



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 01:49 am GMT

PDB ID : 1C9S  
Title : CRYSTAL STRUCTURE OF A COMPLEX OF TRP RNA-BINDING ATTENUATION PROTEIN WITH A 53-BASE SINGLE STRANDED RNA CONTAINING ELEVEN GAG TRIPLETS SEPARATED BY AU DINUCLEOTIDES  
Authors : Antson, A.A.; Dodson, E.J.; Dodson, G.G.; Greaves, R.B.; Chen, X.-P.; Gollnick, P.  
Deposited on : 1999-08-03  
Resolution : 1.90 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

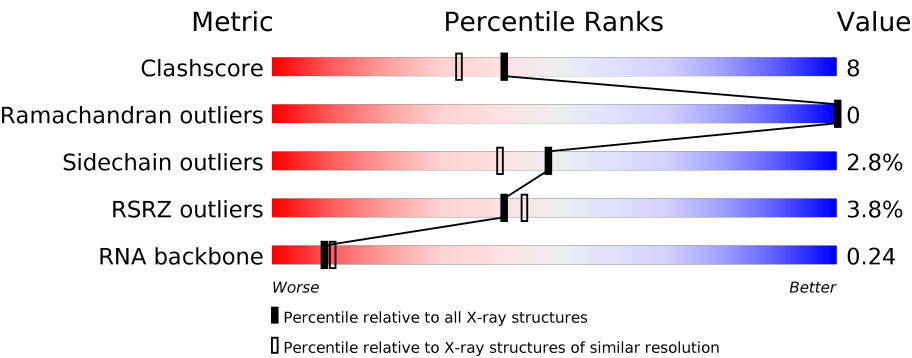
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)
RNA backbone	2435	1002 (2.60-1.20)

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	W	55	<div><div>38%</div><div><div>25%</div><div>56%</div><div>18%</div></div></div>
2	A	74	<div><div>3%</div><div><div>84%</div><div>7%</div><div>7%</div></div></div>
2	B	74	<div><div>3%</div><div><div>72%</div><div>19%</div><div>8%</div></div></div>
2	C	74	<div><div>3%</div><div><div>78%</div><div>12%</div><div>7%</div></div></div>
2	D	74	<div><div>3%</div><div><div>69%</div><div>22%</div><div>7%</div></div></div>
2	E	74	<div><div>76%</div><div><div>16%</div><div>8%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	F	74	 77% 15% • 7%
2	G	74	 80% 12% • 5%
2	H	74	 78% 11% • 7%
2	I	74	 81% 9% •• 7%
2	J	74	 76% 14% • 9%
2	K	74	 78% 12% • 7%
2	L	74	 82% 9% • 5%
2	M	74	 80% 14% ••
2	N	74	 78% 14% • 5%
2	O	74	 80% 12% ••
2	P	74	 81% 9% • 5%
2	Q	74	 78% 11% •• 5%
2	R	74	 77% 15% • 5%
2	S	74	 76% 16% • 5%
2	T	74	 81% 11% • 5%
2	U	74	 74% 16% • 5%
2	V	74	 74% 19% • 5%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14731 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 RNA chain called SINGLE STRANDED RNA (55-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	W	55	Total	C	N	O	P	0	0	0
			1210	539	242	374	55			

- Molecule 2 is a protein called TRP RNA-BINDING ATTENUATION PROTEIN.

