



Full wwPDB EM Validation Report ⓘ

Mar 3, 2025 – 09:10 am GMT

PDB ID : 9IHC
EMDB ID : EMD-52864
Title : CryoEM structure of a synthetic antibody, COP-2, in complex with the C-terminal domain of Clostridium perfringens Enterotoxin
Authors : Pacesa, M.; Goldbach, N.; Vecchio, A.J.; Correia, B.E.
Deposited on : 2025-02-21
Resolution : 2.95 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : **FAILED**
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41

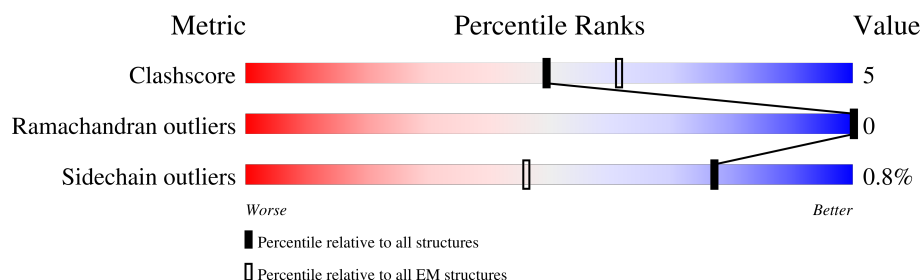
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.95 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	B	134	
2	H	260	
3	L	239	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4288 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Heat-labile enterotoxin B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	119	Total	C	N	O	S	0	0
			944	603	159	181	1		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	191	MET	-	initiating methionine	UNP P01558
B	320	GLY	-	expression tag	UNP P01558
B	321	LEU	-	expression tag	UNP P01558
B	322	VAL	-	expression tag	UNP P01558
B	323	PRO	-	expression tag	UNP P01558
B	324	ARG	-	expression tag	UNP P01558

- Molecule 2 is a protein called COP-2 antibody heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	225	Total	C	N	O	S	0	0
			1692	1072	280	334	6		

- Molecule 3 is a protein called COP-2 antibody light chain.

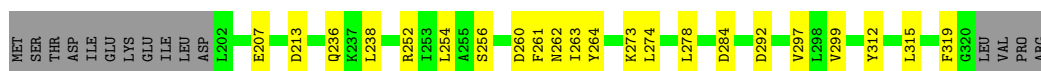
Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	216	Total	C	N	O	S	0	0
			1652	1032	277	337	6		

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. 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. 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: Heat-labile enterotoxin B chain

Chain B: 




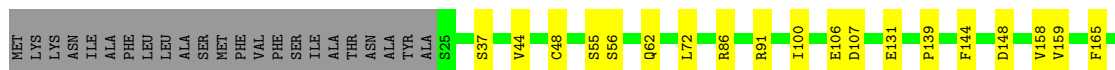
- Molecule 2: COP-2 antibody heavy chain

Chain H: 



- Molecule 3: COP-2 antibody light chain

Chain L: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87280	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor

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	B	0.26	0/965	0.51	0/1312
2	H	0.28	0/1737	0.49	0/2369
3	L	0.30	0/1688	0.50	0/2293
All	All	0.28	0/4390	0.50	0/5974

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	B	944	0	918	13	0
2	H	1692	0	1629	17	0
3	L	1652	0	1601	17	0
All	All	4288	0	4148	46	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 (46) 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:38:VAL:CG2	2:H:44:LEU:HD12	1.76	1.14

