



wwPDB EM Validation Summary Report ⓘ

Mar 17, 2026 – 03:57 PM UTC

PDB ID : 6PIG / pdb_00006pig
EMDB ID : EMD-20350
Title : V. cholerae ThiQ-Cascade complex, closed conformation
Authors : Halpin-Healy, T.; Klompe, S.; Sternberg, S.H.
Deposited on : 2019-06-26
Resolution : 3.50 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 : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
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

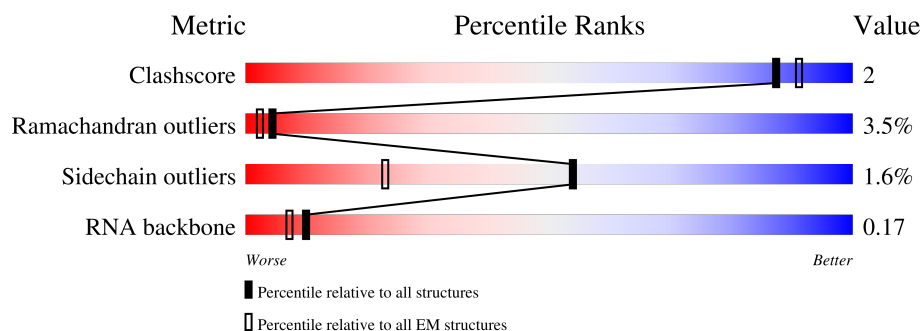
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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
RNA backbone	8273	3508

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	1	60	52% 45% .
2	A	343	88% 9% .
2	B	343	90% 8% ..
2	C	343	91% 6% ..
2	D	343	90% 8% ..
2	E	343	90% 9% .
2	F	343	84% 6% 10%

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Mol	Chain	Length	Quality of chain
3	G	511	85%14% .
4	H	198	84%14% ..
5	I	358	88%10% .
6	J	369	87%11% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 28867 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 RNA chain called RNA (60-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	60	Total	C	N	O	P	0	0
			1271	569	219	424	59		

- Molecule 2 is a protein called cas7 type I-F CRISPR-associated protein Csy3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	343	Total	C	N	O	S	0	0
			2742	1742	471	515	14		
2	B	339	Total	C	N	O	S	0	0
			2714	1727	467	506	14		
2	C	338	Total	C	N	O	S	0	0
			2705	1721	465	505	14		
2	D	338	Total	C	N	O	S	0	0
			2705	1721	465	505	14		
2	E	338	Total	C	N	O	S	0	0
			2705	1721	465	505	14		
2	F	310	Total	C	N	O	S	0	0
			2509	1603	431	461	14		

- Molecule 3 is a protein called cas5_8 naturally occurring fusion protein from *Vibrio cholerae* transposon Tn6677.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	511	Total	C	N	O	S	0	0
			4009	2533	699	757	20		

- Molecule 4 is a protein called type I-F CRISPR-associated endoribonuclease Cas6/Csy4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	197	Total	C	N	O	S	0	0
			1606	1022	285	292	7		

- Molecule 5 is a protein called TniQ monomer 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	357	Total	C	N	O	S	0	0
			2923	1875	508	525	15		

- Molecule 6 is a protein called TniQ monomer 2.

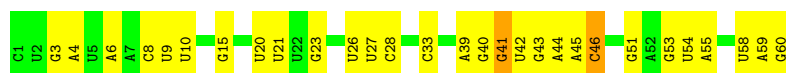
Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	368	Total	C	N	O	S	0	0
			2978	1909	515	538	16		

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.