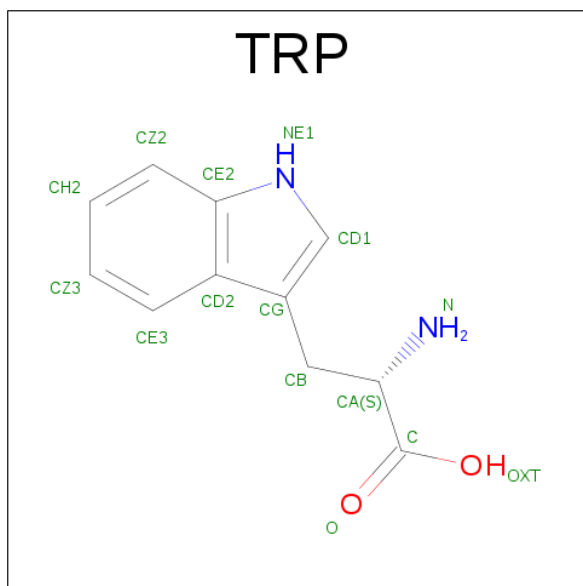
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A	69	Total	C	N	O	8	0	0
			536	336	98	102			
2	B	68	Total	C	N	O	5	1	0
			529	332	96	101			
2	C	69	Total	C	N	O	3	1	0
			537	336	98	103			
2	D	69	Total	C	N	O	4	1	0
			538	338	98	102			
2	E	68	Total	C	N	O	2	1	0
			529	332	96	101			
2	F	69	Total	C	N	O	7	1	0
			538	338	98	102			
2	G	70	Total	C	N	O	4	2	0
			548	344	100	104			
2	H	69	Total	C	N	O	9	1	0
			538	338	98	102			
2	I	69	Total	C	N	O	16	2	0
			540	340	98	102			
2	J	67	Total	C	N	O	8	1	0
			525	330	95	100			
2	K	69	Total	C	N	O	11	1	0
			539	337	98	104			
2	L	70	Total	C	N	O	0	1	0
			544	340	99	105			
2	M	71	Total	C	N	O	0	0	0
			551	344	101	106			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	N	70	Total	C	N	O	0	0	0
			542	338	99	105			
2	O	71	Total	C	N	O	4	1	0
			557	347	104	106			
2	P	70	Total	C	N	O	0	2	0
			549	341	102	106			
2	Q	70	Total	C	N	O	0	0	0
			542	338	99	105			
2	R	70	Total	C	N	O	0	1	0
			548	341	102	105			
2	S	70	Total	C	N	O	0	2	0
			549	341	102	106			
2	T	70	Total	C	N	O	0	1	0
			543	338	99	106			
2	U	70	Total	C	N	O	0	1	0
			548	341	102	105			
2	V	70	Total	C	N	O	0	0	0
			542	338	99	105			

- Molecule 3 is TRYPTOPHAN (three-letter code: TRP) (formula:  $C_{11}H_{12}N_2O_2$ ).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total 15	C 11	N 2	O 2	0	0
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	71	Total O 71 71	0	0
4	B	54	Total O 54 54	0	0
4	C	81	Total O 81 81	0	0
4	D	73	Total O 73 73	0	0
4	E	69	Total O 69 69	0	0
4	F	67	Total O 67 67	0	0
4	G	69	Total O 69 69	0	0
4	H	58	Total O 58 58	0	0
4	I	60	Total O 60 60	0	0
4	J	44	Total O 44 44	0	0
4	K	52	Total O 52 52	0	0
4	L	31	Total O 31 31	0	0
4	M	44	Total O 44 44	0	0
4	N	46	Total O 46 46	0	0
4	O	55	Total O 55 55	0	0
4	P	41	Total O 41 41	0	0
4	Q	46	Total O 46 46	0	0
4	R	59	Total O 59 59	0	0
4	S	45	Total O 45 45	0	0
4	T	47	Total O 47 47	0	0
4	U	50	Total O 50 50	0	0

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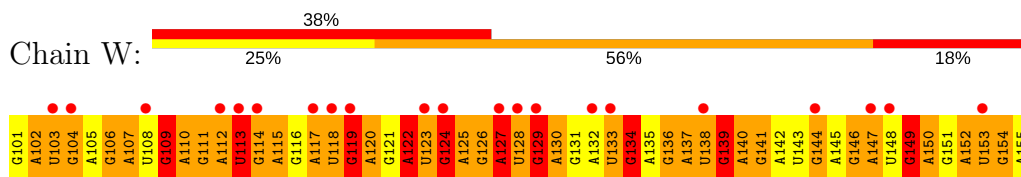
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	V	47	Total 47	O 47	0	0
4	W	55	Total 55	O 55	0	0



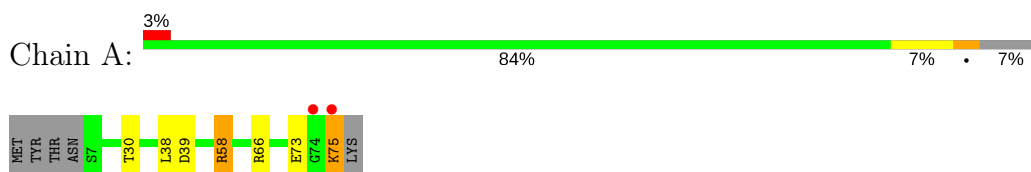
### 3 Residue-property plots [i](#)

