



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:54 PM UTC

PDB ID : 8RY2 / pdb_00008ry2
Title : Crystal Structure of ANV419, a novel IL-2/anti-IL-2 antibody fusion protein
Authors : Rondeau, J.M.; Wirth, E.
Deposited on : 2024-02-08
Resolution : 2.05 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

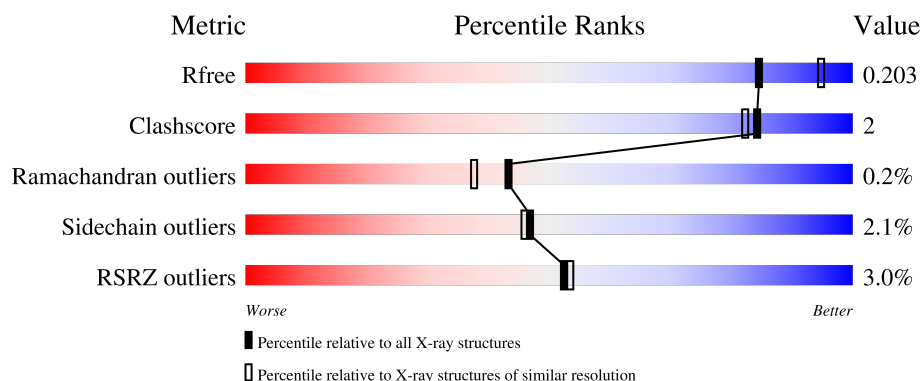
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	224	0% 90% 6% .
1	H	224	2% 87% 8% .
2	B	355	3% 89% 8% .
2	L	355	5% 89% 8% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9060 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 ANV419 heavy-chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1632	1041	267	317	7			
1	H	215	Total	C	N	O	S	0	0	0
			1623	1035	265	316	7			

- Molecule 2 is a protein called ANV419 light-chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	346	Total	C	N	O	S	0	0	0
			2694	1694	450	539	11			
2	L	346	Total	C	N	O	S	0	0	0
			2685	1690	444	539	12			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	116	Total	O	0	0
			116	116		
3	B	89	Total	O	0	0
			89	89		
3	H	128	Total	O	0	0
			128	128		
3	L	93	Total	O	0	0
			93	93		

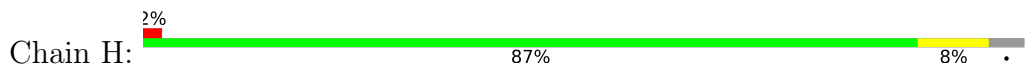
3 Residue-property plots [i](#)

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.

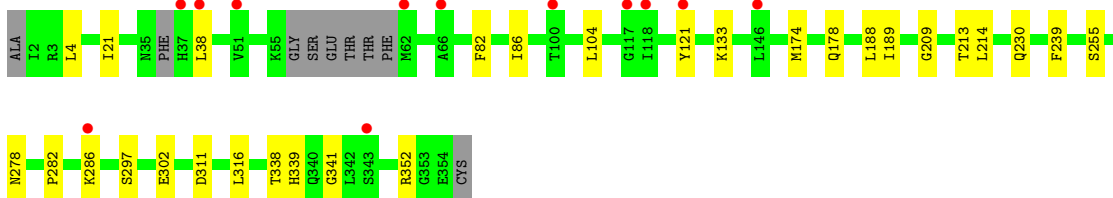
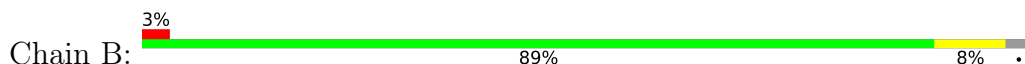
- Molecule 1: ANV419 heavy-chain



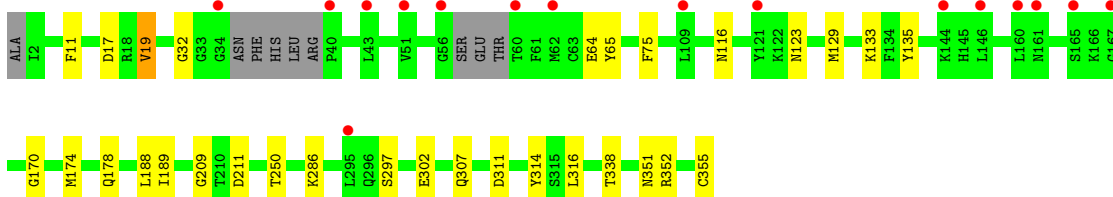
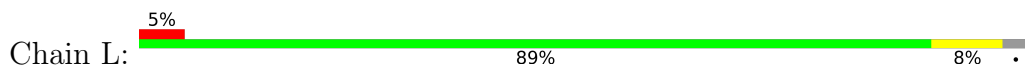
- Molecule 1: ANV419 heavy-chain



