



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 6, 2017 – 11:44 AM EDT

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 : unknown
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

<http://wwpdb.org/validation/2016/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)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029824

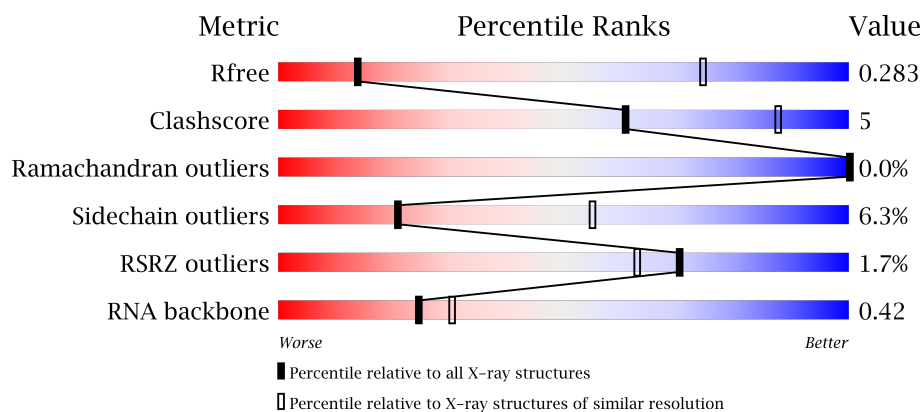
1 Overall quality at a glance

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}	100719	1024 (5.08-3.62)
Clashscore	112137	1021 (5.08-3.70)
Ramachandran outliers	110173	1018 (5.08-3.66)
Sidechain outliers	110143	1000 (5.08-3.66)
RSRZ outliers	101464	1007 (5.08-3.64)
RNA backbone	2435	1036 (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>0.0%</div> <div> <div></div> <div>74%</div> <div>14%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	315	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>13%</div> <div>•</div> <div>11%</div> </div> </div>
1	L	315	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>12%</div> <div>•</div> <div>10%</div> </div> </div>
1	M	315	<div> <div></div> <div> <div></div> <div>73%</div> <div>13%</div> <div>•</div> <div>11%</div> </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 [i](#)

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

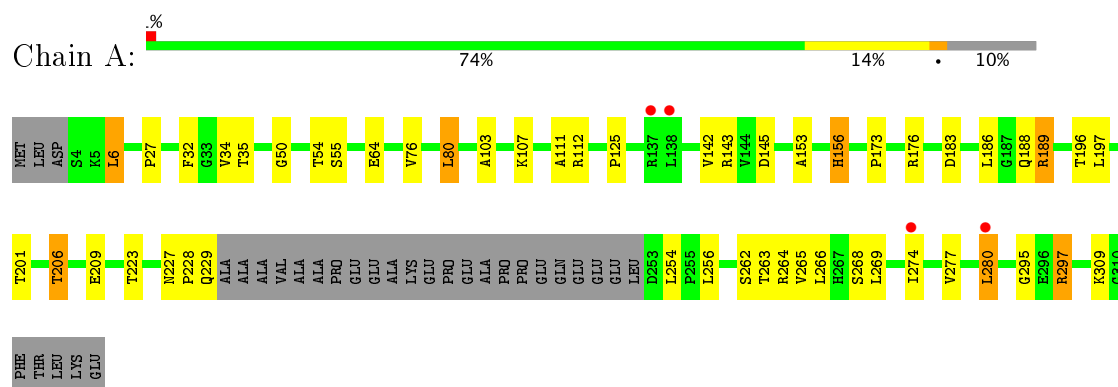
- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

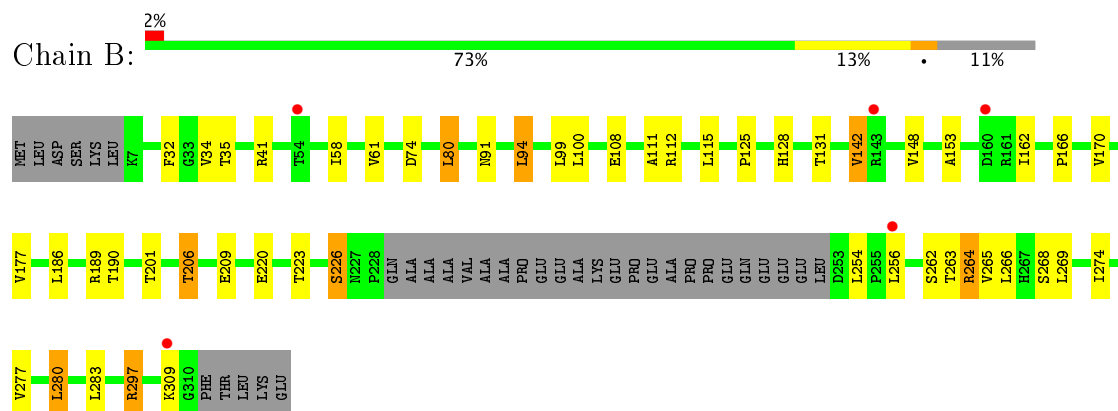
3 Residue-property plots [i](#)

