



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 5, 2016 – 12:13 PM EDT

PDB ID : 5EF2  
Title : RADIATION DAMAGE TO THE TRAP-RNA COMPLEX: DOSE (DWD)  
21.9 MGy  
Authors : Bury, C.S.; McGeehan, J.E.; Garman, E.F.; Shevtsov, M.B.  
Deposited on : 2015-10-23  
Resolution : 1.98 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027457  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

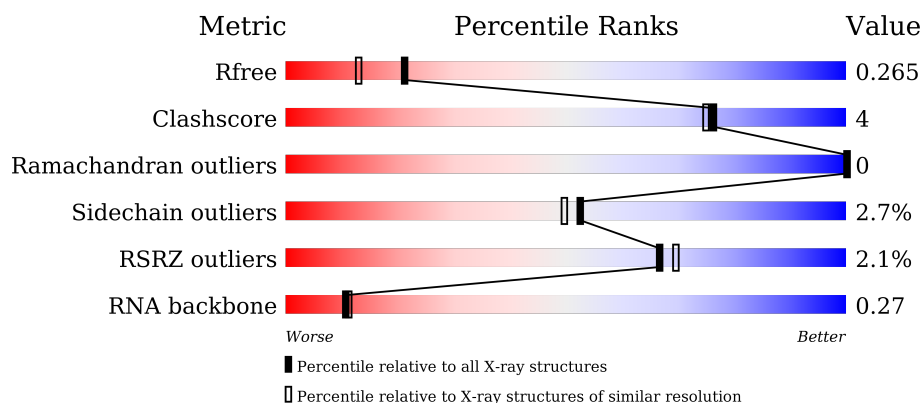
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 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.
















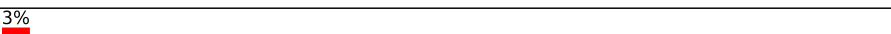





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)
RNA backbone	2183	1000 (2.70-1.26)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	74	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, orange 4%, yellow 12%, green 80%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>4%</span> <span>80%</span> <span>12%</span> <span>7%</span> </div> </div>
1	B	74	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, orange 4%, yellow 14%, green 77%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>4%</span> <span>77%</span> <span>14%</span> <span>8%</span> </div> </div>
1	C	74	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, orange 4%, yellow 12%, green 80%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>4%</span> <span>80%</span> <span>12%</span> <span>7%</span> </div> </div>
1	D	74	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, orange 4%, yellow 12%, green 80%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>4%</span> <span>80%</span> <span>12%</span> <span>7%</span> </div> </div>

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Mol	Chain	Length	Quality of chain
1	E	74	
1	F	74	
1	G	74	
1	H	74	
1	I	74	
1	J	74	
1	K	74	
1	L	74	
1	M	74	
1	N	74	
1	O	74	
1	P	74	
1	Q	74	
1	R	74	
1	S	74	
1	T	74	
1	U	74	
1	V	74	
2	W	55	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13846 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 Transcription attenuation protein MtrB.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	69	Total	C	N	O	0	0	0
			535	334	98	103			
1	B	68	Total	C	N	O	0	0	0
			527	330	96	101			
1	C	69	Total	C	N	O	0	0	0
			535	334	98	103			
1	D	69	Total	C	N	O	0	0	0
			536	336	98	102			
1	E	68	Total	C	N	O	0	0	0
			527	330	96	101			
1	F	69	Total	C	N	O	0	1	0
			542	340	98	104			
1	G	68	Total	C	N	O	0	1	0
			532	333	96	103			
1	H	68	Total	C	N	O	0	0	0
			527	330	96	101			
1	I	68	Total	C	N	O	0	0	0
			527	330	96	101			
1	J	67	Total	C	N	O	0	0	0
			523	328	95	100			
1	K	68	Total	C	N	O	0	0	0
			527	330	96	101			
1	L	70	Total	C	N	O	0	1	0
			547	341	100	106			
1	M	70	Total	C	N	O	0	0	0
			542	338	99	105			
1	N	70	Total	C	N	O	0	0	0
			542	338	99	105			
1	O	70	Total	C	N	O	0	0	0
			542	338	99	105			
1	P	70	Total	C	N	O	0	0	0
			542	338	99	105			

