



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 09:01 PM GMT

PDB ID : 4XLR
Title : Crystal structure of T.aquaticus transcription initiation complex with CarD containing bubble promoter and RNA
Authors : Bae, B.; Darst, S.A.
Deposited on : 2015-01-13
Resolution : 4.30 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
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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) : rb-20026982

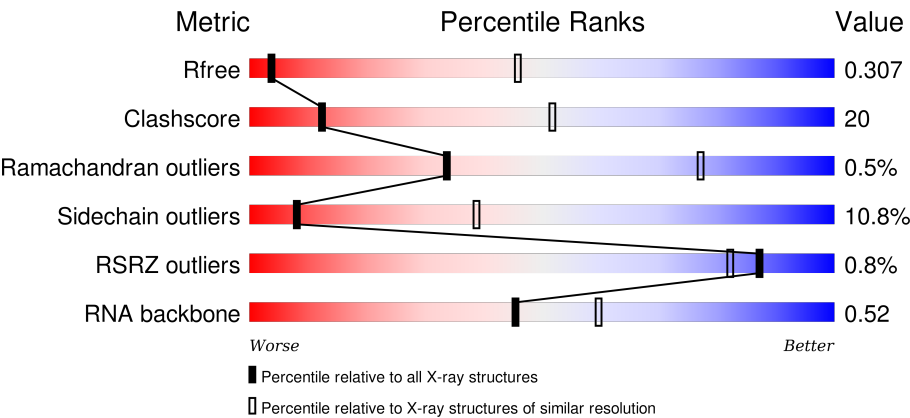
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.30 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	1059 (5.00-3.60)
Clashscore	102246	1166 (5.00-3.60)
Ramachandran outliers	100387	1106 (5.00-3.60)
Sidechain outliers	100360	1089 (5.00-3.60)
RSRZ outliers	91569	1062 (5.00-3.60)
RNA backbone	2183	1087 (5.60-2.80)

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	314	
1	B	314	
1	G	314	
1	H	314	

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Mol	Chain	Length	Quality of chain
2	C	1119	
2	I	1119	%
3	D	1524	
3	J	1524	
4	E	99	
4	K	99	
5	F	347	%
5	L	347	%
6	M	164	3%
6	N	164	3%
7	O	48	8%
7	R	48	2%
8	P	48	8%
8	S	48	2%
9	Q	4	25%
9	T	4	

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 60854 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
			1770	1130	303	334	3			
1	B	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	G	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	H	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1117	Total	C	N	O	S	0	0	0
			8762	5544	1558	1637	23			
2	I	1117	Total	C	N	O	S	0	0	0
			8762	5544	1558	1637	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1490	Total	C	N	O	S	0	0	0
			11761	7439	2088	2196	38			
3	J	1367	Total	C	N	O	S	0	0	0
			10779	6810	1923	2010	36			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	93	Total	C	N	O	S	0	0	0
			768	490	136	138	4			
4	K	93	Total	C	N	O	S	0	0	0
			768	490	136	138	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	345	Total	C	N	O	S	0	0	0
			2787	1758	502	523	4			
5	L	345	Total	C	N	O	S	0	0	0
			2787	1758	502	523	4			

- Molecule 6 is a protein called CarD-like transcriptional regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	M	158	Total	C	N	O	S	0	0	0
			1239	787	229	221	2			
6	N	158	Total	C	N	O	S	0	0	0
			1239	787	229	221	2			

- Molecule 7 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	O	48	Total	C	N	O	P	0	0	0
			988	472	182	287	47			
7	R	48	Total	C	N	O	P	0	0	0
			988	472	182	287	47			

- Molecule 8 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	P	48	Total	C	N	O	P	0	0	0
			985	471	183	284	47			
8	S	48	Total	C	N	O	P	0	0	0
			985	471	183	284	47			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	Q	4	Total	C	N	O	P	0	0	0
			85	38	15	28	4			
9	T	4	Total	C	N	O	P	0	0	0
			85	38	15	28	4			

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

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

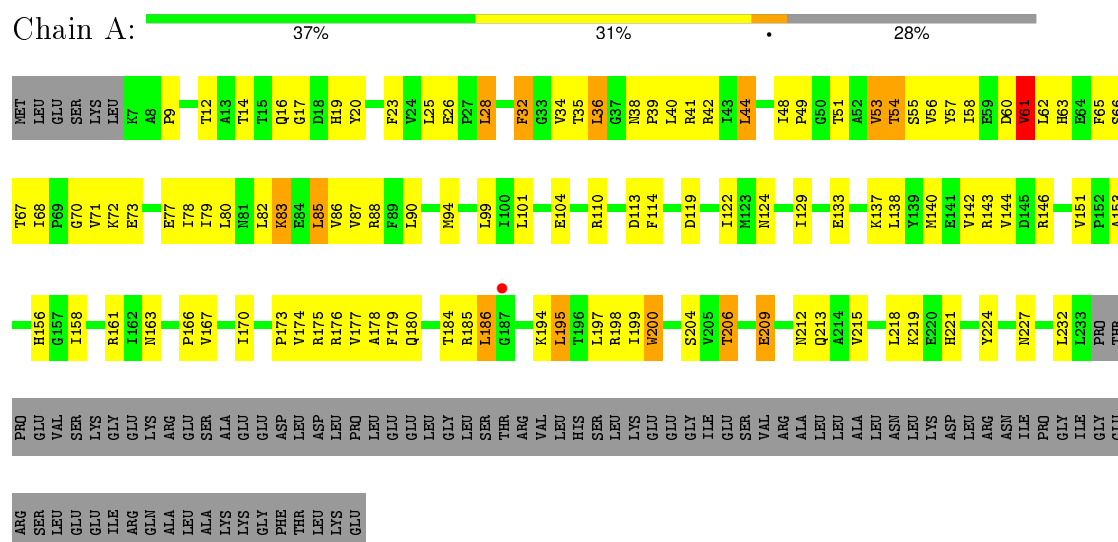
- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