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.

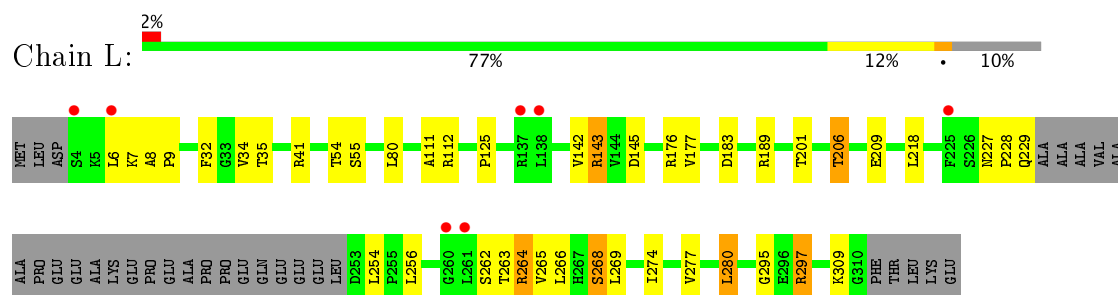
- Molecule 1: DNA-directed RNA polymerase subunit alpha



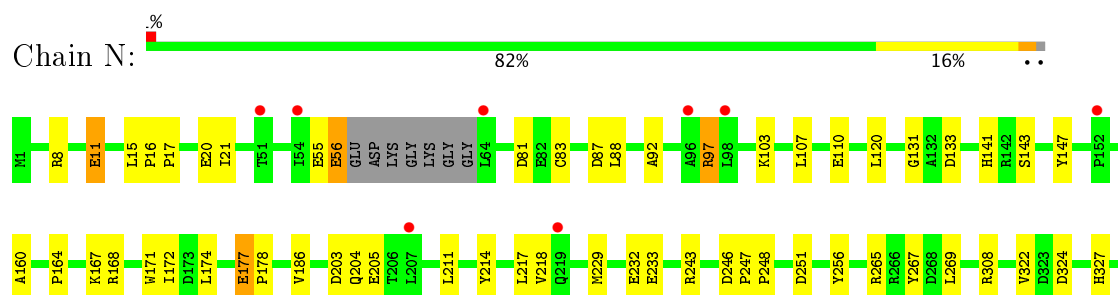
- Molecule 1: DNA-directed RNA polymerase subunit alpha

