wwPDB X-ray Structure Validation Summary Report (i)

Aug 6, 2023 – 09:52 PM EDT

PDB ID	:	1K83
Title	:	Crystal Structure of Yeast RNA Polymerase II Complexed with the Inhibitor Alpha Amanitin
Authors	:	Bushnell, D.A.; Cramer, P.; Kornberg, R.D.
Deposited on	:	2001-10-22
Resolution	:	2.80 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 (i) 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 (i)) were used in the production of this report:

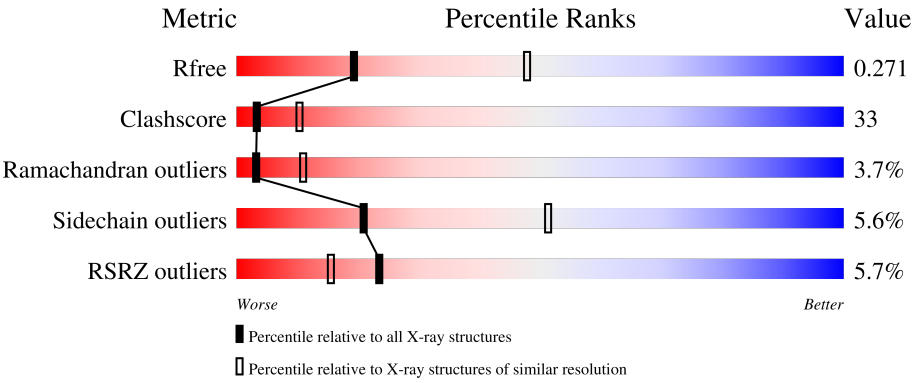
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 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 <=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	1733	4% 40% 33% 5% 21%
2	B	1224	6% 47% 38% · 12%
3	C	318	% 36% 43% · 16%
4	E	215	3% 56% 39% 5% ·
5	F	155	% 25% 27% · 46%

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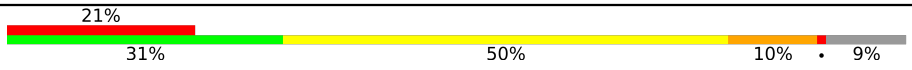
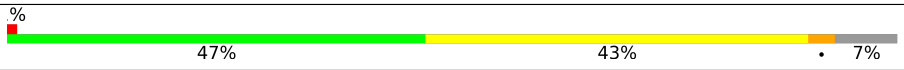
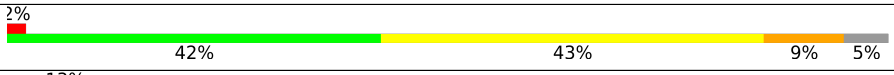
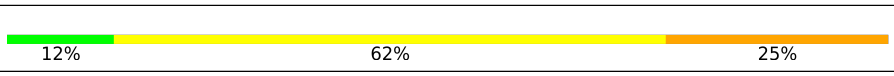
Mol	Chain	Length	Quality of chain
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	M	8	

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 27902 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 II LARGEST SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1366	10751	6785	1871	2036	59	0	0	0

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II 140KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1082	8616	5467	1503	1594	52	0	0	0

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II 45KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	266	2095	1317	348	417	13	0	0	0

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II 27KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	213	1744	1107	308	318	11	0	0	0

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASE II 23KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	84	679	434	115	127	3	0	0	0

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASE II 14.5KD POLYPEP-

TIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II 14.2KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	122	Total	C	N	O	S	0	0	0
			997	613	182	191	11			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASE II 8.3KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II 13.6KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASE II 7.7KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	45	Total	C	N	O	S	0	0	0
			359	221	71	63	4			

- Molecule 11 is a protein called ALPHA AMANITIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	M	8	Total	C	N	O	S	0	0	0
			64	39	10	14	1			

- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	2	Total Zn 2 2	0	0
12	B	1	Total Zn 1 1	0	0
12	C	1	Total Zn 1 1	0	0
12	I	2	Total Zn 2 2	0	0
12	J	1	Total Zn 1 1	0	0
12	L	1	Total Zn 1 1	0	0

- Molecule 13 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total Mn 1 1	0	0

- Molecule 14 is water.