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

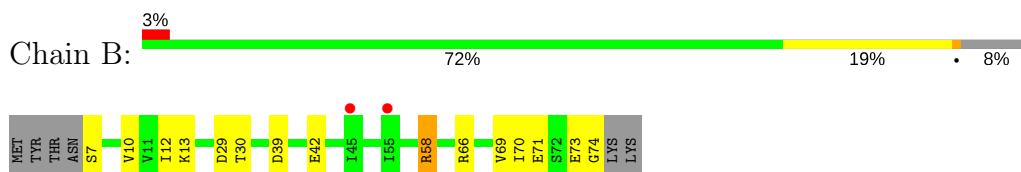
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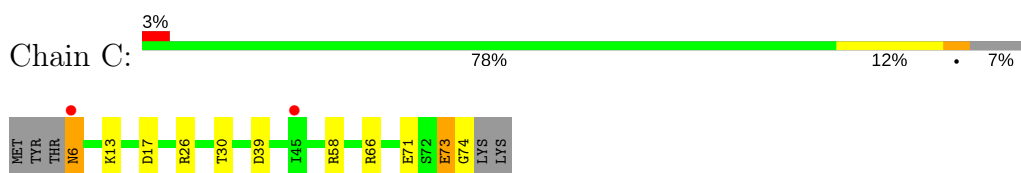
- Molecule 2: TRP RNA-BINDING ATTENUATION PROTEIN



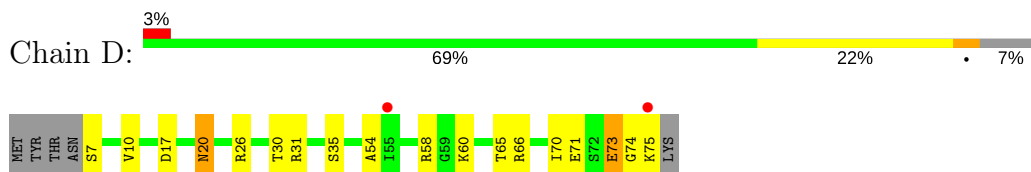
- Molecule 2: TRP RNA-BINDING ATTENUATION PROTEIN



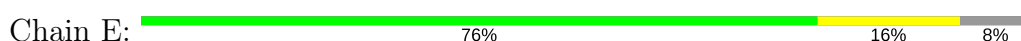
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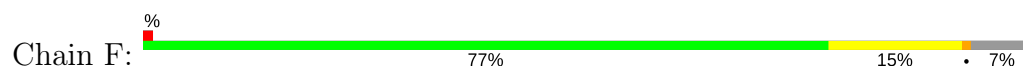


- Molecule 2: TRP RNA-BINDING ATTENUATION PROTEIN

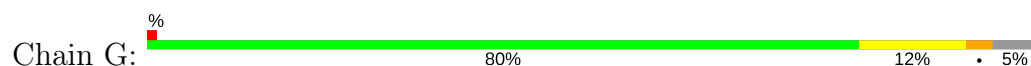




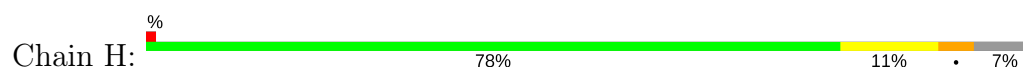
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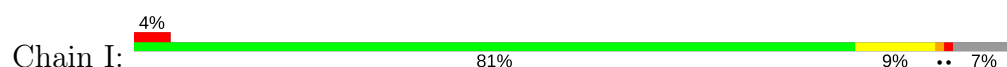
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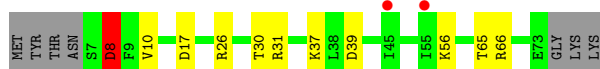
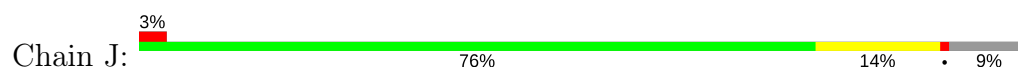
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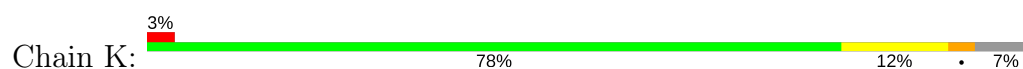
• Molecule 2: TRP RNA-BINDING ATTENUATION PROTEIN



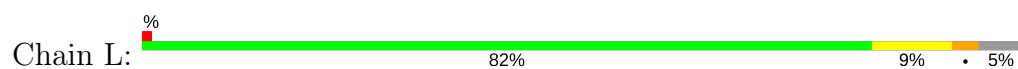
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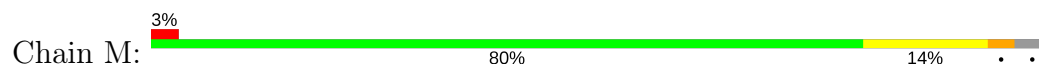


