



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:44 PM GMT

PDB ID : 1QAW  
Title : Regulatory Features of the TRP Operon and the Crystal Structure of the TRP RNA-Binding Attenuation Protein from Bacillus Stearothermophilus.  
Authors : Chen, X.-P.; Antson, A.A.; Yang, M.; Baumann, C.; Dodson, E.J.; Dodson, G.G.; Gollnick, P.  
Deposited on : 1999-03-31  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

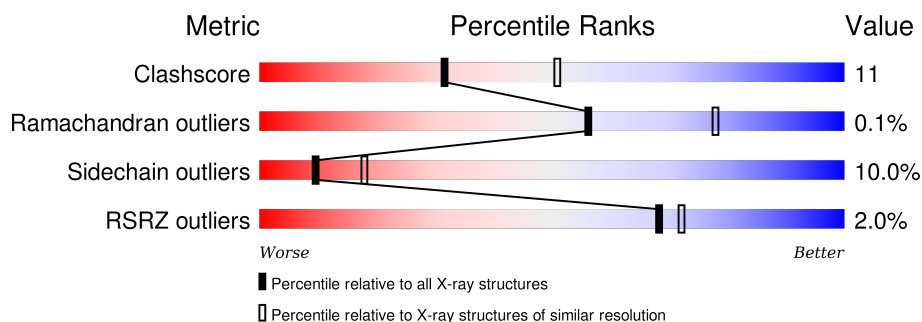
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	
1	B	74	
1	C	74	
1	D	74	
1	E	74	
1	F	74	
1	G	74	

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Mol	Chain	Length	Quality of chain
1	H	74	
1	I	74	
1	J	74	
1	K	74	

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
2	TRP	E	81	-	-	-	X

## 2 Entry composition

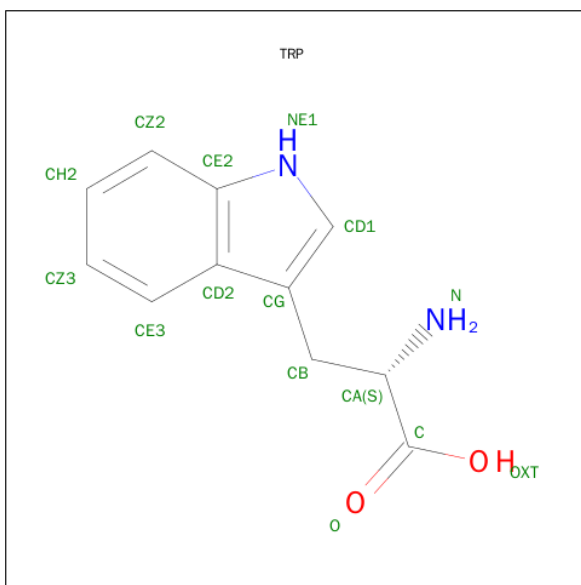
There are 3 unique types of molecules in this entry. The entry contains 6240 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	67	Total	C	N	O	5	1	0
			527	330	95	102			
1	B	70	Total	C	N	O	10	1	0
			550	344	100	106			
1	C	69	Total	C	N	O	5	0	0
			536	336	98	102			
1	D	69	Total	C	N	O	11	0	0
			536	336	98	102			
1	E	69	Total	C	N	O	7	0	0
			536	336	98	102			
1	F	68	Total	C	N	O	10	0	0
			527	330	96	101			
1	G	67	Total	C	N	O	6	1	0
			529	331	98	100			
1	H	68	Total	C	N	O	4	0	0
			527	330	96	101			
1	I	67	Total	C	N	O	30	0	0
			523	328	95	100			
1	J	67	Total	C	N	O	15	0	0
			523	328	95	100			
1	K	68	Total	C	N	O	13	1	0
			531	332	96	103			

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



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	22	Total	O	0	0
			22	22		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	20	Total 20	O 20	0	0
3	C	28	Total 28	O 28	0	0
3	D	37	Total 37	O 37	0	0
3	E	49	Total 49	O 49	0	0
3	F	28	Total 28	O 28	0	0
3	G	19	Total 19	O 19	0	0
3	H	11	Total 11	O 11	0	0
3	I	6	Total 6	O 6	0	0
3	J	5	Total 5	O 5	0	0
3	K	5	Total 5	O 5	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 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 ( $\text{RSRZ} > 2$ ). 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: TRP RNA-BINDING ATTENUATION PROTEIN

Chain A: 



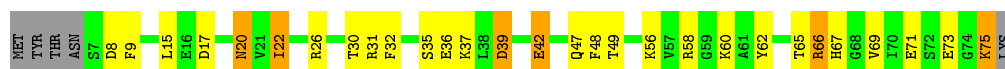
#### • Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN

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

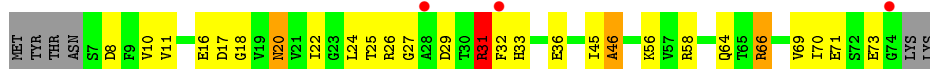
Chain F: 



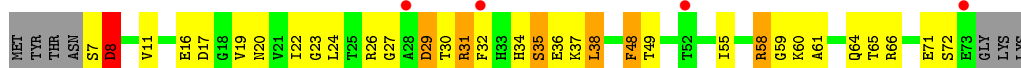
- Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN



