



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 06:03 AM UTC

PDB ID : 9BIR / pdb_00009bir
EMDB ID : EMD-44599
Title : Cryo-EM structure of the mammalian peptide transporter PepT2 bound to cefadroxil
Authors : Parker, J.L.; Deme, J.C.; Lea, S.M.; Newstead, S.
Deposited on : 2024-04-24
Resolution : 3.10 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 : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

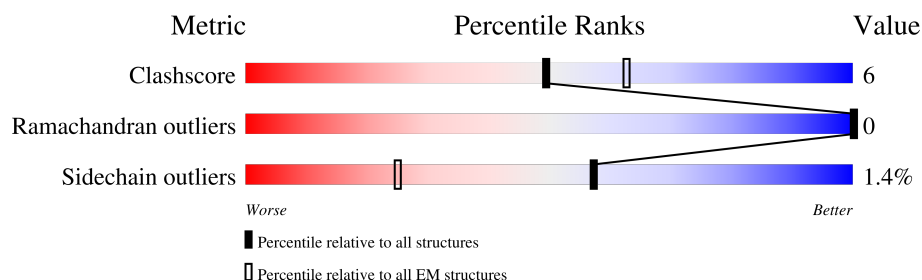
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	A	738	 55% 8% 37%
2	B	131	 79% 14% • 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9383 atoms, of which 4716 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 Solute carrier family 15 member 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	467	7453	2453	3776	583	615	26	0	0

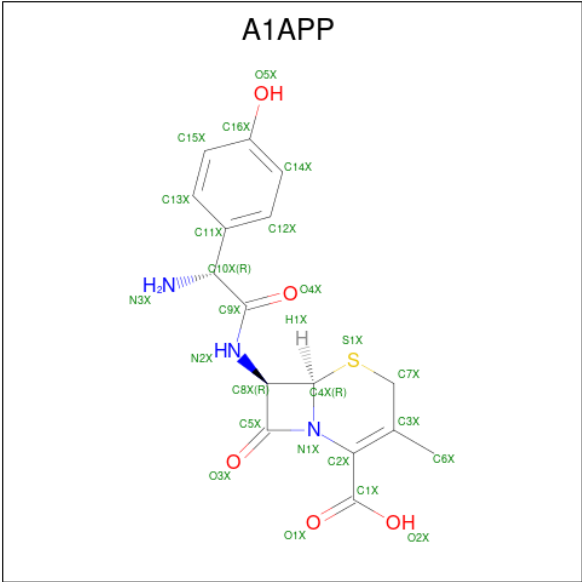
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	730	VAL	-	expression tag	UNP Q63424
A	731	GLU	-	expression tag	UNP Q63424
A	732	GLY	-	expression tag	UNP Q63424
A	733	GLU	-	expression tag	UNP Q63424
A	734	ASN	-	expression tag	UNP Q63424
A	735	LEU	-	expression tag	UNP Q63424
A	736	TYR	-	expression tag	UNP Q63424
A	737	PHE	-	expression tag	UNP Q63424
A	738	GLN	-	expression tag	UNP Q63424

- Molecule 2 is a protein called nanobody.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	123	1889	603	924	174	181	7	0	0

- Molecule 3 is Cefadroxil (CCD ID: A1APP) (formula: C₁₆H₁₇N₃O₅S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	H	N	O	S	0
			41	16	16	3	5	1	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	93759	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 ($e^-/\text{\AA}^2$)	54.8	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1APP

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	0.12	0/3778	0.29	0/5136
2	B	0.11	0/987	0.25	0/1333
All	All	0.12	0/4765	0.28	0/6469

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

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	3677	3776	3776	44	0
2	B	965	924	924	11	0
3	A	25	16	0	2	0
All	All	4667	4716	4700	53	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 6.

