



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:04 PM UTC

PDB ID : 1QAW / pdb_00001qaw
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

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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

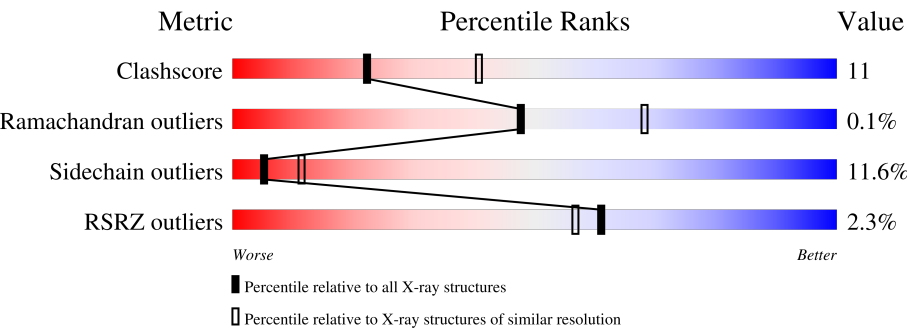
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$. 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	39% 34% 11% 7% 9%
1	B	74	46% 38% 8% 5%
1	C	74	% 51% 32% 9% 7%
1	D	74	49% 35% 9% 7%
1	E	74	3% 51% 31% 7% 7%
1	F	74	47% 35% 9% 8%
1	G	74	43% 31% 14% 9%

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Mol	Chain	Length	Quality of chain
1	H	74	7% 49% 35% 7% 8%
1	I	74	8% 42% 39% 9% 9%
1	J	74	3% 50% 31% 8% 9%
1	K	74	% 42% 28% 18% 8%

2 Entry composition

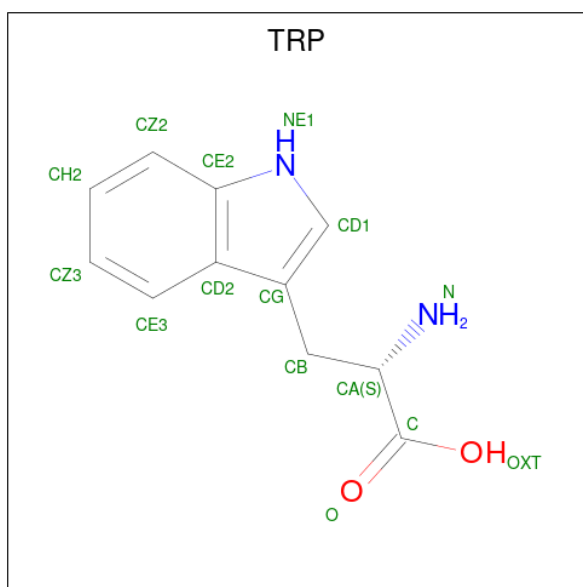
There are 3 unique types of molecules in this entry. The entry contains 6240 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 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		
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		
2	K	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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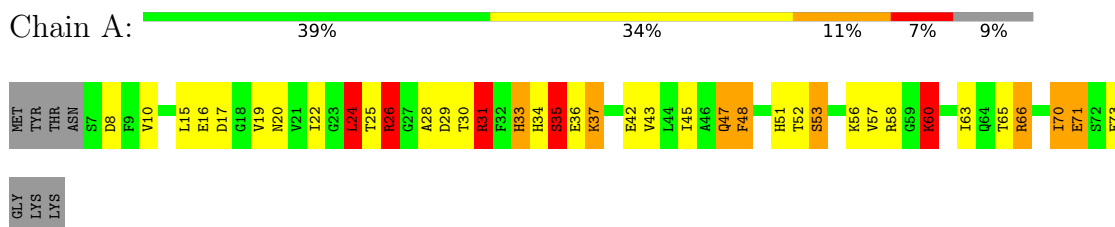
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	20	Total 20	O 20	0	0
3	C	28	Total 28	O 28	0	0
3	D	37	Total 37	O 37	0	0
3	E	49	Total 49	O 49	0	0
3	F	28	Total 28	O 28	0	0
3	G	19	Total 19	O 19	0	0
3	H	11	Total 11	O 11	0	0
3	I	6	Total 6	O 6	0	0
3	J	5	Total 5	O 5	0	0
3	K	5	Total 5	O 5	0	0

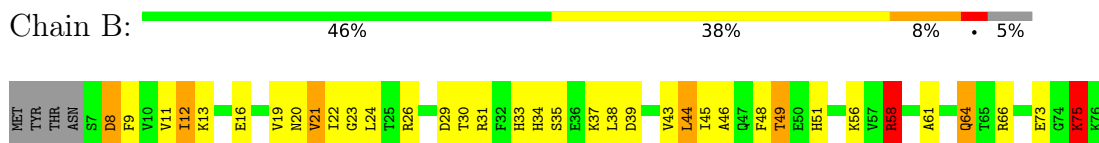
3 Residue-property plots

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 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.