• Molecule 2: TRP RNA-BINDING ATTENUATION PROTEIN

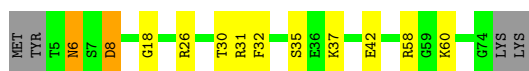
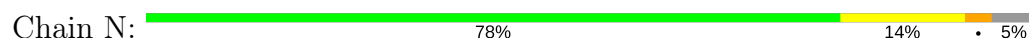




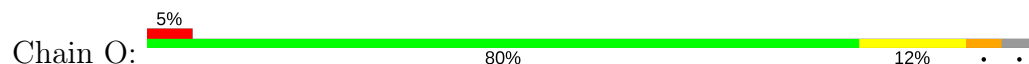
• Molecule 2: TRP RNA-BINDING ATTENUATION PROTEIN



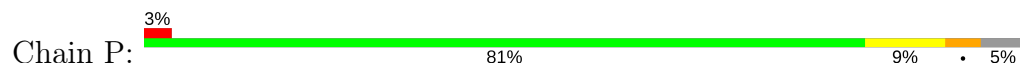
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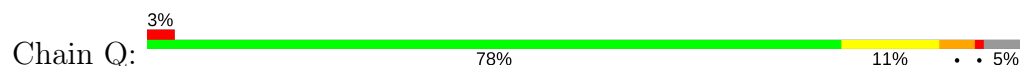
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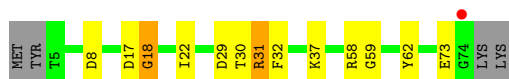
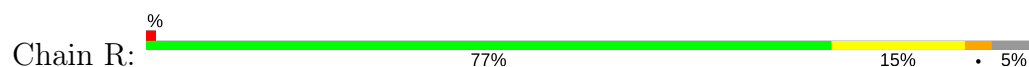
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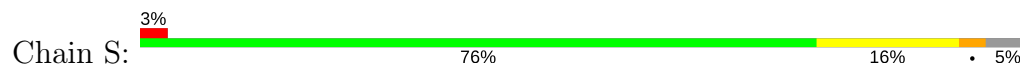
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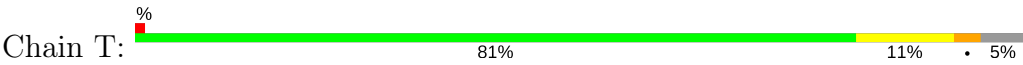


• Molecule 2: TRP RNA-BINDING ATTENUATION PROTEIN





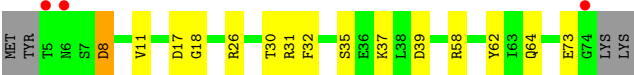
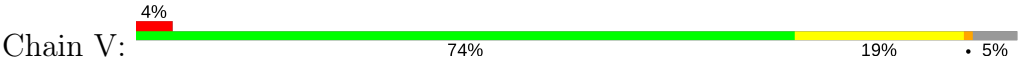
• Molecule 2: TRP RNA-BINDING ATTENUATION PROTEIN



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## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	150.97Å 111.67Å 138.68Å 90.00° 117.77° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 29.48 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.4 (30.00-1.90) 96.5 (29.48-1.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.36 (at 1.91Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.188 , 0.235 0.182 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	22.6	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 61.0	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	0.96	EDS
Total number of atoms	14731	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.26% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	W	0.98	1/1363 (0.1%)	2.38	115/2130 (5.4%)
2	A	0.88	1/543 (0.2%)	1.49	7/728 (1.0%)
2	B	0.75	1/541 (0.2%)	1.39	8/727 (1.1%)
2	C	0.62	0/549	1.35	5/738 (0.7%)
2	D	0.66	0/550	1.50	10/738 (1.4%)
2	E	0.61	0/541	1.34	5/727 (0.7%)
2	F	1.06	2/550 (0.4%)	1.72	9/738 (1.2%)
2	G	0.65	0/565	1.52	9/759 (1.2%)
2	H	1.61	2/550 (0.4%)	1.65	7/738 (0.9%)
2	I	1.80	3/557 (0.5%)	1.83	8/748 (1.1%)
2	J	0.69	1/537 (0.2%)	1.53	12/722 (1.7%)
2	K	1.42	2/551 (0.4%)	1.84	11/739 (1.5%)
2	L	0.49	0/556	1.25	4/748 (0.5%)
2	M	0.50	0/558	1.26	4/749 (0.5%)
2	N	0.48	0/549	1.18	2/738 (0.3%)
2	O	0.59	1/569 (0.2%)	1.23	3/763 (0.4%)
2	P	0.48	0/566	1.29	4/760 (0.5%)
2	Q	0.51	0/549	1.23	4/738 (0.5%)
2	R	0.50	0/560	1.21	4/752 (0.5%)
2	S	0.51	0/566	1.41	11/760 (1.4%)
2	T	0.50	0/555	1.24	2/746 (0.3%)
2	U	0.47	0/560	1.27	4/752 (0.5%)
2	V	0.48	0/549	1.26	6/738 (0.8%)
All	All	0.85	14/13534 (0.1%)	1.56	254/18476 (1.4%)

