



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2018 – 06:52 pm GMT

PDB ID : 5I2D
Title : Crystal structure of T. thermophilus TTHB099 class II transcription activation complex: TAP-RPo
Authors : Feng, Y.; Zhang, Y.; Ebright, R.H.
Deposited on : 2016-02-08
Resolution : 4.41 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 : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

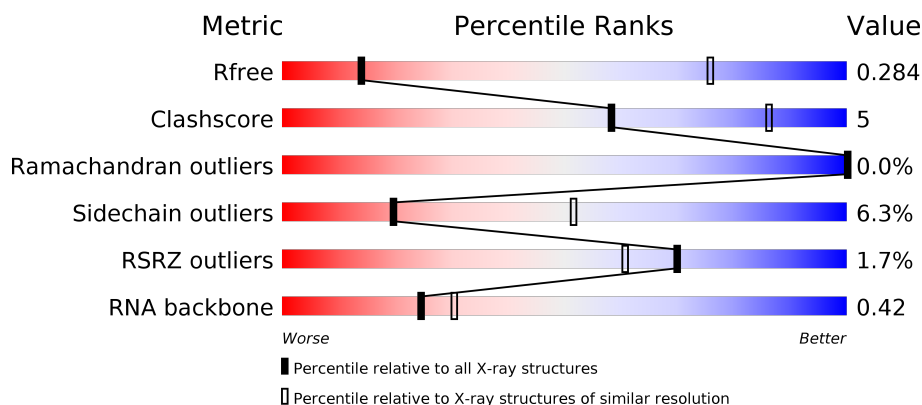
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.41 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}	111664	1058 (5.08-3.70)
Clashscore	122126	1005 (5.08-3.72)
Ramachandran outliers	120053	1078 (5.08-3.70)
Sidechain outliers	120020	1061 (5.08-3.70)
RSRZ outliers	108989	1000 (5.12-3.62)
RNA backbone	2636	1104 (5.90-2.90)

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. 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	315	<div> <div>2%</div> <div>74% 14% • 10%</div> </div>
1	B	315	<div> <div>2%</div> <div>73% 13% • 11%</div> </div>
1	L	315	<div> <div>2%</div> <div>77% 12% • 10%</div> </div>
1	M	315	<div> <div>73% 13% • 11%</div> </div>

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Mol	Chain	Length	Quality of chain
2	C	1119	
2	N	1119	
3	D	1524	
3	O	1524	
4	E	99	
4	P	99	
5	F	443	
5	Q	443	
6	G	215	
6	H	215	
6	R	215	
6	S	215	
7	I	72	
7	T	72	
8	J	72	
8	U	72	
9	K	4	
9	V	4	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 66882 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2231	1421	387	421	2			
1	B	280	Total	C	N	O	S	0	0	0
			2199	1401	381	415	2			
1	L	284	Total	C	N	O	S	0	0	0
			2231	1421	387	421	2			
1	M	280	Total	C	N	O	S	0	0	0
			2199	1401	381	415	2			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0	0
			8770	5548	1564	1634	24			
2	N	1111	Total	C	N	O	S	0	0	0
			8770	5548	1564	1634	24			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1363	Total	C	N	O	S	0	0	0
			10754	6804	1906	2011	33			
3	O	1363	Total	C	N	O	S	0	0	0
			10754	6804	1906	2011	33			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			
4	P	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	346	Total	C	N	O	S	0	0	0
			2807	1770	509	524	4			
5	Q	346	Total	C	N	O	S	0	0	0
			2807	1770	509	524	4			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	initiating methionine	UNP Q5SKW1
F	-18	GLY	-	expression tag	UNP Q5SKW1
F	-17	SER	-	expression tag	UNP Q5SKW1
F	-16	SER	-	expression tag	UNP Q5SKW1
F	-15	HIS	-	expression tag	UNP Q5SKW1
F	-14	HIS	-	expression tag	UNP Q5SKW1
F	-13	HIS	-	expression tag	UNP Q5SKW1
F	-12	HIS	-	expression tag	UNP Q5SKW1
F	-11	HIS	-	expression tag	UNP Q5SKW1
F	-10	HIS	-	expression tag	UNP Q5SKW1
F	-9	SER	-	expression tag	UNP Q5SKW1
F	-8	SER	-	expression tag	UNP Q5SKW1
F	-7	GLY	-	expression tag	UNP Q5SKW1
F	-6	LEU	-	expression tag	UNP Q5SKW1
F	-5	VAL	-	expression tag	UNP Q5SKW1
F	-4	PRO	-	expression tag	UNP Q5SKW1
F	-3	ARG	-	expression tag	UNP Q5SKW1
F	-2	GLY	-	expression tag	UNP Q5SKW1
F	-1	SER	-	expression tag	UNP Q5SKW1
F	0	HIS	-	expression tag	UNP Q5SKW1
Q	-19	MET	-	initiating methionine	UNP Q5SKW1
Q	-18	GLY	-	expression tag	UNP Q5SKW1
Q	-17	SER	-	expression tag	UNP Q5SKW1
Q	-16	SER	-	expression tag	UNP Q5SKW1
Q	-15	HIS	-	expression tag	UNP Q5SKW1
Q	-14	HIS	-	expression tag	UNP Q5SKW1
Q	-13	HIS	-	expression tag	UNP Q5SKW1
Q	-12	HIS	-	expression tag	UNP Q5SKW1
Q	-11	HIS	-	expression tag	UNP Q5SKW1
Q	-10	HIS	-	expression tag	UNP Q5SKW1
Q	-9	SER	-	expression tag	UNP Q5SKW1
Q	-8	SER	-	expression tag	UNP Q5SKW1
Q	-7	GLY	-	expression tag	UNP Q5SKW1
Q	-6	LEU	-	expression tag	UNP Q5SKW1

