



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:41 PM UTC

PDB ID : 6J5G / pdb_00006j5g
Title : Complex structure of MAb 4.2-scFv with tick-borne encephalitis virus envelope protein
Authors : Yang, X.; Qi, J.; Peng, R.; Dai, L.; Gould, E.A.; Tien, P.; Gao, G.F.
Deposited on : 2019-01-10
Resolution : 3.29 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

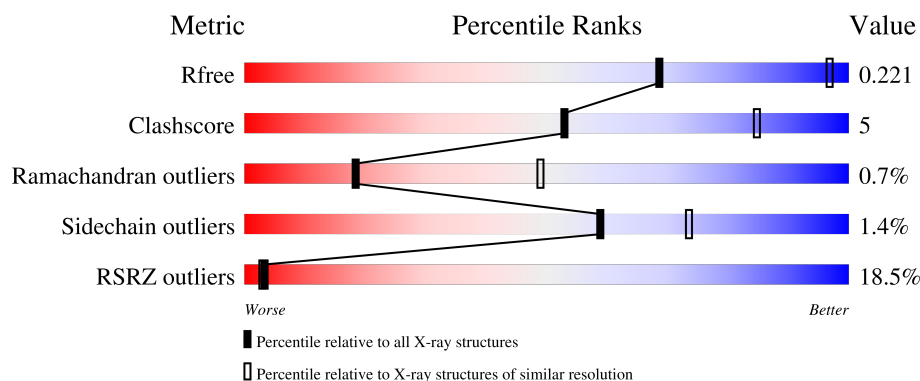
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.29 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	A	407	26% 84% 6% 8%
2	H	120	% 93% 6%
3	L	109	3% 82% 12% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4579 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 Envelope protein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2819	1765	501	533	20			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	402	HIS	-	expression tag	UNP P14336
A	403	HIS	-	expression tag	UNP P14336
A	404	HIS	-	expression tag	UNP P14336
A	405	HIS	-	expression tag	UNP P14336
A	406	HIS	-	expression tag	UNP P14336
A	407	HIS	-	expression tag	UNP P14336

- Molecule 2 is a protein called antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	120	Total	C	N	O	S	0	0	0
			926	586	147	189	4			

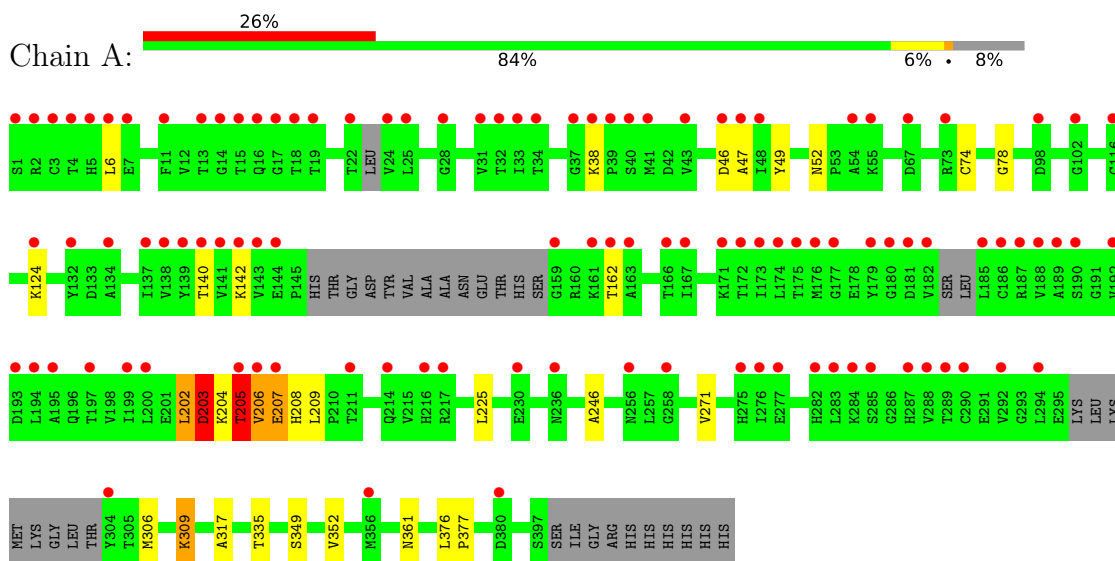
- Molecule 3 is a protein called antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	108	Total	C	N	O	S	0	0	0
			834	530	139	163	2			

