



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 07:50 am BST

PDB ID : 2VXU
Title : Crystal structure of murine reference antibody 125-2H Fab fragment
Authors : Argiriadi, M.A.; Xiang, T.; Wu, C.; Ghayur, T.; Borhani, D.W.
Deposited on : 2008-07-10
Resolution : 2.36 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

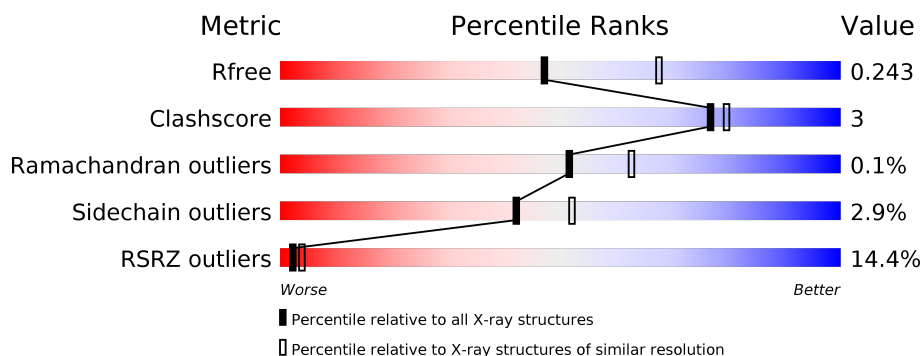
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 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	H	216	<div> <div>19%</div> <div>89%</div> <div>9%</div> </div>
1	I	216	<div> <div>13%</div> <div>92%</div> <div>8%</div> </div>
2	L	214	<div> <div>12%</div> <div>88%</div> <div>11%</div> </div>
2	M	214	<div> <div>14%</div> <div>91%</div> <div>8%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7186 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 MURINE IGG 125-2H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	216	Total	C	N	O	S	0	5	0
			1673	1060	276	329	8			
1	I	216	Total	C	N	O	S	0	5	0
			1671	1059	276	329	7			

- Molecule 2 is a protein called MURINE IGG 125-2H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	5	0
			1696	1049	283	355	9			
2	M	214	Total	C	N	O	S	0	0	0
			1658	1029	277	345	7			

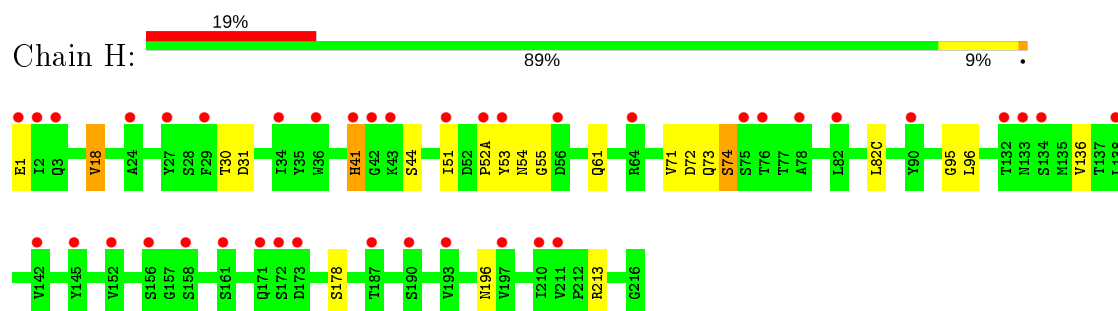
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	135	Total	O	0	0
			135	135		
3	I	121	Total	O	0	0
			121	121		
3	L	109	Total	O	0	0
			109	109		
3	M	123	Total	O	0	0
			123	123		

