



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 5, 2024 – 08:48 AM EST

PDB ID : 1WAP  
Title : TRP RNA-BINDING ATTENUATION PROTEIN IN COMPLEX WITH L-TRYPTOPHAN  
Authors : Antson, A.A.; Dodson, E.J.; Gollnick, P.  
Deposited on : 1995-02-03  
Resolution : 1.80 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

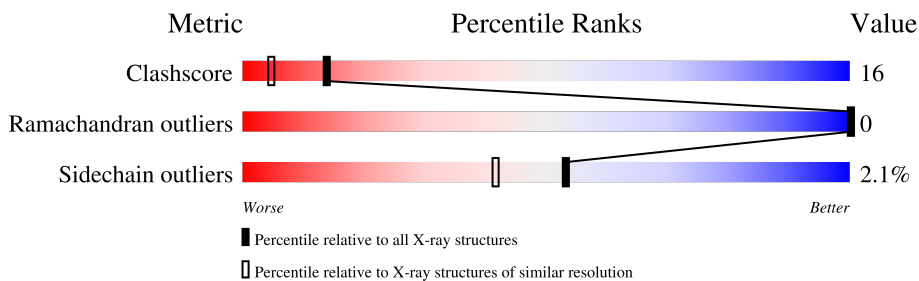
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	75	
1	B	75	
1	C	75	
1	D	75	
1	E	75	
1	F	75	
1	G	75	
1	H	75	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	I	75	 73% 12% 5% 9%
1	J	75	 75% 12% • 11%
1	K	75	 73% 15% • 11%
1	L	75	 76% 11% • 11%
1	M	75	 67% 23% • 9%
1	N	75	 69% 16% • 11%
1	O	75	 57% 28% •• 11%
1	P	75	 72% 16% • 9%
1	Q	75	 67% 19% • 11%
1	R	75	 69% 19% • 11%
1	S	75	 69% 19% •• 9%
1	T	75	 68% 17% • 11%
1	U	75	 64% 23% •• 11%
1	V	75	 75% 13% • 11%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13834 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 TRP RNA-BINDING ATTENUATION PROTEIN.

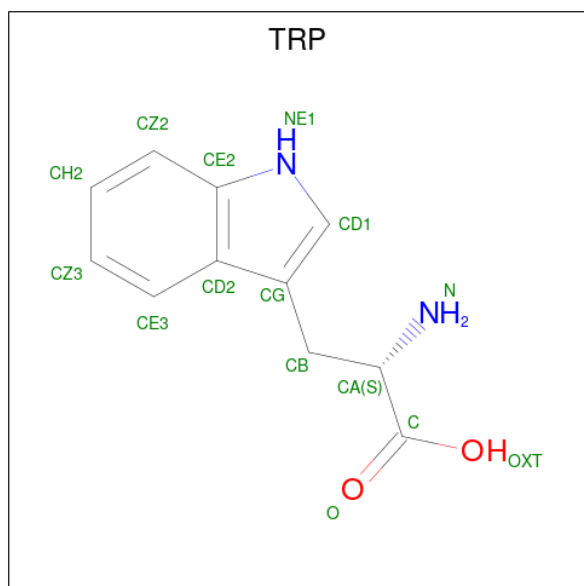
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	68	529	333	91	104	1	0	0	0
1	B	67	519	327	89	102	1	0	0	0
1	C	67	519	327	89	102	1	0	0	0
1	D	67	519	327	89	102	1	0	0	0
1	E	67	519	327	89	102	1	0	0	0
1	F	68	529	333	91	104	1	0	0	0
1	G	67	519	327	89	102	1	0	0	0
1	H	67	519	327	89	102	1	0	0	0
1	I	68	529	333	91	104	1	0	0	0
1	J	67	519	327	89	102	1	0	0	0
1	K	67	519	327	89	102	1	0	0	0
1	L	67	519	327	89	102	1	0	0	0
1	M	68	529	333	91	104	1	0	0	0
1	N	67	519	327	89	102	1	0	0	0
1	O	67	519	327	89	102	1	0	0	0
1	P	68	529	333	91	104	1	0	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	67	Total	C	N	O	S	0	0	0
			519	327	89	102	1			
1	R	67	Total	C	N	O	S	0	0	0
			519	327	89	102	1			
1	S	68	Total	C	N	O	S	0	0	0
			529	333	91	104	1			
1	T	67	Total	C	N	O	S	0	0	0
			519	327	89	102	1			
1	U	67	Total	C	N	O	S	0	0	0
			519	327	89	102	1			
1	V	67	Total	C	N	O	S	0	0	0
			519	327	89	102	1			

- 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		

Continued on next page...

