



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:43 PM UTC

PDB ID : 6MTR / pdb_00006mtr
Title : Crystal structure of VRC43.01 Fab
Authors : Kwon, Y.D.; Druz, A.; Law, W.H.; Peng, D.; Zhang, B.; Doria-Rose, N.A.;
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Deposited on : 2018-10-21
Resolution : 1.80 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

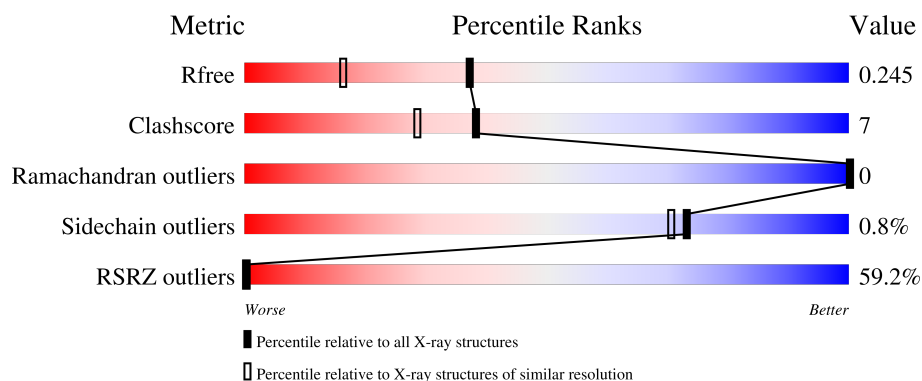
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	H	229	63% 84% 12% .
2	L	215	52% 86% 12% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3338 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 Antibody VRC43.01 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	221	Total	C	N	O	S	0	0	0
			1640	1041	275	320	4			

- Molecule 2 is a protein called Antibody VRC43.01 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	210	Total	C	N	O	S	0	0	0
			1551	976	260	309	6			

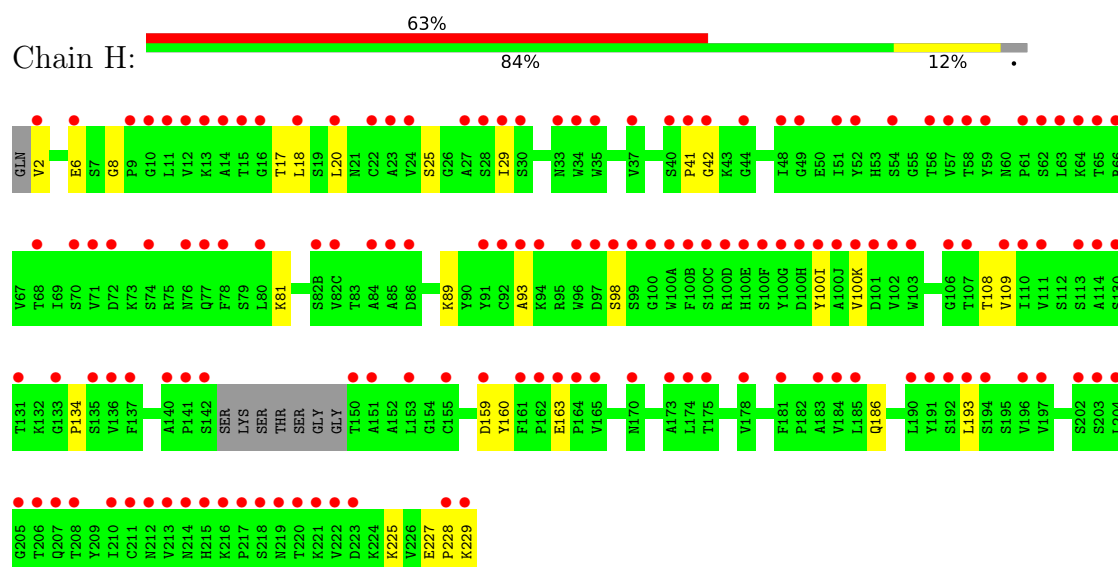
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	64	Total	O	0	0
			64	64		
3	L	83	Total	O	0	0
			83	83		

