



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 08:40 PM UTC

PDB ID : 9EA9 / pdb_00009ea9
Title : Crystal structure of BoNT/A-NTNH-HA70 -VHH_F12-VHH_H7-Fab_NTN
H complex
Authors : Lam, K.H.; Gao, L.; Jin, R.
Deposited on : 2024-11-10
Resolution : 2.93 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

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
Mogul	:	2022.3.0, CSD as543be (2022)
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

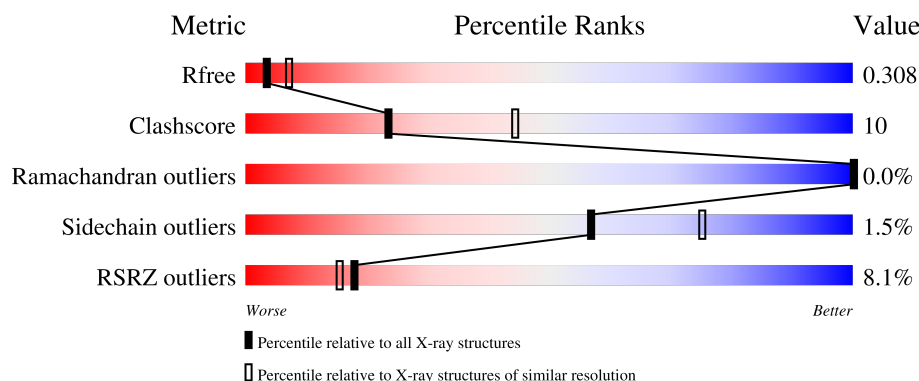
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.93 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	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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	1296	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>23%</div> <div>•</div> </div> </div>
2	B	1194	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>23%</div> <div>••</div> </div> </div>
3	C	128	<div> <div>11%</div> <div> <div></div> <div>64%</div> <div>27%</div> <div>9%</div> </div> </div>
4	F	121	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>19%</div> <div>• 6%</div> </div> </div>
5	D	626	<div> <div>0%</div> <div> <div></div> <div>20%</div> <div>8%</div> <div>72%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	G	626	
5	H	626	
5	I	626	
5	J	626	
6	E	626	
7	K	105	
8	M	117	
9	N	94	
10	L	103	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	SO4	A	1301	-	-	X	-
11	SO4	E	701	-	-	X	-
13	MG	E	705	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 39218 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	1276	Total	C	N	O	S	0	0	0
			10371	6651	1716	1971	33			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	VAL	variant	UNP P0DPI0
A	224	GLN	GLU	conflict	UNP P0DPI0
A	363	ALA	ARG	conflict	UNP P0DPI0
A	366	PHE	TYR	conflict	UNP P0DPI0

- Molecule 2 is a protein called Non-toxic nonhemagglutinin type A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1187	Total	C	N	O	S	0	0	0
			9671	6194	1553	1892	32			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	426	SER	THR	conflict	UNP Q45914
B	1194	PRO	-	expression tag	UNP Q45914

- Molecule 3 is a protein called Nanobody ciA-F12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	117	Total	C	N	O	S	0	0	0
			873	540	153	176	4			

- Molecule 4 is a protein called Nanobody ciA-H7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	114	Total	C	N	O	S	0	0	0
			853	529	151	168	5			

- Molecule 5 is a protein called HA-70.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	169	Total	C	N	O	S	0	0	0
			1376	891	223	260	2			
5	J	421	Total	C	N	O	S	0	0	0
			3366	2121	564	676	5			
5	D	174	Total	C	N	O	S	0	0	0
			1409	914	228	265	2			
5	G	169	Total	C	N	O	S	0	0	0
			1382	894	223	263	2			
5	H	421	Total	C	N	O	S	0	0	0
			3363	2120	562	676	5			

- Molecule 6 is a protein called HA70/A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	421	Total	C	N	O	S	0	0	0
			3358	2115	561	677	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	575	ASP	ILE	conflict	UNP Q8KHU9
E	576	ALA	ASP	conflict	UNP Q8KHU9

- Molecule 7 is a protein called anti-NTNH Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	K	105	Total	C	N	O	S	0	0	0
			803	505	134	162	2			

