



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 25, 2023 – 12:43 PM EDT

PDB ID : 5W1S
Title : X-ray crystal structure of Escherichia coli RNA polymerase and TraR complex
Authors : Murakami, K.S.; Molodtsov, V.
Deposited on : 2017-06-04
Resolution : 3.81 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

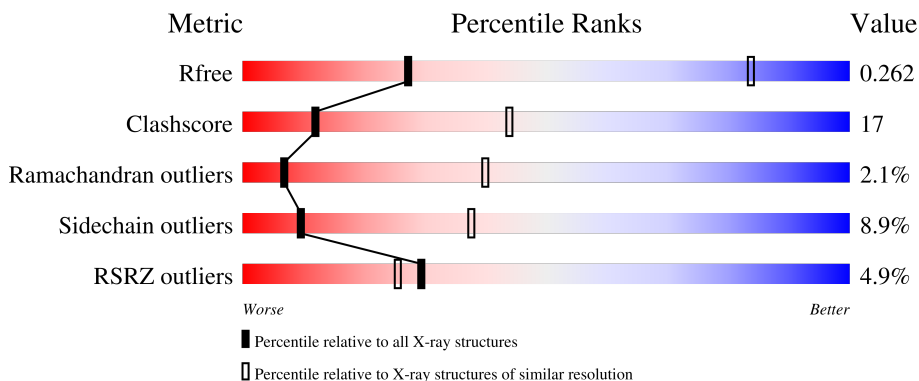
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.81 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	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	329	 2% 45% 41% 10%
1	B	329	 3% 40% 24% 34%
1	G	329	 2% 37% 27% 31%
1	H	329	 6% 42% 22% 34%
2	C	1342	 6% 57% 38%

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Mol	Chain	Length	Quality of chain
2	I	1342	
3	D	1407	
3	J	1407	
4	E	91	
4	K	91	
5	F	613	
5	L	613	
6	M	79	
6	N	79	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 56825 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
			Total	C	N	O	S			
1	A	319	Total	C	N	O	S	0	0	0
			2490	1557	439	486	8			
1	B	217	Total	C	N	O	S	0	0	0
			1677	1047	295	329	6			
1	G	227	Total	C	N	O	S	0	0	0
			1755	1093	311	345	6			
1	H	216	Total	C	N	O	S	0	0	0
			1662	1038	292	326	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	1340	Total	C	N	O	S	0	0	0
			10564	6628	1838	2055	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10566	6629	1840	2054	43			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	1173	Total	C	N	O	S	0	0	0
			9095	5718	1628	1703	46			
3	J	1155	Total	C	N	O	S	0	0	0
			9001	5659	1612	1684	46			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	89	Total	C	N	O	S	0	0	0
			691	421	129	140	1			
4	K	72	Total	C	N	O	S	0	0	0
			573	350	110	112	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	468	Total	C	N	O	S	0	0	0
			3813	2389	678	723	23			
5	L	469	Total	C	N	O	S	0	0	0
			3821	2393	679	726	23			

- Molecule 6 is a protein called Protein TraR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	M	70	Total	C	N	O	S	0	0	0
			557	346	103	103	5			
6	N	69	Total	C	N	O	S	0	0	0
			552	343	102	102	5			

There are 12 discrepancies between the modelled and reference sequences:

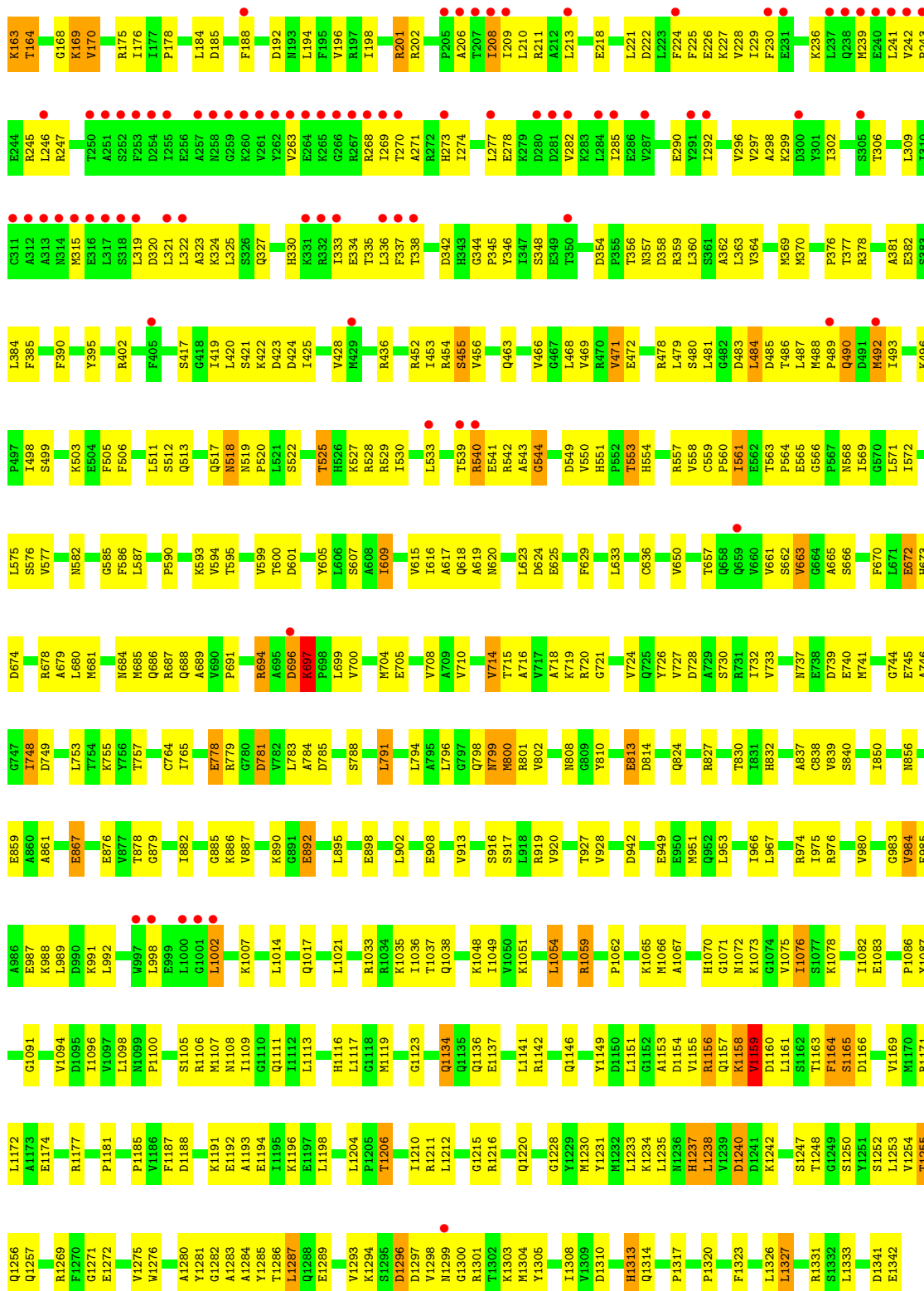
Chain	Residue	Modelled	Actual	Comment	Reference
M	74	HIS	-	expression tag	UNP P41065
M	75	HIS	-	expression tag	UNP P41065
M	76	HIS	-	expression tag	UNP P41065
M	77	HIS	-	expression tag	UNP P41065
M	78	HIS	-	expression tag	UNP P41065
M	79	HIS	-	expression tag	UNP P41065
N	74	HIS	-	expression tag	UNP P41065
N	75	HIS	-	expression tag	UNP P41065
N	76	HIS	-	expression tag	UNP P41065
N	77	HIS	-	expression tag	UNP P41065
N	78	HIS	-	expression tag	UNP P41065
N	79	HIS	-	expression tag	UNP P41065

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	Mg	0	0
			1	1		
7	J	1	Total	Mg	0	0
			1	1		

