



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 11:18 pm BST

PDB ID : 3HUG  
Title : Crystal structure of Mycobacterium tuberculosis anti-sigma factor RslA in complex with -35 promoter binding domain of sigL  
Authors : Thakur, K.G.; Gopal, B.  
Deposited on : 2009-06-14  
Resolution : 2.35 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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
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

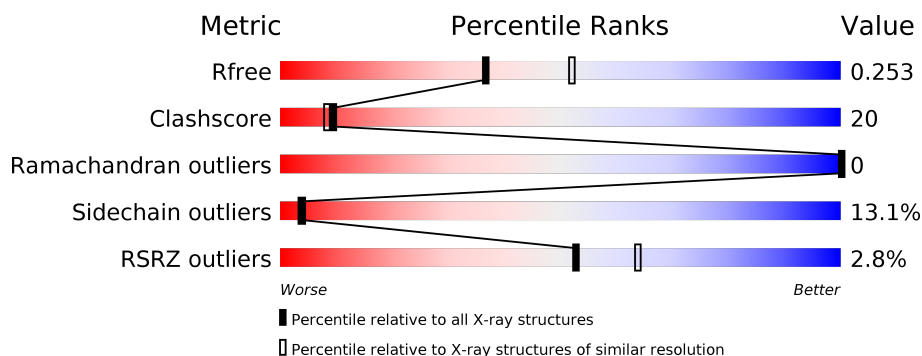
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	92	
1	C	92	
1	E	92	
1	G	92	
1	I	92	
1	K	92	

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Mol	Chain	Length	Quality of chain
1	M	92	
1	O	92	
1	Q	92	
1	S	92	
2	B	108	
2	D	108	
2	F	108	
2	H	108	
2	J	108	
2	L	108	
2	N	108	
2	P	108	
2	R	108	
2	T	108	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	G	6	-	-	X	-
3	SO4	L	109	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10776 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 RNA polymerase sigma factor.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	80	Total	C	N	O	4	1	0
			630	391	119	120			
1	C	77	Total	C	N	O	0	0	0
			598	372	113	113			
1	E	73	Total	C	N	O	0	0	0
			565	353	108	104			
1	G	74	Total	C	N	O	9	0	0
			576	360	109	107			
1	I	77	Total	C	N	O	3	1	0
			606	377	116	113			
1	K	71	Total	C	N	O	0	0	0
			549	343	106	100			
1	M	74	Total	C	N	O	4	0	0
			576	360	109	107			
1	O	73	Total	C	N	O	2	0	0
			569	355	108	106			
1	Q	77	Total	C	N	O	0	0	0
			598	372	113	113			
1	S	73	Total	C	N	O	4	1	0
			577	360	111	106			

There are 130 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	86	MET	-	EXPRESSION TAG	UNP Q7D9D4
A	87	GLY	-	EXPRESSION TAG	UNP Q7D9D4
A	88	SER	-	EXPRESSION TAG	UNP Q7D9D4
A	89	SER	-	EXPRESSION TAG	UNP Q7D9D4
A	90	HIS	-	EXPRESSION TAG	UNP Q7D9D4
A	91	HIS	-	EXPRESSION TAG	UNP Q7D9D4
A	92	HIS	-	EXPRESSION TAG	UNP Q7D9D4
A	93	HIS	-	EXPRESSION TAG	UNP Q7D9D4
A	94	HIS	-	EXPRESSION TAG	UNP Q7D9D4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	95	HIS	-	EXPRESSION TAG	UNP Q7D9D4
A	96	SER	-	EXPRESSION TAG	UNP Q7D9D4
A	97	GLN	-	EXPRESSION TAG	UNP Q7D9D4
A	98	ASP	-	EXPRESSION TAG	UNP Q7D9D4
C	86	MET	-	EXPRESSION TAG	UNP Q7D9D4
C	87	GLY	-	EXPRESSION TAG	UNP Q7D9D4
C	88	SER	-	EXPRESSION TAG	UNP Q7D9D4
C	89	SER	-	EXPRESSION TAG	UNP Q7D9D4
C	90	HIS	-	EXPRESSION TAG	UNP Q7D9D4
C	91	HIS	-	EXPRESSION TAG	UNP Q7D9D4
C	92	HIS	-	EXPRESSION TAG	UNP Q7D9D4
C	93	HIS	-	EXPRESSION TAG	UNP Q7D9D4
C	94	HIS	-	EXPRESSION TAG	UNP Q7D9D4
C	95	HIS	-	EXPRESSION TAG	UNP Q7D9D4
C	96	SER	-	EXPRESSION TAG	UNP Q7D9D4
C	97	GLN	-	EXPRESSION TAG	UNP Q7D9D4
C	98	ASP	-	EXPRESSION TAG	UNP Q7D9D4
E	86	MET	-	EXPRESSION TAG	UNP Q7D9D4
E	87	GLY	-	EXPRESSION TAG	UNP Q7D9D4
E	88	SER	-	EXPRESSION TAG	UNP Q7D9D4
E	89	SER	-	EXPRESSION TAG	UNP Q7D9D4
E	90	HIS	-	EXPRESSION TAG	UNP Q7D9D4
E	91	HIS	-	EXPRESSION TAG	UNP Q7D9D4
E	92	HIS	-	EXPRESSION TAG	UNP Q7D9D4
E	93	HIS	-	EXPRESSION TAG	UNP Q7D9D4
E	94	HIS	-	EXPRESSION TAG	UNP Q7D9D4
E	95	HIS	-	EXPRESSION TAG	UNP Q7D9D4
E	96	SER	-	EXPRESSION TAG	UNP Q7D9D4
E	97	GLN	-	EXPRESSION TAG	UNP Q7D9D4
E	98	ASP	-	EXPRESSION TAG	UNP Q7D9D4
G	86	MET	-	EXPRESSION TAG	UNP Q7D9D4
G	87	GLY	-	EXPRESSION TAG	UNP Q7D9D4
G	88	SER	-	EXPRESSION TAG	UNP Q7D9D4
G	89	SER	-	EXPRESSION TAG	UNP Q7D9D4
G	90	HIS	-	EXPRESSION TAG	UNP Q7D9D4
G	91	HIS	-	EXPRESSION TAG	UNP Q7D9D4
G	92	HIS	-	EXPRESSION TAG	UNP Q7D9D4
G	93	HIS	-	EXPRESSION TAG	UNP Q7D9D4
G	94	HIS	-	EXPRESSION TAG	UNP Q7D9D4
G	95	HIS	-	EXPRESSION TAG	UNP Q7D9D4
G	96	SER	-	EXPRESSION TAG	UNP Q7D9D4
G	97	GLN	-	EXPRESSION TAG	UNP Q7D9D4

