



wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2020 – 03:10 am BST

PDB ID : 1C9B
Title : CRYSTAL STRUCTURE OF A HUMAN TBP CORE DOMAIN-HUMAN
TFIIB CORE DOMAIN COMPLEX BOUND TO AN EXTENDED, MODI-
FIED ADENOVIRAL MAJOR LATE PROMOTER (ADMLP)
Authors : Tsai, F.T.F.; Sigler, P.B.
Deposited on : 1999-08-01
Resolution : 2.65 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

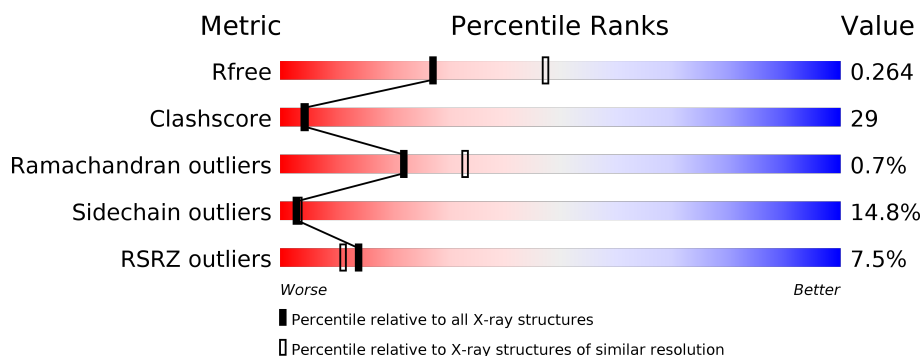
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 ≥ 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	C	18	<div> <div>44%</div> <div>33%</div> <div>22%</div> </div>
1	G	18	<div> <div>39%</div> <div>44%</div> <div>17%</div> </div>
1	K	18	<div> <div>44%</div> <div>39%</div> <div>17%</div> </div>
1	O	18	<div> <div>33%</div> <div>61%</div> <div>6%</div> </div>
1	S	18	<div> <div>44%</div> <div>44%</div> <div>11%</div> </div>
2	D	18	<div> <div>33%</div> <div>50%</div> <div>17%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	18	
2	L	18	
2	P	18	
2	T	18	
3	A	207	
3	E	207	
3	I	207	
3	M	207	
3	Q	207	
4	B	180	
4	F	180	
4	J	180	
4	N	180	
4	R	180	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19199 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 DNA chain called ADMLP TATA-BOX DNA CONTAINING IIB RECOGNITION ELEMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	18	Total	C	N	O	P	0	0	0
			375	177	78	103	17			
1	G	18	Total	C	N	O	P	0	0	0
			375	177	78	103	17			
1	K	18	Total	C	N	O	P	0	0	0
			375	177	78	103	17			
1	O	18	Total	C	N	O	P	0	0	0
			375	177	78	103	17			
1	S	18	Total	C	N	O	P	0	0	0
			375	177	78	103	17			

- Molecule 2 is a DNA chain called ADMLP TATA-BOX DNA CONTAINING IIB RECOGNITION ELEMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	18	Total	C	N	O	P	0	0	0
			357	172	59	109	17			
2	H	18	Total	C	N	O	P	0	0	0
			357	172	59	109	17			
2	L	18	Total	C	N	O	P	0	0	0
			357	172	59	109	17			
2	P	18	Total	C	N	O	P	0	0	0
			357	172	59	109	17			
2	T	18	Total	C	N	O	P	0	0	0
			357	172	59	109	17			

- Molecule 3 is a protein called GENERAL TRANSCRIPTION FACTOR IIB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	207	Total	C	N	O	S	0	0	0
			1615	1017	288	298	12			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	207	Total	C	N	O	S	0	0	0
			1615	1017	288	298	12			
3	I	207	Total	C	N	O	S	0	0	0
			1615	1017	288	298	12			
3	M	207	Total	C	N	O	S	0	0	0
			1615	1017	288	298	12			
3	Q	207	Total	C	N	O	S	0	0	0
			1615	1017	288	298	12			