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	-5	VAL	-	expression tag	UNP Q5SKW1
Q	-4	PRO	-	expression tag	UNP Q5SKW1
Q	-3	ARG	-	expression tag	UNP Q5SKW1
Q	-2	GLY	-	expression tag	UNP Q5SKW1
Q	-1	SER	-	expression tag	UNP Q5SKW1
Q	0	HIS	-	expression tag	UNP Q5SKW1

- Molecule 6 is a protein called Transcriptional regulator, Crp family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	195	Total	C	N	O	S	0	0	0
			1559	974	293	288	4			
6	H	195	Total	C	N	O	S	0	0	0
			1559	974	293	288	4			
6	R	195	Total	C	N	O	S	0	0	0
			1559	974	293	288	4			
6	S	195	Total	C	N	O	S	0	0	0
			1559	974	293	288	4			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-19	MET	-	initiating methionine	UNP Q53W63
G	-18	GLY	-	expression tag	UNP Q53W63
G	-17	SER	-	expression tag	UNP Q53W63
G	-16	SER	-	expression tag	UNP Q53W63
G	-15	HIS	-	expression tag	UNP Q53W63
G	-14	HIS	-	expression tag	UNP Q53W63
G	-13	HIS	-	expression tag	UNP Q53W63
G	-12	HIS	-	expression tag	UNP Q53W63
G	-11	HIS	-	expression tag	UNP Q53W63
G	-10	HIS	-	expression tag	UNP Q53W63
G	-9	SER	-	expression tag	UNP Q53W63
G	-8	SER	-	expression tag	UNP Q53W63
G	-7	GLY	-	expression tag	UNP Q53W63
G	-6	LEU	-	expression tag	UNP Q53W63
G	-5	VAL	-	expression tag	UNP Q53W63
G	-4	PRO	-	expression tag	UNP Q53W63
G	-3	ARG	-	expression tag	UNP Q53W63
G	-2	GLY	-	expression tag	UNP Q53W63
G	-1	SER	-	expression tag	UNP Q53W63
G	0	HIS	-	expression tag	UNP Q53W63

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-19	MET	-	initiating methionine	UNP Q53W63
H	-18	GLY	-	expression tag	UNP Q53W63
H	-17	SER	-	expression tag	UNP Q53W63
H	-16	SER	-	expression tag	UNP Q53W63
H	-15	HIS	-	expression tag	UNP Q53W63
H	-14	HIS	-	expression tag	UNP Q53W63
H	-13	HIS	-	expression tag	UNP Q53W63
H	-12	HIS	-	expression tag	UNP Q53W63
H	-11	HIS	-	expression tag	UNP Q53W63
H	-10	HIS	-	expression tag	UNP Q53W63
H	-9	SER	-	expression tag	UNP Q53W63
H	-8	SER	-	expression tag	UNP Q53W63
H	-7	GLY	-	expression tag	UNP Q53W63
H	-6	LEU	-	expression tag	UNP Q53W63
H	-5	VAL	-	expression tag	UNP Q53W63
H	-4	PRO	-	expression tag	UNP Q53W63
H	-3	ARG	-	expression tag	UNP Q53W63
H	-2	GLY	-	expression tag	UNP Q53W63
H	-1	SER	-	expression tag	UNP Q53W63
H	0	HIS	-	expression tag	UNP Q53W63
R	-19	MET	-	initiating methionine	UNP Q53W63
R	-18	GLY	-	expression tag	UNP Q53W63
R	-17	SER	-	expression tag	UNP Q53W63
R	-16	SER	-	expression tag	UNP Q53W63
R	-15	HIS	-	expression tag	UNP Q53W63
R	-14	HIS	-	expression tag	UNP Q53W63
R	-13	HIS	-	expression tag	UNP Q53W63
R	-12	HIS	-	expression tag	UNP Q53W63
R	-11	HIS	-	expression tag	UNP Q53W63
R	-10	HIS	-	expression tag	UNP Q53W63
R	-9	SER	-	expression tag	UNP Q53W63
R	-8	SER	-	expression tag	UNP Q53W63
R	-7	GLY	-	expression tag	UNP Q53W63
R	-6	LEU	-	expression tag	UNP Q53W63
R	-5	VAL	-	expression tag	UNP Q53W63
R	-4	PRO	-	expression tag	UNP Q53W63
R	-3	ARG	-	expression tag	UNP Q53W63
R	-2	GLY	-	expression tag	UNP Q53W63
R	-1	SER	-	expression tag	UNP Q53W63
R	0	HIS	-	expression tag	UNP Q53W63
S	-19	MET	-	initiating methionine	UNP Q53W63
S	-18	GLY	-	expression tag	UNP Q53W63

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Chain	Residue	Modelled	Actual	Comment	Reference
S	-17	SER	-	expression tag	UNP Q53W63
S	-16	SER	-	expression tag	UNP Q53W63
S	-15	HIS	-	expression tag	UNP Q53W63
S	-14	HIS	-	expression tag	UNP Q53W63
S	-13	HIS	-	expression tag	UNP Q53W63
S	-12	HIS	-	expression tag	UNP Q53W63
S	-11	HIS	-	expression tag	UNP Q53W63
S	-10	HIS	-	expression tag	UNP Q53W63
S	-9	SER	-	expression tag	UNP Q53W63
S	-8	SER	-	expression tag	UNP Q53W63
S	-7	GLY	-	expression tag	UNP Q53W63
S	-6	LEU	-	expression tag	UNP Q53W63
S	-5	VAL	-	expression tag	UNP Q53W63
S	-4	PRO	-	expression tag	UNP Q53W63
S	-3	ARG	-	expression tag	UNP Q53W63
S	-2	GLY	-	expression tag	UNP Q53W63
S	-1	SER	-	expression tag	UNP Q53W63
S	0	HIS	-	expression tag	UNP Q53W63

- Molecule 7 is a DNA chain called DNA (72-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	66	Total	C	N	O	P	0	0	0
			1349	639	246	398	66			
7	T	66	Total	C	N	O	P	0	0	0
			1349	639	246	398	66			

