



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:28 PM GMT

PDB ID : 1XF3
Title : Structure of ligand-free Fab DNA-1 in space group P65
Authors : Schuermann, J.P.; Prewitt, S.P.; Deutscher, S.L.; Tanner, J.J.
Deposited on : 2004-09-13
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

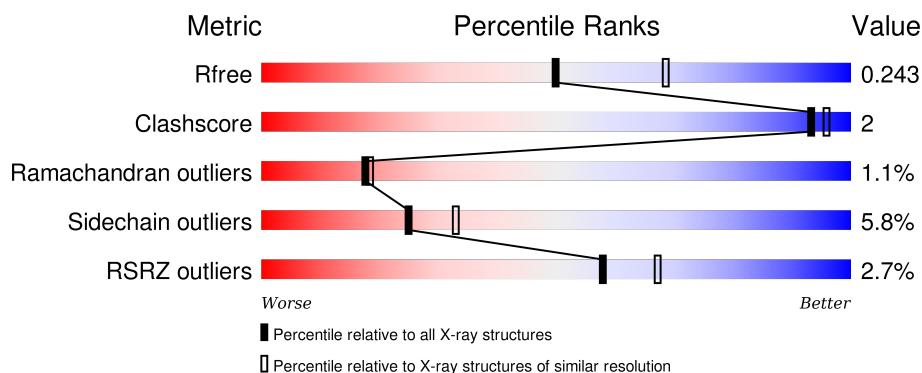
1 Overall quality at a glance

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	214	<div> <div>7%</div> <div>88% 11%</div> </div>
1	L	214	<div> <div>7%</div> <div>85% 13% •</div> </div>
2	B	230	<div> <div>87% 8% 5%</div> </div>
2	H	230	<div> <div>3%</div> <div>82% 10% •• 6%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6457 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 Fab Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	213	Total	C	N	O	S	0	0	0
			1586	991	263	326	6			
1	A	213	Total	C	N	O	S	0	0	0
			1613	1009	272	326	6			

- Molecule 2 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	15	0	0
			1579	998	257	315	9			
2	B	218	Total	C	N	O	S	20	0	0
			1613	1023	258	322	10			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	1	GLN	-	CLONING ARTIFACT	GB 3399661
H	2	VAL	-	CLONING ARTIFACT	GB 3399661
H	3	LYS	-	CLONING ARTIFACT	GB 3399661
H	4	LEU	-	CLONING ARTIFACT	GB 3399661
H	218	HIS	-	EXPRESSION TAG	GB 3399661
H	219	HIS	-	EXPRESSION TAG	GB 3399661
H	220	HIS	-	EXPRESSION TAG	GB 3399661
H	221	HIS	-	EXPRESSION TAG	GB 3399661
H	222	HIS	-	EXPRESSION TAG	GB 3399661
H	223	HIS	-	EXPRESSION TAG	GB 3399661
B	1	GLN	-	CLONING ARTIFACT	GB 3399661
B	2	VAL	-	CLONING ARTIFACT	GB 3399661
B	3	LYS	-	CLONING ARTIFACT	GB 3399661
B	4	LEU	-	CLONING ARTIFACT	GB 3399661
B	218	HIS	-	EXPRESSION TAG	GB 3399661
B	219	HIS	-	EXPRESSION TAG	GB 3399661

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	220	HIS	-	EXPRESSION TAG	GB 3399661
B	221	HIS	-	EXPRESSION TAG	GB 3399661
B	222	HIS	-	EXPRESSION TAG	GB 3399661
B	223	HIS	-	EXPRESSION TAG	GB 3399661

