WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Sep 11, 2023 – 04:53 AM EDT

PDB ID : 4JHA
Title : Crystal Structure of RSV-Neutralizing Human Antibody D25
Authors : Mclellan, J.S.; Chen, M.; Leung, S.; Graepel, K.W.; Du, X.; Yang, Y.; Zhou,
T.; Baxa, U.; Yasuda, E.; Beaumont, T.; Kumar, A.; Modjarrad, K.; Zheng,
Z.; Zhao, M.; Xia, N.; Kwong, P.D.; Graham, B.S.
Deposited on : 2013-03-04
Resolution : 1.60 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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 1.60 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	Percentile Ranks	Value
Rfree		0.255
Clashscore		9
Ramachandran outliers		0.5%
Sidechain outliers		2.7%
RSRZ outliers		31.1%

Worse　　　　　*Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
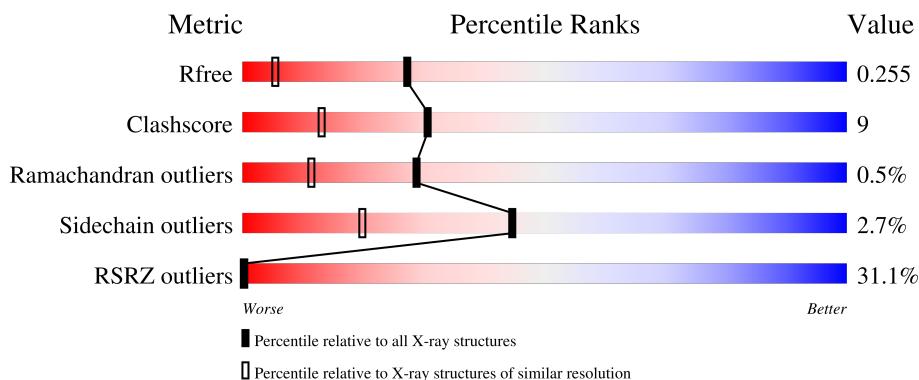
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 <=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	231	26% / 83% / 13% / ··
2	L	214	35% / 75% / 22% / ··
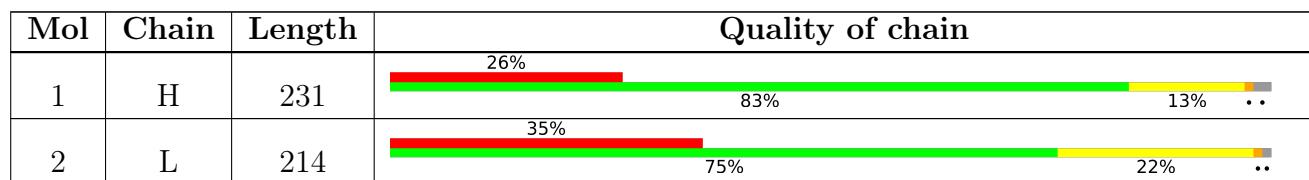
2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3575 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 D25 antigen-binding fragment heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	226	Total 1686	C 1069	N 279	O 330	S 8	0	1	0

- Molecule 2 is a protein called D25 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	211	Total 1619	C 1014	N 269	O 331	S 5	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	141	Total 141	O 141	0	0
3	L	129	Total 129	O 129	0	0

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: D25 antigen-binding fragment heavy chain
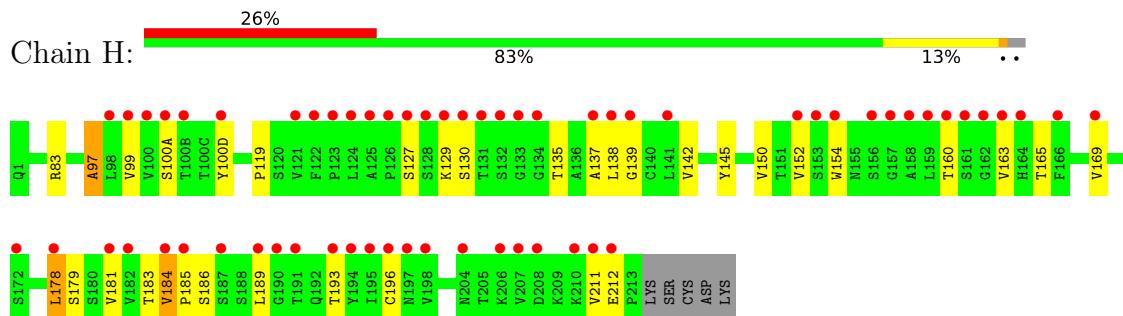
Chain H:

• Molecule 2: D25 light chain

Chain L:
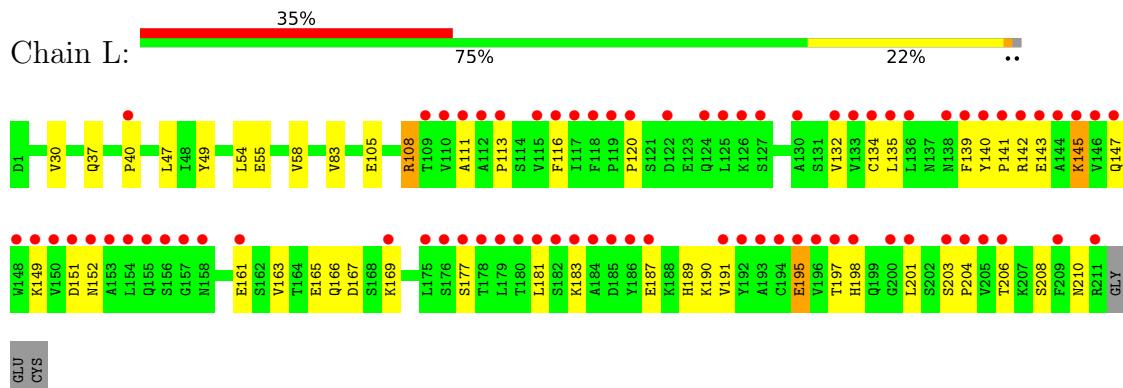
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	108.72Å 108.72Å 139.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.40 – 1.60	Depositor
	35.40 – 1.60	EDS
% Data completeness	98.1 (35.40-1.60)	Depositor
(in resolution range)	98.1 (35.40-1.60)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 1.60Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.240 , 0.255	Depositor
	0.242 , 0.255	DCC
R_{free} test set	3215 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	23.3	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 60.1	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3575	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.38	0/1732	0.61	1/2371 (0.0%)
2	L	0.35	0/1652	0.57	0/2247
All	All	0.37	0/3384	0.59	1/4618 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	178	LEU	CA-CB-CG	5.50	127.96	115.30

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	H	1686	0	1666	22	0
2	L	1619	0	1579	40	1
3	H	141	0	0	8	0
3	L	129	0	0	13	0
All	All	3575	0	3245	60	1

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 9.