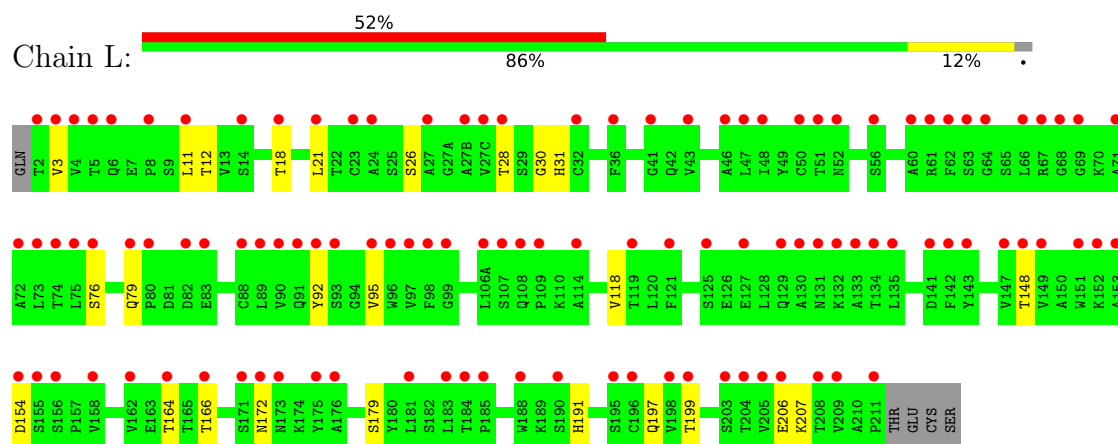
3 Residue-property plots [i](#)

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: Antibody VRC43.01 Fab heavy chain



• Molecule 2: Antibody VRC43.01 Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	163.07Å 54.66Å 66.11Å 90.00° 113.30° 90.00°	Depositor
Resolution (Å)	36.86 – 1.80 36.86 – 1.80	Depositor EDS
% Data completeness (in resolution range)	83.9 (36.86-1.80) 83.9 (36.86-1.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 1.79Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.209 , 0.243 0.223 , 0.245	Depositor DCC
R_{free} test set	2025 reflections (4.05%)	wwPDB-VP
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.003 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3338	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.49% 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	H	0.50	0/1684	0.73	0/2310
2	L	0.54	0/1592	0.72	0/2182
All	All	0.52	0/3276	0.73	0/4492

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	H	1640	0	1569	22	0
2	L	1551	0	1497	22	0
3	H	64	0	0	7	0
3	L	83	0	0	4	0
All	All	3338	0	3066	43	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 7.