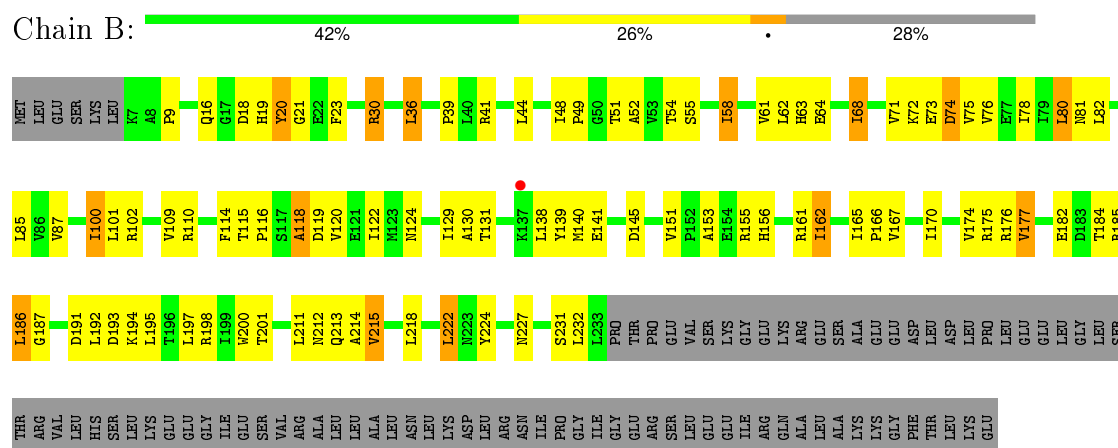
3 Residue-property plots

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

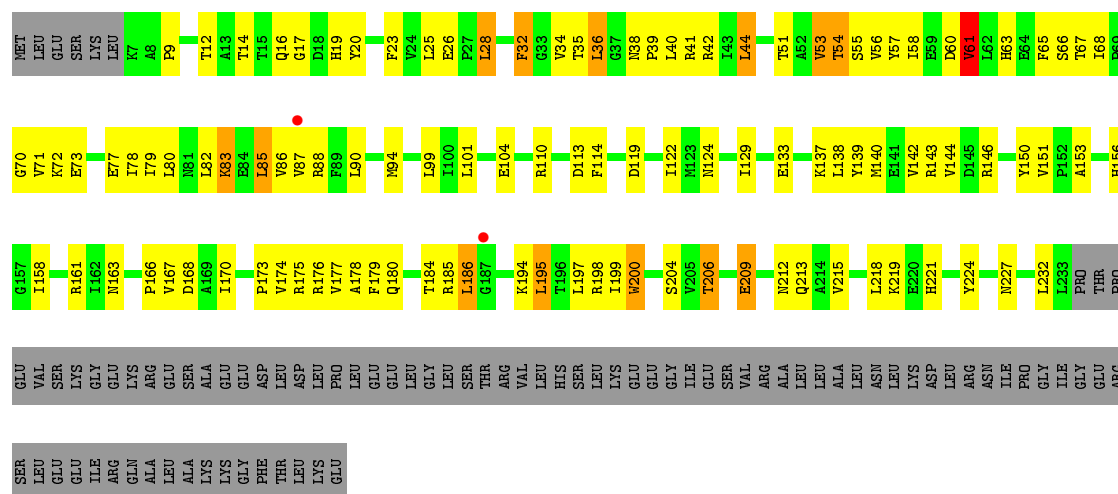


• Molecule 1: DNA-directed RNA polymerase subunit alpha



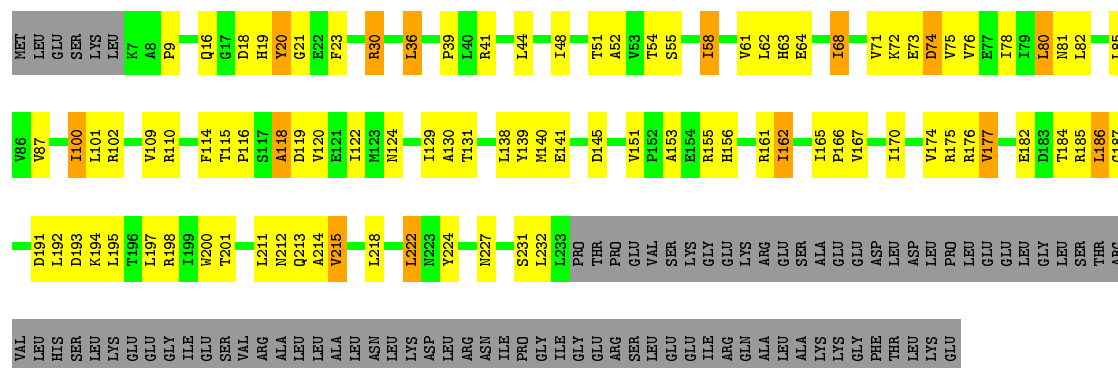
• Molecule 1: DNA-directed RNA polymerase subunit alpha





