



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:11 AM GMT

PDB ID : 2ZP9  
Title : The Nature of the TRAP:Anti-TRAP complex  
Authors : Watanabe, M.; Heddle, J.G.; Unzai, S.; Akashi, S.; Park, S.Y.; Tame, J.R.H.  
Deposited on : 2008-07-08  
Resolution : 3.20 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

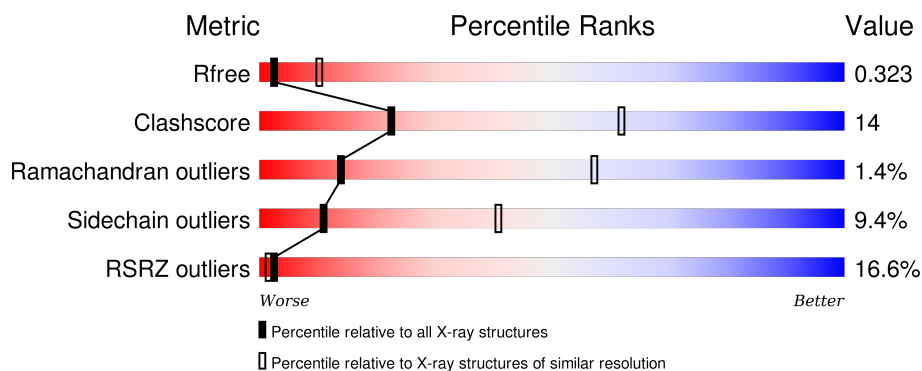
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	81	<div> <div>2%</div> <div>51% 26% • 22%</div> </div>
1	B	81	<div> <div>%</div> <div>51% 26% • 21%</div> </div>
1	F	81	<div> <div>16%</div> <div>60% 17% 22%</div> </div>
1	G	81	<div> <div>9%</div> <div>51% 26% • 22%</div> </div>
1	K	81	<div> <div>9%</div> <div>38% 38% • 22%</div> </div>

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Mol	Chain	Length	Quality of chain
1	L	81	
2	C	53	
2	D	53	
2	E	53	
2	H	53	
2	I	53	
2	J	53	
2	M	53	
2	N	53	
2	O	53	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	TRP	F	100	-	-	X	X
4	TRP	G	100	-	-	X	-
4	TRP	K	100	-	-	-	X
4	TRP	L	100	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5728 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	63	Total	C	N	O	0	0	0
			491	309	91	91			
1	B	64	Total	C	N	O	0	0	0
			499	315	92	92			
1	F	63	Total	C	N	O	0	0	0
			491	309	91	91			
1	G	63	Total	C	N	O	0	0	0
			491	309	91	91			
1	K	63	Total	C	N	O	0	0	0
			491	309	91	91			
1	L	63	Total	C	N	O	0	0	0
			491	309	91	91			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	ALA	-	LINKER	UNP Q9X6J6
A	78	ALA	-	LINKER	UNP Q9X6J6
A	79	ALA	-	LINKER	UNP Q9X6J6
A	80	ALA	-	LINKER	UNP Q9X6J6
A	81	ALA	-	LINKER	UNP Q9X6J6
A	82	ALA	-	LINKER	UNP Q9X6J6
A	83	ALA	-	LINKER	UNP Q9X6J6
B	77	ALA	-	LINKER	UNP Q9X6J6
B	78	ALA	-	LINKER	UNP Q9X6J6
B	79	ALA	-	LINKER	UNP Q9X6J6
B	80	ALA	-	LINKER	UNP Q9X6J6
B	81	ALA	-	LINKER	UNP Q9X6J6
B	82	ALA	-	LINKER	UNP Q9X6J6
B	83	ALA	-	LINKER	UNP Q9X6J6
F	77	ALA	-	LINKER	UNP Q9X6J6
F	78	ALA	-	LINKER	UNP Q9X6J6
F	79	ALA	-	LINKER	UNP Q9X6J6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	80	ALA	-	LINKER	UNP Q9X6J6
F	81	ALA	-	LINKER	UNP Q9X6J6
F	82	ALA	-	LINKER	UNP Q9X6J6
F	83	ALA	-	LINKER	UNP Q9X6J6
G	77	ALA	-	LINKER	UNP Q9X6J6
G	78	ALA	-	LINKER	UNP Q9X6J6
G	79	ALA	-	LINKER	UNP Q9X6J6
G	80	ALA	-	LINKER	UNP Q9X6J6
G	81	ALA	-	LINKER	UNP Q9X6J6
G	82	ALA	-	LINKER	UNP Q9X6J6
G	83	ALA	-	LINKER	UNP Q9X6J6
K	77	ALA	-	LINKER	UNP Q9X6J6
K	78	ALA	-	LINKER	UNP Q9X6J6
K	79	ALA	-	LINKER	UNP Q9X6J6
K	80	ALA	-	LINKER	UNP Q9X6J6
K	81	ALA	-	LINKER	UNP Q9X6J6
K	82	ALA	-	LINKER	UNP Q9X6J6
K	83	ALA	-	LINKER	UNP Q9X6J6
L	77	ALA	-	LINKER	UNP Q9X6J6
L	78	ALA	-	LINKER	UNP Q9X6J6
L	79	ALA	-	LINKER	UNP Q9X6J6
L	80	ALA	-	LINKER	UNP Q9X6J6
L	81	ALA	-	LINKER	UNP Q9X6J6
L	82	ALA	-	LINKER	UNP Q9X6J6
L	83	ALA	-	LINKER	UNP Q9X6J6