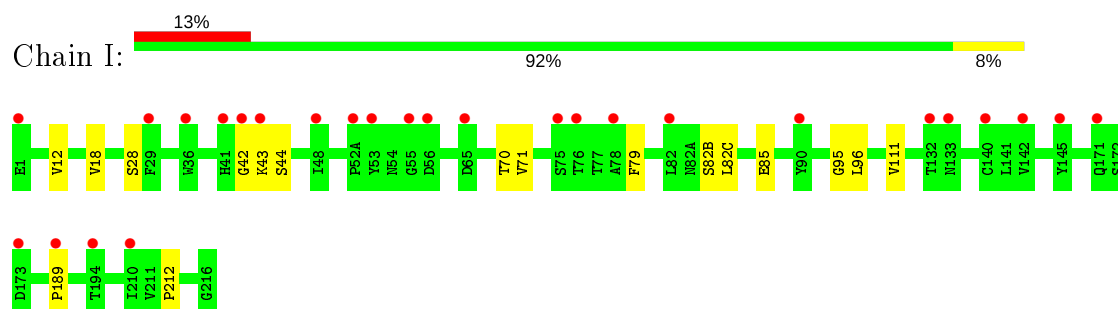
3 Residue-property plots [i](#)

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

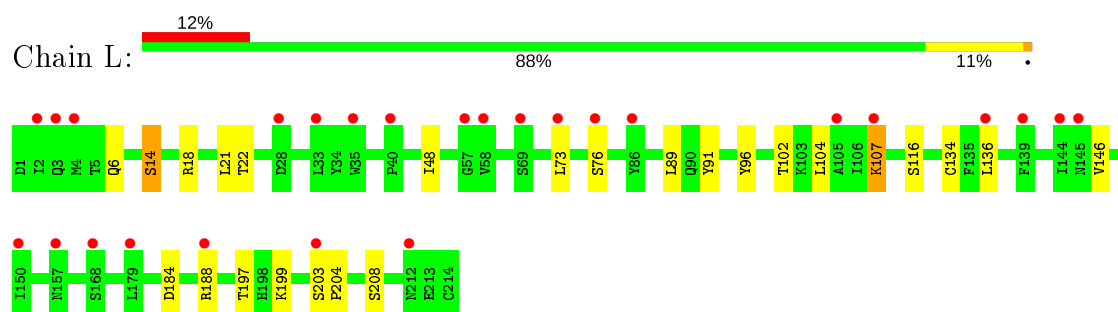
• Molecule 1: MURINE IGG 125-2H



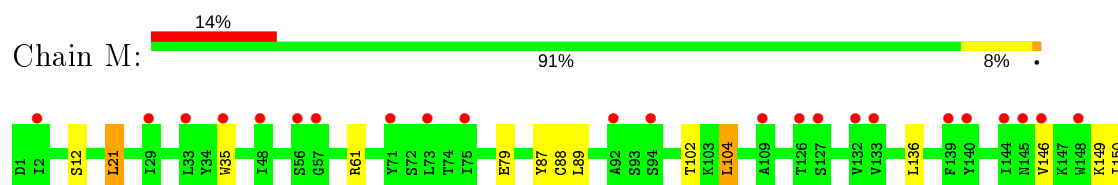
• Molecule 1: MURINE IGG 125-2H

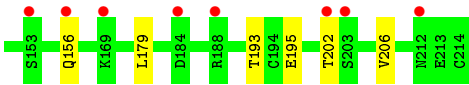


• Molecule 2: MURINE IGG 125-2H



• Molecule 2: MURINE IGG 125-2H





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.06 Å 92.49 Å 137.65 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.42 – 2.36 17.42 – 2.37	Depositor EDS
% Data completeness (in resolution range)	98.2 (17.42-2.36) 97.6 (17.42-2.37)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.57 (at 2.37 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.184 , 0.242 0.189 , 0.243	Depositor DCC
R_{free} test set	2065 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.562	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7186	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.63 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7828e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	H	0.99	13/1718 (0.8%)	0.90	5/2347 (0.2%)
1	I	0.56	0/1716	0.70	0/2344
2	L	0.71	4/1731 (0.2%)	0.69	0/2345
2	M	0.54	0/1693	0.68	1/2294 (0.0%)
All	All	0.72	17/6858 (0.2%)	0.75	6/9330 (0.1%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	74	SER	C-N	12.67	1.63	1.34
1	H	74	SER	CB-OG	12.11	1.57	1.42
2	L	14	SER	CA-CB	10.66	1.69	1.52
2	L	107	LYS	CD-CE	10.12	1.76	1.51
1	H	72	ASP	CB-CG	9.16	1.71	1.51
1	H	31	ASP	CG-OD1	8.95	1.46	1.25
1	H	54	ASN	CB-CG	8.37	1.70	1.51
1	H	55	GLY	N-CA	8.00	1.58	1.46
1	H	54	ASN	CA-C	7.30	1.72	1.52
1	H	54	ASN	CG-ND2	-7.00	1.15	1.32
1	H	72	ASP	CG-OD2	6.68	1.40	1.25
2	L	107	LYS	CB-CG	6.63	1.70	1.52
1	H	72	ASP	CG-OD1	6.51	1.40	1.25
1	H	74	SER	C-O	-6.26	1.11	1.23
1	H	73	GLN	C-N	6.05	1.48	1.34
1	H	53	TYR	CG-CD2	5.77	1.46	1.39
2	L	14	SER	C-O	5.63	1.34	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	31	ASP	CB-CG-OD1	13.24	130.22	118.30
1	H	72	ASP	CB-CG-OD2	-12.54	107.01	118.30
1	H	72	ASP	CB-CG-OD1	8.19	125.67	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	104	LEU	CA-CB-CG	6.37	129.94	115.30
1	H	31	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	H	74	SER	C-N-CA	-5.53	107.87	121.70

