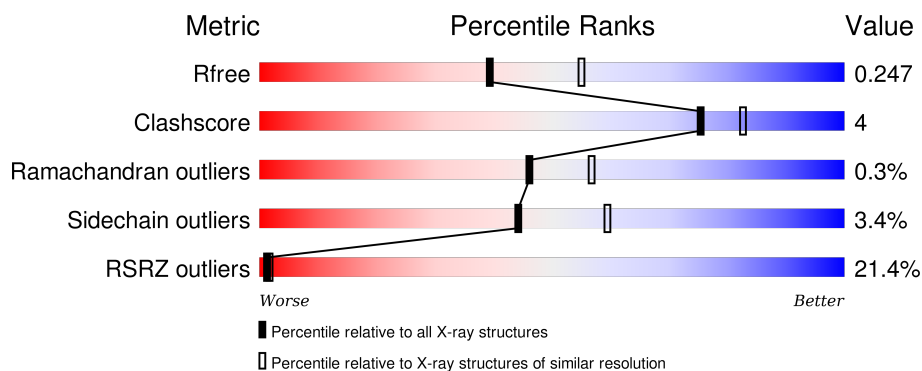
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>16%</div> <div> <div></div> <div>77%</div> <div>9%</div> <div>•</div> <div>13%</div> </div> </div>
2	L	214	<div> <div>18%</div> <div> <div></div> <div>87%</div> <div>13%</div> </div> </div>
3	H	210	<div> <div>27%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>•</div> <div>5%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5598 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	292	Total	C	N	O	S	0	0	0
			2303	1458	382	447	16			

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	213	Total	C	N	O	S	0	0	0
			1616	1019	264	327	6			

- 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
			1459	924	236	293	6			

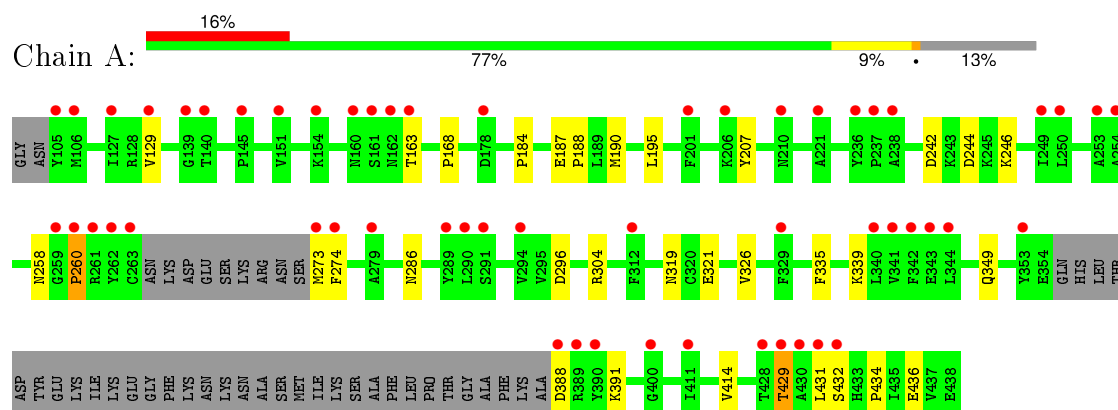
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	175	Total	O	0	0
			175	175		
4	H	34	Total	O	0	0
			34	34		
4	L	11	Total	O	0	0
			11	11		

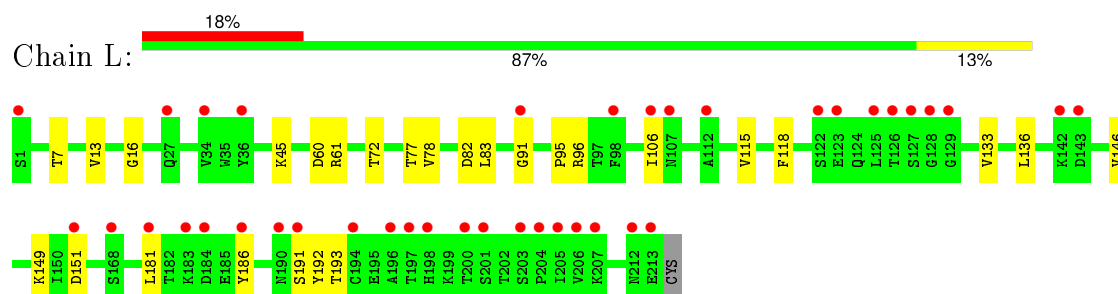
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