*Continued from previous page...*

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	97	Total	O	0	0
			97	97		
3	B	88	Total	O	0	0
			88	88		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	91	Total O 91 91	0	0
3	D	94	Total O 94 94	0	0
3	E	88	Total O 88 88	0	0
3	F	89	Total O 89 89	0	0
3	G	99	Total O 99 99	0	0
3	H	92	Total O 92 92	0	0
3	I	98	Total O 98 98	0	0
3	J	89	Total O 89 89	0	0
3	K	75	Total O 75 75	0	0
3	L	93	Total O 93 93	0	0
3	M	81	Total O 81 81	0	0
3	N	100	Total O 100 100	0	0
3	O	100	Total O 100 100	0	0
3	P	99	Total O 99 99	0	0
3	Q	89	Total O 89 89	0	0
3	R	91	Total O 91 91	0	0
3	S	111	Total O 111 111	0	0
3	T	75	Total O 75 75	0	0
3	U	89	Total O 89 89	0	0
3	V	98	Total O 98 98	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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

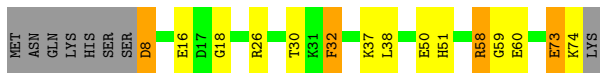
- Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN

Chain A: 



- Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN

Chain B: 



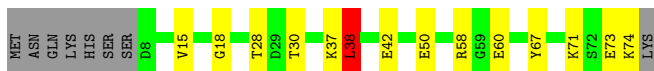
- Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN

Chain C: 



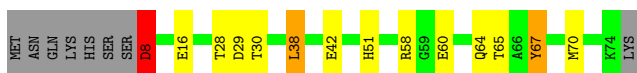
- Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN

Chain D: 



- Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN

Chain E: 



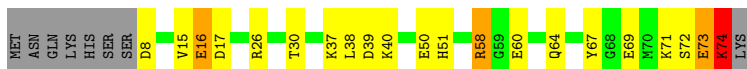
- Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN

Chain F: 

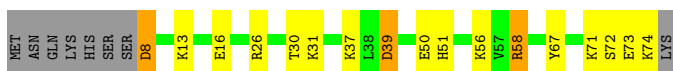




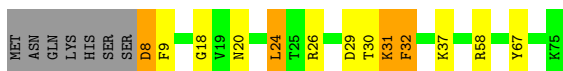
- Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN



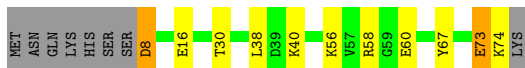
- Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN



- Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN



- Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN



- Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN

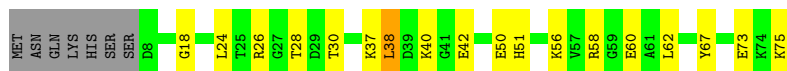


- Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN

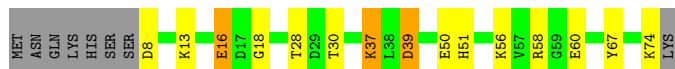


- Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN





● Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN



● Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN



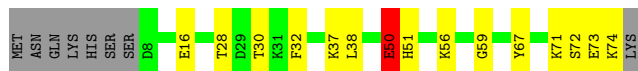
● Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN



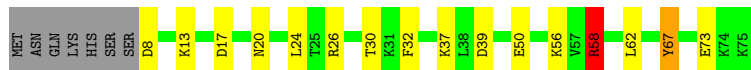
● Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN



● Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN



● Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN



● Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN

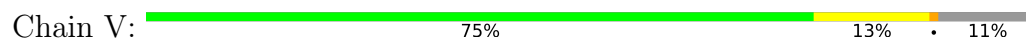




- Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN



- Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	155.91Å 114.44Å 105.67Å 90.00° 117.64° 90.00°	Depositor
Resolution (Å)	10.00 – 1.80	Depositor
% Data completeness (in resolution range)	97.5 (10.00-1.80)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.178 , 0.225	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	13834	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

