



wwPDB EM Validation Summary Report ⓘ

Jul 15, 2025 – 10:10 PM JST

PDB ID : 8JI0 / pdb_00008ji0
EMDB ID : EMD-36303
Title : Cryo-EM structure of the TcsH-CROP in complex with TMPRSS2
Authors : Zhou, R.; Tao, L.; Zhan, X.
Deposited on : 2023-05-25
Resolution : 3.00 Å(reported)

This is a wwPDB EM 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/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 : 4-5-2 with Phenix2.0rc1
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) : 2.44

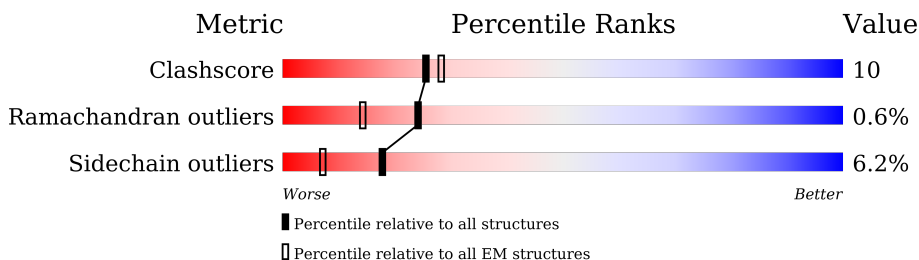
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	424	
2	A	786	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3934 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 Transmembrane protease serine 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	341	Total	C	N	O	S	0	0
			2669	1688	462	496	23		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	69	MET	-	initiating methionine	UNP O15393
B	70	GLY	-	expression tag	UNP O15393
B	71	ILE	-	expression tag	UNP O15393
B	72	LEU	-	expression tag	UNP O15393
B	73	PRO	-	expression tag	UNP O15393
B	74	SER	-	expression tag	UNP O15393
B	75	PRO	-	expression tag	UNP O15393
B	76	GLY	-	expression tag	UNP O15393
B	77	MET	-	expression tag	UNP O15393
B	78	PRO	-	expression tag	UNP O15393
B	79	ALA	-	expression tag	UNP O15393
B	80	LEU	-	expression tag	UNP O15393
B	81	LEU	-	expression tag	UNP O15393
B	82	SER	-	expression tag	UNP O15393
B	83	LEU	-	expression tag	UNP O15393
B	84	VAL	-	expression tag	UNP O15393
B	85	SER	-	expression tag	UNP O15393
B	86	LEU	-	expression tag	UNP O15393
B	87	LEU	-	expression tag	UNP O15393
B	88	SER	-	expression tag	UNP O15393
B	89	VAL	-	expression tag	UNP O15393
B	90	LEU	-	expression tag	UNP O15393
B	91	LEU	-	expression tag	UNP O15393
B	92	MET	-	expression tag	UNP O15393
B	93	GLY	-	expression tag	UNP O15393
B	94	CYS	-	expression tag	UNP O15393
B	95	VAL	-	expression tag	UNP O15393
B	96	ALA	-	expression tag	UNP O15393

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Chain	Residue	Modelled	Actual	Comment	Reference
B	97	GLU	-	expression tag	UNP O15393
B	98	THR	-	expression tag	UNP O15393
B	99	GLY	-	expression tag	UNP O15393
B	100	HIS	-	expression tag	UNP O15393
B	101	HIS	-	expression tag	UNP O15393
B	102	HIS	-	expression tag	UNP O15393
B	103	HIS	-	expression tag	UNP O15393
B	104	HIS	-	expression tag	UNP O15393
B	105	HIS	-	expression tag	UNP O15393
B	255	GLN	ARG	conflict	UNP O15393

- Molecule 2 is a protein called Maltose/maltodextrin-binding periplasmic protein, Hemorrhagic toxin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	157	Total	C	N	O	S	0	0
			1265	824	203	237	1		