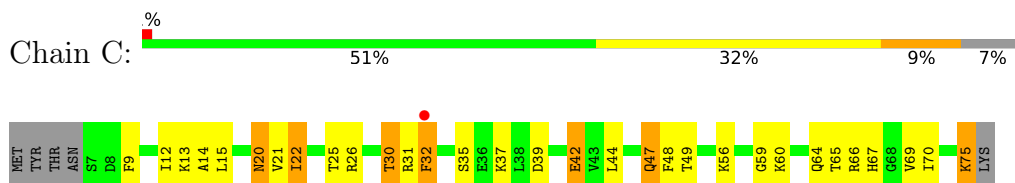
- Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN



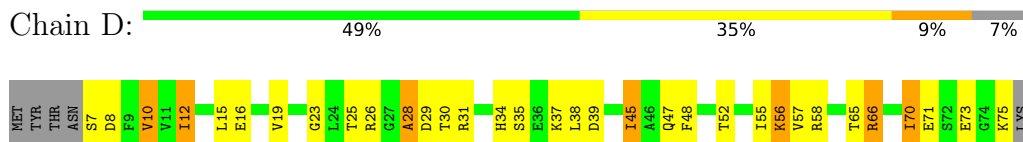
- Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN



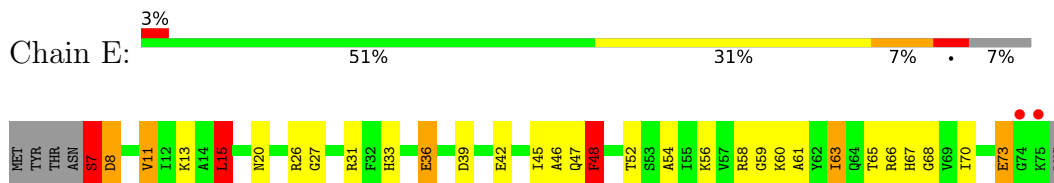
- Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN



- Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN

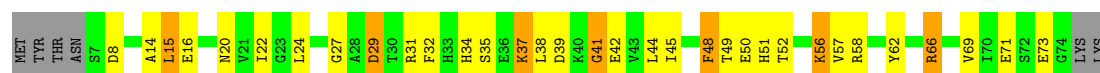


- Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN



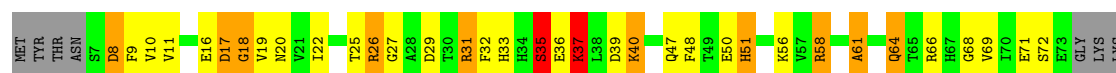
- Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN

Chain F: 



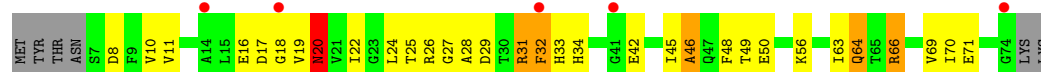
• Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN

Chain G: 



• Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN

Chain H: 

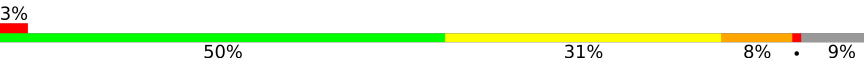


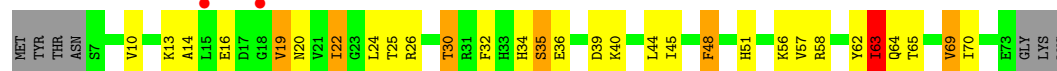
• Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN

Chain I: 



• Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN

Chain J: 



• Molecule 1: TRP RNA-BINDING ATTENUATION PROTEIN

Chain K: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.93Å 117.96Å 147.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.4 (15.00-2.50) 89.8 (15.00-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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.	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.538	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 71.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6240	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	A	0.96	2/539 (0.4%)	2.29	31/724 (4.3%)
1	B	1.13	3/562 (0.5%)	2.47	37/751 (4.9%)
1	C	1.72	2/543 (0.4%)	2.52	33/728 (4.5%)
1	D	1.17	2/543 (0.4%)	2.37	38/728 (5.2%)
1	E	1.16	0/543	2.40	34/728 (4.7%)
1	F	1.08	0/534	2.43	28/717 (3.9%)
1	G	0.96	0/541	2.24	24/726 (3.3%)
1	H	0.75	0/534	2.02	15/717 (2.1%)
1	I	1.09	3/530 (0.6%)	2.15	14/712 (2.0%)
1	J	0.95	2/530 (0.4%)	1.95	9/712 (1.3%)
1	K	0.85	1/543 (0.2%)	2.02	16/729 (2.2%)
All	All	1.10	15/5942 (0.3%)	2.27	279/7972 (3.5%)

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 (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	75	LYS	CE-NZ	31.62	2.44	1.49
1	I	38	LEU	CA-CB	13.06	1.77	1.53
1	J	40	LYS	CA-CB	-13.01	1.32	1.53
1	I	37	LYS	CD-CE	-12.06	1.16	1.52
1	B	37	LYS	CG-CD	-9.28	1.24	1.52
1	B	75	LYS	CG-CD	-8.16	1.27	1.52
1	I	31	ARG	CA-CB	-8.13	1.40	1.53
1	J	32	PHE	CB-CG	-7.85	1.32	1.50
1	A	60	LYS	CE-NZ	7.76	1.72	1.49
1	K	66	ARG	NE-CZ	7.63	1.41	1.33
1	A	37	LYS	CB-CG	7.61	1.75	1.52
1	D	37	LYS	CB-CG	-7.28	1.30	1.52
1	D	75	LYS	CG-CD	7.13	1.73	1.52
1	C	37	LYS	CB-CG	-6.45	1.33	1.52
1	B	49	THR	CA-CB	5.80	1.61	1.53

