



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 7, 2025 – 10:11 AM JST

PDB ID : 8ZH7 / pdb\_00008zh7  
Title : Crystal structure of N-terminal domain of N-methyl-D-aspartate receptor subunit NR1 in complex with patient-derived antibody  
Authors : Nomura, N.; Kumazaki, K.; Amano, Y.  
Deposited on : 2024-05-10  
Resolution : 3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0rc1  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

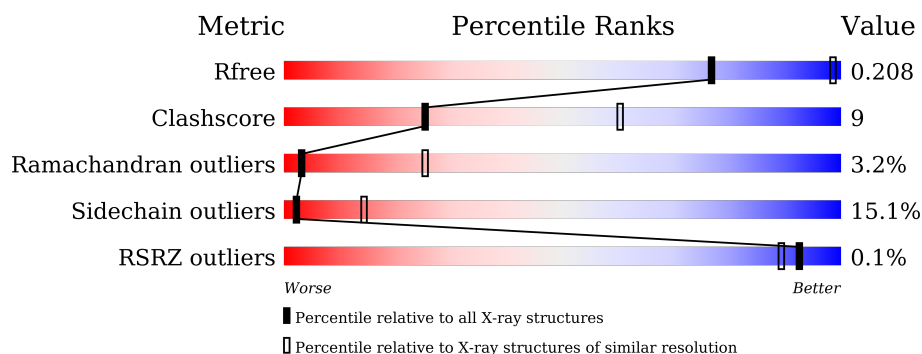
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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))
$R_{free}$	164625	1094 (3.56-3.44)
Clashscore	180529	1045 (3.54-3.46)
Ramachandran outliers	177936	1032 (3.54-3.46)
Sidechain outliers	177891	1033 (3.54-3.46)
RSRZ outliers	164620	1093 (3.56-3.44)

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  $\geq 3$ , 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	384	
1	D	384	
1	G	384	
1	J	384	
2	B	250	
2	E	250	

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Mol	Chain	Length	Quality of chain
2	H	250	 60% 24% • 14%
2	K	250	 63% 21% • 14%
3	C	236	 55% 31% • • 10%
3	F	236	 61% 25% 5% 10%
3	I	236	 64% 24% • 10%
3	L	236	 69% 20% • 10%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24484 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 Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	0	0
			2915	1841	518	544	12			
1	D	371	Total	C	N	O	S	0	0	0
			2915	1841	518	544	12			
1	G	371	Total	C	N	O	S	0	0	0
			2915	1841	518	544	12			
1	J	371	Total	C	N	O	S	0	0	0
			2915	1841	518	544	12			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	394	VAL	-	expression tag	UNP Q05586
A	395	ASP	-	expression tag	UNP Q05586
A	396	GLY	-	expression tag	UNP Q05586
A	397	GLY	-	expression tag	UNP Q05586
A	398	GLY	-	expression tag	UNP Q05586
A	399	GLY	-	expression tag	UNP Q05586
A	400	GLY	-	expression tag	UNP Q05586
A	401	LEU	-	expression tag	UNP Q05586
A	402	VAL	-	expression tag	UNP Q05586
A	403	PRO	-	expression tag	UNP Q05586
A	404	ARG	-	expression tag	UNP Q05586
D	394	VAL	-	expression tag	UNP Q05586
D	395	ASP	-	expression tag	UNP Q05586
D	396	GLY	-	expression tag	UNP Q05586
D	397	GLY	-	expression tag	UNP Q05586
D	398	GLY	-	expression tag	UNP Q05586
D	399	GLY	-	expression tag	UNP Q05586
D	400	GLY	-	expression tag	UNP Q05586
D	401	LEU	-	expression tag	UNP Q05586
D	402	VAL	-	expression tag	UNP Q05586
D	403	PRO	-	expression tag	UNP Q05586