- Molecule 2 is a protein called Tryptophan RNA-binding attenuator protein-inhibitory protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	46	Total	C	N	O	S	0	0	0
			338	212	57	64	5			
2	D	45	Total	C	N	O	S	8	0	0
			334	210	56	63	5			
2	E	49	Total	C	N	O	S	0	0	0
			356	223	60	68	5			
2	H	42	Total	C	N	O	S	25	0	0
			310	197	49	59	5			
2	I	39	Total	C	N	O	S	0	0	0
			290	182	47	57	4			
2	J	41	Total	C	N	O	S	17	0	0
			301	192	48	56	5			
2	M	42	Total	C	N	O	S	25	0	0
			310	197	49	59	5			

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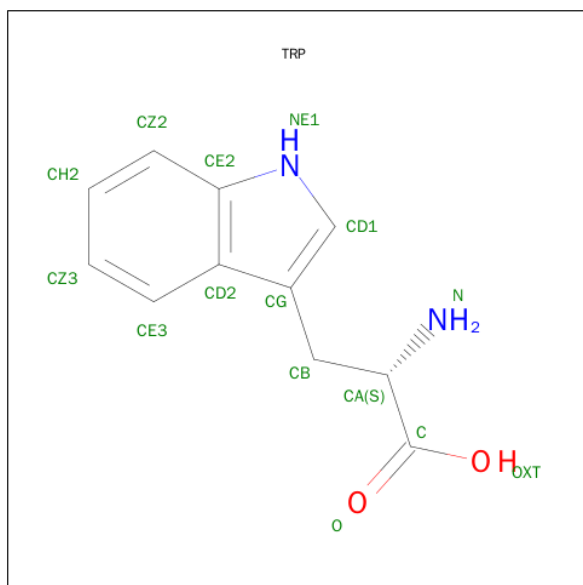
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	17	Total	C	N	O		0	0	0
			139	91	23	25				
2	O	41	Total	C	N	O	S	17	0	0
			301	192	48	56	5			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	1	Total	Zn	0	0
			1	1		
3	I	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		

- Molecule 4 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
4	A	1	Total	C	N	O	0	0
			15	11	2	2		
4	B	1	Total	C	N	O	0	0
			15	11	2	2		

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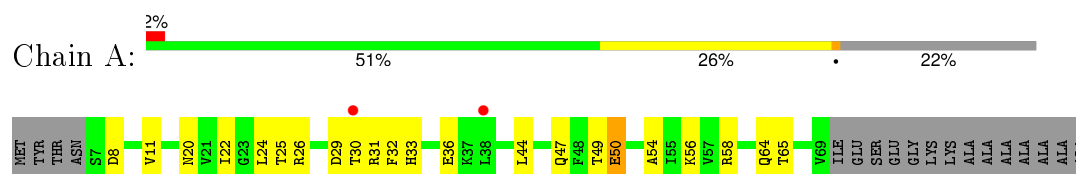
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	F	1	Total	C	N	O	0	0
			15	11	2	2		
4	G	1	Total	C	N	O	0	0
			15	11	2	2		
4	K	1	Total	C	N	O	0	0
			15	11	2	2		
4	L	1	Total	C	N	O	0	0
			15	11	2	2		