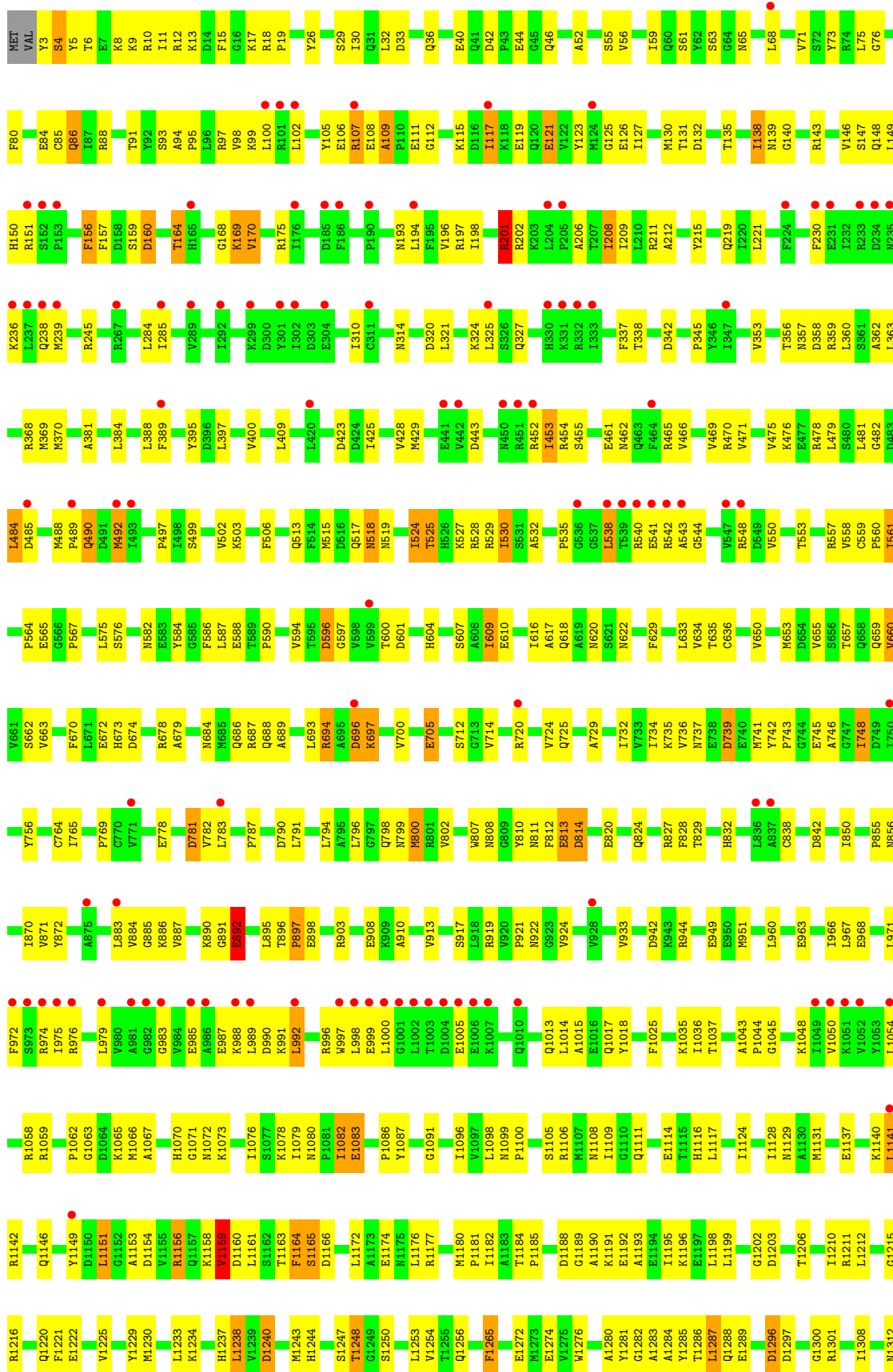
- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	2	Total 2	Zn 2	0	0
8	J	2	Total 2	Zn 2	0	0
8	M	1	Total 1	Zn 1	0	0
8	N	1	Total 1	Zn 1	0	0