- Molecule 8 is a DNA chain called DNA (72-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	66	Total	C	N	O	P	0	0	0
			1367	645	267	390	65			
8	U	66	Total	C	N	O	P	0	0	0
			1367	645	267	390	65			

- Molecule 9 is a RNA chain called RNA (5'-R(*UP*CP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	4	Total	C	N	O	P	0	0	0
			82	38	15	26	3			
9	V	4	Total	C	N	O	P	0	0	0
			82	38	15	26	3			

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	O	2	Total 2	Zn 2	0	0
10	D	2	Total 2	Zn 2	0	0

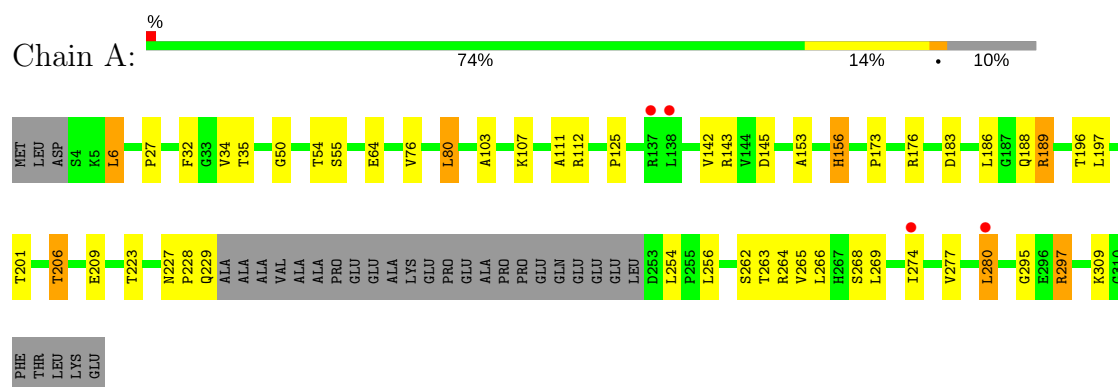
- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	O	1	Total 1	Mg 1	0	0
11	D	1	Total 1	Mg 1	0	0

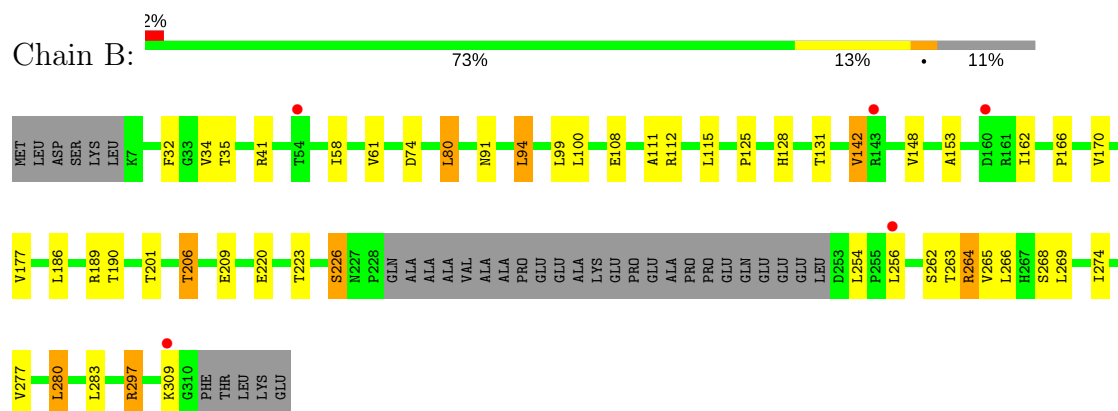
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

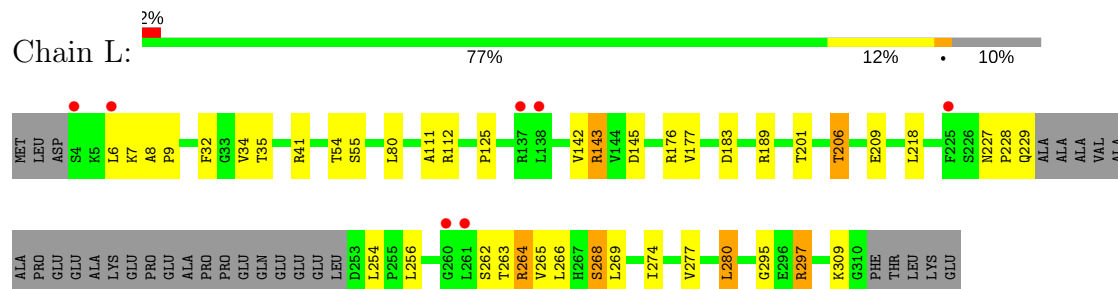
- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 1: DNA-directed RNA polymerase subunit alpha

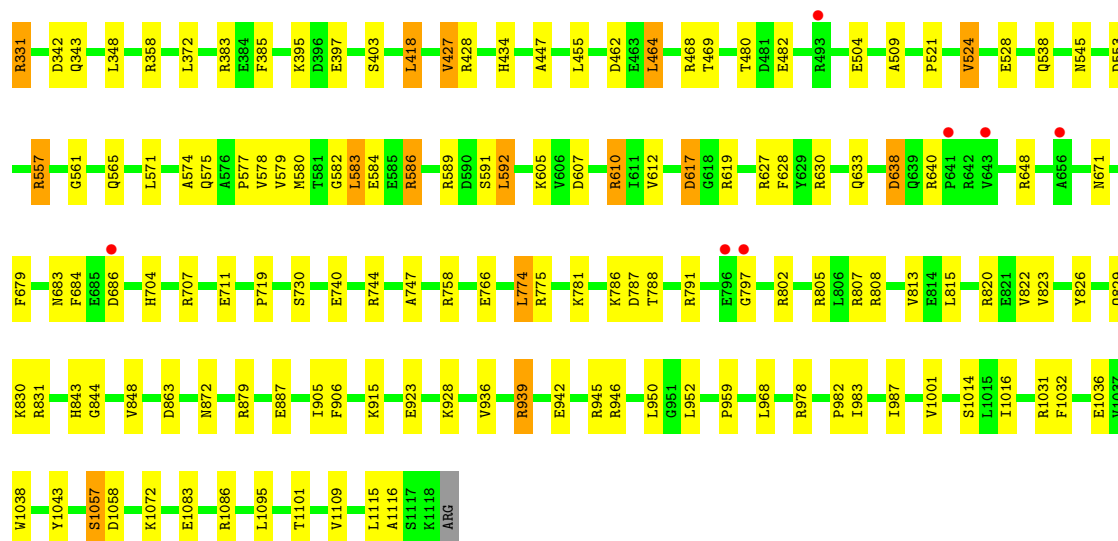
Category	Percentage
Very good	73%
Good	13%
Not good	•
Very bad	11%