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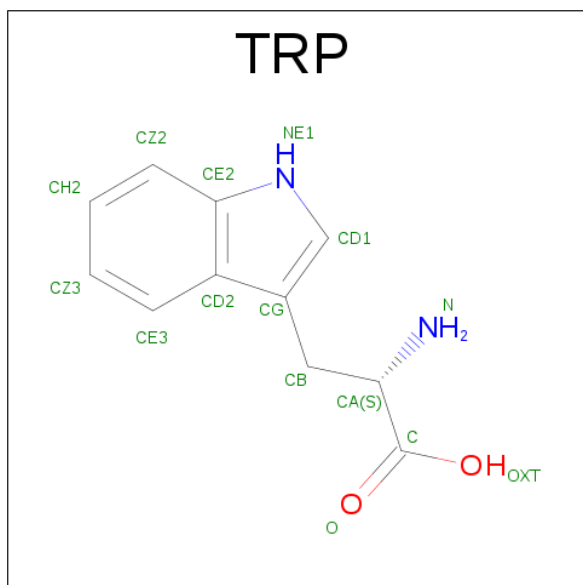
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	Q	70	Total	C	N	O	0	0	0
			542	338	99	105			
1	R	70	Total	C	N	O	0	0	0
			542	338	99	105			
1	S	70	Total	C	N	O	0	0	0
			542	338	99	105			
1	T	70	Total	C	N	O	0	0	0
			542	338	99	105			
1	U	70	Total	C	N	O	0	0	0
			542	338	99	105			
1	V	70	Total	C	N	O	0	0	0
			542	338	99	105			

- Molecule 2 is a RNA chain called (GAGUU)10GAG 53-NUCLEOTIDE RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	W	44	Total	C	N	O	P	0	0	0
			968	429	187	308	44			

- Molecule 3 is TRYPTOPHAN (three-letter code: TRP) (formula: C<sub>11</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub>).



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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	38	Total O 38 38	0	0
4	B	25	Total O 25 25	0	0
4	C	39	Total O 39 39	0	0
4	D	36	Total O 36 36	0	0
4	E	36	Total O 36 36	0	0
4	F	41	Total O 41 41	0	0
4	G	30	Total O 30 30	0	0
4	H	39	Total O 39 39	0	0
4	I	33	Total O 33 33	0	0
4	J	25	Total O 25 25	0	0
4	K	34	Total O 34 34	0	0
4	L	31	Total O 31 31	0	0
4	M	39	Total O 39 39	0	0
4	N	37	Total O 37 37	0	0
4	O	43	Total O 43 43	0	0
4	P	33	Total O 33 33	0	0
4	Q	28	Total O 28 28	0	0
4	R	33	Total O 33 33	0	0
4	S	25	Total O 25 25	0	0
4	T	31	Total O 31 31	0	0
4	U	27	Total O 27 27	0	0
4	V	25	Total O 25 25	0	0

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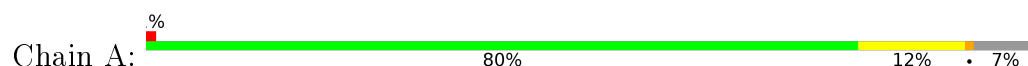
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	W	15	Total	O	0	0
			15	15		



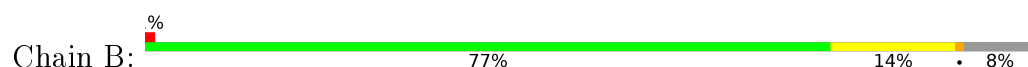
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Transcription attenuation protein MtrB



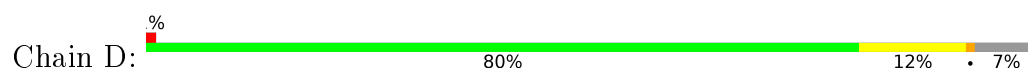
- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB



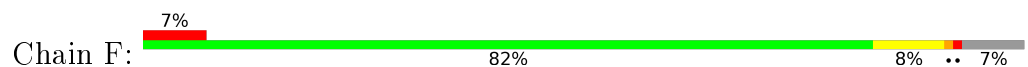
- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB

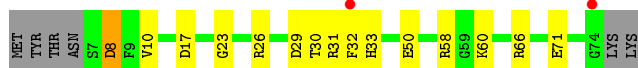
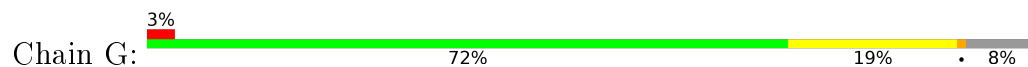


- Molecule 1: Transcription attenuation protein MtrB

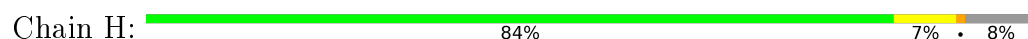




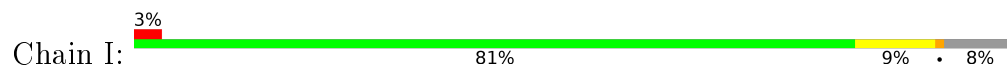
- Molecule 1: Transcription attenuation protein MtrB



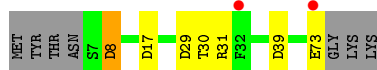
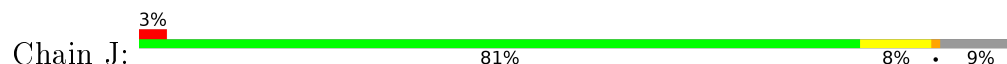
- Molecule 1: Transcription attenuation protein MtrB



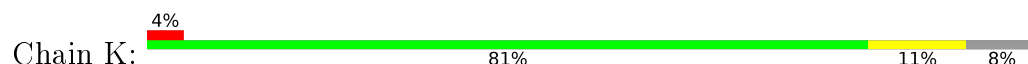
- Molecule 1: Transcription attenuation protein MtrB



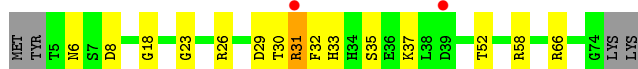
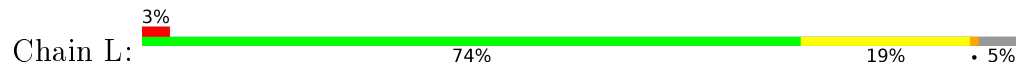
- Molecule 1: Transcription attenuation protein MtrB



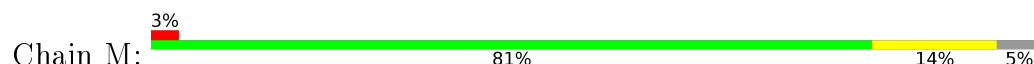
- Molecule 1: Transcription attenuation protein MtrB

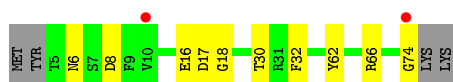


- Molecule 1: Transcription attenuation protein MtrB



- Molecule 1: Transcription attenuation protein MtrB





- Molecule 1: Transcription attenuation protein MtrB

Chain N: 82% 11% • 5%



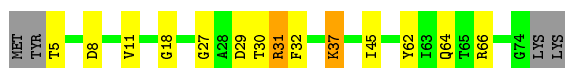
- Molecule 1: Transcription attenuation protein MtrB

Chain O: 86% 7% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain P: 76% 16% • 5%



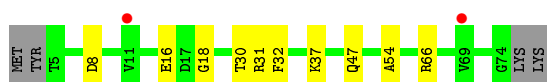
- Molecule 1: Transcription attenuation protein MtrB

Chain Q: 84% 9% • 5%



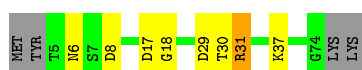
- Molecule 1: Transcription attenuation protein MtrB

Chain R: 3% 81% 14% 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain S: 84% 9% • 5%



