wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 05:54 PM GMT

PDB ID	:	4JKR
Title	:	Crystal Structure of E. coli RNA Polymerase in complex with ppGpp
Authors	:	Zuo, Y.; Wang, Y.; Steitz, T.A.
Deposited on	:	2013-03-11
Resolution	:	4.20 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

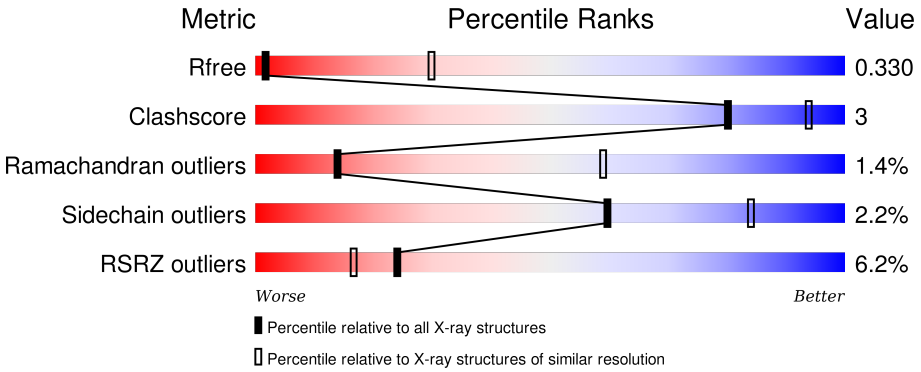
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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}	91344	1039 (4.80-3.60)
Clashscore	102246	1140 (4.80-3.60)
Ramachandran outliers	100387	1083 (4.80-3.60)
Sidechain outliers	100360	1067 (4.80-3.60)
RSRZ outliers	91569	1042 (4.80-3.60)

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 <=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	329	62% 7% 31%
1	B	329	2% 62% 7% 31%
1	G	329	63% 6% 31%
1	H	329	5% 66% 31%
2	C	1342	3% 87% 12%

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Mol	Chain	Length	Quality of chain
2	I	1342	3% 87% 12%
3	D	1416	10% 81% 13% 5%
3	J	1416	10% 80% 14% 6%
4	E	90	% 89% 11%
4	K	90	16% 94% 6%
5	F	628	4% 68% 8% 23%
5	L	628	5% 67% 9% 23%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 58326 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	227	Total	C	N	O	S	0	0	0
			1759	1096	311	346	6			
1	B	227	Total	C	N	O	S	0	0	0
			1759	1096	311	346	6			
1	G	227	Total	C	N	O	S	0	0	0
			1759	1096	311	346	6			
1	H	227	Total	C	N	O	S	0	0	0
			1759	1096	311	346	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0	0
			10569	6631	1841	2054	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10569	6631	1841	2054	43			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE SUBUNIT BETA'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1342	Total	C	N	O	S	0	0	0
			10431	6551	1860	1971	49			
3	J	1338	Total	C	N	O	S	0	0	0
			10401	6533	1854	1965	49			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1408	LEU	-	EXPRESSION TAG	UNP C5A0S8
D	1409	GLU	-	EXPRESSION TAG	UNP C5A0S8
D	1410	VAL	-	EXPRESSION TAG	UNP C5A0S8
D	1411	HIS	-	EXPRESSION TAG	UNP C5A0S8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1412	HIS	-	EXPRESSION TAG	UNP C5A0S8
D	1413	HIS	-	EXPRESSION TAG	UNP C5A0S8
D	1414	HIS	-	EXPRESSION TAG	UNP C5A0S8
D	1415	HIS	-	EXPRESSION TAG	UNP C5A0S8
D	1416	HIS	-	EXPRESSION TAG	UNP C5A0S8
J	1408	LEU	-	EXPRESSION TAG	UNP C5A0S8
J	1409	GLU	-	EXPRESSION TAG	UNP C5A0S8
J	1410	VAL	-	EXPRESSION TAG	UNP C5A0S8
J	1411	HIS	-	EXPRESSION TAG	UNP C5A0S8
J	1412	HIS	-	EXPRESSION TAG	UNP C5A0S8
J	1413	HIS	-	EXPRESSION TAG	UNP C5A0S8
J	1414	HIS	-	EXPRESSION TAG	UNP C5A0S8
J	1415	HIS	-	EXPRESSION TAG	UNP C5A0S8
J	1416	HIS	-	EXPRESSION TAG	UNP C5A0S8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	90	Total	C	N	O	S	0	0	0
			708	430	136	141	1			
4	K	90	Total	C	N	O	S	0	0	0
			708	430	136	141	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	481	Total	C	N	O	S	0	0	0
			3910	2445	699	743	23			
5	L	481	Total	C	N	O	S	0	0	0
			3910	2445	699	743	23			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-14	MET	-	EXPRESSION TAG	UNP P00579
F	-13	ARG	-	EXPRESSION TAG	UNP P00579
F	-12	GLY	-	EXPRESSION TAG	UNP P00579
F	-11	SER	-	EXPRESSION TAG	UNP P00579
F	-10	HIS	-	EXPRESSION TAG	UNP P00579
F	-9	HIS	-	EXPRESSION TAG	UNP P00579
F	-8	HIS	-	EXPRESSION TAG	UNP P00579
F	-7	HIS	-	EXPRESSION TAG	UNP P00579