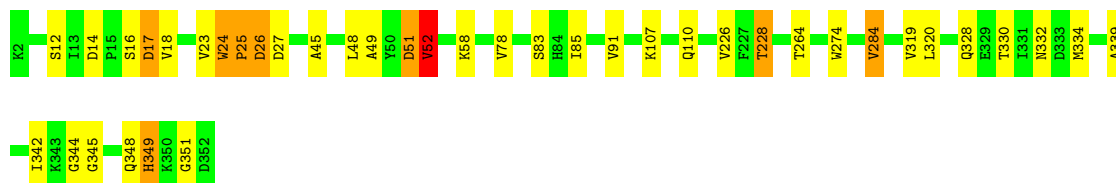
- Molecule 1: RNA (60-MER)

Chain 1: 



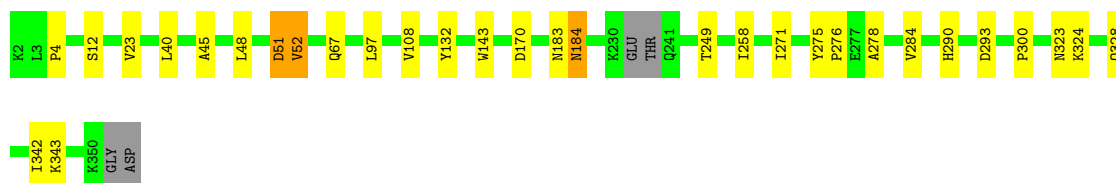
- Molecule 2: cas7 type I-F CRISPR-associated protein Csy3

Chain A: 



- Molecule 2: cas7 type I-F CRISPR-associated protein Csy3

Chain B: 

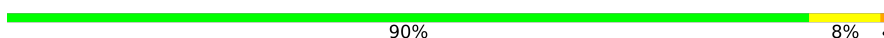


- Molecule 2: cas7 type I-F CRISPR-associated protein Csy3

Chain C: 



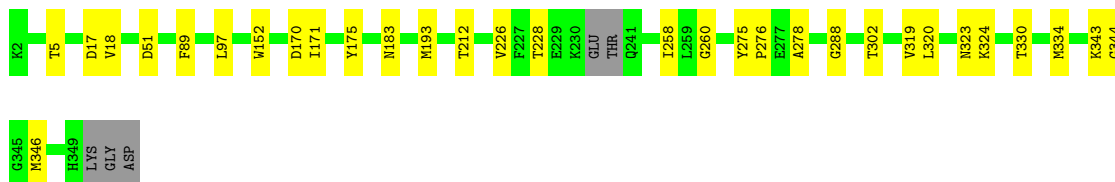
- Molecule 2: cas7 type I-F CRISPR-associated protein Csy3

Chain D: 



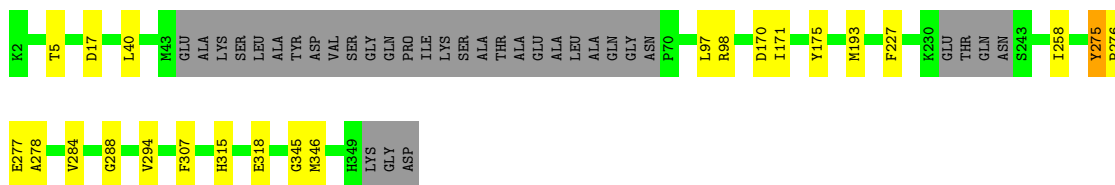
- Molecule 2: cas7 type I-F CRISPR-associated protein Csy3

Chain E: 90% 9%



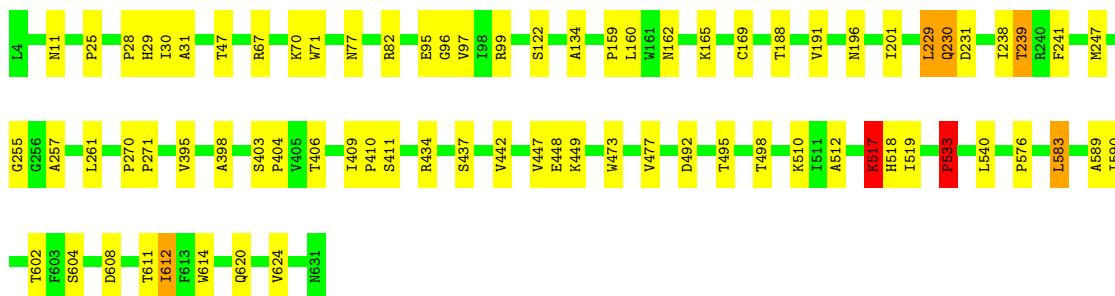
- Molecule 2: cas7 type I-F CRISPR-associated protein Csy3