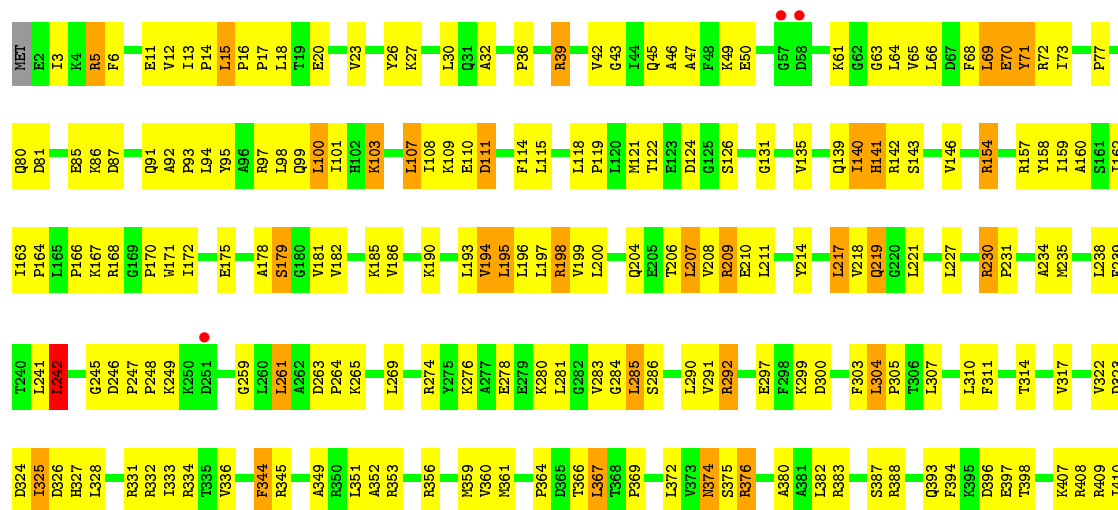
• Molecule 1: DNA-directed RNA polymerase subunit alpha

