



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 04:00 AM UTC

PDB ID : 7QGQ / pdb_00007qgq
EMDB ID : EMD-13957
Title : Extended H/L (SLPH/SLPL) complex from *C. difficile* (CD630 strain) fit into R20291 S-layer negative stain map
Authors : Banerji, O.; Wilson, J.S.; Bullough, P.A.
Deposited on : 2021-12-09
Resolution : Not provided

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

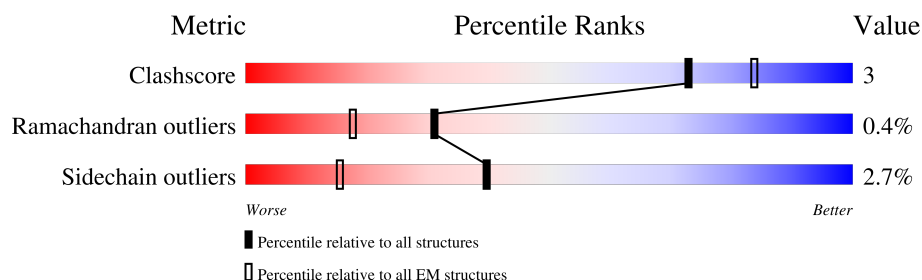
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is unknown.

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.



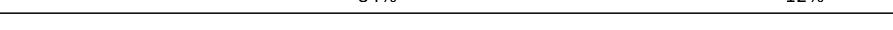
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	B	373	93% 7% .
1	D	373	92% 7% .
1	J	373	93% 6% .
1	K	373	92% 8%
1	L	373	93% 6% .
1	M	373	94% 6%
1	N	373	93% 6% .
1	T	373	92% 7% .
1	U	373	90% 9% .

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Mol	Chain	Length	Quality of chain
1	V	373	 90% 8% .
1	W	373	 90% 8% .
1	X	373	 89% 10% .
2	A	318	 86% 10% .
2	C	318	 89% 9% .
2	E	318	 84% 12% . .
2	F	318	 86% 12% .
2	G	318	 83% 13% .
2	H	318	 87% 11% .
2	I	318	 87% 11% .
2	O	318	 93% 7% .
2	P	318	 88% 9% .
2	Q	318	 87% 9% .
2	R	318	 84% 12% .
2	S	318	 84% 12% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 124044 atoms, of which 62208 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 Precursor of the S-layer proteins.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	B	373	Total	C	H	N	O	S	0	0
			5562	1711	2795	457	594	5		
1	J	373	Total	C	H	N	O	S	0	0
			5562	1711	2795	457	594	5		
1	D	373	Total	C	H	N	O	S	0	0
			5562	1711	2795	457	594	5		
1	T	373	Total	C	H	N	O	S	0	0
			5562	1711	2795	457	594	5		
1	K	373	Total	C	H	N	O	S	0	0
			5562	1711	2795	457	594	5		
1	L	373	Total	C	H	N	O	S	0	0
			5562	1711	2795	457	594	5		
1	U	373	Total	C	H	N	O	S	0	0
			5562	1711	2795	457	594	5		
1	V	373	Total	C	H	N	O	S	0	0
			5562	1711	2795	457	594	5		
1	M	373	Total	C	H	N	O	S	0	0
			5562	1711	2795	457	594	5		
1	N	373	Total	C	H	N	O	S	0	0
			5562	1711	2795	457	594	5		
1	W	373	Total	C	H	N	O	S	0	0
			5562	1711	2795	457	594	5		
1	X	373	Total	C	H	N	O	S	0	0
			5562	1711	2795	457	594	5		

- Molecule 2 is a protein called Precursor of the S-layer proteins.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	318	Total	C	H	N	O	S	0	0
			4775	1490	2389	394	500	2		
2	O	318	Total	C	H	N	O	S	0	0
			4775	1490	2389	394	500	2		
2	A	318	Total	C	H	N	O	S	0	0
			4775	1490	2389	394	500	2		