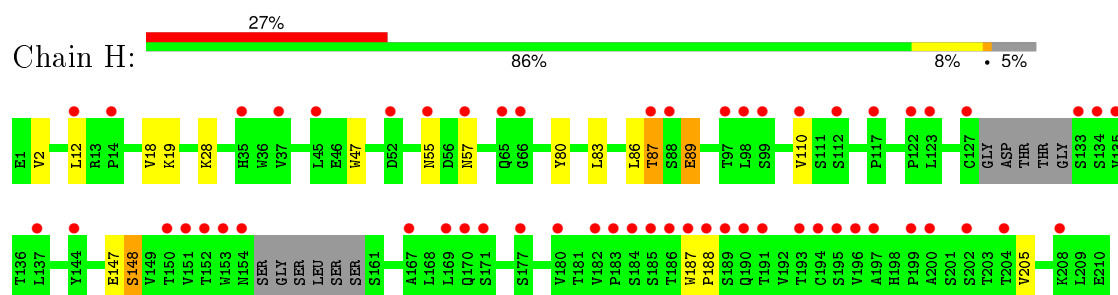
• Molecule 1: Apical membrane antigen 1



• 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	184.91 Å 51.49 Å 95.26 Å 90.00° 108.49° 90.00°	Depositor
Resolution (Å)	27.95 – 2.30 27.95 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (27.95-2.30) 99.4 (27.95-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.62 (at 2.31 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.209 , 0.256 0.202 , 0.247	Depositor DCC
R_{free} test set	1899 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 44.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 38017 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5598	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.45	0/2363	0.58	0/3208
2	L	0.36	0/1655	0.50	0/2260
3	H	0.36	0/1495	0.52	0/2051
All	All	0.40	0/5513	0.54	0/7519

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	A	2303	0	2137	19	0
2	L	1616	0	1494	12	0
3	H	1459	0	1360	11	0
4	A	175	0	0	3	0
4	H	34	0	0	0	0
4	L	11	0	0	1	0
All	All	5598	0	4991	40	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 4.