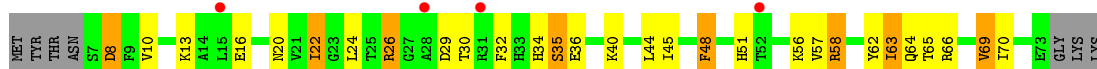
- Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN



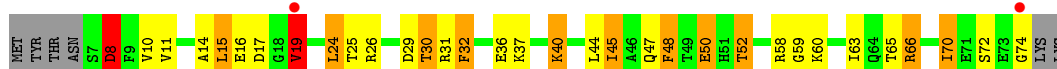
- Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN



- Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN



- Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.93Å 117.96Å 147.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 14.96 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.4 (15.00-2.50) 90.2 (14.96-2.50)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.28 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.215 , 0.299 0.203 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	39.2	Xtriage
Anisotropy	0.538	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 75.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 36543 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6240	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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	0.84	2/539 (0.4%)	1.94	16/724 (2.2%)
1	B	0.85	2/562 (0.4%)	1.99	15/751 (2.0%)
1	C	1.82	2/543 (0.4%)	2.24	28/728 (3.8%)
1	D	0.94	2/543 (0.4%)	2.12	27/728 (3.7%)
1	E	0.87	0/543	2.02	11/728 (1.5%)
1	F	0.83	0/534	1.99	15/717 (2.1%)
1	G	0.74	0/541	1.83	13/726 (1.8%)
1	H	0.58	0/534	1.64	10/717 (1.4%)
1	I	0.96	3/530 (0.6%)	1.88	13/712 (1.8%)
1	J	0.83	2/530 (0.4%)	1.57	10/712 (1.4%)
1	K	0.69	1/543 (0.2%)	1.75	10/729 (1.4%)
All	All	0.96	14/5942 (0.2%)	1.92	168/7972 (2.1%)

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	A	0	6
1	B	0	7
1	C	0	3
1	D	0	2
1	E	0	4
1	F	0	5
1	G	0	3
1	H	0	4
1	I	0	2
1	J	0	3
1	K	0	3
All	All	0	42

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	75	LYS	CE-NZ	38.06	2.44	1.49
1	I	37	LYS	CD-CE	-13.99	1.16	1.51
1	J	32	PHE	CB-CG	-11.04	1.32	1.51
1	I	38	LEU	CA-CB	10.28	1.77	1.53
1	J	40	LYS	CA-CB	-9.56	1.32	1.53
1	A	60	LYS	CE-NZ	9.43	1.72	1.49
1	A	37	LYS	CB-CG	8.42	1.75	1.52
1	B	37	LYS	CG-CD	-8.19	1.24	1.52
1	D	37	LYS	CB-CG	-8.12	1.30	1.52
1	B	75	LYS	CG-CD	-7.20	1.27	1.52
1	C	37	LYS	CB-CG	-7.20	1.33	1.52
1	K	66	ARG	NE-CZ	6.46	1.41	1.33
1	D	75	LYS	CG-CD	6.29	1.73	1.52
1	I	31	ARG	CA-CB	-6.13	1.40	1.53