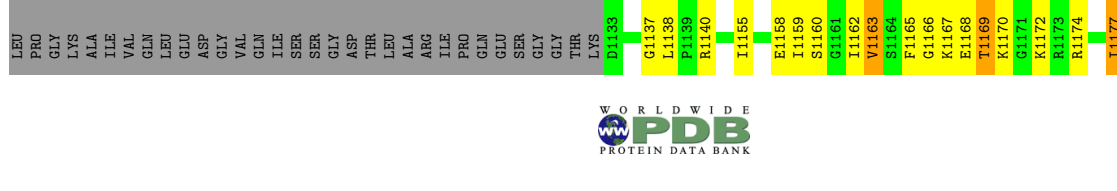
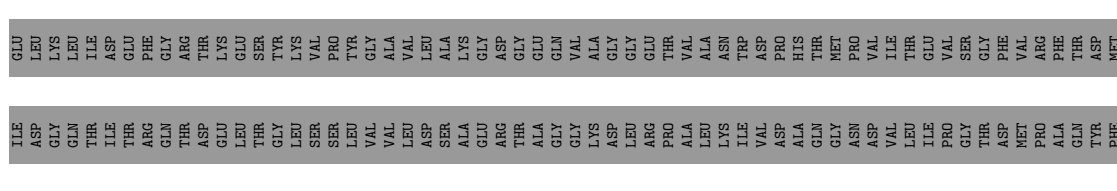
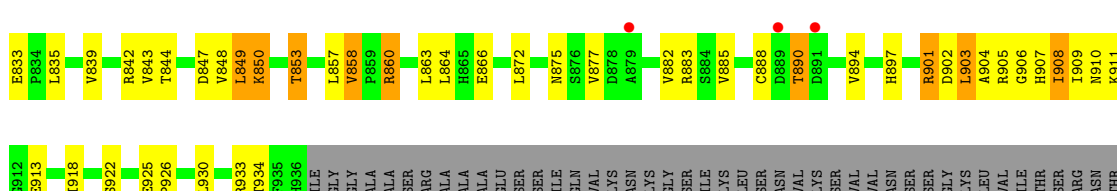
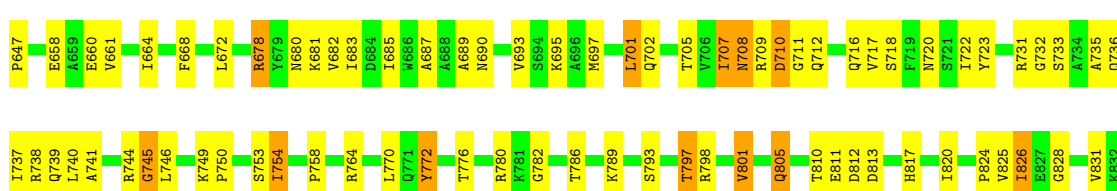
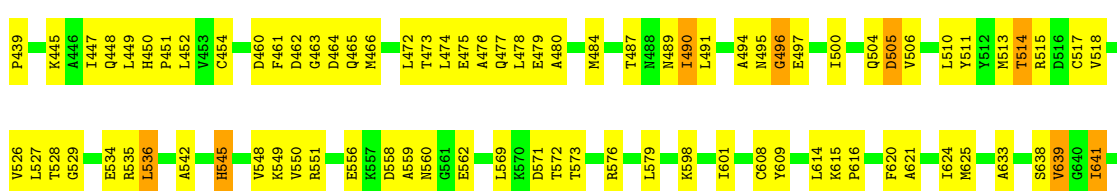
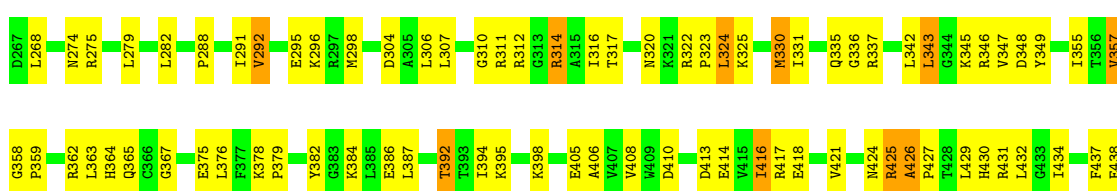
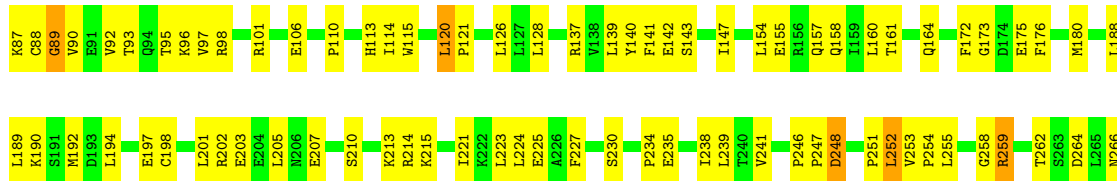
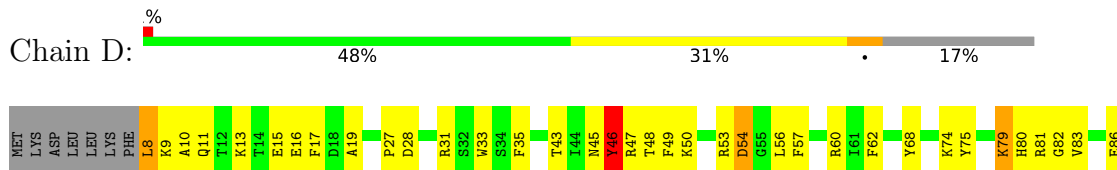
● Molecule 2: DNA-directed RNA polymerase subunit beta

