



## Full wwPDB EM Validation Report ⓘ

Oct 7, 2024 – 02:09 PM JST

PDB ID : 8JI0  
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 Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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) : 2.39

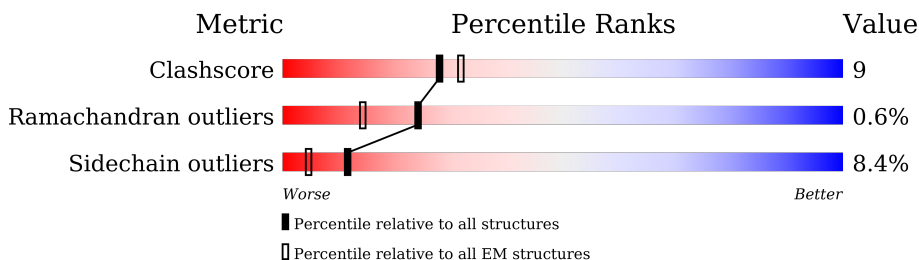
# 1 Overall quality at a glance

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  $\geq 3$ , 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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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



WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

## 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	0.55	8/2740 (0.3%)	0.73	13/3724 (0.3%)
2	A	0.32	0/1307	0.51	1/1771 (0.1%)
All	All	0.49	8/4047 (0.2%)	0.67	14/5495 (0.3%)

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	304	ASN	C-O	-9.70	1.04	1.23
1	B	306	TRP	C-O	-5.90	1.12	1.23
1	B	413	ARG	C-O	-5.83	1.12	1.23
1	B	305	PRO	C-O	-5.83	1.11	1.23
1	B	303	ASN	C-O	-5.65	1.12	1.23
1	B	301	PRO	C-O	-5.64	1.11	1.23
1	B	302	LEU	C-O	-5.50	1.12	1.23
1	B	342	LYS	CG-CD	-5.08	1.35	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	342	LYS	CB-CG-CD	-7.67	91.65	111.60
1	B	305	PRO	N-CD-CG	-7.53	91.91	103.20
1	B	306	TRP	N-CA-CB	-7.40	97.28	110.60
1	B	300	LYS	CB-CA-C	-6.99	96.41	110.40
1	B	305	PRO	CB-CA-C	-6.73	95.17	112.00
2	A	2608	ILE	CB-CA-C	6.71	125.03	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	306	TRP	CB-CA-C	6.55	123.51	110.40
1	B	414	TYR	N-CA-C	-6.50	93.44	111.00
1	B	342	LYS	CB-CA-C	6.20	122.80	110.40
1	B	299	GLU	C-N-CA	6.14	137.04	121.70
1	B	414	TYR	C-N-CA	-5.92	106.90	121.70
1	B	305	PRO	N-CA-CB	-5.23	96.85	102.60
1	B	299	GLU	O-C-N	5.05	130.78	122.70
1	B	413	ARG	CB-CA-C	5.02	120.44	110.40

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

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	60	0
2	A	1265	0	1159	13	0
All	All	3934	0	3720	72	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 9.

