



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 13, 2020 – 02:16 PM BST

PDB ID : 3ZTE
Title : Crystal Structure of the TRP RNA-Binding Attenuation Protein (TRAP) from *Bacillus Licheniformis*.
Authors : Shevtsov, M.B.; Chen, Y.; Gollnick, P.; Antson, A.A.
Deposited on : 2011-07-07
Resolution : 2.41 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.4.dev1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

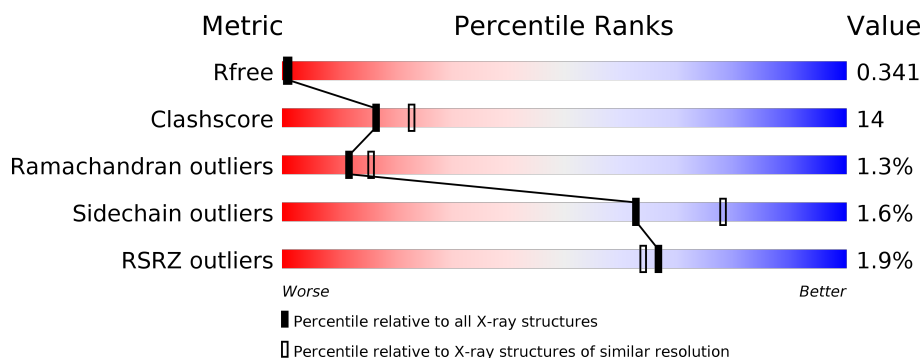
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	78	<div> <div>3%</div> <div> <div></div> <div>63%</div> <div>24%</div> <div>•</div> <div>12%</div> </div> </div>
1	B	78	<div> <div></div> <div> <div>74%</div> <div>13%</div> <div>•</div> <div>12%</div> </div> </div>
1	C	78	<div> <div>4%</div> <div> <div></div> <div>62%</div> <div>26%</div> <div>•</div> <div>12%</div> </div> </div>
1	D	78	<div> <div>3%</div> <div> <div></div> <div>68%</div> <div>19%</div> <div>•</div> <div>12%</div> </div> </div>
1	E	78	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>17%</div> <div>•</div> <div>12%</div> </div> </div>
1	F	78	<div> <div>%</div> <div> <div></div> <div>59%</div> <div>27%</div> <div>•</div> <div>12%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	78	
1	H	78	
1	I	78	
1	J	78	
1	K	78	
1	L	78	
1	M	78	
1	N	78	
1	O	78	
1	P	78	
1	Q	78	
1	R	78	
1	S	78	
1	T	78	
1	U	78	
1	V	78	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 12416 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 TRYPTOPHAN OPERON RNA-BINDING ATTENUATION PROTEIN (TRAP).

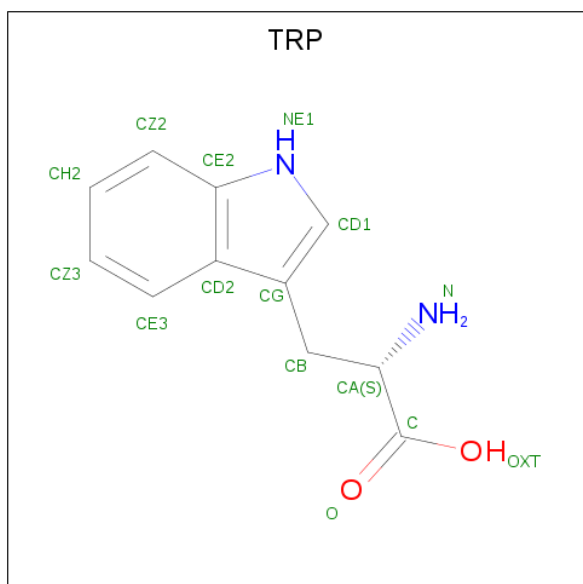
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	69	Total	C	N	O	S	0	0	1
			525	324	94	104	3			
1	B	69	Total	C	N	O	S	0	1	1
			531	328	94	106	3			
1	C	69	Total	C	N	O	S	0	0	1
			525	324	94	104	3			
1	D	69	Total	C	N	O	S	0	0	1
			525	324	94	104	3			
1	E	69	Total	C	N	O	S	0	0	1
			525	324	94	104	3			
1	F	69	Total	C	N	O	S	0	1	1
			531	328	94	106	3			
1	G	69	Total	C	N	O	S	0	0	1
			525	324	94	104	3			
1	H	69	Total	C	N	O	S	0	0	1
			525	324	94	104	3			
1	I	69	Total	C	N	O	S	0	0	1
			525	324	94	104	3			
1	J	70	Total	C	N	O	S	0	0	1
			533	328	96	106	3			
1	K	69	Total	C	N	O	S	0	0	1
			525	324	94	104	3			
1	L	71	Total	C	N	O	S	0	1	1
			545	335	97	110	3			
1	M	69	Total	C	N	O	S	0	0	1
			525	324	94	104	3			
1	N	69	Total	C	N	O	S	0	0	1
			525	324	94	104	3			
1	O	69	Total	C	N	O	S	0	1	1
			533	332	94	104	3			
1	P	69	Total	C	N	O	S	0	1	1
			533	329	97	104	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	69	Total	C	N	O	S	0	0	1
			525	324	94	104	3			
1	R	69	Total	C	N	O	S	0	0	1
			525	324	94	104	3			
1	S	69	Total	C	N	O	S	0	0	1
			525	324	94	104	3			
1	T	69	Total	C	N	O	S	0	0	1
			525	324	94	104	3			
1	U	70	Total	C	N	O	S	0	0	1
			533	328	96	106	3			
1	V	69	Total	C	N	O	S	0	0	1
			525	324	94	104	3			