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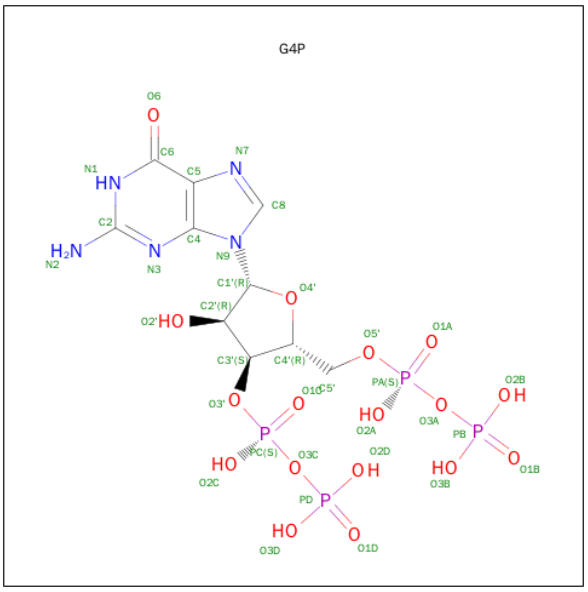
Chain	Residue	Modelled	Actual	Comment	Reference
F	-6	HIS	-	EXPRESSION TAG	UNP P00579
F	-5	HIS	-	EXPRESSION TAG	UNP P00579
F	-4	THR	-	EXPRESSION TAG	UNP P00579
F	-3	ASP	-	EXPRESSION TAG	UNP P00579
F	-2	GLN	-	EXPRESSION TAG	UNP P00579
F	-1	PHE	-	EXPRESSION TAG	UNP P00579
F	0	THR	-	EXPRESSION TAG	UNP P00579
L	-14	MET	-	EXPRESSION TAG	UNP P00579
L	-13	ARG	-	EXPRESSION TAG	UNP P00579
L	-12	GLY	-	EXPRESSION TAG	UNP P00579
L	-11	SER	-	EXPRESSION TAG	UNP P00579
L	-10	HIS	-	EXPRESSION TAG	UNP P00579
L	-9	HIS	-	EXPRESSION TAG	UNP P00579
L	-8	HIS	-	EXPRESSION TAG	UNP P00579
L	-7	HIS	-	EXPRESSION TAG	UNP P00579
L	-6	HIS	-	EXPRESSION TAG	UNP P00579
L	-5	HIS	-	EXPRESSION TAG	UNP P00579
L	-4	THR	-	EXPRESSION TAG	UNP P00579
L	-3	ASP	-	EXPRESSION TAG	UNP P00579
L	-2	GLN	-	EXPRESSION TAG	UNP P00579
L	-1	PHE	-	EXPRESSION TAG	UNP P00579
L	0	THR	-	EXPRESSION TAG	UNP P00579

- Molecule 6 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	J	1	Total Sr 1 1	0	0
6	D	1	Total Sr 1 1	0	0
6	E	1	Total Sr 1 1	0	0
6	I	1	Total Sr 1 1	0	0
6	C	2	Total Sr 2 2	0	0
6	A	1	Total Sr 1 1	0	0
6	F	1	Total Sr 1 1	0	0

- Molecule 7 is GUANOSINE-5',3'-TETRAPHOSPHATE (three-letter code: G4P) (formula: $C_{10}H_{17}N_5O_{17}P_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total C N O P 36 10 5 17 4	0	0
7	K	1	Total C N O P 36 10 5 17 4	0	0

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

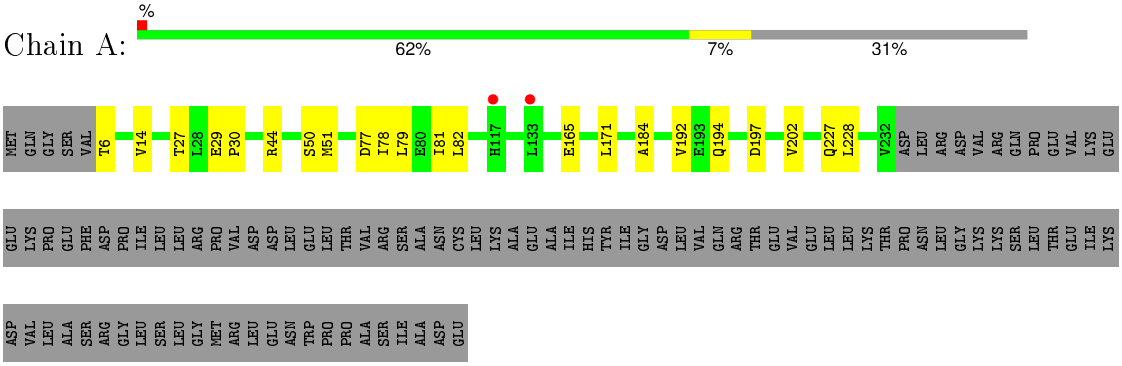
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	J	2	Total Zn 2 2	0	0
8	D	2	Total Zn 2 2	0	0

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 errors 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.