All (60) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

W O R L D W I D E
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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:147:GLN:O	3:L:418:HOH:O	1.82	0.97
2:L:147:GLN:HG2	3:L:418:HOH:O	1.63	0.96
2:L:161:GLU:O	3:L:408:HOH:O	1.89	0.90
1:H:179:SER:OG	3:H:412:HOH:O	1.91	0.87
2:L:203:SER:OG	3:L:420:HOH:O	1.96	0.82
2:L:183:LYS:NZ	3:L:378:HOH:O	2.15	0.79
2:L:120:PRO:HD3	2:L:132:VAL:HG22	1.65	0.77
2:L:187:GLU:OE1	3:L:427:HOH:O	2.05	0.74
1:H:100(A):SER:HB3	1:H:100(D):TYR:HD2	1.49	0.74
2:L:167:ASP:OD1	2:L:169:LYS:HG2	1.89	0.72
2:L:149:LYS:NZ	2:L:152:ASN:O	2.22	0.67
2:L:151:ASP:HA	2:L:191:VAL:HG13	1.79	0.62
1:H:138:LEU:HD13	1:H:211:VAL:HG21	1.81	0.62
2:L:151:ASP:OD2	2:L:189:HIS:ND1	2.33	0.61
2:L:105:GLU:HG3	3:L:388:HOH:O	1.99	0.61
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.83	0.60
1:H:163:VAL:HG13	3:H:435:HOH:O	2.00	0.60
1:H:181:VAL:HG11	2:L:135:LEU:HD22	1.82	0.59
1:H:100(A):SER:HB3	1:H:100(D):TYR:CD2	2.36	0.58
1:H:165:THR:N	3:H:434:HOH:O	2.03	0.57
2:L:116:PHE:HD2	2:L:135:LEU:HD23	1.70	0.56
1:H:142:VAL:HG11	1:H:150:VAL:HG11	1.90	0.53
2:L:198:HIS:CD2	3:L:415:HOH:O	2.61	0.53
2:L:113:PRO:HB3	2:L:139:PHE:CD2	2.45	0.52
1:H:119:PRO:HB3	1:H:145:TYR:HB3	1.92	0.51
1:H:139:GLY:HA2	1:H:154:TRP:CH2	2.46	0.51
1:H:184:VAL:HG22	1:H:185:PRO:HD2	1.92	0.51
2:L:140:TYR:HA	3:L:407:HOH:O	2.11	0.51
1:H:137:ALA:HB2	1:H:183:THR:HG22	1.92	0.51
1:H:137:ALA:N	3:H:433:HOH:O	2.44	0.51
1:H:160:THR:O	1:H:163:VAL:HG22	2.11	0.51
1:H:129:LYS:HE2	2:L:208:SER:O	2.10	0.51
2:L:55:GLU:O	2:L:58:VAL:HG22	2.11	0.51
1:H:186:SER:HA	1:H:189:LEU:HD13	1.92	0.50
1:H:152:VAL:HG22	3:H:432:HOH:O	2.11	0.50
1:H:196:CYS:N	3:H:431:HOH:O	2.45	0.49
2:L:140:TYR:CG	2:L:141:PRO:HA	2.47	0.49
2:L:142:ARG:NH2	2:L:163:VAL:HG11	2.28	0.49
2:L:83:VAL:HG11	2:L:166:GLN:HB3	1.95	0.48
1:H:169:VAL:HA	3:H:364:HOH:O	2.14	0.48
2:L:198:HIS:H	2:L:201:LEU:HD11	1.78	0.48
1:H:97:ALA:C	1:H:99:VAL:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:108:ARG:HH12	2:L:111:ALA:HB2	1.79	0.47
2:L:55:GLU:HG2	3:L:387:HOH:O	2.15	0.46
1:H:127:SER:N	1:H:130:SER:OG	2.42	0.45
2:L:140:TYR:CD1	2:L:141:PRO:HA	2.51	0.45
2:L:142:ARG:CZ	2:L:163:VAL:HG21	2.47	0.44
2:L:40:PRO:HB3	2:L:165:GLU:HG3	1.99	0.43
2:L:195:GLU:HA	2:L:206:THR:HA	2.00	0.43
2:L:165:GLU:OE1	3:L:395:HOH:O	2.21	0.42
2:L:197:THR:HG22	2:L:204:PRO:HB3	2.00	0.42
2:L:134:CYS:HB3	2:L:177:SER:OG	2.20	0.42
2:L:190:LYS:NZ	2:L:210:ASN:CG	2.73	0.42
2:L:190:LYS:NZ	2:L:210:ASN:HB3	2.35	0.41
2:L:190:LYS:HZ3	2:L:210:ASN:CG	2.23	0.41
2:L:145:LYS:HB2	3:L:390:HOH:O	2.21	0.41
1:H:196:CYS:HB3	3:H:431:HOH:O	2.20	0.41
2:L:108:ARG:HB3	3:L:322:HOH:O	2.20	0.41
2:L:54:LEU:HG	2:L:58:VAL:CG2	2.51	0.41
2:L:143:GLU:OE1	2:L:143:GLU:N	2.49	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:49:TYR:OH	2:L:204:PRO:O[8_565]	2.01	0.19

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	225/231 (97%)	217 (96%)	7 (3%)	1 (0%)	34	15
2	L	209/214 (98%)	202 (97%)	6 (3%)	1 (0%)	29	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	434/445 (98%)	419 (96%)	13 (3%)	2 (0%)	29	11

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	97	ALA
2	L	30	VAL

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	192/196 (98%)	186 (97%)	6 (3%)	40	15
2	L	186/188 (99%)	182 (98%)	4 (2%)	52	27
All	All	378/384 (98%)	368 (97%)	10 (3%)	44	21

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	83	ARG
1	H	135	THR
1	H	178	LEU
1	H	184	VAL
1	H	193	THR
1	H	212	GLU
2	L	108	ARG
2	L	145	LYS
2	L	181	LEU
2	L	195	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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	H	226/231 (97%)	1.31	61 (26%)	0	0	17, 32, 135, 157	0
2	L	211/214 (98%)	1.64	75 (35%)	0	0	18, 50, 94, 102	0
All	All	437/445 (98%)	1.47	136 (31%)	0	0	17, 42, 115, 157	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	100	VAL	10.5
2	L	116	PHE	9.5
1	H	138	LEU	9.1
2	L	153	ALA	9.0
1	H	191	THR	8.9
2	L	196	VAL	8.3
1	H	190	GLY	8.2
2	L	200	GLY	7.7
2	L	193	ALA	7.6
2	L	186	TYR	7.6
1	H	126	PRO	7.5
2	L	146	VAL	7.3
1	H	195	ILE	7.3
1	H	161	SER	7.3
1	H	128	SER	7.2
2	L	142	ARG	7.2
2	L	134	CYS	7.0
1	H	181	VAL	6.9
1	H	157	GLY	6.9
1	H	158	ALA	6.8
1	H	124	LEU	6.6
1	H	211	VAL	6.5
1	H	163	VAL	6.5
1	H	131	THR	6.4

