



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:02 PM UTC

PDB ID : 4BXZ / pdb_00004bxz
Title : RNA Polymerase II-Bye1 complex
Authors : Kinkelin, K.; Wozniak, G.G.; Rothbart, S.B.; Lidschreiber, M.; Strahl, B.D.; Cramer, P.
Deposited on : 2013-07-16
Resolution : 4.80 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 ⓘ 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

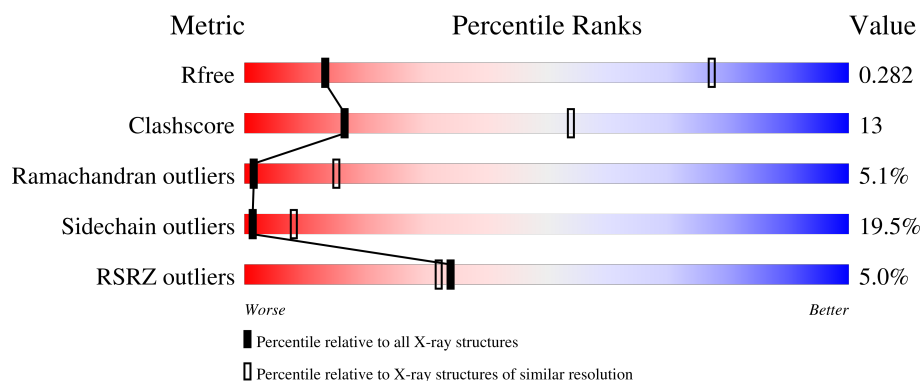
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.80 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}	180053	1018 (5.66-3.94)
Clashscore	190562	1001 (5.60-3.98)
Ramachandran outliers	187476	1104 (5.70-3.90)
Sidechain outliers	187428	1085 (5.70-3.90)
RSRZ outliers	180081	1013 (5.66-3.94)

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	1733	
2	B	1224	
3	C	318	
4	D	221	
5	E	215	

Continued on next page...

Mol	Chain	Length	Quality of chain
6	F	155	26% 25% 2% 46%
7	G	171	60% 36% 3%
8	H	146	9% 42% 38% 10% 9%
9	I	122	7% 54% 39%
10	J	70	6% 44% 40% 6% 7%
11	K	120	2% 62% 27% 8%
12	L	70	14% 36% 20% 9% 34%
13	X	594	4% 16% 81%

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 31509 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 SUBUNIT RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1416	Total	C	N	O	S	0	0	0
			11140	7021	1946	2111	62			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1097	Total	C	N	O	S	0	0	0
			8720	5526	1523	1617	54			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3.

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

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	177	Total	C	N	O	S	0	0	0
			1356	840	241	273	2			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC2.

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

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC3.

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

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC5.

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

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	115	Total	C	N	O	S	0	0	1
			920	590	157	171	2			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 13 is a protein called TRANSCRIPTION FACTOR BYE1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	X	113	Total	C	N	O	0	0	0
			564	338	113	113			

- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

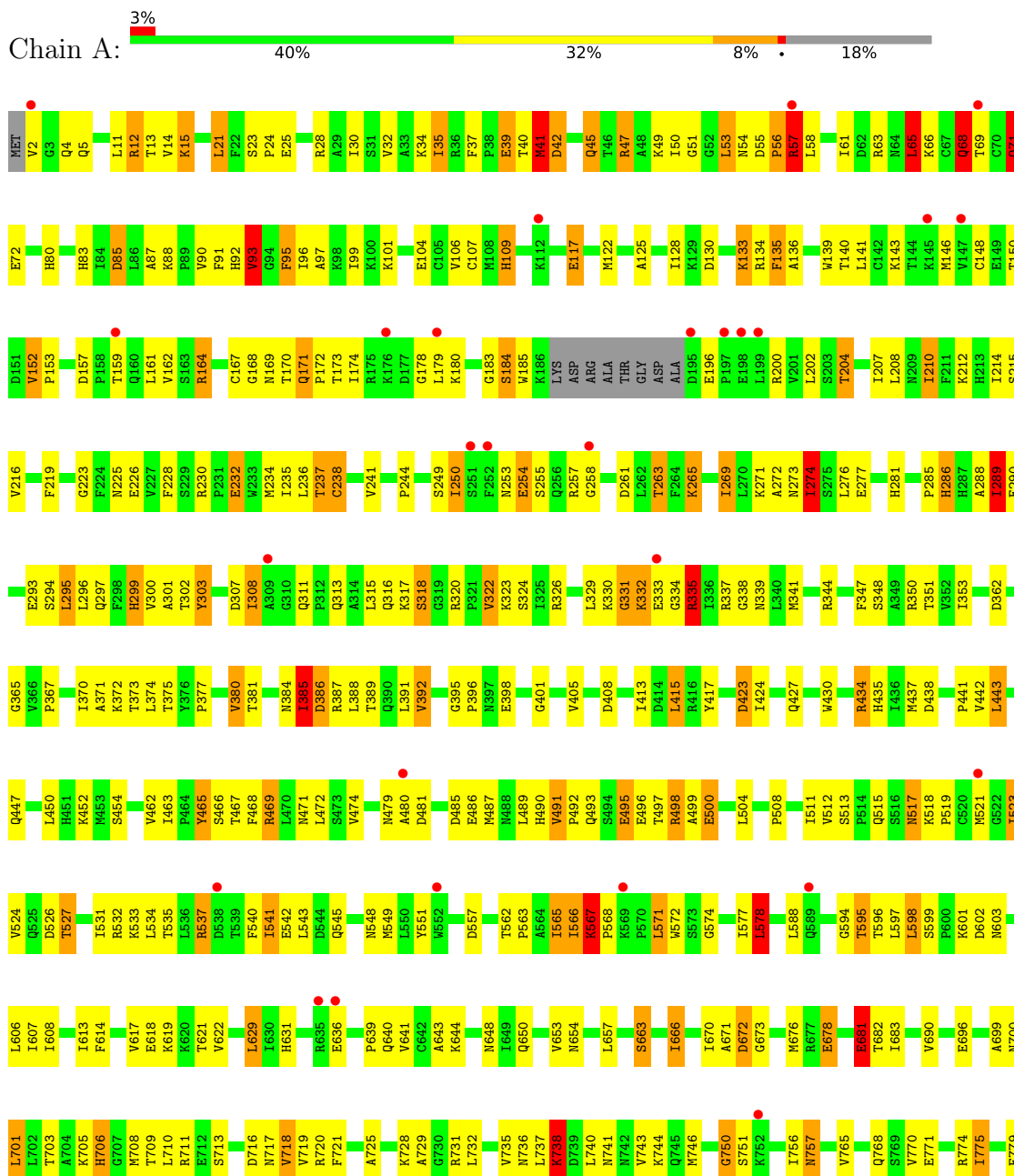
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