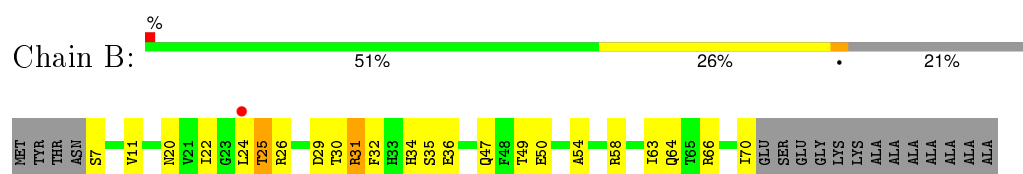
### 3 Residue-property plots [i](#)

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.

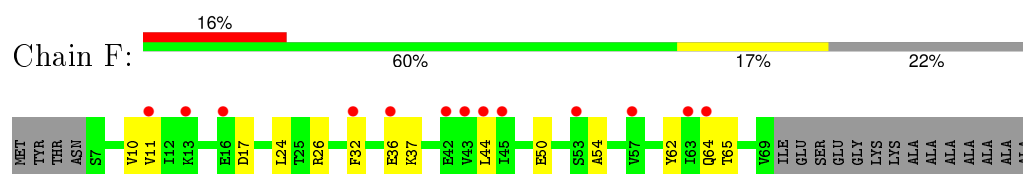
- Molecule 1: Transcription attenuation protein mtrB



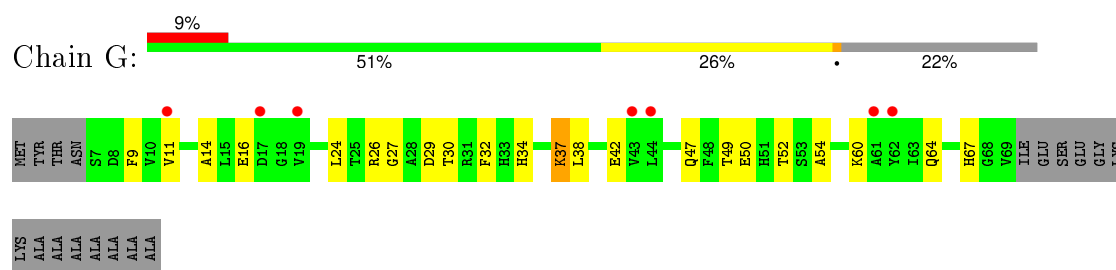
- Molecule 1: Transcription attenuation protein mtrB



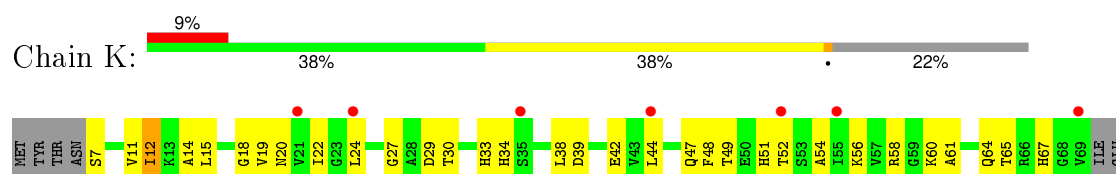
- Molecule 1: Transcription attenuation protein mtrB



- Molecule 1: Transcription attenuation protein mtrB



- Molecule 1: Transcription attenuation protein mtrB





SER  
GLU  
GLY  
LYS  
LYS  
ALA  
ALA  
ALA  
ALA  
ALA  
ALA

- Molecule 1: Transcription attenuation protein mtrB

Chain L: 