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Chain	Residue	Modelled	Actual	Comment	Reference
G	98	ASP	-	EXPRESSION TAG	UNP Q7D9D4
I	86	MET	-	EXPRESSION TAG	UNP Q7D9D4
I	87	GLY	-	EXPRESSION TAG	UNP Q7D9D4
I	88	SER	-	EXPRESSION TAG	UNP Q7D9D4
I	89	SER	-	EXPRESSION TAG	UNP Q7D9D4
I	90	HIS	-	EXPRESSION TAG	UNP Q7D9D4
I	91	HIS	-	EXPRESSION TAG	UNP Q7D9D4
I	92	HIS	-	EXPRESSION TAG	UNP Q7D9D4
I	93	HIS	-	EXPRESSION TAG	UNP Q7D9D4
I	94	HIS	-	EXPRESSION TAG	UNP Q7D9D4
I	95	HIS	-	EXPRESSION TAG	UNP Q7D9D4
I	96	SER	-	EXPRESSION TAG	UNP Q7D9D4
I	97	GLN	-	EXPRESSION TAG	UNP Q7D9D4
I	98	ASP	-	EXPRESSION TAG	UNP Q7D9D4
K	86	MET	-	EXPRESSION TAG	UNP Q7D9D4
K	87	GLY	-	EXPRESSION TAG	UNP Q7D9D4
K	88	SER	-	EXPRESSION TAG	UNP Q7D9D4
K	89	SER	-	EXPRESSION TAG	UNP Q7D9D4
K	90	HIS	-	EXPRESSION TAG	UNP Q7D9D4
K	91	HIS	-	EXPRESSION TAG	UNP Q7D9D4
K	92	HIS	-	EXPRESSION TAG	UNP Q7D9D4
K	93	HIS	-	EXPRESSION TAG	UNP Q7D9D4
K	94	HIS	-	EXPRESSION TAG	UNP Q7D9D4
K	95	HIS	-	EXPRESSION TAG	UNP Q7D9D4
K	96	SER	-	EXPRESSION TAG	UNP Q7D9D4
K	97	GLN	-	EXPRESSION TAG	UNP Q7D9D4
K	98	ASP	-	EXPRESSION TAG	UNP Q7D9D4
M	86	MET	-	EXPRESSION TAG	UNP Q7D9D4
M	87	GLY	-	EXPRESSION TAG	UNP Q7D9D4
M	88	SER	-	EXPRESSION TAG	UNP Q7D9D4
M	89	SER	-	EXPRESSION TAG	UNP Q7D9D4
M	90	HIS	-	EXPRESSION TAG	UNP Q7D9D4
M	91	HIS	-	EXPRESSION TAG	UNP Q7D9D4
M	92	HIS	-	EXPRESSION TAG	UNP Q7D9D4
M	93	HIS	-	EXPRESSION TAG	UNP Q7D9D4
M	94	HIS	-	EXPRESSION TAG	UNP Q7D9D4
M	95	HIS	-	EXPRESSION TAG	UNP Q7D9D4
M	96	SER	-	EXPRESSION TAG	UNP Q7D9D4
M	97	GLN	-	EXPRESSION TAG	UNP Q7D9D4
M	98	ASP	-	EXPRESSION TAG	UNP Q7D9D4
O	86	MET	-	EXPRESSION TAG	UNP Q7D9D4
O	87	GLY	-	EXPRESSION TAG	UNP Q7D9D4