All (279) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	75	LYS	CB-CG-CD	18.42	153.66	111.30
1	I	58	ARG	CD-NE-CZ	16.79	147.90	124.40
1	I	37	LYS	CG-CD-CE	15.24	146.36	111.30
1	C	20	ASN	OD1-CG-ND2	13.63	136.23	122.60
1	J	51	HIS	CA-CB-CG	-13.34	100.46	113.80
1	C	20	ASN	CA-CB-CG	-11.54	101.06	112.60
1	C	75	LYS	CD-CE-NZ	-11.13	76.27	111.90
1	F	73	GLU	CB-CG-CD	10.76	130.88	112.60
1	F	51	HIS	CA-CB-CG	-10.55	103.25	113.80
1	C	32	PHE	CA-CB-CG	10.40	124.20	113.80
1	B	37	LYS	CB-CG-CD	10.31	135.01	111.30
1	G	31	ARG	CD-NE-CZ	10.29	138.81	124.40
1	A	66	ARG	NE-CZ-NH2	10.26	128.43	119.20
1	B	8	ASP	CA-CB-CG	-9.89	102.71	112.60
1	B	29	ASP	CA-CB-CG	-9.41	103.19	112.60
1	F	73	GLU	O-C-N	-9.38	112.29	123.27
1	D	70	ILE	CA-CB-CG2	9.37	126.42	110.50
1	A	73	GLU	CA-C-O	9.34	136.67	120.80
1	H	20	ASN	CA-CB-CG	9.28	121.88	112.60
1	D	75	LYS	CB-CG-CD	-9.27	89.99	111.30
1	K	31	ARG	CD-NE-CZ	9.22	137.31	124.40
1	D	26	ARG	NE-CZ-NH2	9.12	127.41	119.20
1	F	48	PHE	O-C-N	-9.05	112.45	123.04
1	D	70	ILE	CB-CG1-CD1	-8.86	95.19	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	32	PHE	CA-CB-CG	8.72	122.53	113.80
1	F	56	LYS	CA-C-O	-8.59	111.08	120.36
1	B	75	LYS	CB-CA-C	-8.58	95.85	109.84
1	H	26	ARG	CD-NE-CZ	8.39	136.14	124.40
1	C	22	ILE	CA-C-N	8.06	129.36	121.62
1	C	22	ILE	C-N-CA	8.06	129.36	121.62
1	J	40	LYS	N-CA-CB	7.96	122.33	109.28
1	E	20	ASN	CA-CB-CG	-7.93	104.67	112.60
1	C	26	ARG	NH1-CZ-NH2	-7.91	109.02	119.30
1	I	60	LYS	CB-CA-C	7.81	124.57	111.30
1	F	8	ASP	N-CA-C	7.77	120.34	110.24
1	B	26	ARG	CA-C-O	-7.74	111.86	120.69
1	E	39	ASP	CA-CB-CG	-7.72	104.88	112.60
1	E	63	ILE	O-C-N	-7.62	114.95	123.18
1	F	34	HIS	CA-CB-CG	-7.55	106.25	113.80
1	F	32	PHE	CA-CB-CG	7.51	121.31	113.80
1	A	31	ARG	CA-CB-CG	7.51	129.12	114.10
1	D	26	ARG	CA-C-O	-7.40	112.96	121.47
1	D	52	THR	CA-C-O	-7.37	112.37	120.33
1	I	66	ARG	NE-CZ-NH1	-7.35	114.15	121.50
1	J	39	ASP	CA-CB-CG	-7.28	105.32	112.60
1	C	31	ARG	CA-CB-CG	7.27	128.63	114.10
1	D	28	ALA	CA-C-O	-7.24	113.22	120.82
1	E	31	ARG	CD-NE-CZ	-7.23	114.27	124.40
1	C	22	ILE	CA-CB-CG2	7.18	122.72	110.50
1	E	58	ARG	NE-CZ-NH2	7.16	125.64	119.20
1	I	37	LYS	CD-CE-NZ	7.14	134.75	111.90
1	G	33	HIS	N-CA-CB	7.12	121.11	110.65
1	H	49	THR	CA-C-O	-7.08	112.97	121.32
1	D	56	LYS	CA-CB-CG	7.07	128.25	114.10
1	A	37	LYS	CA-CB-CG	-7.06	99.97	114.10
1	D	38	LEU	CA-C-O	-6.96	113.33	120.71
1	I	51	HIS	CA-CB-CG	-6.96	106.84	113.80
1	B	29	ASP	O-C-N	6.93	131.89	123.16
1	I	38	LEU	CB-CA-C	-6.90	97.08	109.71
1	B	39	ASP	N-CA-CB	6.90	120.98	110.70
1	A	31	ARG	NE-CZ-NH2	6.89	125.40	119.20
1	B	75	LYS	CG-CD-CE	6.89	127.14	111.30
1	E	8	ASP	OD1-CG-OD2	6.88	139.42	122.90
1	D	66	ARG	CA-C-O	-6.88	113.26	120.55
1	H	48	PHE	CA-CB-CG	-6.87	106.93	113.80
1	B	22	ILE	N-CA-C	6.80	118.09	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	37	LYS	CA-CB-CG	6.80	127.70	114.10
1	A	66	ARG	NE-CZ-NH1	-6.79	114.70	121.50
1	A	29	ASP	O-C-N	6.78	131.70	123.16
1	C	30	THR	CA-CB-OG1	-6.77	99.45	109.60
1	E	8	ASP	N-CA-CB	-6.75	100.61	110.26
1	C	59	GLY	CA-C-O	-6.73	116.14	122.13
1	H	56	LYS	CA-C-O	-6.72	113.44	120.70
1	B	48	PHE	CA-CB-CG	-6.70	107.10	113.80
1	D	47	GLN	O-C-N	6.69	130.59	123.03
1	A	8	ASP	N-CA-C	6.67	119.90	110.50
1	H	66	ARG	NE-CZ-NH2	6.66	125.19	119.20
1	F	22	ILE	CA-C-N	-6.66	116.34	122.80
1	F	22	ILE	C-N-CA	-6.66	116.34	122.80
1	D	47	GLN	CA-C-O	-6.61	113.60	121.66
1	E	8	ASP	N-CA-C	6.61	119.08	110.43
1	D	75	LYS	N-CA-CB	-6.60	99.28	110.50
1	G	29	ASP	CA-CB-CG	-6.60	106.00	112.60
1	B	58	ARG	NE-CZ-NH1	-6.58	114.92	121.50
1	K	37	LYS	CA-CB-CG	6.58	127.26	114.10
1	B	33	HIS	CA-CB-CG	6.58	120.38	113.80
1	A	17	ASP	CA-C-O	-6.56	114.66	121.87
1	E	54	ALA	CA-C-O	-6.56	112.69	120.43
1	B	33	HIS	N-CA-C	-6.54	105.02	114.12
1	C	22	ILE	O-C-N	-6.53	114.97	122.94
1	E	48	PHE	CA-C-O	-6.51	113.14	120.43