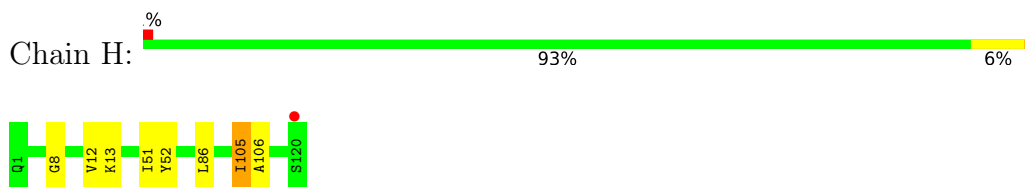
3 Residue-property plots [i](#)

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.

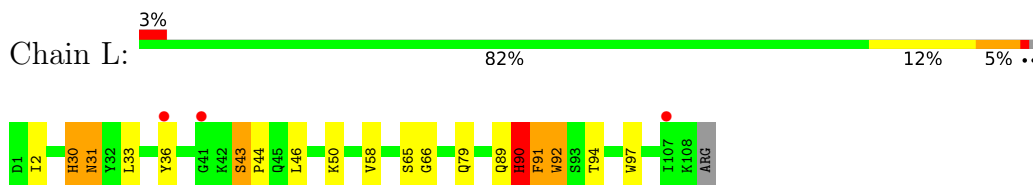
- Molecule 1: Envelope protein E



- Molecule 2: antibody heavy chain



- Molecule 3: antibody 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	135.73Å 100.69Å 140.24Å 90.00° 100.25° 90.00°	Depositor
Resolution (Å)	46.00 – 3.29 46.00 – 3.29	Depositor EDS
% Data completeness (in resolution range)	80.1 (46.00-3.29) 80.1 (46.00-3.29)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 3.32Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.208 , 0.222 0.208 , 0.221	Depositor DCC
R_{free} test set	1136 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å ²)	65.8	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 86.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4579	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% 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	A	0.68	0/2879	1.06	29/3906 (0.7%)
2	H	0.79	0/947	1.12	8/1284 (0.6%)
3	L	0.91	0/857	1.18	11/1165 (0.9%)
All	All	0.75	0/4683	1.09	48/6355 (0.8%)