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Chain	Residue	Modelled	Actual	Comment	Reference
O	88	SER	-	EXPRESSION TAG	UNP Q7D9D4
O	89	SER	-	EXPRESSION TAG	UNP Q7D9D4
O	90	HIS	-	EXPRESSION TAG	UNP Q7D9D4
O	91	HIS	-	EXPRESSION TAG	UNP Q7D9D4
O	92	HIS	-	EXPRESSION TAG	UNP Q7D9D4
O	93	HIS	-	EXPRESSION TAG	UNP Q7D9D4
O	94	HIS	-	EXPRESSION TAG	UNP Q7D9D4
O	95	HIS	-	EXPRESSION TAG	UNP Q7D9D4
O	96	SER	-	EXPRESSION TAG	UNP Q7D9D4
O	97	GLN	-	EXPRESSION TAG	UNP Q7D9D4
O	98	ASP	-	EXPRESSION TAG	UNP Q7D9D4
Q	86	MET	-	EXPRESSION TAG	UNP Q7D9D4
Q	87	GLY	-	EXPRESSION TAG	UNP Q7D9D4
Q	88	SER	-	EXPRESSION TAG	UNP Q7D9D4
Q	89	SER	-	EXPRESSION TAG	UNP Q7D9D4
Q	90	HIS	-	EXPRESSION TAG	UNP Q7D9D4
Q	91	HIS	-	EXPRESSION TAG	UNP Q7D9D4
Q	92	HIS	-	EXPRESSION TAG	UNP Q7D9D4
Q	93	HIS	-	EXPRESSION TAG	UNP Q7D9D4
Q	94	HIS	-	EXPRESSION TAG	UNP Q7D9D4
Q	95	HIS	-	EXPRESSION TAG	UNP Q7D9D4
Q	96	SER	-	EXPRESSION TAG	UNP Q7D9D4
Q	97	GLN	-	EXPRESSION TAG	UNP Q7D9D4
Q	98	ASP	-	EXPRESSION TAG	UNP Q7D9D4
S	86	MET	-	EXPRESSION TAG	UNP Q7D9D4
S	87	GLY	-	EXPRESSION TAG	UNP Q7D9D4
S	88	SER	-	EXPRESSION TAG	UNP Q7D9D4
S	89	SER	-	EXPRESSION TAG	UNP Q7D9D4
S	90	HIS	-	EXPRESSION TAG	UNP Q7D9D4
S	91	HIS	-	EXPRESSION TAG	UNP Q7D9D4
S	92	HIS	-	EXPRESSION TAG	UNP Q7D9D4
S	93	HIS	-	EXPRESSION TAG	UNP Q7D9D4
S	94	HIS	-	EXPRESSION TAG	UNP Q7D9D4
S	95	HIS	-	EXPRESSION TAG	UNP Q7D9D4
S	96	SER	-	EXPRESSION TAG	UNP Q7D9D4
S	97	GLN	-	EXPRESSION TAG	UNP Q7D9D4
S	98	ASP	-	EXPRESSION TAG	UNP Q7D9D4

- Molecule 2 is a protein called PROBABLE CONSERVED MEMBRANE PROTEIN.

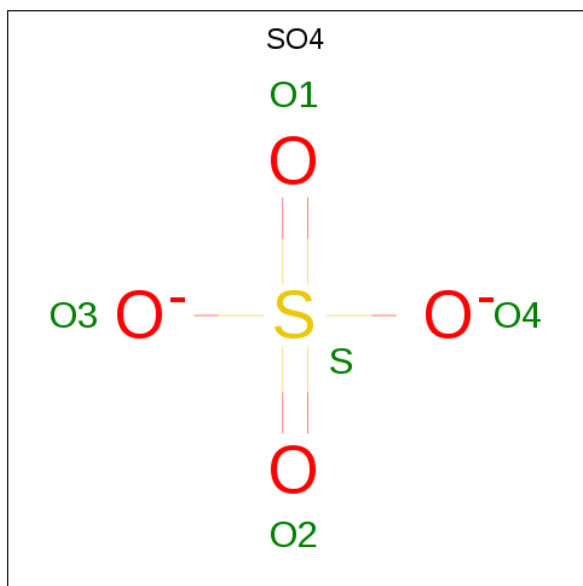
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	62	Total	C	N	O	S	0	0	0
			462	286	82	90	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	62	Total	C	N	O	S	10	0	0
			465	287	82	92	4			
2	F	56	Total	C	N	O	S	10	0	0
			426	264	76	82	4			
2	H	61	Total	C	N	O	S	8	0	0
			459	284	81	90	4			
2	J	64	Total	C	N	O	S	7	0	0
			477	295	84	94	4			
2	L	63	Total	C	N	O	S	11	0	0
			470	290	83	93	4			
2	N	61	Total	C	N	O	S	12	0	0
			459	284	81	90	4			
2	P	60	Total	C	N	O	S	7	0	0
			450	279	80	87	4			
2	R	63	Total	C	N	O	S	4	0	0
			470	290	83	93	4			
2	T	62	Total	C	N	O	S	10	0	0
			465	287	82	92	4			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		
3	M	1	Total	O	S	0	0
			5	4	1		
3	P	1	Total	O	S	0	0
			5	4	1		
3	Q	1	Total	O	S	0	0
			5	4	1		
3	S	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	1	Total	Zn	0	0
			1	1		
4	J	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		
4	H	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		
4	T	1	Total	Zn	0	0
			1	1		
4	N	1	Total	Zn	0	0
			1	1		
4	R	1	Total	Zn	0	0
			1	1		
4	L	1	Total	Zn	0	0
			1	1		
4	F	1	Total	Zn	0	0
			1	1		