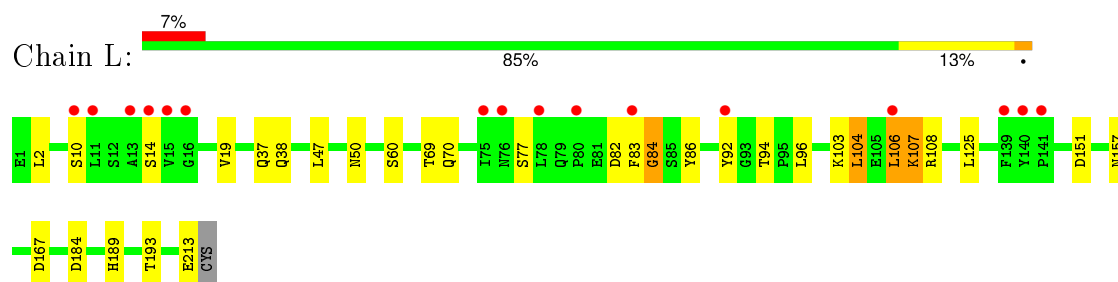
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total	O	0	0
			18	18		
3	B	35	Total	O	0	0
			35	35		
3	H	11	Total	O	0	0
			11	11		
3	L	2	Total	O	0	0
			2	2		

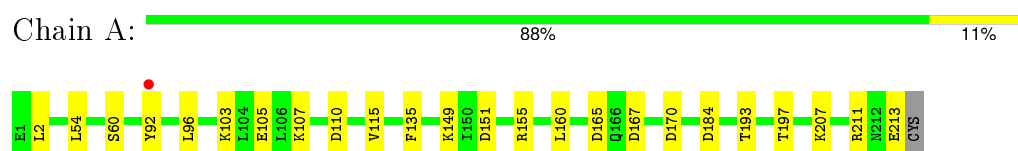
3 Residue-property plots

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.

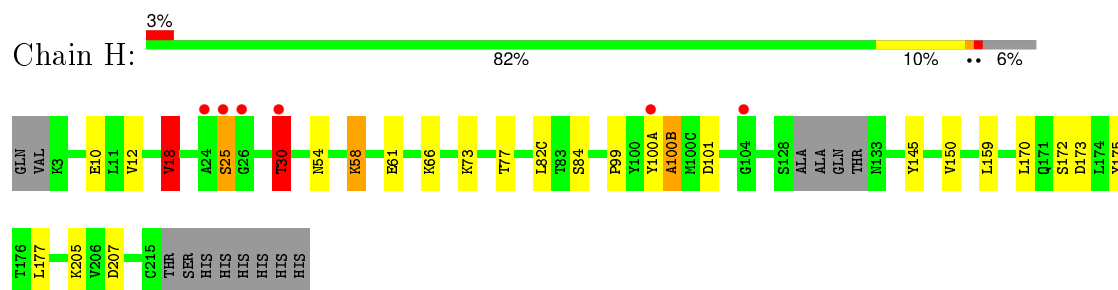
- Molecule 1: Fab Light chain



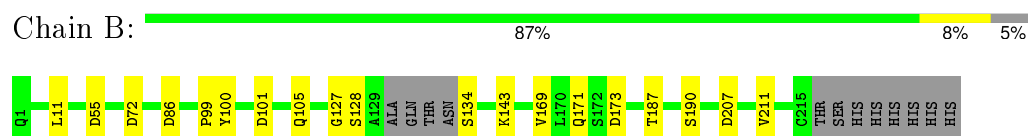
- Molecule 1: Fab Light chain



- Molecule 2: Fab heavy chain



- Molecule 2: Fab heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	201.75 Å 201.75 Å 44.78 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.50 – 2.30 48.46 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.50-2.30) 99.4 (48.46-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.82 (at 2.29 Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.208 , 0.243 0.210 , 0.243	Depositor DCC
R_{free} test set	2323 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	44.3	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.6	EDS
Estimated twinning fraction	0.034 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 46690 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6457	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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 [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	0.45	0/1650	0.73	6/2243 (0.3%)
1	L	0.91	11/1621 (0.7%)	0.76	5/2209 (0.2%)
2	B	0.47	0/1655	0.75	6/2260 (0.3%)
2	H	0.81	3/1619 (0.2%)	0.74	4/2209 (0.2%)
All	All	0.69	14/6545 (0.2%)	0.75	21/8921 (0.2%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	25	SER	CB-OG	17.52	1.65	1.42
1	L	107	LYS	C-O	17.33	1.56	1.23
2	H	30	THR	C-O	11.30	1.44	1.23
1	L	14	SER	CB-OG	8.62	1.53	1.42
2	H	77	THR	C-O	8.39	1.39	1.23
1	L	84	GLY	C-O	7.58	1.35	1.23
1	L	86	TYR	CG-CD2	7.36	1.48	1.39
1	L	107	LYS	C-N	7.31	1.50	1.34
1	L	108	ARG	C-O	6.60	1.35	1.23
1	L	86	TYR	CE1-CZ	6.15	1.46	1.38
1	L	103	LYS	C-O	6.03	1.34	1.23
1	L	19	VAL	C-O	5.41	1.33	1.23
1	L	38	GLN	C-O	5.22	1.33	1.23
1	L	82	ASP	C-O	5.14	1.33	1.23

