



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:14 PM UTC

PDB ID : 5L21 / pdb_00005L21
Title : Crystal structure of BoNT/A receptor binding domain in complex with VHH C2
Authors : Yao, G.; Jin, R.
Deposited on : 2016-07-29
Resolution : 1.68 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

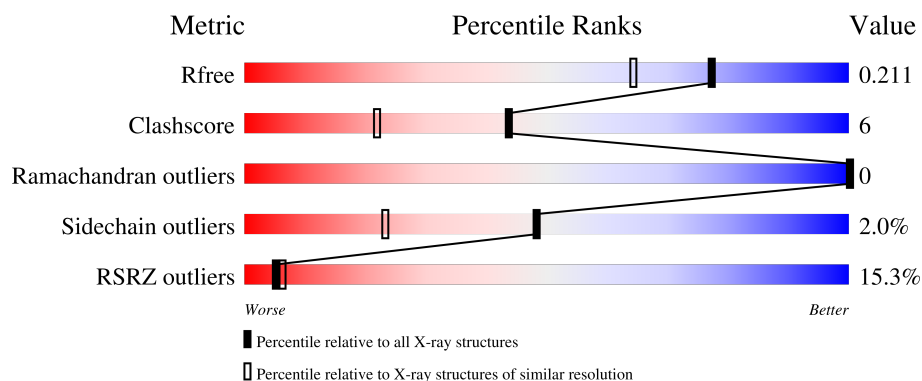
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.68 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	1054 (1.68-1.68)
Clashscore	190562	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

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	428	
2	B	119	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5003 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 Botulinum neurotoxin type A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	0	0
			3499	2231	603	651	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	869	GLY	-	cloning artifact	UNP A5HZZ9
A	870	PRO	-	cloning artifact	UNP A5HZZ9
A	871	MET	-	cloning artifact	UNP A5HZZ9
A	1158	ALA	THR	engineered mutation	UNP A5HZZ9

- Molecule 2 is a protein called VHH-C2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	119	Total	C	N	O	S	0	0	0
			938	592	161	181	4			

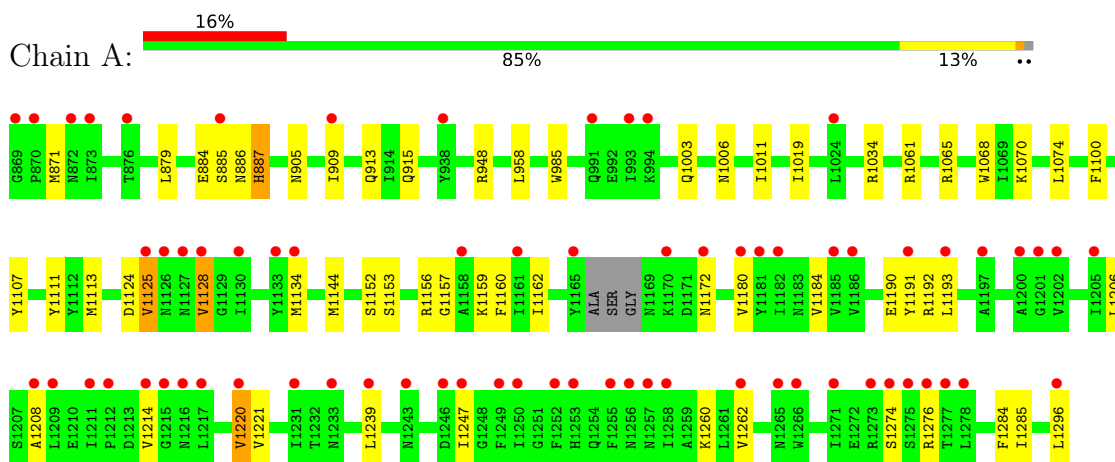
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	448	Total	O	0	0
			448	448		
3	B	118	Total	O	0	0
			118	118		

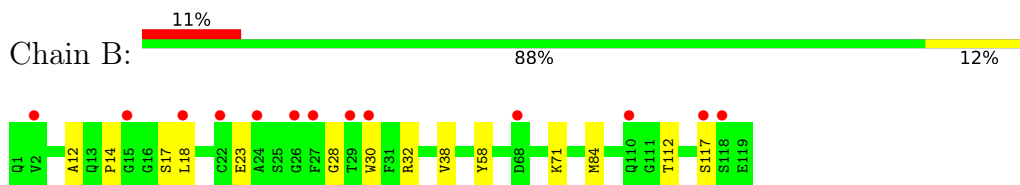
3 Residue-property plots [i](#)

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: Botulinum neurotoxin type A



- Molecule 2: VHH-C2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.10Å 103.72Å 64.70Å 90.00° 93.77° 90.00°	Depositor
Resolution (Å)	35.99 – 1.68 35.99 – 1.68	Depositor EDS
% Data completeness (in resolution range)	99.4 (35.99-1.68) 95.4 (35.99-1.68)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 1.68Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.193 , 0.205 (Not available) , 0.211	Depositor DCC
R_{free} test set	3774 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	19.6	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5003	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.35	0/3572	0.71	2/4829 (0.0%)
2	B	0.39	0/960	0.68	0/1297
All	All	0.36	0/4532	0.70	2/6126 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	958	LEU	N-CA-C	5.84	117.64	111.28
1	A	1247	ILE	N-CA-C	-5.64	107.33	111.90

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	3499	0	3461	45	0
2	B	938	0	898	10	0
3	A	448	0	0	16	3
3	B	118	0	0	3	3
All	All	5003	0	4359	54	3

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 6.