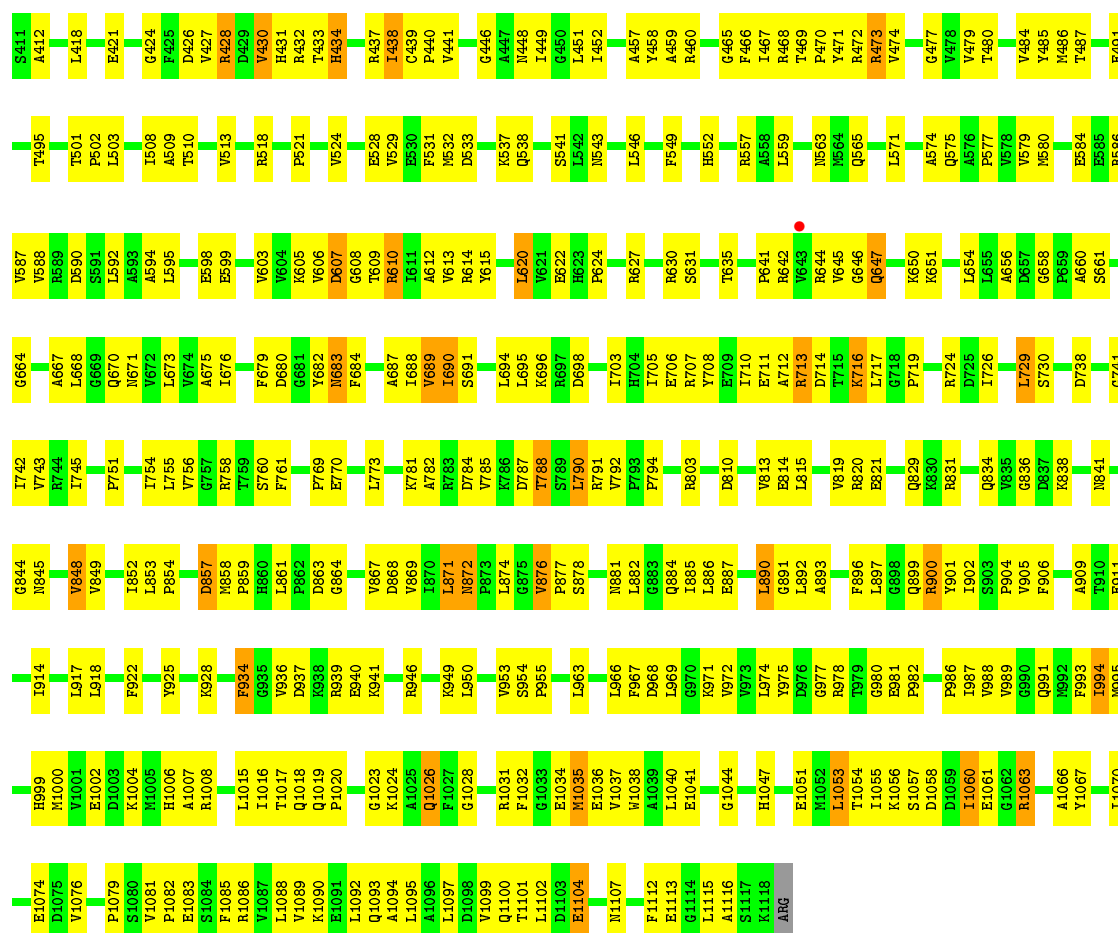
Chain H: 42% 26% 28%



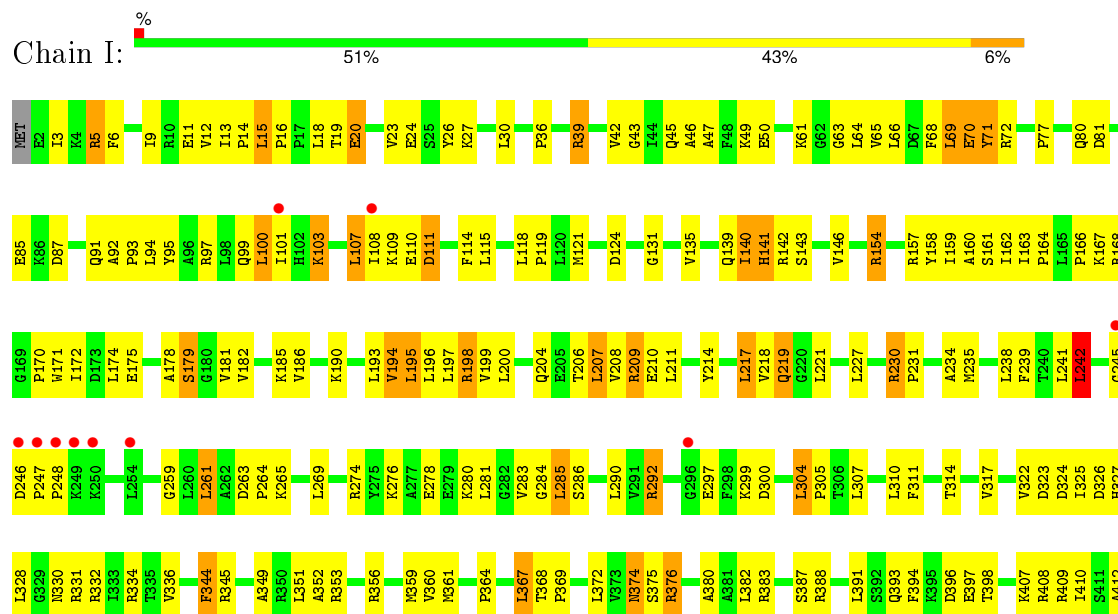
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C: 51% 43% 6%





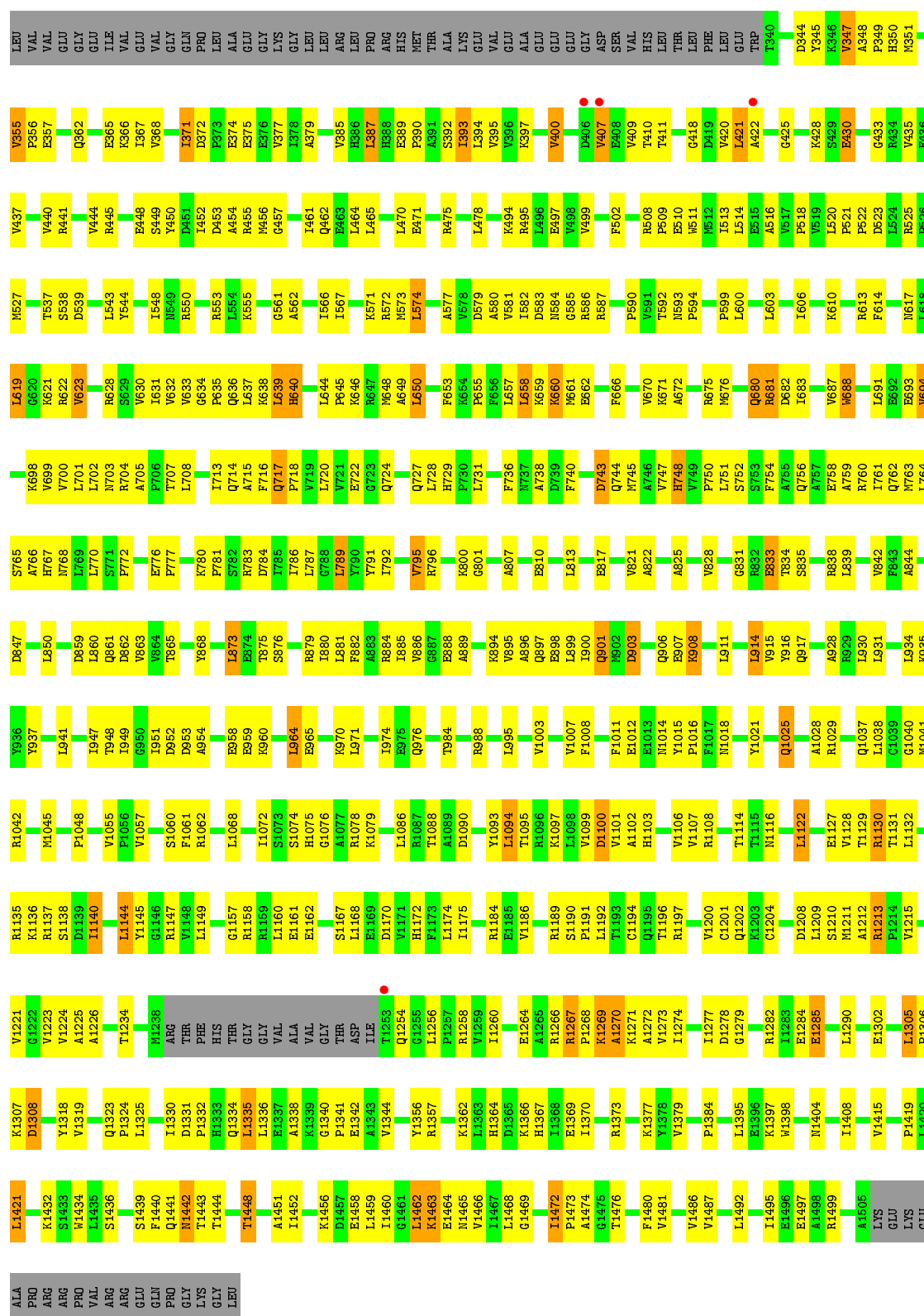
• Molecule 2: DNA-directed RNA polymerase subunit beta