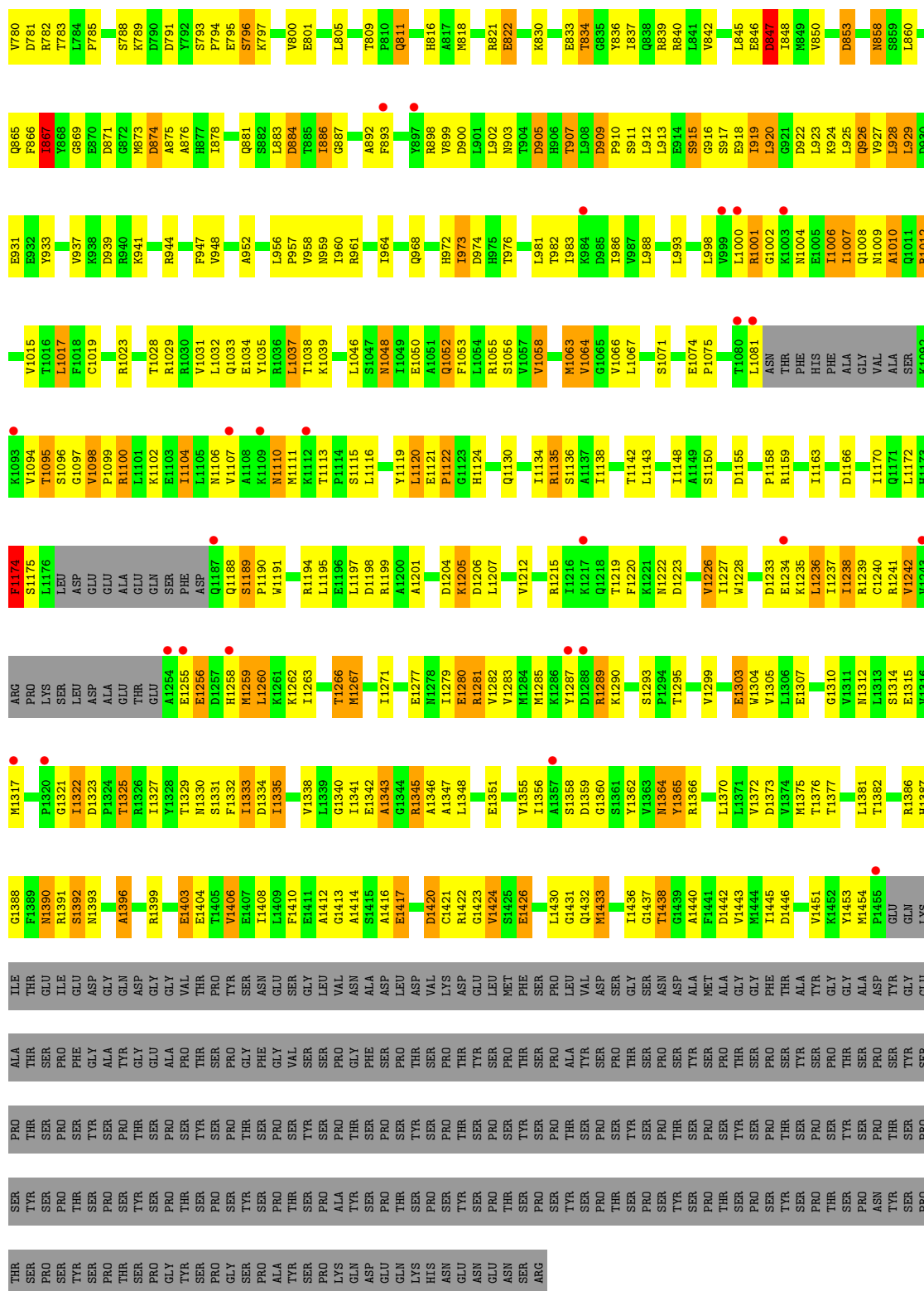
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Mg	0	0
			1	1		