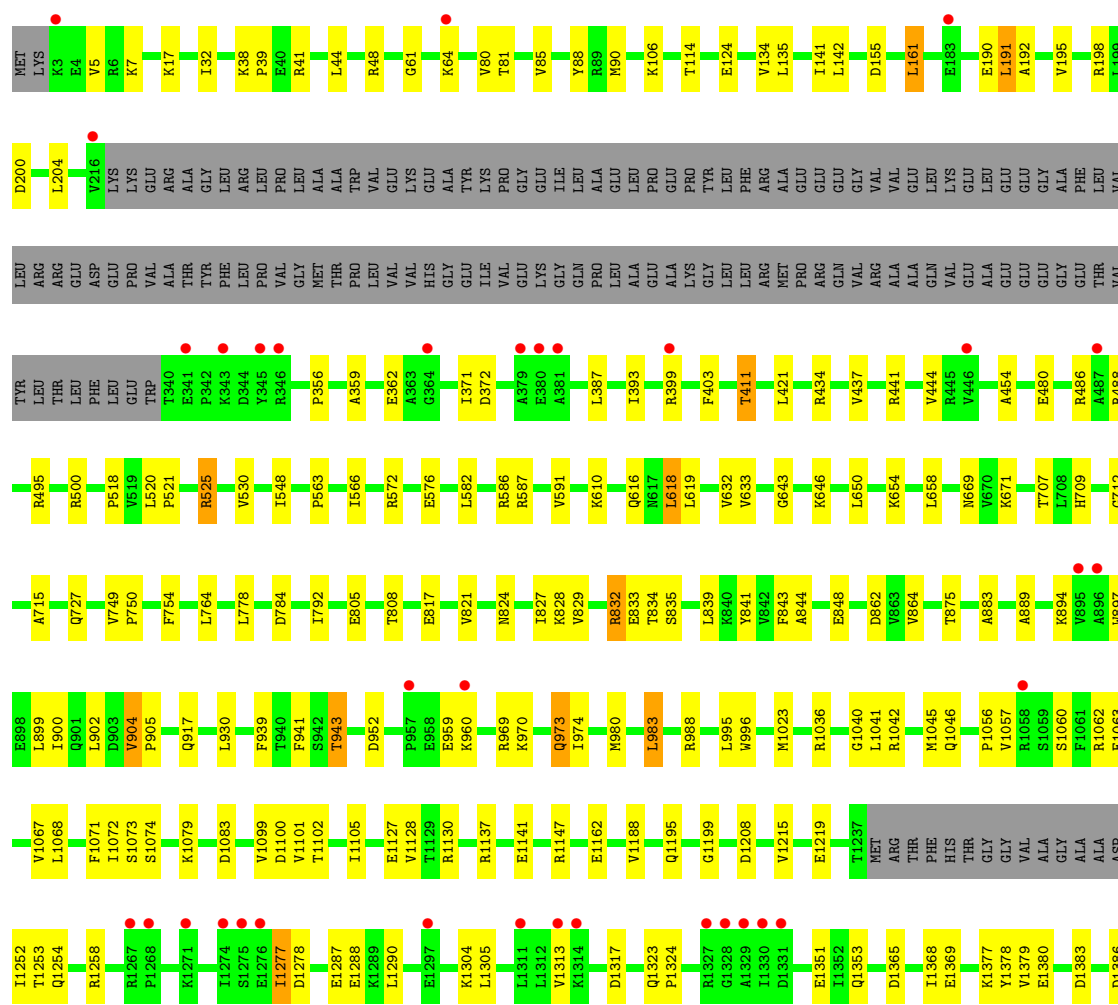
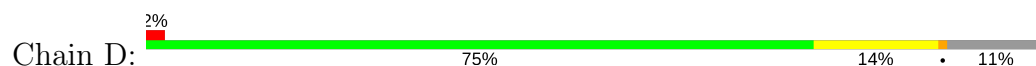
S1057	K830	F679	P536	Q343	D173	M1
D1058	R831	N683	K537	R358	L174	R8
E1083	H843	F684	N545	L372	E177	E11
R1086	H845	H704	R657	R383	M184	L15
V1087	K846	R707	Q575	E384	K185	P16
L1088	V848	Y708	A576	F385	V186	P17
V1089			P577	K395	N187	E20
K1090	D863	E711	V578	D396	L200	I21
A1094	V867	D714	V579	E397	D203	P35
L1095	N872	I726	T581	S403	Q204	K38
L1102	E887	P727	G582	L404	E205	
L1115			L583	R408	L211	T51
A1116	I905	S730	E585	L413	G212	
S1117	F906	R744	R586		A213	
K1118	K915	A747	R589	L418	Y214	
ARG	E923	R758	D590	V427	L217	ASP
	K928	E766	S591	L428	V218	LYS
	F934	P767	L592		D223	GLY
G935			G601	H434	E224	GLY
V936	L774	R775	K605	A447	S225	GLY
R939	R781	K781	D607		M229	L64
E942	A782	V612	R610	L451	R230	D81
R945	R783		V613	L455	E232	D87
L952	K786		R614	D462	E233	A92
V953	D787		Y615	E463	P247	
T954	T788		E616	L464	P248	A96
P955	S789		D617	R468	D251	R97
	L790		G618	T469	R265	K103
P959	R791			T480		E110
L968	G797		R627	D481	L289	
R978	R805		F628	E482	S286	L120
P982	L806		Y629	V483		G131
I983	R808		R630	V484	D300	A132
			Q633	T501	R308	D133
			D638	P502		H141
	V813		Q639	L503	V322	A160
I987	E814		R640	E504	D323	
	L815		P641	A509	D324	P164
V1001	R820		R642		H327	
S1014	E821		R648	P521	L328	K167
R1031	V822		Q670	V524		R168
	V823			E528	R331	
V1038	Q820		A576		D342	V172