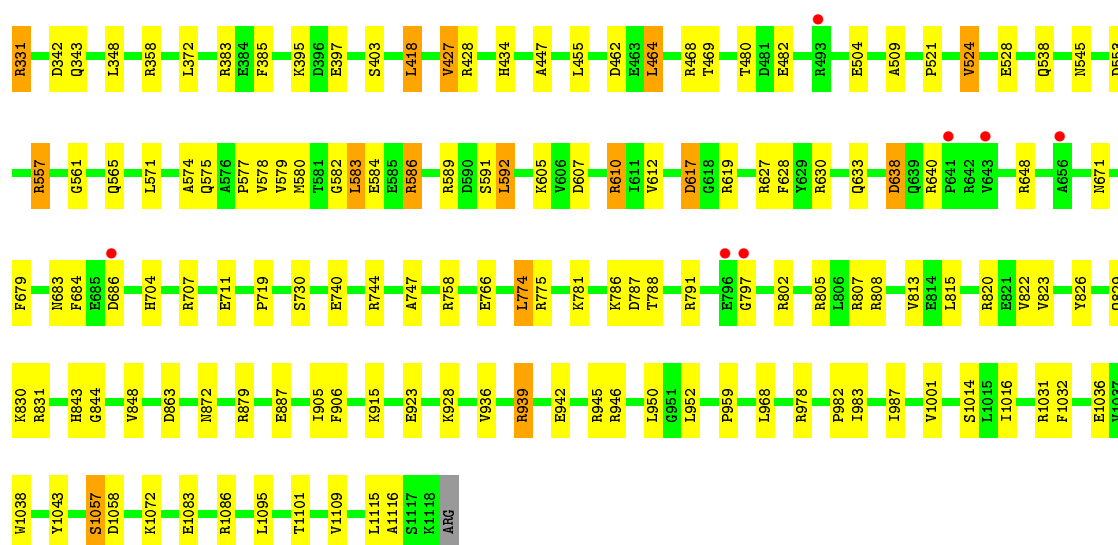


- Molecule 1: DNA-directed RNA polymerase subunit alpha

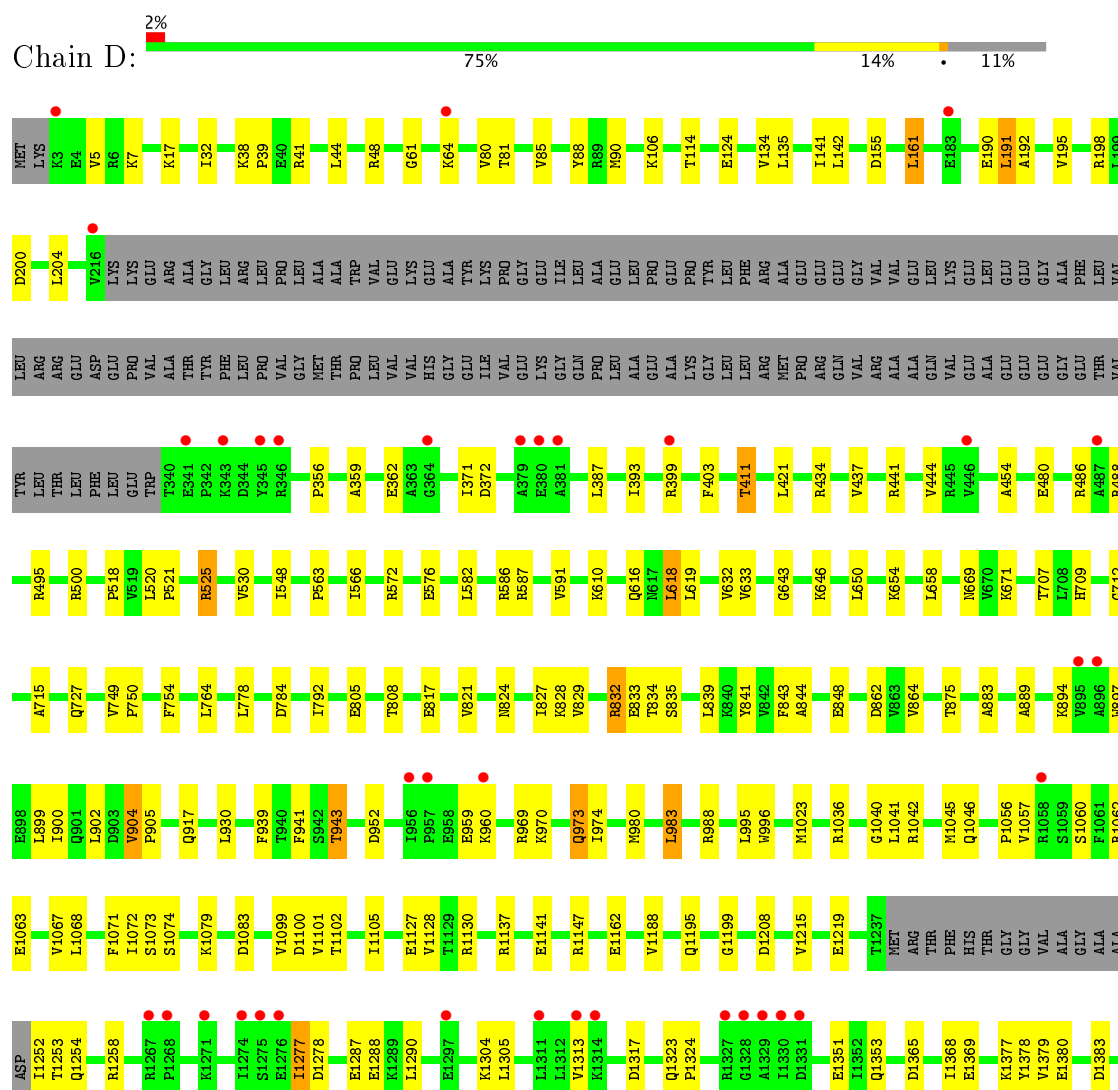


