



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:52 PM UTC

PDB ID : 1IT9 / pdb_00001it9
Title : CRYSTAL STRUCTURE OF AN ANTIGEN-BINDING FRAGMENT
FROM A HUMANIZED VERSION OF THE ANTI-HUMAN FAS ANTI-
BODY HFE7A
Authors : Ito, S.; Takayama, T.; Hanzawa, H.; Takahashi, T.; Miyadai, K.; Serizawa, N.;
Hata, T.; Haruyama, H.
Deposited on : 2002-01-11
Resolution : 2.80 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

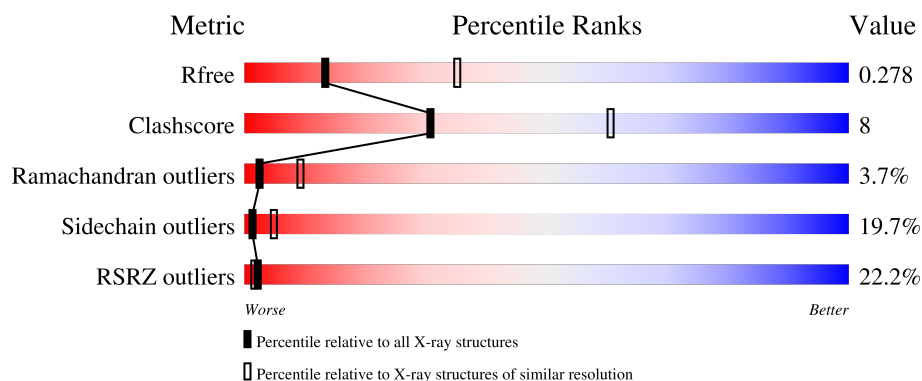
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	L	214	22% 65% 29% 6%
2	H	219	22% 70% 26% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3319 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 HUMANIZED ANTIBODY HFE7A, LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	0	0
			1653	1030	275	343	5			

- Molecule 2 is a protein called HUMANIZED ANTIBODY HFE7A, HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	219	Total	C	N	O	S	0	0	0
			1660	1048	271	334	7			

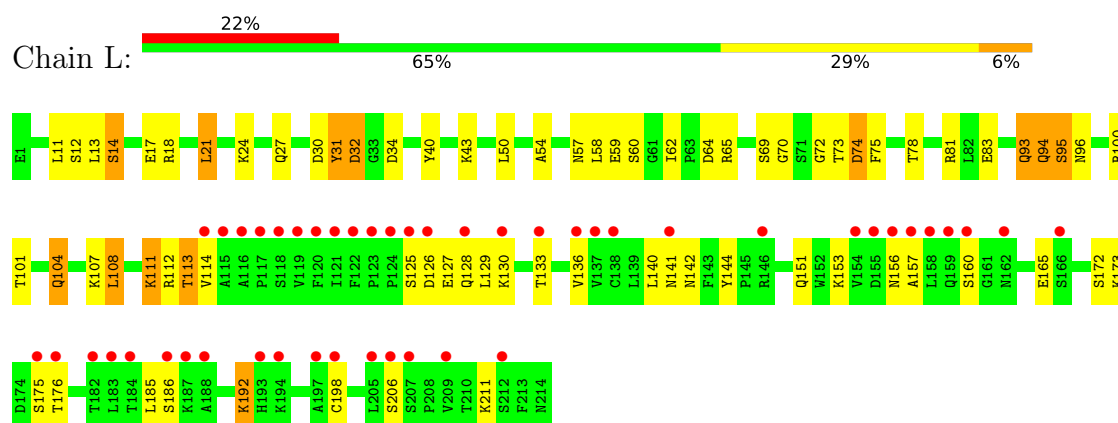
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	3	Total	O	0	0
			3	3		
3	H	3	Total	O	0	0
			3	3		