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Chain	Residue	Modelled	Actual	Comment	Reference
D	404	ARG	-	expression tag	UNP Q05586
G	394	VAL	-	expression tag	UNP Q05586
G	395	ASP	-	expression tag	UNP Q05586
G	396	GLY	-	expression tag	UNP Q05586
G	397	GLY	-	expression tag	UNP Q05586
G	398	GLY	-	expression tag	UNP Q05586
G	399	GLY	-	expression tag	UNP Q05586
G	400	GLY	-	expression tag	UNP Q05586
G	401	LEU	-	expression tag	UNP Q05586
G	402	VAL	-	expression tag	UNP Q05586
G	403	PRO	-	expression tag	UNP Q05586
G	404	ARG	-	expression tag	UNP Q05586
J	394	VAL	-	expression tag	UNP Q05586
J	395	ASP	-	expression tag	UNP Q05586
J	396	GLY	-	expression tag	UNP Q05586
J	397	GLY	-	expression tag	UNP Q05586
J	398	GLY	-	expression tag	UNP Q05586
J	399	GLY	-	expression tag	UNP Q05586
J	400	GLY	-	expression tag	UNP Q05586
J	401	LEU	-	expression tag	UNP Q05586
J	402	VAL	-	expression tag	UNP Q05586
J	403	PRO	-	expression tag	UNP Q05586
J	404	ARG	-	expression tag	UNP Q05586

- Molecule 2 is a protein called Antibody #003-102 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	216	Total	C	N	O	S	0	0	0
			1603	1015	269	315	4			
2	E	216	Total	C	N	O	S	0	0	0
			1603	1015	269	315	4			
2	H	216	Total	C	N	O	S	0	0	0
			1603	1015	269	315	4			
2	K	216	Total	C	N	O	S	0	0	0
			1603	1015	269	315	4			

- Molecule 3 is a protein called Antibody #003-102 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	213	Total	C	N	O	S	0	0	0
			1603	996	268	334	5			

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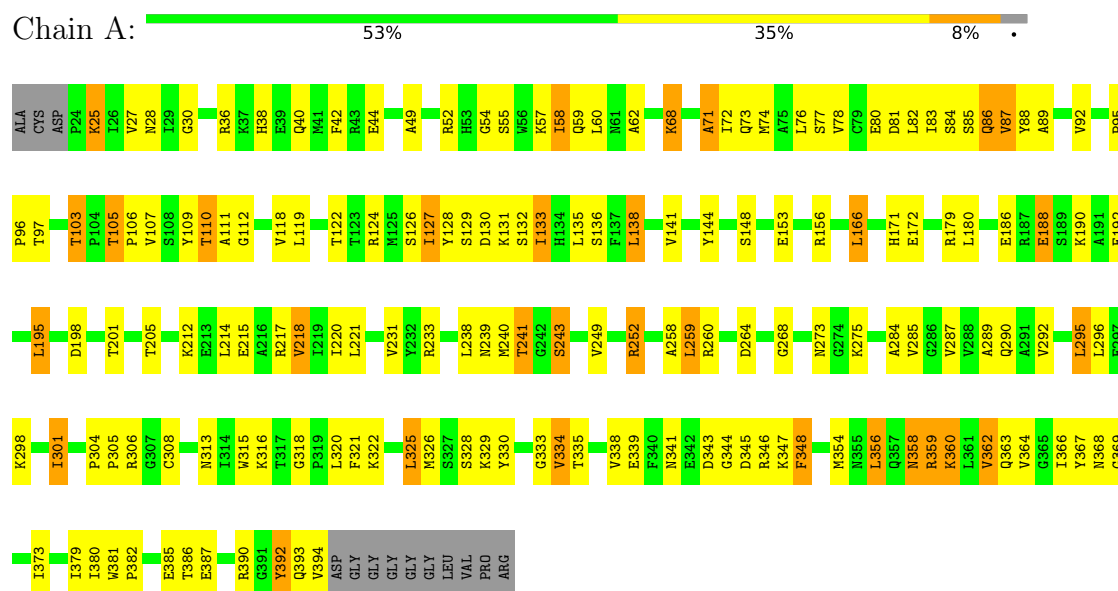
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	213	Total	C	N	O	S	0	0	0
			1603	996	268	334	5			
3	I	213	Total	C	N	O	S	0	0	0
			1603	996	268	334	5			
3	L	213	Total	C	N	O	S	0	0	0
			1603	996	268	334	5			