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1833	MET	-	initiating methionine	UNP P0AEX9
A	1834	ALA	-	expression tag	UNP P0AEX9
A	1835	SER	-	expression tag	UNP P0AEX9
A	1836	MET	-	expression tag	UNP P0AEX9
A	1837	THR	-	expression tag	UNP P0AEX9
A	1838	GLY	-	expression tag	UNP P0AEX9
A	1839	GLY	-	expression tag	UNP P0AEX9
A	1840	GLN	-	expression tag	UNP P0AEX9
A	1841	GLN	-	expression tag	UNP P0AEX9
A	1842	MET	-	expression tag	UNP P0AEX9
A	1843	GLY	-	expression tag	UNP P0AEX9
A	1844	ARG	-	expression tag	UNP P0AEX9
A	1845	GLY	-	expression tag	UNP P0AEX9
A	1846	SER	-	expression tag	UNP P0AEX9
A	1847	HIS	-	expression tag	UNP P0AEX9
A	1848	HIS	-	expression tag	UNP P0AEX9
A	1849	HIS	-	expression tag	UNP P0AEX9
A	1850	HIS	-	expression tag	UNP P0AEX9
A	1851	HIS	-	expression tag	UNP P0AEX9
A	1852	HIS	-	expression tag	UNP P0AEX9
A	1853	HIS	-	expression tag	UNP P0AEX9

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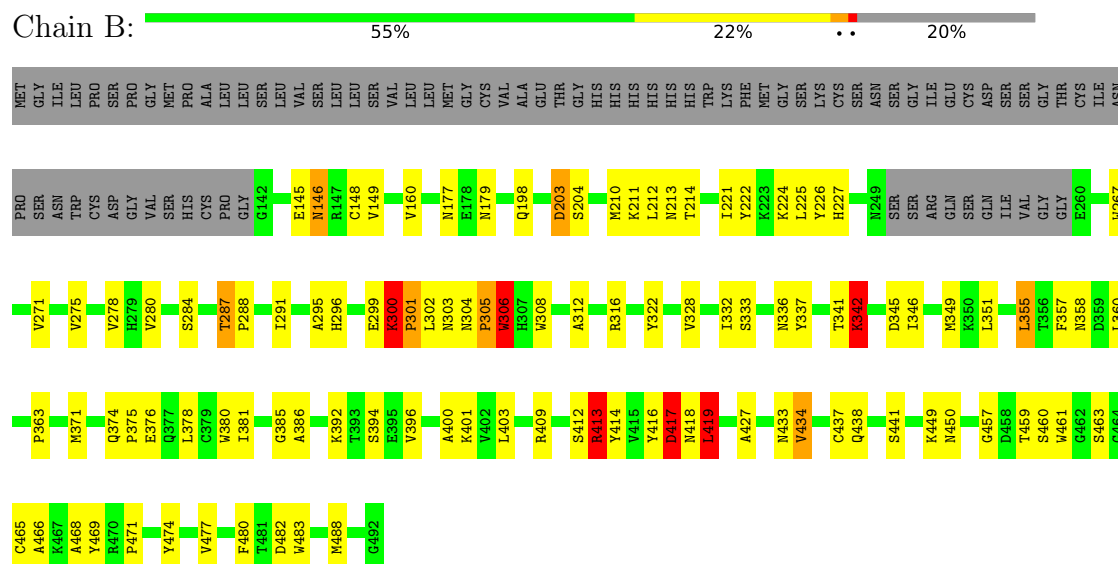
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Chain	Residue	Modelled	Actual	Comment	Reference
A	1854	HIS	-	expression tag	UNP P0AEX9
A	1855	MET	-	expression tag	UNP P0AEX9
A	2222	GLY	-	linker	UNP P0AEX9
A	2223	SER	-	linker	UNP P0AEX9
A	2224	SER	-	linker	UNP P0AEX9
A	2225	SER	-	linker	UNP P0AEX9
A	2226	LEU	-	linker	UNP P0AEX9
A	2227	GLU	-	linker	UNP P0AEX9
A	2228	VAL	-	linker	UNP P0AEX9
A	2229	LEU	-	linker	UNP P0AEX9
A	2230	PHE	-	linker	UNP P0AEX9
A	2231	GLN	-	linker	UNP P0AEX9
A	2232	GLY	-	linker	UNP P0AEX9
A	2233	PRO	-	linker	UNP P0AEX9
A	2234	GLU	-	linker	UNP P0AEX9
A	2235	PHE	-	linker	UNP P0AEX9