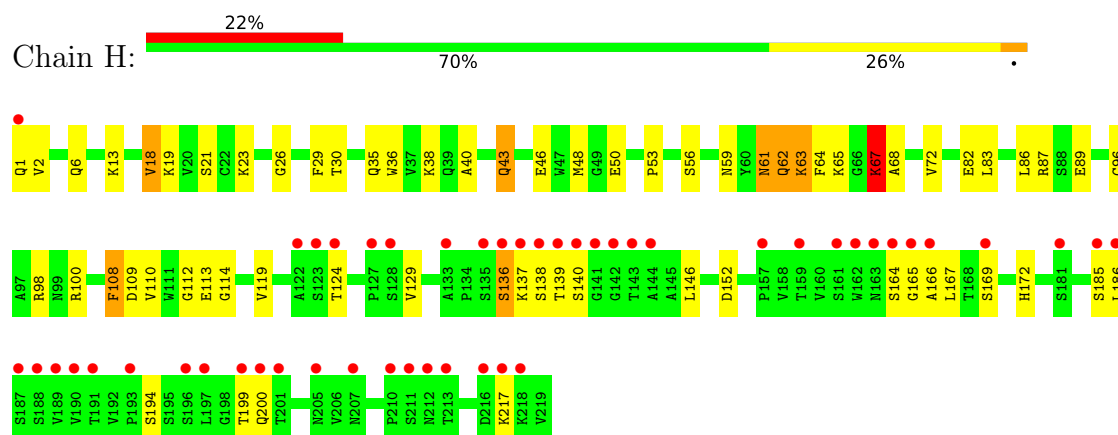
3 Residue-property plots

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: HUMANIZED ANTIBODY HFE7A, LIGHT CHAIN



• Molecule 2: HUMANIZED ANTIBODY HFE7A, HEAVY CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.37Å 82.75Å 104.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.0 (30.00-2.80) 91.0 (30.00-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.53 (at 2.80Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.202 , 0.280 0.202 , 0.278	Depositor DCC
R_{free} test set	1144 reflections (10.31%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 69.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3319	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% 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	L	0.37	0/1688	0.81	1/2291 (0.0%)
2	H	0.37	0/1702	0.85	3/2320 (0.1%)
All	All	0.37	0/3390	0.83	4/4611 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	61	ASN	N-CA-C	-5.46	101.82	109.96
2	H	136	SER	N-CA-C	-5.45	99.20	110.80
1	L	141	ASN	N-CA-C	5.43	117.70	110.53
2	H	67	LYS	N-CA-C	-5.02	106.50	113.18

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	L	1653	0	1587	34	0
2	H	1660	0	1608	20	0
3	H	3	0	0	0	0
3	L	3	0	0	0	0
All	All	3319	0	3195	54	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 8.