- Molecule 2: ANV419 light-chain



- Molecule 2: ANV419 light-chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	37.08Å 90.26Å 96.37Å 87.02° 79.83° 88.23°	Depositor
Resolution (Å)	47.37 – 2.05 47.37 – 2.05	Depositor EDS
% Data completeness (in resolution range)	96.4 (47.37-2.05) 96.4 (47.37-2.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.05Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.190 , 0.224 0.205 , 0.203	Depositor DCC
R_{free} test set	3796 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.579	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 61.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.115 for h,-k,h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9060	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% 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	0.84	0/1674	1.10	3/2277 (0.1%)
1	H	0.84	0/1665	1.09	6/2266 (0.3%)
2	B	0.80	0/2744	1.23	4/3712 (0.1%)
2	L	0.84	0/2735	1.23	4/3699 (0.1%)
All	All	0.83	0/8818	1.18	17/11954 (0.1%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	116	ASN	CA-CB-CG	7.38	119.98	112.60
2	L	17	ASP	CA-CB-CG	6.12	118.72	112.60
2	L	311	ASP	CA-CB-CG	5.99	118.59	112.60
1	A	73	ASP	CA-C-N	5.98	128.62	120.54
1	A	73	ASP	C-N-CA	5.98	128.62	120.54
1	A	61	ASN	N-CA-C	-5.73	101.36	109.96
2	B	311	ASP	CA-CB-CG	5.67	118.27	112.60
1	H	73	ASP	CA-C-N	5.57	129.18	120.82
1	H	73	ASP	C-N-CA	5.57	129.18	120.82
1	H	61	ASN	N-CA-C	-5.44	101.80	109.96
1	H	1	GLU	CA-C-N	5.18	128.03	120.98
1	H	1	GLU	C-N-CA	5.18	128.03	120.98
2	L	75	PHE	CA-CB-CG	5.16	118.96	113.80
2	B	255	SER	N-CA-C	-5.15	100.12	108.41
2	B	121	TYR	CA-C-N	5.08	127.08	120.28
2	B	121	TYR	C-N-CA	5.08	127.08	120.28
1	H	109	ASP	CA-CB-CG	5.08	117.68	112.60

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	A	1632	0	1601	7	0
1	H	1623	0	1588	9	0
2	B	2694	0	2660	13	0
2	L	2685	0	2648	14	0
3	A	116	0	0	0	0
3	B	89	0	0	1	0
3	H	128	0	0	0	0
3	L	93	0	0	1	0
All	All	9060	0	8497	39	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 2.

All (39) 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:L:351:ASN:H	2:L:355:CYS:HB3	1.47	0.78
1:H:164:SER:H	1:H:205:ASN:HD21	1.41	0.68
1:A:55:SER:HB2	2:B:133:LYS:HG3	1.81	0.62
1:H:55:SER:HB2	2:L:133:LYS:HG3	1.83	0.60
2:L:123:ASN:HD21	2:L:129:MET:HE1	1.67	0.60
2:L:178:GLN:HB2	2:L:188:LEU:HD11	1.83	0.59
2:B:178:GLN:HB2	2:B:188:LEU:HD11	1.84	0.58
2:B:82:PHE:CZ	2:B:86:ILE:HD11	2.39	0.57
2:B:339:HIS:CD2	2:B:341:GLY:H	2.25	0.55
2:L:307:GLN:HG3	2:L:314:TYR:CZ	2.42	0.54
1:A:51:ILE:HB	1:A:70:ILE:HG22	1.91	0.53
2:L:211:ASP:HB2	3:L:426:HOH:O	2.08	0.52
2:L:351:ASN:N	2:L:355:CYS:HB3	2.21	0.52
2:B:213:THR:HG23	3:B:418:HOH:O	2.09	0.52
1:H:196:SER:HA	1:H:199:THR:HG22	1.92	0.51
2:B:282:PRO:O	2:B:339:HIS:HE1	1.93	0.51
2:L:32:GLY:HA2	2:L:170:GLY:HA2	1.93	0.49
2:L:11:PHE:HZ	2:L:19:VAL:HG13	1.79	0.48
1:H:164:SER:H	1:H:205:ASN:ND2	2.08	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:HIS:CD2	2:B:278:ASN:HD21	2.32	0.48
1:H:51:ILE:HB	1:H:70:ILE:HG22	1.96	0.47
1:A:172:HIS:HD2	2:B:278:ASN:HD21	1.61	0.47
2:L:286:LYS:HB3	2:L:338:THR:HB	1.95	0.47
1:H:199:THR:HG23	1:H:200:GLN:HG2	1.97	0.46
2:B:286:LYS:HB2	2:B:338:THR:HB	1.97	0.46
2:L:123:ASN:HD21	2:L:129:MET:CE	2.29	0.45
1:A:131:PRO:HD3	1:A:217:LYS:HE2	1.99	0.45
2:B:86:ILE:HD12	2:B:104:LEU:HD21	1.98	0.45
1:A:40:MET:HE3	1:A:43:LYS:HD3	2.01	0.43
1:H:40:MET:HE3	1:H:43:LYS:HD3	2.01	0.43
2:L:65:TYR:CD1	2:L:135:TYR:HB3	2.54	0.42
2:L:302:GLU:HG2	2:L:316:LEU:HD21	2.01	0.42
2:B:302:GLU:HG2	2:B:316:LEU:HD21	2.01	0.42
1:H:99:TRP:CH2	1:H:101:GLY:HA3	2.55	0.41
2:B:230:GLN:HG3	2:B:239:PHE:CE2	2.55	0.41
2:B:21:ILE:HD11	2:B:214:LEU:HD23	2.02	0.41
1:A:99:TRP:CH2	1:A:101:GLY:HA3	2.56	0.41
1:H:2:VAL:HG13	1:H:27:TYR:CD1	2.56	0.40
2:L:123:ASN:ND2	2:L:129:MET:HE1	2.34	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	212/224 (95%)	210 (99%)	2 (1%)	0	100	100
1	H	211/224 (94%)	208 (99%)	3 (1%)	0	100	100
2	B	340/355 (96%)	331 (97%)	8 (2%)	1 (0%)	36	30
2	L	340/355 (96%)	330 (97%)	9 (3%)	1 (0%)	36	30
All	All	1103/1158 (95%)	1079 (98%)	22 (2%)	2 (0%)	43	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	209	GLY
2	B	209	GLY