MET TYR THR ASN S7 V11 G18 G19 N20 V21 I22 G23 L24 T25 A28 F32 H33 H34 K37 L38 E42 V43 L44 Q47 F48 F49 A54 V57 R58 G59 R60 A61 Q64 T65 R66 H67 G68 V69 ILE GLU SER GLU GLY LYS LYS ALA ALA ALA ALA

ALA  
ALA

- Molecule 2: Tryptophan RNA-binding attenuator protein-inhibitory protein

Chain C: 

K1 V2 L8 A11 C12 C15 E16 R17 A18 G19 GLU ILE ILE GLY THR PRO C26 P27 V34 I35 I36 Q39 Q40 Y41 T42 L43 I47 L51 N52 LYS

- Molecule 2: Tryptophan RNA-binding attenuator protein-inhibitory protein

Chain D: 

K1 V2 I3 A4 T5 E9 V10 A11 C12 P13 K14 C15 E16 A17 A18 GLY GLU ILE ILE GLU THR PRO C26 P27 I28 A28 G31 K32 Q33 V34 I35 Q39 L43 L46 I47 H50 L51 N52 LYS

- Molecule 2: Tryptophan RNA-binding attenuator protein-inhibitory protein

Chain E: 

K1 V2 T5 L8 E9 V10 C15 E16 G19 GLU ILE ILE T24 P25 A28 I35 L36 T37 A38 Q39 L43 Q48 N52 LYS

- Molecule 2: Tryptophan RNA-binding attenuator protein-inhibitory protein

Chain H: 

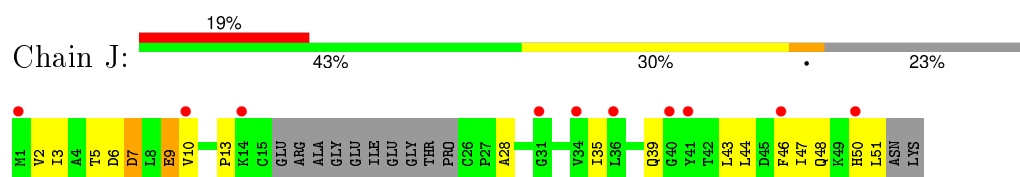
K1 V2 I3 D6 D7 L8 E9 A11 C12 P13 K14 C15 E16 ARG ALA ALA GLY GLU ILE ILE GLY THR PRO C26 P27 A28 C29 S30 G31 K32 G33 V34 I35 L36 L44 D45 F46 K49 H50 L51 ASN LYS

- Molecule 2: Tryptophan RNA-binding attenuator protein-inhibitory protein

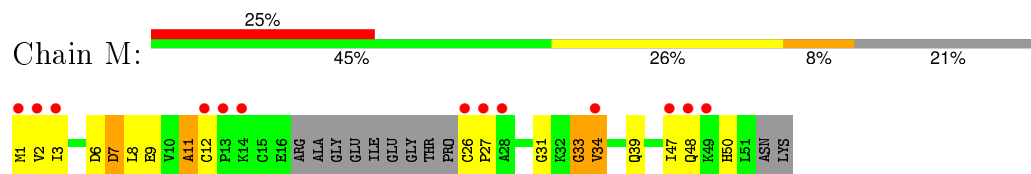
Chain I: 

MET VAL ILE ALA T5 D6 D7 L8 E9 A11 C12 P13 K14 C15 E16 ARG ALA ALA GLY GLU ILE ILE GLY THR PRO C26 P27 A28 K32 G33 V34 I35 L36 T37 A38 Q39 G40 L43 I47 Q48 L51 N52 LYS

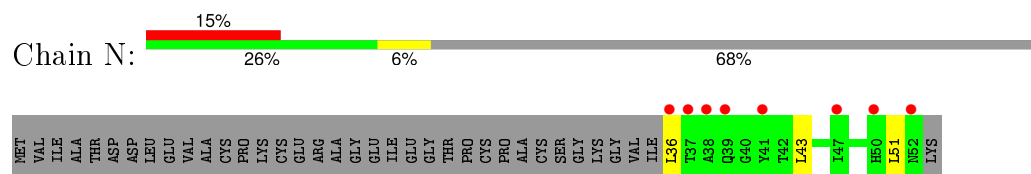
- Molecule 2: Tryptophan RNA-binding attenuator protein-inhibitory protein