All (54) 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:2:VAL:HG11	2:H:98:ARG:NH2	2.03	0.73
1:L:112:ARG:HG3	1:L:112:ARG:HH11	1.56	0.70
1:L:32:ASP:O	1:L:32:ASP:CG	2.36	0.68
2:H:40:ALA:HB3	2:H:43:GLN:HG3	1.76	0.65
1:L:54:ALA:HB3	1:L:57:ASN:HD22	1.62	0.64
1:L:100:ARG:HG2	1:L:100:ARG:HH11	1.60	0.64
2:H:18:VAL:HG22	2:H:86:LEU:HD11	1.79	0.64
1:L:21:LEU:N	1:L:21:LEU:HD23	2.13	0.64
1:L:31:TYR:O	1:L:34:ASP:HB2	2.00	0.62
1:L:112:ARG:NH1	1:L:113:THR:O	2.33	0.61
1:L:40:TYR:HE1	1:L:93:GLN:HE21	1.50	0.60
2:H:6:GLN:HE21	2:H:112:GLY:HA3	1.67	0.60
1:L:112:ARG:HG3	1:L:112:ARG:NH1	2.19	0.57
1:L:13:LEU:HD12	1:L:108:LEU:HD21	1.85	0.57
1:L:94:GLN:HG2	1:L:96:ASN:H	1.69	0.57
1:L:111:LYS:HA	1:L:144:TYR:OH	2.04	0.57
1:L:11:LEU:HD21	1:L:13:LEU:HD11	1.89	0.54
2:H:68:ALA:HA	2:H:82:GLU:O	2.09	0.53
2:H:36:TRP:CZ3	2:H:96:CYS:HB3	2.43	0.53
2:H:6:GLN:NE2	2:H:114:GLY:H	2.07	0.53
2:H:18:VAL:CG2	2:H:86:LEU:HD11	2.38	0.53
2:H:50:GLU:HG2	2:H:59:ASN:HB3	1.92	0.52
1:L:31:TYR:HD2	1:L:32:ASP:OD1	1.94	0.51
1:L:18:ARG:NH1	1:L:78:THR:HG21	2.25	0.50
1:L:30:ASP:O	1:L:31:TYR:HB2	2.12	0.50
1:L:94:GLN:NE2	1:L:101:THR:OG1	2.45	0.49
1:L:12:SER:HB3	1:L:111:LYS:HB2	1.95	0.48
1:L:54:ALA:HB3	1:L:57:ASN:ND2	2.28	0.48
1:L:74:ASP:OD2	1:L:74:ASP:N	2.44	0.48
1:L:112:ARG:HG3	1:L:113:THR:N	2.28	0.48
1:L:100:ARG:HG2	1:L:100:ARG:NH1	2.24	0.48
2:H:61:ASN:O	2:H:63:LYS:N	2.46	0.48
2:H:108:PHE:N	2:H:108:PHE:CD1	2.81	0.48
1:L:59:GLU:O	1:L:62:ILE:HG12	2.15	0.47
1:L:94:GLN:HG2	1:L:95:SER:N	2.29	0.47
1:L:70:GLY:HA3	1:L:75:PHE:HA	1.96	0.47
2:H:48:MET:HE3	2:H:64:PHE:CD2	2.51	0.46
1:L:31:TYR:C	1:L:31:TYR:CD2	2.93	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:94:GLN:HE21	1:L:94:GLN:HB3	1.62	0.46
2:H:2:VAL:HG22	2:H:26:GLY:O	2.16	0.46
2:H:87:ARG:C	2:H:119:VAL:HG11	2.41	0.46
2:H:46:GLU:OE1	2:H:63:LYS:HE2	2.15	0.45
1:L:50:LEU:HD23	1:L:59:GLU:CD	2.41	0.45
2:H:109:ASP:OD1	2:H:110:VAL:N	2.50	0.45
1:L:104:GLN:H	1:L:104:GLN:HG3	1.32	0.44
2:H:35:GLN:HG3	2:H:108:PHE:CD1	2.52	0.44
1:L:59:GLU:HG3	1:L:60:SER:N	2.32	0.44
1:L:14:SER:O	1:L:17:GLU:HB2	2.18	0.44
1:L:31:TYR:CD2	1:L:32:ASP:OD1	2.71	0.43
1:L:113:THR:O	1:L:114:VAL:C	2.61	0.43
2:H:53:PRO:HA	2:H:72:VAL:HG21	2.01	0.42
2:H:67:LYS:O	2:H:83:LEU:HA	2.20	0.41
2:H:6:GLN:HE21	2:H:112:GLY:CA	2.33	0.41
1:L:65:ARG:CZ	1:L:83:GLU:HG3	2.51	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	L	212/214 (99%)	185 (87%)	22 (10%)	5 (2%)	4	17
2	H	217/219 (99%)	186 (86%)	20 (9%)	11 (5%)	1	5
All	All	429/433 (99%)	371 (86%)	42 (10%)	16 (4%)	2	9

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	31	TYR
1	L	157	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	124	THR
2	H	136	SER
2	H	139	THR
2	H	140	SER
2	H	152	ASP
1	L	142	ASN
2	H	62	GLN
2	H	165	GLY
2	H	166	ALA
2	H	137	LYS
1	L	72	GLY
2	H	164	SER
2	H	29	PHE
1	L	192	LYS

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	L	188/188 (100%)	144 (77%)	44 (23%)	1	3
2	H	188/188 (100%)	158 (84%)	30 (16%)	2	9
All	All	376/376 (100%)	302 (80%)	74 (20%)	1	5

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	14	SER
1	L	21	LEU
1	L	24	LYS
1	L	27	GLN
1	L	32	ASP
1	L	43	LYS
1	L	58	LEU
1	L	64	ASP
1	L	69	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	73	THR
1	L	74	ASP
1	L	81	ARG
1	L	93	GLN
1	L	94	GLN
1	L	95	SER
1	L	104	GLN
1	L	107	LYS
1	L	108	LEU
1	L	111	LYS
1	L	113	THR
1	L	125	SER
1	L	126	ASP
1	L	127	GLU
1	L	128	GLN
1	L	129	LEU
1	L	130	LYS
1	L	133	THR
1	L	136	VAL
1	L	140	LEU
1	L	151	GLN
1	L	153	LYS
1	L	156	ASN
1	L	160	SER
1	L	165	GLU
1	L	172	SER
1	L	173	LYS
1	L	175	SER
1	L	176	THR
1	L	185	LEU
1	L	186	SER
1	L	192	LYS
1	L	198	CYS
1	L	206	SER
1	L	211	LYS
2	H	1	GLN
2	H	13	LYS
2	H	18	VAL
2	H	19	LYS
2	H	21	SER
2	H	23	LYS
2	H	30	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	38	LYS
2	H	43	GLN
2	H	56	SER
2	H	62	GLN
2	H	63	LYS
2	H	65	LYS
2	H	67	LYS
2	H	89	GLU
2	H	100	ARG
2	H	108	PHE
2	H	113	GLU
2	H	129	VAL
2	H	138	SER
2	H	146	LEU
2	H	167	LEU
2	H	169	SER
2	H	172	HIS
2	H	185	SER
2	H	186	LEU
2	H	194	SER
2	H	199	THR
2	H	200	GLN
2	H	217	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	27	GLN
1	L	57	ASN
1	L	93	GLN
1	L	94	GLN
1	L	141	ASN
1	L	142	ASN
1	L	156	ASN
1	L	202	HIS
1	L	214	ASN
2	H	6	GLN
2	H	105	ASN
2	H	179	GLN
2	H	200	GLN