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	58	ARG	CD-NE-CZ	17.36	147.90	123.60
1	A	66	ARG	NE-CZ-NH2	16.26	128.43	120.30
1	B	75	LYS	CB-CG-CD	16.18	153.66	111.60
1	C	75	LYS	CD-CE-NZ	-15.40	76.27	111.70
1	E	8	ASP	CB-CG-OD2	-14.59	105.17	118.30
1	D	26	ARG	NE-CZ-NH2	14.22	127.41	120.30
1	D	31	ARG	NE-CZ-NH1	12.68	126.64	120.30
1	C	26	ARG	NE-CZ-NH1	12.39	126.49	120.30
1	I	66	ARG	NE-CZ-NH1	-12.30	114.15	120.30
1	C	31	ARG	NE-CZ-NH2	-12.26	114.17	120.30
1	K	32	PHE	CB-CG-CD1	-11.82	112.53	120.80
1	I	37	LYS	CG-CD-CE	11.49	146.36	111.90
1	A	66	ARG	NE-CZ-NH1	-11.19	114.70	120.30
1	D	58	ARG	NE-CZ-NH1	10.87	125.74	120.30
1	G	31	ARG	CD-NE-CZ	10.86	138.81	123.60
1	B	58	ARG	NE-CZ-NH1	-10.76	114.92	120.30
1	E	58	ARG	NE-CZ-NH2	10.69	125.64	120.30
1	D	31	ARG	NE-CZ-NH2	-10.25	115.17	120.30
1	A	31	ARG	NE-CZ-NH2	10.20	125.40	120.30
1	E	66	ARG	NE-CZ-NH2	-10.13	115.24	120.30
1	I	37	LYS	CD-CE-NZ	10.02	134.75	111.70
1	K	31	ARG	CD-NE-CZ	9.79	137.31	123.60
1	H	66	ARG	NE-CZ-NH2	9.79	125.19	120.30
1	K	32	PHE	CB-CG-CD2	9.71	127.60	120.80
1	G	8	ASP	CB-CG-OD2	-9.58	109.68	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	66	ARG	NE-CZ-NH2	9.50	125.05	120.30
1	G	8	ASP	CB-CG-OD1	9.48	126.84	118.30
1	C	26	ARG	NH1-CZ-NH2	-9.44	109.02	119.40
1	F	39	ASP	CB-CG-OD2	-9.09	110.12	118.30
1	G	26	ARG	NE-CZ-NH2	9.04	124.82	120.30
1	C	58	ARG	NE-CZ-NH1	9.01	124.80	120.30
1	B	37	LYS	CB-CG-CD	9.00	135.01	111.60
1	H	26	ARG	CD-NE-CZ	8.96	136.14	123.60
1	I	58	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	F	29	ASP	CB-CG-OD2	-8.74	110.44	118.30
1	C	39	ASP	CB-CG-OD2	-8.50	110.65	118.30
1	E	8	ASP	OD1-CG-OD2	8.49	139.42	123.30
1	F	66	ARG	NE-CZ-NH1	8.37	124.48	120.30
1	D	75	LYS	CB-CG-CD	-8.31	89.99	111.60
1	E	26	ARG	NE-CZ-NH2	8.29	124.44	120.30
1	C	26	ARG	NE-CZ-NH2	8.15	124.37	120.30
1	A	60	LYS	CD-CE-NZ	-7.94	93.43	111.70
1	A	73	GLU	CA-C-O	7.89	136.67	120.10
1	A	29	ASP	CB-CG-OD2	-7.85	111.23	118.30
1	D	71	GLU	OE1-CD-OE2	-7.83	113.91	123.30
1	D	29	ASP	CB-CG-OD2	7.81	125.33	118.30
1	D	70	ILE	CA-CB-CG2	7.76	126.42	110.90
1	J	32	PHE	CB-CG-CD2	-7.74	115.39	120.80
1	J	51	HIS	CA-CB-CG	-7.73	100.46	113.60
1	F	73	GLU	OE1-CD-OE2	-7.72	114.03	123.30
1	H	26	ARG	NE-CZ-NH2	7.53	124.06	120.30
1	K	8	ASP	CB-CG-OD2	-7.43	111.61	118.30
1	J	8	ASP	CB-CG-OD2	-7.36	111.68	118.30
1	B	75	LYS	CB-CA-C	-7.28	95.85	110.40
1	H	66	ARG	NH1-CZ-NH2	-7.25	111.42	119.40
1	E	15	LEU	CA-CB-CG	7.19	131.83	115.30
1	C	31	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	C	17	ASP	CB-CG-OD1	7.15	124.73	118.30
1	A	31	ARG	CA-CB-CG	7.15	129.12	113.40
1	I	60	LYS	CB-CA-C	7.08	124.57	110.40
1	D	71	GLU	CG-CD-OE1	6.96	132.23	118.30
1	C	31	ARG	CA-CB-CG	6.92	128.63	113.40
1	I	38	LEU	CB-CA-C	-6.91	97.08	110.20
1	F	62	TYR	CB-CG-CD2	-6.85	116.89	121.00
1	D	54	ALA	N-CA-CB	6.81	119.64	110.10
1	D	56	LYS	CA-CB-CG	6.75	128.25	113.40
1	D	70	ILE	CB-CG1-CD1	-6.68	95.19	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	31	ARG	CD-NE-CZ	-6.66	114.27	123.60
1	D	39	ASP	CB-CG-OD1	6.60	124.24	118.30
1	G	66	ARG	NE-CZ-NH2	6.60	123.60	120.30
1	C	62	TYR	CB-CG-CD2	-6.57	117.06	121.00
1	J	40	LYS	N-CA-CB	6.52	122.33	110.60
1	G	37	LYS	CA-CB-CG	6.50	127.70	113.40
1	A	8	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	G	17	ASP	CB-CG-OD1	6.46	124.12	118.30
1	I	26	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	D	58	ARG	CD-NE-CZ	6.46	132.64	123.60
1	F	73	GLU	O-C-N	-6.42	112.29	123.20
1	B	35	SER	N-CA-CB	6.41	120.11	110.50
1	F	48	PHE	O-C-N	-6.40	112.45	122.70
1	J	26	ARG	NE-CZ-NH2	6.37	123.48	120.30
1	K	37	LYS	CA-CB-CG	6.30	127.26	113.40
1	D	26	ARG	NH1-CZ-NH2	-6.29	112.48	119.40
1	D	75	LYS	N-CA-CB	-6.29	99.28	110.60
1	G	24	LEU	CA-CB-CG	6.25	129.68	115.30
1	C	20	ASN	OD1-CG-ND2	6.23	136.23	121.90