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	101	ASP	CB-CG-OD2	8.27	125.74	118.30
1	A	165	ASP	CB-CG-OD2	7.81	125.33	118.30
2	H	101	ASP	CB-CG-OD2	7.68	125.21	118.30
2	B	55	ASP	CB-CG-OD2	6.62	124.25	118.30
2	H	173	ASP	CB-CG-OD2	6.15	123.83	118.30
2	B	72	ASP	CB-CG-OD2	5.98	123.68	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	107	LYS	O-C-N	5.92	132.17	122.70
2	B	207	ASP	CB-CG-OD2	5.82	123.54	118.30
1	L	184	ASP	CB-CG-OD2	5.82	123.54	118.30
2	B	86	ASP	CB-CG-OD2	5.53	123.28	118.30
1	L	107	LYS	CA-C-N	-5.47	105.17	117.20
2	H	18	VAL	CB-CA-C	-5.42	101.10	111.40
1	A	110	ASP	CB-CG-OD2	5.40	123.16	118.30
1	L	108	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	184	ASP	CB-CG-OD2	5.27	123.04	118.30
2	B	173	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	151	ASP	CB-CG-OD2	5.23	123.00	118.30
1	A	170	ASP	CB-CG-OD2	5.22	123.00	118.30
2	H	207	ASP	CB-CG-OD2	5.15	122.94	118.30
1	L	167	ASP	CB-CG-OD2	5.13	122.91	118.30
1	A	167	ASP	CB-CG-OD2	5.05	122.84	118.30

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	1613	0	1520	4	0
1	L	1586	0	1465	6	0
2	B	1613	0	1554	2	0
2	H	1579	0	1508	13	0
3	A	18	0	0	0	0
3	B	35	0	0	0	0
3	H	11	0	0	0	0
3	L	2	0	0	0	0
All	All	6457	0	6047	23	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 2.

All (23) 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:H:25:SER:OG	2:H:25:SER:CB	1.65	1.45
2:H:12:VAL:HG21	2:H:82(C):LEU:HD13	1.63	0.81
2:H:12:VAL:HG11	2:H:18:VAL:HG13	1.73	0.70
2:B:187:THR:O	2:B:190:SER:OG	2.08	0.69
1:L:83:PHE:HA	1:L:104:LEU:HD13	1.84	0.60
2:H:25:SER:HG	2:H:25:SER:CB	2.08	0.59
2:H:18:VAL:HG22	2:H:82(C):LEU:HD11	1.86	0.58
2:H:10:GLU:HG2	2:H:18:VAL:HG11	1.85	0.57
2:H:10:GLU:HG2	2:H:18:VAL:CG1	2.36	0.55
1:A:54:LEU:HD11	1:A:60:SER:HA	1.90	0.53
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.90	0.53
1:L:106:LEU:HD22	1:L:107:LYS:O	2.10	0.52
1:L:94:THR:HG21	2:H:58:LYS:HG2	1.93	0.49
2:H:100(A):TYR:O	2:H:100(B):ALA:HB3	2.16	0.46
1:L:151:ASP:OD2	1:L:189:HIS:ND1	2.40	0.46
2:H:12:VAL:CG2	2:H:82(C):LEU:HD13	2.40	0.45
2:H:145:TYR:CE2	2:H:150:VAL:HG13	2.52	0.45
2:H:30:THR:CG2	2:H:30:THR:O	2.65	0.44
1:A:160:LEU:HD21	2:B:169:VAL:HB	1.99	0.44
2:H:170:LEU:HD13	2:H:175:TYR:CZ	2.55	0.42
1:L:84:GLY:O	1:L:104:LEU:N	2.51	0.41
1:A:149:LYS:HB2	1:A:193:THR:OG1	2.21	0.41
1:A:115:VAL:HA	1:A:135:PHE:O	2.21	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	211/214 (99%)	205 (97%)	5 (2%)	1 (0%)	34	41
1	L	211/214 (99%)	200 (95%)	9 (4%)	2 (1%)	21	24
2	B	214/230 (93%)	205 (96%)	5 (2%)	4 (2%)	10	8