- Molecule 2 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	11	2	2		
2	B	1	Total	C	N	O	0	0
			15	11	2	2		
2	C	1	Total	C	N	O	0	0
			15	11	2	2		
2	D	1	Total	C	N	O	0	0
			15	11	2	2		
2	E	1	Total	C	N	O	0	0
			15	11	2	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	F	1	Total	C	N	O	0	0
			15	11	2	2		
2	G	1	Total	C	N	O	0	0
			15	11	2	2		
2	H	1	Total	C	N	O	0	0
			15	11	2	2		
2	I	1	Total	C	N	O	0	0
			15	11	2	2		
2	J	1	Total	C	N	O	0	0
			15	11	2	2		
2	K	1	Total	C	N	O	0	0
			15	11	2	2		
2	L	1	Total	C	N	O	0	0
			15	11	2	2		
2	M	1	Total	C	N	O	0	0
			15	11	2	2		
2	N	1	Total	C	N	O	0	0
			15	11	2	2		
2	O	1	Total	C	N	O	0	0
			15	11	2	2		
2	P	1	Total	C	N	O	0	0
			15	11	2	2		
2	Q	1	Total	C	N	O	0	0
			15	11	2	2		
2	R	1	Total	C	N	O	0	0
			15	11	2	2		
2	S	1	Total	C	N	O	0	0
			15	11	2	2		
2	T	1	Total	C	N	O	0	0
			15	11	2	2		
2	U	1	Total	C	N	O	0	0
			15	11	2	2		
2	V	1	Total	C	N	O	0	0
			15	11	2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	32	Total	O	0	0
			32	32		
3	B	28	Total	O	0	0
			28	28		

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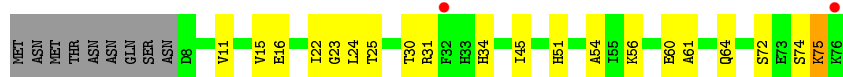
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	16	Total 16	O 16	0	0
3	D	32	Total 32	O 32	0	0
3	E	30	Total 30	O 30	0	0
3	F	22	Total 22	O 22	0	0
3	G	20	Total 20	O 20	0	0
3	H	15	Total 15	O 15	0	0
3	I	23	Total 23	O 23	0	0
3	J	21	Total 21	O 21	0	0
3	K	10	Total 10	O 10	0	0
3	L	26	Total 26	O 26	0	0
3	M	18	Total 18	O 18	0	0
3	N	19	Total 19	O 19	0	0
3	O	25	Total 25	O 25	0	0
3	P	20	Total 20	O 20	0	0
3	Q	16	Total 16	O 16	0	0
3	R	19	Total 19	O 19	0	0
3	S	14	Total 14	O 14	0	0
3	T	23	Total 23	O 23	0	0
3	U	26	Total 26	O 26	0	0
3	V	17	Total 17	O 17	0	0

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: TRYPTOPHAN OPERON RNA-BINDING ATTENUATION PROTEIN (TRAP)