1	F	73	GLU	CB-CG-CD	6.18	130.88	114.20
1	H	66	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	B	29	ASP	CB-CG-OD2	-6.16	112.76	118.30
1	E	29	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	G	31	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	H	58	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	C	67	HIS	CA-C-N	6.12	128.44	116.20
1	C	37	LYS	CA-CB-CG	6.11	126.83	113.40
1	A	37	LYS	CA-CB-CG	-6.10	99.97	113.40
1	K	31	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	F	51	HIS	CA-CB-CG	-6.09	103.25	113.60
1	B	31	ARG	CG-CD-NE	-6.08	99.04	111.80
1	D	8	ASP	CB-CG-OD2	-6.06	112.85	118.30
1	K	29	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	F	58	ARG	CD-NE-CZ	6.02	132.03	123.60
1	B	39	ASP	CB-CG-OD2	-5.97	112.92	118.30
1	D	25	THR	CA-CB-CG2	-5.97	104.04	112.40
1	D	35	SER	N-CA-CB	-5.96	101.56	110.50
1	F	71	GLU	CA-CB-CG	5.92	126.43	113.40
1	B	44	LEU	CA-CB-CG	5.91	128.90	115.30
1	C	22	ILE	CA-CB-CG2	5.91	122.72	110.90
1	C	71	GLU	OE1-CD-OE2	5.89	130.37	123.30
1	A	50[A]	GLU	CA-CB-CG	5.86	126.29	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50[B]	GLU	CA-CB-CG	5.86	126.29	113.40
1	G	33	HIS	N-CA-CB	5.84	121.11	110.60
1	C	8	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	B	39	ASP	N-CA-CB	5.77	120.98	110.60
1	I	8	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	B	29	ASP	O-C-N	5.74	131.89	122.70
1	F	39	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	29	ASP	O-C-N	5.62	131.70	122.70
1	B	26	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	C	56	LYS	CA-CB-CG	5.62	125.75	113.40
1	J	29	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	C	20	ASN	CA-CB-CG	-5.61	101.06	113.40
1	E	54	ALA	N-CA-CB	5.59	117.93	110.10
1	B	38	LEU	CA-CB-CG	5.56	128.09	115.30
1	J	66	ARG	NE-CZ-NH2	5.55	123.08	120.30
1	E	8	ASP	N-CA-CB	-5.55	100.61	110.60
1	D	73	GLU	CA-CB-CG	5.54	125.60	113.40
1	C	62	TYR	CB-CG-CD1	5.53	124.32	121.00
1	C	66	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	29	ASP	CB-CG-OD1	5.51	123.26	118.30
1	K	15	LEU	CA-CB-CG	5.50	127.96	115.30
1	C	31	ARG	CB-CA-C	-5.50	99.41	110.40
1	H	31	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	J	26	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	G	47	GLN	CB-CA-C	-5.38	99.64	110.40
1	D	8	ASP	OD1-CG-OD2	5.37	133.50	123.30
1	G	66	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	A	47	GLN	CB-CA-C	-5.35	99.70	110.40
1	E	65	THR	CA-CB-CG2	-5.35	104.92	112.40
1	I	29	ASP	CB-CG-OD1	5.32	123.09	118.30
1	J	32	PHE	CB-CG-CD1	5.32	124.52	120.80
1	I	60	LYS	CA-CB-CG	5.28	125.02	113.40
1	H	73	GLU	CA-C-N	5.28	126.77	116.20
1	D	65	THR	N-CA-CB	5.25	120.27	110.30
1	C	73	GLU	N-CA-CB	5.23	120.01	110.60
1	D	8	ASP	CB-CG-OD1	-5.21	113.61	118.30
1	A	26	ARG	NE-CZ-NH1	-5.21	117.70	120.30
1	H	56	LYS	CA-CB-CG	5.19	124.83	113.40
1	C	17	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	F	29	ASP	CB-CA-C	-5.17	100.05	110.40
1	K	24	LEU	CA-CB-CG	5.17	127.19	115.30
1	G	50	GLU	OE1-CD-OE2	-5.17	117.10	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	52	THR	O-C-N	5.16	130.95	122.70
1	C	73	GLU	CA-C-N	-5.13	105.94	116.20
1	C	69	VAL	CA-CB-CG2	5.13	118.60	110.90
1	D	19	VAL	CG1-CB-CG2	5.11	119.08	110.90
1	J	58	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	B	26	ARG	NE-CZ-NH1	-5.09	117.75	120.30
1	F	62	TYR	CB-CG-CD1	5.09	124.05	121.00
1	D	43	VAL	CA-CB-CG1	5.08	118.52	110.90
1	K	24	LEU	CB-CG-CD1	5.08	119.64	111.00
1	B	75	LYS	CG-CD-CE	5.08	127.14	111.90
1	F	56	LYS	O-C-N	5.07	130.81	122.70
1	I	29	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	H	36	GLU	OE1-CD-OE2	5.05	129.35	123.30
1	D	32	PHE	CB-CG-CD1	5.04	124.33	120.80
1	C	36	GLU	OE1-CD-OE2	5.04	129.35	123.30
1	A	31	ARG	CD-NE-CZ	-5.04	116.55	123.60
1	C	71	GLU	CG-CD-OE2	-5.04	108.23	118.30