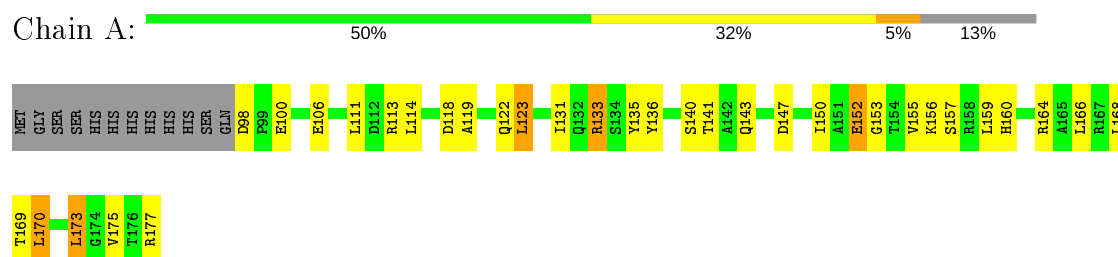
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	22	Total O 22 22	0	0
5	B	3	Total O 3 3	0	0
5	C	20	Total O 20 20	0	0
5	D	9	Total O 9 9	0	0
5	E	17	Total O 17 17	0	0
5	F	8	Total O 8 8	0	0
5	G	17	Total O 17 17	0	0
5	H	4	Total O 4 4	0	0
5	I	19	Total O 19 19	0	0
5	J	9	Total O 9 9	0	0
5	K	15	Total O 15 15	0	0
5	L	7	Total O 7 7	0	0
5	M	15	Total O 15 15	0	0
5	N	5	Total O 5 5	0	0
5	O	13	Total O 13 13	0	0
5	P	9	Total O 9 9	0	0
5	Q	30	Total O 30 30	0	0
5	R	9	Total O 9 9	0	0
5	S	25	Total O 25 25	0	0
5	T	13	Total O 13 13	0	0

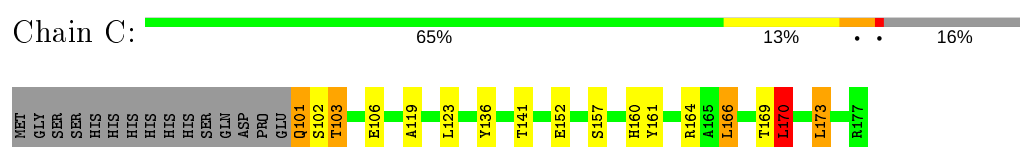
### 3 Residue-property plots

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.

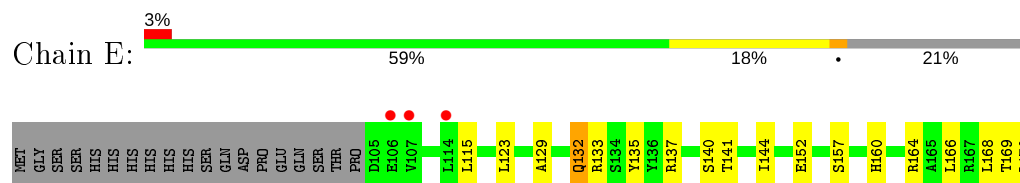
- Molecule 1: RNA polymerase sigma factor



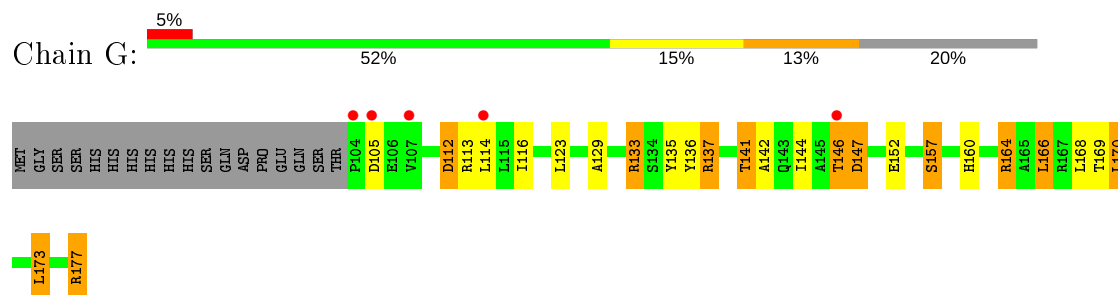
- Molecule 1: RNA polymerase sigma factor