All (54) 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:A:1134:MET:SD	1:A:1193:LEU:HD13	2.02	0.97
1:A:1113:MET:SD	3:A:1313:HOH:O	2.34	0.85
1:A:1006:ASN:CG	3:A:1304:HOH:O	2.24	0.79
1:A:1172:ASN:N	3:A:1301:HOH:O	2.04	0.78
1:A:1162:ILE:HG23	1:A:1180:VAL:HG21	1.66	0.78
1:A:1134:MET:SD	1:A:1193:LEU:CD1	2.73	0.77
1:A:1144:MET:SD	3:A:1736:HOH:O	2.43	0.76
1:A:1107:TYR:O	3:A:1302:HOH:O	2.05	0.73
2:B:12:ALA:HB2	2:B:18:LEU:HD11	1.70	0.73
1:A:1006:ASN:CB	3:A:1304:HOH:O	2.36	0.73
1:A:1134:MET:HE1	1:A:1184:VAL:HG21	1.70	0.73
1:A:1152:SER:OG	3:A:1304:HOH:O	2.07	0.72
1:A:1134:MET:CE	1:A:1184:VAL:HG21	2.20	0.72
1:A:1190:GLU:OE1	3:A:1305:HOH:O	2.08	0.70
1:A:1157:GLY:O	3:A:1306:HOH:O	2.12	0.67
1:A:1006:ASN:HB3	3:A:1304:HOH:O	1.97	0.65
1:A:1124:ASP:OD2	3:A:1307:HOH:O	2.16	0.63
1:A:1034:ARG:NH1	3:A:1314:HOH:O	2.31	0.62
2:B:23:GLU:HG3	2:B:84:MET:HG2	1.82	0.62
1:A:1156:ARG:NH1	3:A:1317:HOH:O	2.33	0.61
2:B:28:GLY:O	3:B:201:HOH:O	2.16	0.59
1:A:1160:PHE:HB2	3:A:1313:HOH:O	2.02	0.58
2:B:14:PRO:HD3	2:B:117:SER:O	2.05	0.57
1:A:1153:SER:OG	1:A:1156:ARG:NH2	2.38	0.56
1:A:885:SER:O	1:A:886:ASN:HB2	2.06	0.56
1:A:1134:MET:HE3	1:A:1208:ALA:HB2	1.88	0.54
2:B:12:ALA:CB	2:B:18:LEU:HD11	2.37	0.54
1:A:1107:TYR:CD1	1:A:1162:ILE:HG22	2.47	0.49
1:A:1128:VAL:HG11	1:A:1191:TYR:CE1	2.47	0.48
2:B:32:ARG:HD2	3:B:206:HOH:O	2.12	0.48
1:A:985:TRP:CD2	1:A:1019:ILE:HG21	2.49	0.48
1:A:1003:GLN:HA	1:A:1011:ILE:HD11	1.96	0.47
1:A:1192:ARG:HG2	1:A:1214:VAL:HG21	1.96	0.47
1:A:948:ARG:HB3	1:A:1068:TRP:HB2	1.97	0.46
1:A:1134:MET:HE2	1:A:1184:VAL:HG21	1.95	0.46
1:A:1180:VAL:HG12	1:A:1221:VAL:O	2.16	0.46
2:B:71:LYS:NZ	3:B:210:HOH:O	2.49	0.46
1:A:1220:VAL:O	1:A:1239:LEU:HD12	2.15	0.45
1:A:1274:SER:OG	1:A:1276:ARG:HG2	2.17	0.45
1:A:884:GLU:O	1:A:885:SER:C	2.57	0.44
1:A:1156:ARG:HH22	1:A:1296:LEU:HD13	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:884:GLU:O	1:A:887:HIS:ND1	2.49	0.43
1:A:1193:LEU:HD11	1:A:1206:LEU:HB3	1.99	0.43
1:A:1260:LYS:NZ	3:A:1344:HOH:O	2.52	0.42
2:B:17:SER:C	2:B:18:LEU:HD12	2.43	0.42
1:A:905:ASN:HB3	1:A:915:GLN:HB3	2.00	0.42
2:B:38:VAL:HG22	2:B:58:TYR:HB3	2.02	0.42
1:A:1134:MET:CE	1:A:1193:LEU:HD13	2.50	0.41
1:A:879:LEU:HB3	1:A:1074:LEU:HB2	2.03	0.41
1:A:913:GLN:HG2	1:A:1070:LYS:HD3	2.02	0.41
1:A:1100:PHE:HB2	1:A:1285:ILE:HG12	2.03	0.41
1:A:1159:LYS:HE3	2:B:30:TRP:CZ3	2.56	0.40
1:A:1125:VAL:HG13	3:A:1352:HOH:O	2.22	0.40
1:A:1111:TYR:CG	1:A:1284:PHE:HB3	2.57	0.40