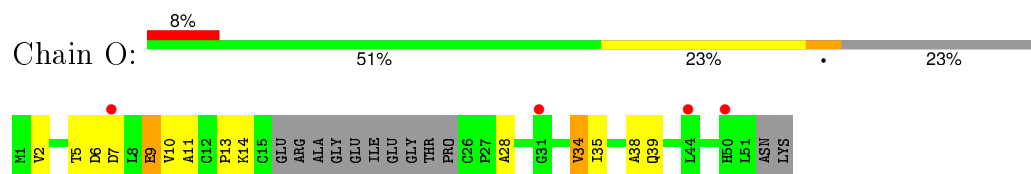
- Molecule 2: Tryptophan RNA-binding attenuator protein-inhibitory protein



- Molecule 2: Tryptophan RNA-binding attenuator protein-inhibitory protein



- Molecule 2: Tryptophan RNA-binding attenuator protein-inhibitory protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	197.13 Å   197.13 Å   56.66 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	20.00 – 3.20 37.25 – 3.20	Depositor EDS
% Data completeness (in resolution range)	91.0 (20.00-3.20) 90.8 (37.25-3.20)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.93 (at 3.18 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.303 , 0.325 0.302 , 0.323	Depositor DCC
$R_{free}$ test set	984 reflections (5.41%)	DCC
Wilson B-factor (Å <sup>2</sup> )	93.3	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 91.2	EDS
Estimated twinning fraction	0.439 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 19198 reflections	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	5728	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.46	0/498	0.62	0/669
1	B	0.53	0/506	0.67	0/680
1	F	0.38	0/498	0.55	0/669
1	G	0.42	0/498	0.58	0/669
1	K	0.39	0/498	0.57	0/669
1	L	0.37	0/498	0.55	0/669
2	C	0.38	0/341	0.59	0/459
2	D	1.41	3/337 (0.9%)	2.27	4/454 (0.9%)
2	E	0.44	0/360	0.60	0/486
2	H	0.91	3/313 (1.0%)	3.48	8/422 (1.9%)
2	I	0.41	0/293	0.57	0/395
2	J	1.48	2/304 (0.7%)	1.08	3/410 (0.7%)
2	M	0.75	3/313 (1.0%)	3.26	5/422 (1.2%)
2	N	0.42	0/141	0.50	0/190
2	O	1.77	2/304 (0.7%)	1.66	5/410 (1.2%)
All	All	0.78	13/5702 (0.2%)	1.42	25/7673 (0.3%)

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
2	D	0	1
2	H	0	2
2	J	0	2
2	M	0	3
2	O	0	1
All	All	0	9

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	7	ASP	C-N	-27.86	0.69	1.34
2	J	7	ASP	C-N	-22.03	0.83	1.34
2	D	34	VAL	C-N	17.88	1.75	1.34
2	D	35	ILE	C-N	-14.52	1.00	1.34
2	J	9	GLU	C-N	-11.23	1.08	1.34

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	9	GLU	O-C-N	-64.52	19.48	122.70
2	H	9	GLU	O-C-N	-61.24	24.71	122.70
2	D	34	VAL	O-C-N	-36.43	64.41	122.70
2	H	33	GLY	O-C-N	-26.49	80.32	122.70
2	D	34	VAL	CA-C-N	24.14	170.30	117.20

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	35	ILE	Mainchain
2	H	33	GLY	Mainchain,Peptide
2	J	7	ASP	Mainchain
2	J	9	GLU	Mainchain
2	M	11	ALA	Mainchain

## 5.2 Too-close contacts [i](#)

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	491	0	497	18	1
1	B	499	0	508	15	0
1	F	491	0	497	8	0
1	G	491	0	497	21	0
1	K	491	0	497	22	0
1	L	491	0	497	13	0
2	C	338	0	343	12	0
2	D	334	0	337	15	0
2	E	356	0	358	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	310	0	316	12	0
2	I	290	0	285	12	0
2	J	301	0	306	14	0
2	M	310	0	317	10	0
2	N	139	0	140	2	0
2	O	301	0	310	8	0
3	C	1	0	0	1	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	I	1	0	0	1	0
3	J	1	0	0	0	0
4	A	15	0	9	5	0
4	B	15	0	9	2	1
4	F	15	0	9	6	0
4	G	15	0	9	10	0
4	K	15	0	9	2	0
4	L	15	0	9	1	0
All	All	5728	0	5759	151	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 14.