1	I	66	ARG	NE-CZ-NH2	6.50	125.05	119.20
1	A	26	ARG	CA-C-O	-6.49	113.30	120.69
1	A	22	ILE	N-CA-C	6.46	117.42	107.99
1	K	16	GLU	CA-C-O	-6.42	114.41	121.28
1	A	52	THR	CA-C-N	6.38	132.40	122.26
1	A	52	THR	C-N-CA	6.38	132.40	122.26
1	G	18	GLY	CA-C-N	-6.37	111.84	120.95
1	G	18	GLY	C-N-CA	-6.37	111.84	120.95
1	C	37	LYS	CA-CB-CG	6.37	126.83	114.10
1	B	19	VAL	CA-C-O	-6.35	113.55	121.11
1	B	20	ASN	CA-C-O	6.34	127.29	120.38
1	A	33	HIS	N-CA-C	-6.32	106.16	114.31
1	D	48	PHE	CA-CB-CG	-6.31	107.49	113.80
1	C	44	LEU	O-C-N	-6.31	115.80	123.30
1	F	56	LYS	O-C-N	6.31	130.81	123.30
1	F	35	SER	CA-C-O	6.30	127.13	120.33
1	F	52	THR	CA-C-O	-6.29	113.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	20	ASN	CA-CB-CG	6.28	118.88	112.60
1	E	46	ALA	N-CA-C	6.28	119.72	109.24
1	J	63	ILE	N-CA-C	6.28	116.90	108.11
1	J	32	PHE	CA-CB-CG	6.26	120.06	113.80
1	D	19	VAL	CA-C-O	-6.25	115.15	121.59
1	G	26	ARG	NE-CZ-NH2	6.25	124.82	119.20
1	C	14	ALA	O-C-N	-6.21	115.28	122.93
1	E	63	ILE	N-CA-C	6.20	117.40	108.48
1	F	50	GLU	CB-CG-CD	6.19	123.13	112.60
1	A	35	SER	CA-C-O	-6.19	113.90	120.40
1	F	71	GLU	CA-CB-CG	6.16	126.43	114.10
1	G	47	GLN	CB-CA-C	-6.16	99.64	109.80
1	A	47	GLN	CB-CA-C	-6.12	99.70	109.80
1	D	35	SER	N-CA-CB	-6.11	101.56	110.84
1	J	14	ALA	CA-C-O	6.10	127.83	120.81
1	C	21	VAL	CA-C-N	6.09	129.98	122.37
1	C	21	VAL	C-N-CA	6.09	129.98	122.37
1	J	25	THR	N-CA-CB	6.09	119.03	109.83
1	E	7	SER	CA-C-N	6.08	131.15	120.87
1	E	7	SER	C-N-CA	6.08	131.15	120.87
1	G	18	GLY	CA-C-O	-6.07	112.75	120.03
1	B	35	SER	N-CA-CB	6.06	120.11	110.65
1	H	66	ARG	NH1-CZ-NH2	-6.06	111.42	119.30
1	K	13	LYS	CA-C-O	6.05	126.98	120.32
1	F	57	VAL	O-C-N	-6.04	116.73	123.26
1	D	71	GLU	CG-CD-OE1	6.01	132.23	118.40
1	E	33	HIS	ND1-CE1-NE2	6.00	114.40	108.40
1	C	31	ARG	CB-CA-C	-6.00	99.41	111.17
1	E	54	ALA	CA-C-N	-5.98	114.63	122.94
1	E	54	ALA	C-N-CA	-5.98	114.63	122.94
1	H	28	ALA	CA-C-O	-5.95	113.54	120.20
1	D	52	THR	O-C-N	5.93	130.95	123.12
1	E	59	GLY	CA-C-O	5.93	126.72	122.45
1	A	24	LEU	CA-C-N	5.93	129.18	120.82
1	A	24	LEU	C-N-CA	5.93	129.18	120.82
1	E	15	LEU	N-CA-C	-5.90	104.74	112.41
1	B	31	ARG	CG-CD-NE	-5.89	99.04	112.00
1	B	20	ASN	O-C-N	-5.88	116.35	123.29
1	D	58	ARG	CD-NE-CZ	5.88	132.64	124.40
1	B	16	GLU	CA-C-O	-5.88	114.99	121.28
1	C	32	PHE	CA-C-O	-5.87	113.68	120.49
1	D	35	SER	O-C-N	-5.86	115.39	123.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	63	ILE	N-CA-C	5.85	116.36	108.17
1	G	39	ASP	CB-CA-C	5.84	120.05	109.83
1	B	35	SER	CA-C-O	-5.84	114.05	120.30
1	C	56	LYS	CA-CB-CG	5.83	125.75	114.10
1	E	26	ARG	NE-CZ-NH2	5.83	124.44	119.20
1	E	67	HIS	CA-C-O	-5.83	112.23	119.28
1	K	53	SER	CA-CB-OG	5.81	122.72	111.10
1	B	64	GLN	O-C-N	-5.79	116.41	123.30
1	A	60	LYS	CD-CE-NZ	-5.77	93.43	111.90
1	G	17	ASP	CA-CB-CG	5.77	118.37	112.60
1	E	8	ASP	CB-CG-OD2	-5.75	105.17	118.40
1	K	26	ARG	CA-C-O	-5.75	114.13	120.69
1	C	26	ARG	NE-CZ-NH2	5.75	124.37	119.20
1	D	73	GLU	CA-CB-CG	5.75	125.60	114.10
1	J	19	VAL	CA-C-O	-5.75	115.67	121.59
1	H	64	GLN	OE1-CD-NE2	5.73	128.33	122.60
1	A	71	GLU	CA-C-O	-5.73	114.23	120.36
1	A	63	ILE	N-CA-C	5.73	116.13	108.11
1	B	13	LYS	CA-C-O	-5.72	114.18	120.30
1	C	67	HIS	CA-C-O	-5.70	111.65	119.12
1	G	61	ALA	N-CA-C	5.69	118.73	109.06
1	K	52	THR	N-CA-C	5.67	117.65	108.41
1	I	31	ARG	CB-CA-C	5.67	119.11	109.99
1	A	31	ARG	CD-NE-CZ	-5.61	116.55	124.40
1	C	12	ILE	O-C-N	-5.61	117.25	123.20
1	B	22	ILE	N-CA-CB	-5.60	104.27	110.99
1	B	11	VAL	N-CA-C	5.60	116.16	107.99
1	D	57	VAL	O-C-N	-5.59	117.31	123.18
1	C	31	ARG	NE-CZ-NH2	-5.59	114.17	119.20
1	F	49	THR	N-CA-C	5.59	117.12	109.18
1	C	30	THR	CA-C-O	-5.57	114.34	120.30
1	A	43	VAL	N-CA-C	5.57	115.87	107.80
1	K	8	ASP	CA-C-O	5.56	128.32	121.87
1	K	11	VAL	N-CA-CB	-5.54	104.48	111.46
1	A	37	LYS	CB-CG-CD	5.54	124.04	111.30
1	F	29	ASP	CB-CA-C	-5.53	100.05	109.51