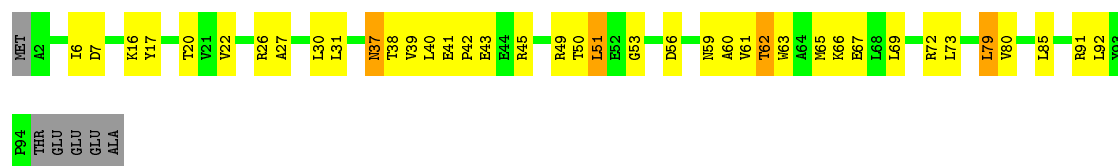
Response	Percentage
Yes	49%
No	37%
Don't know	1%
No answer	10%





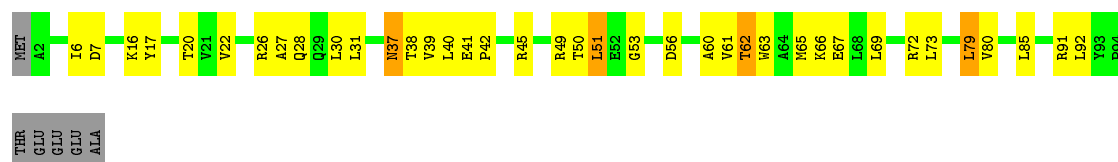
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 55% 35% 6%



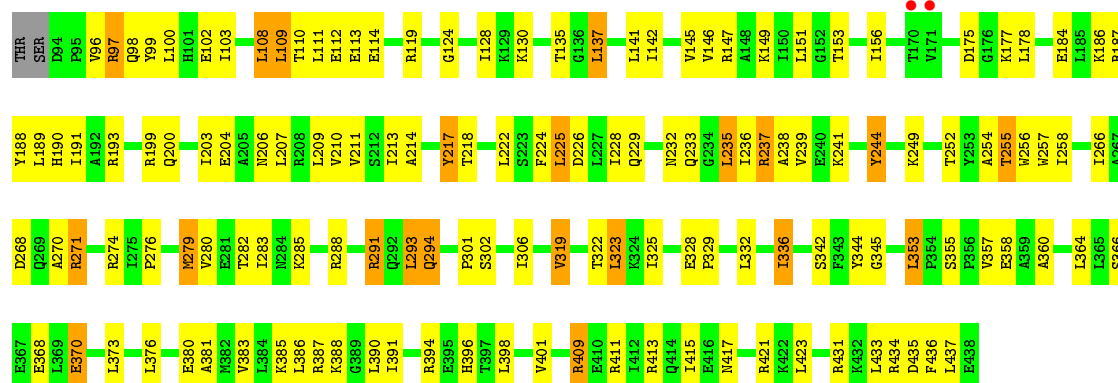
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain K: 56% 34% 6%



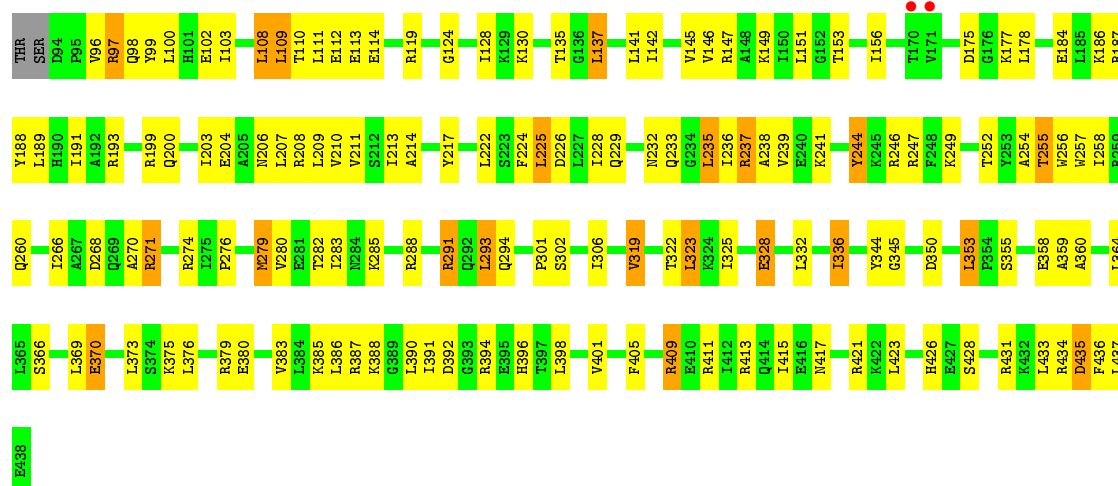
- Molecule 5: RNA polymerase sigma factor SigA