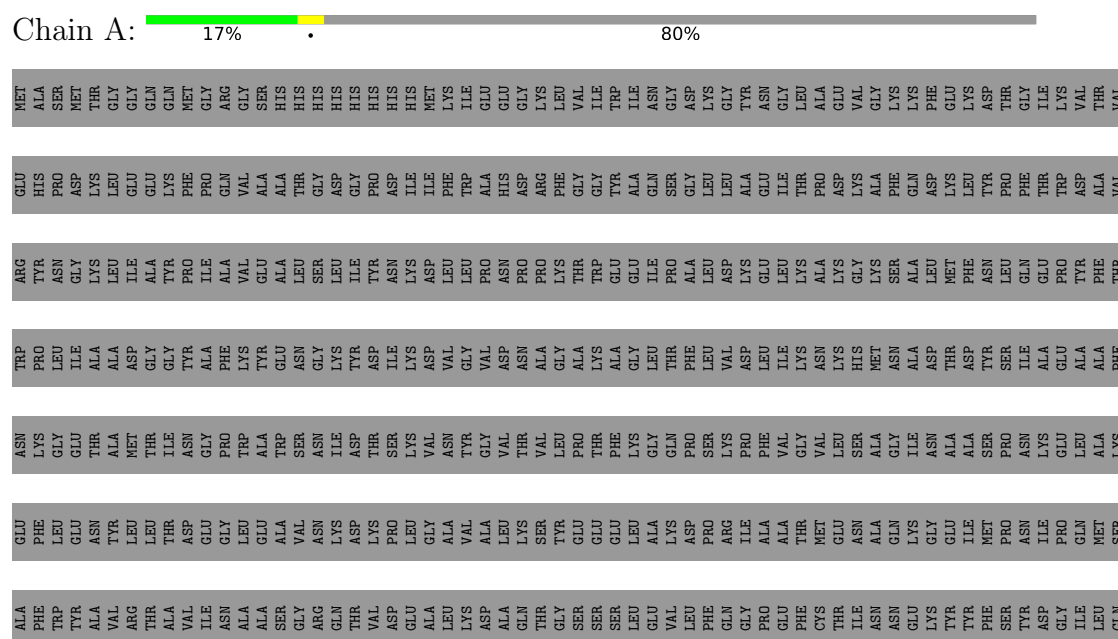
3 Residue-property plots

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. 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: Transmembrane protease serine 2