- Molecule 4 is a protein called TATA BOX BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	180	Total	C	N	O	S	0	0	0
			1427	925	252	243	7			
4	F	180	Total	C	N	O	S	0	0	0
			1427	925	252	243	7			
4	J	180	Total	C	N	O	S	0	0	0
			1427	925	252	243	7			
4	N	180	Total	C	N	O	S	0	0	0
			1427	925	252	243	7			
4	R	180	Total	C	N	O	S	0	0	0
			1427	925	252	243	7			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	158	GLY	SER	CONFLICT	UNP P20226
F	158	GLY	SER	CONFLICT	UNP P20226
J	158	GLY	SER	CONFLICT	UNP P20226
N	158	GLY	SER	CONFLICT	UNP P20226
R	158	GLY	SER	CONFLICT	UNP P20226

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	15	Total	O	0	0
			15	15		
5	D	15	Total	O	0	0
			15	15		
5	G	7	Total	O	0	0
			7	7		

Continued on next page...

Continued from previous page...

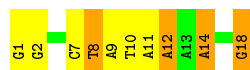
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	14	Total 14	O 14	0	0
5	K	7	Total 7	O 7	0	0
5	L	8	Total 8	O 8	0	0
5	O	7	Total 7	O 7	0	0
5	P	9	Total 9	O 9	0	0
5	S	4	Total 4	O 4	0	0
5	T	4	Total 4	O 4	0	0
5	A	28	Total 28	O 28	0	0
5	B	44	Total 44	O 44	0	0
5	E	56	Total 56	O 56	0	0
5	F	29	Total 29	O 29	0	0
5	I	12	Total 12	O 12	0	0
5	J	22	Total 22	O 22	0	0
5	M	15	Total 15	O 15	0	0
5	N	14	Total 14	O 14	0	0
5	Q	10	Total 10	O 10	0	0
5	R	9	Total 9	O 9	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: ADMLP TATA-BOX DNA CONTAINING IIB RECOGNITION ELEMENT

Chain C: 



- Molecule 1: ADMLP TATA-BOX DNA CONTAINING IIB RECOGNITION ELEMENT

Chain G: 



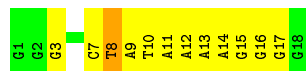
- Molecule 1: ADMLP TATA-BOX DNA CONTAINING IIB RECOGNITION ELEMENT

Chain K: 



- Molecule 1: ADMLP TATA-BOX DNA CONTAINING IIB RECOGNITION ELEMENT

Chain O: 

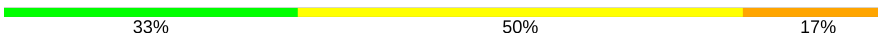


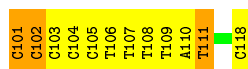
- Molecule 1: ADMLP TATA-BOX DNA CONTAINING IIB RECOGNITION ELEMENT

Chain S: 



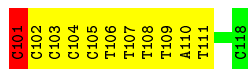
- Molecule 2: ADMLP TATA-BOX DNA CONTAINING IIB RECOGNITION ELEMENT

Chain D: 



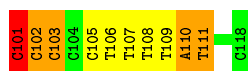
- Molecule 2: ADMLP TATA-BOX DNA CONTAINING IIB RECOGNITION ELEMENT

Chain H: 39% 56% 6%



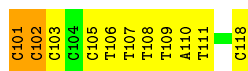
- Molecule 2: ADMLP TATA-BOX DNA CONTAINING IIB RECOGNITION ELEMENT

Chain L: 44% 28% 22% 6%



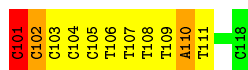
- Molecule 2: ADMLP TATA-BOX DNA CONTAINING IIB RECOGNITION ELEMENT

Chain P: 39% 50% 11%



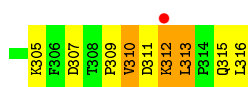
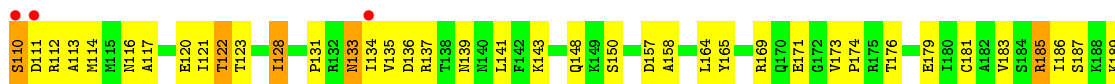
- Molecule 2: ADMLP TATA-BOX DNA CONTAINING IIB RECOGNITION ELEMENT