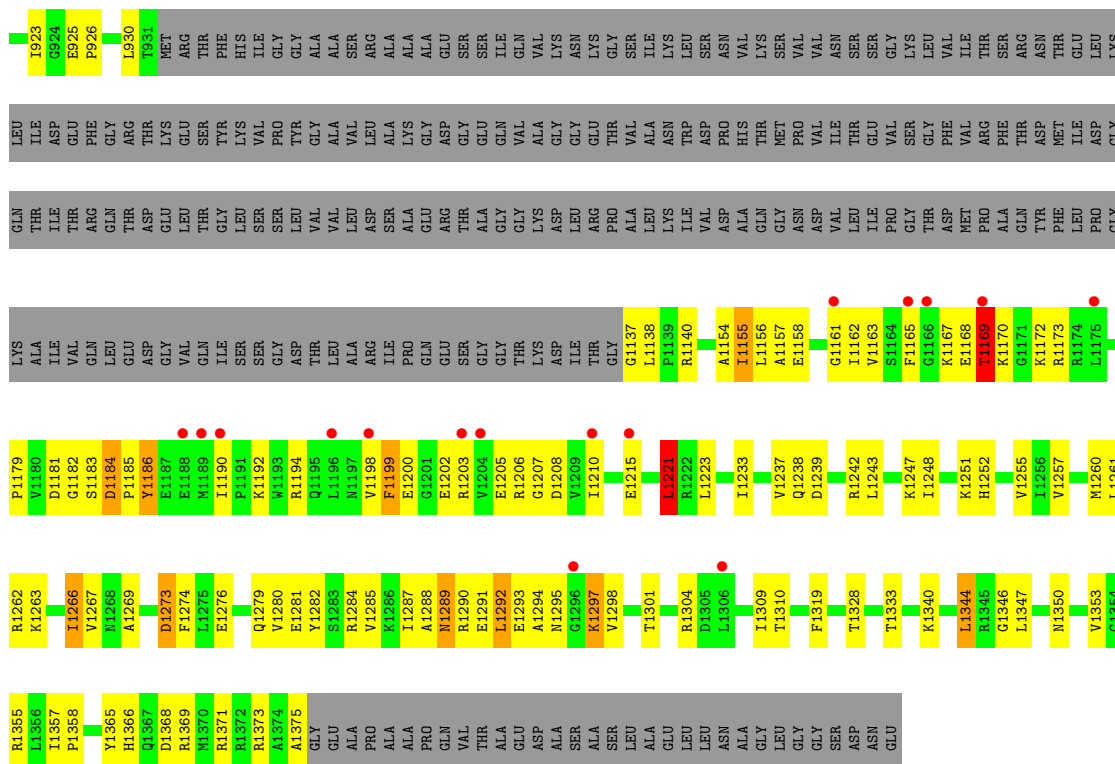




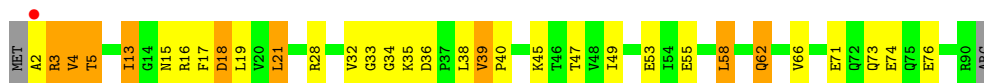


• Molecule 3: DNA-directed RNA polymerase subunit beta'

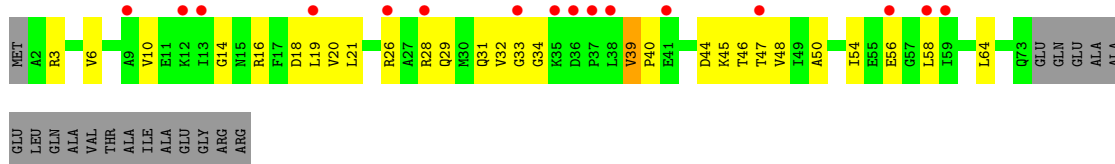




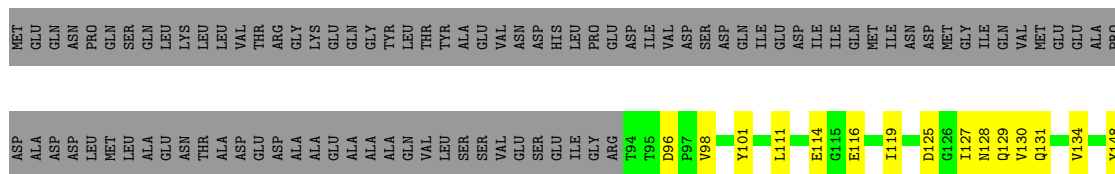
• Molecule 4: DNA-directed RNA polymerase subunit omega