- Molecule 2: Maltose/maltodextrin-binding periplasmic protein,Hemorrhagic toxin



T2581	PHE	ILE	ASN	GLY
I2603	LYS	ASP	GLY	TYR
I2608	GLY	LYS	LYS	ILE
D2609	PRO	LYS	TYR	THR
Q2813	ASP	LYS	ILE	GLY
I2616	PHE	TYR	ASP	GLY
TYR	GLU	PHE	ASN	ARG
GLY	TYR	ASN	LEU	
	PHE	ASN	SER	PHE
	ALA	ASN	LYS	TYR
	PRO	THR	ALA	PHE
	ALA	ILE	VAL	ASP
	ASN	THR	GLY	SER
	HIS	ALA	TRP	ASN
	ASN	THR	GLN	ASN
	ASN	GLY	THR	ASP
	ASN	TRP	ILE	SER
	GLU	GLN	ASP	LYS
	GLU	ALA	GLY	MET
	GLY	ILE	LYS	THR
	GLN	ASP	LYS	THR
	SER	GLY	TYR	GLY
	ILE	LYS	TYR	VAL
	THR	LYS	PHE	PHE
	TYR	TYR	LYS	LYS
Q2460	+	TYR	PRO	GLY
H2489	+	PHE	ASN	PRO
F2490	+	PRO	THR	ASN
F2491	+	ASN	ALA	GLY
I2499	+	THR	ILE	PHE
G2500	+	ALA	GLU	THR
G2500	+	ALA	ALA	TYR
G2500	+	THR	MET	PHE
T2506	+	THR	GLY	ALA
T2506	+	SER	TRP	PRO
N2511	+	ILE	TRP	PRO
L2518	+	GLY	GLN	ALA
L2518	+	TYR	ALA	ALA
L2518	+	THR	ILE	ASN
V2523	+	THR	ASP	TYR
V2523	+	THR	GLY	ASN
G2526	+	ILE	LYS	ASN
G2526	+	ASN	ASN	ASN
G2529	+	SER	LEU	LEU
F2530	+	LYS	TYR	GLU
E2531	+	PHE	TYR	GLY
E2531	+	ASN	ASN	GLN
S2547	+	PHE	PRO	ALA
I2548	+	ASN	THR	ILE
T2549	+	ASN	THR	VAL
Y2550	+	ASP	ALA	TYR
Y2550	+	GLY	ILE	GLN
Y2550	+	GLY	ALA	ASN
F2554	+	ILE	THR	LYS
F2554	+	MET	THR	PHE
R2561	+	GLN	THR	LEU
Y2562	+	LEU	GLY	THR
Y2562	+	GLY	TRP	ILE
Y2562	+	GLN	GLN	ASN
Y2562	+	VAL	THR	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	760140	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

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	B	0.69	13/2740 (0.5%)	0.85	31/3724 (0.8%)
2	A	0.25	1/1307 (0.1%)	0.38	0/1771
All	All	0.59	14/4047 (0.3%)	0.73	31/5495 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	304	ASN	C-O	-13.12	1.04	1.23
1	B	301	PRO	C-O	-10.18	1.11	1.24
1	B	306	TRP	C-O	-9.69	1.12	1.24
1	B	305	PRO	C-O	-9.51	1.11	1.24
1	B	303	ASN	C-O	-8.29	1.12	1.24

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	414	TYR	N-CA-C	-14.00	93.44	114.16
1	B	306	TRP	N-CA-CB	-10.38	97.28	110.98
1	B	305	PRO	CB-CA-C	-9.93	95.17	111.56
1	B	306	TRP	CB-CA-C	8.68	123.51	109.27
1	B	342	LYS	CB-CG-CD	-8.54	91.65	111.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	300	LYS	Mainchain
1	B	306	TRP	Mainchain

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	2669	0	2561	65	0
2	A	1265	0	1159	13	0
All	All	3934	0	3720	77	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 77 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:B:300:LYS:HB3	1:B:301:PRO:CD	1.94	0.98
1:B:300:LYS:O	1:B:300:LYS:NZ	2.03	0.90
1:B:300:LYS:HB3	1:B:301:PRO:HD3	1.54	0.90
1:B:419:LEU:HD23	1:B:461:TRP:CH2	2.06	0.90
1:B:371:MET:O	1:B:449:LYS:NZ	2.07	0.88

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	337/424 (80%)	300 (89%)	34 (10%)	3 (1%)	14	49
2	A	155/786 (20%)	145 (94%)	10 (6%)	0	100	100
All	All	492/1210 (41%)	445 (90%)	44 (9%)	3 (1%)	24	57

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	300	LYS
1	B	145	GLU
1	B	305	PRO

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 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	290/360 (81%)	267 (92%)	23 (8%)	10	35
2	A	128/637 (20%)	125 (98%)	3 (2%)	45	75
All	All	418/997 (42%)	392 (94%)	26 (6%)	18	45

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	381	ILE
1	B	418	ASN
2	A	2581	THR
1	B	417	ASP
1	B	419	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	327	GLN
1	B	418	ASN
2	A	2552	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.