Chain T: 39% 44% 11% 6%



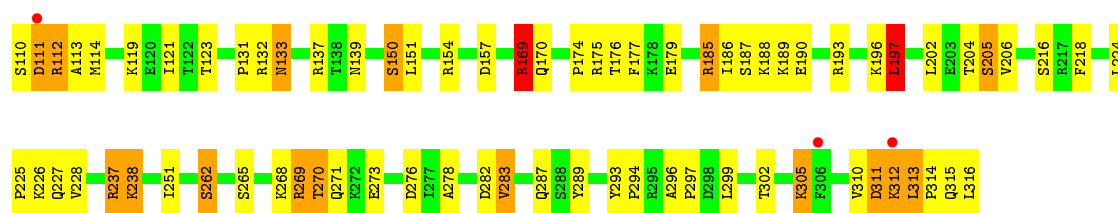
- Molecule 3: GENERAL TRANSCRIPTION FACTOR IIB

Chain A: 2% 59% 33% 8%

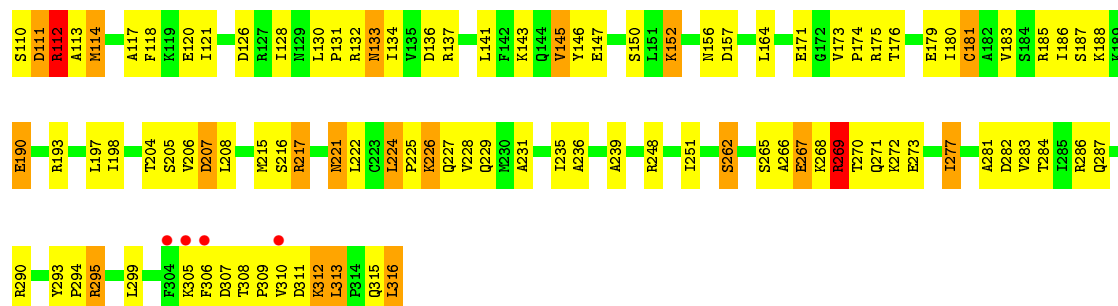


- Molecule 3: GENERAL TRANSCRIPTION FACTOR IIB

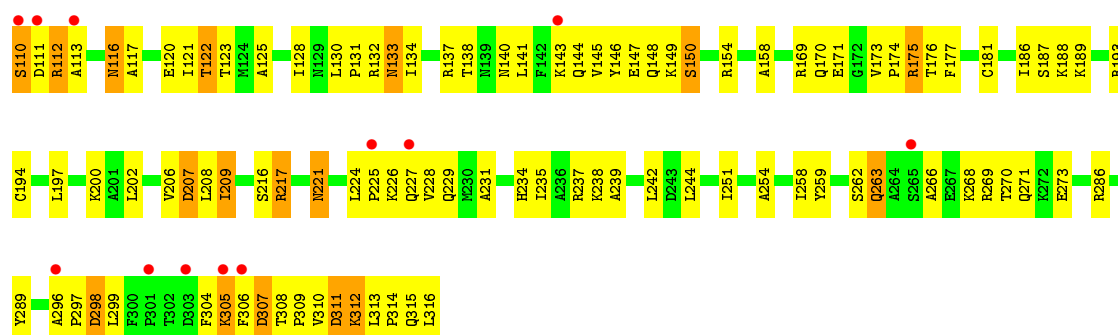
Chain E: 64% 27% 8%



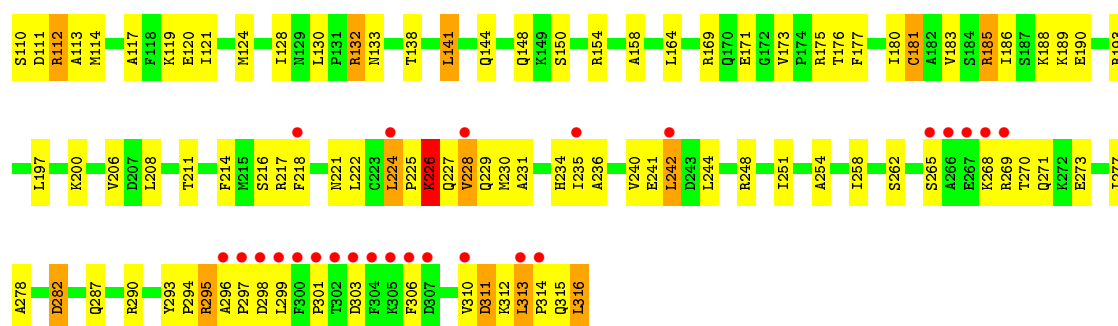
● Molecule 3: GENERAL TRANSCRIPTION FACTOR IIB