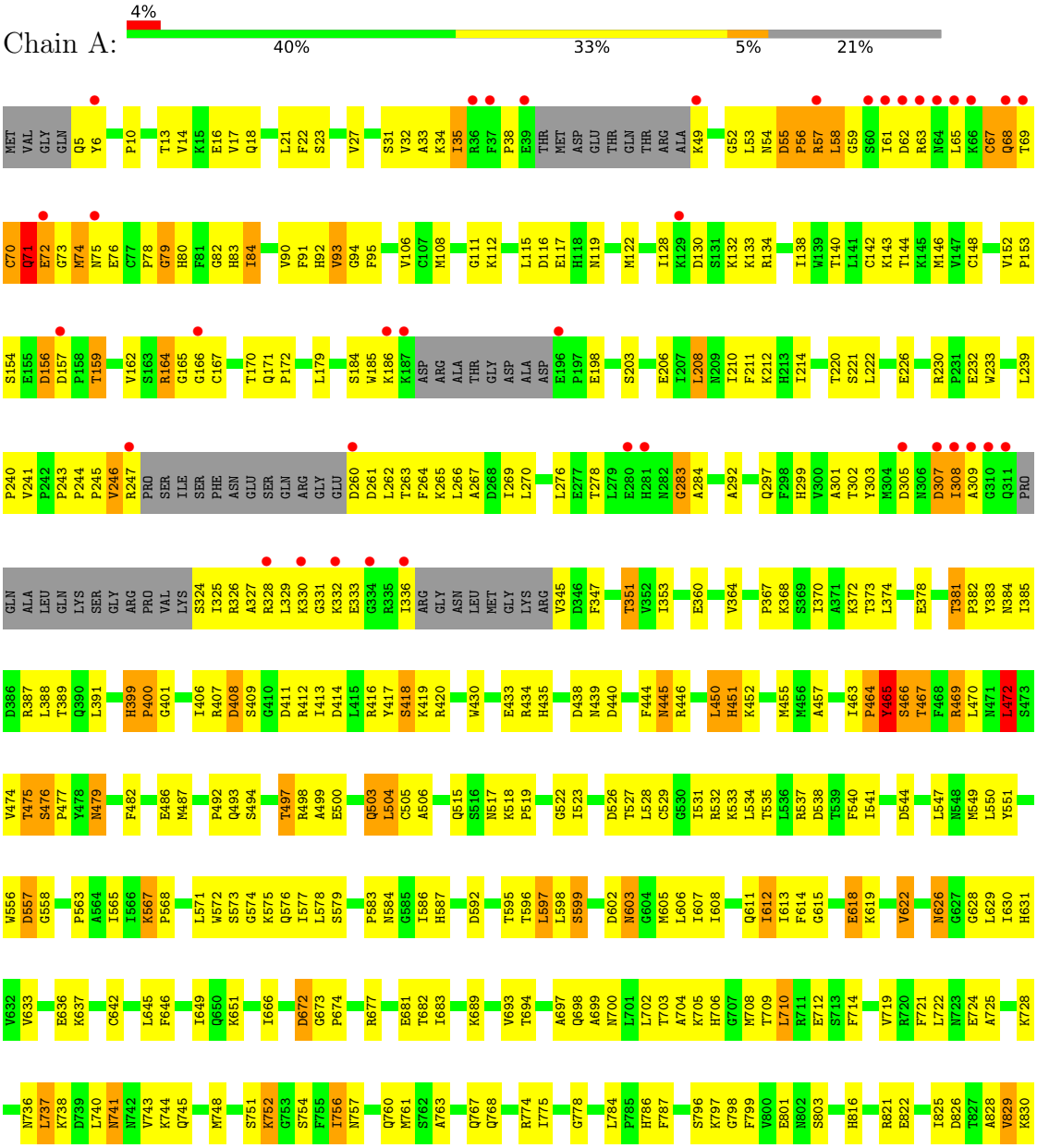
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	31	Total O 31 31	0	0
14	B	23	Total O 23 23	0	0
14	C	3	Total O 3 3	0	0
14	E	6	Total O 6 6	0	0
14	F	4	Total O 4 4	0	0
14	J	1	Total O 1 1	0	0
14	M	1	Total O 1 1	0	0