- Molecule 8 is a protein called anti-NTNH Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	M	117	Total	C	N	O	S	0	0	0
			881	557	144	176	4			

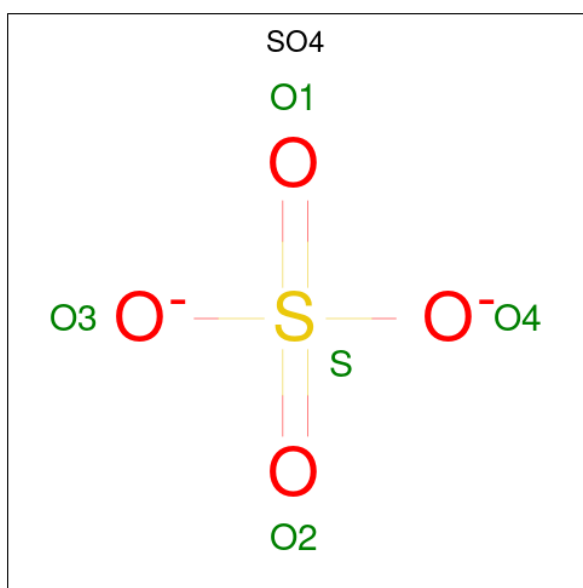
- Molecule 9 is a protein called anti-NTNH Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	N	94	Total	C	N	O	S	8	0	0
			634	399	104	129	2			

- Molecule 10 is a protein called anti-NTNH Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	103	Total	C	N	O	S	0	0	0
			752	460	129	160	3			

- Molecule 11 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	O	S	0	0
			5	4	1		
11	A	1	Total	O	S	0	0
			5	4	1		
11	A	1	Total	O	S	0	0
			5	4	1		
11	A	1	Total	O	S	0	0
			5	4	1		
11	B	1	Total	O	S	0	0
			5	4	1		
11	B	1	Total	O	S	0	0
			5	4	1		
11	B	1	Total	O	S	0	0
			5	4	1		
11	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	D	1	Total	O	S	0	0
			5	4	1		
11	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	1	Total	Zn	0	0
			1	1		

- Molecule 13 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	1	Total	Mg	0	0
			1	1		
13	B	1	Total	Mg	0	0
			1	1		
13	J	1	Total	Mg	0	0
			1	1		
13	E	6	Total	Mg	0	0
			6	6		
13	H	1	Total	Mg	0	0
			1	1		

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	25	Total	O	0	0
			25	25		
14	B	15	Total	O	0	0
			15	15		
14	F	4	Total	O	0	0
			4	4		
14	I	3	Total	O	0	0
			3	3		
14	J	2	Total	O	0	0
			2	2		
14	D	3	Total	O	0	0
			3	3		
14	E	8	Total	O	0	0
			8	8		