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Mol	Chain	Residues	Atoms						AltConf	Trace
2	P	318	Total 4775	C 1490	H 2389	N 394	O 500	S 2	0	0
2	Q	318	Total 4775	C 1490	H 2389	N 394	O 500	S 2	0	0
2	E	318	Total 4775	C 1490	H 2389	N 394	O 500	S 2	0	0
2	F	318	Total 4775	C 1490	H 2389	N 394	O 500	S 2	0	0
2	R	318	Total 4775	C 1490	H 2389	N 394	O 500	S 2	0	0
2	S	318	Total 4775	C 1490	H 2389	N 394	O 500	S 2	0	0
2	G	318	Total 4775	C 1490	H 2389	N 394	O 500	S 2	0	0
2	H	318	Total 4775	C 1490	H 2389	N 394	O 500	S 2	0	0
2	I	318	Total 4775	C 1490	H 2389	N 394	O 500	S 2	0	0

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: Precursor of the S-layer proteins

Chain B:  93% 7% .



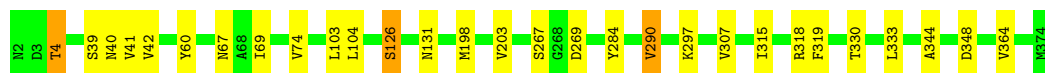
- Molecule 1: Precursor of the S-layer proteins

Chain J:  93% 6% .



- Molecule 1: Precursor of the S-layer proteins

Chain D:  92% 7% .



- Molecule 1: Precursor of the S-layer proteins

Chain T:  92% 7% .



- Molecule 1: Precursor of the S-layer proteins

Chain K:  92% 8% .



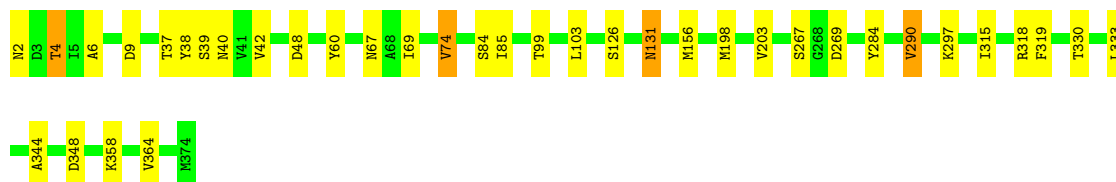
- Molecule 1: Precursor of the S-layer proteins

Chain L:  93% 6% .



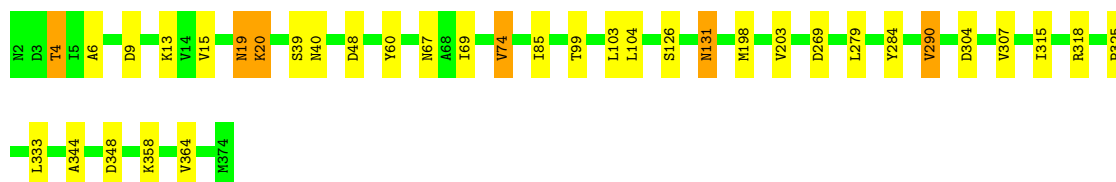
- Molecule 1: Precursor of the S-layer proteins

Chain U: 90% 9% .



- Molecule 1: Precursor of the S-layer proteins

Chain V: 90% 8% .



- Molecule 1: Precursor of the S-layer proteins

Chain M: 94% 6% .



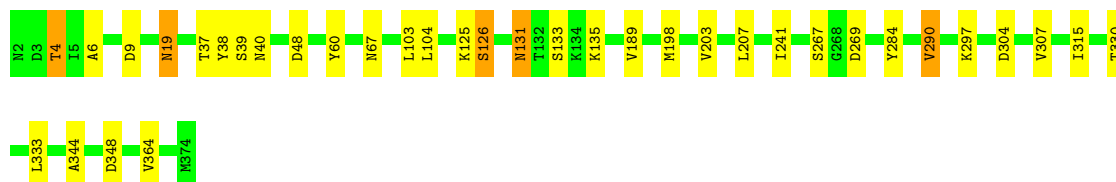
- Molecule 1: Precursor of the S-layer proteins

Chain N: 93% 6% .