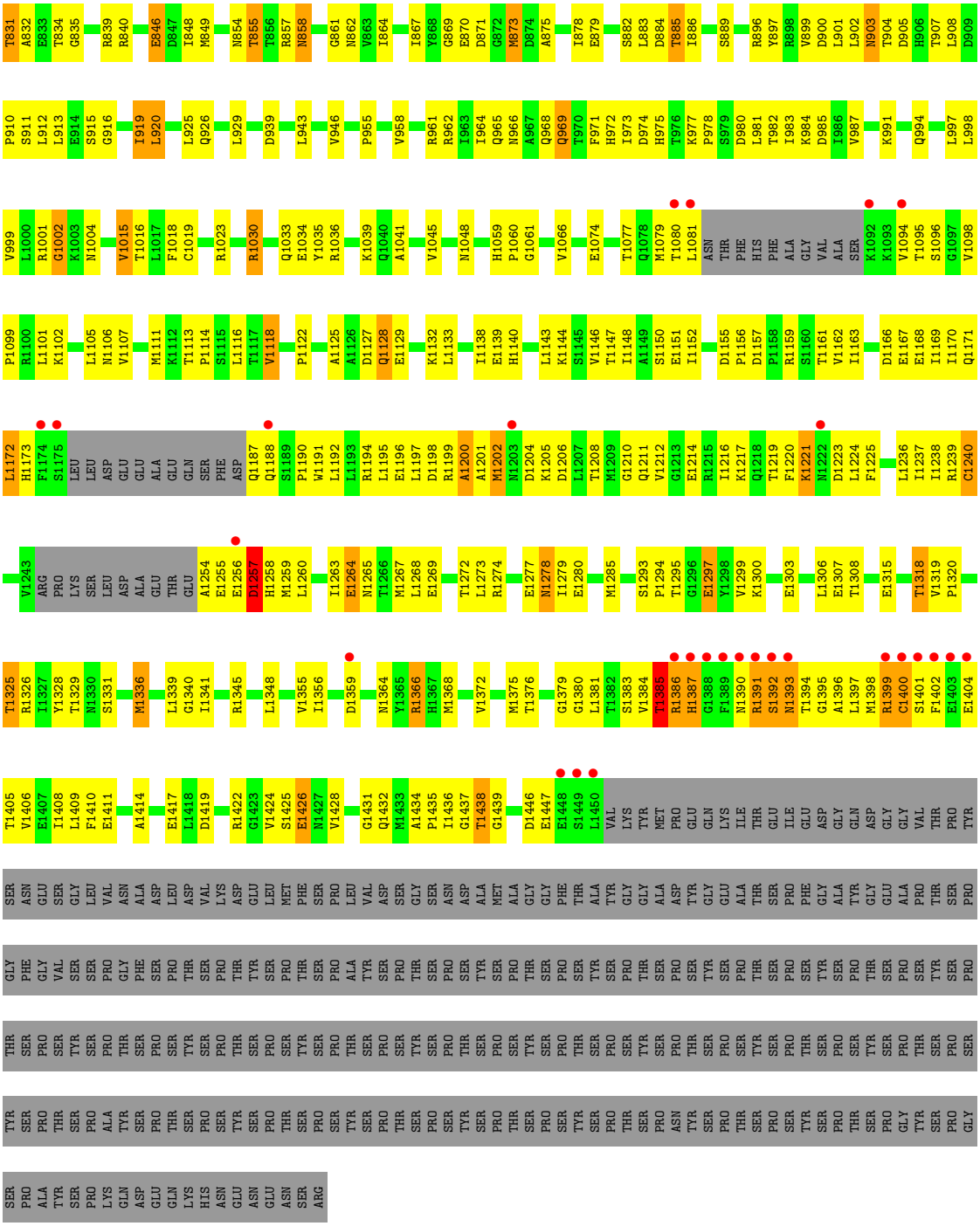
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DNA-DIRECTED RNA POLYMERASE II LARGEST SUBUNIT