Chain F: 59% 35% 6%

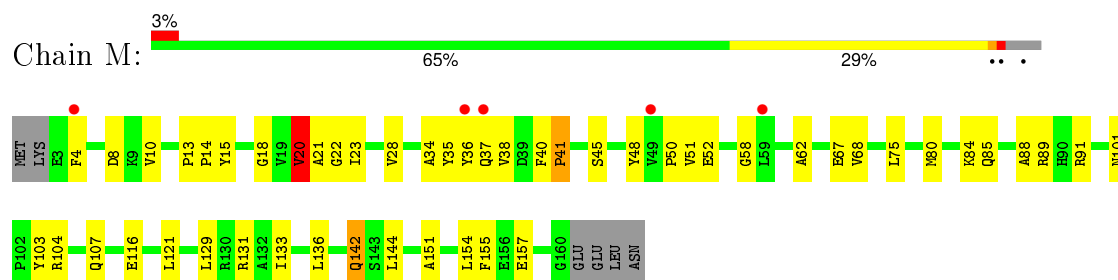


- Molecule 5: RNA polymerase sigma factor SigA

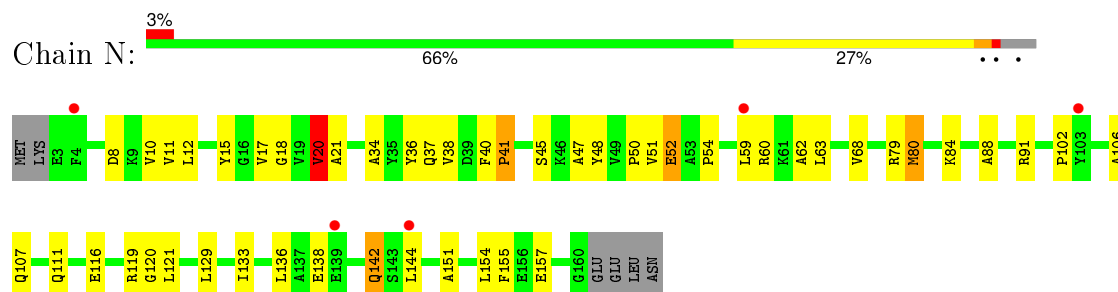
Chain L: 57% 36% 6%



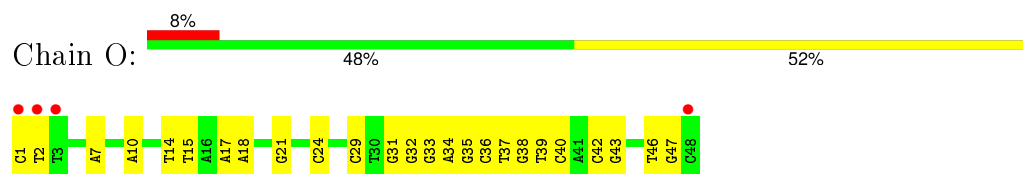
- Molecule 6: CarD-like transcriptional regulator



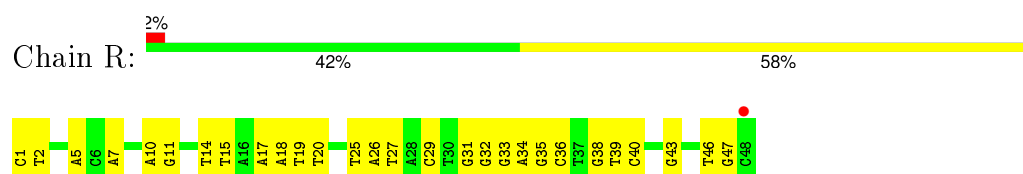
- Molecule 6: CarD-like transcriptional regulator



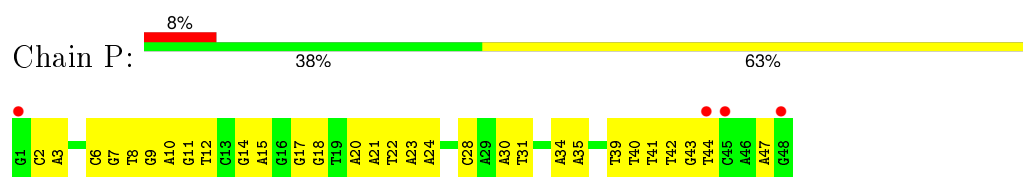
- Molecule 7: DNA (48-MER)