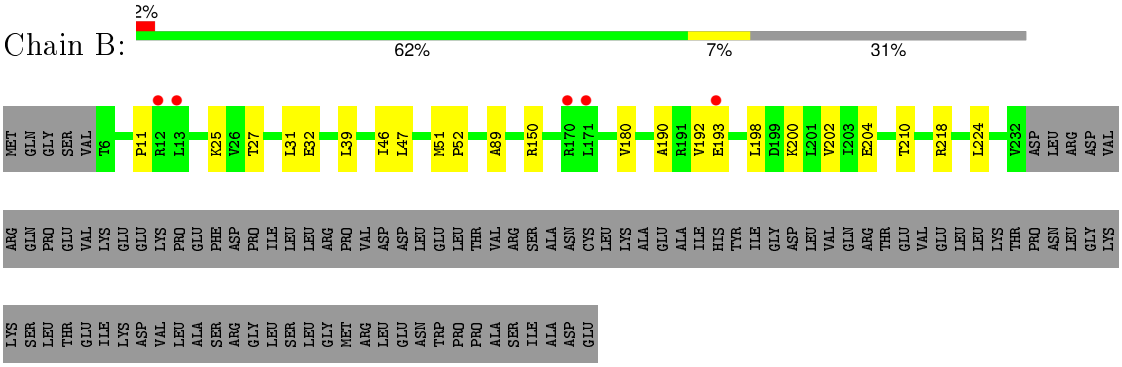
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



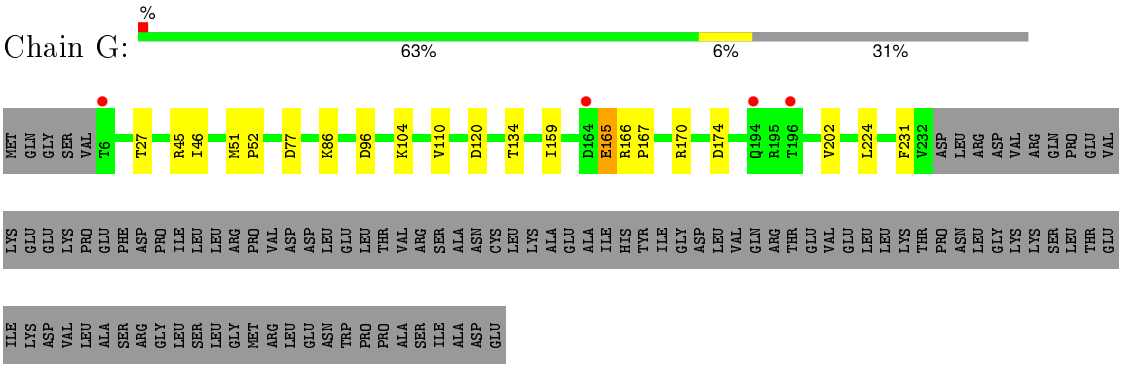
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B:



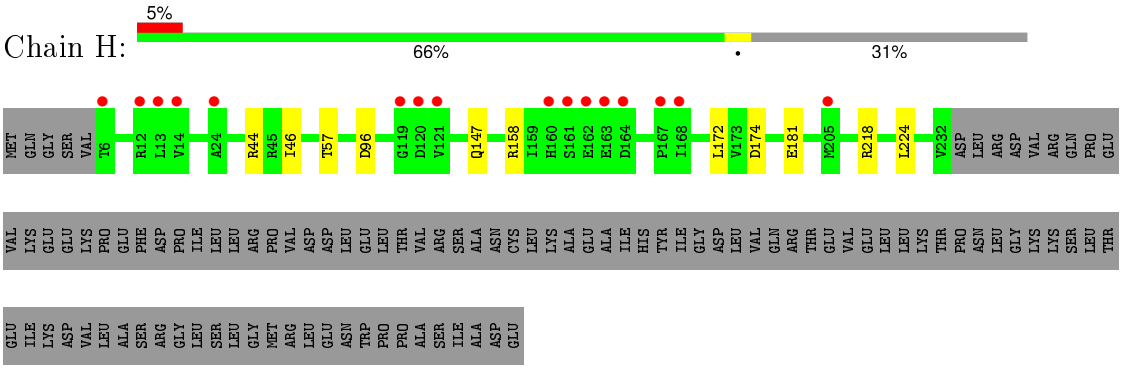
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain G:



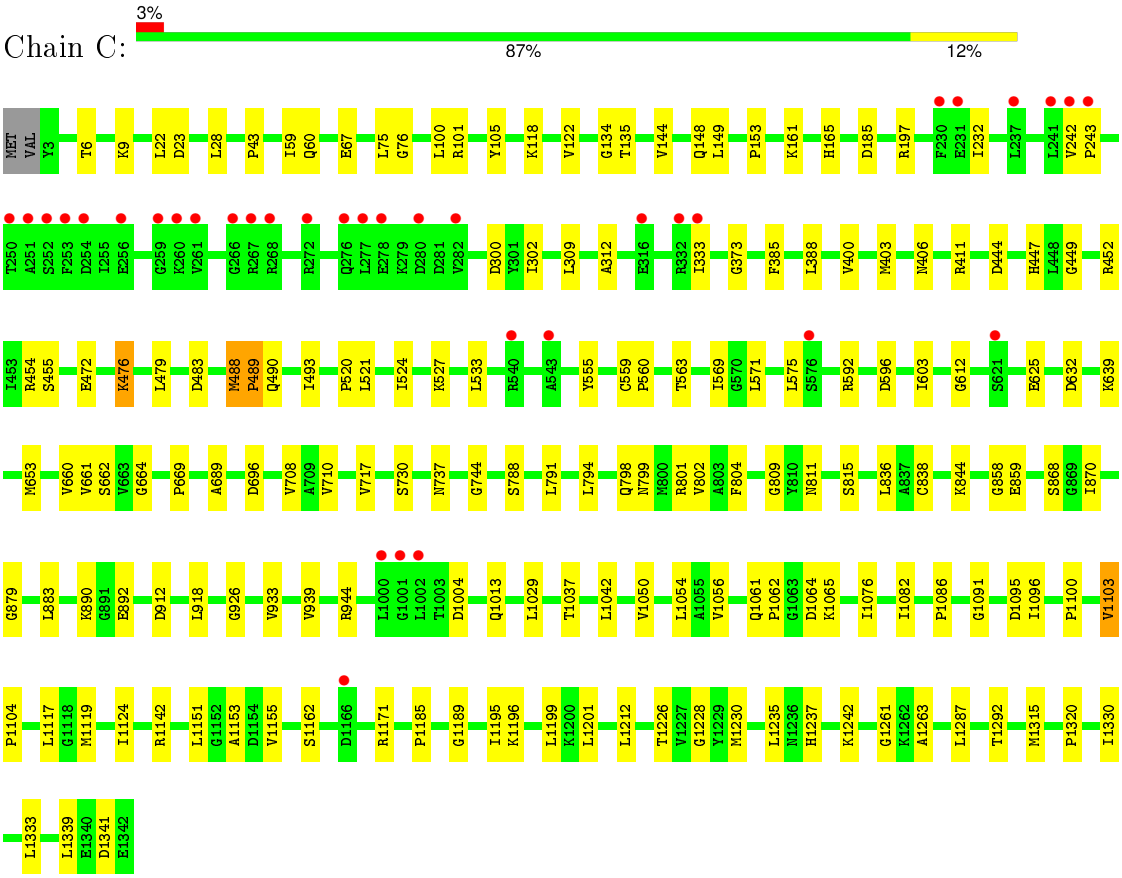
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain H:



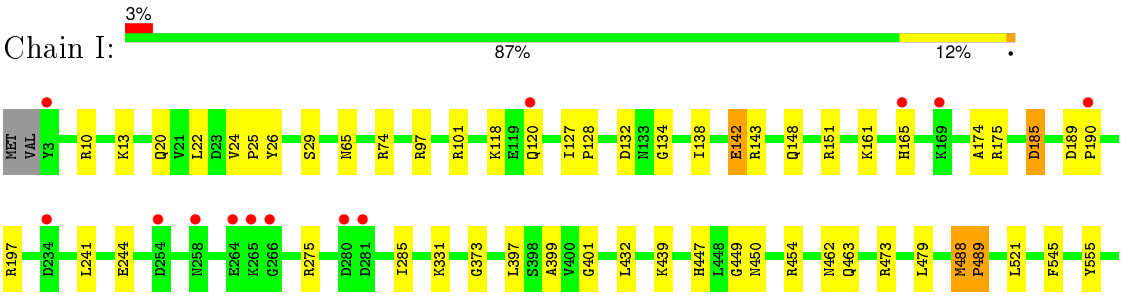
• Molecule 2: DNA-directed RNA polymerase subunit beta

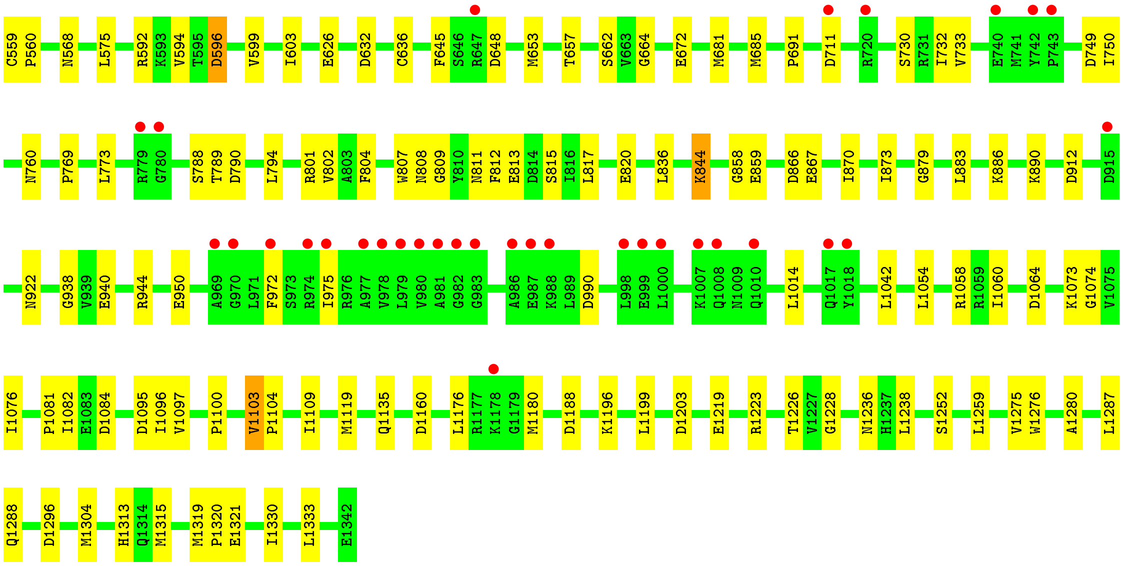
Chain C:



• Molecule 2: DNA-directed RNA polymerase subunit beta

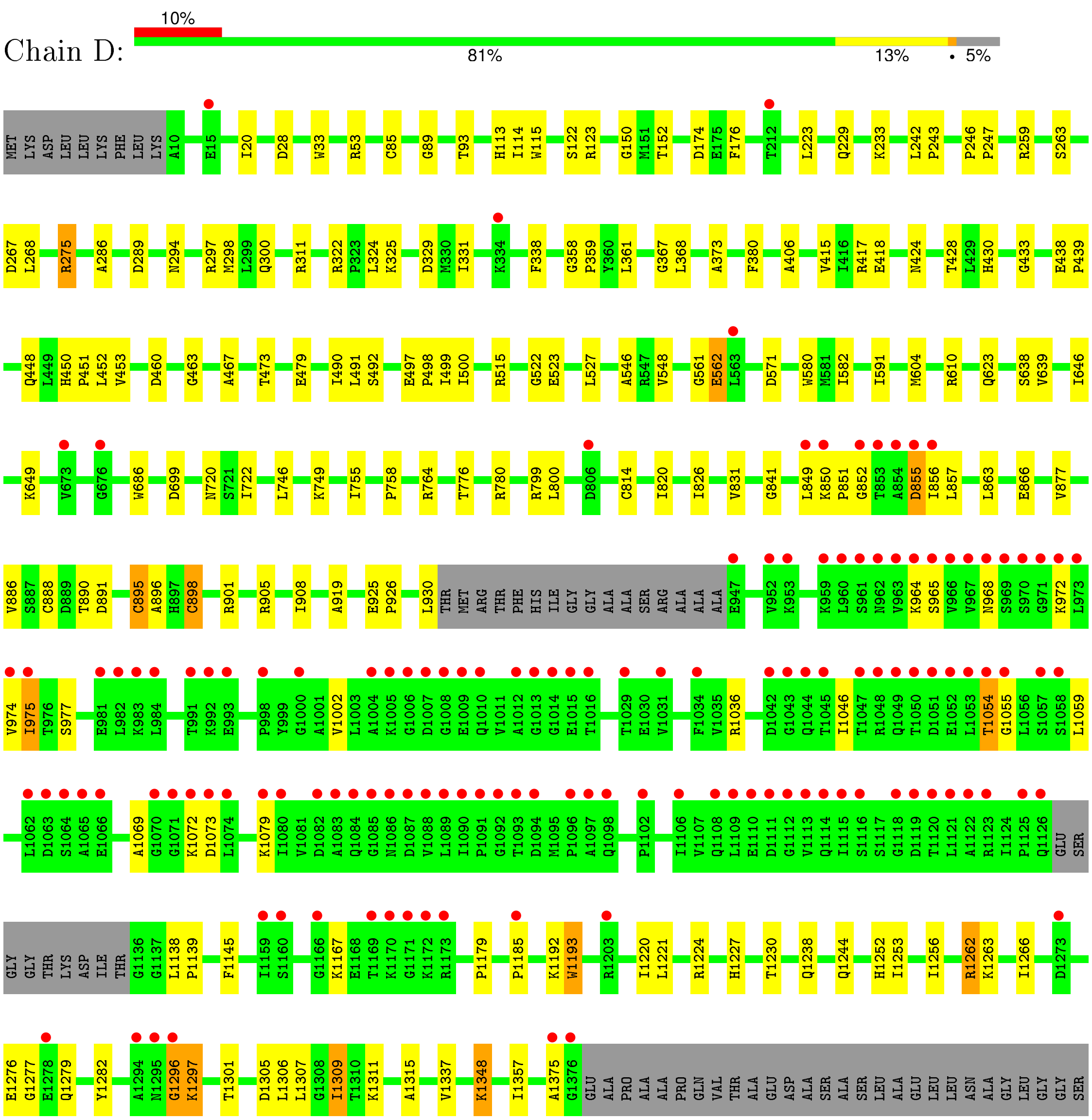
Chain I:





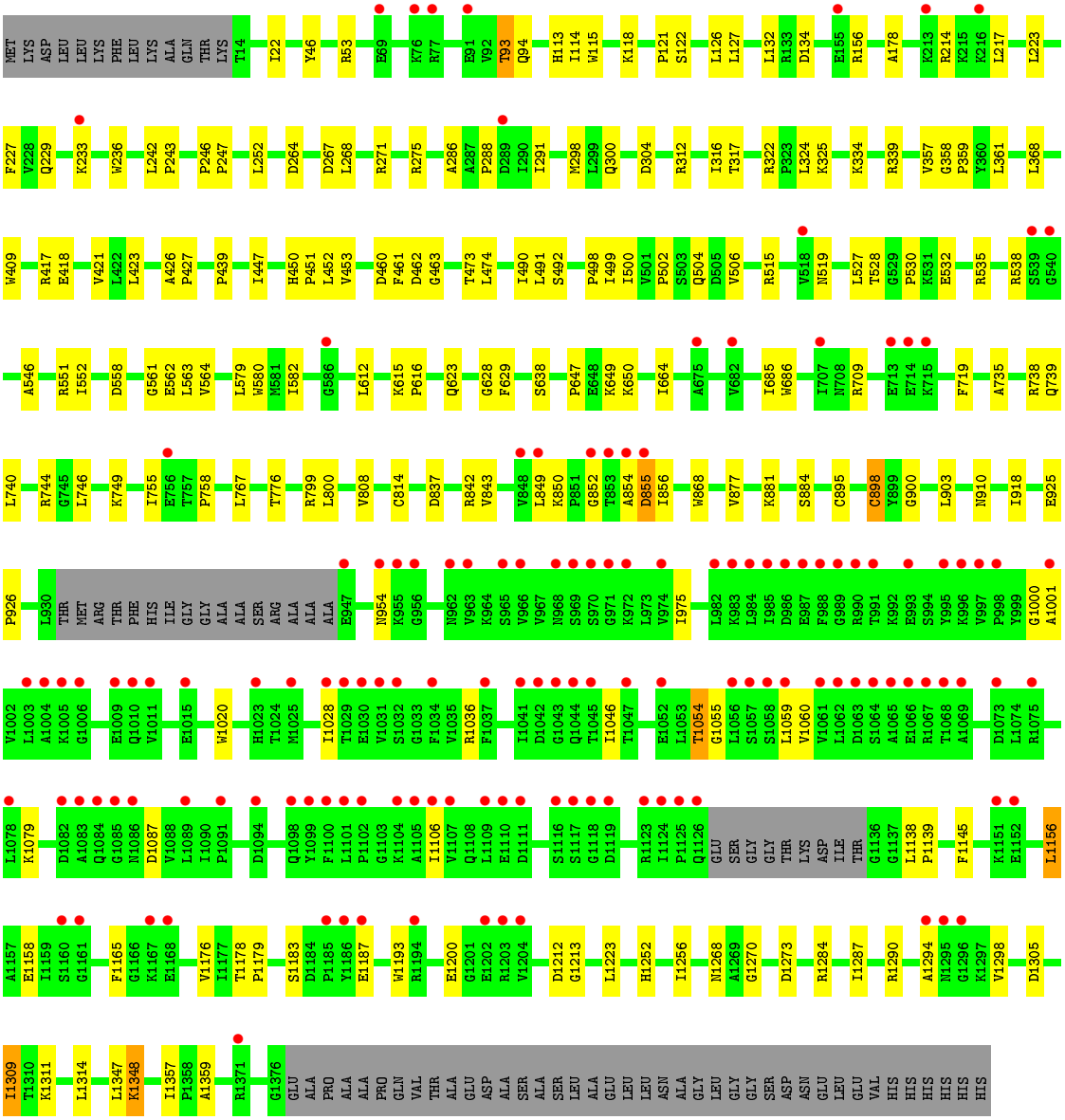
- Molecule 3: DNA-DIRECTED RNA POLYMERASE SUBUNIT BETA'