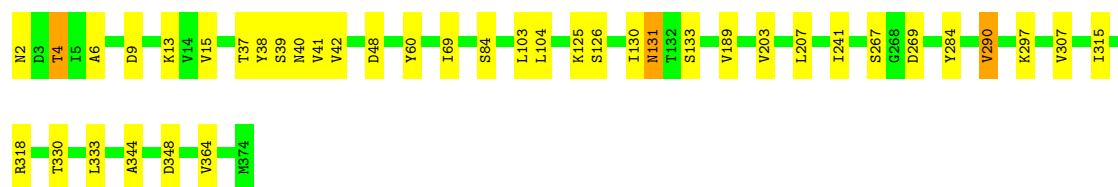
- Molecule 1: Precursor of the S-layer proteins

Chain W: 90% 8% .



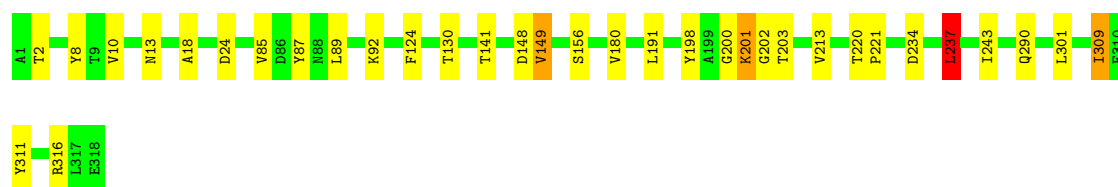
- Molecule 1: Precursor of the S-layer proteins

Chain X:  89% 10%



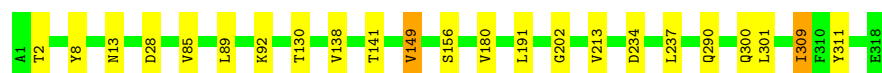
- Molecule 2: Precursor of the S-layer proteins

Chain C:  89% 9%



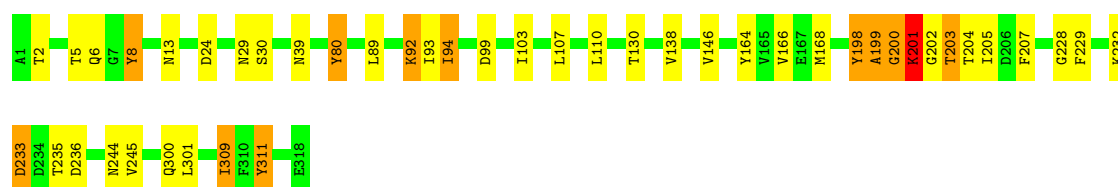
- Molecule 2: Precursor of the S-layer proteins

Chain O:  93% 7%



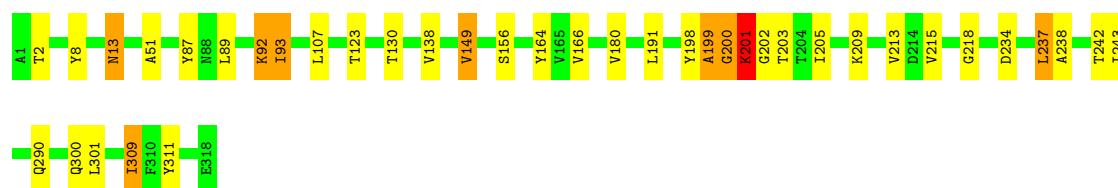
- Molecule 2: Precursor of the S-layer proteins

Chain A:  86% 10%



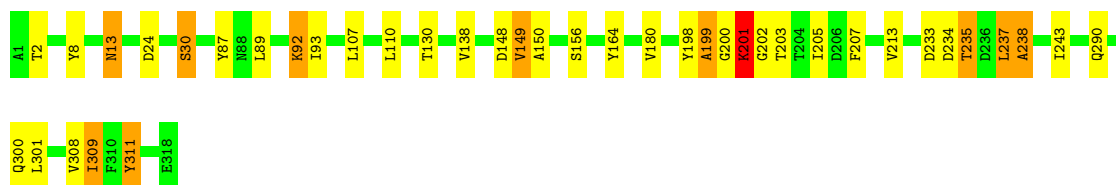
- Molecule 2: Precursor of the S-layer proteins