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Mol	Chain	Res	Type	RSRZ
2	L	194	CYS	6.1
2	L	184	ALA	6.1
2	L	127	SER	6.0
1	H	166	PHE	5.8
1	H	132	SER	5.7
2	L	152	ASN	5.7
1	H	206	LYS	5.7
2	L	117	ILE	5.6
2	L	147	GLN	5.5
2	L	181	LEU	5.5
1	H	99	VAL	5.4
2	L	126	LYS	5.3
1	H	133	GLY	5.3
1	H	197	ASN	5.2
2	L	175	LEU	5.2
1	H	134	GLY	5.2
1	H	122	PHE	5.2
1	H	137	ALA	5.0
2	L	133	VAL	5.0
1	H	98	LEU	4.7
2	L	197	THR	4.7
1	H	125	ALA	4.7
2	L	136	LEU	4.7
2	L	192	TYR	4.4
1	H	198	VAL	4.4
1	H	160	THR	4.3
2	L	205	VAL	4.3
1	H	193	THR	4.3
2	L	157	GLY	4.3
1	H	172	SER	4.2
1	H	204	ASN	4.2
1	H	129	LYS	4.2
1	H	178	LEU	4.2
2	L	118	PHE	4.2
1	H	152	VAL	4.2
1	H	187	SER	4.2
2	L	122	ASP	4.1
2	L	179	LEU	4.1
2	L	148	TRP	4.0
2	L	115	VAL	4.0
2	L	198	HIS	4.0
2	L	178	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	H	156	SER	4.0
2	L	169	LYS	4.0
1	H	212	GLU	4.0
2	L	183	LYS	3.9
2	L	151	ASP	3.9
2	L	120	PRO	3.9
1	H	182	VAL	3.9
2	L	143	GLU	3.9
2	L	119	PRO	3.8
2	L	155	GLN	3.8
1	H	154	TRP	3.8
2	L	201	LEU	3.8
2	L	132	VAL	3.7
2	L	191	VAL	3.7
2	L	138	ASN	3.6
2	L	158	ASN	3.6
2	L	139	PHE	3.6
1	H	127	SER	3.5
2	L	206	THR	3.5
1	H	189	LEU	3.5
2	L	150	VAL	3.4
2	L	113	PRO	3.4
1	H	184	VAL	3.4
1	H	123	PRO	3.4
2	L	187	GLU	3.3
2	L	109	THR	3.3
2	L	130	ALA	3.3
2	L	144	ALA	3.2
2	L	182	SER	3.2
1	H	153	SER	3.2
2	L	111	ALA	3.2
2	L	125	LEU	3.2
1	H	194	TYR	3.2
2	L	112	ALA	3.1
1	H	185	PRO	3.1
1	H	207	VAL	3.1
2	L	141	PRO	3.1
2	L	176	SER	3.0
2	L	135	LEU	3.0
2	L	149	LYS	2.9
2	L	204	PRO	2.9
2	L	110	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
2	L	195	GLU	2.7
1	H	210	LYS	2.7
2	L	177	SER	2.7
1	H	130	SER	2.6
1	H	139	GLY	2.6
1	H	208	ASP	2.6
1	H	100(B)	THR	2.6
1	H	100(A)	SER	2.6
1	H	159	LEU	2.6
2	L	156	SER	2.6
1	H	196	CYS	2.6
2	L	140	TYR	2.5
2	L	209	PHE	2.5
2	L	185	ASP	2.4
1	H	169	VAL	2.4
1	H	164	HIS	2.3
2	L	203	SER	2.3
1	H	141	LEU	2.2
2	L	40	PRO	2.2
2	L	211	ARG	2.2
1	H	100(D)	TYR	2.2
1	H	121	VAL	2.2
2	L	145	LYS	2.1
2	L	161	GLU	2.1
1	H	162	GLY	2.1
2	L	180	THR	2.1
2	L	154	LEU	2.0
2	L	124	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 monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.