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	W	0	2
2	A	1	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
2	D	0	4
2	G	0	1
2	H	0	1
2	I	0	4
2	K	0	2
2	L	0	1
2	Q	0	2
2	R	0	3
2	U	0	2
All	All	1	24

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	66	ARG	NE-CZ	35.26	1.78	1.33
2	H	66	ARG	NE-CZ	34.09	1.77	1.33
2	K	66	ARG	NE-CZ	27.42	1.68	1.33
2	F	75	LYS	CB-CG	18.30	2.02	1.52
2	I	73	GLU	CG-CD	-17.47	1.25	1.51

The worst 5 of 254 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	66	ARG	CD-NE-CZ	-24.60	89.16	123.60
2	K	75	LYS	N-CA-CB	-23.56	68.19	110.60
2	I	66	ARG	CD-NE-CZ	-23.05	91.33	123.60
2	F	58	ARG	NE-CZ-NH1	-19.92	110.34	120.30
2	A	75	LYS	N-CA-CB	18.29	143.53	110.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	75	LYS	CA

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	73	GLU	Mainchain
2	C	73	GLU	Mainchain
2	D	54	ALA	Mainchain
1	W	122	A	Sidechain

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Mol	Chain	Res	Type	Group
1	W	127	A	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	W	1210	0	594	81	0
2	A	536	0	541	4	0
2	B	529	0	533	8	0
2	C	537	0	539	6	0
2	D	538	0	546	5	0
2	E	529	0	533	12	0
2	F	538	0	546	4	0
2	G	548	0	557	5	0
2	H	538	0	546	6	0
2	I	540	0	551	3	0
2	J	525	0	530	5	0
2	K	539	0	541	5	0
2	L	544	0	546	7	0
2	M	551	0	554	12	0
2	N	542	0	541	13	0
2	O	557	0	563	13	0
2	P	549	0	551	10	0
2	Q	542	0	541	10	0
2	R	548	0	550	10	0
2	S	549	0	551	12	0
2	T	543	0	542	15	0
2	U	548	0	550	16	0
2	V	542	0	541	10	0
3	A	30	0	18	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	0
3	O	15	0	9	1	0
3	P	15	0	9	1	0
3	Q	15	0	9	1	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	1	0
3	V	15	0	9	1	0
4	A	71	0	0	1	0
4	B	54	0	0	2	0
4	C	81	0	0	4	0
4	D	73	0	0	2	2
4	E	69	0	0	6	0
4	F	67	0	0	2	0
4	G	69	0	0	2	2
4	H	58	0	0	5	0
4	I	60	0	0	2	0
4	J	44	0	0	1	0
4	K	52	0	0	1	0
4	L	31	0	0	2	0
4	M	44	0	0	6	1
4	N	46	0	0	3	0
4	O	55	0	0	3	0
4	P	41	0	0	3	0
4	Q	46	0	0	6	0
4	R	59	0	0	0	0
4	S	45	0	0	1	0
4	T	47	0	0	3	0
4	U	50	0	0	3	0
4	V	47	0	0	4	0
4	W	55	0	0	2	0
All	All	14731	0	12794	210	3

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 8.

The worst 5 of 210 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:M:73:GLU:CD	4:M:118:HOH:O	1.90	1.08
2:E:71:GLU:HG3	4:E:141:HOH:O	1.51	1.07
1:W:112:A:H2'	1:W:113:U:H5'	1.31	1.06
2:E:71:GLU:CG	4:E:141:HOH:O	2.05	1.04
2:E:71:GLU:CD	4:E:141:HOH:O	1.96	1.02

All (3) 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)
4:M:117:HOH:O	4:M:117:HOH:O[2_555]	1.10	1.10
4:D:94:HOH:O	4:G:137:HOH:O[4_546]	1.81	0.39
4:D:102:HOH:O	4:G:138:HOH:O[4_546]	1.92	0.28