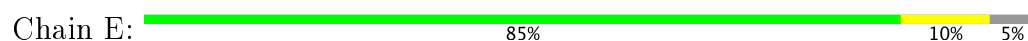
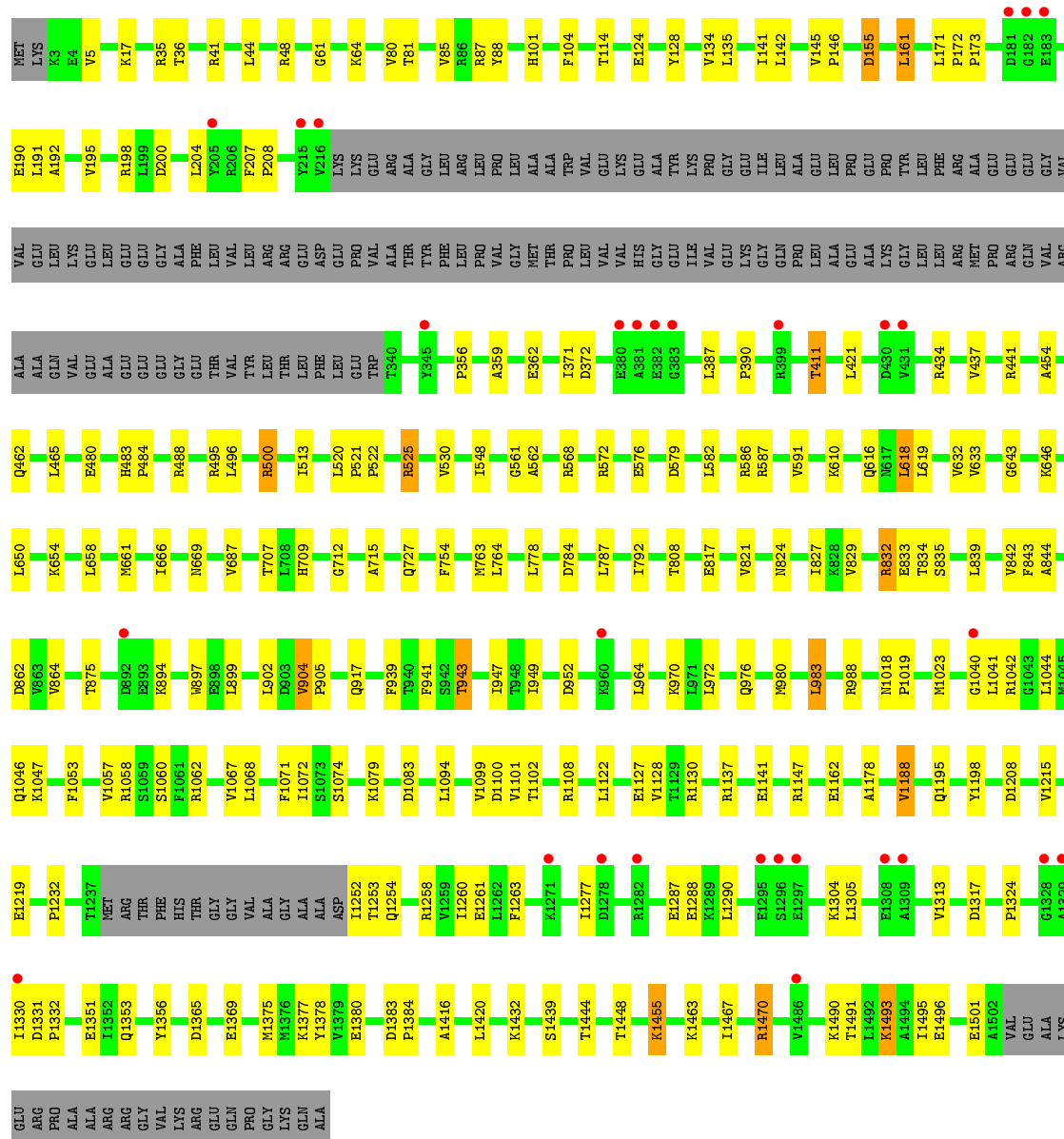
- Molecule 1: DNA-directed RNA polymerase subunit alpha