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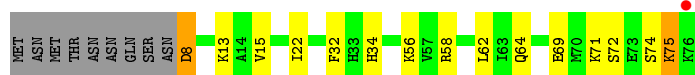
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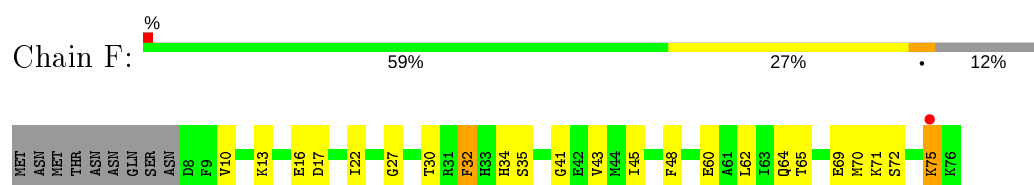
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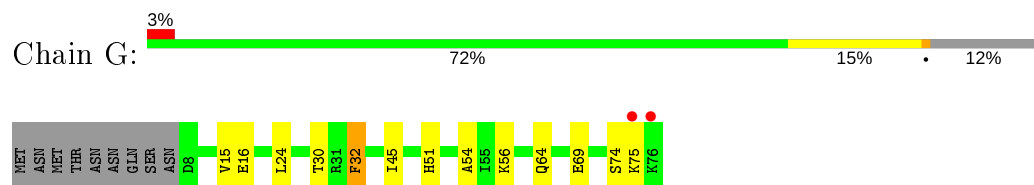
- Molecule 1: TRYPTOPHAN OPERON RNA-BINDING ATTENUATION PROTEIN (TRAP)



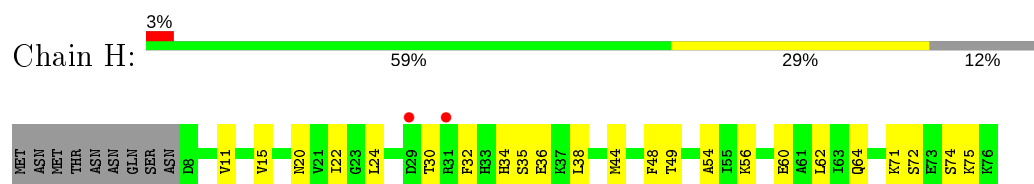
- Molecule 1: TRYPTOPHAN OPERON RNA-BINDING ATTENUATION PROTEIN (TRAP)



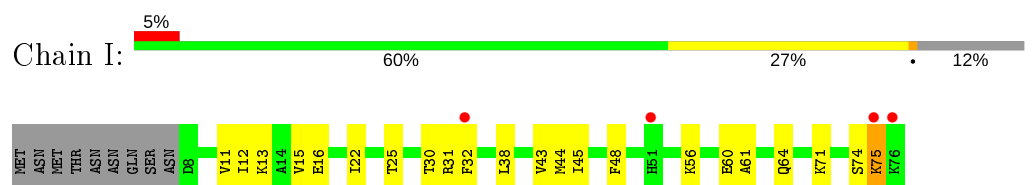
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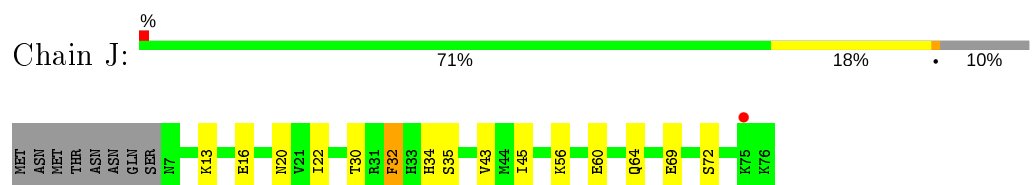
- Molecule 1: TRYPTOPHAN OPERON RNA-BINDING ATTENUATION PROTEIN (TRAP)



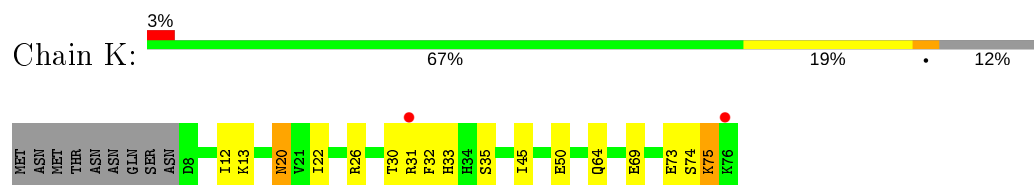
- Molecule 1: TRYPTOPHAN OPERON RNA-BINDING ATTENUATION PROTEIN (TRAP)