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	376	LEU	CA-C-N	9.96	126.83	119.66
1	A	376	LEU	C-N-CA	9.96	126.83	119.66
2	H	8	GLY	CA-C-N	8.33	128.27	119.85
2	H	8	GLY	C-N-CA	8.33	128.27	119.85
1	A	52	ASN	CA-C-N	8.27	128.22	120.03
1	A	52	ASN	C-N-CA	8.27	128.22	120.03
3	L	58	VAL	CA-C-N	8.03	128.03	119.76
3	L	58	VAL	C-N-CA	8.03	128.03	119.76
1	A	271	VAL	CA-C-N	7.86	127.88	119.78
1	A	271	VAL	C-N-CA	7.86	127.88	119.78
3	L	43	SER	CA-C-N	7.47	127.52	119.90
3	L	43	SER	C-N-CA	7.47	127.52	119.90
2	H	52	TYR	CA-C-N	7.46	127.17	119.56
2	H	52	TYR	C-N-CA	7.46	127.17	119.56
2	H	13	LYS	CA-C-N	7.17	127.21	119.90
2	H	13	LYS	C-N-CA	7.17	127.21	119.90
1	A	38	LYS	CA-C-N	7.12	127.29	120.31
1	A	38	LYS	C-N-CA	7.12	127.29	120.31
1	A	349	SER	CA-C-N	7.04	129.17	121.00
1	A	349	SER	C-N-CA	7.04	129.17	121.00
1	A	246	ALA	CA-C-N	6.96	127.21	119.90
1	A	246	ALA	C-N-CA	6.96	127.21	119.90
1	A	74	CYS	CA-C-N	6.54	128.02	119.84
1	A	74	CYS	C-N-CA	6.54	128.02	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	92	TRP	N-CA-C	6.41	119.69	109.24
1	A	377	PRO	CA-C-N	6.34	126.72	119.93
1	A	377	PRO	C-N-CA	6.34	126.72	119.93
3	L	94	THR	CA-C-N	6.17	126.73	120.38
3	L	94	THR	C-N-CA	6.17	126.73	120.38
2	H	105	ILE	CB-CA-C	-6.16	103.92	112.36
1	A	225	LEU	CA-C-N	6.06	126.00	119.76
1	A	225	LEU	C-N-CA	6.06	126.00	119.76
3	L	90	HIS	N-CA-C	6.05	119.40	108.69
1	A	209	LEU	CA-C-N	-5.76	114.02	119.90
1	A	209	LEU	C-N-CA	-5.76	114.02	119.90
1	A	361	ASN	CA-C-N	5.72	127.00	119.84
1	A	361	ASN	C-N-CA	5.72	127.00	119.84
1	A	317	ALA	CA-C-N	5.62	126.87	119.84
1	A	317	ALA	C-N-CA	5.62	126.87	119.84
1	A	78	GLY	CA-C-N	5.56	127.51	120.51
1	A	78	GLY	C-N-CA	5.56	127.51	120.51
1	A	203	ASP	N-CA-C	-5.41	103.48	110.19
2	H	105	ILE	N-CA-C	5.33	117.53	111.88
1	A	49	TYR	N-CA-C	5.19	116.18	108.60
3	L	79	GLN	CA-C-N	5.13	124.92	119.28
3	L	79	GLN	C-N-CA	5.13	124.92	119.28
1	A	352	VAL	N-CA-C	5.05	115.12	107.80
3	L	91	PHE	N-CA-C	5.02	118.43	111.55

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	A	2819	0	2718	19	0
2	H	926	0	883	6	0
3	L	834	0	802	24	0
All	All	4579	0	4403	45	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 5.