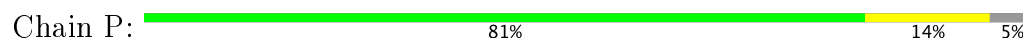
• Molecule 3: DNA-directed RNA polymerase subunit beta'



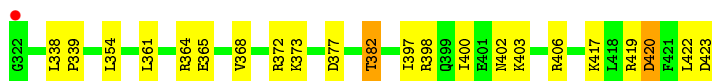
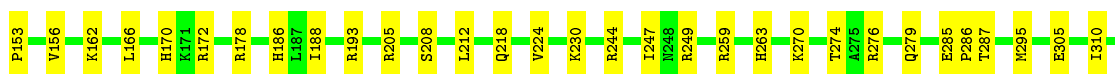
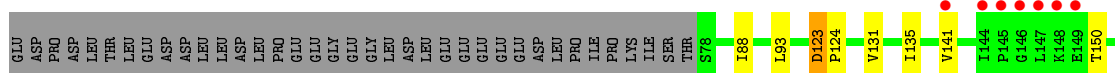




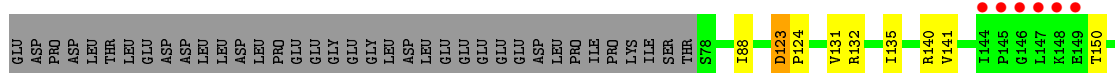
- Molecule 4: DNA-directed RNA polymerase subunit omega



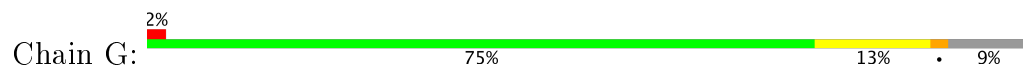
- Molecule 5: RNA polymerase sigma factor SigA



- Molecule 5: RNA polymerase sigma factor SigA



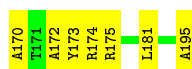
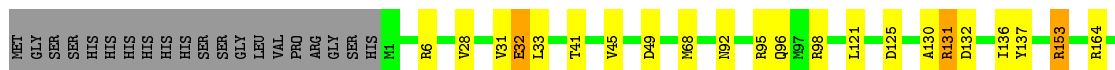
- Molecule 6: Transcriptional regulator, Crp family





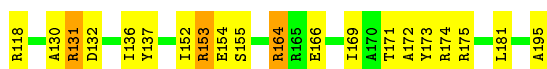
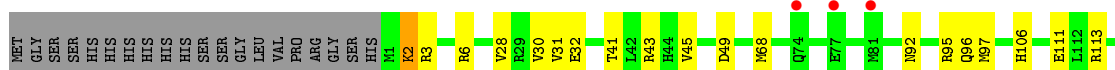
- Molecule 6: Transcriptional regulator, Crp family

Chain H: 77% 12% 9%



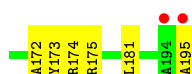
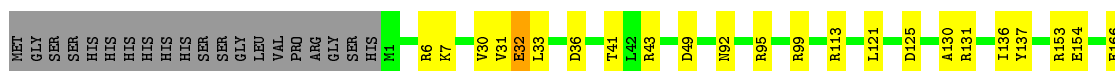
- Molecule 6: Transcriptional regulator, Crp family

Chain R: 73% 16% 9%



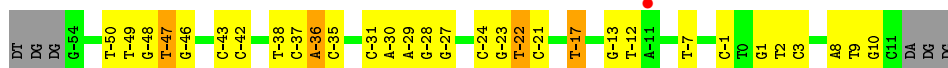
- Molecule 6: Transcriptional regulator, Crp family

Chain S: 77% 13% 9%



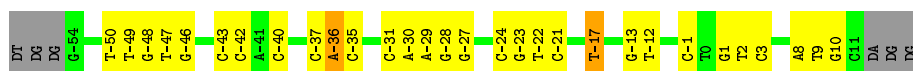
- Molecule 7: DNA (72-MER)

Chain I: 49% 38% 6% 8%



- Molecule 7: DNA (72-MER)

Chain T: 50% 39% 8%



- Molecule 8: DNA (72-MER)

Chain J: 50% 39% 8%



● Molecule 8: DNA (72-MER)



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



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



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 0.239 , 0.283	Depositor DCC
R_{free} test set	1771 reflections (2.51%)	DCC
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.*

¹ Intensities estimated from amplitudes.