All (53) 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:262:ALA:O	1:A:276:LYS:NZ	2.22	0.71
1:A:331:ASN:O	1:A:608:ILE:N	2.26	0.69
1:A:302:VAL:HG11	1:A:645:LEU:HD12	1.75	0.68
1:A:117:LEU:HD23	1:A:159:GLY:HA3	1.77	0.67
1:A:98:ILE:HG13	1:A:651:LEU:HD21	1.78	0.66
1:A:110:LYS:NZ	1:A:170:ASP:OD2	2.26	0.62
1:A:333:ASP:OD1	1:A:334:LEU:N	2.34	0.61
1:A:98:ILE:HD11	1:A:651:LEU:HD11	1.83	0.60
1:A:266:ARG:HE	1:A:276:LYS:HE2	1.69	0.57
1:A:330:MET:HE3	1:A:401:ILE:HD11	1.87	0.56
2:B:123:VAL:HG23	2:B:123:VAL:O	2.06	0.55
1:A:622:GLU:OE2	3:A:801:A1APP:N3X	2.40	0.55
2:B:87:VAL:HG23	2:B:89:ARG:H	1.71	0.53
2:B:33:ASP:N	2:B:99:ALA:O	2.40	0.52
1:A:113:THR:HG22	1:A:117:LEU:HD22	1.92	0.52
1:A:136:LEU:H	1:A:136:LEU:HD23	1.75	0.52
1:A:609:ALA:O	1:A:610:TRP:HB2	2.12	0.50
1:A:273:ASP:O	1:A:274:LEU:HD12	2.11	0.49
1:A:284:ALA:O	1:A:293:ILE:HD11	2.13	0.48
1:A:103:ILE:O	1:A:107:TRP:O	2.32	0.48
2:B:31:ASP:OD2	2:B:100:ARG:NH1	2.47	0.48
1:A:63:MET:SD	1:A:67:LEU:HD13	2.56	0.46
1:A:305:LEU:HD21	1:A:377:LEU:HD21	1.99	0.45
2:B:52:SER:O	2:B:72:ARG:NH1	2.50	0.45
1:A:67:LEU:HD11	1:A:150:LEU:HD21	1.99	0.44
1:A:156:GLY:O	1:A:160:ILE:HG12	2.17	0.44
1:A:309:LEU:N	1:A:310:PRO:CD	2.80	0.44
1:A:110:LYS:O	1:A:111:PHE:HB3	2.17	0.43
1:A:687:LEU:O	1:A:691:VAL:HG23	2.18	0.43
1:A:653:VAL:HG21	3:A:801:A1APP:C6X	2.49	0.43
2:B:67:ARG:NE	2:B:67:ARG:HA	2.34	0.43
1:A:157:THR:HG22	1:A:161:LYS:HE3	2.01	0.43
1:A:308:PRO:HD3	1:A:692:MET:HE1	2.00	0.43
1:A:609:ALA:C	1:A:611:GLN:H	2.27	0.43
1:A:295:ASP:N	1:A:295:ASP:OD1	2.52	0.42
1:A:79:GLU:OE2	2:B:54:SER:OG	2.36	0.42
1:A:276:LYS:HB3	1:A:283:TRP:HB2	2.00	0.42
1:A:198:SER:O	1:A:202:THR:HG23	2.19	0.42
2:B:64:MET:O	2:B:65:LYS:C	2.62	0.42
1:A:649:TRP:O	1:A:652:THR:OG1	2.29	0.42
1:A:211:CYS:HB2	1:A:216:CYS:HA	2.02	0.42
1:A:63:MET:HE3	1:A:63:MET:HB3	1.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:SER:OG	2:B:103:TRP:NE1	2.51	0.42
2:B:90:ASP:OD1	2:B:90:ASP:C	2.62	0.41
1:A:308:PRO:CD	1:A:692:MET:HE1	2.50	0.41
1:A:79:GLU:O	1:A:83:THR:OG1	2.32	0.41
1:A:302:VAL:HG11	1:A:645:LEU:CD1	2.49	0.41
1:A:96:THR:N	1:A:97:PRO:CD	2.84	0.41
1:A:332:GLY:HA2	1:A:608:ILE:HB	2.03	0.41
1:A:276:LYS:HA	1:A:283:TRP:HB2	2.02	0.40
2:B:22:CYS:N	2:B:79:MET:O	2.45	0.40
1:A:57:ARG:O	1:A:58:PHE:C	2.65	0.40
1:A:107:TRP:O	1:A:108:LEU:HB2	2.21	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	A	463/738 (63%)	420 (91%)	43 (9%)	0	100	100
2	B	121/131 (92%)	108 (89%)	13 (11%)	0	100	100
All	All	584/869 (67%)	528 (90%)	56 (10%)	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	A	394/639 (62%)	390 (99%)	4 (1%)	68	79
2	B	101/107 (94%)	98 (97%)	3 (3%)	36	65
All	All	495/746 (66%)	488 (99%)	7 (1%)	57	76

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	THR
1	A	181	THR
1	A	211	CYS
1	A	276	LYS
2	B	80	PHE
2	B	87	VAL
2	B	108	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	3	GLN
2	B	74	ASN

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 ⓘ

1 ligand is modelled in this entry.