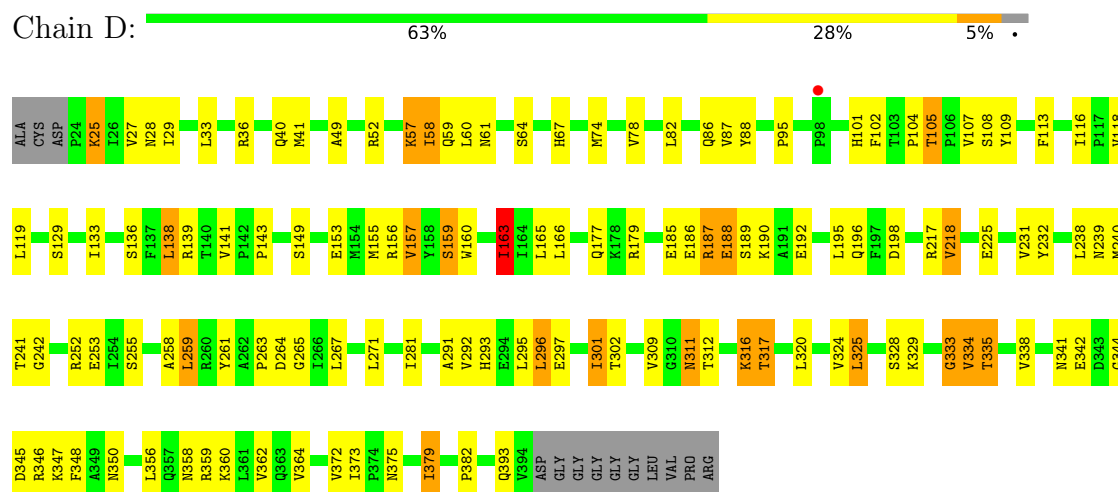
### 3 Residue-property plots

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: Glutamate receptor ionotropic, NMDA 1