² Theoretical 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

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:683:ASN:HB3	2:N:872:ASN:HB2	1.69	0.74
2:N:630:ARG:CZ	2:N:707:ARG:HD3	2.17	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%)	55	89
3	O	1357/1524 (89%)	1339 (99%)	17 (1%)	1 (0%)	55	89
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%)	11	40
1	B	245/273 (90%)	223 (91%)	22 (9%)	11	41
1	L	249/273 (91%)	227 (91%)	22 (9%)	12	42
1	M	245/273 (90%)	225 (92%)	20 (8%)	13	46
2	C	936/941 (100%)	877 (94%)	59 (6%)	21	55
2	N	936/941 (100%)	876 (94%)	60 (6%)	20	54
3	D	1152/1279 (90%)	1086 (94%)	66 (6%)	24	58
3	O	1152/1279 (90%)	1087 (94%)	65 (6%)	25	59
4	E	83/88 (94%)	82 (99%)	1 (1%)	75	88
4	P	83/88 (94%)	82 (99%)	1 (1%)	75	88
5	F	301/388 (78%)	273 (91%)	28 (9%)	10	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	Q	301/388 (78%)	273 (91%)	28 (9%)	10	40
6	G	155/172 (90%)	150 (97%)	5 (3%)	44	72
6	H	155/172 (90%)	152 (98%)	3 (2%)	62	82
6	R	155/172 (90%)	150 (97%)	5 (3%)	44	72
6	S	155/172 (90%)	151 (97%)	4 (3%)	51	76
All	All	6552/7172 (91%)	6140 (94%)	412 (6%)	21	55

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 67	40, 111, 176, 252	0
1	B	280/315 (88%)	-0.17	5 (1%) 69 61	25, 117, 187, 259	0
1	L	284/315 (90%)	-0.22	7 (2%) 58 49	24, 117, 191, 242	0
1	M	280/315 (88%)	-0.30	0 100 100	39, 117, 182, 232	0
2	C	1111/1119 (99%)	-0.18	13 (1%) 79 71	10, 94, 167, 243	0
2	N	1111/1119 (99%)	-0.11	15 (1%) 75 67	3, 99, 174, 254	0
3	D	1363/1524 (89%)	-0.13	37 (2%) 55 46	6, 80, 179, 266	1 (0%)
3	O	1363/1524 (89%)	-0.14	29 (2%) 64 56	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%)	-0.37	0 100 100	19, 74, 143, 182	0
5	F	346/443 (78%)	-0.20	8 (2%) 61 53	27, 107, 192, 270	0
5	Q	346/443 (78%)	-0.26	8 (2%) 61 53	17, 104, 188, 271	0
6	G	195/215 (90%)	-0.21	4 (2%) 64 56	8, 64, 155, 220	0
6	H	195/215 (90%)	-0.25	0 100 100	14, 86, 160, 231	0
6	R	195/215 (90%)	-0.18	3 (1%) 74 66	7, 63, 151, 234	0
6	S	195/215 (90%)	-0.31	2 (1%) 82 75	17, 82, 163, 268	0
7	I	66/72 (91%)	-0.07	1 (1%) 74 66	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%)	-0.07	0 100 100	40, 145, 238, 270	0
8	U	66/72 (91%)	-0.08	0 100 100	52, 137, 230, 280	0
9	K	4/4 (100%)	1.17	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	136 (1%) 70 63	3, 94, 182, 302	2 (0%)

The worst 5 of 136 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	148	LYS	8.7
5	F	146	GLY	6.0
5	Q	148	LYS	6.0
3	D	380	GLU	6.0
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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
10	ZN	D	2001	1/1	0.98	0.14	-0.63	52,52,52,52	0
10	ZN	O	2001	1/1	0.98	0.13	-0.63	53,53,53,53	0
10	ZN	O	2002	1/1	0.93	0.07	-1.16	65,65,65,65	0
10	ZN	D	2002	1/1	0.97	0.04	-1.61	49,49,49,49	0
11	MG	D	2003	1/1	0.98	0.40	-	18,18,18,18	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.