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 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	L	214/214 (100%)	0.75	47 (21%) 2 2	3, 21, 35, 54	101 (47%)
2	H	219/219 (100%)	0.68	49 (22%) 2 1	1, 23, 39, 64	98 (44%)
All	All	433/433 (100%)	0.72	96 (22%) 2 1	1, 21, 38, 64	199 (45%)

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	137	LYS	5.7
1	L	159	GLN	4.4
1	L	160	SER	4.3
1	L	125	SER	4.3
2	H	165	GLY	4.2
1	L	115	ALA	4.1
1	L	193	HIS	3.9
1	L	124	PRO	3.9
2	H	164	SER	3.8
1	L	121	ILE	3.7
1	L	162	ASN	3.7
1	L	155	ASP	3.7
1	L	206	SER	3.6
1	L	207	SER	3.6
2	H	188	SER	3.5
2	H	139	THR	3.5
2	H	199	THR	3.5
2	H	211	SER	3.4
1	L	118	SER	3.4
2	H	191	THR	3.3
1	L	157	ALA	3.2
1	L	158	LEU	3.2
2	H	169	SER	3.2
2	H	207	ASN	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	212	ASN	3.2
2	H	201	THR	3.2
2	H	187	SER	3.1
2	H	189	VAL	3.1
2	H	138	SER	3.1
2	H	193	PRO	3.0
2	H	163	ASN	3.0
2	H	216	ASP	2.9
1	L	188	ALA	2.9
1	L	154	VAL	2.9
2	H	128	SER	2.9
2	H	213	THR	2.9
1	L	116	ALA	2.8
2	H	205	ASN	2.8
1	L	176	THR	2.8
1	L	186	SER	2.8
1	L	183	LEU	2.7
1	L	136	VAL	2.7
1	L	197	ALA	2.7
1	L	205	LEU	2.7
2	H	143	THR	2.7
2	H	218	LYS	2.7
1	L	184	THR	2.7
1	L	126	ASP	2.7
1	L	212	SER	2.7
2	H	144	ALA	2.6
2	H	196	SER	2.6
2	H	210	PRO	2.6
2	H	161	SER	2.6
1	L	209	VAL	2.5
2	H	186	LEU	2.5
2	H	159	THR	2.5
2	H	135	SER	2.5
2	H	157	PRO	2.5
2	H	185	SER	2.5
1	L	122	PHE	2.5
2	H	217	LYS	2.5
1	L	138	CYS	2.5
1	L	117	PRO	2.4
2	H	162	TRP	2.4
1	L	146	ARG	2.4
2	H	140	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	182	THR	2.4
2	H	197	LEU	2.3
1	L	114	VAL	2.3
1	L	156	ASN	2.3
1	L	130	LYS	2.3
1	L	137	VAL	2.3
2	H	142	GLY	2.3
2	H	122	ALA	2.2
2	H	133	ALA	2.2
2	H	123	SER	2.2
2	H	200	GLN	2.2
2	H	181	SER	2.2
1	L	119	VAL	2.2
2	H	136	SER	2.2
1	L	120	PHE	2.2
1	L	187	LYS	2.2
2	H	1	GLN	2.1
2	H	127	PRO	2.1
2	H	124	THR	2.1
2	H	141	GLY	2.1
1	L	123	PRO	2.1
1	L	166	SER	2.1
1	L	194	LYS	2.1
2	H	190	VAL	2.1
1	L	133	THR	2.1
1	L	198	CYS	2.1
1	L	141	ASN	2.1
2	H	166	ALA	2.1
1	L	175	SER	2.0
1	L	128	GLN	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 ⓘ

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.