All (40) 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	2.01	0.93
1:A:258:ASN:O	1:A:260:PRO:HD3	1.88	0.73
3:H:55:ASN:HB2	3:H:57:ASN:HB2	1.73	0.69
2:L:16:GLY:O	2:L:77:THR:HG22	1.93	0.69
1:A:242:ASP:HB2	1:A:286:ASN:HB3	1.83	0.61
2:L:149:LYS:HB2	2:L:193:THR:HB	1.84	0.59
1:A:429:THR:HG22	1:A:431:LEU:H	1.67	0.58
3:H:87:THR:HG22	3:H:89:GLU:H	1.73	0.53
1:A:335:PHE:HD1	1:A:434:PRO:HB2	1.75	0.52
1:A:429:THR:HB	1:A:432:SER:OG	2.10	0.52
2:L:115:VAL:HG22	2:L:136:LEU:HD22	1.93	0.50
1:A:187:GLU:HA	1:A:188:PRO:C	2.32	0.49
1:A:190:MET:HG3	3:H:2:VAL:HG21	1.94	0.49
3:H:147:GLU:O	3:H:148:SER:CB	2.61	0.48
1:A:429:THR:CG2	1:A:431:LEU:H	2.25	0.48
3:H:19:LYS:HD2	3:H:80:TYR:HB3	1.96	0.48
1:A:335:PHE:CD1	1:A:434:PRO:HB2	2.49	0.47
1:A:168:PRO:HB3	1:A:184:PRO:HA	1.95	0.47
1:A:429:THR:HG22	1:A:431:LEU:N	2.28	0.47
1:A:349:GLN:NE2	4:A:497:HOH:O	2.47	0.47
2:L:118:PHE:HB2	2:L:133:VAL:HG13	1.97	0.46
3:H:12:LEU:O	3:H:110:VAL:HA	2.17	0.45
2:L:83:LEU:HD13	2:L:106:ILE:HG12	1.99	0.44
1:A:244:ASP:HB3	1:A:246:LYS:HG3	1.99	0.44
1:A:129:VAL:HG11	1:A:349:GLN:HG2	2.00	0.43
2:L:61:ARG:NH1	2:L:82:ASP:OD1	2.52	0.42
2:L:136:LEU:HD11	2:L:146:VAL:HG22	2.02	0.42
1:A:391:LYS:NZ	4:A:591:HOH:O	2.52	0.42
2:L:151:ASP:HA	2:L:191:SER:HB3	2.02	0.41
1:A:388:ASP:N	1:A:391:LYS:HE2	2.36	0.41
4:A:440:HOH:O	3:H:28:LYS:HE3	2.19	0.41
2:L:91:GLY:HA2	2:L:96:ARG:HD3	2.01	0.41
2:L:95:PRO:HA	3:H:47:TRP:CZ3	2.56	0.41
2:L:186:TYR:HA	2:L:192:TYR:OH	2.21	0.41
3:H:187:TRP:HA	3:H:188:PRO:HA	1.87	0.41
3:H:87:THR:HG22	3:H:89:GLU:N	2.35	0.41
1:A:335:PHE:CE2	1:A:339:LYS:HE2	2.57	0.40
2:L:45:LYS:HE2	4:L:215:HOH:O	2.20	0.40
1:A:207:TYR:OH	1:A:296:ASP:OD1	2.32	0.40
3:H:12:LEU:HD13	3:H:18:VAL:HB	2.03	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	286/336 (85%)	274 (96%)	11 (4%)	1 (0%)	46	57
2	L	211/214 (99%)	205 (97%)	6 (3%)	0	100	100
3	H	193/210 (92%)	186 (96%)	6 (3%)	1 (0%)	34	41
All	All	690/760 (91%)	665 (96%)	23 (3%)	2 (0%)	46	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	148	SER
1	A	260	PRO

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	248/296 (84%)	239 (96%)	9 (4%)	42	57
2	L	175/191 (92%)	169 (97%)	6 (3%)	44	59
3	H	157/183 (86%)	152 (97%)	5 (3%)	46	62
All	All	580/670 (87%)	560 (97%)	20 (3%)	44	59