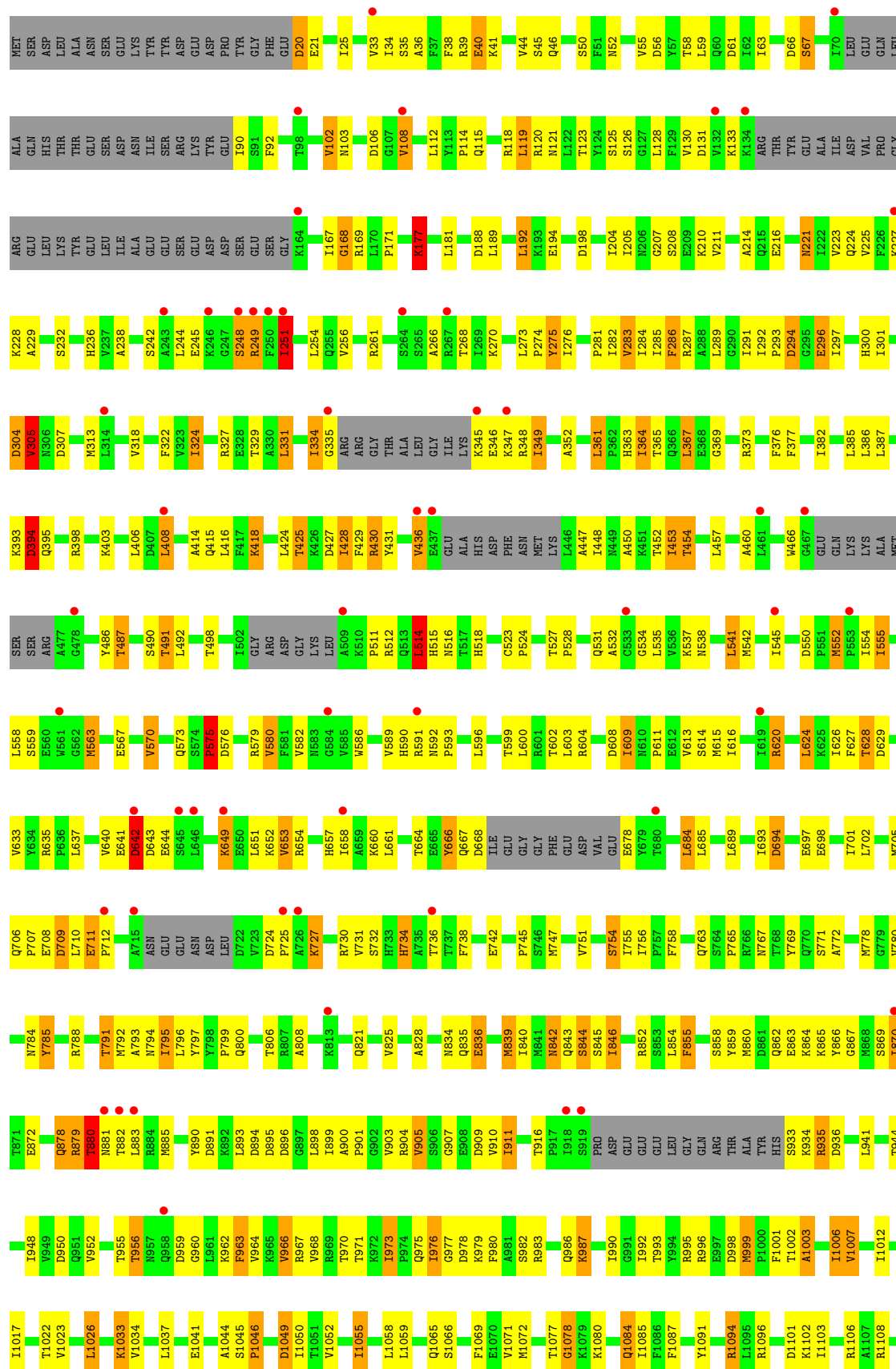
3 Residue-property plots

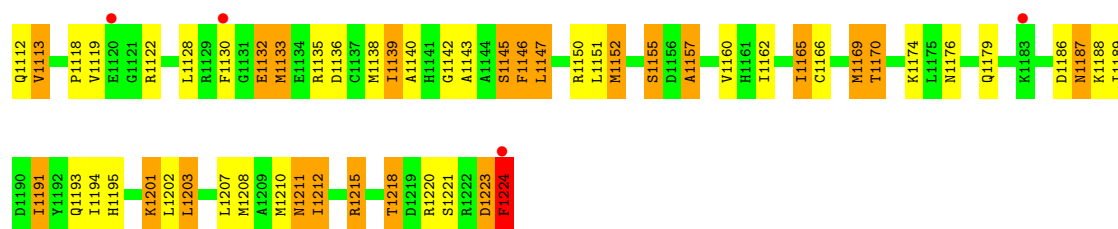
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 SUBUNIT RPB1