## 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	
2	A	67/74 (90%)	67 (100%)	0	0	100	100
2	B	67/74 (90%)	67 (100%)	0	0	100	100
2	C	68/74 (92%)	68 (100%)	0	0	100	100
2	D	68/74 (92%)	68 (100%)	0	0	100	100
2	E	67/74 (90%)	67 (100%)	0	0	100	100
2	F	68/74 (92%)	68 (100%)	0	0	100	100
2	G	70/74 (95%)	70 (100%)	0	0	100	100
2	H	68/74 (92%)	68 (100%)	0	0	100	100
2	I	69/74 (93%)	69 (100%)	0	0	100	100
2	J	66/74 (89%)	66 (100%)	0	0	100	100
2	K	68/74 (92%)	68 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	69/74 (93%)	69 (100%)	0	0	100	100
2	M	69/74 (93%)	69 (100%)	0	0	100	100
2	N	68/74 (92%)	68 (100%)	0	0	100	100
2	O	70/74 (95%)	70 (100%)	0	0	100	100
2	P	70/74 (95%)	70 (100%)	0	0	100	100
2	Q	68/74 (92%)	68 (100%)	0	0	100	100
2	R	69/74 (93%)	68 (99%)	1 (1%)	0	100	100
2	S	70/74 (95%)	70 (100%)	0	0	100	100
2	T	69/74 (93%)	69 (100%)	0	0	100	100
2	U	69/74 (93%)	69 (100%)	0	0	100	100
2	V	68/74 (92%)	68 (100%)	0	0	100	100
All	All	1505/1628 (92%)	1504 (100%)	1 (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	
2	A	57/62 (92%)	56 (98%)	1 (2%)	64	60
2	B	57/62 (92%)	55 (96%)	2 (4%)	41	30
2	C	58/62 (94%)	57 (98%)	1 (2%)	66	62
2	D	58/62 (94%)	56 (97%)	2 (3%)	42	32
2	E	57/62 (92%)	57 (100%)	0	100	100
2	F	58/62 (94%)	56 (97%)	2 (3%)	42	32
2	G	60/62 (97%)	59 (98%)	1 (2%)	66	62
2	H	58/62 (94%)	57 (98%)	1 (2%)	66	62
2	I	59/62 (95%)	59 (100%)	0	100	100
2	J	57/62 (92%)	56 (98%)	1 (2%)	64	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	58/62 (94%)	56 (97%)	2 (3%)	42	32
2	L	59/62 (95%)	58 (98%)	1 (2%)	66	62
2	M	59/62 (95%)	57 (97%)	2 (3%)	42	32
2	N	58/62 (94%)	55 (95%)	3 (5%)	27	16
2	O	60/62 (97%)	56 (93%)	4 (7%)	19	9
2	P	60/62 (97%)	57 (95%)	3 (5%)	28	17
2	Q	58/62 (94%)	54 (93%)	4 (7%)	18	8
2	R	59/62 (95%)	58 (98%)	1 (2%)	66	62
2	S	60/62 (97%)	60 (100%)	0	100	100
2	T	59/62 (95%)	56 (95%)	3 (5%)	28	16
2	U	59/62 (95%)	57 (97%)	2 (3%)	42	32
2	V	58/62 (94%)	56 (97%)	2 (3%)	42	32
All	All	1286/1364 (94%)	1248 (97%)	38 (3%)	49	37

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	N	8	ASP
2	O	37	LYS
2	U	8	ASP
2	O	6	ASN
2	O	75	LYS

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

Mol	Chain	Res	Type
2	L	6	ASN
2	M	6	ASN
2	P	6	ASN
2	I	20	ASN
2	O	6	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	W	54/55 (98%)	21 (38%)	0

5 of 21 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	W	105	A
1	W	109	G
1	W	110	A
1	W	113	U
1	W	114	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