The worst 5 of 151 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:27:GLY:H	4:G:100:TRP:HB2	1.18	1.09
2:I:15:CYS:HG	3:I:54:ZN:ZN	0.84	0.90
2:C:12:CYS:HG	3:C:54:ZN:ZN	0.64	0.89
4:G:100:TRP:HA	1:K:49:THR:CB	2.09	0.83
4:G:100:TRP:HA	1:K:49:THR:OG1	1.79	0.81

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:A:49:THR:OG1	4:B:100:TRP:OXT[6_555]	2.15	0.05

## 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	61/81 (75%)	60 (98%)	1 (2%)	0	100	100
1	B	62/81 (76%)	61 (98%)	1 (2%)	0	100	100
1	F	61/81 (75%)	58 (95%)	3 (5%)	0	100	100
1	G	61/81 (75%)	60 (98%)	1 (2%)	0	100	100
1	K	61/81 (75%)	59 (97%)	1 (2%)	1 (2%)	12	54
1	L	61/81 (75%)	60 (98%)	1 (2%)	0	100	100
2	C	42/53 (79%)	38 (90%)	3 (7%)	1 (2%)	7	43
2	D	41/53 (77%)	33 (80%)	6 (15%)	2 (5%)	3	22
2	E	45/53 (85%)	40 (89%)	4 (9%)	1 (2%)	8	45
2	H	38/53 (72%)	34 (90%)	3 (8%)	1 (3%)	7	40
2	I	35/53 (66%)	33 (94%)	1 (3%)	1 (3%)	6	36
2	J	37/53 (70%)	34 (92%)	1 (3%)	2 (5%)	2	19
2	M	38/53 (72%)	34 (90%)	3 (8%)	1 (3%)	7	40
2	N	15/53 (28%)	15 (100%)	0	0	100	100
2	O	37/53 (70%)	36 (97%)	1 (3%)	0	100	100
All	All	695/963 (72%)	655 (94%)	30 (4%)	10 (1%)	14	57

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	16	GLU
2	E	16	GLU
2	H	34	VAL
2	I	35	ILE
2	M	34	VAL

### 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	52/62 (84%)	47 (90%)	5 (10%)	10	39
1	B	53/62 (86%)	49 (92%)	4 (8%)	17	55
1	F	52/62 (84%)	50 (96%)	2 (4%)	40	78
1	G	52/62 (84%)	48 (92%)	4 (8%)	16	54
1	K	52/62 (84%)	46 (88%)	6 (12%)	7	30
1	L	52/62 (84%)	50 (96%)	2 (4%)	40	78
2	C	37/43 (86%)	32 (86%)	5 (14%)	5	22
2	D	37/43 (86%)	30 (81%)	7 (19%)	2	10
2	E	39/43 (91%)	35 (90%)	4 (10%)	9	36
2	H	35/43 (81%)	31 (89%)	4 (11%)	7	31
2	I	33/43 (77%)	28 (85%)	5 (15%)	3	17
2	J	34/43 (79%)	31 (91%)	3 (9%)	12	45
2	M	35/43 (81%)	33 (94%)	2 (6%)	25	67
2	N	15/43 (35%)	14 (93%)	1 (7%)	20	60
2	O	34/43 (79%)	31 (91%)	3 (9%)	12	45
All	All	612/759 (81%)	555 (91%)	57 (9%)	11	41

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	17	ASP
2	H	2	VAL
2	M	48	GLN
1	F	37	LYS
1	G	30	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:



Mol	Chain	Res	Type
2	I	48	GLN
2	J	39	GLN
1	L	67	HIS
1	G	47	GLN
2	M	39	GLN

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 for Mogul analysis.