All (43) 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:H:227:GLU:HG2	1:H:228:PRO:HD2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:164:THR:HG22	2:L:179:SER:OG	1.92	0.69
1:H:186:GLN:NE2	3:H:302:HOH:O	2.26	0.68
1:H:225:LYS:NZ	3:H:303:HOH:O	2.27	0.68
2:L:79:GLN:NE2	3:L:303:HOH:O	2.25	0.67
2:L:154:ASP:OD1	2:L:191:HIS:HB3	1.95	0.67
1:H:98:SER:HB2	1:H:100(I):TYR:HE1	1.62	0.64
2:L:12:THR:OG1	3:L:301:HOH:O	2.15	0.64
2:L:172:ASN:ND2	3:L:305:HOH:O	2.34	0.59
1:H:8:GLY:HA3	1:H:20:LEU:HD23	1.85	0.59
1:H:159:ASP:OD1	1:H:186:GLN:NE2	2.35	0.59
2:L:11:LEU:HD12	2:L:21:LEU:HD23	1.84	0.59
2:L:118:VAL:O	2:L:207:LYS:NZ	2.37	0.58
2:L:28:THR:HG23	2:L:30:GLY:H	1.69	0.58
1:H:18:LEU:HD13	1:H:109:VAL:HG11	1.88	0.55
2:L:18:THR:HG22	2:L:76:SER:HA	1.88	0.55
2:L:28:THR:HG22	2:L:31:HIS:CE1	2.43	0.54
2:L:28:THR:HG22	2:L:31:HIS:ND1	2.22	0.54
2:L:92:TYR:O	2:L:95:VAL:HG22	2.08	0.54
1:H:93:ALA:HB1	1:H:100(K):VAL:CG1	2.38	0.54
1:H:229:LYS:HA	3:H:304:HOH:O	2.08	0.52
2:L:154:ASP:OD2	2:L:191:HIS:HD2	1.92	0.52
2:L:197:GLN:HG2	2:L:206:GLU:HG2	1.91	0.52
1:H:17:THR:HG21	1:H:81:LYS:HE3	1.93	0.50
2:L:3:VAL:HG22	2:L:26:SER:HB3	1.93	0.49
1:H:89:LYS:HD2	1:H:108:THR:OG1	2.14	0.47
1:H:41:PRO:HD2	3:H:310:HOH:O	2.14	0.47
1:H:93:ALA:HB1	1:H:100(K):VAL:HG11	1.97	0.46
2:L:197:GLN:HE21	2:L:206:GLU:CD	2.24	0.46
1:H:41:PRO:CD	3:H:310:HOH:O	2.65	0.45
2:L:11:LEU:HD12	2:L:21:LEU:CD2	2.46	0.45
1:H:108:THR:HG23	3:H:347:HOH:O	2.16	0.45
1:H:42:GLY:HA3	2:L:166:THR:HG21	1.99	0.45
2:L:21:LEU:HB3	3:L:337:HOH:O	2.17	0.45
1:H:93:ALA:HB1	1:H:100(K):VAL:HG13	2.00	0.44
2:L:28:THR:HG23	2:L:30:GLY:N	2.33	0.43
1:H:160:TYR:HE2	1:H:163:GLU:O	2.01	0.43
2:L:148:THR:OG1	2:L:199:THR:HB	2.19	0.42
2:L:197:GLN:NE2	2:L:206:GLU:OE2	2.51	0.42
1:H:98:SER:HB2	1:H:100(I):TYR:CE1	2.50	0.42
1:H:134:PRO:HB3	1:H:160:TYR:HB3	2.02	0.41
1:H:228:PRO:HD3	3:H:339:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:2:VAL:HA	1:H:25:SER:O	2.21	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	217/229 (95%)	206 (95%)	11 (5%)	0	100	100
2	L	208/215 (97%)	203 (98%)	5 (2%)	0	100	100
All	All	425/444 (96%)	409 (96%)	16 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	181/196 (92%)	178 (98%)	3 (2%)	53	45
2	L	172/180 (96%)	172 (100%)	0	100	100
All	All	353/376 (94%)	350 (99%)	3 (1%)	73	70

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	6	GLU
1	H	29	ILE
1	H	193	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	21	ASN
2	L	53	ASN
2	L	200	HIS

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	H	221/229 (96%)	2.47	144 (65%) 0 0	31, 53, 81, 129	0
2	L	210/215 (97%)	2.18	111 (52%) 0 0	32, 49, 72, 81	0
All	All	431/444 (97%)	2.33	255 (59%) 0 0	31, 50, 76, 129	0