- Molecule 1: RNA polymerase sigma factor

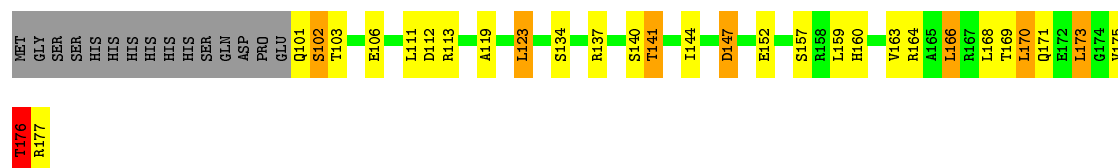


- Molecule 1: RNA polymerase sigma factor

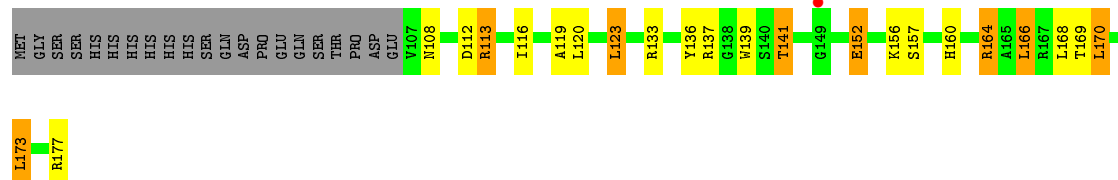


- Molecule 1: RNA polymerase sigma factor





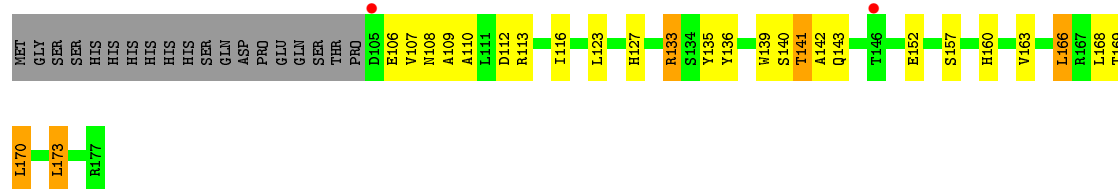
- Molecule 1: RNA polymerase sigma factor



- Molecule 1: RNA polymerase sigma factor



- Molecule 1: RNA polymerase sigma factor



- Molecule 1: RNA polymerase sigma factor

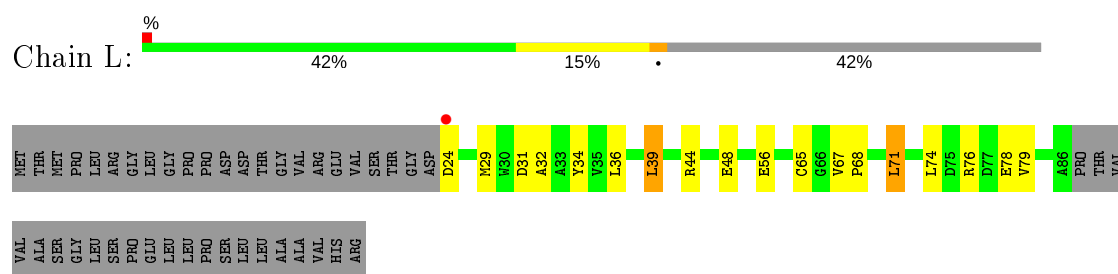


- Molecule 1: RNA polymerase sigma factor

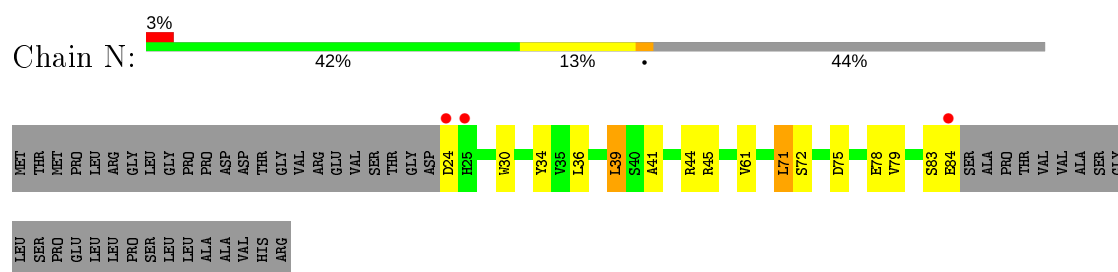


- Molecule 2: PROBABLE CONSERVED MEMBRANE PROTEIN

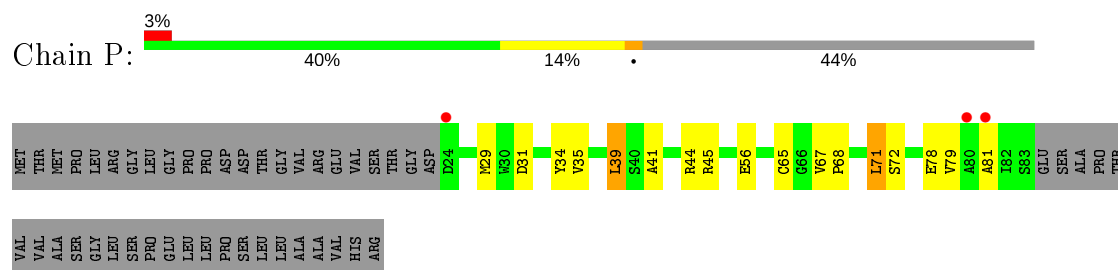




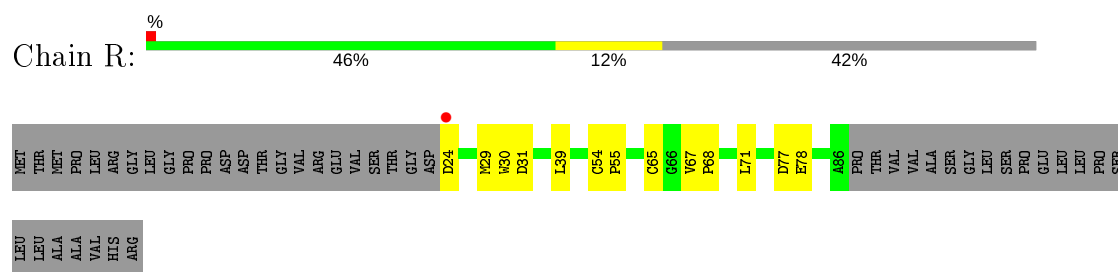
• Molecule 2: PROBABLE CONSERVED MEMBRANE PROTEIN