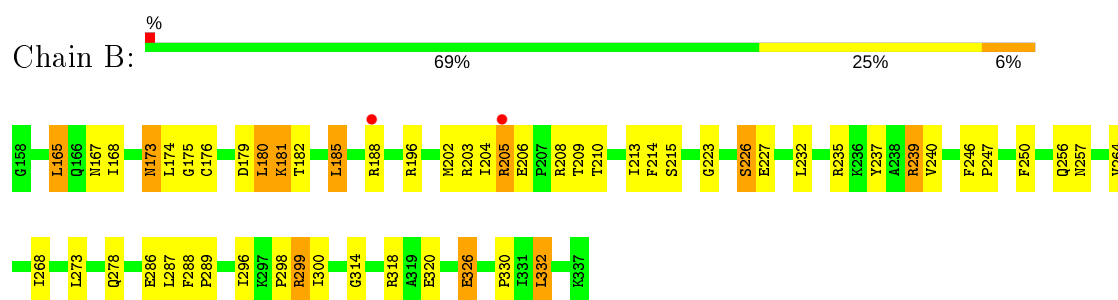
● Molecule 3: GENERAL TRANSCRIPTION FACTOR IIB



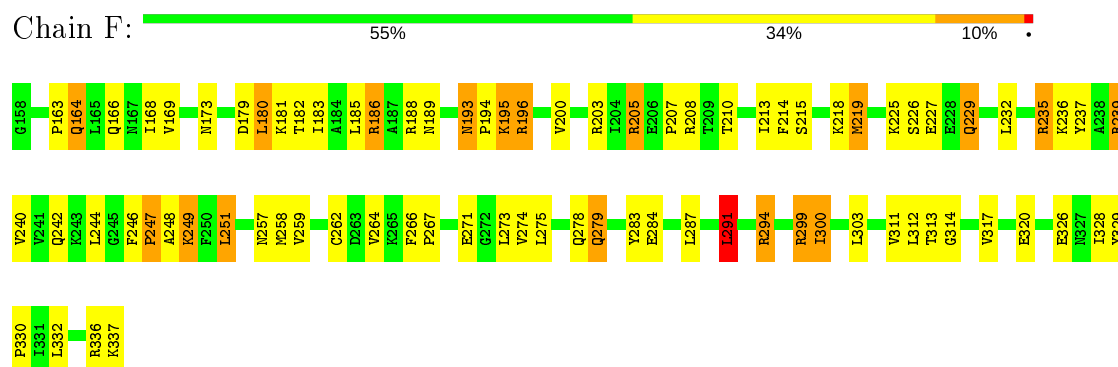
● Molecule 3: GENERAL TRANSCRIPTION FACTOR IIB