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	26	ARG	Mainchain
1	A	28	ALA	Mainchain
1	A	35	SER	Mainchain
1	A	37	LYS	Mainchain
1	A	56	LYS	Mainchain
1	A	57	VAL	Mainchain
1	B	23	GLY	Mainchain
1	B	44	LEU	Mainchain
1	B	46	ALA	Mainchain
1	B	49	THR	Mainchain
1	B	64	GLN	Mainchain
1	B	73	GLU	Mainchain
1	B	75	LYS	Mainchain
1	C	35	SER	Mainchain
1	C	49	THR	Mainchain
1	C	65	THR	Mainchain
1	D	28	ALA	Mainchain
1	D	66	ARG	Mainchain
1	E	15	LEU	Mainchain
1	E	42	GLU	Mainchain

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Mol	Chain	Res	Type	Group
1	E	48	PHE	Mainchain
1	E	65	THR	Mainchain
1	F	15	LEU	Mainchain
1	F	29	ASP	Mainchain
1	F	41	GLY	Mainchain
1	F	48	PHE	Mainchain
1	F	62	TYR	Mainchain
1	G	18	GLY	Mainchain
1	G	25	THR	Mainchain
1	G	37	LYS	Mainchain
1	H	22	ILE	Mainchain
1	H	32	PHE	Mainchain
1	H	46	ALA	Mainchain
1	H	71	GLU	Mainchain
1	I	48	PHE	Mainchain
1	I	49	THR	Mainchain
1	J	22	ILE	Mainchain
1	J	35	SER	Mainchain
1	J	48	PHE	Mainchain
1	K	19	VAL	Mainchain
1	K	48	PHE	Mainchain
1	K	52	THR	Mainchain