- Molecule 1: Transcription attenuation protein MtrB

Chain T: 4% 81% 12% • 5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.21Å 111.16Å 138.28Å 90.00° 117.39° 90.00°	Depositor
Resolution (Å)	59.69 – 1.98 59.68 – 1.98	Depositor EDS
% Data completeness (in resolution range)	98.9 (59.69-1.98) 99.2 (59.68-1.98)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.22 (at 1.98Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.234 , 0.264 0.241 , 0.265	Depositor DCC
$R_{free}$ test set	12743 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.7	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13846	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.90% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 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	A	1.29	2/542 (0.4%)	1.30	5/728 (0.7%)
1	B	1.31	1/534 (0.2%)	1.34	6/717 (0.8%)
1	C	1.17	0/542	1.18	5/728 (0.7%)
1	D	1.10	0/543	1.25	7/728 (1.0%)
1	E	1.34	1/534 (0.2%)	1.30	9/717 (1.3%)
1	F	1.27	1/552 (0.2%)	1.21	3/740 (0.4%)
1	G	1.32	3/542 (0.6%)	1.45	9/728 (1.2%)
1	H	1.28	1/534 (0.2%)	1.21	4/717 (0.6%)
1	I	1.30	4/534 (0.7%)	1.17	3/717 (0.4%)
1	J	1.26	1/530 (0.2%)	1.30	6/712 (0.8%)
1	K	1.24	1/534 (0.2%)	1.14	0/717
1	L	1.22	1/557 (0.2%)	1.21	5/749 (0.7%)
1	M	1.30	3/549 (0.5%)	1.29	7/738 (0.9%)
1	N	1.41	0/549	1.17	1/738 (0.1%)
1	O	1.34	0/549	1.24	3/738 (0.4%)
1	P	1.38	2/549 (0.4%)	1.28	4/738 (0.5%)
1	Q	1.32	1/549 (0.2%)	1.23	4/738 (0.5%)
1	R	1.29	2/549 (0.4%)	1.23	4/738 (0.5%)
1	S	1.19	0/549	1.23	4/738 (0.5%)
1	T	1.25	1/549 (0.2%)	1.11	3/738 (0.4%)
1	U	1.22	1/549 (0.2%)	1.23	4/738 (0.5%)
1	V	1.29	2/549 (0.4%)	1.13	2/738 (0.3%)
2	W	1.09	7/1078 (0.6%)	1.25	13/1661 (0.8%)
All	All	1.26	35/13046 (0.3%)	1.24	111/17739 (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	D	0	1
1	R	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	2

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	W	146	G	C8-N7	20.53	1.43	1.30
2	W	146	G	C5-C4	9.78	1.45	1.38
1	I	71	GLU	CD-OE2	8.41	1.34	1.25
1	J	73	GLU	CD-OE1	7.42	1.33	1.25
2	W	146	G	N1-C2	7.40	1.43	1.37