## 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	0.67	0/535	1.43	4/715 (0.6%)
1	B	0.66	0/525	1.50	7/704 (1.0%)
1	C	0.66	0/525	1.39	7/704 (1.0%)
1	D	0.64	0/525	1.30	2/704 (0.3%)
1	E	0.66	0/525	1.39	5/704 (0.7%)
1	F	0.68	0/535	1.38	7/715 (1.0%)
1	G	0.69	0/525	1.47	9/704 (1.3%)
1	H	0.68	0/525	1.34	3/704 (0.4%)
1	I	0.72	0/535	1.47	6/715 (0.8%)
1	J	0.71	0/525	1.56	3/704 (0.4%)
1	K	0.70	0/525	1.59	6/704 (0.9%)
1	L	0.66	0/525	1.34	4/704 (0.6%)
1	M	0.72	0/535	1.48	6/715 (0.8%)
1	N	0.70	0/525	1.31	3/704 (0.4%)
1	O	0.71	0/525	1.42	7/704 (1.0%)
1	P	0.69	0/535	1.36	4/715 (0.6%)
1	Q	0.70	0/525	1.48	8/704 (1.1%)
1	R	0.70	0/525	1.44	6/704 (0.9%)
1	S	0.73	0/535	1.67	9/715 (1.3%)
1	T	0.70	0/525	1.50	6/704 (0.9%)
1	U	0.71	0/525	1.35	5/704 (0.7%)
1	V	0.67	0/525	1.23	1/704 (0.1%)
All	All	0.69	0/11610	1.43	118/15554 (0.8%)

There are no bond length outliers.

The worst 5 of 118 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	58	ARG	NE-CZ-NH1	17.93	129.26	120.30
1	J	58	ARG	CD-NE-CZ	16.61	146.85	123.60
1	K	58	ARG	CD-NE-CZ	16.01	146.02	123.60
1	S	58	ARG	CD-NE-CZ	14.52	143.93	123.60
1	I	26	ARG	NE-CZ-NH1	12.66	126.63	120.30

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	529	0	537	14	0
1	B	519	0	524	22	0
1	C	519	0	524	26	0
1	D	519	0	524	16	0
1	E	519	0	524	12	0
1	F	529	0	537	21	0
1	G	519	0	524	26	0
1	H	519	0	524	18	0
1	I	529	0	537	16	0
1	J	519	0	524	13	0
1	K	519	0	524	12	0
1	L	519	0	524	7	0
1	M	529	0	537	19	0
1	N	519	0	524	28	0
1	O	519	0	524	26	0
1	P	529	0	537	17	0
1	Q	519	0	524	22	0
1	R	519	0	524	16	0
1	S	529	0	537	24	0
1	T	519	0	524	14	0
1	U	519	0	524	21	0
1	V	519	0	524	16	0
2	A	15	0	9	1	0
2	B	15	0	9	1	0
2	C	15	0	9	1	0
2	D	15	0	9	1	0
2	E	15	0	9	1	0
2	F	15	0	9	1	0
2	G	15	0	9	1	0
2	H	15	0	9	1	0
2	I	15	0	9	3	0
2	J	15	0	9	1	0
2	K	15	0	9	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	15	0	9	0	0
2	M	15	0	9	0	0
2	N	15	0	9	1	0
2	O	15	0	9	1	0
2	P	15	0	9	1	0
2	Q	15	0	9	1	0
2	R	15	0	9	1	0
2	S	15	0	9	1	0
2	T	15	0	9	1	0
2	U	15	0	9	1	0
2	V	15	0	9	1	0
3	A	97	0	0	7	2
3	B	88	0	0	6	0
3	C	91	0	0	5	0
3	D	94	0	0	7	0
3	E	88	0	0	4	1
3	F	89	0	0	4	0
3	G	99	0	0	14	0
3	H	92	0	0	8	0
3	I	98	0	0	11	0
3	J	89	0	0	4	1
3	K	75	0	0	8	0
3	L	93	0	0	2	0
3	M	81	0	0	8	2
3	N	100	0	0	15	0
3	O	100	0	0	15	1
3	P	99	0	0	6	0
3	Q	89	0	0	11	1
3	R	91	0	0	9	0
3	S	111	0	0	5	0
3	T	75	0	0	12	0
3	U	89	0	0	14	0
3	V	98	0	0	5	0
All	All	13834	0	11804	373	5

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 16.

The worst 5 of 373 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:F:24:LEU:HD11	1:F:32:PHE:CE1	1.59	1.35
1:G:37:LYS:HG2	3:G:163:HOH:O	1.30	1.31
1:K:51:HIS:HB3	3:K:137:HOH:O	1.31	1.29
1:G:74:LYS:HA	3:G:136:HOH:O	1.22	1.29
1:D:15:VAL:CG2	1:D:60:GLU:HG2	1.63	1.26

All (5) 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)
3:O:175:HOH:O	3:O:175:HOH:O[2_656]	1.78	0.42
3:E:116:HOH:O	3:E:116:HOH:O[2_555]	1.91	0.29
3:A:92:HOH:O	3:Q:113:HOH:O[4_556]	2.08	0.12
3:J:144:HOH:O	3:M:120:HOH:O[4_555]	2.09	0.11
3:A:129:HOH:O	3:M:129:HOH:O[3_455]	2.17	0.03