## 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	527	0	527	25	0
1	B	550	0	556	15	1
1	C	536	0	541	11	0
1	D	536	0	541	4	0
1	E	536	0	541	6	0
1	F	527	0	528	9	0
1	G	529	0	534	16	0
1	H	527	0	528	10	0
1	I	523	0	525	18	0
1	J	523	0	525	16	0
1	K	531	0	530	23	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	15	0	9	3	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	0	0
2	G	30	0	18	1	0
2	H	15	0	9	1	0
2	I	15	0	9	1	0
2	J	15	0	9	0	0
2	K	15	0	9	3	0
3	A	22	0	0	0	0
3	B	20	0	0	1	0
3	C	28	0	0	0	0
3	D	37	0	0	0	0
3	E	49	0	0	2	0
3	F	28	0	0	0	0
3	G	19	0	0	0	0
3	H	11	0	0	0	0
3	I	6	0	0	0	0
3	J	5	0	0	0	0
3	K	5	0	0	0	0
All	All	6240	0	5975	125	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 11.

All (125) 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:A:66:ARG:HH12	1:B:66:ARG:HD2	1.23	0.99
1:B:66:ARG:HH22	1:C:66:ARG:HE	1.12	0.94
1:I:20:ASN:HD22	1:I:58:ARG:HH21	0.97	0.94
1:B:66:ARG:NH2	1:C:66:ARG:HE	1.65	0.93
1:J:22:ILE:HD12	1:J:56:LYS:HD3	1.65	0.79
1:A:66:ARG:NH1	1:B:66:ARG:HD2	1.97	0.79
1:G:56:LYS:HZ3	1:G:58[A]:ARG:HH21	1.31	0.78
1:C:39:ASP:O	1:C:42:GLU:HG3	1.86	0.76
1:A:31:ARG:HH21	1:A:33:HIS:HA	1.51	0.76
1:G:56:LYS:NZ	1:G:58[A]:ARG:HH21	1.85	0.74
1:B:66:ARG:HH22	1:C:66:ARG:NE	1.85	0.74
1:B:51:HIS:ND1	3:B:85:HOH:O	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:20:ASN:ND2	1:I:58:ARG:HH21	1.81	0.73
1:I:20:ASN:HD22	1:I:58:ARG:NH2	1.81	0.71
1:F:66:ARG:HH12	1:G:66:ARG:HD2	1.56	0.69
1:A:10:VAL:HG12	1:A:65:THR:HG22	1.77	0.65
1:B:30:THR:HG1	2:B:81:TRP:N	1.96	0.64
1:E:7:SER:O	3:E:101:HOH:O	2.15	0.64
1:K:30:THR:HG23	2:K:81:TRP:HB2	1.79	0.63
1:K:19:VAL:HG13	1:K:59:GLY:HA3	1.81	0.62
1:I:19:VAL:HG22	1:I:59:GLY:HA3	1.81	0.61
1:I:11:VAL:HB	1:I:64:GLN:HB2	1.81	0.61
1:G:48:PHE:HZ	1:H:45:ILE:HG22	1.67	0.59
1:K:60:LYS:HA	1:K:72:SER:O	2.03	0.59
1:I:34:HIS:NE2	1:I:36:GLU:HB2	2.18	0.59
1:A:15:LEU:HB2	1:A:60:LYS:HG3	1.85	0.59
1:E:73:GLU:O	1:F:41:GLY:HA3	2.05	0.57
1:I:22:ILE:CG2	1:I:32:PHE:HB2	2.35	0.57
1:K:11:VAL:HG22	1:K:45:ILE:HG23	1.85	0.57
1:K:10:VAL:HG12	1:K:65:THR:HG22	1.88	0.56
1:A:30:THR:HG1	2:A:81:TRP:N	2.03	0.56
1:G:16:GLU:HA	1:G:40:LYS:HG3	1.88	0.55
1:J:62:TYR:CZ	1:J:69:VAL:HG11	2.41	0.55
1:A:45:ILE:HD13	1:K:10:VAL:HG11	1.88	0.55
1:C:9:PHE:HB3	1:C:47:GLN:HG2	1.89	0.54
1:K:63:ILE:HB	1:K:70:ILE:O	2.07	0.54
1:K:24:LEU:HD23	1:K:30:THR:HG22	1.90	0.54
1:C:30:THR:HG1	2:C:81:TRP:N	2.06	0.54
1:G:61:ALA:HB3	1:G:72:SER:OG	2.08	0.53
1:A:24:LEU:HD12	1:A:24:LEU:N	2.24	0.53
1:A:31:ARG:HH21	1:A:33:HIS:CA	2.20	0.53
1:F:66:ARG:HH21	1:F:66:ARG:HG2	1.74	0.53
1:E:60:LYS:HG2	3:E:107:HOH:O	2.09	0.53
1:H:27:GLY:O	2:H:81:TRP:N	2.42	0.52
1:I:61:ALA:HB3	1:I:72:SER:OG	2.09	0.52
1:B:66:ARG:NH2	1:C:66:ARG:NE	2.47	0.52
1:A:20:ASN:ND2	1:A:35:SER:OG	2.35	0.52
1:I:22:ILE:HG21	1:I:32:PHE:HB2	1.92	0.51
1:J:56:LYS:HE2	1:J:58:ARG:NH1	2.25	0.51
1:A:31:ARG:NH2	1:A:33:HIS:HA	2.23	0.51
1:K:36:GLU:HG2	1:K:44:LEU:HD22	1.93	0.51
1:J:24:LEU:HD23	1:J:30:THR:CG2	2.41	0.51
1:J:20:ASN:ND2	1:J:35:SER:OG	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:11:VAL:HB	1:G:64:GLN:HB2	1.93	0.50
1:G:26:ARG:HD2	1:G:50:GLU:O	2.11	0.50
1:K:16:GLU:CA	1:K:40:LYS:HG3	2.40	0.50
1:B:21:VAL:HG21	1:B:44:LEU:HD23	1.93	0.50
1:I:22:ILE:HG23	1:I:34:HIS:O	2.11	0.50
1:A:26:ARG:HB2	1:A:53:SER:HB3	1.93	0.50
1:A:34:HIS:HE2	1:A:36:GLU:HB2	1.77	0.49
1:I:27:GLY:O	2:I:81:TRP:N	2.46	0.49
1:E:66:ARG:HH21	1:F:66:ARG:HD2	1.77	0.49
1:A:10:VAL:HG11	1:B:45:ILE:HD13	1.94	0.48
1:C:48:PHE:HZ	1:D:45:ILE:HG22	1.77	0.48
1:J:57:VAL:HG21	1:J:63:ILE:CD1	2.44	0.48
1:A:15:LEU:HB2	1:A:60:LYS:CG	2.43	0.48
1:B:12:ILE:O	1:B:43:VAL:HA	2.13	0.48
1:J:48:PHE:HB3	1:K:47:GLN:OE1	2.14	0.48
1:G:48:PHE:CZ	1:H:45:ILE:HG22	2.49	0.47
1:K:14:ALA:HB1	1:K:19:VAL:HG21	1.95	0.47
1:H:10:VAL:HG23	1:H:10:VAL:O	2.15	0.47
1:H:11:VAL:HB	1:H:64:GLN:HB2	1.96	0.47
1:A:15:LEU:HD12	1:A:60:LYS:HD2	1.96	0.47
1:A:16:GLU:OE1	1:A:60:LYS:HB3	2.15	0.47
1:K:30:THR:CG2	2:K:81:TRP:HB2	2.45	0.47
1:A:30:THR:HG23	2:A:81:TRP:HB2	1.96	0.47
1:A:19:VAL:HG13	1:A:58:ARG:O	2.16	0.46
1:A:42:GLU:OE2	1:K:58:ARG:HG3	2.16	0.46
1:G:16:GLU:HG3	1:G:17:ASP:O	2.16	0.46
1:K:16:GLU:HA	1:K:40:LYS:HG3	1.97	0.46
1:I:48:PHE:HZ	1:J:45:ILE:HG22	1.80	0.46
1:I:16:GLU:HG3	1:I:17:ASP:O	2.16	0.46
1:B:56:LYS:HE2	1:B:58:ARG:NH2	2.30	0.45
1:F:14:ALA:HB2	1:F:38:LEU:HB2	1.98	0.45
1:J:10:VAL:CG1	1:J:65:THR:HG22	2.46	0.45
1:B:38:LEU:HD21	1:B:44:LEU:HB2	1.97	0.45
1:G:27:GLY:O	2:G:82:TRP:N	2.50	0.45
1:I:22:ILE:HG22	1:I:23:GLY:N	2.32	0.45
1:K:8:ASP:OD2	1:K:66:ARG:HD3	2.17	0.45
1:I:71:GLU:O	1:J:13:LYS:HE3	2.17	0.45
1:A:45:ILE:HG22	1:K:48:PHE:HZ	1.82	0.44
1:C:15:LEU:HB2	1:C:60:LYS:HD3	1.99	0.44
1:I:30:THR:HB	1:J:34:HIS:CE1	2.52	0.44
1:J:36:GLU:HG2	1:J:44:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:THR:HG1	2:D:81:TRP:N	2.15	0.44
1:D:10:VAL:HG23	1:D:12:ILE:CD1	2.48	0.44
1:G:56:LYS:NZ	1:G:58[A]:ARG:NH2	2.62	0.43
1:I:55:ILE:O	1:J:44:LEU:HD12	2.18	0.43
1:E:11:VAL:O	1:E:63:ILE:HA	2.18	0.43
1:I:34:HIS:CG	1:I:35:SER:N	2.86	0.43
1:A:47:GLN:HB3	1:A:48:PHE:O	2.18	0.43
1:A:15:LEU:HD12	1:A:60:LYS:HG3	2.00	0.43
1:A:47:GLN:OE1	1:K:26:ARG:NH2	2.51	0.43
1:C:30:THR:HG21	1:D:34:HIS:CD2	2.54	0.43
1:H:10:VAL:HG22	1:H:46:ALA:O	2.19	0.42
1:F:27:GLY:HA2	1:G:51:HIS:CE1	2.54	0.42
1:H:18:GLY:O	1:H:20:ASN:ND2	2.53	0.42
1:K:30:THR:HG1	2:K:81:TRP:N	2.18	0.42
1:B:56:LYS:HE2	1:B:58:ARG:HH21	1.85	0.42
1:F:66:ARG:NH1	1:G:66:ARG:HD2	2.29	0.42
1:G:22:ILE:HG13	1:G:35:SER:HB2	2.02	0.42
1:J:26:ARG:HD3	1:K:50[A]:GLU:OE1	2.20	0.41
1:B:24:LEU:N	1:B:24:LEU:HD12	2.36	0.41
1:A:30:THR:CG2	2:A:81:TRP:HB2	2.51	0.41
1:E:48:PHE:HZ	1:F:45:ILE:HG22	1.86	0.41
1:C:22:ILE:HD13	1:C:22:ILE:HG21	1.86	0.41
1:K:60:LYS:HB2	1:K:74:GLY:H	1.86	0.41
1:K:16:GLU:N	1:K:40:LYS:HG3	2.35	0.41
1:H:31:ARG:NH2	1:H:33:HIS:HA	2.35	0.41
1:H:25:THR:HG23	1:H:31:ARG:O	2.21	0.40
1:H:16:GLU:HG3	1:H:17:ASP:O	2.21	0.40
1:J:63:ILE:HB	1:J:70:ILE:CG2	2.50	0.40
1:K:25:THR:OG1	1:K:30:THR:HA	2.21	0.40
1:F:56:LYS:NZ	1:G:36:GLU:OE2	2.52	0.40
1:J:10:VAL:HG12	1:J:65:THR:HG22	2.02	0.40