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	180/187 (96%)	176 (98%)	4 (2%)	45	44
1	H	179/187 (96%)	176 (98%)	3 (2%)	53	53
2	B	308/315 (98%)	302 (98%)	6 (2%)	50	50
2	L	307/315 (98%)	300 (98%)	7 (2%)	44	42
All	All	974/1004 (97%)	954 (98%)	20 (2%)	47	46

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ILE
1	A	146	LEU
1	A	187	SER
1	A	195	SER
2	B	4	LEU
2	B	38	LEU
2	B	174	MET
2	B	189	ILE
2	B	297	SER
2	B	352	ARG
1	H	51	ILE
1	H	146	LEU
1	H	195	SER
2	L	19	VAL
2	L	64	GLU
2	L	174	MET
2	L	189	ILE
2	L	250	THR

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Mol	Chain	Res	Type
2	L	297	SER
2	L	352	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
2	B	120	ASN
2	B	123	ASN
2	B	164	GLN
2	B	179	GLN
2	B	220	GLN
2	B	278	ASN
2	B	299	ASN
2	B	330	HIS
2	B	339	HIS
1	H	39	GLN
1	H	205	ASN
2	L	120	ASN
2	L	123	ASN
2	L	164	GLN
2	L	179	GLN
2	L	220	GLN
2	L	299	ASN
2	L	301	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 ⓘ

There are no oligosaccharides 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	A	216/224 (96%)	0.09	2 (0%) 81 83	35, 57, 89, 132	0
1	H	215/224 (95%)	-0.01	4 (1%) 66 68	33, 50, 81, 108	0
2	B	346/355 (97%)	0.52	12 (3%) 47 48	51, 82, 139, 153	0
2	L	346/355 (97%)	0.43	16 (4%) 37 37	46, 77, 125, 163	0
All	All	1123/1158 (96%)	0.31	34 (3%) 52 53	33, 71, 129, 163	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	56	GLY	3.7
2	L	34	GLY	3.2
2	L	40	PRO	3.2
2	B	38	LEU	3.1
1	H	104	TYR	2.9
2	L	121	TYR	2.8
2	L	167	GLY	2.8
2	L	295	LEU	2.6
2	B	121	TYR	2.6
2	L	165	SER	2.6
1	H	135	SER	2.6
2	L	43	LEU	2.6
2	L	160	LEU	2.5
1	A	41	PRO	2.5
1	A	43	LYS	2.5
2	B	118	ILE	2.3
2	B	146	LEU	2.3
2	L	51	VAL	2.3
2	L	62	MET	2.2
2	B	62	MET	2.2
2	L	109	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	L	60	THR	2.1
2	B	66	ALA	2.1
1	H	43	LYS	2.1
2	B	37	HIS	2.1
2	B	51	VAL	2.1
2	B	343	SER	2.1
2	L	146	LEU	2.0
1	H	199	THR	2.0
2	B	286	LYS	2.0
2	L	161	ASN	2.0
2	L	144	LYS	2.0
2	B	100	THR	2.0
2	B	117	GLY	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.