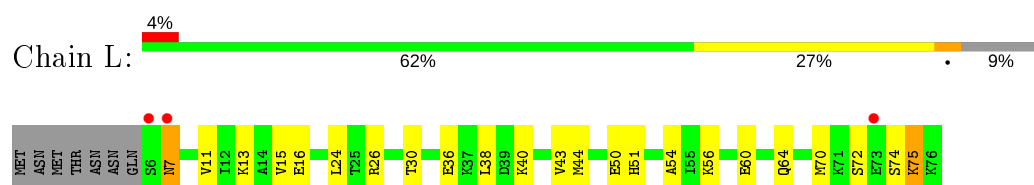
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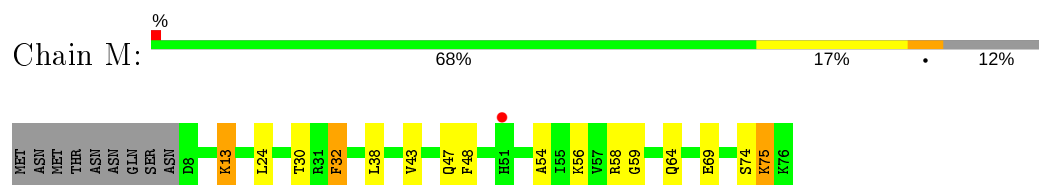
- Molecule 1: TRYPTOPHAN OPERON RNA-BINDING ATTENUATION PROTEIN (TRAP)



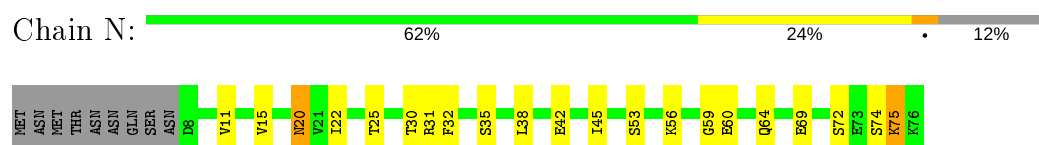
- Molecule 1: TRYPTOPHAN OPERON RNA-BINDING ATTENUATION PROTEIN (TRAP)



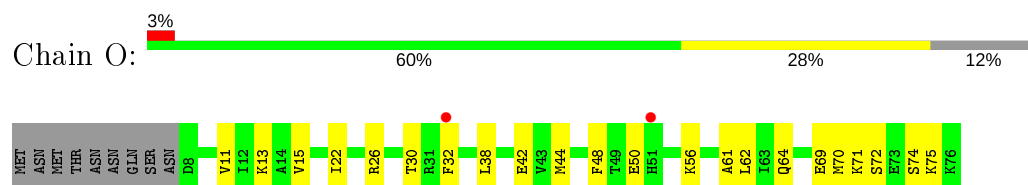
● Molecule 1: TRYPTOPHAN OPERON RNA-BINDING ATTENUATION PROTEIN (TRAP)



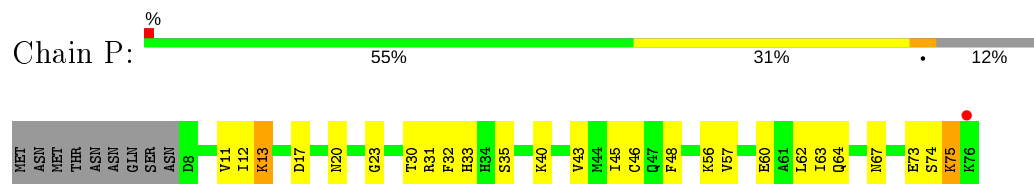
● Molecule 1: TRYPTOPHAN OPERON RNA-BINDING ATTENUATION PROTEIN (TRAP)



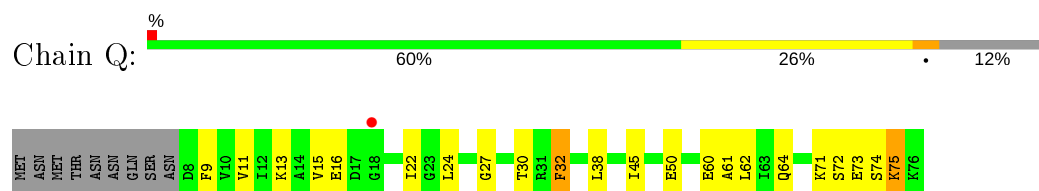
● Molecule 1: TRYPTOPHAN OPERON RNA-BINDING ATTENUATION PROTEIN (TRAP)