1	E	36	GLU	O-C-N	-5.53	117.02	123.27
1	B	22	ILE	O-C-N	-5.53	116.89	123.03
1	E	26	ARG	CD-NE-CZ	-5.52	116.67	124.40
1	C	64	GLN	OE1-CD-NE2	-5.51	117.09	122.60
1	I	33	HIS	N-CA-CB	5.51	119.01	110.80
1	K	25	THR	N-CA-C	5.51	118.01	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	42	GLU	CA-C-O	-5.47	115.60	121.56
1	I	60	LYS	CA-CB-CG	5.46	125.02	114.10
1	K	58	ARG	CA-C-O	5.46	126.32	120.32
1	C	20	ASN	N-CA-CB	-5.46	102.14	110.65
1	F	58	ARG	CD-NE-CZ	5.45	132.03	124.40
1	C	47	GLN	CB-CG-CD	-5.45	103.34	112.60
1	B	9	PHE	CA-CB-CG	-5.44	108.36	113.80
1	F	44	LEU	N-CA-CB	5.44	119.09	110.55
1	B	34	HIS	CA-C-N	-5.44	115.33	123.00
1	B	34	HIS	C-N-CA	-5.44	115.33	123.00
1	H	42	GLU	CB-CG-CD	5.44	121.85	112.60
1	K	17	ASP	CA-CB-CG	-5.44	107.16	112.60
1	I	8	ASP	N-CA-C	5.43	122.36	110.80
1	D	25	THR	CA-C-O	-5.41	115.25	121.19
1	H	26	ARG	NE-CZ-NH2	5.40	124.06	119.20
1	G	71	GLU	N-CA-CB	5.40	119.05	110.57
1	I	38	LEU	N-CA-CB	-5.40	101.61	110.68
1	B	37	LYS	CG-CD-CE	5.38	123.69	111.30
1	D	65	THR	N-CA-CB	5.37	120.27	111.31
1	E	61	ALA	N-CA-C	5.37	117.55	109.23
1	H	56	LYS	CA-CB-CG	5.36	124.83	114.10
1	D	65	THR	CA-C-O	-5.36	115.45	121.40
1	G	35	SER	CA-C-N	-5.36	115.55	123.05
1	G	35	SER	C-N-CA	-5.36	115.55	123.05
1	G	19	VAL	CB-CA-C	5.35	117.48	111.59
1	K	33	HIS	N-CA-C	-5.35	107.41	114.31
1	C	13	LYS	CA-C-O	-5.34	114.44	120.32
1	B	8	ASP	N-CA-C	5.33	122.14	110.80
1	K	12	ILE	N-CA-C	5.32	115.52	107.75
1	C	75	LYS	N-CA-CB	5.32	119.54	110.50
1	H	32	PHE	CA-C-O	-5.32	115.76	121.56
1	A	52	THR	N-CA-CB	-5.32	102.35	110.65
1	D	39	ASP	N-CA-CB	5.32	118.70	110.46
1	G	64	GLN	N-CA-C	5.30	117.16	108.52
1	E	68	GLY	CA-C-O	-5.30	117.15	121.76
1	D	8	ASP	N-CA-C	5.30	117.17	110.33
1	C	25	THR	CA-C-N	5.28	128.37	120.87
1	C	25	THR	C-N-CA	5.28	128.37	120.87
1	A	70	ILE	N-CA-CB	-5.28	104.07	111.19
1	F	49	THR	CA-CB-OG1	5.26	117.49	109.60
1	G	8	ASP	N-CA-C	5.25	117.50	110.35
1	D	26	ARG	NH1-CZ-NH2	-5.24	112.48	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	12	ILE	N-CA-CB	5.24	118.94	111.82
1	B	49	THR	CB-CA-C	-5.24	100.78	113.19
1	E	13	LYS	O-C-N	-5.24	117.11	123.29
1	A	29	ASP	CA-C-N	-5.23	115.39	122.77
1	A	29	ASP	C-N-CA	-5.23	115.39	122.77
1	G	9	PHE	CA-CB-CG	-5.23	108.57	113.80
1	H	34	HIS	CA-CB-CG	-5.21	108.58	113.80
1	J	30	THR	CB-CA-C	-5.21	101.80	110.14
1	E	36	GLU	CA-C-O	5.21	126.11	120.43
1	F	37	LYS	CA-C-N	-5.21	115.38	122.93
1	F	37	LYS	C-N-CA	-5.21	115.38	122.93
1	E	70	ILE	CA-C-O	-5.20	116.08	120.96
1	B	21	VAL	CB-CA-C	-5.20	104.69	111.81
1	C	22	ILE	CB-CA-C	-5.20	104.67	110.96
1	E	52	THR	N-CA-C	5.18	117.25	108.02
1	D	16	GLU	O-C-N	-5.18	118.33	123.46
1	F	42	GLU	O-C-N	5.18	129.17	123.16
1	D	29	ASP	CA-C-O	-5.17	115.37	121.16
1	B	61	ALA	O-C-N	-5.17	117.36	123.25
1	B	75	LYS	N-CA-CB	5.17	117.96	109.95
1	F	24	LEU	CA-C-N	5.17	128.18	120.95
1	F	24	LEU	C-N-CA	5.17	128.18	120.95
1	D	56	LYS	CG-CD-CE	5.16	123.17	111.30
1	A	25	THR	N-CA-C	5.15	117.77	110.10
1	D	25	THR	N-CA-C	5.15	117.69	110.23
1	D	31	ARG	NE-CZ-NH1	5.14	126.64	121.50
1	A	51	HIS	CA-CB-CG	-5.13	108.67	113.80
1	D	45	ILE	CA-C-O	-5.13	114.83	120.48
1	K	25	THR	CB-CA-C	-5.12	101.45	109.70
1	E	70	ILE	CA-CB-CG2	5.12	119.20	110.50
1	I	28	ALA	CA-C-O	-5.12	114.32	120.10
1	D	23	GLY	CA-C-O	-5.11	116.69	121.18
1	G	51	HIS	CA-CB-CG	-5.10	108.70	113.80
1	F	20	ASN	N-CA-CB	5.09	119.24	110.68
1	F	39	ASP	CA-CB-CG	-5.09	107.51	112.60
1	G	68	GLY	O-C-N	-5.09	117.97	123.00
1	G	40	LYS	CA-C-O	-5.08	116.11	120.88
1	E	47	GLN	CA-CB-CG	5.07	124.23	114.10
1	D	30	THR	CA-C-O	-5.06	115.08	120.40
1	E	11	VAL	CA-C-O	5.05	125.83	120.48
1	A	48	PHE	N-CA-C	-5.03	102.33	110.32
1	B	12	ILE	N-CA-C	5.03	115.09	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	55	ILE	CA-C-O	-5.03	114.79	120.67
1	E	27	GLY	N-CA-C	5.02	118.09	111.52
1	B	75	LYS	CA-CB-CG	5.01	124.13	114.10