Chain D:



- Molecule 3: DNA-DIRECTED RNA POLYMERASE SUBUNIT BETA'

Chain J:

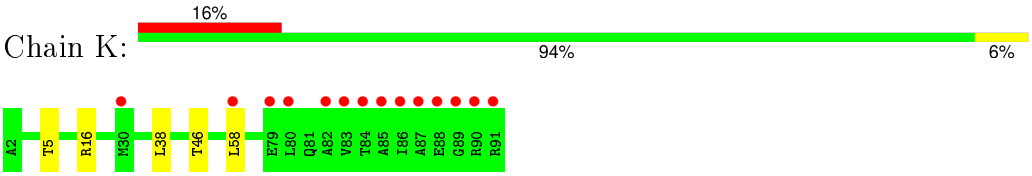


- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:

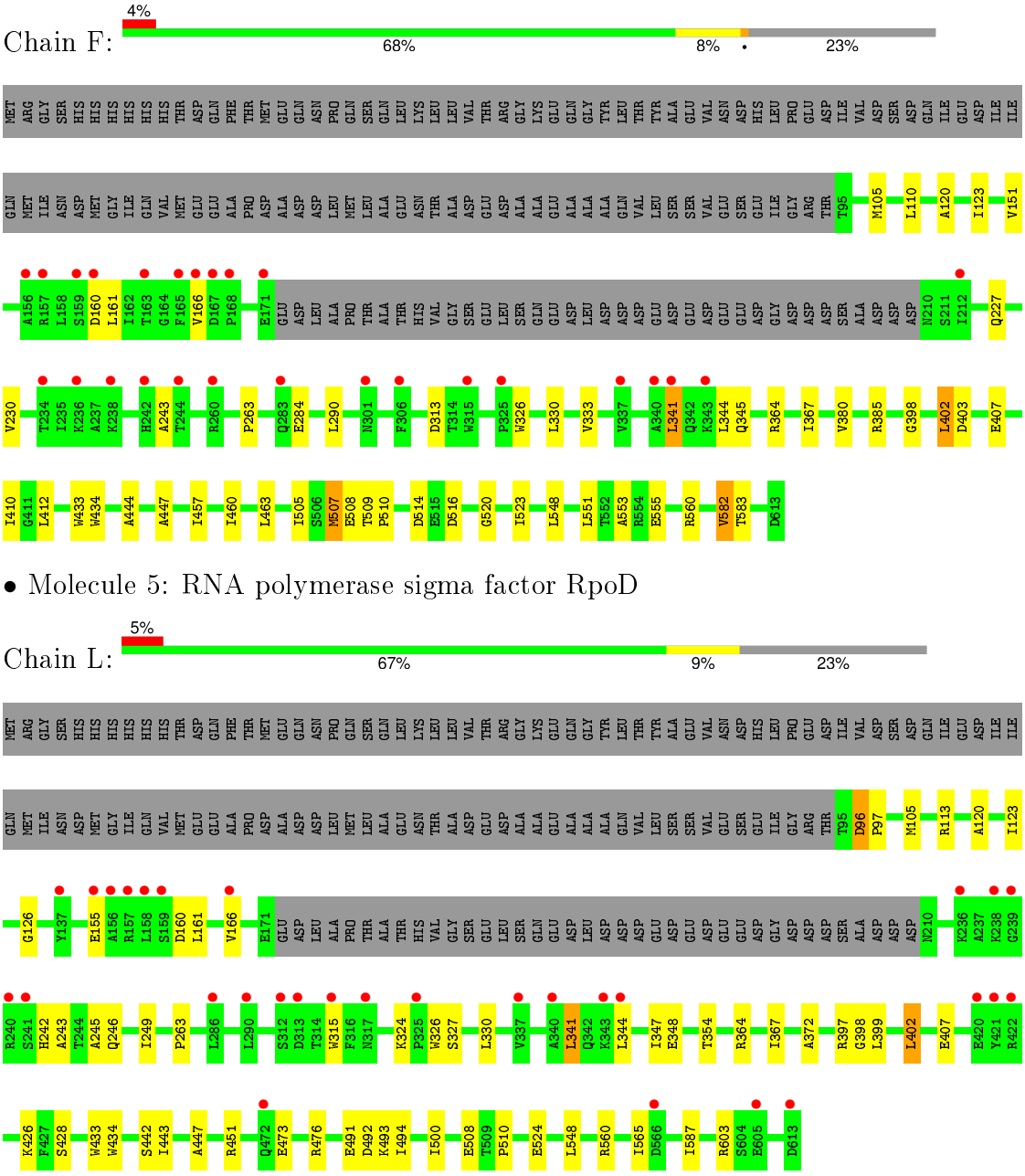
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain K:



• Molecule 5: RNA polymerase sigma factor RpoD

Chain F:



• Molecule 5: RNA polymerase sigma factor RpoD

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	187.57Å 206.16Å 311.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.97 – 4.20 39.94 – 4.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.97-4.20) 99.7 (39.94-4.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 4.13Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.247 , 0.318 0.260 , 0.330	Depositor DCC
R_{free} test set	4401 reflections (5.25%)	DCC
Wilson B-factor (Å^2)	167.3	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 203.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 88171 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	58326	wwPDB-VP
Average B, all atoms (Å^2)	280.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: G4P, SR, ZN

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	0.45	0/1781	0.49	1/2414 (0.0%)
1	B	0.43	0/1781	0.51	1/2414 (0.0%)
1	G	0.41	0/1781	0.47	0/2414
1	H	0.40	0/1781	0.47	0/2414
2	C	0.50	0/10738	0.54	1/14489 (0.0%)
2	I	0.42	2/10738 (0.0%)	0.49	0/14489
3	D	0.50	5/10588 (0.0%)	0.53	2/14295 (0.0%)
3	J	0.45	7/10558 (0.1%)	0.51	1/14255 (0.0%)
4	E	0.53	0/710	0.56	0/956
4	K	0.39	0/710	0.51	0/956
5	F	0.45	3/3964 (0.1%)	0.52	0/5330
5	L	0.43	4/3964 (0.1%)	0.49	0/5330
All	All	0.46	21/59094 (0.0%)	0.51	6/79756 (0.0%)

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	479	GLU	CD-OE1	-6.85	1.18	1.25
2	I	807	TRP	CD2-CE2	5.79	1.48	1.41
3	D	580	TRP	CD2-CE2	5.54	1.48	1.41
3	D	33	TRP	CD2-CE2	5.48	1.48	1.41
3	J	868	TRP	CD2-CE2	5.42	1.47	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	218	ARG	NE-CZ-NH2	-6.97	116.81	120.30
2	C	1341	ASP	CB-CG-OD1	6.31	123.98	118.30
3	D	479	GLU	OE1-CD-OE2	-6.14	115.94	123.30
3	D	855	ASP	CB-CG-OD2	5.23	123.00	118.30
3	J	855	ASP	CB-CG-OD2	5.21	122.99	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	1759	0	1785	10	0
1	B	1759	0	1785	14	0
1	G	1759	0	1785	11	0
1	H	1759	0	1785	5	0
2	C	10569	0	10582	75	0
2	I	10569	0	10582	77	0
3	D	10431	0	10649	104	0
3	J	10401	0	10616	103	0
4	E	708	0	719	5	0
4	K	708	0	719	3	0
5	F	3910	0	3970	23	0
5	L	3910	0	3970	22	0
6	A	1	0	0	0	0
6	C	2	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
7	D	36	0	11	1	0
7	K	36	0	11	0	0
8	D	2	0	0	1	0
8	J	2	0	0	0	0
All	All	58326	0	58969	404	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 3.

The worst 5 of 404 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)
3:J:895:CYS:HB2	3:J:898:CYS:SG	1.76	1.24
3:D:888:CYS:SG	3:D:895:CYS:SG	2.60	0.99
3:J:895:CYS:CB	3:J:898:CYS:SG	2.53	0.97
3:J:895:CYS:N	3:J:898:CYS:SG	2.42	0.93
3:D:898:CYS:O	3:D:898:CYS:SG	2.29	0.90

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	225/329 (68%)	216 (96%)	6 (3%)	3 (1%)	15 60
1	B	225/329 (68%)	213 (95%)	12 (5%)	0	100 100
1	G	225/329 (68%)	214 (95%)	10 (4%)	1 (0%)	39 80
1	H	225/329 (68%)	217 (96%)	7 (3%)	1 (0%)	39 80
2	C	1338/1342 (100%)	1208 (90%)	107 (8%)	23 (2%)	11 56
2	I	1338/1342 (100%)	1186 (89%)	131 (10%)	21 (2%)	12 57
3	D	1336/1416 (94%)	1206 (90%)	110 (8%)	20 (2%)	13 58
3	J	1332/1416 (94%)	1207 (91%)	111 (8%)	14 (1%)	17 64
4	E	88/90 (98%)	82 (93%)	5 (6%)	1 (1%)	17 64
4	K	88/90 (98%)	83 (94%)	5 (6%)	0	100 100
5	F	477/628 (76%)	432 (91%)	36 (8%)	9 (2%)	10 54
5	L	477/628 (76%)	442 (93%)	27 (6%)	8 (2%)	11 56
All	All	7374/8268 (89%)	6706 (91%)	567 (8%)	101 (1%)	14 59