## 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	66/75 (88%)	66 (100%)	0	0	100	100
1	B	65/75 (87%)	65 (100%)	0	0	100	100
1	C	65/75 (87%)	65 (100%)	0	0	100	100
1	D	65/75 (87%)	65 (100%)	0	0	100	100
1	E	65/75 (87%)	65 (100%)	0	0	100	100
1	F	66/75 (88%)	66 (100%)	0	0	100	100
1	G	65/75 (87%)	65 (100%)	0	0	100	100
1	H	65/75 (87%)	65 (100%)	0	0	100	100
1	I	66/75 (88%)	66 (100%)	0	0	100	100
1	J	65/75 (87%)	65 (100%)	0	0	100	100

*Continued on next page...*



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	65/75 (87%)	64 (98%)	1 (2%)	0	100	100
1	L	65/75 (87%)	65 (100%)	0	0	100	100
1	M	66/75 (88%)	66 (100%)	0	0	100	100
1	N	65/75 (87%)	65 (100%)	0	0	100	100
1	O	65/75 (87%)	65 (100%)	0	0	100	100
1	P	66/75 (88%)	65 (98%)	1 (2%)	0	100	100
1	Q	65/75 (87%)	65 (100%)	0	0	100	100
1	R	65/75 (87%)	65 (100%)	0	0	100	100
1	S	66/75 (88%)	66 (100%)	0	0	100	100
1	T	65/75 (87%)	65 (100%)	0	0	100	100
1	U	65/75 (87%)	65 (100%)	0	0	100	100
1	V	65/75 (87%)	64 (98%)	1 (2%)	0	100	100
All	All	1436/1650 (87%)	1433 (100%)	3 (0%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	57/64 (89%)	56 (98%)	1 (2%)	59	48
1	B	56/64 (88%)	56 (100%)	0	100	100
1	C	56/64 (88%)	54 (96%)	2 (4%)	35	20
1	D	56/64 (88%)	54 (96%)	2 (4%)	35	20
1	E	56/64 (88%)	54 (96%)	2 (4%)	35	20
1	F	57/64 (89%)	56 (98%)	1 (2%)	59	48
1	G	56/64 (88%)	54 (96%)	2 (4%)	35	20
1	H	56/64 (88%)	55 (98%)	1 (2%)	59	48
1	I	57/64 (89%)	55 (96%)	2 (4%)	36	21

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	56/64 (88%)	54 (96%)	2 (4%)	35	20
1	K	56/64 (88%)	56 (100%)	0	100	100
1	L	56/64 (88%)	54 (96%)	2 (4%)	35	20
1	M	57/64 (89%)	57 (100%)	0	100	100
1	N	56/64 (88%)	55 (98%)	1 (2%)	59	48
1	O	56/64 (88%)	54 (96%)	2 (4%)	35	20
1	P	57/64 (89%)	57 (100%)	0	100	100
1	Q	56/64 (88%)	56 (100%)	0	100	100
1	R	56/64 (88%)	55 (98%)	1 (2%)	59	48
1	S	57/64 (89%)	55 (96%)	2 (4%)	36	21
1	T	56/64 (88%)	54 (96%)	2 (4%)	35	20
1	U	56/64 (88%)	54 (96%)	2 (4%)	35	20
1	V	56/64 (88%)	56 (100%)	0	100	100
All	All	1238/1408 (88%)	1211 (98%)	27 (2%)	53	39

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	73	GLU
1	N	37	LYS
1	T	37	LYS
1	L	60	GLU
1	O	16	GLU