23 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	181	-	11,16,16	0.99	1 (9%)	11,22,22	0.70	0
3	TRP	A	81	-	11,16,16	0.74	0	11,22,22	1.12	0
3	TRP	B	81	-	11,16,16	0.84	1 (9%)	11,22,22	0.97	0
3	TRP	C	81	-	11,16,16	0.65	0	11,22,22	0.91	0
3	TRP	D	81	-	11,16,16	0.66	0	11,22,22	1.26	1 (9%)
3	TRP	E	81	-	11,16,16	0.78	0	11,22,22	1.23	1 (9%)
3	TRP	F	81	-	11,16,16	0.69	0	11,22,22	1.15	1 (9%)
3	TRP	G	81	-	11,16,16	0.71	0	11,22,22	1.31	1 (9%)
3	TRP	H	81	-	11,16,16	0.67	0	11,22,22	1.25	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	TRP	I	81	-	11,16,16	0.76	0	11,22,22	1.28	2 (18%)
3	TRP	J	81	-	11,16,16	0.79	0	11,22,22	1.19	0
3	TRP	K	81	-	11,16,16	0.70	0	11,22,22	1.27	1 (9%)
3	TRP	L	81	-	11,16,16	0.68	0	11,22,22	0.83	0
3	TRP	M	81	-	11,16,16	0.79	0	11,22,22	1.00	0
3	TRP	N	81	-	11,16,16	0.66	0	11,22,22	0.80	0
3	TRP	O	81	-	11,16,16	0.72	0	11,22,22	1.21	1 (9%)
3	TRP	P	81	-	11,16,16	0.73	0	11,22,22	1.51	2 (18%)
3	TRP	Q	81	-	11,16,16	0.77	0	11,22,22	1.04	0
3	TRP	R	81	-	11,16,16	0.70	0	11,22,22	0.99	1 (9%)
3	TRP	S	81	-	11,16,16	0.72	0	11,22,22	1.08	1 (9%)
3	TRP	T	81	-	11,16,16	0.80	0	11,22,22	0.65	0
3	TRP	U	81	-	11,16,16	0.74	0	11,22,22	0.73	0
3	TRP	V	81	-	11,16,16	0.69	0	11,22,22	0.87	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	181	-	-	0/3/8/8	0/2/2/2
3	TRP	A	81	-	-	0/3/8/8	0/2/2/2
3	TRP	B	81	-	-	0/3/8/8	0/2/2/2
3	TRP	C	81	-	-	0/3/8/8	0/2/2/2
3	TRP	D	81	-	-	0/3/8/8	0/2/2/2
3	TRP	E	81	-	-	0/3/8/8	0/2/2/2
3	TRP	F	81	-	-	0/3/8/8	0/2/2/2
3	TRP	G	81	-	-	0/3/8/8	0/2/2/2
3	TRP	H	81	-	-	0/3/8/8	0/2/2/2
3	TRP	I	81	-	-	0/3/8/8	0/2/2/2
3	TRP	J	81	-	-	0/3/8/8	0/2/2/2
3	TRP	K	81	-	-	0/3/8/8	0/2/2/2
3	TRP	L	81	-	-	0/3/8/8	0/2/2/2
3	TRP	M	81	-	-	0/3/8/8	0/2/2/2
3	TRP	N	81	-	-	0/3/8/8	0/2/2/2
3	TRP	O	81	-	-	0/3/8/8	0/2/2/2
3	TRP	P	81	-	-	0/3/8/8	0/2/2/2
3	TRP	Q	81	-	-	0/3/8/8	0/2/2/2
3	TRP	R	81	-	-	0/3/8/8	0/2/2/2
3	TRP	S	81	-	-	0/3/8/8	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TRP	T	81	-	-	0/3/8/8	0/2/2/2
3	TRP	U	81	-	-	0/3/8/8	0/2/2/2
3	TRP	V	81	-	-	0/3/8/8	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	181	TRP	CZ2-CE2	-2.02	1.38	1.41
3	B	81	TRP	CH2-CZ3	2.11	1.43	1.38

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	81	TRP	CH2-CZ2-CE2	-2.76	115.92	120.07
3	O	81	TRP	CH2-CZ2-CE2	-2.58	116.18	120.07
3	I	81	TRP	CZ3-CE3-CD2	-2.54	117.25	120.88
3	H	81	TRP	CZ3-CE3-CD2	-2.50	117.31	120.88
3	P	81	TRP	CZ3-CE3-CD2	-2.48	117.34	120.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