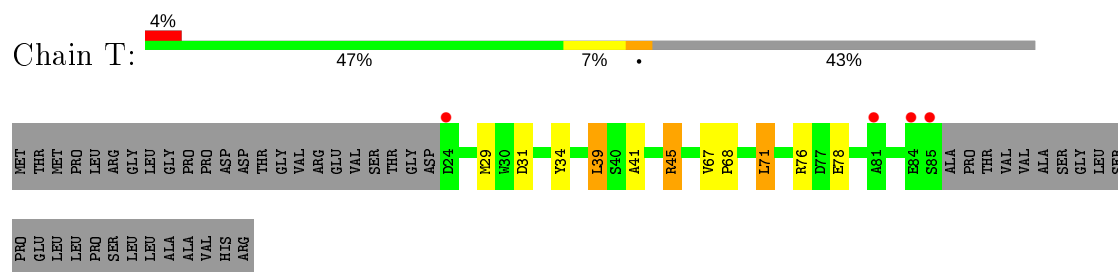
• Molecule 2: PROBABLE CONSERVED MEMBRANE PROTEIN



• Molecule 2: PROBABLE CONSERVED MEMBRANE PROTEIN



• Molecule 2: PROBABLE CONSERVED MEMBRANE PROTEIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.07Å 166.77Å 178.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.88 – 2.35 41.88 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.5 (41.88-2.35) 99.5 (41.88-2.35)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.54 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.211 , 0.260 0.211 , 0.253	Depositor DCC
$R_{free}$ test set	5171 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.2	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 32.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10776	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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, SO4

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	0.60	0/641	0.72	0/870
1	C	0.53	0/605	0.73	1/821 (0.1%)
1	E	0.63	0/571	0.75	0/774
1	G	0.58	1/583 (0.2%)	0.75	1/790 (0.1%)
1	I	0.57	0/616	0.73	1/835 (0.1%)
1	K	0.57	0/555	0.76	0/752
1	M	0.59	0/583	0.72	0/790
1	O	0.50	0/575	0.68	0/779
1	Q	0.54	0/605	0.78	1/821 (0.1%)
1	S	0.66	0/586	0.72	0/793
2	B	0.59	0/471	0.68	0/640
2	D	0.61	0/474	0.81	1/644 (0.2%)
2	F	0.68	1/435 (0.2%)	0.72	0/591
2	H	0.48	0/468	0.73	1/636 (0.2%)
2	J	0.60	0/487	0.67	0/663
2	L	0.59	0/479	0.69	0/651
2	N	0.60	0/468	0.66	0/636
2	P	0.47	0/459	0.63	0/624
2	R	0.58	0/479	0.67	0/651
2	T	0.54	0/474	0.65	0/644
All	All	0.58	2/10614 (0.0%)	0.72	6/14405 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	105	ASP	CA-CB	-5.41	1.42	1.53
2	F	77	ASP	CB-CG	-5.04	1.41	1.51

The worst 5 of 6 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	147	ASP	CB-CA-C	-5.94	98.53	110.40
1	C	170	LEU	CA-CB-CG	5.78	128.58	115.30
2	H	84	GLU	N-CA-CB	5.50	120.50	110.60
2	D	58	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	I	176	THR	CB-CA-C	-5.07	97.90	111.60

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	630	0	639	26	0
1	C	598	0	609	34	0
1	E	565	0	578	19	0
1	G	576	0	590	38	0
1	I	606	0	622	44	0
1	K	549	0	563	42	0
1	M	576	0	590	24	0
1	O	569	0	582	34	0
1	Q	598	0	609	30	0
1	S	577	0	595	29	0
2	B	462	0	433	22	0
2	D	465	0	432	21	0
2	F	426	0	395	17	0
2	H	459	0	427	25	0
2	J	477	0	444	20	0
2	L	470	0	437	37	0
2	N	459	0	427	19	0
2	P	450	0	421	24	0
2	R	470	0	437	19	0
2	T	465	0	432	24	0
3	A	5	0	0	0	0
3	C	5	0	0	0	0
3	G	5	0	0	3	0
3	I	10	0	0	1	0
3	L	5	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	M	5	0	0	0	0
3	P	5	0	0	0	0
3	Q	5	0	0	0	0
3	S	5	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
4	J	1	0	0	0	0
4	L	1	0	0	0	0
4	N	1	0	0	0	0
4	P	1	0	0	0	0
4	R	1	0	0	0	0
4	T	1	0	0	0	0
5	A	22	0	0	4	0
5	B	3	0	0	0	0
5	C	20	0	0	0	0
5	D	9	0	0	0	0
5	E	17	0	0	2	0
5	F	8	0	0	2	0
5	G	17	0	0	0	0
5	H	4	0	0	0	0
5	I	19	0	0	2	0
5	J	9	0	0	1	0
5	K	15	0	0	1	0
5	L	7	0	0	0	0
5	M	15	0	0	1	0
5	N	5	0	0	0	0
5	O	13	0	0	1	0
5	P	9	0	0	0	0
5	Q	30	0	0	2	0
5	R	9	0	0	1	0
5	S	25	0	0	3	0
5	T	13	0	0	1	0
All	All	10776	0	10262	405	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 20.