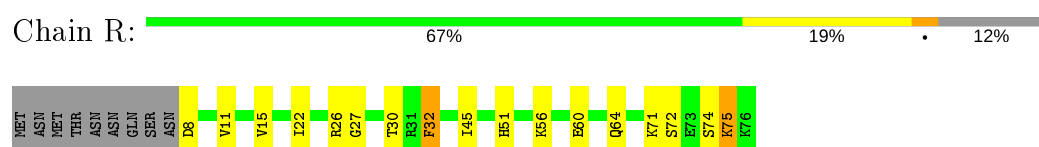
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4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	145.43 Å 145.43 Å 183.07 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.83 – 2.41 44.83 – 2.41	Depositor EDS
% Data completeness (in resolution range)	96.5 (44.83-2.41) 96.5 (44.83-2.41)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.47 (at 2.39 Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.281 , 0.346 0.276 , 0.341	Depositor DCC
R_{free} test set	3709 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12416	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.26 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5969e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.31	0/530	0.42	0/710
1	B	0.31	0/539	0.47	0/722
1	C	0.32	0/530	0.46	0/710
1	D	0.33	0/530	0.46	0/710
1	E	0.33	0/530	0.47	0/710
1	F	0.32	0/539	0.44	0/722
1	G	0.31	0/530	0.44	0/710
1	H	0.32	0/530	0.46	0/710
1	I	0.31	0/530	0.45	0/710
1	J	0.31	0/538	0.43	0/721
1	K	0.32	0/530	0.47	0/710
1	L	0.31	0/553	0.45	0/741
1	M	0.32	0/530	0.46	0/710
1	N	0.33	0/530	0.46	0/710
1	O	0.32	0/542	0.44	0/726
1	P	0.32	0/541	0.46	0/724
1	Q	0.32	0/530	0.43	0/710
1	R	0.32	0/530	0.45	0/710
1	S	0.32	0/530	0.47	0/710
1	T	0.32	0/530	0.45	0/710
1	U	0.32	0/538	0.45	0/721
1	V	0.32	0/530	0.46	0/710
All	All	0.32	0/11740	0.45	0/15727

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	525	0	524	20	0
1	B	531	0	530	13	0
1	C	525	0	524	14	0
1	D	525	0	524	16	0
1	E	525	0	524	12	0
1	F	531	0	530	20	0
1	G	525	0	524	15	0
1	H	525	0	524	27	0
1	I	525	0	524	23	0
1	J	533	0	530	12	0
1	K	525	0	524	13	0
1	L	545	0	541	19	0
1	M	525	0	524	14	0
1	N	525	0	524	17	0
1	O	533	0	533	17	0
1	P	533	0	537	20	0
1	Q	525	0	524	26	0
1	R	525	0	524	21	0
1	S	525	0	524	21	0
1	T	525	0	524	18	0
1	U	533	0	530	15	0
1	V	525	0	524	15	0
2	A	15	0	9	0	0
2	B	15	0	9	1	0
2	C	15	0	9	0	0
2	D	15	0	9	2	0
2	E	15	0	9	1	0
2	F	15	0	9	0	0
2	G	15	0	9	1	0
2	H	15	0	9	2	0
2	I	15	0	9	1	0
2	J	15	0	9	1	0
2	K	15	0	9	1	0
2	L	15	0	9	1	0
2	M	15	0	9	1	0
2	N	15	0	9	1	0
2	O	15	0	9	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	15	0	9	2	0
2	Q	15	0	9	1	0
2	R	15	0	9	2	0
2	S	15	0	9	1	0
2	T	15	0	9	2	0
2	U	15	0	9	1	0
2	V	15	0	9	2	0
3	A	32	0	0	1	0
3	B	28	0	0	4	0
3	C	16	0	0	0	0
3	D	32	0	0	1	0
3	E	30	0	0	2	0
3	F	22	0	0	0	0
3	G	20	0	0	0	0
3	H	15	0	0	1	0
3	I	23	0	0	1	0
3	J	21	0	0	2	0
3	K	10	0	0	0	0
3	L	26	0	0	2	0
3	M	18	0	0	0	0
3	N	19	0	0	0	0
3	O	25	0	0	1	0
3	P	20	0	0	2	0
3	Q	16	0	0	1	0
3	R	19	0	0	1	0
3	S	14	0	0	1	0
3	T	23	0	0	1	0
3	U	26	0	0	0	0
3	V	17	0	0	0	0
All	All	12416	0	11789	337	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 14.

The worst 5 of 337 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:J:32:PHE:HE2	1:J:35:SER:HG	1.06	0.98
1:M:32:PHE:H	1:M:32:PHE:HD1	1.11	0.93
1:R:56:LYS:HE3	1:S:38:LEU:HD23	1.52	0.90
1:N:74:SER:O	1:N:75:LYS:HB2	1.68	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:74:SER:O	1:M:75:LYS:HB2	1.72	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 X-ray entries followed by that with respect to entries of similar resolution.