The worst 5 of 111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	8	ASP	CB-CG-OD2	-13.82	105.86	118.30
1	A	31	ARG	NE-CZ-NH2	-12.48	114.06	120.30
1	M	8	ASP	CB-CG-OD2	-10.73	108.64	118.30
2	W	124	U	O5'-P-OP1	-10.73	96.05	105.70
1	B	40	LYS	CD-CE-NZ	-10.55	87.43	111.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	74	GLY	Peptide
1	R	47	GLN	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	A	535	0	534	3	0
1	B	527	0	528	3	0
1	C	535	0	534	5	0
1	D	536	0	541	2	0
1	E	527	0	528	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	542	0	547	5	0
1	G	532	0	532	3	1
1	H	527	0	528	4	0
1	I	527	0	528	3	0
1	J	523	0	525	1	0
1	K	527	0	528	6	0
1	L	547	0	547	9	0
1	M	542	0	541	5	0
1	N	542	0	541	6	0
1	O	542	0	541	4	0
1	P	542	0	541	8	0
1	Q	542	0	541	6	0
1	R	542	0	541	5	0
1	S	542	0	541	4	0
1	T	542	0	541	7	0
1	U	542	0	541	6	0
1	V	542	0	541	5	0
2	W	968	0	484	27	0
3	A	15	0	9	1	0
3	B	15	0	9	1	0
3	C	15	0	9	1	0
3	D	15	0	9	1	0
3	E	15	0	9	1	0
3	F	15	0	9	1	0
3	G	15	0	9	1	0
3	H	15	0	9	1	0
3	I	15	0	9	1	0
3	J	15	0	9	1	0
3	K	15	0	9	1	0
3	L	15	0	9	1	0
3	M	15	0	9	1	0
3	N	15	0	9	0	0
3	O	15	0	9	1	0
3	P	15	0	9	1	0
3	Q	15	0	9	0	0
3	R	15	0	9	1	0
3	S	15	0	9	1	0
3	T	15	0	9	1	0
3	U	15	0	9	0	0
3	V	15	0	9	0	0
4	A	38	0	0	1	0
4	B	25	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	39	0	0	1	0
4	D	36	0	0	0	0
4	E	36	0	0	0	0
4	F	41	0	0	1	0
4	G	30	0	0	0	0
4	H	39	0	0	2	0
4	I	33	0	0	1	0
4	J	25	0	0	0	0
4	K	34	0	0	2	0
4	L	31	0	0	2	0
4	M	39	0	0	0	0
4	N	37	0	0	1	0
4	O	43	0	0	2	0
4	P	33	0	0	1	0
4	Q	28	0	0	2	0
4	R	33	0	0	0	0
4	S	25	0	0	0	0
4	T	31	0	0	0	0
4	U	27	0	0	0	0
4	V	25	0	0	2	0
4	W	15	0	0	0	0
All	All	13846	0	12492	98	1

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 4.

The worst 5 of 98 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:G:23:GLY:O	1:G:32:PHE:O	1.64	1.14
1:Q:18:GLY:HA2	2:W:131:G:O6	1.76	0.85
1:K:20:ASN:ND2	1:K:35:SER:HB3	1.93	0.84
1:U:66:ARG:HG3	1:U:66:ARG:HH11	1.45	0.81
1:O:33:HIS:CE1	1:O:52:THR:OG1	2.36	0.78

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:50:GLU:OE2	1:G:50:GLU:OE2[2_555]	1.89	0.31

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	67/74 (90%)	67 (100%)	0	0	100	100
1	B	66/74 (89%)	66 (100%)	0	0	100	100
1	C	67/74 (90%)	67 (100%)	0	0	100	100
1	D	67/74 (90%)	67 (100%)	0	0	100	100
1	E	66/74 (89%)	66 (100%)	0	0	100	100
1	F	68/74 (92%)	68 (100%)	0	0	100	100
1	G	67/74 (90%)	65 (97%)	2 (3%)	0	100	100
1	H	66/74 (89%)	65 (98%)	1 (2%)	0	100	100
1	I	66/74 (89%)	66 (100%)	0	0	100	100
1	J	65/74 (88%)	65 (100%)	0	0	100	100
1	K	66/74 (89%)	66 (100%)	0	0	100	100
1	L	69/74 (93%)	68 (99%)	1 (1%)	0	100	100
1	M	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	N	68/74 (92%)	68 (100%)	0	0	100	100
1	O	68/74 (92%)	68 (100%)	0	0	100	100
1	P	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	Q	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
1	R	68/74 (92%)	68 (100%)	0	0	100	100
1	S	68/74 (92%)	68 (100%)	0	0	100	100
1	T	68/74 (92%)	68 (100%)	0	0	100	100
1	U	68/74 (92%)	68 (100%)	0	0	100	100
1	V	68/74 (92%)	68 (100%)	0	0	100	100
All	All	1480/1628 (91%)	1473 (100%)	7 (0%)	0	100	100

There are no Ramachandran outliers to report.