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
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

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Mol	Chain	Res	Type	Group
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	7	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	22	1
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	0	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	2	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	124	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 (124) 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	1.32	0.77
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:51:HIS:ND1	3:B:85:HOH:O	2.20	0.74
1:B:66:ARG:HH22	1:C:66:ARG:NE	1.85	0.74
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: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:I:34:HIS:NE2	1:I:36:GLU:HB2	2.18	0.59
1:K:60:LYS:HA	1:K:72:SER:O	2.03	0.59
1:A:15:LEU:HB2	1:A:60:LYS:HG3	1.85	0.59
1:B:30:THR:HG1	2:B:81:TRP:N	2.01	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:30:THR:HG1	2:A:81:TRP:N	2.06	0.53
1:A:31:ARG:HH21	1:A:33:HIS:CA	2.20	0.53
1:E:60:LYS:HG2	3:E:107:HOH:O	2.09	0.53
1:F:66:ARG:HG2	1:F:66:ARG:HH21	1.74	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:G:11:VAL:HB	1:G:64:GLN:HB2	1.93	0.50
1:J:20:ASN:ND2	1:J:35:SER:OG	2.44	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:A:26:ARG:HB2	1:A:53:SER:HB3	1.93	0.50
1:I:22:ILE:HG23	1:I:34:HIS:O	2.11	0.50
1:A:34:HIS:HE2	1:A:36:GLU:HB2	1.77	0.49
1:C:30:THR:HG1	2:C:81:TRP:N	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:H:10:VAL:HG23	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:A:30:THR:HG23	2:A:81:TRP:HB2	1.96	0.47
1:K:30:THR:CG2	2:K:81:TRP:HB2	2.45	0.47
1:D:56:LYS:NZ	1:E:36:GLU:OE2	2.47	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:I:48:PHE:HZ	1:J:45:ILE:HG22	1.80	0.46
1:K:16:GLU:HA	1:K:40:LYS:HG3	1.97	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: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
1:I:22:ILE:HG22	1:I:23:GLY:N	2.32	0.44
1:D:10:VAL:HG23	1:D:12:ILE:CD1	2.48	0.44
1:E:11:VAL:O	1:E:63:ILE:HA	2.18	0.43
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:A:47:GLN:HB3	1:A:48:PHE:O	2.18	0.43
1:I:34:HIS:CG	1:I:35:SER:N	2.86	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:B:56:LYS:HE2	1:B:58:ARG:HH21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:22:ILE:HD13	1:C:22:ILE:HG21	1.86	0.41
1:E:48:PHE:HZ	1:F:45:ILE:HG22	1.86	0.41
1:H:31:ARG:NH2	1:H:33:HIS:HA	2.35	0.41
1:K:16:GLU:N	1:K:40:LYS:HG3	2.35	0.41
1:K:60:LYS:HB2	1:K:74:GLY:H	1.86	0.41
1:H:16:GLU:HG3	1:H:17:ASP:O	2.21	0.40
1:H:25:THR:HG23	1:H:31:ARG:O	2.21	0.40
1:J:63:ILE:HB	1:J:70:ILE:CG2	2.50	0.40
1:F:56:LYS:NZ	1:G:36:GLU:OE2	2.52	0.40
1:K:25:THR:OG1	1:K:30:THR:HA	2.21	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 [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	66/74 (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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	8	16
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%)	48	68