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

Mol	Chain	Res	Type
1	A	163	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	195	LEU
1	A	273	MET
1	A	274	PHE
1	A	319	ASN
1	A	321	GLU
1	A	326	VAL
1	A	414	VAL
1	A	429	THR
2	L	7	THR
2	L	13	VAL
2	L	60	ASP
2	L	72	THR
2	L	78	VAL
2	L	181	LEU
3	H	83	LEU
3	H	86	LEU
3	H	87	THR
3	H	89	GLU
3	H	205	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	349	GLN
2	L	107	ASN
2	L	145	ASN
3	H	55	ASN
3	H	77	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 carbohydrates 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, 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	292/336 (86%)	1.04	55 (18%) 2 2	30, 35, 48, 58	0
2	L	213/214 (99%)	1.10	39 (18%) 2 2	33, 37, 40, 41	0
3	H	199/210 (94%)	1.45	57 (28%) 1 1	32, 38, 43, 46	0
All	All	704/760 (92%)	1.17	151 (21%) 1 2	30, 37, 44, 58	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	262	TYR	7.1
3	H	187	TRP	6.0
3	H	194	CYS	5.9
1	A	259	GLY	5.9
3	H	195	SER	5.7
1	A	105	TYR	5.5
3	H	193	THR	5.5
1	A	261	ARG	5.5
2	L	206	VAL	5.4
3	H	171	SER	5.4
1	A	390	TYR	5.2
3	H	191	THR	5.1
1	A	353	TYR	5.0
3	H	65	GLN	5.0
2	L	34	VAL	4.8
1	A	388	ASP	4.7
3	H	189	SER	4.3
3	H	153	TRP	4.3
3	H	66	GLY	4.2
2	L	200	THR	4.1
3	H	186	THR	4.0
1	A	151	VAL	4.0
1	A	289	TYR	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	198	HIS	3.9
1	A	127	ILE	3.9
3	H	152	THR	3.9
1	A	249	ILE	3.9
1	A	237	PRO	3.8
2	L	196	ALA	3.7
1	A	263	CYS	3.7
2	L	212	ASN	3.6
3	H	137	LEU	3.6
3	H	184	SER	3.6
3	H	185	SER	3.6
1	A	238	ALA	3.6
3	H	196	VAL	3.6
2	L	128	GLY	3.6
1	A	221	ALA	3.6
3	H	110	VAL	3.5
1	A	106	MET	3.5
2	L	204	PRO	3.5
3	H	117	PRO	3.5
3	H	182	VAL	3.5
1	A	430	ALA	3.5
3	H	197	ALA	3.5
2	L	205	ILE	3.5
2	L	203	SER	3.4
2	L	190	ASN	3.4
1	A	411	ILE	3.4
2	L	191	SER	3.4
1	A	341	VAL	3.4
2	L	194	CYS	3.4
3	H	37	VAL	3.4
2	L	197	THR	3.3
2	L	127	SER	3.3
2	L	98	PHE	3.3
1	A	160	ASN	3.3
2	L	125	LEU	3.3
3	H	144	TYR	3.3
3	H	169	LEU	3.3
1	A	279	ALA	3.2
3	H	167	ALA	3.2
3	H	150	THR	3.2
1	A	274	PHE	3.1
3	H	134	SER	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	H	202	SER	3.0
1	A	342	PHE	3.0
3	H	199	PRO	3.0
2	L	184	ASP	3.0
3	H	183	PRO	3.0
1	A	389	ARG	3.0
1	A	162	ASN	3.0
2	L	112	ALA	3.0
2	L	201	SER	2.9
1	A	428	THR	2.9
1	A	163	THR	2.9
1	A	206	LYS	2.8
3	H	133	SER	2.8
1	A	429	THR	2.8
2	L	151	ASP	2.7
3	H	204	THR	2.7
3	H	123	LEU	2.7
1	A	290	LEU	2.7
2	L	181	LEU	2.6
3	H	208	LYS	2.6
1	A	236	TYR	2.6
2	L	123	GLU	2.6
2	L	143	ASP	2.6
3	H	177	SER	2.6
3	H	180	VAL	2.6
1	A	260	PRO	2.6
2	L	129	GLY	2.5
3	H	99	SER	2.5
1	A	431	LEU	2.5
1	A	210	ASN	2.5
3	H	190	GLN	2.5
2	L	186	TYR	2.5
1	A	139	GLY	2.5
2	L	1	SER	2.5
3	H	55	ASN	2.5
1	A	344	LEU	2.4
1	A	432	SER	2.4
2	L	107	ASN	2.4
1	A	312	PHE	2.4
1	A	145	PRO	2.4
2	L	122	SER	2.4
3	H	87	THR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	253	ALA	2.3
3	H	97	THR	2.3
1	A	400	GLY	2.3
3	H	98	LEU	2.3
1	A	154	LYS	2.3
2	L	183	LYS	2.3
3	H	127	CYS	2.3
3	H	45	LEU	2.3
1	A	201	PHE	2.2
3	H	154	ASN	2.2
3	H	12	LEU	2.2
3	H	151	VAL	2.2
3	H	112	SER	2.2
2	L	27	GLN	2.2
2	L	142	LYS	2.2
2	L	91	GLY	2.2
1	A	273	MET	2.2
2	L	126	THR	2.2
2	L	168	SER	2.2
3	H	188	PRO	2.2
3	H	170	GLN	2.2
2	L	36	TYR	2.2
2	L	207	LYS	2.2
3	H	122	PRO	2.1
1	A	161	SER	2.1
3	H	35	HIS	2.1
1	A	140	THR	2.1
1	A	178	ASP	2.1
3	H	135	VAL	2.1
1	A	254	ALA	2.1
3	H	52	ASP	2.1
1	A	129	VAL	2.1
3	H	200	ALA	2.1
3	H	14	PRO	2.1
3	H	88	SER	2.1
2	L	106	ILE	2.1
1	A	250	LEU	2.0
1	A	291	SER	2.0
3	H	57	ASN	2.0
1	A	329	PHE	2.0
1	A	294	VAL	2.0
1	A	343	GLU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	213	GLU	2.0
1	A	340	LEU	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 carbohydrates 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.