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	$\# Z  > 2$
4	TRP	A	100	-	12,16,16	0.95	0	7,22,22	0.97	0
4	TRP	B	100	-	12,16,16	0.97	0	7,22,22	1.14	0
4	TRP	F	100	-	12,16,16	0.78	0	7,22,22	1.03	0
4	TRP	G	100	-	12,16,16	0.75	0	7,22,22	1.05	0
4	TRP	K	100	-	12,16,16	0.73	0	7,22,22	1.00	0
4	TRP	L	100	-	12,16,16	0.72	0	7,22,22	1.01	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
4	TRP	A	100	-	-	0/3/8/8	0/2/2/2
4	TRP	B	100	-	-	0/3/8/8	0/2/2/2
4	TRP	F	100	-	-	0/3/8/8	0/2/2/2
4	TRP	G	100	-	-	0/3/8/8	0/2/2/2
4	TRP	K	100	-	-	0/3/8/8	0/2/2/2
4	TRP	L	100	-	-	0/3/8/8	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	100	TRP	5	0
4	B	100	TRP	2	1
4	F	100	TRP	6	0
4	G	100	TRP	10	0
4	K	100	TRP	2	0
4	L	100	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	63/81 (77%)	0.82	2 (3%) 51 36	83, 86, 88, 90	0
1	B	64/81 (79%)	0.71	1 (1%) 74 62	81, 86, 88, 90	0
1	F	63/81 (77%)	1.10	13 (20%) 1 1	84, 86, 89, 95	0
1	G	63/81 (77%)	1.00	7 (11%) 7 4	84, 86, 89, 97	0
1	K	63/81 (77%)	0.81	7 (11%) 7 4	83, 86, 89, 96	0
1	L	63/81 (77%)	1.34	15 (23%) 1 1	84, 86, 89, 97	0
2	C	46/53 (86%)	0.98	6 (13%) 5 3	85, 86, 87, 90	3 (6%)
2	D	44/53 (83%)	1.37	8 (18%) 2 1	82, 86, 86, 87	11 (25%)
2	E	49/53 (92%)	0.83	3 (6%) 25 13	77, 86, 86, 88	7 (14%)
2	H	38/53 (71%)	1.75	10 (26%) 1 0	85, 86, 86, 86	2 (5%)
2	I	39/53 (73%)	2.09	14 (35%) 0 0	85, 86, 86, 87	8 (20%)
2	J	39/53 (73%)	1.07	10 (25%) 1 0	86, 86, 87, 88	3 (7%)
2	M	38/53 (71%)	2.50	13 (34%) 0 0	85, 86, 87, 88	2 (5%)
2	N	17/53 (32%)	2.25	8 (47%) 0 0	85, 86, 86, 87	1 (5%)
2	O	39/53 (73%)	0.95	4 (10%) 9 5	85, 86, 87, 88	3 (7%)
All	All	728/963 (75%)	1.20	121 (16%) 2 1	77, 86, 88, 97	40 (5%)

The worst 5 of 121 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	MET	12.2
2	I	52	ASN	12.1
2	H	1	MET	9.1
2	M	12	CYS	9.0
2	I	27	PRO	7.2

## 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
4	TRP	F	100	15/15	0.85	0.45	1.69	92,92,93,93	0
4	TRP	K	100	15/15	0.76	0.46	1.09	122,122,122,122	0
4	TRP	L	100	15/15	0.86	0.41	0.81	111,111,112,112	0
4	TRP	B	100	15/15	0.87	0.34	0.49	66,68,69,70	0
3	ZN	E	54	1/1	0.99	0.29	0.11	70,70,70,70	0
3	ZN	J	54	1/1	0.94	0.23	-0.35	118,118,118,118	0
4	TRP	A	100	15/15	0.95	0.29	-0.45	56,57,58,58	0
3	ZN	D	54	1/1	0.97	0.25	-0.45	123,123,123,123	0
3	ZN	C	54	1/1	0.84	0.17	-0.89	133,133,133,133	0
3	ZN	I	54	1/1	0.87	0.23	-1.00	140,140,140,140	0
4	TRP	G	100	15/15	0.89	0.20	-1.28	93,93,93,93	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.