All (45) 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:106:ALA:HA	3:L:91:PHE:CE1	2.08	0.88
1:A:124:LYS:HA	1:A:203:ASP:CG	2.00	0.87
3:L:2:ILE:HG21	3:L:90:HIS:CD2	2.11	0.85
1:A:142:LYS:HE2	1:A:162:THR:OG1	1.78	0.83
2:H:106:ALA:HA	3:L:91:PHE:HE1	1.43	0.81
1:A:124:LYS:HA	1:A:203:ASP:OD2	1.85	0.75
3:L:90:HIS:ND1	3:L:90:HIS:O	2.21	0.74
3:L:33:LEU:C	3:L:33:LEU:HD23	2.14	0.72
3:L:2:ILE:HB	3:L:90:HIS:NE2	2.07	0.69
1:A:206:VAL:O	1:A:208:HIS:N	2.26	0.69
3:L:36:TYR:CE2	3:L:46:LEU:HD13	2.28	0.68
1:A:205:THR:O	1:A:207:GLU:N	2.27	0.67
1:A:204:LYS:O	1:A:205:THR:HG23	1.96	0.66
1:A:202:LEU:HD23	1:A:202:LEU:N	2.13	0.63
3:L:31:ASN:HD22	3:L:31:ASN:N	1.97	0.62
3:L:2:ILE:CB	3:L:90:HIS:NE2	2.65	0.59
3:L:2:ILE:CG2	3:L:90:HIS:CD2	2.85	0.58
3:L:33:LEU:HD23	3:L:33:LEU:O	2.05	0.56
2:H:105:ILE:C	3:L:91:PHE:CD1	2.83	0.56
1:A:335:THR:O	1:A:335:THR:HG23	2.06	0.55
2:H:106:ALA:CA	3:L:91:PHE:CE1	2.85	0.54
3:L:30:HIS:O	3:L:31:ASN:HB2	2.10	0.52
1:A:124:LYS:O	1:A:203:ASP:HB2	2.09	0.52
3:L:90:HIS:ND1	3:L:90:HIS:C	2.68	0.52
3:L:30:HIS:C	3:L:31:ASN:HD22	2.20	0.49
1:A:47:ALA:HB3	1:A:140:THR:HG22	1.97	0.47
3:L:90:HIS:O	3:L:90:HIS:CG	2.67	0.46
3:L:89:GLN:HG2	3:L:90:HIS:N	2.31	0.46
1:A:46:ASP:HB3	1:A:140:THR:HG23	1.97	0.46
1:A:6:LEU:HD23	1:A:6:LEU:N	2.30	0.46
3:L:90:HIS:HD1	3:L:92:TRP:H	1.65	0.45
1:A:205:THR:O	1:A:206:VAL:C	2.59	0.45
1:A:140:THR:HG23	1:A:140:THR:O	2.16	0.45
1:A:47:ALA:HB3	1:A:140:THR:CG2	2.47	0.45
1:A:124:LYS:HD3	1:A:203:ASP:OD2	2.18	0.44
3:L:90:HIS:C	3:L:90:HIS:HD1	2.25	0.44
3:L:31:ASN:N	3:L:31:ASN:ND2	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LEU:N	1:A:202:LEU:CD2	2.82	0.42
1:A:309:LYS:H	1:A:309:LYS:HG2	1.69	0.42
3:L:91:PHE:HA	3:L:97:TRP:CE3	2.55	0.42
2:H:51:ILE:O	2:H:51:ILE:HG23	2.21	0.41
3:L:43:SER:HA	3:L:44:PRO:HD3	1.97	0.41
3:L:65:SER:OG	3:L:66:GLY:N	2.53	0.41
1:A:306:MET:HE3	1:A:306:MET:HB2	1.72	0.40
2:H:12:VAL:HG21	2:H:86:LEU:HD12	2.03	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	363/407 (89%)	338 (93%)	22 (6%)	3 (1%)	16	45
2	H	118/120 (98%)	111 (94%)	7 (6%)	0	100	100
3	L	106/109 (97%)	97 (92%)	8 (8%)	1 (1%)	14	43
All	All	587/636 (92%)	546 (93%)	37 (6%)	4 (1%)	18	49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	205	THR
1	A	206	VAL
1	A	207	GLU
3	L	30	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	A	296/337 (88%)	292 (99%)	4 (1%)	59	73
2	H	99/99 (100%)	99 (100%)	0	100	100
3	L	91/92 (99%)	88 (97%)	3 (3%)	33	59
All	All	486/528 (92%)	479 (99%)	7 (1%)	59	73

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	202	LEU
1	A	203	ASP
1	A	205	THR
1	A	309	LYS
3	L	31	ASN
3	L	50	LYS
3	L	90	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	39	GLN
2	H	77	ASN
3	L	30	HIS
3	L	31	ASN
3	L	38	GLN