22 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	81	TRP	1	0
3	B	81	TRP	1	0
3	C	81	TRP	1	0
3	D	81	TRP	1	0
3	E	81	TRP	1	0
3	F	81	TRP	1	0
3	G	81	TRP	1	0
3	H	81	TRP	1	0
3	I	81	TRP	1	0
3	J	81	TRP	1	0
3	K	81	TRP	1	0
3	L	81	TRP	1	0
3	M	81	TRP	1	0
3	N	81	TRP	1	0
3	O	81	TRP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	81	TRP	1	0
3	Q	81	TRP	1	0
3	R	81	TRP	1	0
3	S	81	TRP	1	0
3	T	81	TRP	1	0
3	U	81	TRP	1	0
3	V	81	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	W	55/55 (100%)	1.34	21 (38%) 0 0	37, 55, 81, 84	0
2	A	69/74 (93%)	-0.04	2 (2%) 52 56	17, 23, 41, 49	2 (2%)
2	B	68/74 (91%)	-0.10	2 (2%) 52 56	15, 22, 35, 44	1 (1%)
2	C	69/74 (93%)	-0.27	2 (2%) 52 56	15, 21, 37, 53	1 (1%)
2	D	69/74 (93%)	-0.18	2 (2%) 52 56	15, 20, 29, 43	1 (1%)
2	E	68/74 (91%)	-0.14	0 100 100	16, 21, 37, 40	1 (1%)
2	F	69/74 (93%)	-0.07	1 (1%) 75 78	16, 22, 38, 47	2 (2%)
2	G	70/74 (94%)	-0.06	1 (1%) 75 78	16, 21, 39, 45	1 (1%)
2	H	69/74 (93%)	-0.19	1 (1%) 75 78	17, 23, 38, 53	3 (4%)
2	I	69/74 (93%)	-0.03	3 (4%) 36 39	19, 25, 38, 50	5 (7%)
2	J	67/74 (90%)	-0.15	2 (2%) 51 54	19, 25, 36, 46	3 (4%)
2	K	69/74 (93%)	0.04	2 (2%) 52 56	19, 24, 38, 51	4 (5%)
2	L	70/74 (94%)	-0.23	1 (1%) 75 78	21, 26, 39, 45	0
2	M	71/74 (95%)	-0.22	2 (2%) 53 57	21, 26, 39, 62	0
2	N	70/74 (94%)	-0.25	0 100 100	21, 26, 38, 43	0
2	O	71/74 (95%)	-0.10	4 (5%) 25 28	20, 26, 38, 67	1 (1%)
2	P	70/74 (94%)	-0.26	2 (2%) 52 56	20, 26, 39, 45	0
2	Q	70/74 (94%)	-0.14	2 (2%) 52 56	20, 26, 38, 45	0
2	R	70/74 (94%)	-0.27	1 (1%) 75 78	19, 25, 36, 45	0
2	S	70/74 (94%)	-0.24	2 (2%) 52 56	19, 25, 35, 49	0
2	T	70/74 (94%)	-0.21	1 (1%) 75 78	19, 25, 38, 47	0
2	U	70/74 (94%)	-0.19	3 (4%) 36 39	20, 26, 38, 46	0
2	V	70/74 (94%)	-0.18	3 (4%) 36 39	21, 26, 38, 49	0
All	All	1583/1683 (94%)	-0.11	60 (3%) 41 45	15, 25, 42, 84	25 (1%)

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	74	GLY	3.4
2	O	75	LYS	3.3
2	L	74	GLY	3.0
2	H	75	LYS	2.9
1	W	128	U	2.8

## 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	T	81	15/15	0.96	0.12	1.05	20,20,22,22	0
3	TRP	L	81	15/15	0.97	0.12	0.79	18,22,23,23	0
3	TRP	Q	81	15/15	0.96	0.11	0.72	18,19,20,22	0
3	TRP	R	81	15/15	0.98	0.10	0.50	19,20,22,22	0
3	TRP	U	81	15/15	0.97	0.09	0.16	21,22,24,24	0
3	TRP	O	81	15/15	0.97	0.10	0.14	20,21,23,23	0
3	TRP	N	81	15/15	0.97	0.10	0.08	19,21,24,25	0
3	TRP	K	81	15/15	0.91	0.10	0.01	18,22,24,25	0
3	TRP	B	81	15/15	0.97	0.11	0.00	16,18,19,19	0
3	TRP	M	81	15/15	0.97	0.08	-0.02	20,21,22,23	0
3	TRP	V	81	15/15	0.97	0.09	-0.05	20,23,24,25	0
3	TRP	S	81	15/15	0.97	0.09	-0.14	18,20,22,24	0
3	TRP	D	81	15/15	0.97	0.09	-0.18	14,16,18,18	0
3	TRP	C	81	15/15	0.97	0.09	-0.18	16,17,19,19	0
3	TRP	F	81	15/15	0.98	0.09	-0.23	15,18,20,20	0
3	TRP	A	181	15/15	0.97	0.08	-0.37	16,18,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	TRP	H	81	15/15	0.97	0.07	-0.40	15,19,21,22	0
3	TRP	I	81	15/15	0.97	0.08	-0.45	15,20,25,26	0
3	TRP	P	81	15/15	0.97	0.08	-0.47	18,20,21,22	0
3	TRP	E	81	15/15	0.98	0.07	-0.50	14,15,17,17	0
3	TRP	G	81	15/15	0.97	0.08	-0.62	16,17,20,21	0
3	TRP	J	81	15/15	0.97	0.08	-0.66	20,23,24,24	0
3	TRP	A	81	15/15	0.96	0.07	-0.79	18,20,21,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.