Chain P:  88% 9%

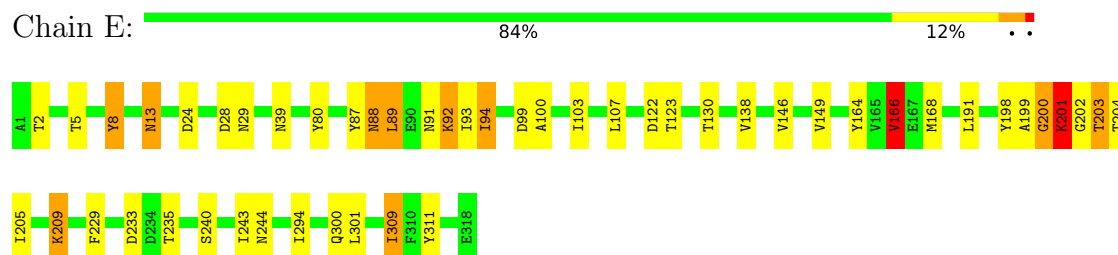


- Molecule 2: Precursor of the S-layer proteins

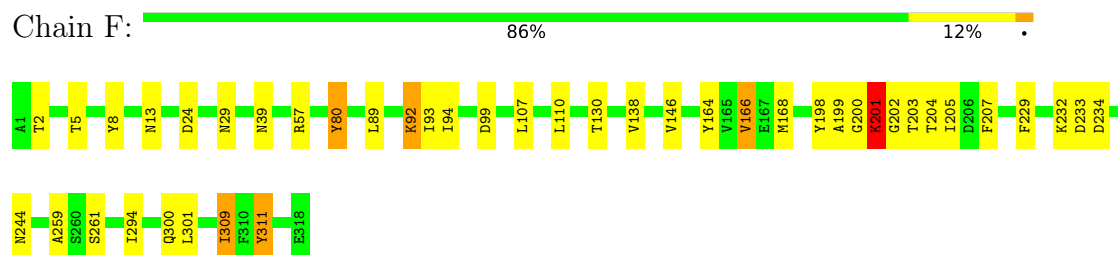
Chain Q:  87% 9%



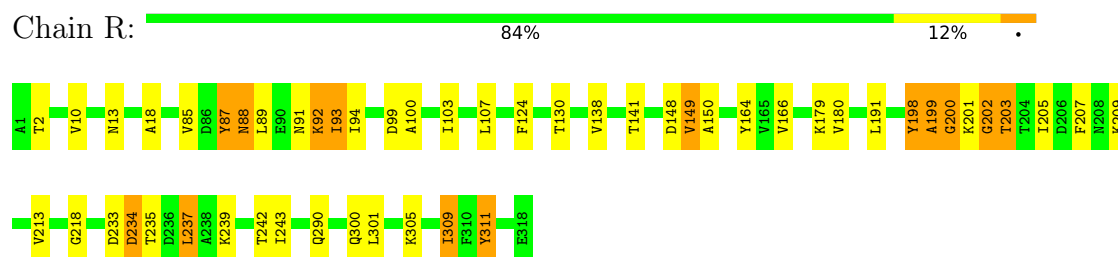
- Molecule 2: Precursor of the S-layer proteins



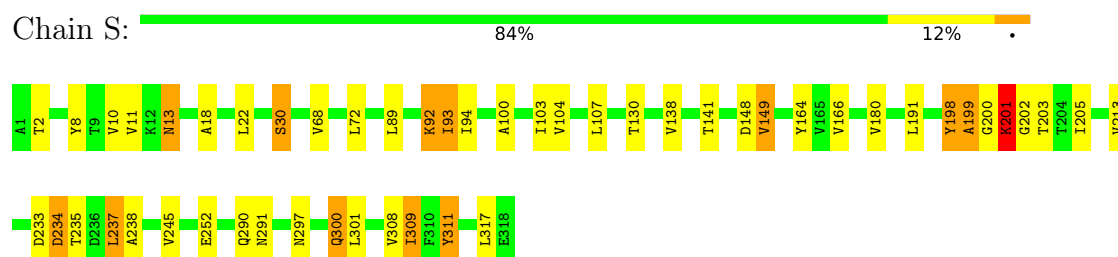
- Molecule 2: Precursor of the S-layer proteins