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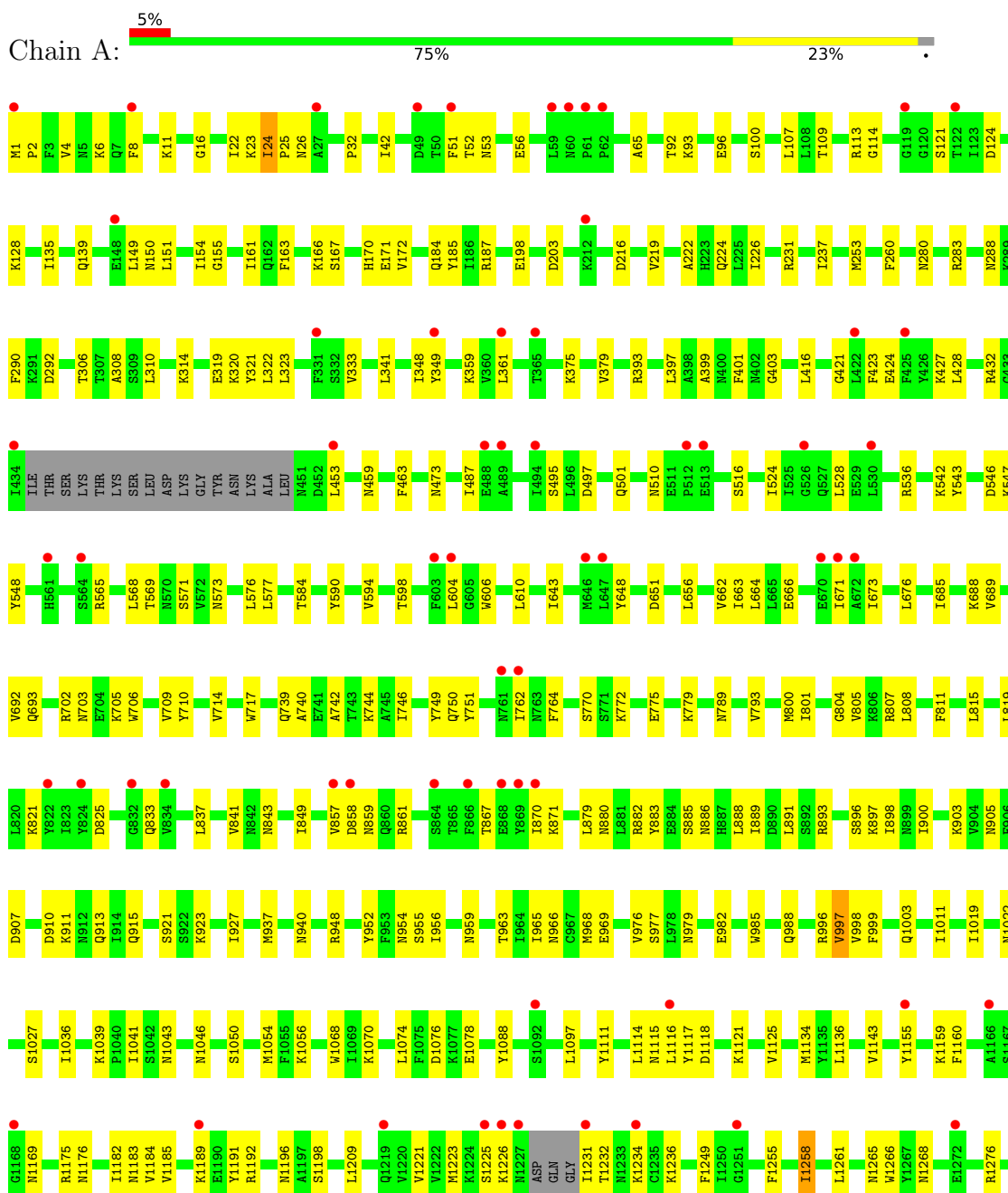
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	G	2	Total	O	0	0
			2	2		
14	H	2	Total	O	0	0
			2	2		
14	M	1	Total	O	0	0
			1	1		