5 of 101 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	488	MET

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Mol	Chain	Res	Type
2	C	489	PRO
2	C	555	TYR
2	C	569	ILE
5	F	243	ALA

5.3.2 Protein sidechains (i)

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	195/286 (68%)	192 (98%)	3 (2%)	72	89
1	B	195/286 (68%)	195 (100%)	0	100	100
1	G	195/286 (68%)	191 (98%)	4 (2%)	61	85
1	H	195/286 (68%)	193 (99%)	2 (1%)	82	91
2	C	1155/1157 (100%)	1133 (98%)	22 (2%)	65	86
2	I	1155/1157 (100%)	1122 (97%)	33 (3%)	50	79
3	D	1123/1177 (95%)	1098 (98%)	25 (2%)	60	84
3	J	1120/1177 (95%)	1090 (97%)	30 (3%)	52	80
4	E	74/74 (100%)	72 (97%)	2 (3%)	52	80
4	K	74/74 (100%)	73 (99%)	1 (1%)	74	89
5	F	427/554 (77%)	419 (98%)	8 (2%)	65	86
5	L	427/554 (77%)	415 (97%)	12 (3%)	51	80
All	All	6335/7068 (90%)	6193 (98%)	142 (2%)	60	84

5 of 142 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	96	ASP
2	I	632	ASP
5	L	105	MET
2	I	13	LYS
2	I	331	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	406	GLN
2	I	46	GLN
3	J	1279	GLN
1	H	41	ASN
2	I	447	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 12 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
7	G4P	D	2001	-	29,38,38	1.43	4 (13%)	42,61,61	1.93	10 (23%)
7	G4P	K	101	-	29,38,38	1.30	3 (10%)	42,61,61	1.77	8 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	G4P	D	2001	-	-	0/23/43/43	0/3/3/3
7	G4P	K	101	-	-	0/23/43/43	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	2001	G4P	PB-O2B	-2.25	1.46	1.54
7	K	101	G4P	C5-C4	2.98	1.47	1.40
7	D	2001	G4P	O4'-C1'	3.26	1.45	1.41
7	D	2001	G4P	C5-C4	3.29	1.47	1.40
7	D	2001	G4P	C6-C5	3.35	1.47	1.41

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	2001	G4P	PA-O3A-PB	-4.59	117.28	132.67
7	D	2001	G4P	C4-C5-N7	-4.11	105.70	109.48
7	K	101	G4P	PC-O3C-PD	-3.81	119.91	132.67
7	K	101	G4P	C5-C6-N1	-3.76	118.44	123.59
7	D	2001	G4P	PC-O3C-PD	-3.72	120.21	132.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	2001	G4P	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	227/329 (68%)	-0.10	2 (0%) 85 80	148, 217, 322, 411	0
1	B	227/329 (68%)	0.03	5 (2%) 65 55	155, 276, 386, 464	0
1	G	227/329 (68%)	-0.05	4 (1%) 71 62	195, 272, 381, 487	0
1	H	227/329 (68%)	0.34	16 (7%) 19 14	209, 313, 434, 551	0
2	C	1340/1342 (99%)	-0.10	35 (2%) 59 48	116, 219, 400, 608	0
2	I	1340/1342 (99%)	0.01	46 (3%) 49 38	158, 257, 405, 600	0
3	D	1342/1416 (94%)	0.34	137 (10%) 9 7	114, 234, 543, 696	0
3	J	1338/1416 (94%)	0.43	141 (10%) 8 7	158, 266, 556, 725	0
4	E	90/90 (100%)	-0.09	1 (1%) 82 75	147, 230, 311, 405	0
4	K	90/90 (100%)	0.80	14 (15%) 3 4	217, 322, 517, 666	0
5	F	481/628 (76%)	0.07	26 (5%) 29 22	153, 297, 481, 614	0
5	L	481/628 (76%)	0.16	30 (6%) 24 17	182, 318, 469, 601	0
All	All	7410/8268 (89%)	0.15	457 (6%) 24 17	114, 258, 482, 725	0

The worst 5 of 457 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	1073	ASP	24.1
3	J	1118	GLY	18.8
3	J	1125	PRO	17.5
3	D	983	LYS	16.7
3	J	1057	SER	12.6

6.2 Non-standard residues in protein, DNA, RNA chains

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, 95^{th} 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
7	G4P	D	2001	36/36	0.90	0.32	-0.23	125,188,244,266	0
7	G4P	K	101	36/36	0.76	0.25	-0.64	158,256,299,307	0
8	ZN	D	2003	1/1	0.88	0.12	-1.15	245,245,245,245	0
8	ZN	J	1502	1/1	0.84	0.12	-1.44	256,256,256,256	0
8	ZN	D	2002	1/1	0.94	0.04	-2.07	261,261,261,261	0
8	ZN	J	1501	1/1	0.96	0.03	-2.27	249,249,249,249	0
6	SR	I	1401	1/1	0.77	0.39	-	346,346,346,346	0
6	SR	J	1503	1/1	0.95	0.31	-	322,322,322,322	0
6	SR	D	2004	1/1	0.94	0.17	-	288,288,288,288	0
6	SR	F	701	1/1	0.94	0.44	-	239,239,239,239	0
6	SR	A	401	1/1	0.90	0.14	-	261,261,261,261	0
6	SR	C	1402	1/1	0.96	0.62	-	212,212,212,212	0
6	SR	C	1401	1/1	0.85	0.44	-	303,303,303,303	0
6	SR	E	101	1/1	0.70	0.27	-	328,328,328,328	0

6.5 Other polymers (i)

There are no such residues in this entry.