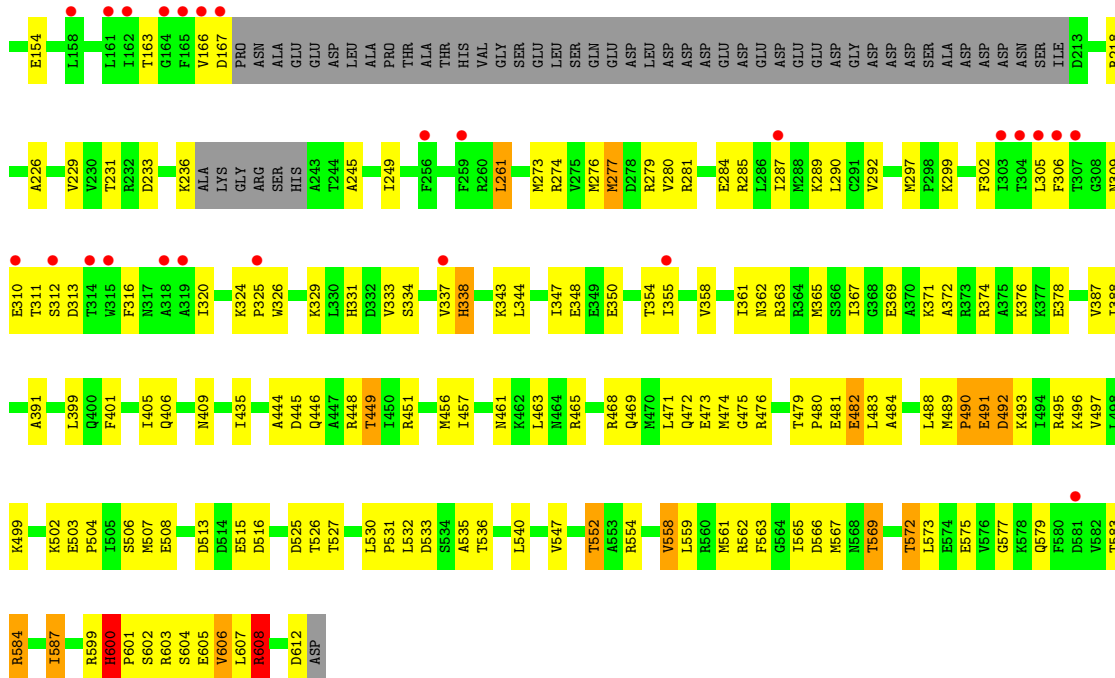


• Molecule 4: DNA-directed RNA polymerase subunit omega

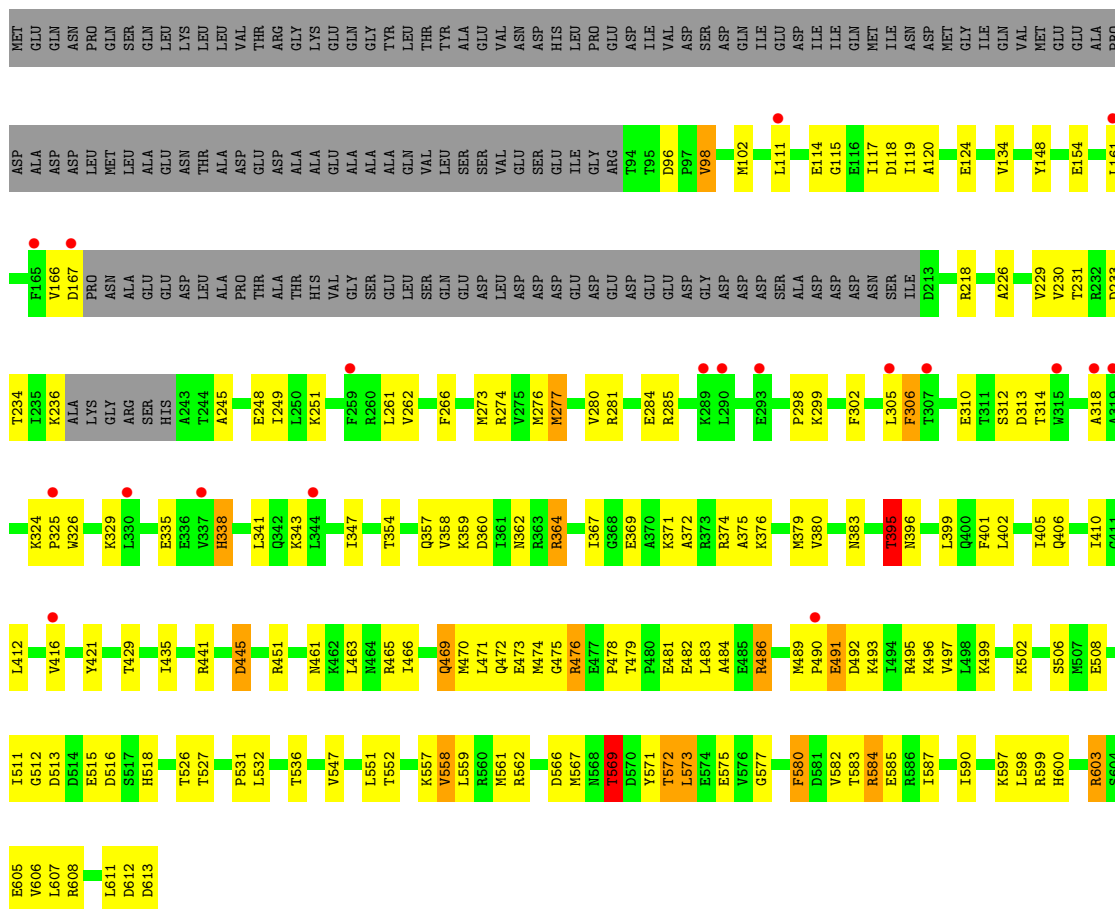


• Molecule 5: RNA polymerase sigma factor RpoD

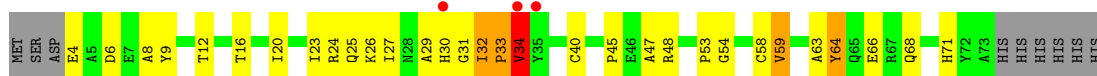




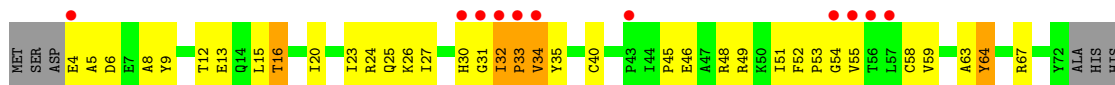
● Molecule 5: RNA polymerase sigma factor RpoD



- Molecule 6: Protein TraR



- Molecule 6: Protein TraR



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	186.48Å 206.04Å 310.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.84 – 3.81 49.84 – 3.81	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.84-3.81) 86.5 (49.84-3.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.60 (at 3.77Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.208 , 0.262 0.208 , 0.262	Depositor DCC
R_{free} test set	2000 reflections (1.70%)	wwPDB-VP
Wilson B-factor (Å ²)	156.4	Xtrriage
Anisotropy	0.169	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 180.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	56825	wwPDB-VP
Average B, all atoms (Å ²)	239.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.29	0/2524	0.63	1/3421 (0.0%)
1	B	0.30	0/1697	0.60	0/2300
1	G	0.28	0/1777	0.59	0/2408
1	H	0.29	0/1681	0.63	2/2278 (0.1%)
2	C	0.30	0/10733	0.58	1/14482 (0.0%)
2	I	0.29	0/10735	0.56	0/14484
3	D	0.31	0/9235	0.59	0/12472
3	J	0.29	0/9140	0.56	2/12341 (0.0%)
4	E	0.27	0/693	0.52	0/935
4	K	0.26	0/575	0.43	0/774
5	F	0.28	0/3864	0.54	1/5194 (0.0%)
5	L	0.27	0/3872	0.53	0/5205
6	M	0.34	0/567	0.64	1/766 (0.1%)
6	N	0.37	0/562	0.64	1/759 (0.1%)
All	All	0.29	0/57655	0.57	9/77819 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	2
2	I	0	2
3	D	0	2
3	J	0	2
5	F	0	1
All	All	0	9

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	LEU	CA-CB-CG	6.11	129.35	115.30
6	M	32	ILE	C-N-CD	-6.10	107.18	120.60
1	H	29	GLU	C-N-CD	-5.98	107.44	120.60
3	J	1221	LEU	CA-CB-CG	5.83	128.71	115.30
6	N	32	ILE	C-N-CD	-5.66	108.16	120.60