3 Residue-property plots

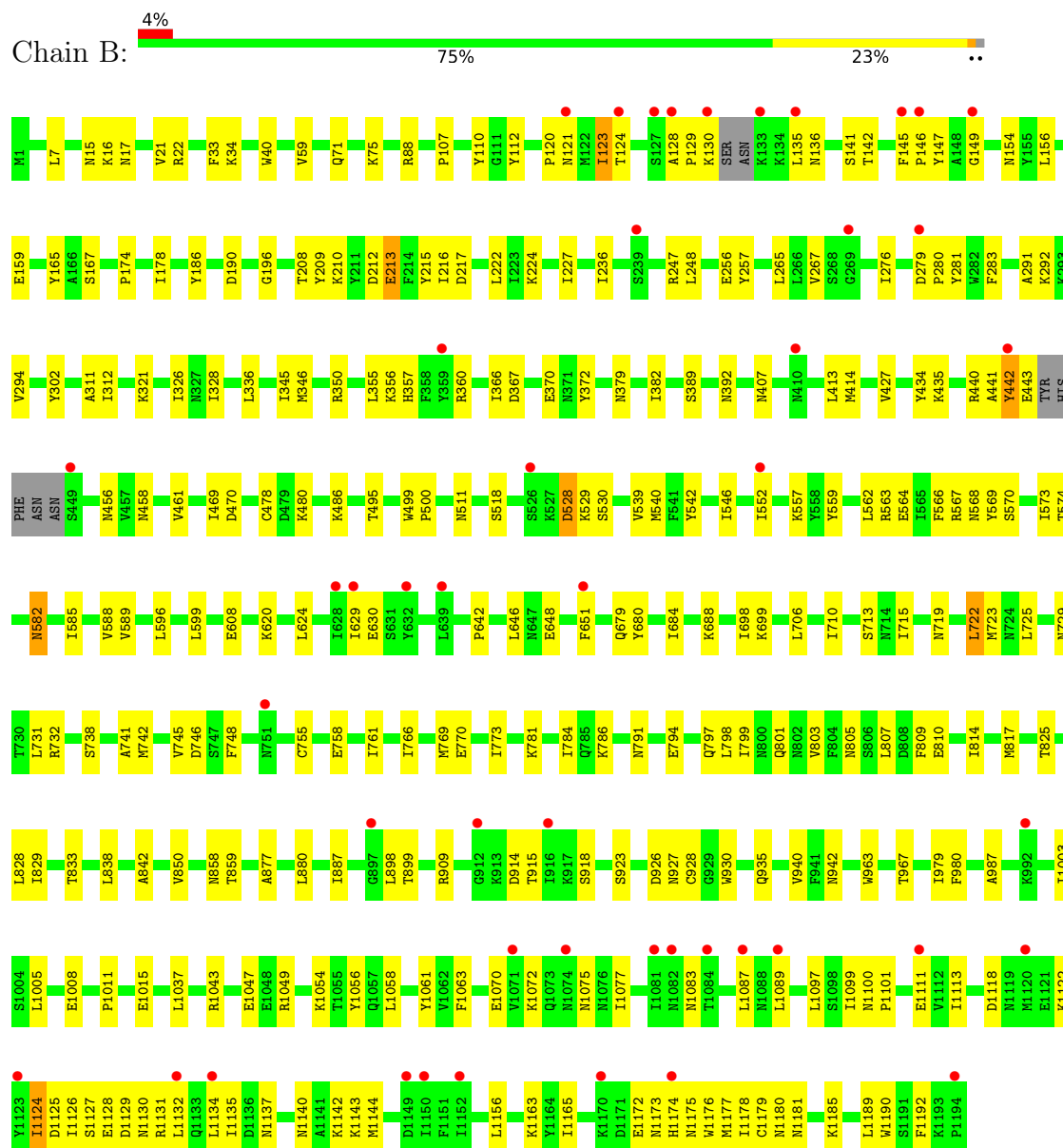
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Botulinum neurotoxin type A

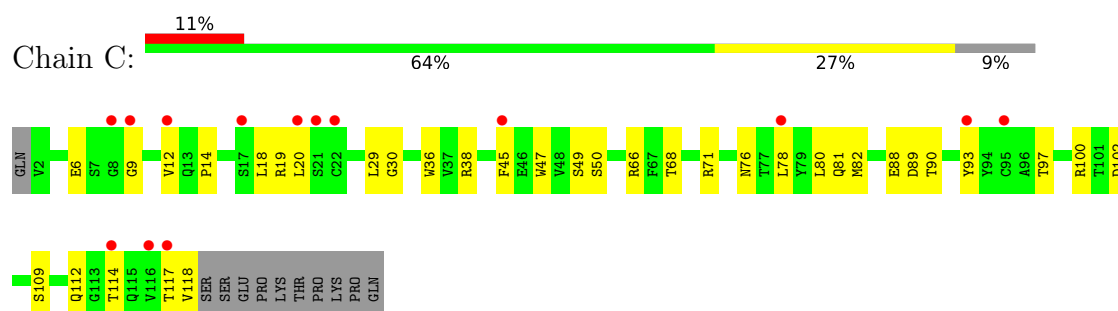




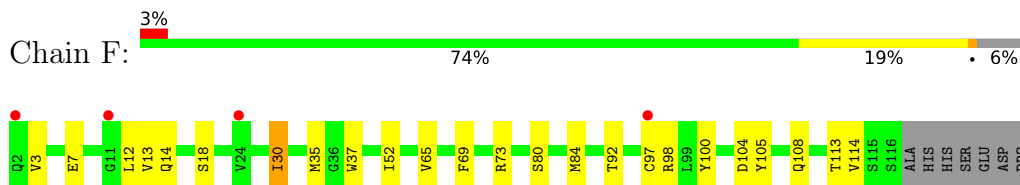
• Molecule 2: Non-toxic nonhemagglutinin type A