All (255) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	100(C)	SER	8.7
1	H	100(B)	PHE	8.0
1	H	212	ASN	7.0
1	H	100(A)	TRP	6.4
2	L	153	ALA	5.6
1	H	65	THR	5.5
2	L	2	THR	5.1
2	L	106(A)	LEU	5.0
2	L	119	THR	4.9
1	H	155	CYS	4.9
1	H	99	SER	4.9
1	H	63	LEU	4.9
1	H	96	TRP	4.8
1	H	82(C)	VAL	4.8
2	L	27	ALA	4.7
1	H	150	THR	4.6
1	H	100(K)	VAL	4.6
1	H	62	SER	4.5
1	H	57	VAL	4.4
2	L	107	SER	4.4
1	H	223	ASP	4.4
2	L	188	TRP	4.3
2	L	88	CYS	4.2
1	H	100(G)	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
2	L	43	VAL	4.1
1	H	214	ASN	4.1
1	H	92	CYS	4.0
1	H	211	CYS	4.0
2	L	5	THR	4.0
2	L	211	PRO	4.0
1	H	184	VAL	4.0
1	H	131	THR	3.9
1	H	153	LEU	3.9
2	L	21	LEU	3.9
1	H	100	GLY	3.9
1	H	84	ALA	3.9
1	H	175	THR	3.8
1	H	29	ILE	3.8
2	L	4	VAL	3.8
2	L	90	VAL	3.8
2	L	50	CYS	3.8
2	L	203	SER	3.7
2	L	206	GLU	3.7
2	L	121	PHE	3.7
1	H	111	VAL	3.7
1	H	220	THR	3.7
2	L	27(C)	VAL	3.6
1	H	100(F)	SER	3.6
1	H	40	SER	3.5
1	H	27	ALA	3.5
2	L	209	VAL	3.5
2	L	156	SER	3.5
2	L	204	THR	3.5
1	H	100(J)	ALA	3.4
1	H	102	VAL	3.4
2	L	162	VAL	3.4
1	H	51	ILE	3.4
2	L	60	ALA	3.3
2	L	92	TYR	3.3
2	L	67	ARG	3.3
1	H	164	PRO	3.3
1	H	206	THR	3.3
2	L	158	VAL	3.3
1	H	35	TRP	3.3
1	H	42	GLY	3.3
2	L	27(B)	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	H	85	ALA	3.2
2	L	68	GLY	3.2
1	H	58	THR	3.2
2	L	184	THR	3.2
2	L	11	LEU	3.2
1	H	140	ALA	3.2
1	H	178	VAL	3.2
1	H	202	SER	3.2
2	L	63	SER	3.2
1	H	181	PHE	3.2
2	L	66	LEU	3.1
2	L	176	ALA	3.1
2	L	28	THR	3.1
1	H	9	PRO	3.1
1	H	61	PRO	3.1
2	L	196	CYS	3.1
2	L	64	GLY	3.1
2	L	148	THR	3.1
1	H	163	GLU	3.1
1	H	205	GLY	3.0
1	H	2	VAL	3.0
1	H	165	VAL	3.0
1	H	68	THR	3.0
1	H	210	ILE	3.0
1	H	228	PRO	3.0
1	H	197	VAL	3.0
2	L	133	ALA	3.0
1	H	64	LYS	3.0
2	L	80	PRO	3.0
1	H	213	VAL	2.9
1	H	215	HIS	2.9
1	H	161	PHE	2.9
2	L	79	GLN	2.9
2	L	73	LEU	2.9
1	H	100(E)	HIS	2.9
2	L	190	SER	2.9
2	L	98	PHE	2.9
1	H	219	ASN	2.9
2	L	71	ALA	2.9
2	L	154	ASP	2.9
1	H	218	SER	2.9
1	H	114	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	136	VAL	2.8
1	H	229	LYS	2.8
1	H	11	LEU	2.8
2	L	171	SER	2.8
2	L	91	GLN	2.8
1	H	93	ALA	2.8
1	H	217	PRO	2.8
2	L	89	LEU	2.8
1	H	170	ASN	2.8
1	H	34	TRP	2.8
1	H	10	GLY	2.8
1	H	78	PHE	2.8
1	H	82(B)	SER	2.8
2	L	125	SER	2.8
2	L	173	ASN	2.7
2	L	164	THR	2.7
2	L	130	ALA	2.7
1	H	185	LEU	2.7
2	L	47	LEU	2.7
1	H	77	GLN	2.7