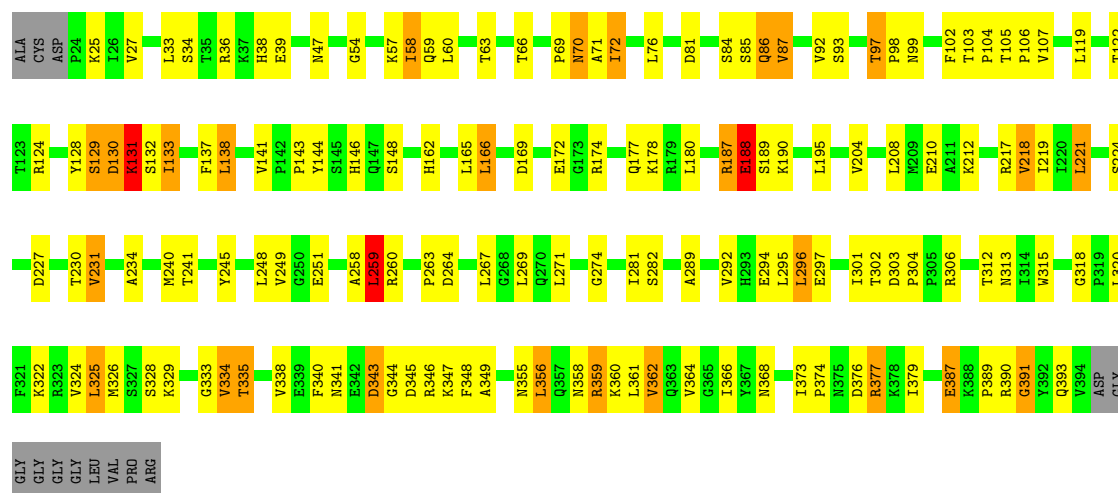


- Molecule 1: Glutamate receptor ionotropic, NMDA 1



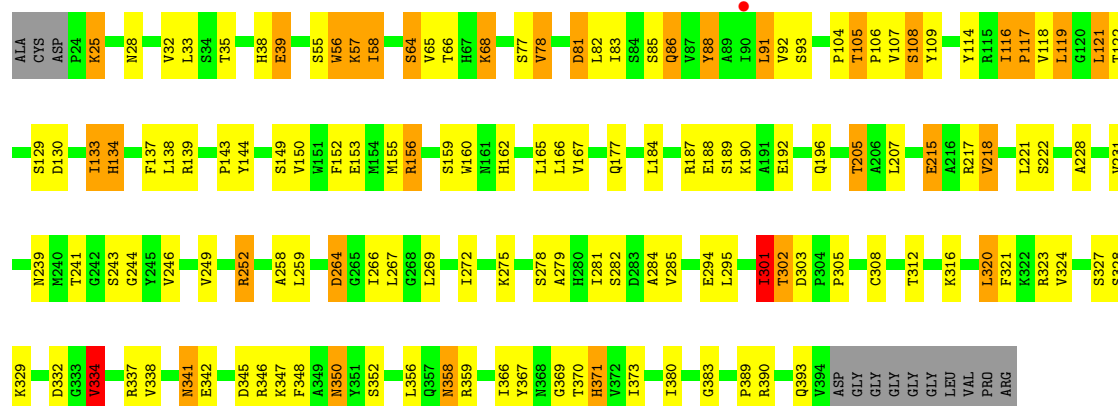
- Molecule 1: Glutamate receptor ionotropic, NMDA 1

Chain G:  57% 32% 7% ..



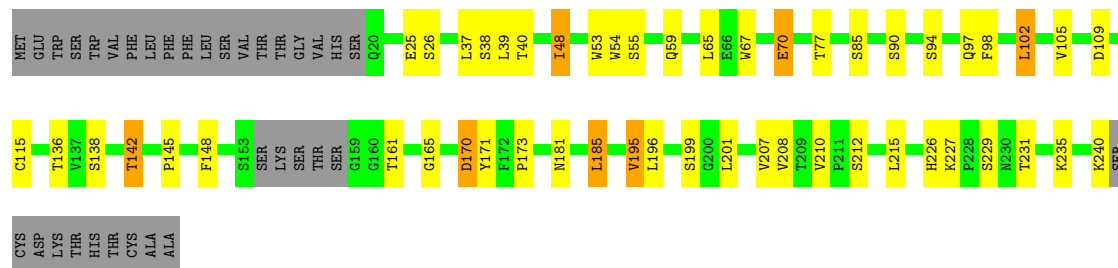
- Molecule 1: Glutamate receptor ionotropic, NMDA 1

Chain J:  60% 28% 8% ..



- Molecule 2: Antibody #003-102 heavy chain

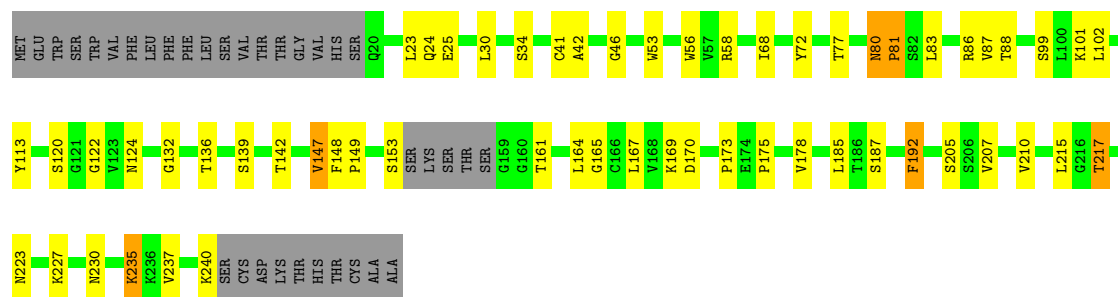
Chain B:  66% 18% 14% ..