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%)	50 (88%)	7 (12%)	4	10
1	B	59/62 (95%)	57 (97%)	2 (3%)	32	60
1	C	57/62 (92%)	51 (90%)	6 (10%)	6	14
1	D	57/62 (92%)	53 (93%)	4 (7%)	14	29
1	E	57/62 (92%)	51 (90%)	6 (10%)	6	14
1	F	56/62 (90%)	50 (89%)	6 (11%)	6	13
1	G	57/62 (92%)	49 (86%)	8 (14%)	3	7
1	H	56/62 (90%)	45 (80%)	11 (20%)	1	2
1	I	56/62 (90%)	47 (84%)	9 (16%)	2	4
1	J	56/62 (90%)	51 (91%)	5 (9%)	9	20
1	K	57/62 (92%)	46 (81%)	11 (19%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	625/682 (92%)	550 (88%)	75 (12%)	5 10

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	31	ARG
1	A	35	SER
1	A	53	SER
1	A	60	LYS
1	A	70	ILE
1	A	71	GLU
1	B	8	ASP
1	B	58	ARG
1	C	20	ASN
1	C	32	PHE
1	C	42	GLU
1	C	69	VAL
1	C	70	ILE
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	45	ILE
1	E	56	LYS
1	E	73	GLU
1	F	15	LEU
1	F	16	GLU
1	F	31	ARG
1	F	37	LYS
1	F	66	ARG
1	F	69	VAL
1	G	8	ASP
1	G	10	VAL
1	G	31	ARG
1	G	35	SER
1	G	37	LYS
1	G	58[A]	ARG

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Mol	Chain	Res	Type
1	G	58[B]	ARG
1	G	69	VAL
1	H	8	ASP
1	H	19	VAL
1	H	20	ASN
1	H	24	LEU
1	H	29	ASP
1	H	31	ARG
1	H	50	GLU
1	H	63	ILE
1	H	66	ARG
1	H	69	VAL
1	H	70	ILE
1	I	7	SER
1	I	19	VAL
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	I	69	VAL
1	J	16	GLU
1	J	19	VAL
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	45	ILE
1	K	50[A]	GLU
1	K	50[B]	GLU
1	K	52	THR
1	K	69	VAL
1	K	70	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	B	20	ASN
1	B	33	HIS
1	B	64	GLN
1	C	64	GLN
1	D	64	GLN
1	F	20	ASN
1	H	20	ASN
1	I	20	ASN
1	J	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 oligosaccharides 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	B	81	-	15,16,16	0.82	0	18,22,22	0.95	1 (5%)
2	TRP	D	81	-	15,16,16	0.67	0	18,22,22	1.00	1 (5%)
2	TRP	J	81	-	15,16,16	0.57	0	18,22,22	0.91	2 (11%)
2	TRP	C	81	-	15,16,16	0.73	0	18,22,22	0.74	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TRP	I	81	-	15,16,16	0.55	0	18,22,22	0.56	0
2	TRP	K	81	-	15,16,16	0.94	1 (6%)	18,22,22	1.03	1 (5%)
2	TRP	G	82	-	15,16,16	0.79	0	18,22,22	0.95	2 (11%)
2	TRP	G	81	-	15,16,16	0.99	1 (6%)	18,22,22	0.86	0
2	TRP	A	81	-	15,16,16	0.87	0	18,22,22	1.35	3 (16%)
2	TRP	E	81	-	15,16,16	0.82	0	18,22,22	0.70	0
2	TRP	H	81	-	15,16,16	0.70	0	18,22,22	0.61	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
2	TRP	B	81	-	-	1/8/8/8	0/2/2/2
2	TRP	D	81	-	-	0/8/8/8	0/2/2/2
2	TRP	J	81	-	-	2/8/8/8	0/2/2/2
2	TRP	C	81	-	-	1/8/8/8	0/2/2/2
2	TRP	I	81	-	-	1/8/8/8	0/2/2/2
2	TRP	K	81	-	-	3/8/8/8	0/2/2/2
2	TRP	G	82	-	-	1/8/8/8	0/2/2/2
2	TRP	G	81	-	-	1/8/8/8	0/2/2/2
2	TRP	A	81	-	-	2/8/8/8	0/2/2/2
2	TRP	E	81	-	-	1/8/8/8	0/2/2/2
2	TRP	H	81	-	-	1/8/8/8	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	81	TRP	O-C	2.23	1.28	1.22
2	G	81	TRP	O-C	2.02	1.28	1.22