All (3) 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)
3:A:1748:HOH:O	3:B:316:HOH:O[2_645]	2.10	0.10
3:A:1326:HOH:O	3:B:271:HOH:O[2_645]	2.16	0.04
3:A:1741:HOH:O	3:B:250:HOH:O[1_455]	2.17	0.03

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	421/428 (98%)	407 (97%)	14 (3%)	0	100	100
2	B	117/119 (98%)	115 (98%)	2 (2%)	0	100	100
All	All	538/547 (98%)	522 (97%)	16 (3%)	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	A	392/393 (100%)	383 (98%)	9 (2%)	44	18
2	B	100/100 (100%)	99 (99%)	1 (1%)	68	52
All	All	492/493 (100%)	482 (98%)	10 (2%)	48	23

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

Mol	Chain	Res	Type
1	A	871	MET
1	A	887	HIS
1	A	909	ILE
1	A	1061	ARG
1	A	1065	ARG
1	A	1125	VAL
1	A	1128	VAL
1	A	1220	VAL
1	A	1262	VAL
2	B	112	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	905	ASN
1	A	935	ASN
1	A	1026	ASN
1	A	1046	ASN
1	A	1052	ASN
1	A	1106	GLN
1	A	1256	ASN

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	A	425/428 (99%)	0.78	70 (16%) 4 5	13, 31, 67, 106	0
2	B	119/119 (100%)	0.71	13 (10%) 10 13	19, 36, 63, 93	0
All	All	544/547 (99%)	0.76	83 (15%) 5 6	13, 33, 65, 106	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1200	ALA	5.4
1	A	1262	VAL	5.0
1	A	1202	VAL	4.9
1	A	1125	VAL	4.8
2	B	22	CYS	4.7
1	A	1165	TYR	4.5
1	A	1212	PRO	4.4
2	B	30	TRP	4.3
1	A	1275	SER	4.2
1	A	1128	VAL	4.2
1	A	1296	LEU	4.1
1	A	1266	TRP	4.1
1	A	1271	ILE	3.9
1	A	1211	ILE	3.8
1	A	1209	LEU	3.7
1	A	1273	ARG	3.6
1	A	1247	ILE	3.6
1	A	870	PRO	3.6
1	A	1185	VAL	3.5
1	A	1191	TYR	3.4
1	A	1231	ILE	3.4
1	A	1024	LEU	3.4
1	A	1257	ASN	3.3
1	A	993	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	1181	TYR	3.3
1	A	1214	VAL	3.3
2	B	26	GLY	3.2
1	A	1133	TYR	3.2
1	A	869	GLY	3.2
1	A	1130	ILE	3.2
1	A	1250	ILE	3.1
1	A	1274	SER	3.1
2	B	118	SER	3.0
2	B	2	VAL	3.0
2	B	117	SER	3.0
1	A	1217	LEU	3.0
1	A	1201	GLY	2.9
1	A	873	ILE	2.9
1	A	1258	ILE	2.9
1	A	1265	ASN	2.8
1	A	1172	ASN	2.7
1	A	1220	VAL	2.6
1	A	1277	THR	2.6
1	A	1252	PHE	2.6
1	A	1180	VAL	2.6
1	A	1161	ILE	2.6
2	B	24	ALA	2.6
2	B	110	GLN	2.5
1	A	1276	ARG	2.5
1	A	1255	PHE	2.5
1	A	876	THR	2.5
1	A	1127	ASN	2.5
1	A	1186	VAL	2.5
1	A	1256	ASN	2.4
1	A	1193	LEU	2.4
2	B	27	PHE	2.4
1	A	938	TYR	2.4
1	A	1158	ALA	2.3
1	A	1246	ASP	2.3
1	A	994	LYS	2.3
1	A	1134	MET	2.3
1	A	1243	ASN	2.3
1	A	1215	GLY	2.3
1	A	1197	ALA	2.3
1	A	1239	LEU	2.3
1	A	1205	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1208	ALA	2.2
2	B	18	LEU	2.2
1	A	909	ILE	2.2
1	A	1253	HIS	2.2
1	A	1170	LYS	2.2
1	A	1182	ILE	2.2
2	B	29	THR	2.2
1	A	872	ASN	2.1
1	A	1233	ASN	2.1
1	A	1126	ASN	2.1
1	A	1216	ASN	2.1
1	A	885	SER	2.1
1	A	1278	LEU	2.1
1	A	1249	PHE	2.1
2	B	15	GLY	2.0
1	A	991	GLN	2.0
2	B	68	ASP	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.