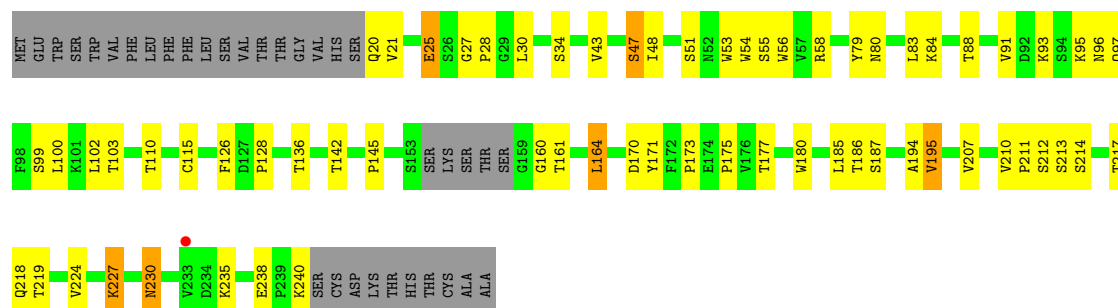
- Molecule 2: Antibody #003-102 heavy chain

Chain E:  63% 21% 14% ..

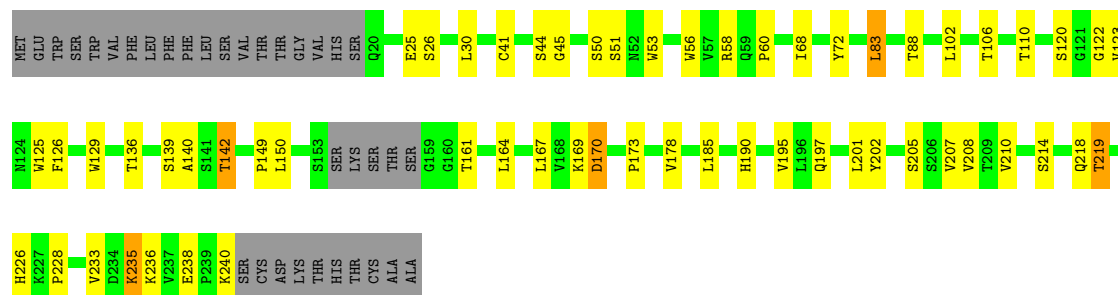




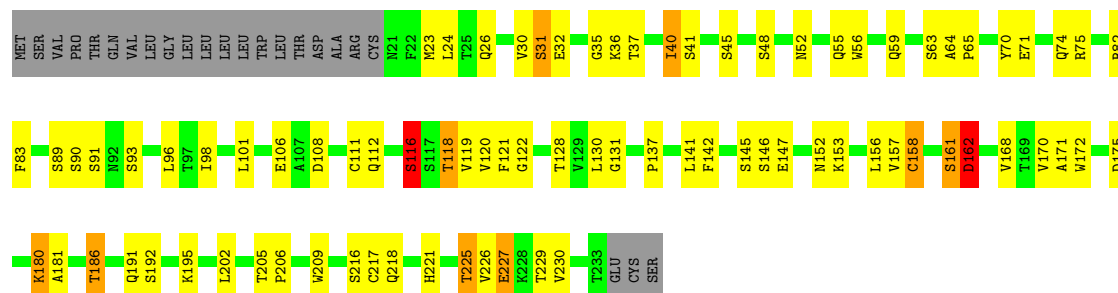
• Molecule 2: Antibody #003-102 heavy chain