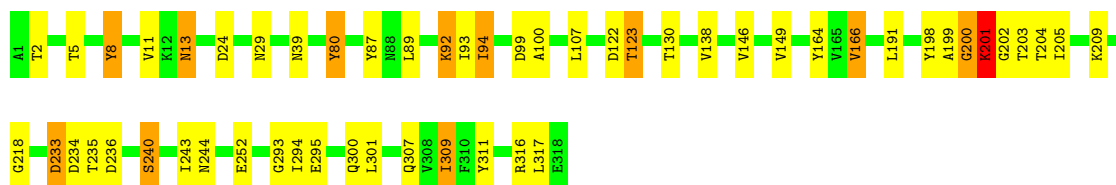
- Molecule 2: Precursor of the S-layer proteins



- Molecule 2: Precursor of the S-layer proteins



- Molecule 2: Precursor of the S-layer proteins



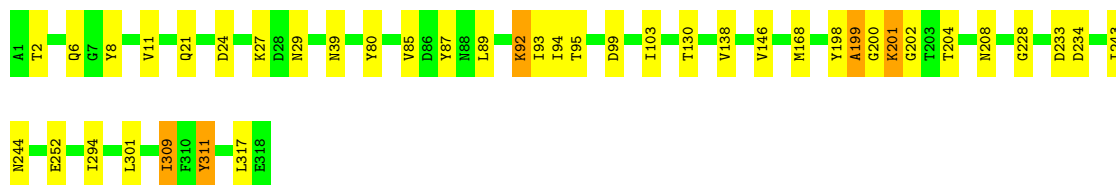
- Molecule 2: Precursor of the S-layer proteins

Chain H: 87% 11% .



- Molecule 2: Precursor of the S-layer proteins

Chain I: 87% 11% .



4 Experimental information

Property	Value	Source
EM reconstruction method	CRYSTALLOGRAPHY	Depositor
Imposed symmetry	3D CRYSTAL, $a=80$ Å, $b=80$ Å, $c=160$ Å, $\alpha=90^\circ$, $\beta=90^\circ$, $\gamma=100^\circ$, space group=P 1 1 2	Depositor
Number of images used	Not provided	
Resolution determination method	DIFFRACTION PATTERN/LAYERLINES	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	0.1	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN ULTRASCAN 4000 (4k 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	0.81	3/2790 (0.1%)	1.50	17/3774 (0.5%)
1	D	0.81	4/2790 (0.1%)	1.44	12/3774 (0.3%)
1	J	0.79	2/2790 (0.1%)	1.45	18/3774 (0.5%)
1	K	0.80	4/2790 (0.1%)	1.47	13/3774 (0.3%)
1	L	0.78	2/2790 (0.1%)	1.43	8/3774 (0.2%)
1	M	0.82	4/2790 (0.1%)	1.46	12/3774 (0.3%)
1	N	0.83	4/2790 (0.1%)	1.47	16/3774 (0.4%)
1	T	0.78	2/2790 (0.1%)	1.41	12/3774 (0.3%)
1	U	0.77	2/2790 (0.1%)	1.43	15/3774 (0.4%)
1	V	0.77	1/2790 (0.0%)	1.42	14/3774 (0.4%)
1	W	0.80	1/2790 (0.0%)	1.46	20/3774 (0.5%)
1	X	0.81	3/2790 (0.1%)	1.47	18/3774 (0.5%)
2	A	0.80	0/2412	1.49	21/3261 (0.6%)
2	C	0.77	0/2412	1.37	11/3261 (0.3%)
2	E	0.79	0/2412	1.51	22/3261 (0.7%)
2	F	0.78	0/2412	1.46	17/3261 (0.5%)
2	G	0.80	0/2412	1.49	23/3261 (0.7%)
2	H	0.79	0/2412	1.42	12/3261 (0.4%)
2	I	0.78	0/2412	1.42	16/3261 (0.5%)
2	O	0.78	0/2412	1.36	3/3261 (0.1%)
2	P	0.82	0/2412	1.47	15/3261 (0.5%)
2	Q	0.80	0/2412	1.45	18/3261 (0.6%)
2	R	0.82	0/2412	1.51	21/3261 (0.6%)
2	S	0.80	0/2412	1.48	23/3261 (0.7%)
All	All	0.80	32/62424 (0.1%)	1.45	377/84420 (0.4%)