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	109	ALA	Peptide
2	C	236	LYS	Peptide
3	D	1184	ASP	Peptide
3	D	901	ARG	Peptide
5	F	600	HIS	Peptide

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	2490	0	2542	120	0
1	B	1677	0	1703	61	0
1	G	1755	0	1773	78	0
1	H	1662	0	1687	59	0
2	C	10564	0	10571	426	0
2	I	10566	0	10576	351	0
3	D	9095	0	9222	385	0
3	J	9001	0	9167	375	0
4	E	691	0	695	26	0
4	K	573	0	587	20	0
5	F	3813	0	3880	119	0
5	L	3821	0	3884	109	0
6	M	557	0	547	31	0
6	N	552	0	542	44	0
7	D	1	0	0	0	0
7	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	2	0	0	0	0
8	J	2	0	0	0	0
8	M	1	0	0	0	0
8	N	1	0	0	0	0
All	All	56825	0	57376	1966	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 17.

The worst 5 of 1966 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:45:ARG:HG2	1:B:38:THR:HB	1.42	1.02
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.42	1.01
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.38	1.00
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.44	0.99
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.46	0.96

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	317/329 (96%)	247 (78%)	52 (16%)	18 (6%)	1	21
1	B	213/329 (65%)	194 (91%)	15 (7%)	4 (2%)	8	42
1	G	225/329 (68%)	199 (88%)	20 (9%)	6 (3%)	5	35
1	H	212/329 (64%)	196 (92%)	12 (6%)	4 (2%)	8	42
2	C	1338/1342 (100%)	1201 (90%)	118 (9%)	19 (1%)	11	46
2	I	1338/1342 (100%)	1197 (90%)	120 (9%)	21 (2%)	9	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	1169/1407 (83%)	1038 (89%)	104 (9%)	27 (2%)	6	38
3	J	1151/1407 (82%)	1026 (89%)	99 (9%)	26 (2%)	6	38
4	E	87/91 (96%)	80 (92%)	5 (6%)	2 (2%)	6	38
4	K	70/91 (77%)	61 (87%)	8 (11%)	1 (1%)	11	46
5	F	462/613 (75%)	426 (92%)	28 (6%)	8 (2%)	9	43
5	L	463/613 (76%)	425 (92%)	30 (6%)	8 (2%)	9	43
6	M	68/79 (86%)	56 (82%)	7 (10%)	5 (7%)	1	16
6	N	67/79 (85%)	56 (84%)	6 (9%)	5 (8%)	1	15
All	All	7180/8380 (86%)	6402 (89%)	624 (9%)	154 (2%)	7	40