All (72) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:TYR:OH	1:B:471:PRO:O	1.91	0.88
2:A:2506:THR:OG1	2:A:2511:ASN:OD1	1.97	0.82
2:A:2603:ILE:HD12	2:A:2603:ILE:O	1.81	0.81
1:B:419:LEU:HD23	1:B:461:TRP:CZ2	2.17	0.80
1:B:328:VAL:HG21	1:B:349:MET:HE3	1.64	0.79
1:B:419:LEU:CD2	1:B:461:TRP:CH2	2.66	0.79
2:A:2550:TYR:OH	2:A:2554:PHE:O	2.00	0.79
1:B:437:CYS:SG	1:B:438:GLN:N	2.63	0.72
1:B:291:ILE:HD12	1:B:351:LEU:HD21	1.71	0.71
1:B:457:GLY:HA2	1:B:477:VAL:HG23	1.77	0.67
1:B:463:SER:O	1:B:463:SER:OG	2.15	0.64
1:B:291:ILE:CD1	1:B:351:LEU:HD21	2.28	0.64
1:B:385:GLY:O	1:B:394:SER:N	2.31	0.63
2:A:2561:ARG:NE	2:A:2609:ASP:O	2.32	0.62
1:B:295:ALA:N	1:B:345:ASP:OD1	2.33	0.61
1:B:322:TYR:OH	2:A:2489:HIS:ND1	2.33	0.60
1:B:203:ASP:N	1:B:203:ASP:OD1	2.33	0.60
1:B:211:LYS:N	1:B:226:TYR:O	2.38	0.57
1:B:482:ASP:OD1	1:B:483:TRP:N	2.37	0.57
1:B:177:ASN:OD1	1:B:179:ASN:N	2.35	0.56
1:B:465:CYS:O	1:B:466:ALA:HB3	2.05	0.56
1:B:346:ILE:HG21	1:B:480:PHE:CD2	2.42	0.54
1:B:358:ASN:OD1	1:B:360:LEU:N	2.36	0.54
1:B:413:ARG:HB3	1:B:417:ASP:HB2	1.91	0.53
2:A:2613:GLN:HA	2:A:2613:GLN:OE1	2.08	0.53
1:B:342:LYS:O	1:B:345:ASP:HB2	2.08	0.53
1:B:336:ASN:OD1	1:B:336:ASN:O	2.27	0.52
1:B:146:ASN:OD1	1:B:146:ASN:N	2.44	0.50
1:B:278:VAL:O	1:B:280:VAL:HG23	2.12	0.50
1:B:271:VAL:HG12	1:B:312:ALA:HB2	1.93	0.50
1:B:275:VAL:HB	1:B:280:VAL:HG21	1.94	0.50
2:A:2531:GLU:OE2	2:A:2547:SER:OG	2.26	0.49
1:B:468:ALA:O	1:B:469:TYR:HB2	2.13	0.49
1:B:328:VAL:HG21	1:B:349:MET:CE	2.38	0.48
1:B:380:TRP:CZ2	1:B:401:LYS:HD2	2.49	0.48
2:A:2523:VAL:HG21	2:A:2562:TYR:CD2	2.48	0.48
1:B:213:ASN:O	1:B:224:LYS:NZ	2.39	0.46
2:A:2609:ASP:OD1	2:A:2609:ASP:N	2.48	0.46
1:B:450:ASN:OD1	1:B:450:ASN:O	2.33	0.46
1:B:288:PRO:O	1:B:355:LEU:N	2.37	0.46
1:B:400:ALA:HB1	1:B:434:VAL:HG13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:PHE:CZ	1:B:363:PRO:HG3	2.52	0.45
1:B:149:VAL:HG12	1:B:160:VAL:HG22	1.98	0.44
1:B:222:TYR:HA	1:B:225:LEU:CD2	2.48	0.44
1:B:386:ALA:HB2	1:B:392:LYS:O	2.18	0.44
2:A:2499:ILE:HG22	2:A:2500:GLY:N	2.33	0.43
1:B:465:CYS:O	1:B:466:ALA:CB	2.66	0.43
1:B:376:GLU:OE1	1:B:403:LEU:HD23	2.19	0.43
1:B:392:LYS:N	1:B:392:LYS:HD2	2.33	0.43
1:B:433:ASN:O	1:B:434:VAL:HG23	2.19	0.43
1:B:221:ILE:O	1:B:225:LEU:HD22	2.19	0.43
1:B:267:TRP:CZ2	1:B:380:TRP:CE3	3.07	0.42
1:B:409:ARG:NE	1:B:409:ARG:HA	2.34	0.42
1:B:213:ASN:OD1	1:B:214:THR:N	2.53	0.42
1:B:222:TYR:HA	1:B:225:LEU:HD23	2.02	0.42
2:A:2491:PHE:CE2	2:A:2518:LEU:HD13	2.55	0.41
1:B:210:MET:HB3	1:B:225:LEU:HB3	2.02	0.41
1:B:300:LYS:HA	1:B:300:LYS:HD2	1.48	0.41
1:B:221:ILE:HG23	1:B:222:TYR:CE1	2.55	0.41
1:B:374:GLN:HB2	1:B:375:PRO:HD2	2.01	0.41
1:B:212:LEU:HG	1:B:213:ASN:N	2.36	0.41
1:B:427:ALA:HB3	1:B:474:TYR:CE1	2.56	0.41
2:A:2523:VAL:HB	2:A:2562:TYR:CE2	2.55	0.41
2:A:2526:GLY:N	2:A:2529:GLY:O	2.46	0.41
1:B:275:VAL:HG23	1:B:308:TRP:CE3	2.56	0.41
1:B:296:HIS:ND1	1:B:342:LYS:HE2	2.36	0.41
1:B:316:ARG:NE	1:B:396:VAL:HG12	2.35	0.41

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%)	259 (89%)	31 (11%)	5	22
2	A	128/637 (20%)	124 (97%)	4 (3%)	35	68
All	All	418/997 (42%)	383 (92%)	35 (8%)	11	33

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	146	ASN
1	B	148	CYS
1	B	188	MET
1	B	204	SER
1	B	222	TYR
1	B	227	HIS
1	B	231	CYS
1	B	284	SER
1	B	287	THR
1	B	306	TRP
1	B	329	GLU
1	B	332	ILE
1	B	333	SER

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Mol	Chain	Res	Type
1	B	342	LYS
1	B	355	LEU
1	B	381	ILE
1	B	382	SER
1	B	392	LYS
1	B	401	LYS
1	B	413	ARG
1	B	417	ASP
1	B	418	ASN
1	B	419	LEU
1	B	434	VAL
1	B	437	CYS
1	B	441	SER
1	B	451	ASN
1	B	459	THR
1	B	460	SER
1	B	470	ARG
1	B	478	MET
2	A	2507	LEU
2	A	2565	ASP
2	A	2581	THR
2	A	2600	ASP

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

### 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 [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.