Chain F: 84% 6% 10%



- Molecule 3: cas5_8 naturally occurring fusion protein from Vibrio cholerae transposon Tn6677

Chain G: 85% 14%



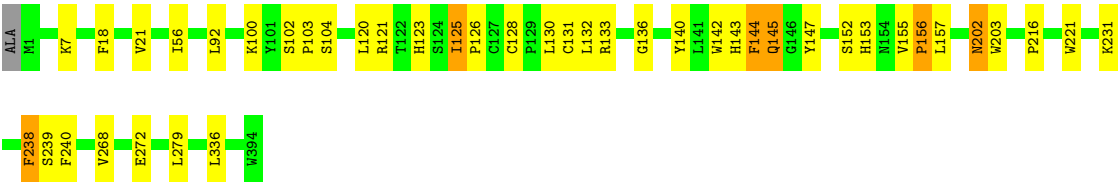
- Molecule 4: type I-F CRISPR-associated endoribonuclease Cas6/Csy4

Chain H: 84% 14%

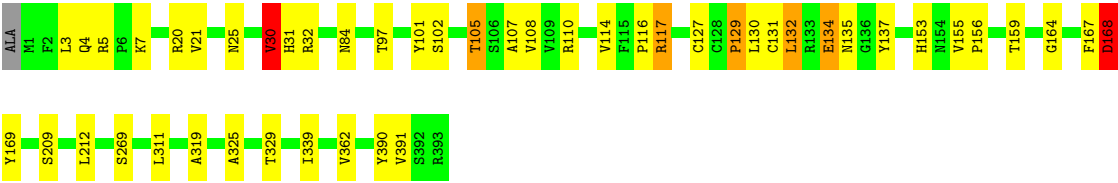
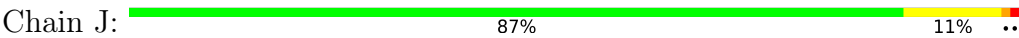


- Molecule 5: ThiQ monomer 1

Chain I: 88% 10%



• Molecule 6: ThiQ monomer 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
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	1	0.36	0/1419	0.72	1/2209 (0.0%)
2	A	1.06	0/2813	1.41	0/3821
2	B	1.06	0/2785	1.40	2/3783 (0.1%)
2	C	1.06	0/2776	1.40	1/3772 (0.0%)
2	D	1.05	0/2776	1.38	2/3772 (0.1%)
2	E	1.05	0/2776	1.38	0/3772
2	F	1.05	0/2577	1.37	0/3498
3	G	1.08	0/4098	1.41	2/5563 (0.0%)
4	H	1.08	0/1643	1.45	0/2216
5	I	1.06	0/3005	1.45	2/4071 (0.0%)
6	J	1.06	0/3060	1.46	2/4150 (0.0%)
All	All	1.04	0/29728	1.38	12/40627 (0.0%)

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
2	A	0	3
2	B	0	4
2	D	0	3
2	E	0	4
2	F	0	1
3	G	0	13
4	H	0	4
5	I	0	13
6	J	0	9
All	All	0	54

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	533	PRO	N-CA-CB	-6.43	96.50	103.25
2	C	276	PRO	N-CA-CB	-6.07	96.88	103.25
2	B	67	GLN	CA-C-N	5.74	125.43	119.92
2	B	67	GLN	C-N-CA	5.74	125.43	119.92
3	G	201	ILE	CA-C-O	-5.37	117.44	121.68

There are no chirality outliers.