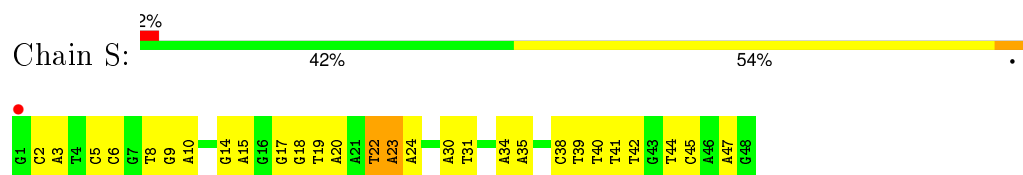
- Molecule 7: DNA (48-MER)



- Molecule 8: DNA (48-MER)



- Molecule 8: DNA (48-MER)



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	289.84Å 289.84Å 536.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.56 – 4.30 39.56 – 4.30	Depositor EDS
% Data completeness (in resolution range)	94.8 (39.56-4.30) 94.8 (39.56-4.30)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 4.28Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1839)	Depositor
R, R_{free}	0.275 , 0.310 0.268 , 0.307	Depositor DCC
R_{free} test set	7326 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	165.1	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 123.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Outliers	0 of 146564 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	60854	wwPDB-VP
Average B, all atoms (Å ²)	179.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.29	0/1804	0.52	0/2455
1	B	0.27	0/1804	0.49	0/2455
1	G	0.30	0/1804	0.52	0/2455
1	H	0.27	0/1804	0.49	0/2455
2	C	0.29	0/8929	0.51	1/12074 (0.0%)
2	I	0.29	0/8929	0.51	1/12074 (0.0%)
3	D	0.29	0/11963	0.50	0/16165
3	J	0.28	0/10959	0.49	0/14802
4	E	0.27	0/783	0.53	0/1054
4	K	0.27	0/783	0.53	0/1054
5	F	0.34	0/2829	0.54	0/3804
5	L	0.33	0/2829	0.54	0/3804
6	M	0.35	0/1267	0.55	0/1719
6	N	0.35	0/1267	0.55	0/1719
7	O	0.59	0/1109	0.92	0/1712
7	R	0.56	0/1109	0.92	0/1712
8	P	0.64	0/1106	0.88	0/1706
8	S	0.61	0/1106	0.90	2/1706 (0.1%)
9	Q	0.24	0/94	0.71	0/144
9	T	0.24	0/94	0.76	0/144
All	All	0.33	0/62372	0.55	4/85213 (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	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	J	0	1
6	M	0	2
6	N	0	2
All	All	0	10

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	23	DA	O5'-P-OP1	-6.61	99.75	105.70
2	C	242	LEU	CA-CB-CG	5.68	128.36	115.30
2	I	242	LEU	CA-CB-CG	5.57	128.10	115.30
8	S	22	DT	OP1-P-O3'	5.13	116.48	105.20

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	360	VAL	Peptide
2	C	71	TYR	Mainchain
3	D	1270	ALA	Peptide
2	I	360	VAL	Peptide
2	I	71	TYR	Mainchain

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	1770	0	1799	87	0
1	B	1770	0	1799	66	0
1	G	1770	0	1799	88	0
1	H	1770	0	1799	65	0
2	C	8762	0	8854	435	0
2	I	8762	0	8854	436	0
3	D	11761	0	11976	537	0
3	J	10779	0	10993	490	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	768	0	784	38	0
4	K	768	0	784	36	0
5	F	2787	0	2866	122	0
5	L	2787	0	2866	127	0
6	M	1239	0	1259	38	0
6	N	1239	0	1259	39	0
7	O	988	0	544	30	0
7	R	988	0	544	38	0
8	P	985	0	543	36	0
8	S	985	0	543	30	0
9	Q	85	0	43	1	0
9	T	85	0	43	2	0
10	D	2	0	0	0	0
10	J	2	0	0	0	0
11	D	1	0	0	0	0
11	J	1	0	0	0	0
All	All	60854	0	59951	2363	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 2363 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:D:73:CYS:HB3	3:D:76:CYS:SG	1.97	1.04
3:J:73:CYS:HB3	3:J:76:CYS:SG	1.97	1.04
3:D:105:VAL:HA	3:D:112:ILE:HD11	1.55	0.89
3:D:412:GLY:HA2	3:D:434:ARG:HD3	1.55	0.89
3:J:105:VAL:HA	3:J:112:ILE:HD11	1.55	0.88

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	225/314 (72%)	191 (85%)	32 (14%)	2 (1%)	21	67
1	B	225/314 (72%)	196 (87%)	27 (12%)	2 (1%)	21	67
1	G	225/314 (72%)	190 (84%)	33 (15%)	2 (1%)	21	67
1	H	225/314 (72%)	196 (87%)	27 (12%)	2 (1%)	21	67
2	C	1115/1119 (100%)	974 (87%)	137 (12%)	4 (0%)	39	80
2	I	1115/1119 (100%)	974 (87%)	137 (12%)	4 (0%)	39	80
3	D	1486/1524 (98%)	1306 (88%)	171 (12%)	9 (1%)	30	74
3	J	1361/1524 (89%)	1200 (88%)	156 (12%)	5 (0%)	39	80
4	E	91/99 (92%)	82 (90%)	9 (10%)	0	100	100
4	K	91/99 (92%)	82 (90%)	9 (10%)	0	100	100
5	F	343/347 (99%)	301 (88%)	41 (12%)	1 (0%)	46	83
5	L	343/347 (99%)	300 (88%)	42 (12%)	1 (0%)	46	83
6	M	156/164 (95%)	143 (92%)	11 (7%)	2 (1%)	15	60
6	N	156/164 (95%)	142 (91%)	12 (8%)	2 (1%)	15	60
All	All	7157/7762 (92%)	6277 (88%)	844 (12%)	36 (0%)	34	77