### 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	57/62 (92%)	56 (98%)	1 (2%)	66	67
1	B	56/62 (90%)	53 (95%)	3 (5%)	27	19
1	C	57/62 (92%)	55 (96%)	2 (4%)	43	38
1	D	57/62 (92%)	56 (98%)	1 (2%)	66	67
1	E	56/62 (90%)	54 (96%)	2 (4%)	42	36
1	F	58/62 (94%)	55 (95%)	3 (5%)	29	20
1	G	57/62 (92%)	54 (95%)	3 (5%)	28	20
1	H	56/62 (90%)	56 (100%)	0	100	100
1	I	56/62 (90%)	55 (98%)	1 (2%)	66	67
1	J	56/62 (90%)	55 (98%)	1 (2%)	66	67
1	K	56/62 (90%)	55 (98%)	1 (2%)	66	67
1	L	59/62 (95%)	58 (98%)	1 (2%)	68	69
1	M	58/62 (94%)	58 (100%)	0	100	100
1	N	58/62 (94%)	56 (97%)	2 (3%)	44	39
1	O	58/62 (94%)	56 (97%)	2 (3%)	44	39
1	P	58/62 (94%)	56 (97%)	2 (3%)	44	39
1	Q	58/62 (94%)	56 (97%)	2 (3%)	44	39
1	R	58/62 (94%)	57 (98%)	1 (2%)	68	69
1	S	58/62 (94%)	57 (98%)	1 (2%)	68	69
1	T	58/62 (94%)	56 (97%)	2 (3%)	44	39
1	U	58/62 (94%)	56 (97%)	2 (3%)	44	39
1	V	58/62 (94%)	56 (97%)	2 (3%)	44	39
All	All	1261/1364 (92%)	1226 (97%)	35 (3%)	52	48

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	8	ASP
1	N	8	ASP
1	U	37	LYS
1	J	8	ASP
1	K	70	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	6	ASN
1	S	6	ASN
1	O	33	HIS
1	M	64	GLN
1	O	20	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	W	33/55 (60%)	12 (36%)	0

5 of 12 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	W	107	A
2	W	112	A
2	W	117	A
2	W	127	A
2	W	132	A

There are no RNA pucker outliers to report.

## 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 carbohydrates 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$
3	TRP	A	101	-	12,16,16	1.52	3 (25%)	8,22,22	0.97	0
3	TRP	B	101	-	12,16,16	1.20	2 (16%)	8,22,22	1.18	1 (12%)
3	TRP	C	101	-	12,16,16	1.18	1 (8%)	8,22,22	1.21	1 (12%)
3	TRP	D	101	-	12,16,16	1.16	1 (8%)	8,22,22	1.02	0
3	TRP	E	101	-	12,16,16	1.53	3 (25%)	8,22,22	1.45	2 (25%)
3	TRP	F	101	-	12,16,16	1.42	2 (16%)	8,22,22	1.52	1 (12%)
3	TRP	G	101	-	12,16,16	1.10	1 (8%)	8,22,22	1.34	1 (12%)
3	TRP	H	101	-	12,16,16	1.58	1 (8%)	8,22,22	1.13	1 (12%)
3	TRP	I	101	-	12,16,16	1.36	2 (16%)	8,22,22	1.09	1 (12%)
3	TRP	J	101	-	12,16,16	1.48	2 (16%)	8,22,22	1.28	0
3	TRP	K	101	-	12,16,16	1.07	2 (16%)	8,22,22	1.05	0
3	TRP	L	101	-	12,16,16	0.89	1 (8%)	8,22,22	1.11	0
3	TRP	M	101	-	12,16,16	1.09	1 (8%)	8,22,22	1.29	1 (12%)
3	TRP	N	101	-	12,16,16	1.06	2 (16%)	8,22,22	0.96	0
3	TRP	O	101	-	12,16,16	1.41	3 (25%)	8,22,22	1.05	0
3	TRP	P	101	-	12,16,16	1.26	2 (16%)	8,22,22	1.28	1 (12%)
3	TRP	Q	101	-	12,16,16	1.15	2 (16%)	8,22,22	1.16	1 (12%)
3	TRP	R	101	-	12,16,16	0.67	0	8,22,22	0.95	0
3	TRP	S	101	-	12,16,16	0.80	0	8,22,22	1.32	1 (12%)
3	TRP	T	101	-	12,16,16	1.26	3 (25%)	8,22,22	0.78	0
3	TRP	U	101	-	12,16,16	1.26	2 (16%)	8,22,22	0.87	0
3	TRP	V	101	-	12,16,16	1.27	1 (8%)	8,22,22	0.90	0