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	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	J	0	2
1	K	0	1
1	L	0	1
1	M	0	1
1	T	0	1
1	U	0	1
2	A	0	4
2	C	0	4
2	E	0	3
2	F	0	3
2	G	0	2
2	H	0	3
2	I	0	2
2	O	0	2
2	P	0	1
2	Q	0	2
2	R	0	2
2	S	0	2
All	All	0	39

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	40	ASN	CA-C	8.40	1.63	1.52
1	M	40	ASN	CA-C	8.17	1.63	1.52
1	D	40	ASN	CA-C	7.93	1.62	1.52
1	M	41	VAL	N-CA	7.17	1.55	1.46
1	N	41	VAL	N-CA	7.15	1.55	1.46

The worst 5 of 377 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	40	ASN	N-CA-C	18.00	138.31	112.94
1	K	40	ASN	N-CA-C	16.25	135.85	112.94
1	X	40	ASN	N-CA-C	16.09	133.32	112.41
1	D	40	ASN	N-CA-C	15.44	134.71	112.94
1	N	40	ASN	N-CA-C	15.25	135.75	113.02

There are no chirality outliers.

5 of 39 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	61	TYR	Sidechain
2	C	311	TYR	Sidechain
2	C	316	ARG	Sidechain
2	C	8	TYR	Sidechain
2	C	87	TYR	Sidechain

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	2767	2795	2792	20	0
1	D	2767	2795	2792	10	0
1	J	2767	2795	2792	18	0
1	K	2767	2795	2792	19	0
1	L	2767	2795	2792	17	0
1	M	2767	2795	2792	12	0
1	N	2767	2795	2792	13	0
1	T	2767	2795	2792	10	0
1	U	2767	2795	2792	18	0
1	V	2767	2795	2792	23	0
1	W	2767	2795	2792	14	0
1	X	2767	2795	2792	20	0
2	A	2386	2389	2389	38	0
2	C	2386	2389	2389	11	0
2	E	2386	2389	2389	45	0
2	F	2386	2389	2389	28	0
2	G	2386	2389	2389	40	0
2	H	2386	2389	2389	22	0
2	I	2386	2389	2389	19	0
2	O	2386	2389	2389	4	0
2	P	2386	2389	2389	24	0
2	Q	2386	2389	2389	26	0
2	R	2386	2389	2389	39	0
2	S	2386	2389	2389	32	0
All	All	61836	62208	62172	409	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 3.

The worst 5 of 409 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:P:237:LEU:HD13	2:P:243:ILE:HG22	1.51	0.89
2:S:309:ILE:HD13	1:X:4:THR:H	1.45	0.80
1:B:4:THR:H	2:A:309:ILE:HD13	1.47	0.79
1:K:4:THR:H	2:F:309:ILE:HD13	1.49	0.78
2:Q:309:ILE:HD13	1:U:4:THR:H	1.49	0.77