• Molecule 3: Nanobody ciA-F12



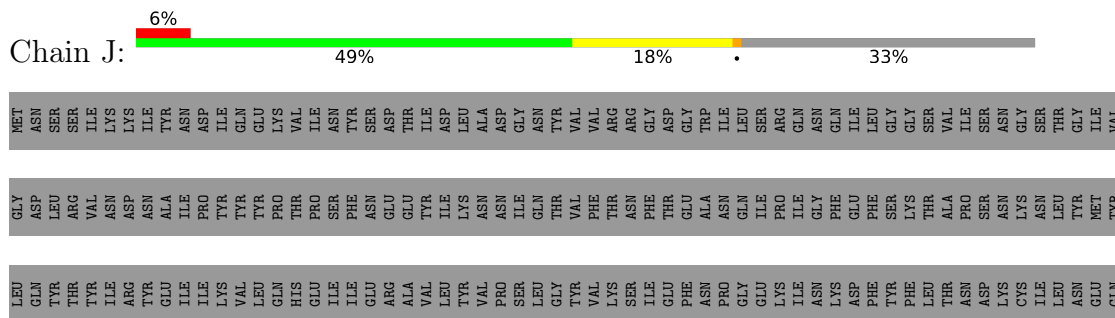
- Molecule 4: Nanobody ciA-H7



- Molecule 5: HA-70

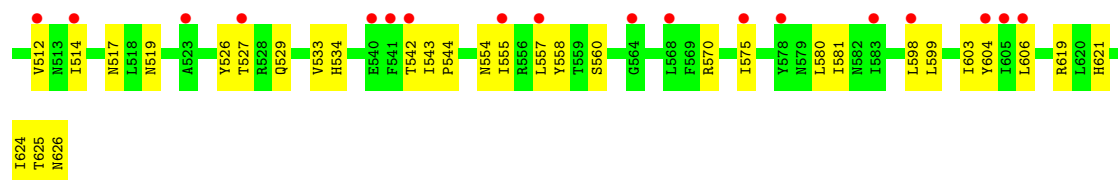


- Molecule 5: HA-70

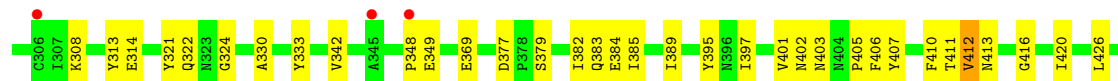
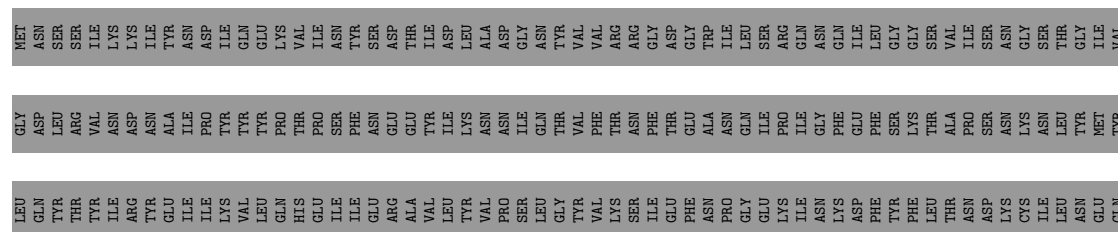




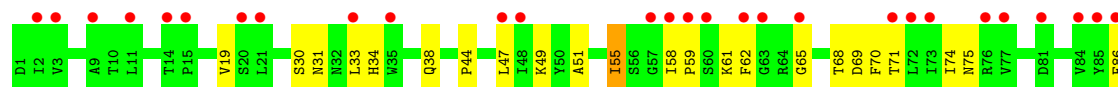
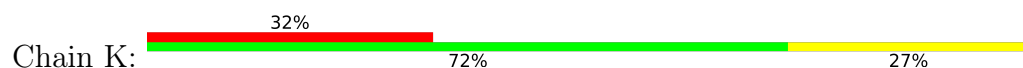