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
3	A1APP	A	801	-	25,27,27	0.54	0	35,40,40	0.47	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1APP	A	801	-	-	4/16/45/45	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	A1APP	C11X-C10X-C9X-N2X
3	A	801	A1APP	C11X-C10X-C9X-O4X
3	A	801	A1APP	O1X-C1X-C2X-C3X
3	A	801	A1APP	N3X-C10X-C9X-O4X

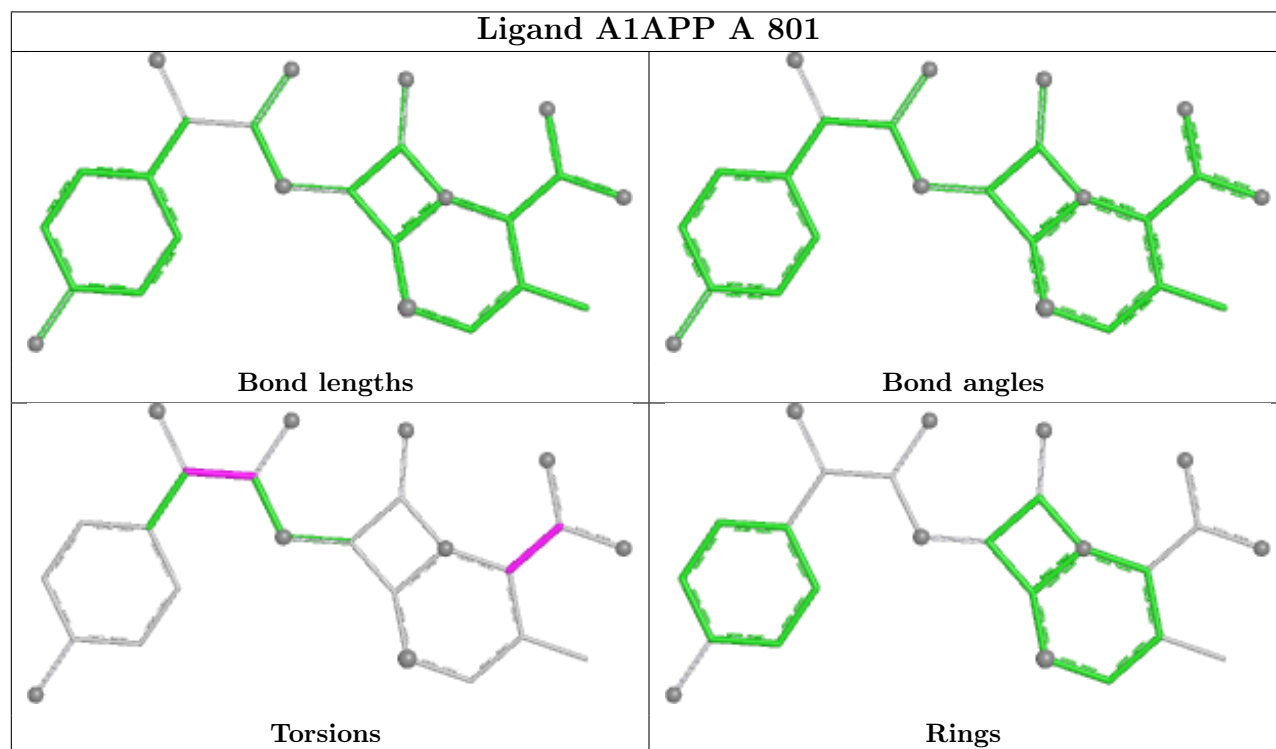
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	A1APP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 Map visualisation

This section contains visualisations of the EMDB entry EMD-44599. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.