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
3	TRP	A	101	-	-	0/3/8/8	0/2/2/2
3	TRP	B	101	-	-	0/3/8/8	0/2/2/2
3	TRP	C	101	-	-	0/3/8/8	0/2/2/2
3	TRP	D	101	-	-	0/3/8/8	0/2/2/2
3	TRP	E	101	-	-	0/3/8/8	0/2/2/2
3	TRP	F	101	-	-	0/3/8/8	0/2/2/2
3	TRP	G	101	-	-	0/3/8/8	0/2/2/2
3	TRP	H	101	-	-	0/3/8/8	0/2/2/2
3	TRP	I	101	-	-	0/3/8/8	0/2/2/2
3	TRP	J	101	-	-	0/3/8/8	0/2/2/2
3	TRP	K	101	-	-	0/3/8/8	0/2/2/2
3	TRP	L	101	-	-	0/3/8/8	0/2/2/2
3	TRP	M	101	-	-	0/3/8/8	0/2/2/2
3	TRP	N	101	-	-	0/3/8/8	0/2/2/2
3	TRP	O	101	-	-	0/3/8/8	0/2/2/2
3	TRP	P	101	-	-	0/3/8/8	0/2/2/2
3	TRP	Q	101	-	-	0/3/8/8	0/2/2/2
3	TRP	R	101	-	-	0/3/8/8	0/2/2/2
3	TRP	S	101	-	-	0/3/8/8	0/2/2/2
3	TRP	T	101	-	-	0/3/8/8	0/2/2/2
3	TRP	U	101	-	-	0/3/8/8	0/2/2/2
3	TRP	V	101	-	-	0/3/8/8	0/2/2/2

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	101	TRP	CD1-CG	-2.04	1.31	1.37
3	A	101	TRP	CZ2-CE2	2.01	1.45	1.41
3	N	101	TRP	CH2-CZ3	2.01	1.43	1.38
3	T	101	TRP	CH2-CZ3	2.05	1.43	1.38
3	O	101	TRP	CD1-NE1	2.08	1.40	1.36