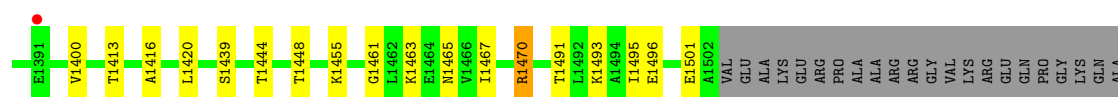
- Molecule 2: DNA-directed RNA polymerase subunit beta

Category	Count
P1	1
R8	1
E11	1
L15	1
P16	1
P17	1
E20	1
L21	1
T51	1
I54	1
E55	1
E56	1
ASP	1
LYS	1
GLY	1
LYS	1
GLY	1
L64	1
D81	1
P82	1
C83	1
D87	1
L88	1
A92	1
A96	1
R97	1
L98	1
K103	1
L107	1
E110	1
L120	1
G131	1
A132	1
D133	1
H141	1
H142	1
S143	1
Y147	1
P152	1
A160	1
P164	1
K167	1
R168	1
W171	1
I172	1
D173	1
L174	1
E177	1
P178	1
V196	1
D203	1
Q204	1
E205	1
T206	1
L207	1
L211	1
Y214	1
L218	1
P217	1
Q219	1
M229	1
E232	1
E233	1
R243	1
D246	1
P247	1
P248	1
D251	1
Y256	1
R265	1
E266	1
Y267	1
D268	1
L269	1
R308	1
V322	1
R323	1
D324	1
H327	1

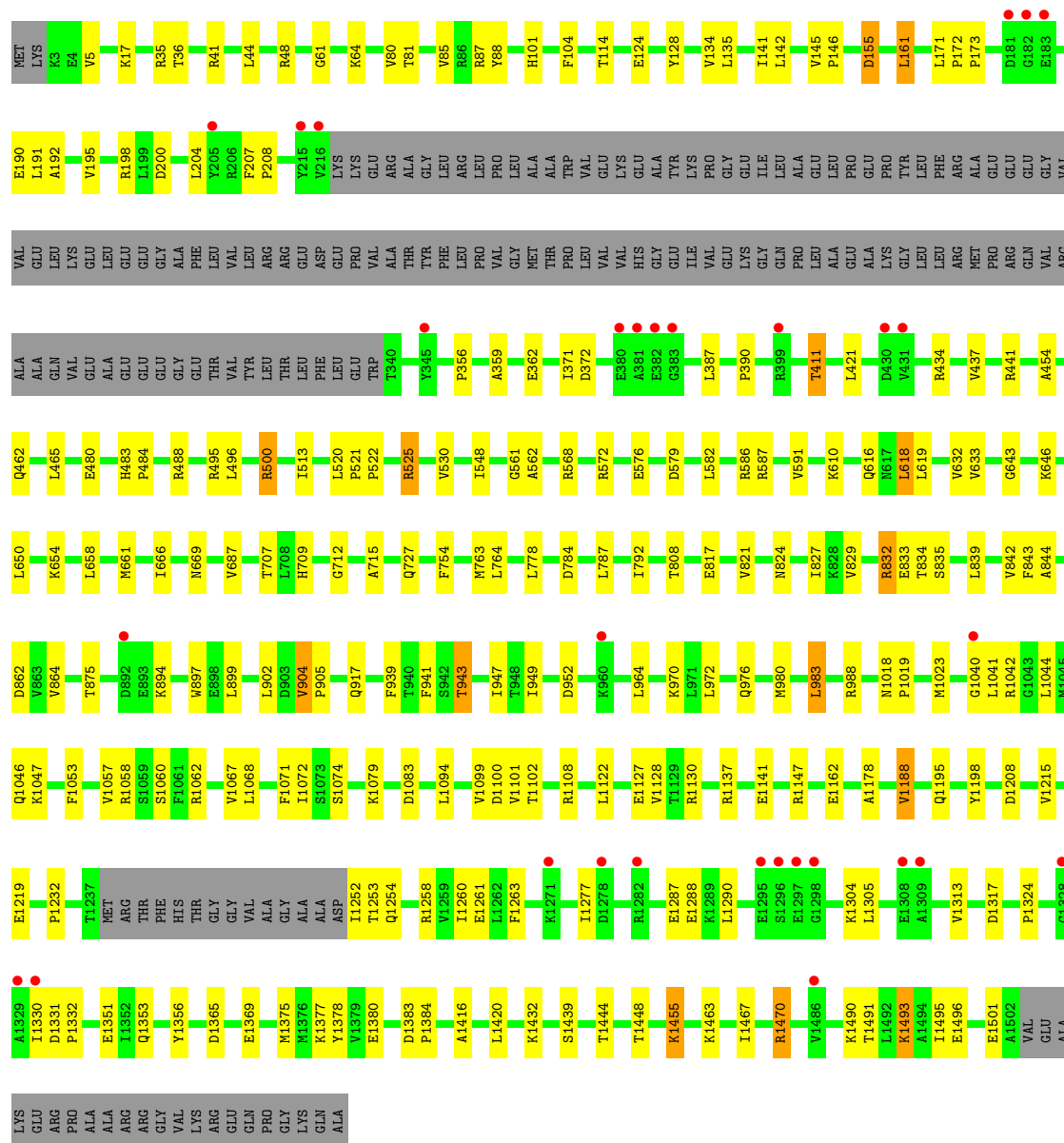
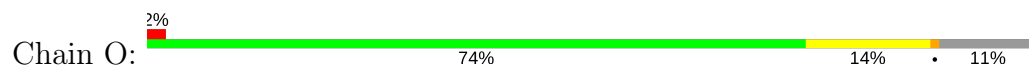