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	H	1673	0	1623	7	0
1	I	1671	0	1624	9	0
2	L	1696	0	1604	17	0
2	M	1658	0	1583	9	0
3	H	135	0	0	1	0
3	I	121	0	0	0	0
3	L	109	0	0	1	0
3	M	123	0	0	0	0
All	All	7186	0	6434	39	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 (39) 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)
2:L:107:LYS:CE	2:L:107:LYS:CD	1.76	1.63
2:L:21:LEU:HD22	2:L:102:THR:HG21	1.54	0.86
1:H:96[A]:LEU:HD13	2:L:89:LEU:HD21	1.59	0.84
2:L:107:LYS:CE	2:L:107:LYS:CG	2.61	0.79
1:I:95[B]:GLY:O	1:I:96[B]:LEU:HB2	1.97	0.65
2:M:21:LEU:HD22	2:M:102:THR:HG21	1.79	0.62
2:M:150:ILE:HD11	2:M:179:LEU:HD21	1.83	0.59
1:I:42[B]:GLY:O	1:I:43[B]:LYS:HB2	2.03	0.58
1:I:18:VAL:HG22	1:I:82(C):LEU:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:107:LYS:NZ	2:L:107:LYS:CD	2.65	0.57
2:L:184:ASP:O	2:L:188:ARG:HG3	2.06	0.56
1:H:213:ARG:NH2	3:H:2134:HOH:O	2.39	0.55
1:I:85:GLU:N	1:I:85:GLU:OE1	2.35	0.55
2:M:61:ARG:CZ	2:M:79:GLU:HG3	2.40	0.52
2:L:199:LYS:NZ	3:L:2099:HOH:O	2.39	0.51
2:L:136:LEU:HD21	2:L:146:VAL:HG22	1.94	0.50
2:M:195:GLU:HG2	2:M:206:VAL:HG22	1.92	0.50
2:L:18:ARG:HG3	2:L:76:SER:HA	1.95	0.49
1:H:95[B]:GLY:O	1:H:96[B]:LEU:HB2	2.13	0.49
2:L:48:ILE:HD12	2:L:73:LEU:CD1	2.43	0.48
1:H:18:VAL:HB	1:H:82(C):LEU:HD11	1.96	0.48
2:L:21:LEU:HD21	2:L:104:LEU:HD21	1.96	0.46
2:M:35:TRP:CZ3	2:M:88:CYS:HB3	2.50	0.46
2:M:149:LYS:HB2	2:M:193:THR:HB	1.98	0.46
1:H:30:THR:HA	1:H:52(A):PRO:HB2	1.98	0.45
2:L:91:TYR:HA	2:L:96:TYR:CD1	2.50	0.45
1:H:51:ILE:HD13	1:H:71:VAL:HG13	2.00	0.44
1:I:189:PRO:HB3	1:I:212:PRO:HG3	1.99	0.43
2:M:146:VAL:HA	2:M:195:GLU:O	2.18	0.43
2:M:136:LEU:N	2:M:136:LEU:HD12	2.34	0.43
1:I:12:VAL:O	1:I:111:VAL:HA	2.19	0.42
1:I:95[B]:GLY:O	1:I:96[B]:LEU:CB	2.66	0.42
2:L:6:GLN:HA	2:L:22:THR:O	2.20	0.41
1:H:96[B]:LEU:HD13	2:L:89:LEU:HD21	2.02	0.41
2:L:203:SER:HA	2:L:204:PRO:HD2	1.93	0.41
2:L:116:SER:O	2:L:134[B]:CYS:HA	2.20	0.40
2:L:116:SER:O	2:L:134[A]:CYS:HA	2.21	0.40
1:I:43[B]:LYS:HB3	2:M:87:TYR:OH	2.21	0.40
1:I:70:THR:OG1	1:I:79:PHE:HB2	2.22	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	H	219/216 (101%)	211 (96%)	6 (3%)	2 (1%)	17	17
1	I	219/216 (101%)	211 (96%)	8 (4%)	0	100	100
2	L	217/214 (101%)	212 (98%)	5 (2%)	0	100	100
2	M	212/214 (99%)	208 (98%)	4 (2%)	0	100	100
All	All	867/860 (101%)	842 (97%)	23 (3%)	2 (0%)	51	56