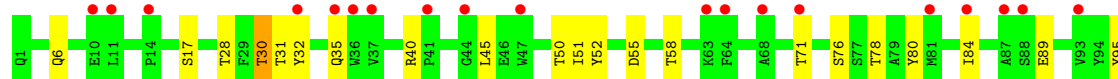
• Molecule 6: HA70/A1

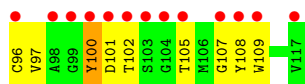


• Molecule 7: anti-NTNH Fab

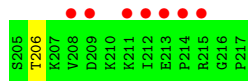
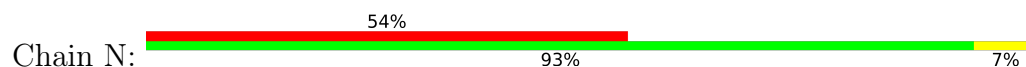


• Molecule 8: anti-NTNH Fab

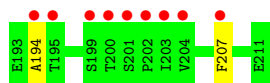
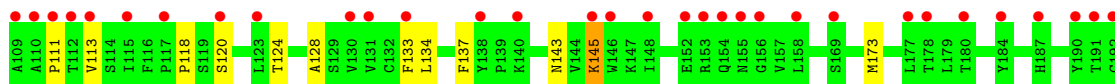
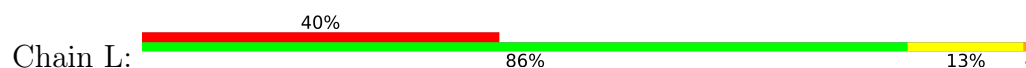




● Molecule 9: anti-NTNH Fab



● Molecule 10: anti-NTNH Fab



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 ₂ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	203.65Å 203.65Å 479.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.61 – 2.93 99.61 – 2.93	Depositor EDS
% Data completeness (in resolution range)	99.9 (99.61-2.93) 99.9 (99.61-2.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.21rc1_5107	Depositor
R, R_{free}	0.286 , 0.308 0.287 , 0.308	Depositor DCC
R_{free} test set	2000 reflections (0.93%)	wwPDB-VP
Wilson B-factor (Å ²)	54.9	Xtriage
Anisotropy	0.535	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	39218	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.00% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ZN, MG

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	0.14	0/10590	0.32	0/14338
2	B	0.15	0/9876	0.34	0/13390
3	C	0.16	0/893	0.34	0/1213
4	F	0.15	0/867	0.35	0/1167
5	D	0.16	0/1442	0.37	0/1959
5	G	0.11	0/1414	0.32	0/1919
5	H	0.14	0/3426	0.36	0/4662
5	I	0.13	0/1408	0.36	0/1911
5	J	0.13	0/3429	0.36	0/4667
6	E	0.13	0/3421	0.35	0/4657
7	K	0.29	0/821	0.50	0/1116
8	M	0.15	0/902	0.34	0/1226
9	N	0.11	0/650	0.33	0/900
10	L	0.13	0/768	0.31	0/1047
All	All	0.14	0/39907	0.34	0/54172

There are no bond length outliers.

There are no bond angle outliers.

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	10371	0	10228	199	0
2	B	9671	0	9434	189	0
3	C	873	0	812	20	0
4	F	853	0	830	17	0
5	D	1409	0	1375	41	0
5	G	1382	0	1357	38	0
5	H	3363	0	3265	73	0
5	I	1376	0	1348	35	0
5	J	3366	0	3267	84	0
6	E	3358	0	3253	69	0
7	K	803	0	766	30	0
8	M	881	0	834	23	0
9	N	634	0	579	4	0
10	L	752	0	650	10	0
11	A	20	0	0	3	0
11	B	20	0	0	1	0
11	D	5	0	0	0	0
11	E	5	0	0	4	0
12	A	1	0	0	0	0
13	A	1	0	0	0	0
13	B	1	0	0	0	0
13	E	6	0	0	0	0
13	H	1	0	0	0	0
13	J	1	0	0	0	0
14	A	25	0	0	4	0
14	B	15	0	0	3	0
14	D	3	0	0	1	0
14	E	8	0	0	3	0
14	F	4	0	0	0	0
14	G	2	0	0	0	0
14	H	2	0	0	1	0
14	I	3	0	0	0	0
14	J	2	0	0	0	0
14	M	1	0	0	0	0
All	All	39218	0	37998	785	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 10.