• Molecule 3: DNA-directed RNA polymerase subunit beta'

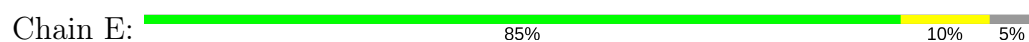




• Molecule 3: DNA-directed RNA polymerase subunit beta'



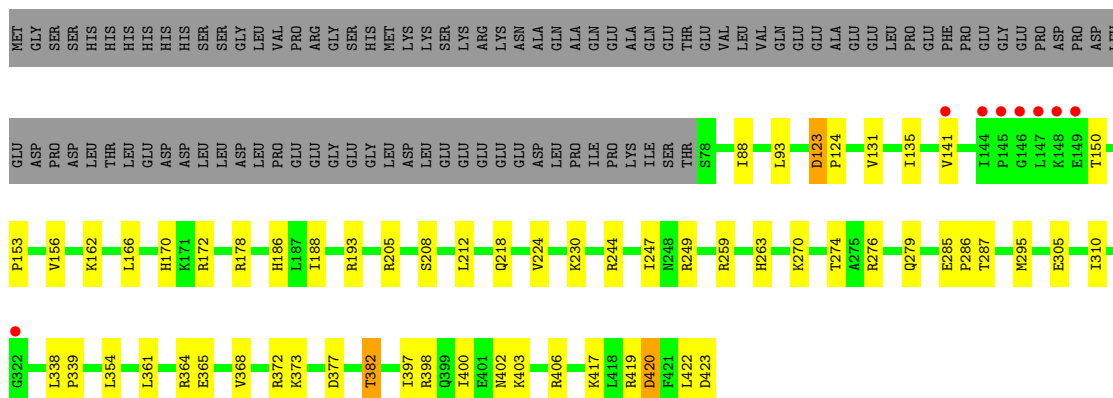
• Molecule 4: DNA-directed RNA polymerase subunit omega



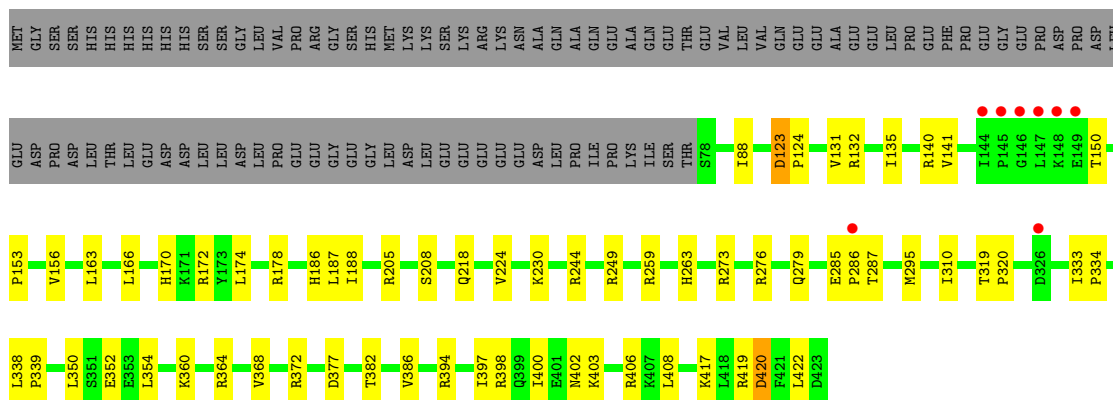
• Molecule 4: DNA-directed RNA polymerase subunit omega

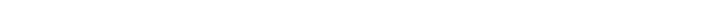
MET	A2	V13	D14	L19	R45	P46	T50	L51	E52	K66	E67	L68	L69	T70	V80	D83	E88	M89	V95	GLU	ARG	GLU	GLU
-----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Chain F:  2% 64% 13% 22%




- Chain Q: 

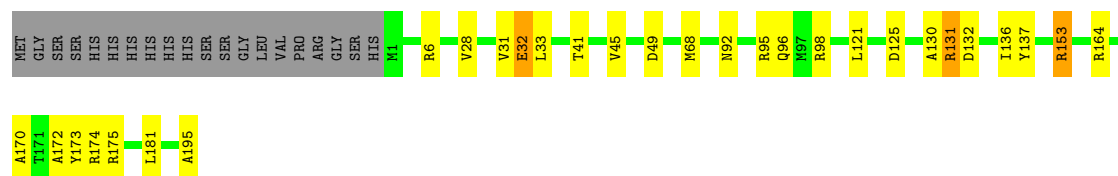


- Chain G:  2% 75% 13% 9%




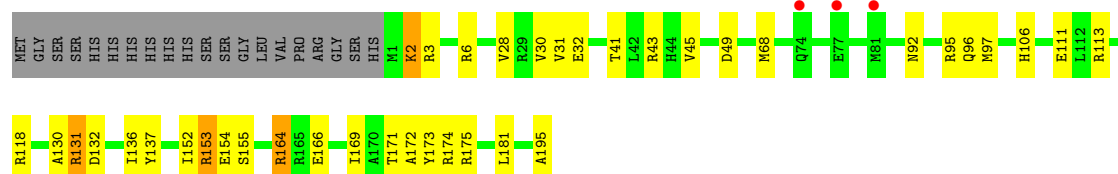
- Molecule 6: Transcriptional regulator, Crp family

Chain H: 