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	VAL
3	D	681	ARG
3	D	683	ILE
3	D	1128	VAL
1	G	53	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	194/270 (72%)	171 (88%)	23 (12%)	6	34
1	B	194/270 (72%)	167 (86%)	27 (14%)	4	29
1	G	194/270 (72%)	171 (88%)	23 (12%)	6	34
1	H	194/270 (72%)	167 (86%)	27 (14%)	4	29
2	C	931/936 (100%)	820 (88%)	111 (12%)	6	34
2	I	931/936 (100%)	820 (88%)	111 (12%)	6	34
3	D	1252/1281 (98%)	1115 (89%)	137 (11%)	8	38
3	J	1150/1281 (90%)	1033 (90%)	117 (10%)	9	40
4	E	83/88 (94%)	77 (93%)	6 (7%)	18	57
4	K	83/88 (94%)	77 (93%)	6 (7%)	18	57
5	F	296/299 (99%)	267 (90%)	29 (10%)	10	43
5	L	296/299 (99%)	267 (90%)	29 (10%)	10	43
6	M	127/133 (96%)	122 (96%)	5 (4%)	39	74
6	N	127/133 (96%)	122 (96%)	5 (4%)	39	74
All	All	6052/6554 (92%)	5396 (89%)	656 (11%)	8	39

5 of 656 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	1497	GLU
1	H	74	ASP
3	J	1462	LEU
5	F	108	LEU
1	G	12	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 109 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	294	GLN
2	I	434	HIS
5	L	269	GLN
5	F	295	GLN
1	H	81	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
9	Q	3/4 (75%)	2 (66%)	0
9	T	3/4 (75%)	0	0
All	All	6/8 (75%)	2 (33%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	Q	2	C
9	Q	3	G

There are no RNA pucker outliers to report.

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 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 [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, 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	227/314 (72%)	-0.23	1 (0%) 93 90	144, 176, 208, 241	0
1	B	227/314 (72%)	-0.41	1 (0%) 93 90	143, 164, 196, 228	0
1	G	227/314 (72%)	-0.03	2 (0%) 85 80	148, 188, 218, 252	0
1	H	227/314 (72%)	-0.34	0 100 100	145, 175, 207, 241	0
2	C	1117/1119 (99%)	-0.19	4 (0%) 93 90	144, 172, 211, 253	0
2	I	1117/1119 (99%)	-0.20	15 (1%) 79 71	144, 182, 221, 270	0
3	D	1490/1524 (97%)	-0.23	3 (0%) 95 94	117, 162, 195, 251	0
3	J	1367/1524 (89%)	-0.20	6 (0%) 93 90	120, 171, 204, 250	0
4	E	93/99 (93%)	-0.23	0 100 100	144, 165, 194, 217	0
4	K	93/99 (93%)	-0.23	0 100 100	144, 179, 206, 228	0
5	F	345/347 (99%)	-0.17	2 (0%) 90 86	144, 179, 222, 245	0
5	L	345/347 (99%)	-0.17	2 (0%) 90 86	145, 187, 225, 258	0
6	M	158/164 (96%)	0.17	5 (3%) 51 40	159, 207, 235, 243	0
6	N	158/164 (96%)	0.42	5 (3%) 51 40	171, 215, 240, 267	0
7	O	48/48 (100%)	0.34	4 (8%) 14 11	157, 217, 256, 270	0
7	R	48/48 (100%)	-0.22	1 (2%) 67 57	163, 207, 251, 276	0
8	P	48/48 (100%)	0.38	4 (8%) 14 11	161, 219, 260, 270	0
8	S	48/48 (100%)	-0.09	1 (2%) 67 57	167, 212, 250, 261	0
9	Q	4/4 (100%)	0.94	1 (25%) 1 2	175, 177, 186, 189	0
9	T	4/4 (100%)	-0.17	0 100 100	165, 183, 184, 196	0
All	All	7391/7962 (92%)	-0.18	57 (0%) 87 82	117, 174, 219, 276	0

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	187	GLY	4.7
2	I	246	ASP	4.4
3	J	216	LEU	3.4
3	D	1253	THR	3.4
7	O	1	DC	3.4

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(\AA^2)	Q<0.9
11	MG	J	2003	1/1	0.96	0.19	0.07	270,270,270,270	0
10	ZN	J	2001	1/1	0.89	0.14	-0.20	277,277,277,277	0
10	ZN	D	2002	1/1	0.92	0.16	-0.92	237,237,237,237	0
10	ZN	J	2002	1/1	0.95	0.07	-1.14	157,157,157,157	0
10	ZN	D	2001	1/1	0.98	0.10	-1.29	116,116,116,116	0
11	MG	D	2003	1/1	0.97	0.09	-1.89	283,283,283,283	0

6.5 Other polymers [i](#)

There are no such residues in this entry.