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:B:75:LYS:NZ	1:K:17:ASP:OD2[3_545]	1.53	0.67

## 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	66/74 (89%)	64 (97%)	2 (3%)	0	100	100
1	B	69/74 (93%)	67 (97%)	2 (3%)	0	100	100
1	C	67/74 (90%)	64 (96%)	3 (4%)	0	100	100
1	D	67/74 (90%)	67 (100%)	0	0	100	100
1	E	67/74 (90%)	65 (97%)	2 (3%)	0	100	100
1	F	66/74 (89%)	66 (100%)	0	0	100	100
1	G	66/74 (89%)	65 (98%)	1 (2%)	0	100	100
1	H	66/74 (89%)	65 (98%)	1 (2%)	0	100	100
1	I	65/74 (88%)	62 (95%)	2 (3%)	1 (2%)	13	22
1	J	65/74 (88%)	62 (95%)	3 (5%)	0	100	100
1	K	67/74 (90%)	66 (98%)	1 (2%)	0	100	100
All	All	731/814 (90%)	713 (98%)	17 (2%)	1 (0%)	56	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	8	ASP

### 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%)	52 (91%)	5 (9%)	12	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	59/62 (95%)	56 (95%)	3 (5%)	29	52
1	C	57/62 (92%)	53 (93%)	4 (7%)	19	34
1	D	57/62 (92%)	53 (93%)	4 (7%)	19	34
1	E	57/62 (92%)	53 (93%)	4 (7%)	19	34
1	F	56/62 (90%)	50 (89%)	6 (11%)	8	15
1	G	57/62 (92%)	50 (88%)	7 (12%)	6	11
1	H	56/62 (90%)	48 (86%)	8 (14%)	4	7
1	I	56/62 (90%)	48 (86%)	8 (14%)	4	7
1	J	56/62 (90%)	51 (91%)	5 (9%)	12	23
1	K	57/62 (92%)	46 (81%)	11 (19%)	2	3
All	All	625/682 (92%)	560 (90%)	65 (10%)	9	16

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	31	ARG
1	A	35	SER
1	A	53	SER
1	A	60	LYS
1	B	8	ASP
1	B	58	ARG
1	B	66	ARG
1	C	20	ASN
1	C	32	PHE
1	C	42	GLU
1	C	75	LYS
1	D	7	SER
1	D	10	VAL
1	D	15	LEU
1	D	70	ILE
1	E	7	SER
1	E	8	ASP
1	E	15	LEU
1	E	73	GLU
1	F	15	LEU
1	F	16	GLU
1	F	31	ARG

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Mol	Chain	Res	Type
1	F	37	LYS
1	F	66	ARG
1	F	69	VAL
1	G	8	ASP
1	G	31	ARG
1	G	32	PHE
1	G	35	SER
1	G	37	LYS
1	G	58[A]	ARG
1	G	58[B]	ARG
1	H	8	ASP
1	H	20	ASN
1	H	24	LEU
1	H	29	ASP
1	H	31	ARG
1	H	66	ARG
1	H	69	VAL
1	H	70	ILE
1	I	7	SER
1	I	8	ASP
1	I	24	LEU
1	I	29	ASP
1	I	31	ARG
1	I	35	SER
1	I	38	LEU
1	I	65	THR
1	J	8	ASP
1	J	16	GLU
1	J	63	ILE
1	J	64	GLN
1	J	69	VAL
1	K	8	ASP
1	K	15	LEU
1	K	19	VAL
1	K	30	THR
1	K	32	PHE
1	K	40	LYS
1	K	45	ILE
1	K	50[A]	GLU
1	K	50[B]	GLU
1	K	52	THR
1	K	70	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	H	20	ASN
1	I	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