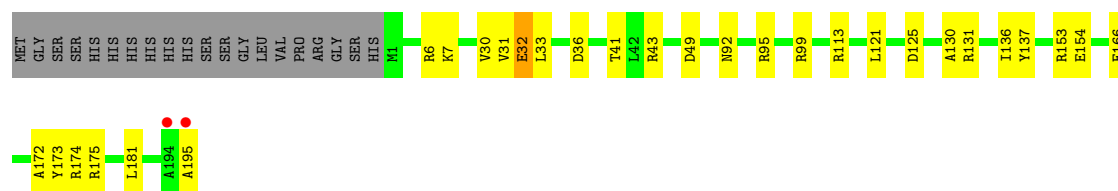
- Molecule 6: Transcriptional regulator, Crp family

Chain R: 



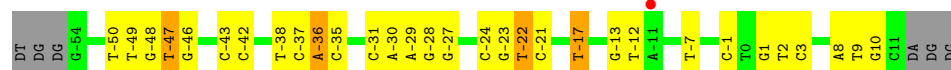
- Molecule 6: Transcriptional regulator, Crp family

Chain S: 



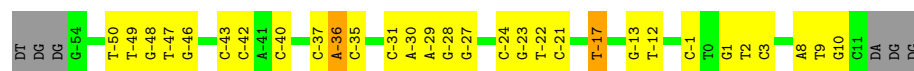
- Molecule 7: DNA (72-MER)

Chain I: 



- Molecule 7: DNA (72-MER)

Chain T: 



- Molecule 8: DNA (72-MER)

Chain J: 



- Molecule 8: DNA (72-MER)

Chain U:

51%

38%

• 8%



● Molecule 9: RNA (5'-R(*UP*CP*GP*A)-3')

Chain K:

50%

25%

25%



● Molecule 9: RNA (5'-R(*UP*CP*GP*A)-3')

Chain V:

75%

25%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	171.49Å 105.45Å 374.58Å 90.00° 102.39° 90.00°	Depositor
Resolution (Å)	49.31 – 4.41 49.39 – 4.41	Depositor EDS
% Data completeness (in resolution range)	85.8 (49.31-4.41) 84.9 (49.39-4.41)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 4.45Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.241 , 0.284 0.242 , 0.284	Depositor DCC
R_{free} test set	2033 reflections (2.49%)	wwPDB-VP
Wilson B-factor (Å ²)	156.7	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 69.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	66882	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.62 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.6653e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.21	0/2265	0.42	0/3069
1	B	0.21	0/2233	0.43	0/3027
1	L	0.21	0/2265	0.42	0/3069
1	M	0.21	0/2233	0.43	0/3027
2	C	0.21	0/8937	0.40	0/12087
2	N	0.21	0/8937	0.40	0/12087
3	D	0.20	0/10937	0.39	0/14781
3	O	0.20	0/10937	0.39	0/14781
4	E	0.21	0/775	0.37	0/1045
4	P	0.20	0/775	0.37	0/1045
5	F	0.21	0/2852	0.38	0/3837
5	Q	0.21	0/2852	0.38	0/3837
6	G	0.21	0/1580	0.41	0/2129
6	H	0.21	0/1580	0.40	0/2129
6	R	0.21	0/1580	0.41	0/2129
6	S	0.21	0/1580	0.40	0/2129
7	I	0.44	0/1511	1.06	8/2329 (0.3%)
7	T	0.44	0/1511	1.05	5/2329 (0.2%)
8	J	0.45	0/1538	0.98	5/2376 (0.2%)
8	U	0.45	0/1538	0.97	5/2376 (0.2%)
9	K	0.17	0/91	0.77	0/140
9	V	0.17	0/91	0.81	0/140
All	All	0.24	0/68598	0.50	23/93898 (0.0%)

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	-10	DC	O4'-C4'-C3'	-7.85	101.29	106.00
8	U	-10	DC	O4'-C4'-C3'	-7.61	101.43	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	U	1	DC	O4'-C1'-N1	6.45	112.52	108.00
8	J	1	DC	O4'-C1'-N1	6.44	112.51	108.00
7	T	10	DG	C4'-C3'-C2'	-6.23	97.49	103.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2231	0	2313	21	0
1	B	2199	0	2276	24	0
1	L	2231	0	2313	17	0
1	M	2199	0	2276	24	0
2	C	8770	0	8874	101	0
2	N	8770	0	8874	97	0
3	D	10754	0	10975	107	0
3	O	10754	0	10975	113	0
4	E	761	0	778	7	0
4	P	761	0	778	10	0
5	F	2807	0	2882	29	0
5	Q	2807	0	2882	31	0
6	G	1559	0	1587	24	0
6	H	1559	0	1587	20	0
6	R	1559	0	1587	29	0
6	S	1559	0	1587	18	0
7	I	1349	0	741	25	0
7	T	1349	0	741	27	0
8	J	1367	0	739	32	0
8	U	1367	0	739	28	0
9	K	82	0	44	2	0
9	V	82	0	44	2	0
10	D	2	0	0	0	0
10	O	2	0	0	0	0
11	D	1	0	0	0	0
11	O	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	66882	0	65592	692	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 5.