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	101	TRP	CZ3-CE3-CD2	-3.04	116.66	120.88
3	S	101	TRP	CH2-CZ2-CE2	-2.58	116.02	120.07
3	M	101	TRP	CH2-CZ2-CE2	-2.57	116.04	120.07
3	E	101	TRP	CZ3-CE3-CD2	-2.46	117.46	120.88
3	G	101	TRP	CZ3-CE3-CD2	-2.45	117.49	120.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	101	TRP	1	0
3	B	101	TRP	1	0
3	C	101	TRP	1	0
3	D	101	TRP	1	0
3	E	101	TRP	1	0
3	F	101	TRP	1	0
3	G	101	TRP	1	0
3	H	101	TRP	1	0
3	I	101	TRP	1	0
3	J	101	TRP	1	0
3	K	101	TRP	1	0
3	L	101	TRP	1	0
3	M	101	TRP	1	0
3	O	101	TRP	1	0
3	P	101	TRP	1	0
3	R	101	TRP	1	0
3	S	101	TRP	1	0
3	T	101	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	69/74 (93%)	0.37	1 (1%) 78 80	33, 45, 61, 86	1 (1%)
1	B	68/74 (91%)	0.43	1 (1%) 76 79	32, 43, 58, 65	0
1	C	69/74 (93%)	0.54	3 (4%) 39 43	32, 43, 65, 71	2 (2%)
1	D	69/74 (93%)	0.51	1 (1%) 78 80	32, 44, 64, 71	1 (1%)
1	E	68/74 (91%)	0.48	0 100 100	32, 42, 58, 66	0
1	F	69/74 (93%)	0.58	5 (7%) 18 22	30, 41, 65, 75	1 (1%)
1	G	68/74 (91%)	0.37	2 (2%) 55 58	32, 42, 59, 66	1 (1%)
1	H	68/74 (91%)	0.31	0 100 100	33, 42, 59, 67	1 (1%)
1	I	68/74 (91%)	0.39	2 (2%) 55 58	34, 44, 64, 72	1 (1%)
1	J	67/74 (90%)	0.37	2 (2%) 54 57	35, 44, 60, 67	1 (1%)
1	K	68/74 (91%)	0.40	3 (4%) 38 42	33, 44, 61, 67	1 (1%)
1	L	70/74 (94%)	0.41	2 (2%) 55 58	34, 45, 64, 71	2 (2%)
1	M	70/74 (94%)	0.52	2 (2%) 55 58	32, 44, 57, 68	0
1	N	70/74 (94%)	0.36	0 100 100	30, 39, 55, 60	0
1	O	70/74 (94%)	0.19	0 100 100	30, 38, 54, 59	0
1	P	70/74 (94%)	0.31	0 100 100	29, 38, 56, 57	0
1	Q	70/74 (94%)	0.57	0 100 100	30, 42, 55, 60	0
1	R	70/74 (94%)	0.70	2 (2%) 55 58	32, 43, 59, 68	0
1	S	70/74 (94%)	0.45	0 100 100	33, 44, 61, 65	1 (1%)
1	T	70/74 (94%)	0.51	3 (4%) 39 43	32, 45, 61, 70	0
1	U	70/74 (94%)	0.45	1 (1%) 78 80	34, 45, 62, 66	0
1	V	70/74 (94%)	0.42	2 (2%) 55 58	34, 46, 62, 68	1 (1%)
2	W	44/55 (80%)	0.39	1 (2%) 64 67	62, 74, 83, 94	0
All	All	1565/1683 (92%)	0.44	33 (2%) 67 69	29, 44, 65, 94	14 (0%)



The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	74	GLY	5.7
1	G	32	PHE	4.7
1	K	32	PHE	3.8
1	J	32	PHE	3.5
1	M	74	GLY	3.4

## 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	TRP	K	101	15/15	0.95	0.14	0.77	36,38,41,45	0
3	TRP	D	101	15/15	0.93	0.14	0.40	38,39,44,44	0
3	TRP	J	101	15/15	0.95	0.12	0.14	36,40,45,46	0
3	TRP	E	101	15/15	0.95	0.13	0.13	33,37,40,44	0
3	TRP	A	101	15/15	0.95	0.12	0.03	35,40,43,49	0
3	TRP	V	101	15/15	0.96	0.12	-0.18	37,41,43,48	0
3	TRP	P	101	15/15	0.96	0.11	-0.19	28,32,35,36	0
3	TRP	F	101	15/15	0.94	0.10	-0.58	36,38,42,43	0
3	TRP	I	101	15/15	0.96	0.10	-0.72	38,42,44,45	0
3	TRP	C	101	15/15	0.95	0.10	-0.83	39,41,47,47	0
3	TRP	H	101	15/15	0.94	0.10	-0.87	40,42,45,47	0
3	TRP	U	101	15/15	0.95	0.10	-0.91	36,41,44,45	0
3	TRP	Q	101	15/15	0.95	0.09	-0.96	33,35,39,39	0
3	TRP	T	101	15/15	0.94	0.10	-1.09	36,40,43,44	0
3	TRP	G	101	15/15	0.97	0.08	-1.12	36,40,43,44	0
3	TRP	B	101	15/15	0.95	0.10	-1.12	35,40,43,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	TRP	L	101	15/15	0.95	0.09	-1.13	36,41,46,46	0
3	TRP	N	101	15/15	0.94	0.09	-1.16	32,36,38,38	0
3	TRP	M	101	15/15	0.96	0.08	-1.16	34,38,41,43	0
3	TRP	O	101	15/15	0.95	0.09	-1.33	32,35,39,39	0
3	TRP	R	101	15/15	0.95	0.10	-1.62	34,38,42,42	0
3	TRP	S	101	15/15	0.94	0.09	-1.64	33,37,41,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.