5 of 54 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	24	TRP	Peptide
2	A	26	ASP	Peptide
2	A	348	GLN	Peptide
2	B	183	ASN	Peptide
2	B	184	ASN	Peptide

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	1	1271	0	643	3	0
2	A	2742	0	2663	17	0
2	B	2714	0	2643	10	0
2	C	2705	0	2630	7	0
2	D	2705	0	2630	10	0
2	E	2705	0	2630	10	0
2	F	2509	0	2447	7	0
3	G	4009	0	3977	22	0
4	H	1606	0	1594	13	0
5	I	2923	0	2837	4	0
6	J	2978	0	2889	15	0
All	All	28867	0	27583	111	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 2.

The worst 5 of 111 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)
4:H:152:LEU:O	4:H:164:ARG:NH1	2.33	0.62
4:H:154:GLU:O	4:H:163:PHE:O	2.17	0.62
6:J:20:ARG:HD2	6:J:132:LEU:HD13	1.82	0.62
6:J:132:LEU:O	6:J:132:LEU:HD12	1.98	0.62
2:D:249:THR:HG23	2:D:258:ILE:HD12	1.83	0.59

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	
2	A	339/343 (99%)	292 (86%)	34 (10%)	13 (4%)	2	20
2	B	335/343 (98%)	287 (86%)	41 (12%)	7 (2%)	5	31
2	C	334/343 (97%)	294 (88%)	32 (10%)	8 (2%)	4	29
2	D	334/343 (97%)	289 (86%)	38 (11%)	7 (2%)	5	31
2	E	334/343 (97%)	280 (84%)	48 (14%)	6 (2%)	6	34
2	F	304/343 (89%)	256 (84%)	41 (14%)	7 (2%)	5	30
3	G	505/511 (99%)	393 (78%)	89 (18%)	23 (5%)	2	17
4	H	195/198 (98%)	141 (72%)	45 (23%)	9 (5%)	2	17
5	I	349/358 (98%)	252 (72%)	74 (21%)	23 (7%)	1	11
6	J	362/369 (98%)	276 (76%)	72 (20%)	14 (4%)	2	20
All	All	3391/3494 (97%)	2760 (81%)	514 (15%)	117 (4%)	4	23

5 of 117 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	17	ASP
2	A	25	PRO
2	A	58	LYS

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Mol	Chain	Res	Type
2	A	349	HIS
2	B	184	ASN

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	
2	A	300/301 (100%)	297 (99%)	3 (1%)	68	75
2	B	297/301 (99%)	292 (98%)	5 (2%)	53	70
2	C	296/301 (98%)	289 (98%)	7 (2%)	43	64
2	D	296/301 (98%)	293 (99%)	3 (1%)	68	75
2	E	296/301 (98%)	293 (99%)	3 (1%)	68	75
2	F	277/301 (92%)	272 (98%)	5 (2%)	51	69
3	G	451/451 (100%)	444 (98%)	7 (2%)	55	70
4	H	177/178 (99%)	174 (98%)	3 (2%)	53	70
5	I	322/322 (100%)	316 (98%)	6 (2%)	50	68
6	J	323/323 (100%)	317 (98%)	6 (2%)	50	68
All	All	3035/3080 (98%)	2987 (98%)	48 (2%)	54	70

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	406	THR
4	H	159	THR
3	G	442	VAL
3	G	533	PRO
5	I	92	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
5	I	338	GLN

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Mol	Chain	Res	Type
6	J	23	ASN
6	J	320	ASN
2	D	138	ASN
2	D	135	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	59/60 (98%)	27 (45%)	0

5 of 27 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	3	G
1	1	8	C
1	1	9	U
1	1	10	U
1	1	15	G

There are no RNA pucker outliers to report.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	I	3
6	J	2
3	G	2
2	A	1

The worst 5 of 8 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	172:SER	C	195:GLU	N	29.87
1	I	162:SER	C	193:GLY	N	29.40
1	G	276:ASN	C	384:ASN	N	23.55
1	A	231:GLU	C	240:THR	N	12.70
1	G	49:LYS	C	60:ALA	N	12.32

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-20350. 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.