5 of 154 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	107	ILE
1	A	136	GLU
1	A	162	GLU
1	A	167	PRO

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	278/286 (97%)	226 (81%)	52 (19%)	1	11
1	B	186/286 (65%)	171 (92%)	15 (8%)	11	41
1	G	193/286 (68%)	169 (88%)	24 (12%)	4	24
1	H	183/286 (64%)	172 (94%)	11 (6%)	19	50
2	C	1154/1157 (100%)	1052 (91%)	102 (9%)	10	38
2	I	1154/1157 (100%)	1058 (92%)	96 (8%)	11	40
3	D	962/1168 (82%)	882 (92%)	80 (8%)	11	40
3	J	960/1168 (82%)	876 (91%)	84 (9%)	10	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	72/75 (96%)	63 (88%)	9 (12%)	4	24
4	K	62/75 (83%)	59 (95%)	3 (5%)	25	56
5	F	417/540 (77%)	387 (93%)	30 (7%)	14	45
5	L	418/540 (77%)	380 (91%)	38 (9%)	9	36
6	M	59/68 (87%)	55 (93%)	4 (7%)	16	47
6	N	59/68 (87%)	56 (95%)	3 (5%)	24	54
All	All	6157/7160 (86%)	5606 (91%)	551 (9%)	9	38

5 of 551 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	641	ILE
3	J	847	ASP
3	J	573	THR
5	L	405	ILE
3	D	425	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
3	J	206	ASN
6	M	71	HIS
3	J	680	ASN
3	J	1295	ASN
3	D	320	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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 [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 [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, 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	319/329 (96%)	-0.01	8 (2%) 57 49	152, 220, 344, 468	0
1	B	217/329 (65%)	-0.05	9 (4%) 37 31	140, 238, 332, 383	0
1	G	227/329 (68%)	-0.06	7 (3%) 49 40	204, 264, 358, 416	0
1	H	216/329 (65%)	0.41	19 (8%) 10 8	204, 298, 387, 432	0
2	C	1340/1342 (99%)	0.23	83 (6%) 20 16	104, 197, 403, 528	0
2	I	1340/1342 (99%)	0.38	109 (8%) 12 10	127, 264, 377, 485	0
3	D	1173/1407 (83%)	-0.07	12 (1%) 82 76	101, 174, 294, 419	0
3	J	1155/1407 (82%)	0.07	34 (2%) 51 42	125, 213, 329, 431	0
4	E	89/91 (97%)	-0.34	1 (1%) 80 74	160, 216, 269, 393	0
4	K	72/91 (79%)	1.28	16 (22%) 0 0	227, 323, 429, 470	0
5	F	468/613 (76%)	0.08	25 (5%) 26 23	137, 239, 365, 477	0
5	L	469/613 (76%)	-0.06	19 (4%) 37 31	162, 251, 379, 489	0
6	M	70/79 (88%)	0.12	3 (4%) 35 30	226, 315, 399, 479	0
6	N	69/79 (87%)	0.45	11 (15%) 1 2	325, 403, 501, 568	0
All	All	7224/8380 (86%)	0.14	356 (4%) 29 25	101, 230, 372, 568	0

The worst 5 of 356 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	338	THR	14.4
2	C	252	SER	10.7
2	C	241	LEU	9.4
3	J	1198	VAL	9.2
2	C	251	ALA	9.1

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 monosaccharides 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
7	MG	D	2001	1/1	0.42	0.18	251,251,251,251	0
8	ZN	N	101	1/1	0.78	0.06	465,465,465,465	0
8	ZN	M	101	1/1	0.84	0.04	468,468,468,468	0
8	ZN	J	2002	1/1	0.87	0.15	229,229,229,229	0
8	ZN	D	2002	1/1	0.94	0.15	182,182,182,182	0
8	ZN	D	2003	1/1	0.97	0.49	334,334,334,334	0
7	MG	J	2001	1/1	0.98	0.47	170,170,170,170	0
8	ZN	J	2003	1/1	0.99	0.24	126,126,126,126	0

6.5 Other polymers [i](#)

There are no such residues in this entry.