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	371/373 (100%)	363 (98%)	6 (2%)	2 (0%)	24	24
1	D	371/373 (100%)	365 (98%)	6 (2%)	0	100	100
1	J	371/373 (100%)	361 (97%)	8 (2%)	2 (0%)	24	24
1	K	371/373 (100%)	364 (98%)	6 (2%)	1 (0%)	36	36
1	L	371/373 (100%)	364 (98%)	6 (2%)	1 (0%)	36	36
1	M	371/373 (100%)	363 (98%)	7 (2%)	1 (0%)	36	36
1	N	371/373 (100%)	364 (98%)	6 (2%)	1 (0%)	36	36
1	T	371/373 (100%)	363 (98%)	8 (2%)	0	100	100
1	U	371/373 (100%)	363 (98%)	7 (2%)	1 (0%)	36	36
1	V	371/373 (100%)	361 (97%)	10 (3%)	0	100	100
1	W	371/373 (100%)	361 (97%)	9 (2%)	1 (0%)	36	36
1	X	371/373 (100%)	363 (98%)	7 (2%)	1 (0%)	36	36
2	A	316/318 (99%)	308 (98%)	7 (2%)	1 (0%)	36	36
2	C	316/318 (99%)	309 (98%)	5 (2%)	2 (1%)	21	21
2	E	316/318 (99%)	308 (98%)	7 (2%)	1 (0%)	36	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	316/318 (99%)	308 (98%)	7 (2%)	1 (0%)	36	36
2	G	316/318 (99%)	309 (98%)	6 (2%)	1 (0%)	36	36
2	H	316/318 (99%)	309 (98%)	6 (2%)	1 (0%)	36	36
2	I	316/318 (99%)	308 (98%)	7 (2%)	1 (0%)	36	36
2	O	316/318 (99%)	309 (98%)	6 (2%)	1 (0%)	36	36
2	P	316/318 (99%)	309 (98%)	4 (1%)	3 (1%)	14	14
2	Q	316/318 (99%)	309 (98%)	4 (1%)	3 (1%)	14	14
2	R	316/318 (99%)	308 (98%)	6 (2%)	2 (1%)	21	21
2	S	316/318 (99%)	309 (98%)	5 (2%)	2 (1%)	21	21
All	All	8244/8292 (99%)	8058 (98%)	156 (2%)	30 (0%)	31	30

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	149	VAL
2	O	149	VAL
2	A	201	LYS
2	P	149	VAL
2	P	201	LYS

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	312/312 (100%)	309 (99%)	3 (1%)	68	68
1	D	312/312 (100%)	305 (98%)	7 (2%)	45	45
1	J	312/312 (100%)	309 (99%)	3 (1%)	68	68
1	K	312/312 (100%)	308 (99%)	4 (1%)	61	61
1	L	312/312 (100%)	308 (99%)	4 (1%)	61	61
1	M	312/312 (100%)	308 (99%)	4 (1%)	61	61
1	N	312/312 (100%)	308 (99%)	4 (1%)	61	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	T	312/312 (100%)	305 (98%)	7 (2%)	45	45
1	U	312/312 (100%)	305 (98%)	7 (2%)	45	45
1	V	312/312 (100%)	305 (98%)	7 (2%)	45	45
1	W	312/312 (100%)	306 (98%)	6 (2%)	50	50
1	X	312/312 (100%)	306 (98%)	6 (2%)	50	50
2	A	259/259 (100%)	250 (96%)	9 (4%)	32	32
2	C	259/259 (100%)	248 (96%)	11 (4%)	26	26
2	E	259/259 (100%)	249 (96%)	10 (4%)	28	28
2	F	259/259 (100%)	250 (96%)	9 (4%)	32	32
2	G	259/259 (100%)	249 (96%)	10 (4%)	28	28
2	H	259/259 (100%)	251 (97%)	8 (3%)	35	35
2	I	259/259 (100%)	251 (97%)	8 (3%)	35	35
2	O	259/259 (100%)	247 (95%)	12 (5%)	24	24
2	P	259/259 (100%)	248 (96%)	11 (4%)	26	26
2	Q	259/259 (100%)	247 (95%)	12 (5%)	24	24
2	R	259/259 (100%)	246 (95%)	13 (5%)	22	22
2	S	259/259 (100%)	246 (95%)	13 (5%)	22	22
All	All	6852/6852 (100%)	6664 (97%)	188 (3%)	40	39

5 of 188 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	309	ILE
2	G	13	ASN
2	R	130	THR
2	S	13	ASN
2	G	301	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 100 such sidechains are listed below:

Mol	Chain	Res	Type
1	U	338	ASN
2	S	131	GLN
1	X	206	GLN
1	V	338	ASN

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Mol	Chain	Res	Type
2	F	300	GLN

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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13957. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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.