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 [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	A	373/407 (91%)	1.40	107 (28%) 1 1	30, 138, 230, 282	0
2	H	120/120 (100%)	-0.06	1 (0%) 82 68	26, 45, 74, 92	0
3	L	108/109 (99%)	-0.09	3 (2%) 55 36	27, 43, 84, 113	0
All	All	601/636 (94%)	0.84	111 (18%) 3 3	26, 83, 221, 282	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	24	VAL	8.3
1	A	5	HIS	7.4
1	A	290	CYS	6.7
1	A	206	VAL	6.4
1	A	159	GLY	6.4
1	A	192	VAL	6.4
1	A	186	CYS	5.9
1	A	188	VAL	5.6
1	A	189	ALA	5.6
1	A	141	VAL	5.4
1	A	4	THR	5.1
1	A	16	GLN	5.0
1	A	172	THR	5.0
1	A	34	THR	5.0
1	A	137	ILE	4.8
1	A	15	THR	4.8
1	A	1	SER	4.6
1	A	173	ILE	4.5
1	A	161	LYS	4.4
1	A	140	THR	4.4
1	A	258	GLY	4.2
1	A	187	ARG	4.1
1	A	28	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	185	LEU	4.0
1	A	285	SER	4.0
1	A	134	ALA	4.0
1	A	11	PHE	3.9
1	A	124	LYS	3.8
1	A	171	LYS	3.8
1	A	22	THR	3.8
1	A	214	GLN	3.7
1	A	289	THR	3.7
1	A	31	VAL	3.7
1	A	47	ALA	3.7
1	A	190	SER	3.6
1	A	356	MET	3.6
1	A	25	LEU	3.6
1	A	177	GLY	3.6
1	A	139	TYR	3.6
1	A	163	ALA	3.5
1	A	38	LYS	3.5
1	A	6	LEU	3.5
1	A	276	ILE	3.4
1	A	236	ASN	3.4
1	A	284	LYS	3.4
1	A	40	SER	3.4
1	A	287	HIS	3.3
1	A	179	TYR	3.2
1	A	211	THR	3.2
1	A	18	THR	3.2
1	A	143	VAL	3.2
1	A	98	ASP	3.1
1	A	43	VAL	3.1
3	L	107	ILE	3.1
1	A	182	VAL	3.1
1	A	176	MET	3.1
1	A	181	ASP	3.1
1	A	193	ASP	3.1
1	A	132	TYR	3.0
1	A	283	LEU	3.0
1	A	282	HIS	3.0
1	A	216	HIS	2.9
1	A	67	ASP	2.9
1	A	73	ARG	2.9
1	A	39	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	41	MET	2.9
1	A	46	ASP	2.8
1	A	292	VAL	2.8
1	A	13	THR	2.8
1	A	380	ASP	2.8
1	A	2	ARG	2.8
1	A	54	ALA	2.8
3	L	36	TYR	2.7
1	A	256	ASN	2.7
1	A	167	ILE	2.7
1	A	162	THR	2.7
1	A	14	GLY	2.7
1	A	138	VAL	2.7
1	A	304	TYR	2.6
1	A	294	LEU	2.6
1	A	180	GLY	2.6
1	A	207	GLU	2.6
1	A	116	CYS	2.6
1	A	37	GLY	2.6
1	A	230	GLU	2.6
1	A	275	HIS	2.5
1	A	199	ILE	2.5
1	A	174	LEU	2.5
2	H	120	SER	2.5
1	A	48	ILE	2.5
1	A	277	GLU	2.5
1	A	166	THR	2.5
1	A	200	LEU	2.4
1	A	144	GLU	2.4
1	A	32	THR	2.4
1	A	175	THR	2.4
1	A	55	LYS	2.4
1	A	33	ILE	2.3
1	A	197	THR	2.3
1	A	194	LEU	2.3
1	A	142	LYS	2.2
1	A	17	GLY	2.2
1	A	7	GLU	2.2
1	A	19	THR	2.2
1	A	102	GLY	2.2
1	A	3	CYS	2.2
3	L	41	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	288	VAL	2.1
1	A	195	ALA	2.1
1	A	217	ARG	2.0
1	A	205	THR	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.