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	67/78 (86%)	66 (98%)	0	1 (2%)	10	13
1	B	68/78 (87%)	65 (96%)	2 (3%)	1 (2%)	10	13
1	C	67/78 (86%)	66 (98%)	0	1 (2%)	10	13
1	D	67/78 (86%)	65 (97%)	2 (3%)	0	100	100
1	E	67/78 (86%)	65 (97%)	1 (2%)	1 (2%)	10	13
1	F	68/78 (87%)	65 (96%)	2 (3%)	1 (2%)	10	13
1	G	67/78 (86%)	66 (98%)	1 (2%)	0	100	100
1	H	67/78 (86%)	63 (94%)	4 (6%)	0	100	100
1	I	67/78 (86%)	64 (96%)	2 (3%)	1 (2%)	10	13
1	J	68/78 (87%)	66 (97%)	2 (3%)	0	100	100
1	K	67/78 (86%)	65 (97%)	1 (2%)	1 (2%)	10	13
1	L	70/78 (90%)	67 (96%)	1 (1%)	2 (3%)	4	3
1	M	67/78 (86%)	65 (97%)	1 (2%)	1 (2%)	10	13
1	N	67/78 (86%)	66 (98%)	0	1 (2%)	10	13
1	O	68/78 (87%)	67 (98%)	1 (2%)	0	100	100
1	P	68/78 (87%)	67 (98%)	0	1 (2%)	10	13
1	Q	67/78 (86%)	66 (98%)	0	1 (2%)	10	13
1	R	67/78 (86%)	66 (98%)	0	1 (2%)	10	13
1	S	67/78 (86%)	64 (96%)	1 (2%)	2 (3%)	4	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	T	67/78 (86%)	64 (96%)	2 (3%)	1 (2%)	10	13
1	U	68/78 (87%)	67 (98%)	0	1 (2%)	10	13
1	V	67/78 (86%)	66 (98%)	0	1 (2%)	10	13
All	All	1483/1716 (86%)	1441 (97%)	23 (2%)	19 (1%)	12	16

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	75	LYS
1	C	75	LYS
1	I	75	LYS
1	K	75	LYS
1	L	7	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 X-ray entries followed by that with respect to entries of similar resolution.

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	58/68 (85%)	58 (100%)	0	100	100
1	B	59/68 (87%)	59 (100%)	0	100	100
1	C	58/68 (85%)	56 (97%)	2 (3%)	37	54
1	D	58/68 (85%)	57 (98%)	1 (2%)	60	77
1	E	58/68 (85%)	56 (97%)	2 (3%)	37	54
1	F	59/68 (87%)	58 (98%)	1 (2%)	60	77
1	G	58/68 (85%)	57 (98%)	1 (2%)	60	77
1	H	58/68 (85%)	58 (100%)	0	100	100
1	I	58/68 (85%)	58 (100%)	0	100	100
1	J	59/68 (87%)	58 (98%)	1 (2%)	60	77
1	K	58/68 (85%)	56 (97%)	2 (3%)	37	54
1	L	61/68 (90%)	60 (98%)	1 (2%)	62	78
1	M	58/68 (85%)	56 (97%)	2 (3%)	37	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	58/68 (85%)	57 (98%)	1 (2%)	60	77
1	O	59/68 (87%)	59 (100%)	0	100	100
1	P	59/68 (87%)	58 (98%)	1 (2%)	60	77
1	Q	58/68 (85%)	56 (97%)	2 (3%)	37	54
1	R	58/68 (85%)	57 (98%)	1 (2%)	60	77
1	S	58/68 (85%)	58 (100%)	0	100	100
1	T	58/68 (85%)	58 (100%)	0	100	100
1	U	59/68 (87%)	58 (98%)	1 (2%)	60	77
1	V	58/68 (85%)	56 (97%)	2 (3%)	37	54
All	All	1285/1496 (86%)	1264 (98%)	21 (2%)	62	78

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	31	ARG
1	M	13	LYS
1	R	32	PHE
1	K	20	ASN
1	U	32	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	20	ASN
1	L	7	ASN
1	S	47	GLN
1	J	20	ASN
1	O	20	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 monosaccharides in this entry.