11 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	A	81	-	12,16,16	0.84	0	7,22,22	1.58	1 (14%)
2	TRP	B	81	-	12,16,16	0.73	0	7,22,22	1.48	2 (28%)
2	TRP	C	81	-	12,16,16	0.95	1 (8%)	7,22,22	0.84	0
2	TRP	D	81	-	12,16,16	0.85	0	7,22,22	0.99	0
2	TRP	E	81	-	12,16,16	0.78	0	7,22,22	0.92	0
2	TRP	G	81	-	12,16,16	0.68	0	7,22,22	1.40	1 (14%)
2	TRP	G	82	-	12,16,16	0.73	0	7,22,22	1.27	1 (14%)
2	TRP	H	81	-	12,16,16	0.67	0	7,22,22	0.80	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	TRP	I	81	-	12,16,16	0.66	0	7,22,22	0.98	0
2	TRP	J	81	-	12,16,16	0.74	0	7,22,22	1.35	1 (14%)
2	TRP	K	81	-	12,16,16	0.65	0	7,22,22	1.11	1 (14%)

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	A	81	-	-	0/3/8/8	0/2/2/2
2	TRP	B	81	-	-	0/3/8/8	0/2/2/2
2	TRP	C	81	-	-	0/3/8/8	0/2/2/2
2	TRP	D	81	-	-	0/3/8/8	0/2/2/2
2	TRP	E	81	-	-	0/3/8/8	0/2/2/2
2	TRP	G	81	-	-	0/3/8/8	0/2/2/2
2	TRP	G	82	-	-	0/3/8/8	0/2/2/2
2	TRP	H	81	-	-	0/3/8/8	0/2/2/2
2	TRP	I	81	-	-	0/3/8/8	0/2/2/2
2	TRP	J	81	-	-	0/3/8/8	0/2/2/2
2	TRP	K	81	-	-	0/3/8/8	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	81	TRP	CZ3-CE3	2.02	1.41	1.36

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	81	TRP	CB-CG-CD1	-3.44	123.71	127.97
2	G	82	TRP	CZ3-CE3-CD2	-2.56	117.26	120.88
2	B	81	TRP	CZ3-CE3-CD2	-2.54	117.28	120.88
2	G	81	TRP	CH2-CZ2-CE2	-2.28	116.41	120.06
2	B	81	TRP	CH2-CZ2-CE2	-2.25	116.45	120.06
2	J	81	TRP	CZ3-CE3-CD2	-2.11	117.90	120.88
2	K	81	TRP	CB-CG-CD1	-2.04	125.45	127.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	81	TRP	3	0
2	B	81	TRP	1	0
2	C	81	TRP	1	0
2	D	81	TRP	1	0
2	G	82	TRP	1	0
2	H	81	TRP	1	0
2	I	81	TRP	1	0
2	K	81	TRP	3	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	67/74 (90%)	-0.27	0 100 100	42, 59, 74, 80	2 (2%)
1	B	70/74 (94%)	-0.39	1 (1%) 78 80	36, 51, 65, 85	3 (4%)
1	C	69/74 (93%)	-0.64	0 100 100	31, 43, 63, 75	2 (2%)
1	D	69/74 (93%)	-0.76	0 100 100	30, 37, 52, 65	3 (4%)
1	E	69/74 (93%)	-0.67	1 (1%) 78 80	29, 37, 52, 75	2 (2%)
1	F	68/74 (91%)	-0.60	0 100 100	33, 44, 58, 69	2 (2%)
1	G	67/74 (90%)	-0.43	0 100 100	41, 54, 67, 78	1 (1%)
1	H	68/74 (91%)	0.22	3 (4%) 38 43	54, 71, 88, 92	1 (1%)
1	I	67/74 (90%)	0.38	4 (5%) 25 28	65, 80, 90, 96	7 (10%)
1	J	67/74 (90%)	0.40	4 (5%) 25 28	63, 77, 90, 93	3 (4%)
1	K	68/74 (91%)	0.10	2 (2%) 55 60	52, 69, 82, 88	3 (4%)
All	All	749/814 (92%)	-0.24	15 (2%) 68 72	29, 57, 85, 96	29 (3%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	75	LYS	4.1
1	I	28	ALA	3.9
1	J	28	ALA	3.8
1	J	15	LEU	3.6
1	K	74	GLY	3.1
1	I	32	PHE	3.0
1	J	31	ARG	2.7
1	B	76	LYS	2.7
1	H	32	PHE	2.6
1	H	74	GLY	2.6
1	J	52	THR	2.4
1	I	52	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	28	ALA	2.1
1	K	19	VAL	2.1
1	I	73	GLU	2.0

## 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
2	TRP	E	81	15/15	0.97	0.17	2.08	28,39,43,44	0
2	TRP	H	81	15/15	0.90	0.23	1.09	74,79,88,90	0
2	TRP	J	81	15/15	0.90	0.21	0.56	67,69,74,75	0
2	TRP	I	81	15/15	0.91	0.22	0.42	70,74,82,83	0
2	TRP	K	81	15/15	0.93	0.16	0.40	41,52,61,62	0
2	TRP	B	81	15/15	0.98	0.14	0.26	24,37,46,47	0
2	TRP	G	81	15/15	0.96	0.13	0.06	29,44,51,53	0
2	TRP	C	81	15/15	0.99	0.10	0.01	20,32,39,40	0
2	TRP	G	82	15/15	0.94	0.16	-0.08	53,59,66,69	0
2	TRP	A	81	15/15	0.96	0.13	-0.21	38,45,50,51	0
2	TRP	D	81	15/15	0.99	0.10	-0.23	25,30,36,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.