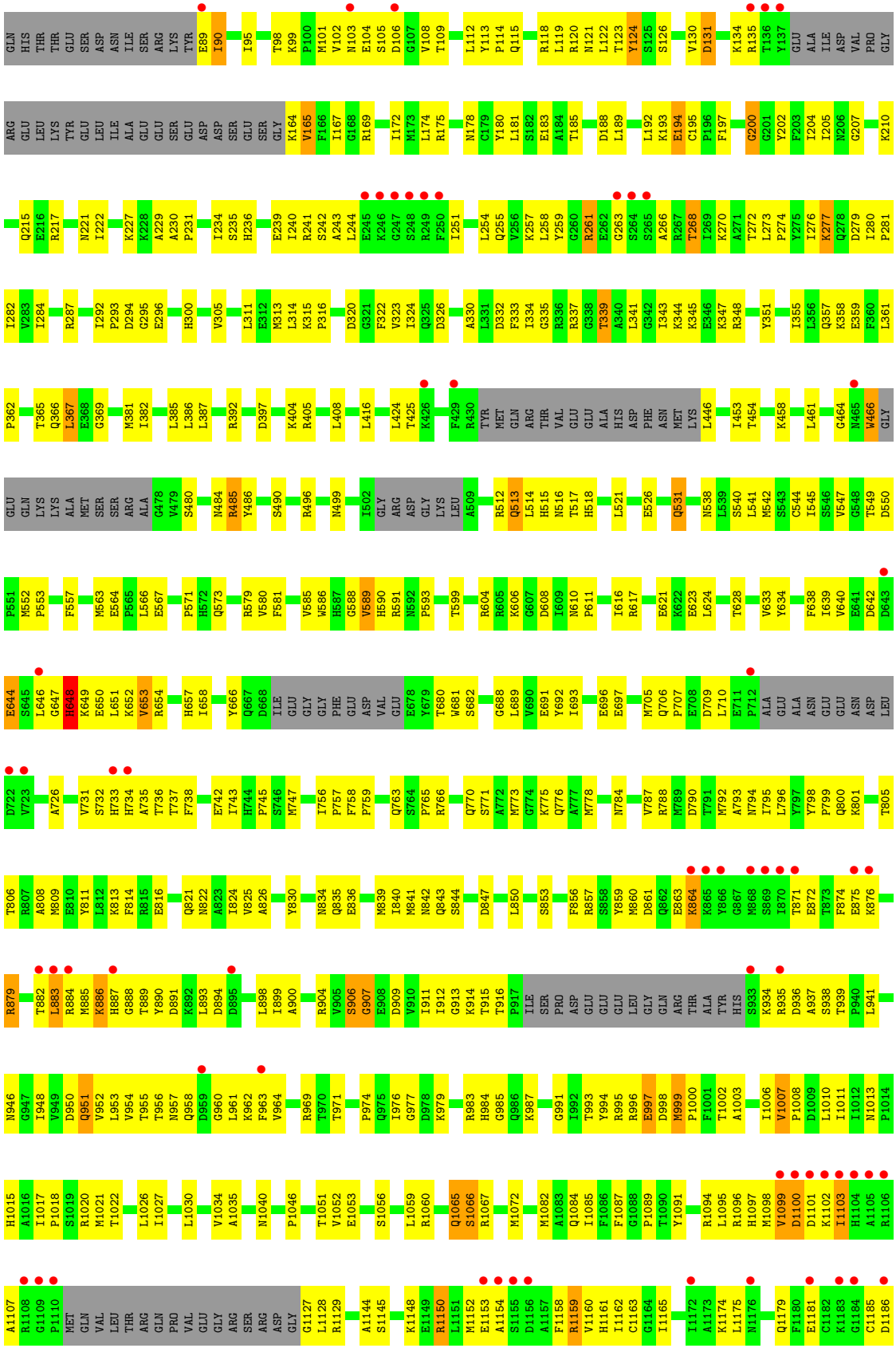
Chain A:





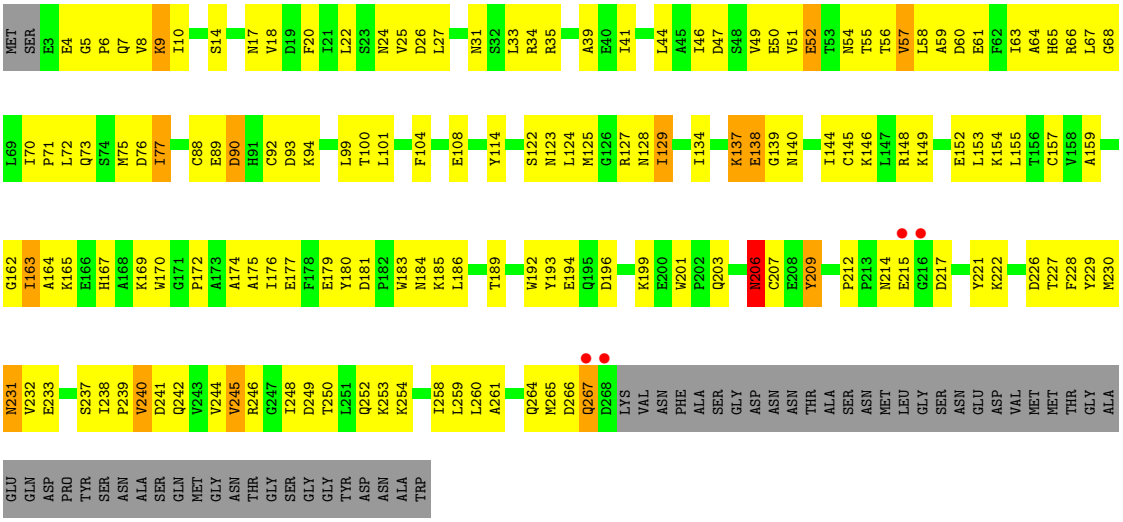
• Molecule 2: DNA-DIRECTED RNA POLYMERASE II 140KD POLYPEPTIDE

Chain B:



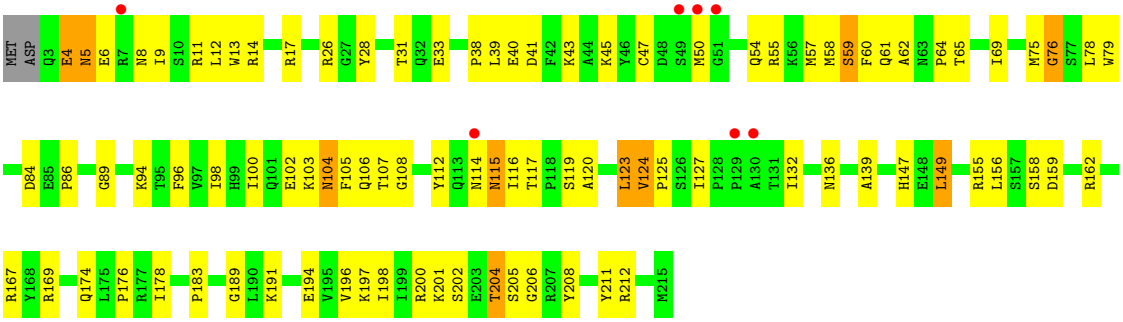
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II 45KD POLYPEPTIDE

Chain C:



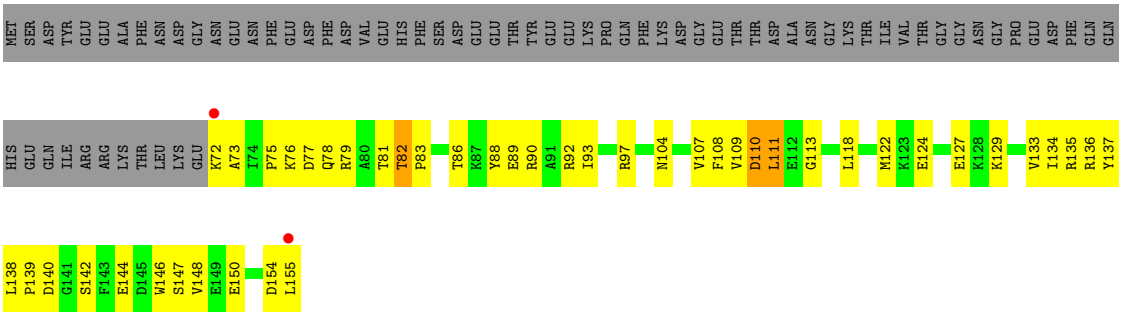
• Molecule 4: DNA-DIRECTED RNA POLYMERASE II 27KD POLYPEPTIDE

Chain E:



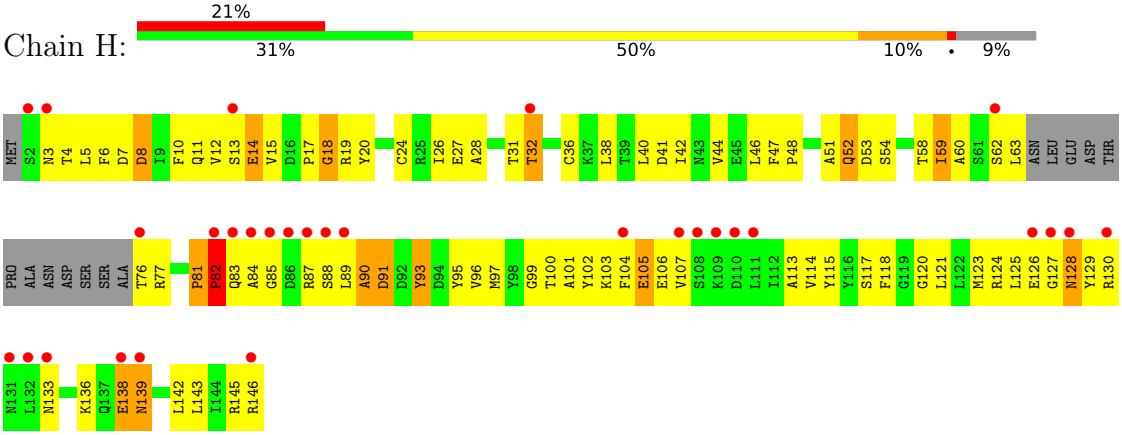
• Molecule 5: DNA-DIRECTED RNA POLYMERASE II 23KD POLYPEPTIDE

Chain F:



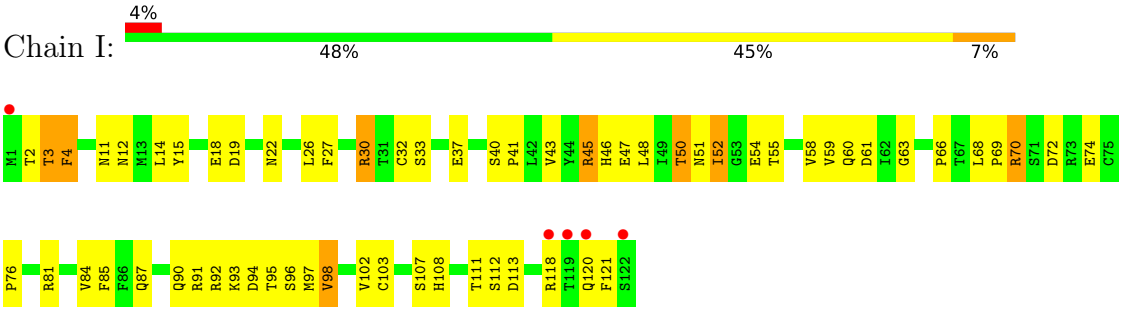
• Molecule 6: DNA-DIRECTED RNA POLYMERASE II 14.5KD POLYPEPTIDE

Chain H:



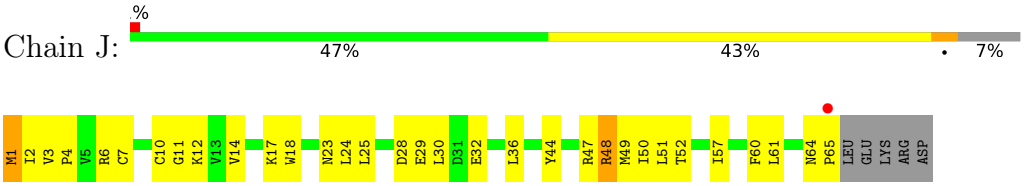
• Molecule 7: DNA-DIRECTED RNA POLYMERASE II 14.2KD POLYPEPTIDE

Chain I:



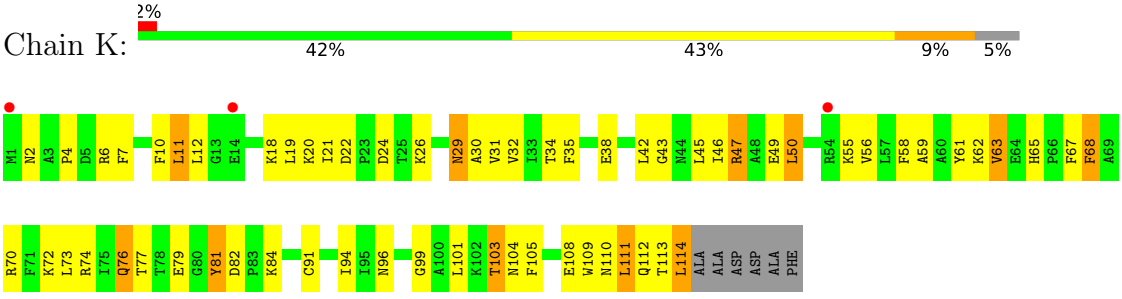
• Molecule 8: DNA-DIRECTED RNA POLYMERASE II 8.3KD POLYPEPTIDE

Chain J:



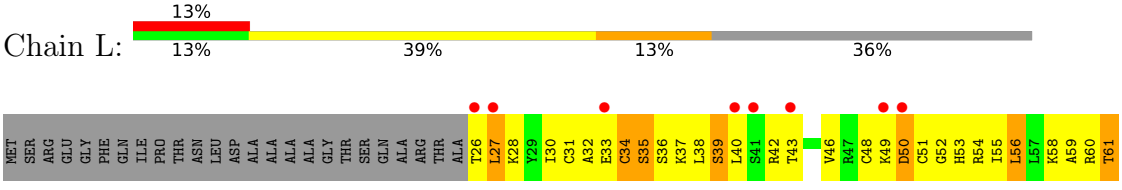
• Molecule 9: DNA-DIRECTED RNA POLYMERASE II 13.6KD POLYPEPTIDE

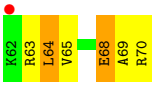
Chain K:



• Molecule 10: DNA-DIRECTED RNA POLYMERASE II 7.7KD POLYPEPTIDE

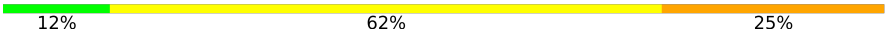
Chain L:





• Molecule 11: ALPHA AMANITIN

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	122.51Å 222.48Å 374.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.80) 93.4 (20.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 2.79Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.280 0.221 , 0.271	Depositor DCC
R_{free} test set	3507 reflections (2.80%)	wwPDB-VP
Wilson B-factor (Å^2)	50.5	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 47.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	27902	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% 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, 0.333 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: CSX, ZN, HYP, MN, TRX, ILX