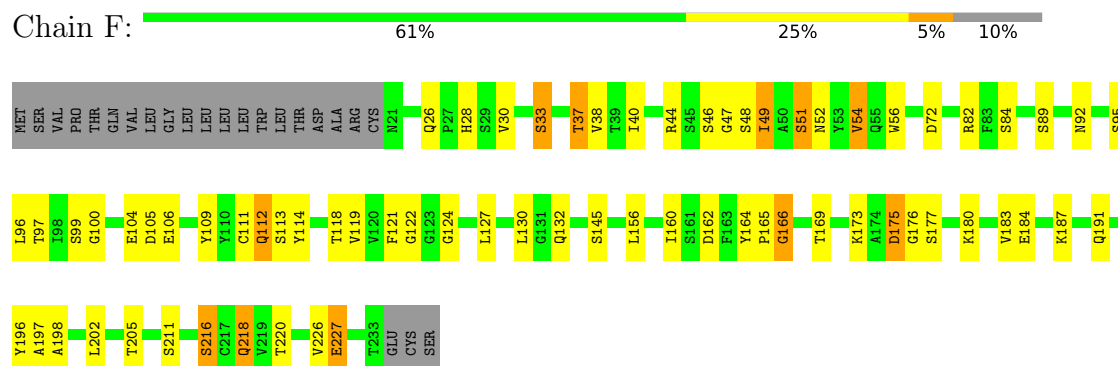
• Molecule 2: Antibody #003-102 heavy chain



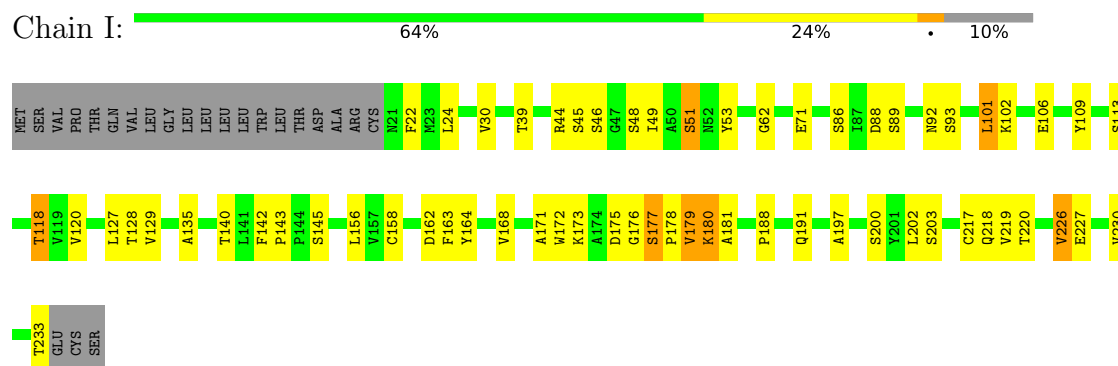
• Molecule 3: Antibody #003-102 light chain



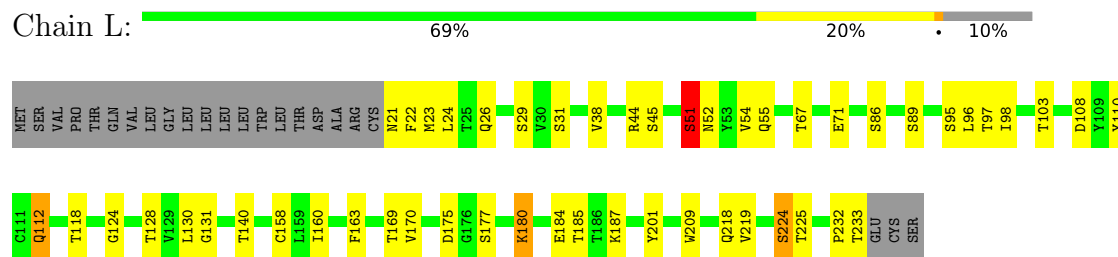
- Molecule 3: Antibody #003-102 light chain