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

Mol	Chain	Res	Type
1	V	20	ASN
1	S	20	ASN
1	M	20	ASN
1	K	20	ASN
1	O	20	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	V	81	-	14,16,16	0.77	0	16,22,22	0.96	0
2	TRP	T	81	-	14,16,16	0.80	0	16,22,22	0.98	1 (6%)
2	TRP	M	81	-	14,16,16	0.85	0	16,22,22	1.14	1 (6%)
2	TRP	F	81	-	14,16,16	0.80	0	16,22,22	1.09	1 (6%)
2	TRP	B	81	-	14,16,16	0.82	0	16,22,22	1.03	1 (6%)
2	TRP	E	81	-	14,16,16	0.88	0	16,22,22	1.16	2 (12%)
2	TRP	L	81	-	14,16,16	0.76	0	16,22,22	1.16	1 (6%)
2	TRP	N	81	-	14,16,16	0.89	0	16,22,22	0.47	0
2	TRP	H	81	-	14,16,16	0.80	0	16,22,22	1.65	2 (12%)
2	TRP	G	81	-	14,16,16	0.84	0	16,22,22	0.89	0
2	TRP	A	81	-	14,16,16	1.02	1 (7%)	16,22,22	1.16	2 (12%)
2	TRP	R	81	-	14,16,16	0.90	0	16,22,22	1.28	1 (6%)
2	TRP	D	81	-	14,16,16	0.97	0	16,22,22	0.99	1 (6%)
2	TRP	K	81	-	14,16,16	0.88	0	16,22,22	1.15	2 (12%)
2	TRP	I	81	-	14,16,16	0.91	0	16,22,22	1.14	2 (12%)
2	TRP	U	81	-	14,16,16	0.89	0	16,22,22	1.49	3 (18%)
2	TRP	P	81	-	14,16,16	0.74	0	16,22,22	0.96	0
2	TRP	J	81	-	14,16,16	0.66	0	16,22,22	1.26	3 (18%)
2	TRP	O	81	-	14,16,16	0.84	0	16,22,22	1.11	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	TRP	S	81	-	14,16,16	1.01	1 (7%)	16,22,22	0.64	0
2	TRP	Q	81	-	14,16,16	0.93	0	16,22,22	1.04	1 (6%)
2	TRP	C	81	-	14,16,16	1.07	0	16,22,22	1.06	1 (6%)

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	V	81	-	-	1/7/8/8	0/2/2/2
2	TRP	T	81	-	-	1/7/8/8	0/2/2/2
2	TRP	M	81	-	-	1/7/8/8	0/2/2/2
2	TRP	F	81	-	-	1/7/8/8	0/2/2/2
2	TRP	B	81	-	-	1/7/8/8	0/2/2/2
2	TRP	E	81	-	-	1/7/8/8	0/2/2/2
2	TRP	L	81	-	-	0/7/8/8	0/2/2/2
2	TRP	N	81	-	-	1/7/8/8	0/2/2/2
2	TRP	H	81	-	-	1/7/8/8	0/2/2/2
2	TRP	G	81	-	-	2/7/8/8	0/2/2/2
2	TRP	A	81	-	-	0/7/8/8	0/2/2/2
2	TRP	R	81	-	-	1/7/8/8	0/2/2/2
2	TRP	D	81	-	-	0/7/8/8	0/2/2/2
2	TRP	K	81	-	-	1/7/8/8	0/2/2/2
2	TRP	I	81	-	-	0/7/8/8	0/2/2/2
2	TRP	U	81	-	-	0/7/8/8	0/2/2/2
2	TRP	P	81	-	-	1/7/8/8	0/2/2/2
2	TRP	J	81	-	-	0/7/8/8	0/2/2/2
2	TRP	O	81	-	-	1/7/8/8	0/2/2/2
2	TRP	S	81	-	-	1/7/8/8	0/2/2/2
2	TRP	Q	81	-	-	1/7/8/8	0/2/2/2
2	TRP	C	81	-	-	1/7/8/8	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	81	TRP	CZ2-CE2	-2.14	1.38	1.41
2	A	81	TRP	CZ2-CE2	-2.01	1.38	1.41

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	81	TRP	OXT-C-O	-4.78	113.24	124.09
2	M	81	TRP	CB-CG-CD1	-3.04	124.21	127.97
2	U	81	TRP	CH2-CZ2-CE2	-2.91	115.90	120.08
2	R	81	TRP	CH2-CZ2-CE2	-2.75	116.13	120.08
2	J	81	TRP	CB-CG-CD1	-2.73	124.59	127.97

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	M	81	TRP	OXT-C-CA-N
2	H	81	TRP	O-C-CA-N
2	C	81	TRP	OXT-C-CA-N
2	E	81	TRP	OXT-C-CA-N
2	V	81	TRP	OXT-C-CA-N

There are no ring outliers.

20 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	V	81	TRP	1	0
2	T	81	TRP	1	0
2	F	81	TRP	1	0
2	B	81	TRP	1	0
2	E	81	TRP	1	0
2	N	81	TRP	1	0
2	H	81	TRP	1	0
2	G	81	TRP	1	0
2	A	81	TRP	1	0
2	R	81	TRP	1	0
2	D	81	TRP	1	0
2	K	81	TRP	1	0
2	I	81	TRP	3	0
2	U	81	TRP	1	0
2	P	81	TRP	1	0
2	J	81	TRP	1	0
2	O	81	TRP	1	0
2	S	81	TRP	1	0
2	Q	81	TRP	1	0
2	C	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

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.