The worst 5 of 405 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:152:GLU:OE1	1:A:156:LYS:HE3	1.39	1.20
1:E:164:ARG:HD3	5:E:181:HOH:O	1.45	1.16
1:S:177:ARG:CG	1:S:177:ARG:HH11	1.63	1.12
1:S:157:SER:CB	2:T:29:MET:HE2	1.79	1.12
1:S:157:SER:HB2	2:T:29:MET:CE	1.83	1.08

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	79/92 (86%)	79 (100%)	0	0	100	100
1	C	75/92 (82%)	74 (99%)	1 (1%)	0	100	100
1	E	71/92 (77%)	71 (100%)	0	0	100	100
1	G	72/92 (78%)	69 (96%)	3 (4%)	0	100	100
1	I	76/92 (83%)	76 (100%)	0	0	100	100
1	K	69/92 (75%)	69 (100%)	0	0	100	100
1	M	72/92 (78%)	71 (99%)	1 (1%)	0	100	100
1	O	71/92 (77%)	70 (99%)	1 (1%)	0	100	100
1	Q	75/92 (82%)	75 (100%)	0	0	100	100
1	S	72/92 (78%)	72 (100%)	0	0	100	100
2	B	60/108 (56%)	58 (97%)	2 (3%)	0	100	100
2	D	60/108 (56%)	60 (100%)	0	0	100	100
2	F	54/108 (50%)	53 (98%)	1 (2%)	0	100	100
2	H	59/108 (55%)	58 (98%)	1 (2%)	0	100	100
2	J	62/108 (57%)	61 (98%)	1 (2%)	0	100	100
2	L	61/108 (56%)	61 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	59/108 (55%)	56 (95%)	3 (5%)	0	100	100
2	P	58/108 (54%)	57 (98%)	1 (2%)	0	100	100
2	R	61/108 (56%)	61 (100%)	0	0	100	100
2	T	60/108 (56%)	59 (98%)	1 (2%)	0	100	100
All	All	1326/2000 (66%)	1310 (99%)	16 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	65/75 (87%)	53 (82%)	12 (18%)	1	1
1	C	61/75 (81%)	55 (90%)	6 (10%)	8	7
1	E	56/75 (75%)	47 (84%)	9 (16%)	2	1
1	G	58/75 (77%)	44 (76%)	14 (24%)	0	0
1	I	62/75 (83%)	51 (82%)	11 (18%)	2	1
1	K	54/75 (72%)	43 (80%)	11 (20%)	1	1
1	M	58/75 (77%)	52 (90%)	6 (10%)	7	6
1	O	57/75 (76%)	50 (88%)	7 (12%)	4	4
1	Q	61/75 (81%)	53 (87%)	8 (13%)	4	4
1	S	58/75 (77%)	48 (83%)	10 (17%)	2	1
2	B	45/83 (54%)	40 (89%)	5 (11%)	6	5
2	D	46/83 (55%)	40 (87%)	6 (13%)	4	4
2	F	42/83 (51%)	37 (88%)	5 (12%)	5	4
2	H	45/83 (54%)	40 (89%)	5 (11%)	6	5
2	J	47/83 (57%)	44 (94%)	3 (6%)	17	18
2	L	46/83 (55%)	42 (91%)	4 (9%)	10	9
2	N	45/83 (54%)	40 (89%)	5 (11%)	6	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	44/83 (53%)	41 (93%)	3 (7%)	16	16
2	R	46/83 (55%)	43 (94%)	3 (6%)	17	18
2	T	46/83 (55%)	43 (94%)	3 (6%)	17	18
All	All	1042/1580 (66%)	906 (87%)	136 (13%)	4	4

5 of 136 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	71	LEU
1	K	108	ASN
1	S	114	LEU
1	I	111	LEU
1	I	170	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	160	HIS
2	H	26	HIS
1	Q	171	GLN
1	G	171	GLN
2	H	25	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 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 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 for Mogul analysis.

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	$\# Z  > 2$
3	SO4	M	4	-	4,4,4	0.18	0	6,6,6	0.39	0
3	SO4	S	7	-	4,4,4	0.14	0	6,6,6	0.14	0
3	SO4	C	5	-	4,4,4	0.18	0	6,6,6	0.38	0
3	SO4	I	9	-	4,4,4	0.17	0	6,6,6	0.15	0
3	SO4	A	3	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	I	10	-	4,4,4	0.23	0	6,6,6	0.11	0
3	SO4	Q	1	-	4,4,4	0.09	0	6,6,6	0.32	0
3	SO4	P	109	-	4,4,4	0.10	0	6,6,6	0.31	0
3	SO4	G	6	-	4,4,4	0.13	0	6,6,6	0.12	0
3	SO4	L	109	-	4,4,4	0.20	0	6,6,6	0.53	0

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.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	9	SO4	1	0
3	G	6	SO4	3	0
3	L	109	SO4	2	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 (i)