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	212/230 (92%)	201 (95%)	9 (4%)	2 (1%)	21	24
All	All	848/888 (96%)	811 (96%)	28 (3%)	9 (1%)	17	18

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	99	PRO
2	B	128	SER
1	L	77	SER
1	A	92	TYR
2	B	100	TYR
2	H	100(B)	ALA
1	L	92	TYR
2	B	127	GLY
2	H	99	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	176/188 (94%)	166 (94%)	10 (6%)	25	34
1	L	171/188 (91%)	158 (92%)	13 (8%)	16	20
2	B	181/200 (90%)	175 (97%)	6 (3%)	45	61
2	H	174/200 (87%)	162 (93%)	12 (7%)	19	24
All	All	702/776 (90%)	661 (94%)	41 (6%)	25	33

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	2	LEU
1	L	10	SER
1	L	50	ASN
1	L	60	SER
1	L	69	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	70	GLN
1	L	96	LEU
1	L	104	LEU
1	L	106	LEU
1	L	125	LEU
1	L	157	ASN
1	L	193	THR
1	L	213	GLU
2	H	18	VAL
2	H	30	THR
2	H	54	ASN
2	H	58	LYS
2	H	61	GLU
2	H	66	LYS
2	H	73	LYS
2	H	84	SER
2	H	159	LEU
2	H	172	SER
2	H	177	LEU
2	H	205	LYS
1	A	2	LEU
1	A	96	LEU
1	A	103	LYS
1	A	105	GLU
1	A	107	LYS
1	A	155	ARG
1	A	197	THR
1	A	207	LYS
1	A	211	ARG
1	A	213	GLU
2	B	11	LEU
2	B	105	GLN
2	B	134	SER
2	B	143	LYS
2	B	171	GLN
2	B	211	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	38	GLN
1	L	89	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	157	ASN
1	L	161	ASN
2	H	39	GLN
2	H	54	ASN
2	H	164	HIS
2	H	171	GLN
1	A	89	GLN
1	A	137	ASN
1	A	161	ASN
1	A	190	ASN

5.3.3 RNA [i](#)

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 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](#)

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	213/214 (99%)	-0.14	1 (0%) 91 94	5, 16, 31, 40	0
1	L	213/214 (99%)	0.50	16 (7%) 17 24	18, 28, 35, 42	0
2	B	214/230 (93%)	-0.18	0 100 100	6, 12, 20, 30	0
2	H	213/230 (92%)	0.12	6 (2%) 56 66	10, 21, 28, 36	0
All	All	853/888 (96%)	0.08	23 (2%) 58 67	5, 19, 33, 42	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	24	ALA	6.4
1	L	75	ILE	5.3
1	L	80	PRO	3.5
2	H	30	THR	3.5
2	H	100(A)	TYR	3.3
1	L	15	VAL	3.3
1	L	11	LEU	3.2
1	A	92	TYR	3.0
1	L	140	TYR	3.0
1	L	106	LEU	3.0
1	L	141	PRO	3.0
2	H	25	SER	2.9
1	L	16	GLY	2.9
1	L	139	PHE	2.8
2	H	26	GLY	2.6
1	L	14	SER	2.5
1	L	10	SER	2.4
1	L	83	PHE	2.3
1	L	13	ALA	2.3
2	H	104	GLY	2.3
1	L	76	ASN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	78	LEU	2.2
1	L	92	TYR	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 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.