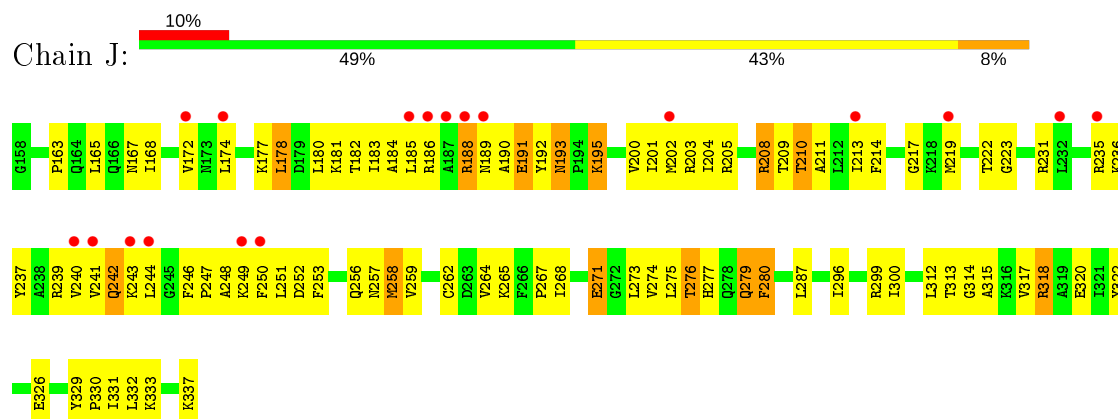
● Molecule 4: TATA BOX BINDING PROTEIN



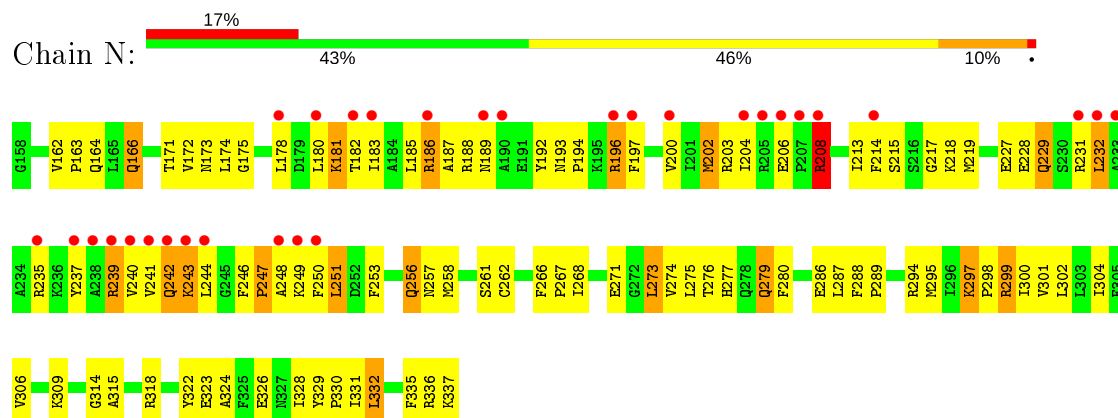
- Molecule 4: TATA BOX BINDING PROTEIN



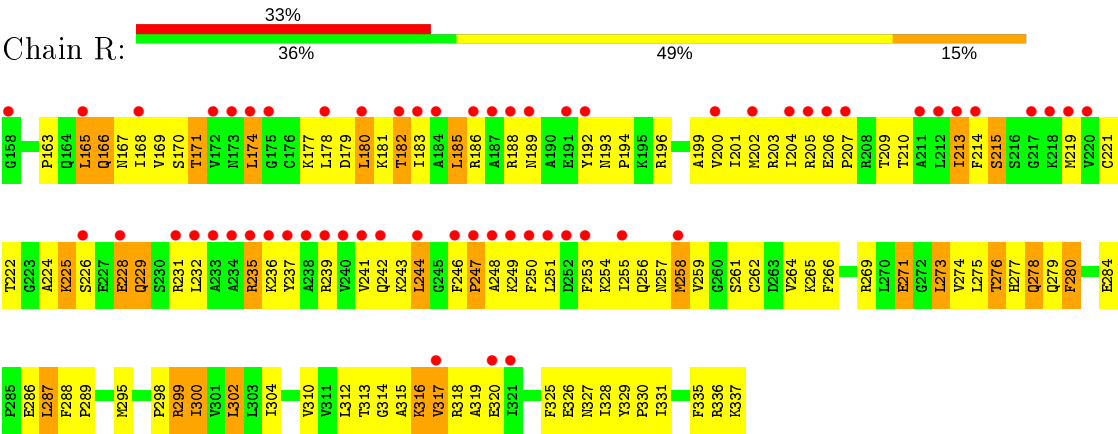
- Molecule 4: TATA BOX BINDING PROTEIN



- Molecule 4: TATA BOX BINDING PROTEIN



● Molecule 4: TATA BOX BINDING PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	118.45Å 122.30Å 140.22Å 90.00° 113.08° 90.00°	Depositor
Resolution (Å)	50.00 – 2.65 46.74 – 2.66	Depositor EDS
% Data completeness (in resolution range)	91.0 (50.00-2.65) 94.7 (46.74-2.66)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.65Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.229 , 0.260 0.234 , 0.264	Depositor DCC
R_{free} test set	5030 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19199	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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	C	1.10	0/423	1.07	0/653
1	G	1.03	0/423	1.06	0/653
1	K	0.96	0/423	1.05	0/653
1	O	0.94	0/423	1.07	0/653
1	S	0.88	0/423	1.04	0/653
2	D	1.01	0/397	1.08	0/609
2	H	1.09	0/397	1.14	1/609 (0.2%)
2	L	0.85	0/397	1.08	1/609 (0.2%)
2	P	0.88	0/397	1.09	0/609
2	T	0.86	0/397	1.07	1/609 (0.2%)
3	A	0.67	1/1639 (0.1%)	0.78	1/2209 (0.0%)
3	E	0.68	0/1639	0.73	2/2209 (0.1%)
3	I	0.64	0/1639	0.73	1/2209 (0.0%)
3	M	0.62	1/1639 (0.1%)	0.72	0/2209
3	Q	0.68	1/1639 (0.1%)	0.79	2/2209 (0.1%)
4	B	0.77	0/1453	0.84	0/1953
4	F	0.68	0/1453	0.85	2/1953 (0.1%)
4	J	0.65	0/1453	0.80	0/1953
4	N	0.69	0/1453	0.82	2/1953 (0.1%)
4	R	0.73	0/1453	0.76	0/1953
All	All	0.75	3/19560 (0.0%)	0.86	13/27120 (0.0%)

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	C	0	4
1	G	0	3
1	K	0	4
1	O	0	2
1	S	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	3
2	H	0	1
2	L	0	5
2	P	0	2
2	T	0	3
3	I	0	1