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	41[A]	HIS
1	H	41[B]	HIS

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	H	191/187 (102%)	181 (95%)	10 (5%)	23	27
1	I	190/187 (102%)	186 (98%)	4 (2%)	53	65
2	L	196/191 (103%)	193 (98%)	3 (2%)	65	76
2	M	191/191 (100%)	185 (97%)	6 (3%)	40	48
All	All	768/756 (102%)	745 (97%)	23 (3%)	42	50

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	1	GLU
1	H	18	VAL
1	H	41[A]	HIS
1	H	41[B]	HIS
1	H	44	SER
1	H	61	GLN

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Mol	Chain	Res	Type
1	H	74	SER
1	H	136	VAL
1	H	178	SER
1	H	196	ASN
1	I	28	SER
1	I	44	SER
1	I	71	VAL
1	I	82(B)	SER
2	L	14	SER
2	L	197	THR
2	L	208	SER
2	M	12	SER
2	M	21	LEU
2	M	89	LEU
2	M	104	LEU
2	M	156	GLN
2	M	202	THR

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

Mol	Chain	Res	Type
1	H	171	GLN
1	I	73	GLN
1	I	131	GLN
2	L	212	ASN
2	M	156	GLN
2	M	190	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 [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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	74:SER	C	75:SER	N	1.63