- Molecule 3: Antibody #003-102 light chain



- Molecule 3: Antibody #003-102 light chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	287.01Å 287.01Å 53.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.71 – 3.50 49.71 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.71-3.50) 99.9 (49.71-3.50)	Depositor EDS
$R_{merge}$	0.27	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.14 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.186 , 0.227 0.170 , 0.208	Depositor DCC
$R_{free}$ test set	3158 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	120.4	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 74.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.032 for -h,-k,l 0.024 for h,-h-k,-l 0.017 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	24484	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	132.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.83	0/2978	1.14	7/4040 (0.2%)
1	D	0.80	0/2978	1.14	13/4040 (0.3%)
1	G	0.80	0/2978	1.13	6/4040 (0.1%)
1	J	0.89	0/2978	1.18	12/4040 (0.3%)
2	B	0.82	0/1645	1.06	3/2250 (0.1%)
2	E	0.85	0/1645	1.14	9/2250 (0.4%)
2	H	0.91	0/1645	1.19	13/2250 (0.6%)
2	K	0.83	1/1645 (0.1%)	1.00	1/2250 (0.0%)
3	C	0.84	0/1641	1.13	6/2240 (0.3%)
3	F	0.89	0/1641	1.08	4/2240 (0.2%)
3	I	0.86	0/1641	1.10	5/2240 (0.2%)
3	L	0.82	0/1641	1.06	2/2240 (0.1%)
All	All	0.84	1/25056 (0.0%)	1.12	81/34120 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	G	0	1
3	C	0	1
3	I	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	60	PRO	CA-C	5.74	1.55	1.51

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	64	ALA	CA-C-N	8.84	130.89	119.84
3	C	64	ALA	C-N-CA	8.84	130.89	119.84
2	H	177	THR	N-CA-C	8.25	122.10	108.49
1	D	350	ASN	N-CA-C	8.04	121.28	110.35
1	A	344	GLY	N-CA-C	-7.79	101.70	112.13

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	186	THR	Peptide
1	D	333	GLY	Peptide
1	G	391	GLY	Peptide
3	I	143	PRO	Peptide

## 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	2915	0	2914	75	0
1	D	2915	0	2914	57	0
1	G	2915	0	2914	73	0
1	J	2915	0	2914	77	0
2	B	1603	0	1574	23	0
2	E	1603	0	1574	23	0
2	H	1603	0	1574	18	0
2	K	1603	0	1574	19	0
3	C	1603	0	1540	41	0
3	F	1603	0	1540	32	0
3	I	1603	0	1540	27	0
3	L	1603	0	1540	19	0
All	All	24484	0	24112	460	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 9.

The worst 5 of 460 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:D:138:LEU:HA	1:D:345:ASP:OD1	1.73	0.87
1:A:138:LEU:HA	1:A:345:ASP:OD1	1.75	0.85
3:I:171:ALA:HB3	3:I:218:GLN:HB3	1.58	0.85
1:D:143:PRO:HD3	1:D:346:ARG:HG2	1.60	0.83
3:F:173:LYS:HB2	3:F:216:SER:HB2	1.66	0.76