5.6 Ligand geometry

22 ligands are 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$
2	TRP	M	80	-	12,16,16	1.14	0	12,22,22	1.25	2 (16%)
2	TRP	U	80	-	12,16,16	1.19	1 (8%)	12,22,22	1.32	2 (16%)
2	TRP	P	80	-	12,16,16	1.15	0	12,22,22	1.25	2 (16%)
2	TRP	C	80	-	12,16,16	1.16	0	12,22,22	1.35	2 (16%)
2	TRP	G	80	-	12,16,16	1.16	0	12,22,22	1.20	1 (8%)
2	TRP	B	80	-	12,16,16	1.15	0	12,22,22	1.28	2 (16%)
2	TRP	A	80	-	12,16,16	1.17	0	12,22,22	1.33	2 (16%)
2	TRP	S	80	-	12,16,16	1.14	0	12,22,22	1.25	2 (16%)
2	TRP	H	80	-	12,16,16	1.19	0	12,22,22	1.25	2 (16%)
2	TRP	O	80	-	12,16,16	1.19	0	12,22,22	1.33	2 (16%)
2	TRP	J	80	-	12,16,16	1.18	0	12,22,22	1.26	2 (16%)
2	TRP	T	80	-	12,16,16	1.15	0	12,22,22	1.23	2 (16%)
2	TRP	F	80	-	12,16,16	1.14	0	12,22,22	1.16	1 (8%)
2	TRP	N	80	-	12,16,16	1.18	0	12,22,22	1.29	2 (16%)
2	TRP	I	80	-	12,16,16	1.14	0	12,22,22	1.28	2 (16%)
2	TRP	V	80	-	12,16,16	1.16	0	12,22,22	1.22	2 (16%)
2	TRP	D	80	-	12,16,16	1.16	0	12,22,22	1.21	2 (16%)
2	TRP	K	80	-	12,16,16	1.16	0	12,22,22	1.27	2 (16%)
2	TRP	L	80	-	12,16,16	1.18	0	12,22,22	1.29	2 (16%)
2	TRP	R	80	-	12,16,16	1.17	0	12,22,22	1.18	1 (8%)
2	TRP	Q	80	-	12,16,16	1.15	0	12,22,22	1.22	2 (16%)
2	TRP	E	80	-	12,16,16	1.15	0	12,22,22	1.39	2 (16%)

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
2	TRP	M	80	-	-	0/3/8/8	0/2/2/2
2	TRP	U	80	-	-	0/3/8/8	0/2/2/2
2	TRP	P	80	-	-	0/3/8/8	0/2/2/2
2	TRP	C	80	-	-	0/3/8/8	0/2/2/2
2	TRP	G	80	-	-	0/3/8/8	0/2/2/2
2	TRP	B	80	-	-	0/3/8/8	0/2/2/2
2	TRP	A	80	-	-	0/3/8/8	0/2/2/2
2	TRP	S	80	-	-	0/3/8/8	0/2/2/2
2	TRP	H	80	-	-	0/3/8/8	0/2/2/2
2	TRP	O	80	-	-	0/3/8/8	0/2/2/2
2	TRP	J	80	-	-	0/3/8/8	0/2/2/2
2	TRP	T	80	-	-	0/3/8/8	0/2/2/2
2	TRP	F	80	-	-	0/3/8/8	0/2/2/2
2	TRP	N	80	-	-	0/3/8/8	0/2/2/2
2	TRP	I	80	-	-	0/3/8/8	0/2/2/2
2	TRP	V	80	-	-	0/3/8/8	0/2/2/2
2	TRP	D	80	-	-	0/3/8/8	0/2/2/2
2	TRP	K	80	-	-	0/3/8/8	0/2/2/2
2	TRP	L	80	-	-	0/3/8/8	0/2/2/2
2	TRP	R	80	-	-	0/3/8/8	0/2/2/2
2	TRP	Q	80	-	-	0/3/8/8	0/2/2/2
2	TRP	E	80	-	-	0/3/8/8	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	80	TRP	CD2-CE2	2.01	1.48	1.42

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	80	TRP	CE3-CD2-CE2	2.88	121.99	118.17
2	A	80	TRP	CE3-CD2-CE2	2.73	121.79	118.17
2	C	80	TRP	CE3-CD2-CE2	2.72	121.77	118.17
2	O	80	TRP	CE3-CD2-CE2	2.71	121.76	118.17
2	L	80	TRP	CE3-CD2-CE2	2.67	121.71	118.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

19 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	80	TRP	1	0
2	U	80	TRP	1	0
2	P	80	TRP	2	0
2	G	80	TRP	1	0
2	B	80	TRP	1	0
2	S	80	TRP	1	0
2	H	80	TRP	2	0
2	O	80	TRP	2	0
2	J	80	TRP	1	0
2	T	80	TRP	2	0
2	N	80	TRP	1	0
2	I	80	TRP	1	0
2	V	80	TRP	2	0
2	D	80	TRP	2	0
2	K	80	TRP	1	0
2	L	80	TRP	1	0
2	R	80	TRP	2	0
2	Q	80	TRP	1	0
2	E	80	TRP	1	0