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	81	TRP	CA-CB-CG	-2.97	107.85	113.49
2	D	81	TRP	CA-CB-CG	2.97	119.12	113.49
2	A	81	TRP	CA-CB-CG	-2.90	107.99	113.49
2	A	81	TRP	CG-CD1-NE1	-2.79	107.25	110.31
2	A	81	TRP	CE2-NE1-CD1	2.57	111.36	109.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	81	TRP	CA-CB-CG	-2.48	108.79	113.49
2	J	81	TRP	CH2-CZ3-CE3	2.21	122.96	120.24
2	G	82	TRP	CA-CB-CG	-2.15	109.41	113.49
2	B	81	TRP	CA-CB-CG	2.09	117.45	113.49
2	G	82	TRP	CH2-CZ3-CE3	2.01	122.72	120.24
2	C	81	TRP	CA-CB-CG	-2.01	109.68	113.49

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	81	TRP	OXT-C-CA-N
2	A	81	TRP	OXT-C-CA-N
2	G	81	TRP	OXT-C-CA-N
2	G	82	TRP	OXT-C-CA-N
2	H	81	TRP	OXT-C-CA-N
2	C	81	TRP	OXT-C-CA-N
2	A	81	TRP	O-C-CA-N
2	J	81	TRP	OXT-C-CA-N
2	B	81	TRP	OXT-C-CA-N
2	K	81	TRP	O-C-CA-N
2	E	81	TRP	OXT-C-CA-N
2	I	81	TRP	OXT-C-CA-N
2	K	81	TRP	OXT-C-CA-CB
2	J	81	TRP	O-C-CA-N

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	81	TRP	1	0
2	C	81	TRP	1	0
2	I	81	TRP	1	0
2	K	81	TRP	2	0
2	G	82	TRP	1	0
2	A	81	TRP	3	0
2	H	81	TRP	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95th 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 ²)	Q<0.9
1	A	67/74 (90%)	0.10	0 100 100	34, 59, 74, 80	3 (4%)
1	B	70/74 (94%)	-0.19	0 100 100	30, 51, 63, 85	4 (5%)
1	C	69/74 (93%)	-0.45	1 (1%) 73 70	30, 43, 63, 66	2 (2%)
1	D	69/74 (93%)	-0.71	0 100 100	23, 36, 51, 65	3 (4%)
1	E	69/74 (93%)	-0.48	2 (2%) 53 49	29, 37, 52, 70	2 (2%)
1	F	68/74 (91%)	-0.46	0 100 100	20, 42, 58, 69	2 (2%)
1	G	67/74 (90%)	-0.08	0 100 100	27, 53, 67, 78	2 (2%)
1	H	68/74 (91%)	0.55	5 (7%) 20 18	39, 71, 88, 92	1 (1%)
1	I	67/74 (90%)	0.96	6 (8%) 15 13	31, 77, 90, 96	7 (10%)
1	J	67/74 (90%)	0.80	2 (2%) 52 48	38, 77, 90, 93	3 (4%)
1	K	68/74 (91%)	0.56	1 (1%) 72 68	34, 68, 82, 88	4 (5%)
All	All	749/814 (92%)	0.05	17 (2%) 61 57	20, 56, 85, 96	33 (4%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	74	GLY	4.3
1	I	60	LYS	3.9
1	I	41	GLY	3.3
1	H	41	GLY	3.2
1	I	61	ALA	2.9
1	H	74	GLY	2.7
1	H	18	GLY	2.6
1	J	18	GLY	2.6
1	H	32	PHE	2.5
1	I	28	ALA	2.4
1	E	75	LYS	2.4
1	H	14	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	74	GLY	2.3
1	J	15	LEU	2.3
1	C	32	PHE	2.3
1	I	18	GLY	2.2
1	I	32	PHE	2.2

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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
2	TRP	H	81	15/15	0.91	0.13	74,79,88,90	0
2	TRP	I	81	15/15	0.91	0.12	70,74,82,83	0
2	TRP	J	81	15/15	0.91	0.12	67,69,74,75	0
2	TRP	K	81	15/15	0.92	0.12	41,52,61,62	0
2	TRP	G	82	15/15	0.93	0.10	53,59,66,69	0
2	TRP	G	81	15/15	0.95	0.07	29,44,51,53	0
2	TRP	A	81	15/15	0.95	0.08	38,45,50,51	0
2	TRP	E	81	15/15	0.97	0.06	28,39,43,44	0
2	TRP	C	81	15/15	0.98	0.06	20,32,39,40	0
2	TRP	D	81	15/15	0.98	0.04	25,30,36,36	0
2	TRP	B	81	15/15	0.98	0.05	24,37,46,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.