The worst 5 of 692 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)
6:G:164:ARG:NH1	6:G:171:THR:OG1	2.20	0.75
8:U:15:DG:H2"	8:U:16:DC:H5"	1.66	0.75
2:N:630:ARG:CZ	2:N:707:ARG:HD3	2.17	0.74
2:N:683:ASN:HB3	2:N:872:ASN:HB2	1.69	0.74
6:R:164:ARG:NH1	6:R:171:THR:OG1	2.21	0.73

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	
1	A	280/315 (89%)	269 (96%)	11 (4%)	0	100	100
1	B	276/315 (88%)	264 (96%)	12 (4%)	0	100	100
1	L	280/315 (89%)	269 (96%)	11 (4%)	0	100	100
1	M	276/315 (88%)	264 (96%)	12 (4%)	0	100	100
2	C	1107/1119 (99%)	1090 (98%)	17 (2%)	0	100	100
2	N	1107/1119 (99%)	1088 (98%)	19 (2%)	0	100	100
3	D	1357/1524 (89%)	1337 (98%)	19 (1%)	1 (0%)	53	87
3	O	1357/1524 (89%)	1339 (99%)	17 (1%)	1 (0%)	53	87
4	E	92/99 (93%)	89 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	P	92/99 (93%)	89 (97%)	3 (3%)	0	100	100
5	F	344/443 (78%)	337 (98%)	7 (2%)	0	100	100
5	Q	344/443 (78%)	337 (98%)	7 (2%)	0	100	100
6	G	193/215 (90%)	190 (98%)	3 (2%)	0	100	100
6	H	193/215 (90%)	190 (98%)	3 (2%)	0	100	100
6	R	193/215 (90%)	190 (98%)	3 (2%)	0	100	100
6	S	193/215 (90%)	190 (98%)	3 (2%)	0	100	100
All	All	7684/8490 (90%)	7532 (98%)	150 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	530	VAL
3	O	530	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	249/273 (91%)	226 (91%)	23 (9%)	10	36
1	B	245/273 (90%)	223 (91%)	22 (9%)	10	38
1	L	249/273 (91%)	227 (91%)	22 (9%)	11	39
1	M	245/273 (90%)	225 (92%)	20 (8%)	12	43
2	C	936/941 (100%)	877 (94%)	59 (6%)	20	51
2	N	936/941 (100%)	876 (94%)	60 (6%)	19	51
3	D	1152/1279 (90%)	1086 (94%)	66 (6%)	23	55
3	O	1152/1279 (90%)	1087 (94%)	65 (6%)	23	56
4	E	83/88 (94%)	82 (99%)	1 (1%)	74	87
4	P	83/88 (94%)	82 (99%)	1 (1%)	74	87
5	F	301/388 (78%)	273 (91%)	28 (9%)	10	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	Q	301/388 (78%)	273 (91%)	28 (9%)	10	36
6	G	155/172 (90%)	150 (97%)	5 (3%)	42	68
6	H	155/172 (90%)	152 (98%)	3 (2%)	60	80
6	R	155/172 (90%)	150 (97%)	5 (3%)	42	68
6	S	155/172 (90%)	151 (97%)	4 (3%)	49	73
All	All	6552/7172 (91%)	6140 (94%)	412 (6%)	20	51

5 of 412 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	295	MET
1	M	80	LEU
5	Q	186	HIS
5	F	398	ARG
1	L	34	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
6	G	108	GLN
1	L	128	HIS
3	O	1172	HIS
4	E	33	HIS
3	O	1195	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
9	K	3/4 (75%)	1 (33%)	0
9	V	3/4 (75%)	1 (33%)	0
All	All	6/8 (75%)	2 (33%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	K	2	C
9	V	2	C

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	284/315 (90%)	-0.13	4 (1%) 75 66	40, 111, 176, 252	0
1	B	280/315 (88%)	-0.16	5 (1%) 68 59	25, 117, 187, 259	0
1	L	284/315 (90%)	-0.21	7 (2%) 57 47	24, 117, 191, 242	0
1	M	280/315 (88%)	-0.29	0 100 100	39, 117, 182, 232	0
2	C	1111/1119 (99%)	-0.18	14 (1%) 77 68	10, 94, 167, 243	0
2	N	1111/1119 (99%)	-0.11	15 (1%) 75 66	3, 99, 174, 254	0
3	D	1363/1524 (89%)	-0.13	36 (2%) 56 45	6, 80, 179, 266	1 (0%)
3	O	1363/1524 (89%)	-0.14	30 (2%) 62 52	6, 79, 187, 278	1 (0%)
4	E	94/99 (94%)	-0.26	0 100 100	8, 68, 147, 194	0
4	P	94/99 (94%)	-0.36	0 100 100	19, 74, 143, 182	0
5	F	346/443 (78%)	-0.20	8 (2%) 60 51	27, 107, 192, 270	0
5	Q	346/443 (78%)	-0.26	8 (2%) 60 51	17, 104, 188, 271	0
6	G	195/215 (90%)	-0.21	4 (2%) 63 54	8, 64, 155, 220	0
6	H	195/215 (90%)	-0.24	0 100 100	14, 86, 160, 231	0
6	R	195/215 (90%)	-0.18	3 (1%) 73 64	7, 63, 151, 234	0
6	S	195/215 (90%)	-0.31	2 (1%) 82 74	17, 82, 163, 268	0
7	I	66/72 (91%)	-0.06	1 (1%) 73 64	60, 135, 247, 283	0
7	T	66/72 (91%)	-0.11	0 100 100	60, 134, 217, 302	0
8	J	66/72 (91%)	-0.06	0 100 100	40, 145, 238, 270	0
8	U	66/72 (91%)	-0.07	0 100 100	52, 137, 230, 280	0
9	K	4/4 (100%)	1.18	0 100 100	71, 79, 107, 113	0
9	V	4/4 (100%)	1.15	0 100 100	62, 74, 97, 217	0
All	All	8008/8786 (91%)	-0.17	137 (1%) 70 61	3, 94, 182, 302	2 (0%)

The worst 5 of 137 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	148	LYS	8.6
5	F	146	GLY	6.1
3	D	380	GLU	6.0
5	Q	148	LYS	5.8
5	F	147	LEU	5.7

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. 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(\AA^2)	Q<0.9
10	ZN	O	2002	1/1	0.93	0.08	65,65,65,65	0
10	ZN	D	2002	1/1	0.97	0.04	49,49,49,49	0
10	ZN	D	2001	1/1	0.98	0.14	52,52,52,52	0
11	MG	D	2003	1/1	0.98	0.39	18,18,18,18	0
10	ZN	O	2001	1/1	0.98	0.14	53,53,53,53	0
11	MG	O	2003	1/1	0.99	0.38	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.