4	N	0	1
All	All	0	31

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	181	CYS	CB-SG	-7.45	1.69	1.82
3	Q	181	CYS	CB-SG	-5.49	1.72	1.81
3	M	181	CYS	CB-SG	-5.07	1.73	1.81

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	169	ARG	NE-CZ-NH1	11.56	126.08	120.30
4	N	235	ARG	NE-CZ-NH1	7.09	123.85	120.30
4	F	291	LEU	CA-CB-CG	6.97	131.34	115.30
4	N	235	ARG	CG-CD-NE	-6.24	98.70	111.80
3	I	269	ARG	CG-CD-NE	-5.89	99.44	111.80

There are no chirality outliers.

5 of 31 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	12	DA	Sidechain
1	C	14	DA	Sidechain
1	C	18	DG	Sidechain
1	C	8	DT	Sidechain
2	D	101	DC	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	375	0	202	17	0
1	G	375	0	202	20	0
1	K	375	0	202	9	0
1	O	375	0	202	14	0
1	S	375	0	202	13	0
2	D	357	0	205	12	0
2	H	357	0	205	13	0
2	L	357	0	205	14	0
2	P	357	0	205	19	0
2	T	357	0	205	24	0
3	A	1615	0	1670	90	0
3	E	1615	0	1670	65	0
3	I	1615	0	1670	117	0
3	M	1615	0	1670	115	0
3	Q	1615	0	1670	91	0
4	B	1427	0	1517	46	0
4	F	1427	0	1517	103	0
4	J	1427	0	1517	93	0
4	N	1427	0	1517	111	0
4	R	1427	0	1517	137	0
5	A	28	0	0	4	0
5	B	44	0	0	2	0
5	C	15	0	0	2	0
5	D	15	0	0	0	0
5	E	56	0	0	2	0
5	F	29	0	0	1	0
5	G	7	0	0	1	0
5	H	14	0	0	0	0
5	I	12	0	0	2	0
5	J	22	0	0	0	0
5	K	7	0	0	1	0
5	L	8	0	0	0	0
5	M	15	0	0	1	0
5	N	14	0	0	2	0
5	O	7	0	0	1	0
5	P	9	0	0	0	0
5	Q	10	0	0	0	0
5	R	9	0	0	1	0
5	S	4	0	0	0	0
5	T	4	0	0	0	0
All	All	19199	0	17970	1074	0

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 29.

The worst 5 of 1074 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)
4:N:193:ASN:HB3	4:N:196:ARG:NE	1.37	1.35
4:N:193:ASN:CB	4:N:196:ARG:HE	1.47	1.26
3:Q:224:LEU:CD2	3:Q:228:VAL:HG21	1.67	1.23
4:N:188:ARG:HG3	4:N:189:ASN:H	1.04	1.20
1:G:11:DA:H2''	1:G:12:DA:H5'	1.22	1.16

There are no symmetry-related clashes.