1	H	207	GLN	2.7
1	H	98	SER	2.7
1	H	113	SER	2.7
1	H	130	SER	2.7
2	L	166	THR	2.7
1	H	30	SER	2.6
2	L	23	CYS	2.6
1	H	12	VAL	2.6
2	L	208	THR	2.6
1	H	6	GLU	2.6
1	H	72	ASP	2.6
1	H	159	ASP	2.6
2	L	183	LEU	2.6
1	H	222	VAL	2.6
1	H	110	ILE	2.6
1	H	14	ALA	2.6
1	H	162	PRO	2.6
2	L	109	PRO	2.6
1	H	106	GLY	2.6
1	H	204	LEU	2.6
1	H	37	VAL	2.6
1	H	100(I)	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	173	ALA	2.6
2	L	127	GLU	2.6
1	H	15	THR	2.5
2	L	62	PHE	2.5
1	H	70	SER	2.5
2	L	135	LEU	2.5
2	L	83	GLU	2.5
2	L	129	GLN	2.5
2	L	69	GLY	2.5
1	H	28	SER	2.5
2	L	142	PHE	2.5
2	L	172	ASN	2.5
2	L	6	GLN	2.5
2	L	134	THR	2.5
1	H	216	LYS	2.5
1	H	221	LYS	2.5
2	L	155	SER	2.5
2	L	3	VAL	2.5
2	L	149	VAL	2.5
2	L	51	THR	2.5
2	L	82	ASP	2.4
2	L	32	CYS	2.4
1	H	52	TYR	2.4
1	H	107	THR	2.4
1	H	194	SER	2.4
1	H	196	VAL	2.4
2	L	18	THR	2.4
2	L	131	ASN	2.4
2	L	141	ASP	2.4
1	H	103	TRP	2.4
1	H	190	LEU	2.4
1	H	193	LEU	2.4
1	H	76	ASN	2.4
1	H	48	ILE	2.4
2	L	95	VAL	2.4
2	L	93	SER	2.4
2	L	46	ALA	2.4
1	H	100(D)	ARG	2.4
2	L	132	LYS	2.4
1	H	24	VAL	2.4
2	L	198	VAL	2.4
1	H	16	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	135	SER	2.3
2	L	76	SER	2.3
2	L	72	ALA	2.3
2	L	74	THR	2.3
2	L	36	PHE	2.3
1	H	203	SER	2.3
2	L	56	SER	2.3
1	H	86	ASP	2.3
1	H	97	ASP	2.3
1	H	151	ALA	2.3
2	L	24	ALA	2.3
2	L	151	TRP	2.3
1	H	71	VAL	2.3
1	H	109	VAL	2.3
2	L	97	VAL	2.3
1	H	49	GLY	2.3
1	H	13	LYS	2.3
1	H	54	SER	2.3
2	L	195	SER	2.3
1	H	91	TYR	2.3
1	H	94	LYS	2.3
1	H	100(H)	ASP	2.3
2	L	96	TRP	2.2
2	L	185	PRO	2.2
2	L	99	GLY	2.2
2	L	143	TYR	2.2
1	H	41	PRO	2.2
1	H	23	ALA	2.2
1	H	192	SER	2.2
1	H	44	GLY	2.2
1	H	133	GLY	2.2
2	L	108	GLN	2.2
2	L	52	ASN	2.2
1	H	22	CYS	2.2
1	H	20	LEU	2.2
2	L	41	GLY	2.2
2	L	152	LYS	2.2
2	L	8	PRO	2.2
1	H	101	ASP	2.1
2	L	114	ALA	2.1
1	H	66	ARG	2.1
1	H	80	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	56	THR	2.1
1	H	191	TYR	2.1
2	L	175	TYR	2.1
2	L	205	VAL	2.1
1	H	33	ASN	2.1
1	H	174	LEU	2.1
1	H	142	SER	2.1
1	H	141	PRO	2.1
1	H	183	ALA	2.1
2	L	147	VAL	2.1
2	L	61	ARG	2.1
1	H	208	THR	2.1
2	L	199	THR	2.1
1	H	59	TYR	2.1
1	H	137	PHE	2.1
2	L	48	ILE	2.1
1	H	18	LEU	2.0
2	L	75	LEU	2.0
2	L	181	LEU	2.0
1	H	74	SER	2.0
2	L	14	SER	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 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.