The worst 5 of 785 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)
10:L:143:ASN:HB3	10:L:145:LYS:HE2	1.47	0.96
5:J:584:GLN:HG3	5:J:587:LEU:HD11	1.48	0.92
5:I:54:ASN:HD22	5:I:114:ASN:H	1.22	0.87
1:A:903:LYS:HG3	1:A:921:SER:HB2	1.55	0.87
2:B:120:PRO:HB3	2:B:146:PRO:HD2	1.57	0.87

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	1270/1296 (98%)	1236 (97%)	34 (3%)	0	100	100
2	B	1181/1194 (99%)	1133 (96%)	48 (4%)	0	100	100
3	C	115/128 (90%)	113 (98%)	2 (2%)	0	100	100
4	F	112/121 (93%)	110 (98%)	1 (1%)	1 (1%)	14	34
5	D	172/626 (28%)	164 (95%)	8 (5%)	0	100	100
5	G	167/626 (27%)	161 (96%)	6 (4%)	0	100	100
5	H	419/626 (67%)	399 (95%)	20 (5%)	0	100	100
5	I	167/626 (27%)	156 (93%)	11 (7%)	0	100	100
5	J	419/626 (67%)	401 (96%)	18 (4%)	0	100	100
6	E	419/626 (67%)	403 (96%)	16 (4%)	0	100	100
7	K	103/105 (98%)	91 (88%)	12 (12%)	0	100	100
8	M	115/117 (98%)	108 (94%)	7 (6%)	0	100	100
9	N	90/94 (96%)	88 (98%)	2 (2%)	0	100	100
10	L	101/103 (98%)	101 (100%)	0	0	100	100
All	All	4850/6914 (70%)	4664 (96%)	185 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	30	ILE

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	1152/1177 (98%)	1140 (99%)	12 (1%)	68	81
2	B	1101/1113 (99%)	1088 (99%)	13 (1%)	63	78
3	C	90/103 (87%)	90 (100%)	0	100	100
4	F	90/97 (93%)	90 (100%)	0	100	100
5	D	153/572 (27%)	147 (96%)	6 (4%)	28	53
5	G	153/572 (27%)	153 (100%)	0	100	100
5	H	381/572 (67%)	375 (98%)	6 (2%)	55	74
5	I	151/572 (26%)	147 (97%)	4 (3%)	40	65
5	J	381/572 (67%)	373 (98%)	8 (2%)	47	70
6	E	380/571 (66%)	374 (98%)	6 (2%)	55	74
7	K	91/94 (97%)	89 (98%)	2 (2%)	45	69
8	M	90/94 (96%)	87 (97%)	3 (3%)	33	58
9	N	68/83 (82%)	66 (97%)	2 (3%)	37	62
10	L	79/95 (83%)	77 (98%)	2 (2%)	42	66
All	All	4360/6287 (69%)	4296 (98%)	64 (2%)	57	75

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	M	30	THR
8	M	100	TYR
2	B	1124	ILE
2	B	828	LEU
9	N	138	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
5	H	365	ASN
5	H	446	ASN
8	M	35	GLN
2	B	694	GLN
2	B	507	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 ⓘ