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	A	369/384 (96%)	288 (78%)	64 (17%)	17 (5%)	2	18
1	D	369/384 (96%)	313 (85%)	49 (13%)	7 (2%)	6	34
1	G	369/384 (96%)	295 (80%)	54 (15%)	20 (5%)	1	14
1	J	369/384 (96%)	298 (81%)	56 (15%)	15 (4%)	2	20
2	B	212/250 (85%)	191 (90%)	20 (9%)	1 (0%)	25	59
2	E	212/250 (85%)	182 (86%)	23 (11%)	7 (3%)	3	25
2	H	212/250 (85%)	171 (81%)	34 (16%)	7 (3%)	3	25
2	K	212/250 (85%)	183 (86%)	26 (12%)	3 (1%)	9	40
3	C	211/236 (89%)	183 (87%)	21 (10%)	7 (3%)	3	25
3	F	211/236 (89%)	185 (88%)	20 (10%)	6 (3%)	4	27
3	I	211/236 (89%)	178 (84%)	28 (13%)	5 (2%)	5	30
3	L	211/236 (89%)	185 (88%)	21 (10%)	5 (2%)	5	30
All	All	3168/3480 (91%)	2652 (84%)	416 (13%)	100 (3%)	3	25

5 of 100 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	GLN

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Mol	Chain	Res	Type
1	A	393	GLN
3	C	116	SER
3	C	162	ASP
1	D	188	GLU

### 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	318/325 (98%)	255 (80%)	63 (20%)	1	6
1	D	318/325 (98%)	263 (83%)	55 (17%)	1	9
1	G	318/325 (98%)	251 (79%)	67 (21%)	1	5
1	J	318/325 (98%)	264 (83%)	54 (17%)	1	10
2	B	184/215 (86%)	162 (88%)	22 (12%)	4	20
2	E	184/215 (86%)	167 (91%)	17 (9%)	7	29
2	H	184/215 (86%)	162 (88%)	22 (12%)	4	20
2	K	184/215 (86%)	157 (85%)	27 (15%)	2	15
3	C	185/206 (90%)	160 (86%)	25 (14%)	3	18
3	F	185/206 (90%)	164 (89%)	21 (11%)	4	22
3	I	185/206 (90%)	167 (90%)	18 (10%)	6	27
3	L	185/206 (90%)	162 (88%)	23 (12%)	4	20
All	All	2748/2984 (92%)	2334 (85%)	414 (15%)	2	14

5 of 414 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	190	LYS
2	H	214	SER
3	L	96	LEU
1	G	230	THR
1	G	356	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	86	GLN
3	L	26	GLN
1	J	162	HIS
1	J	358	ASN
3	L	132	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	371/384 (96%)	-0.97	0 <span>100</span> <span>100</span>	77, 121, 155, 209	0
1	D	371/384 (96%)	-0.89	1 (0%) <span>90</span> <span>82</span>	82, 130, 186, 225	0
1	G	371/384 (96%)	-1.00	0 <span>100</span> <span>100</span>	81, 118, 149, 192	0
1	J	371/384 (96%)	-0.77	1 (0%) <span>90</span> <span>82</span>	71, 131, 185, 291	0
2	B	216/250 (86%)	-0.99	0 <span>100</span> <span>100</span>	90, 127, 155, 183	0
2	E	216/250 (86%)	-0.98	0 <span>100</span> <span>100</span>	100, 135, 165, 212	0
2	H	216/250 (86%)	-0.88	1 (0%) <span>87</span> <span>75</span>	103, 131, 170, 198	0
2	K	216/250 (86%)	-1.03	0 <span>100</span> <span>100</span>	93, 124, 149, 163	0
3	C	213/236 (90%)	-1.00	0 <span>100</span> <span>100</span>	96, 130, 157, 175	0
3	F	213/236 (90%)	-0.89	0 <span>100</span> <span>100</span>	105, 146, 181, 200	0
3	I	213/236 (90%)	-0.99	0 <span>100</span> <span>100</span>	97, 142, 173, 190	0
3	L	213/236 (90%)	-1.02	0 <span>100</span> <span>100</span>	94, 133, 160, 173	0
All	All	3200/3480 (91%)	-0.94	3 (0%) <span>92</span> <span>89</span>	71, 129, 169, 291	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	90	ILE	4.0
2	H	233	VAL	2.9
1	D	98	PRO	2.6

### 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 monosaccharides 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.