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:38:VAL:HG21	2:H:44:LEU:HD12	1.29	1.11
2:H:38:VAL:HG21	2:H:44:LEU:CD1	1.86	1.04
2:H:38:VAL:CG2	2:H:44:LEU:CD1	2.47	0.86
1:B:207:GLU:HG2	1:B:238:LEU:HD11	1.77	0.66
2:H:38:VAL:HG21	2:H:44:LEU:HD13	1.77	0.63
2:H:43:SER:HA	2:H:109:MET:O	1.99	0.62
3:L:55:SER:O	3:L:91:ARG:NE	2.37	0.57
2:H:130:ASN:ND2	3:L:56:SER:OG	2.36	0.57
3:L:196:ASP:OD2	3:L:196:ASP:N	2.37	0.56
3:L:106:GLU:OE2	3:L:106:GLU:N	2.36	0.56
1:B:263:ILE:HG22	1:B:274:LEU:HB2	1.88	0.56
3:L:55:SER:OG	3:L:56:SER:N	2.38	0.56
3:L:169:GLU:OE1	3:L:225:GLN:NE2	2.39	0.55
2:H:165:PRO:HG3	2:H:177:LEU:HB3	1.89	0.54
2:H:120:TYR:O	2:H:145:GLY:HA2	2.07	0.53
1:B:213:ASP:OD2	1:B:213:ASP:N	2.38	0.51
3:L:86:ARG:NE	3:L:107:ASP:OD2	2.44	0.51
3:L:170:ALA:HB2	3:L:224:HIS:HD2	1.76	0.49
1:B:264:TYR:HB2	1:B:297:VAL:HB	1.95	0.48
1:B:254:LEU:HB2	1:B:315:LEU:HB3	1.97	0.47
1:B:263:ILE:O	1:B:274:LEU:N	2.49	0.46
3:L:62:GLN:HB2	3:L:72:LEU:HD11	1.97	0.46
2:H:117:THR:HG23	2:H:149:THR:HA	1.97	0.46
3:L:148:ASP:OD1	3:L:148:ASP:N	2.48	0.46
2:H:66:ALA:HB3	2:H:69:LYS:HB2	1.98	0.45
2:H:38:VAL:HG23	2:H:44:LEU:CD1	2.41	0.45
1:B:254:LEU:HD13	1:B:315:LEU:HD23	1.99	0.45
1:B:261:PHE:HA	1:B:299:VAL:O	2.17	0.45
2:H:117:THR:HA	2:H:148:VAL:O	2.16	0.44
3:L:139:PRO:HB3	3:L:165:PHE:HB3	1.98	0.44
1:B:252:ARG:HB2	1:B:319:PHE:HE1	1.82	0.44
2:H:202:VAL:HG23	2:H:221:VAL:HG22	2.00	0.44
3:L:171:LYS:HB3	3:L:171:LYS:HE3	1.75	0.43
3:L:44:VAL:HG22	3:L:100:ILE:HB	1.99	0.43
2:H:113:ARG:NE	2:H:115:GLU:OE2	2.51	0.43
3:L:158:VAL:HG23	3:L:205:LEU:HB3	2.01	0.42
1:B:273:LYS:HE3	1:B:273:LYS:HB2	1.81	0.42
2:H:248:LYS:HB2	2:H:248:LYS:HE2	1.82	0.41
2:H:139:LEU:O	2:H:142:TRP:NE1	2.54	0.41
3:L:37:SER:HA	3:L:131:GLU:HG2	2.03	0.41
3:L:144:PHE:HB2	3:L:159:VAL:HB	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:SER:HA	1:B:284:ASP:OD2	2.22	0.40
3:L:86:ARG:NH2	3:L:107:ASP:OD1	2.44	0.40
1:B:236:GLN:O	1:B:312:TYR:OH	2.35	0.40
1:B:260:ASP:HB3	1:B:278:LEU:HA	2.04	0.40

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 PDB entries followed by that with respect to all EM entries.

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	B	117/134 (87%)	115 (98%)	2 (2%)	0	100	100
2	H	221/260 (85%)	218 (99%)	3 (1%)	0	100	100
3	L	214/239 (90%)	208 (97%)	6 (3%)	0	100	100
All	All	552/633 (87%)	541 (98%)	11 (2%)	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 PDB entries followed by that with respect to all EM entries.

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	B	102/118 (86%)	100 (98%)	2 (2%)	50	72
2	H	189/218 (87%)	188 (100%)	1 (0%)	86	93
3	L	190/208 (91%)	189 (100%)	1 (0%)	86	93

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	481/544 (88%)	477 (99%)	4 (1%)	77	88

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	262	ASN
1	B	292	ASP
2	H	255	CYS
3	L	48	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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.