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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	69/78 (88%)	0.30	2 (2%) 51 49	22, 33, 44, 53	0
1	B	69/78 (88%)	0.14	0 100 100	23, 34, 45, 52	0
1	C	69/78 (88%)	0.28	3 (4%) 35 32	22, 30, 46, 63	0
1	D	69/78 (88%)	0.08	2 (2%) 51 49	20, 29, 37, 46	0
1	E	69/78 (88%)	0.03	1 (1%) 75 73	21, 28, 36, 45	0
1	F	69/78 (88%)	0.16	1 (1%) 75 73	23, 34, 47, 60	0
1	G	69/78 (88%)	0.40	2 (2%) 51 49	26, 34, 47, 52	0
1	H	69/78 (88%)	0.38	2 (2%) 51 49	24, 32, 45, 53	1 (1%)
1	I	69/78 (88%)	0.26	4 (5%) 23 21	25, 34, 47, 51	0
1	J	70/78 (89%)	0.24	1 (1%) 75 73	24, 34, 44, 50	0
1	K	69/78 (88%)	0.32	2 (2%) 51 49	21, 31, 41, 53	1 (1%)
1	L	71/78 (91%)	0.37	3 (4%) 36 34	24, 33, 47, 52	0
1	M	69/78 (88%)	0.15	1 (1%) 75 73	24, 33, 46, 53	0
1	N	69/78 (88%)	0.13	0 100 100	21, 31, 44, 54	0
1	O	69/78 (88%)	0.09	2 (2%) 51 49	21, 29, 38, 45	0
1	P	69/78 (88%)	0.15	1 (1%) 75 73	22, 30, 38, 47	0
1	Q	69/78 (88%)	0.26	1 (1%) 75 73	23, 35, 46, 51	0
1	R	69/78 (88%)	0.08	0 100 100	25, 33, 44, 50	0
1	S	69/78 (88%)	0.15	1 (1%) 75 73	19, 33, 45, 61	0
1	T	69/78 (88%)	0.10	0 100 100	24, 34, 45, 51	0
1	U	70/78 (89%)	-0.09	0 100 100	21, 31, 42, 50	0
1	V	69/78 (88%)	0.08	0 100 100	22, 31, 39, 46	0
All	All	1522/1716 (88%)	0.19	29 (1%) 66 64	19, 32, 46, 63	2 (0%)

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	76	LYS	11.5
1	C	76	LYS	6.6
1	K	76	LYS	6.1
1	G	76	LYS	5.2
1	L	6	SER	4.7

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	TRP	N	80	15/15	0.88	0.19	21,22,26,27	0
2	TRP	T	80	15/15	0.89	0.17	23,26,31,33	0
2	TRP	O	80	15/15	0.90	0.20	28,30,32,33	0
2	TRP	J	80	15/15	0.91	0.20	22,25,26,27	0
2	TRP	I	80	15/15	0.91	0.16	28,31,35,35	0
2	TRP	D	80	15/15	0.91	0.14	25,26,28,29	0
2	TRP	B	80	15/15	0.92	0.15	24,26,30,30	0
2	TRP	A	80	15/15	0.92	0.16	23,25,27,27	0
2	TRP	Q	80	15/15	0.92	0.14	22,27,34,35	0
2	TRP	H	80	15/15	0.93	0.14	18,20,26,27	0
2	TRP	L	80	15/15	0.93	0.14	20,25,27,27	0
2	TRP	R	80	15/15	0.93	0.15	27,29,31,31	0
2	TRP	M	80	15/15	0.93	0.14	27,29,31,33	0
2	TRP	C	80	15/15	0.94	0.14	16,22,24,24	0
2	TRP	F	80	15/15	0.94	0.13	22,24,28,29	0
2	TRP	U	80	15/15	0.94	0.16	23,25,27,28	0
2	TRP	P	80	15/15	0.94	0.15	13,16,22,23	0
2	TRP	E	80	15/15	0.94	0.14	12,17,21,21	0
2	TRP	G	80	15/15	0.95	0.15	25,27,31,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	TRP	V	80	15/15	0.95	0.16	19,21,26,27	0
2	TRP	S	80	15/15	0.95	0.13	20,23,24,27	0
2	TRP	K	80	15/15	0.95	0.14	14,22,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.