### 6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	80/92 (86%)	-0.16	0 <span style="border: 1px solid blue;">100</span> <span style="border: 1px solid blue;">100</span>	32, 41, 57, 62	1 (1%)
1	C	77/92 (83%)	-0.09	0 <span style="border: 1px solid blue;">100</span> <span style="border: 1px solid blue;">100</span>	32, 40, 63, 74	0
1	E	73/92 (79%)	0.10	3 (4%) <span style="border: 1px solid red;">37</span> <span style="border: 1px solid gray;">49</span>	37, 46, 58, 77	0
1	G	74/92 (80%)	0.18	5 (6%) <span style="border: 1px solid red;">17</span> <span style="border: 1px solid red;">25</span>	37, 48, 63, 67	2 (2%)
1	I	77/92 (83%)	-0.04	0 <span style="border: 1px solid blue;">100</span> <span style="border: 1px solid blue;">100</span>	35, 42, 59, 71	1 (1%)
1	K	71/92 (77%)	-0.04	1 (1%) <span style="border: 1px solid blue;">75</span> <span style="border: 1px solid blue;">83</span>	33, 41, 54, 57	0
1	M	74/92 (80%)	-0.12	1 (1%) <span style="border: 1px solid blue;">75</span> <span style="border: 1px solid blue;">83</span>	33, 46, 70, 80	2 (2%)
1	O	73/92 (79%)	0.18	2 (2%) <span style="border: 1px solid gray;">54</span> <span style="border: 1px solid gray;">64</span>	35, 50, 71, 82	4 (5%)
1	Q	77/92 (83%)	0.01	0 <span style="border: 1px solid blue;">100</span> <span style="border: 1px solid blue;">100</span>	34, 41, 57, 66	0
1	S	73/92 (79%)	-0.25	1 (1%) <span style="border: 1px solid blue;">75</span> <span style="border: 1px solid blue;">83</span>	30, 37, 45, 54	2 (2%)
2	B	62/108 (57%)	0.32	7 (11%) <span style="border: 1px solid red;">5</span> <span style="border: 1px solid red;">8</span>	36, 50, 60, 68	0
2	D	62/108 (57%)	-0.06	1 (1%) <span style="border: 1px solid blue;">72</span> <span style="border: 1px solid blue;">80</span>	32, 47, 56, 71	3 (4%)
2	F	56/108 (51%)	0.19	2 (3%) <span style="border: 1px solid red;">42</span> <span style="border: 1px solid gray;">55</span>	40, 49, 63, 73	6 (10%)
2	H	61/108 (56%)	0.14	2 (3%) <span style="border: 1px solid red;">46</span> <span style="border: 1px solid gray;">59</span>	37, 51, 76, 79	2 (3%)
2	J	64/108 (59%)	0.06	1 (1%) <span style="border: 1px solid blue;">72</span> <span style="border: 1px solid blue;">80</span>	34, 44, 64, 69	2 (3%)
2	L	63/108 (58%)	0.00	1 (1%) <span style="border: 1px solid blue;">72</span> <span style="border: 1px solid blue;">80</span>	35, 44, 59, 70	3 (4%)
2	N	61/108 (56%)	0.25	3 (4%) <span style="border: 1px solid red;">29</span> <span style="border: 1px solid red;">42</span>	37, 48, 70, 73	3 (4%)
2	P	60/108 (55%)	0.20	3 (5%) <span style="border: 1px solid red;">28</span> <span style="border: 1px solid red;">41</span>	37, 49, 79, 81	2 (3%)
2	R	63/108 (58%)	-0.11	1 (1%) <span style="border: 1px solid blue;">72</span> <span style="border: 1px solid blue;">80</span>	33, 43, 53, 69	1 (1%)
2	T	62/108 (57%)	0.13	4 (6%) <span style="border: 1px solid red;">18</span> <span style="border: 1px solid red;">27</span>	32, 43, 66, 77	3 (4%)
All	All	1363/2000 (68%)	0.04	38 (2%) <span style="border: 1px solid gray;">53</span> <span style="border: 1px solid gray;">64</span>	30, 45, 66, 82	37 (2%)

The worst 5 of 38 RSRZ outliers are listed below:



Mol	Chain	Res	Type	RSRZ
2	F	24	ASP	4.7
1	E	107	VAL	4.6
1	G	107	VAL	4.2
2	N	24	ASP	3.6
2	B	86	ALA	3.5

## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	I	10	5/5	0.87	0.32	93,93,93,93	0
3	SO4	P	109	5/5	0.88	0.16	106,106,106,107	0
3	SO4	S	7	5/5	0.89	0.17	81,81,81,82	5
3	SO4	G	6	5/5	0.93	0.18	99,99,99,99	0
3	SO4	C	5	5/5	0.94	0.17	49,49,50,51	5
3	SO4	A	3	5/5	0.95	0.21	79,79,80,80	0
3	SO4	M	4	5/5	0.95	0.10	65,65,66,66	5
3	SO4	I	9	5/5	0.96	0.12	60,60,62,62	5
3	SO4	Q	1	5/5	0.98	0.12	53,54,55,55	0
3	SO4	L	109	5/5	0.98	0.13	61,62,62,62	0
4	ZN	F	109	1/1	0.99	0.01	47,47,47,47	0
4	ZN	D	109	1/1	0.99	0.02	41,41,41,41	0
4	ZN	B	109	1/1	0.99	0.04	42,42,42,42	0
4	ZN	L	110	1/1	0.99	0.03	42,42,42,42	0
4	ZN	J	109	1/1	0.99	0.02	42,42,42,42	0
4	ZN	N	109	1/1	1.00	0.02	43,43,43,43	0
4	ZN	R	109	1/1	1.00	0.02	40,40,40,40	0
4	ZN	T	109	1/1	1.00	0.02	38,38,38,38	0
4	ZN	P	110	1/1	1.00	0.01	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ZN	H	109	1/1	1.00	0.02	47,47,47,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.