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	0.42	0/10940	0.68	2/14792 (0.0%)
2	B	0.42	0/8786	0.68	1/11847 (0.0%)
3	C	0.40	0/2133	0.66	0/2891
4	E	0.40	0/1780	0.67	0/2395
5	F	0.46	0/691	0.67	0/933
6	H	0.36	0/1086	0.68	0/1470
7	I	0.48	0/1016	0.68	0/1365
8	J	0.44	0/541	0.70	0/727
9	K	0.39	0/937	0.62	0/1265
10	L	0.47	0/361	0.71	0/478
11	M	2.39	1/22 (4.5%)	1.63	0/26
All	All	0.42	1/28293 (0.0%)	0.68	3/38189 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	7	ASN	CA-C	5.26	1.66	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	200	GLY	N-CA-C	5.82	127.64	113.10
1	A	798	GLY	N-CA-C	5.55	126.98	113.10
1	A	472	LEU	CA-CB-CG	-5.01	103.78	115.30

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	10751	0	10819	759	0
2	B	8616	0	8645	586	0
3	C	2095	0	2051	165	0
4	E	1744	0	1772	87	0
5	F	679	0	701	55	0
6	H	1068	0	1040	115	0
7	I	997	0	953	75	0
8	J	532	0	542	56	0
9	K	919	0	929	71	0
10	L	359	0	382	61	1
11	M	64	0	51	7	0
12	A	2	0	0	0	0
12	B	1	0	0	0	0
12	C	1	0	0	0	0
12	I	2	0	0	0	0
12	J	1	0	0	0	0
12	L	1	0	0	0	0
13	A	1	0	0	0	0
14	A	31	0	0	1	0
14	B	23	0	0	5	0
14	C	3	0	0	0	0
14	E	6	0	0	1	0
14	F	4	0	0	0	0
14	J	1	0	0	0	0
14	M	1	0	0	0	0
All	All	27902	0	27885	1826	1

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 33.

The worst 5 of 1826 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:1161:THR:HG22	1:A:1163:ILE:H	1.09	1.15
2:B:1051:THR:HG22	2:B:1053:GLU:H	1.17	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:871:THR:HG22	2:B:872:GLU:H	1.09	1.09
1:A:855:THR:HG21	1:A:857:ARG:HE	1.10	1.08
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.33	1.07

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:28:LYS:NZ	10:L:28:LYS:NZ[3_655]	2.05	0.15

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	1348/1733 (78%)	1160 (86%)	134 (10%)	54 (4%)	3 9
2	B	1062/1224 (87%)	931 (88%)	107 (10%)	24 (2%)	6 21
3	C	264/318 (83%)	223 (84%)	30 (11%)	11 (4%)	3 9
4	E	211/215 (98%)	180 (85%)	23 (11%)	8 (4%)	3 10
5	F	82/155 (53%)	71 (87%)	10 (12%)	1 (1%)	13 39
6	H	129/146 (88%)	88 (68%)	23 (18%)	18 (14%)	0 0
7	I	120/122 (98%)	102 (85%)	16 (13%)	2 (2%)	9 29
8	J	63/70 (90%)	58 (92%)	5 (8%)	0	100 100
9	K	112/120 (93%)	98 (88%)	13 (12%)	1 (1%)	17 46
10	L	43/70 (61%)	23 (54%)	13 (30%)	7 (16%)	0 0
11	M	4/8 (50%)	4 (100%)	0	0	100 100
All	All	3438/4181 (82%)	2938 (86%)	374 (11%)	126 (4%)	3 11

5 of 126 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	ASP
1	A	56	PRO
1	A	399	HIS
1	A	464	PRO
1	A	465	TYR

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	1196/1520 (79%)	1116 (93%)	80 (7%)	16 43
2	B	940/1061 (89%)	899 (96%)	41 (4%)	28 61
3	C	234/274 (85%)	221 (94%)	13 (6%)	21 51
4	E	195/197 (99%)	190 (97%)	5 (3%)	46 79
5	F	74/137 (54%)	71 (96%)	3 (4%)	30 64
6	H	117/128 (91%)	114 (97%)	3 (3%)	46 79
7	I	116/116 (100%)	108 (93%)	8 (7%)	15 41
8	J	60/65 (92%)	57 (95%)	3 (5%)	24 56
9	K	99/102 (97%)	88 (89%)	11 (11%)	6 19
10	L	40/57 (70%)	34 (85%)	6 (15%)	3 9
11	M	2/2 (100%)	2 (100%)	0	100 100
All	All	3073/3659 (84%)	2900 (94%)	173 (6%)	21 51