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	
3	A	205/207 (99%)	195 (95%)	8 (4%)	2 (1%)	15	23
3	E	205/207 (99%)	192 (94%)	11 (5%)	2 (1%)	15	23
3	I	205/207 (99%)	194 (95%)	9 (4%)	2 (1%)	15	23
3	M	205/207 (99%)	191 (93%)	13 (6%)	1 (0%)	29	43
3	Q	205/207 (99%)	191 (93%)	12 (6%)	2 (1%)	15	23
4	B	178/180 (99%)	167 (94%)	11 (6%)	0	100	100
4	F	178/180 (99%)	162 (91%)	15 (8%)	1 (1%)	25	37
4	J	178/180 (99%)	163 (92%)	14 (8%)	1 (1%)	25	37
4	N	178/180 (99%)	159 (89%)	17 (10%)	2 (1%)	14	21
4	R	178/180 (99%)	162 (91%)	15 (8%)	1 (1%)	25	37
All	All	1915/1935 (99%)	1776 (93%)	125 (6%)	14 (1%)	22	33

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	312	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	M	312	LYS
3	E	312	LYS
3	I	112	ARG
3	Q	312	LYS

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	
3	A	176/176 (100%)	155 (88%)	21 (12%)	5	7
3	E	176/176 (100%)	149 (85%)	27 (15%)	2	3
3	I	176/176 (100%)	148 (84%)	28 (16%)	2	2
3	M	176/176 (100%)	152 (86%)	24 (14%)	3	5
3	Q	176/176 (100%)	152 (86%)	24 (14%)	3	5
4	B	154/154 (100%)	136 (88%)	18 (12%)	5	7
4	F	154/154 (100%)	132 (86%)	22 (14%)	3	3
4	J	154/154 (100%)	133 (86%)	21 (14%)	3	5
4	N	154/154 (100%)	126 (82%)	28 (18%)	1	1
4	R	154/154 (100%)	123 (80%)	31 (20%)	1	1
All	All	1650/1650 (100%)	1406 (85%)	244 (15%)	3	3

5 of 244 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	I	277	ILE
4	J	333	LYS
4	R	228	GLU
3	I	305	LYS
4	J	210	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
3	I	139	ASN
4	J	193	ASN
4	R	166	GLN
3	I	156	ASN
3	I	263	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](#)

There are no ligands in this entry.

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, 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	C	18/18 (100%)	0.13	0	100	100	27, 41, 52, 58	0
1	G	18/18 (100%)	-0.06	0	100	100	25, 43, 50, 57	0
1	K	18/18 (100%)	-0.17	0	100	100	32, 45, 52, 59	0
1	O	18/18 (100%)	-0.16	0	100	100	29, 44, 58, 65	0
1	S	18/18 (100%)	-0.30	0	100	100	33, 49, 58, 62	0
2	D	18/18 (100%)	0.08	0	100	100	25, 37, 52, 53	0
2	H	18/18 (100%)	-0.01	0	100	100	26, 40, 50, 50	0
2	L	18/18 (100%)	-0.23	0	100	100	31, 42, 54, 55	0
2	P	18/18 (100%)	-0.30	0	100	100	31, 45, 51, 53	0
2	T	18/18 (100%)	-0.44	0	100	100	36, 47, 54, 55	0
3	A	207/207 (100%)	0.15	4 (1%)	66	63	31, 49, 66, 75	0
3	E	207/207 (100%)	0.33	3 (1%)	75	73	25, 45, 65, 71	0
3	I	207/207 (100%)	0.20	4 (1%)	66	63	33, 52, 68, 72	0
3	M	207/207 (100%)	0.45	12 (5%)	23	19	34, 54, 69, 75	0
3	Q	207/207 (100%)	0.60	25 (12%)	4	3	34, 53, 69, 75	0
4	B	180/180 (100%)	0.38	2 (1%)	80	79	23, 42, 62, 72	0
4	F	180/180 (100%)	0.15	0	100	100	25, 46, 65, 73	0
4	J	180/180 (100%)	0.44	18 (10%)	7	5	30, 49, 66, 73	0
4	N	180/180 (100%)	0.68	31 (17%)	1	1	32, 53, 69, 74	0
4	R	180/180 (100%)	1.51	60 (33%)	0	0	35, 56, 70, 75	0
All	All	2115/2115 (100%)	0.43	159 (7%)	14	11	23, 49, 68, 75	0

The worst 5 of 159 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	110	SER	9.7
4	R	237	TYR	7.5
3	M	110	SER	6.9
4	R	241	VAL	6.1
3	Q	301	PRO	5.8

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.