Of 21 ligands modelled in this entry, 11 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	SO4	A	1301	-	4,4,4	0.64	0	6,6,6	0.09	0
11	SO4	A	1304	-	4,4,4	0.72	0	6,6,6	0.39	0
11	SO4	A	1302	-	4,4,4	0.67	0	6,6,6	0.18	0
11	SO4	B	1203	-	4,4,4	0.67	0	6,6,6	0.08	0
11	SO4	D	701	-	4,4,4	0.68	0	6,6,6	0.38	0
11	SO4	A	1303	-	4,4,4	0.67	0	6,6,6	0.05	0
11	SO4	B	1201	-	4,4,4	0.67	0	6,6,6	0.07	0
11	SO4	E	701	-	4,4,4	1.04	0	6,6,6	1.39	1 (16%)
11	SO4	B	1204	-	4,4,4	0.73	0	6,6,6	0.42	0
11	SO4	B	1202	-	4,4,4	0.66	0	6,6,6	0.22	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	E	701	SO4	O4-S-O3	3.06	125.39	108.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	1301	SO4	3	0
11	E	701	SO4	4	0
11	B	1202	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	N	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	132:PRO	C	137:SER	N	10.71

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	1276/1296 (98%)	0.59	66 (5%)	33 27	35, 63, 101, 165	0
2	B	1187/1194 (99%)	0.46	47 (3%)	42 34	27, 53, 95, 176	0
3	C	117/128 (91%)	0.95	14 (11%)	9 8	56, 94, 129, 158	0
4	F	114/121 (94%)	0.49	4 (3%)	47 39	55, 68, 90, 95	0
5	D	174/626 (27%)	0.52	7 (4%)	42 34	28, 48, 87, 133	0
5	G	169/626 (26%)	0.69	6 (3%)	46 38	40, 61, 92, 113	0
5	H	421/626 (67%)	0.87	44 (10%)	11 11	32, 82, 127, 170	0
5	I	169/626 (26%)	0.50	5 (2%)	52 44	28, 49, 79, 107	0
5	J	421/626 (67%)	0.83	35 (8%)	17 15	36, 71, 124, 159	0
6	E	421/626 (67%)	0.48	9 (2%)	63 54	24, 42, 86, 169	0
7	K	105/105 (100%)	1.69	34 (32%)	1 1	96, 141, 175, 214	0
8	M	117/117 (100%)	1.39	32 (27%)	1 1	84, 116, 146, 155	0
9	N	93/94 (98%)	2.27	51 (54%)	0 0	131, 179, 209, 218	0
10	L	103/103 (100%)	1.86	41 (39%)	1 0	168, 206, 234, 274	0
All	All	4887/6914 (70%)	0.70	395 (8%)	18 15	24, 62, 150, 274	0

The worst 5 of 395 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	L	201	SER	6.4
9	N	188	SER	5.9
10	L	111	PRO	5.5
7	K	102	LEU	5.1
1	A	1225	SER	5.0

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
13	MG	E	705	1/1	0.60	0.88	89,89,89,89	1
11	SO4	B	1204	5/5	0.68	0.14	75,77,108,134	0
11	SO4	A	1304	5/5	0.74	0.11	96,100,111,132	0
13	MG	A	1306	1/1	0.81	0.29	36,36,36,36	0
11	SO4	B	1203	5/5	0.82	0.14	55,70,82,87	0
11	SO4	E	701	5/5	0.83	0.23	66,67,86,90	0
11	SO4	D	701	5/5	0.86	0.10	64,66,79,88	0
13	MG	E	707	1/1	0.86	0.29	20,20,20,20	0
11	SO4	A	1303	5/5	0.87	0.12	67,69,84,106	0
13	MG	B	1205	1/1	0.87	0.22	40,40,40,40	0
11	SO4	B	1201	5/5	0.88	0.08	59,70,88,91	0
11	SO4	B	1202	5/5	0.88	0.10	45,57,60,69	0
11	SO4	A	1301	5/5	0.89	0.12	63,64,82,90	0
11	SO4	A	1302	5/5	0.89	0.13	63,66,73,79	0
13	MG	E	703	1/1	0.90	0.14	20,20,20,20	0
13	MG	E	704	1/1	0.93	0.25	30,30,30,30	0
13	MG	H	701	1/1	0.93	0.21	14,14,14,14	0
13	MG	E	702	1/1	0.94	0.17	24,24,24,24	0
13	MG	J	701	1/1	0.94	0.23	34,34,34,34	0
12	ZN	A	1305	1/1	0.96	0.04	129,129,129,129	0
13	MG	E	706	1/1	0.97	0.41	49,49,49,49	1

6.5 Other polymers [i](#)

There are no such residues in this entry.