5 of 173 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1065	GLN
6	H	91	ASP
2	B	1211	ASN
3	C	206	ASN
7	I	70	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	786	ASN
3	C	65	HIS
2	B	1015	HIS
2	B	1177	HIS
3	C	131	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)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
11	HYP	M	8	11	6,8,9	0.95	0	5,10,12	1.49	1 (20%)
11	ILX	M	1	11	8,9,10	2.41	3 (37%)	9,11,13	2.02	3 (33%)
11	CSX	M	6	11	3,6,7	2.97	2 (66%)	1,6,8	0.50	0
11	TRX	M	2	11	14,16,17	2.58	6 (42%)	15,22,24	1.79	6 (40%)

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
11	HYP	M	8	11	-	0/0/11/13	0/1/1/1
11	ILX	M	1	11	-	2/11/12/14	-
11	CSX	M	6	11	-	1/1/5/7	-
11	TRX	M	2	11	-	0/4/6/8	0/2/2/2

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	2	TRX	CZ2-CH2	5.63	1.47	1.37
11	M	1	ILX	CB-CA	5.03	1.60	1.54
11	M	2	TRX	CZ2-CE2	4.72	1.49	1.41
11	M	6	CSX	CB-CA	4.24	1.63	1.53
11	M	1	ILX	OG1-CG1	3.10	1.49	1.43

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	M	1	ILX	CB-CA-C	-3.65	108.02	112.94
11	M	1	ILX	CG2-CB-CG1	-3.48	105.72	111.17
11	M	2	TRX	CB-CA-C	3.19	117.45	111.47
11	M	2	TRX	OH2-CH2-CZ3	-2.88	111.82	120.02
11	M	2	TRX	CH2-CZ2-CE2	-2.77	116.37	119.29

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	M	6	CSX	N-CA-CB-SG
11	M	1	ILX	C-CA-CB-CG2
11	M	1	ILX	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	M	1	ILX	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 9 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, 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	1366/1733 (78%)	-0.05	66 (4%) 30 21	18, 48, 107, 137	0
2	B	1082/1224 (88%)	-0.03	71 (6%) 18 11	20, 46, 105, 128	0
3	C	266/318 (83%)	-0.11	4 (1%) 73 68	30, 53, 83, 124	0
4	E	213/215 (99%)	-0.00	7 (3%) 46 36	22, 59, 99, 109	0
5	F	84/155 (54%)	-0.26	2 (2%) 59 49	24, 44, 67, 82	0
6	H	133/146 (91%)	1.12	30 (22%) 0 0	64, 94, 122, 125	0
7	I	122/122 (100%)	-0.00	5 (4%) 37 27	30, 51, 89, 106	0
8	J	65/70 (92%)	-0.41	1 (1%) 73 68	26, 47, 76, 85	0
9	K	114/120 (95%)	-0.18	3 (2%) 56 46	31, 60, 79, 97	0
10	L	45/70 (64%)	1.01	9 (20%) 1 0	49, 86, 108, 110	0
11	M	4/8 (50%)	0.86	0 100 100	73, 80, 83, 84	0
All	All	3494/4181 (83%)	-0.00	198 (5%) 23 15	18, 50, 105, 137	0

The worst 5 of 198 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	69	THR	14.9
1	A	1390	ASN	10.9
2	B	882	THR	8.9
2	B	866	TYR	8.3
1	A	1389	PHE	8.2

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

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^{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	B-factors(Å^2)	Q<0.9
11	CSX	M	6	7/8	0.74	0.24	80,82,84,86	0
11	ILX	M	1	10/11	0.84	0.33	72,74,79,80	0
11	TRX	M	2	15/16	0.88	0.23	75,77,79,80	0
11	HYP	M	8	8/9	0.91	0.20	70,72,72,73	0

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, 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	B-factors(Å^2)	Q<0.9
13	MN	A	3009	1/1	0.72	0.35	149,149,149,149	0
12	ZN	L	3005	1/1	0.89	0.06	86,86,86,86	0
12	ZN	I	3004	1/1	0.96	0.07	62,62,62,62	0
12	ZN	A	3008	1/1	0.97	0.12	81,81,81,81	0
12	ZN	A	3006	1/1	0.97	0.10	64,64,64,64	0
12	ZN	B	3007	1/1	0.99	0.07	64,64,64,64	0
12	ZN	J	3001	1/1	0.99	0.12	46,46,46,46	0
12	ZN	C	3002	1/1	0.99	0.09	49,49,49,49	0
12	ZN	I	3003	1/1	0.99	0.08	45,45,45,45	0

6.5 Other polymers (i)

There are no such residues in this entry.