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	H	216/216 (100%)	1.11	40 (18%) ⓘ ⓘ	40, 49, 58, 64	0
1	I	216/216 (100%)	0.94	27 (12%) ⓘ ⓘ	39, 48, 55, 60	0
2	L	214/214 (100%)	0.94	26 (12%) ⓘ ⓘ	43, 50, 55, 61	0
2	M	214/214 (100%)	0.99	31 (14%) ⓘ ⓘ	41, 48, 53, 56	0
All	All	860/860 (100%)	0.99	124 (14%) ⓘ ⓘ	39, 49, 55, 64	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	42	GLY	5.8
2	M	202	THR	5.1
1	H	132	THR	4.7
1	H	1	GLU	4.5
2	L	33	LEU	4.0
1	I	53	TYR	3.9
2	M	33	LEU	3.9
2	L	40	PRO	3.8
2	L	57	GLY	3.8
2	L	2	ILE	3.7
2	M	29	ILE	3.7
1	H	193	VAL	3.7
1	I	41[A]	HIS	3.7
1	I	65	ASP	3.6
1	H	210	ILE	3.5
2	M	139	PHE	3.4
1	I	1	GLU	3.4
2	M	35	TRP	3.4
1	I	75	SER	3.4
1	I	171	GLN	3.3
1	H	43	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
2	L	212	ASN	3.2
2	M	203	SER	3.2
2	M	132	VAL	3.2
1	I	43[A]	LYS	3.1
1	H	53	TYR	3.1
1	H	133	ASN	3.1
2	M	75	ILE	3.1
1	I	42[A]	GLY	3.1
1	H	41[A]	HIS	3.0
2	M	57	GLY	3.0
2	L	203	SER	3.0
1	H	56	ASP	3.0
1	H	51	ILE	3.0
2	L	139	PHE	3.0
2	M	184	ASP	2.9
1	I	82	LEU	2.9
2	L	179	LEU	2.9
1	I	145	TYR	2.9
2	L	58	VAL	2.9
2	M	145	ASN	2.8
1	H	29	PHE	2.8
2	M	71	TYR	2.8
1	H	190	SER	2.7
1	H	173	ASP	2.7
1	I	210	ILE	2.7
1	I	78	ALA	2.7
2	L	145	ASN	2.7
1	H	171	GLN	2.7
2	L	86	TYR	2.7
2	L	73	LEU	2.7
2	M	212	ASN	2.6
1	H	90	TYR	2.6
1	I	48	ILE	2.6
2	L	35	TRP	2.6
1	H	211	VAL	2.6
2	M	92	ALA	2.6
1	H	36	TRP	2.6
2	L	76	SER	2.6
2	M	169	LYS	2.6
1	H	187	THR	2.5
1	H	142	VAL	2.5
1	H	75	SER	2.5

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Mol	Chain	Res	Type	RSRZ
2	L	69	SER	2.5
1	I	76	THR	2.5
1	I	173	ASP	2.5
2	M	156	GLN	2.5
1	H	172	SER	2.5
1	I	132	THR	2.5
2	L	136	LEU	2.5
2	L	168	SER	2.5
1	I	55	GLY	2.5
1	I	189	PRO	2.5
1	H	34	ILE	2.5
2	L	107	LYS	2.5
2	L	150	ILE	2.5
2	L	144	ILE	2.4
2	M	73	LEU	2.4
1	H	161	SER	2.4
1	I	133	ASN	2.4
1	I	56	ASP	2.4
1	H	197	VAL	2.4
2	M	146	VAL	2.4
1	H	2	ILE	2.4
1	H	82	LEU	2.4
2	L	4	MET	2.4
1	I	194	THR	2.4
2	L	157	ASN	2.4
2	M	48	ILE	2.3
1	I	90	TYR	2.3
1	I	36	TRP	2.3
2	M	148	TRP	2.3
1	H	78	ALA	2.3
2	M	188	ARG	2.3
2	M	126	THR	2.3
2	M	133	VAL	2.3
2	L	105	ALA	2.3
2	L	3	GLN	2.3
2	M	94	SER	2.3
1	H	145	TYR	2.2
1	H	156	SER	2.2
2	M	127	SER	2.2
2	M	153	SER	2.2
2	M	2	ILE	2.2
1	H	52(A)	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
2	M	144	ILE	2.2
1	H	138	LEU	2.2
1	H	134	SER	2.2
1	H	27	TYR	2.2
1	I	140	CYS	2.2
2	L	28	ASP	2.2
1	H	3	GLN	2.2
1	I	29	PHE	2.1
2	M	56	SER	2.1
1	H	152	VAL	2.1
2	L	188	ARG	2.1
2	M	109	ALA	2.1
1	H	158	SER	2.1
1	H	76	THR	2.1
2	M	140	TYR	2.1
1	I	142	VAL	2.1
1	I	52(A)	PRO	2.0
1	H	64	ARG	2.0
1	H	24	ALA	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.