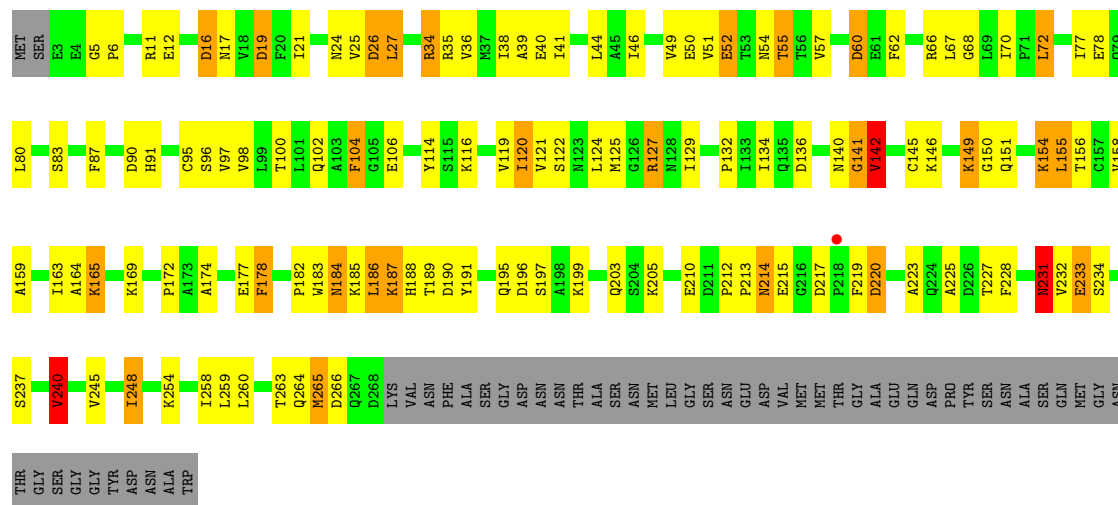






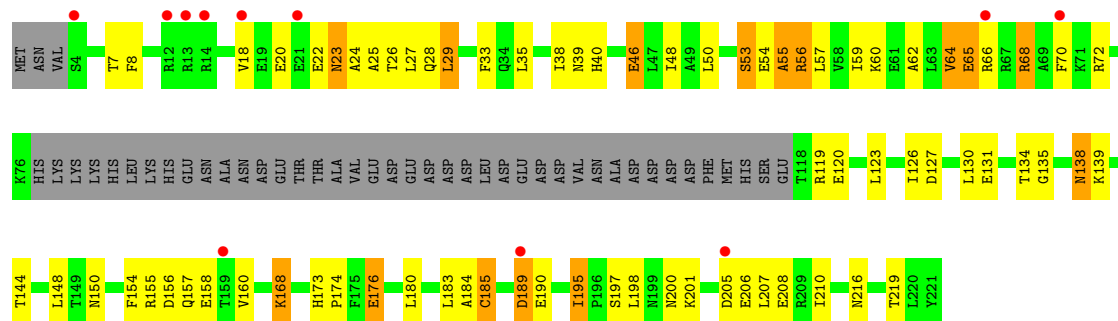
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

Chain C: 43% 31% 8% 16%



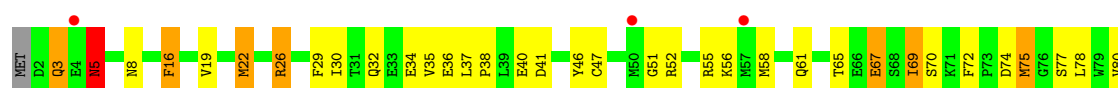
• Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4

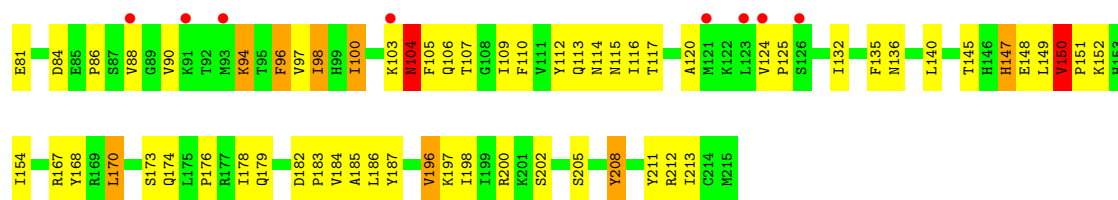
Chain D: 5% 46% 28% 7% 20%



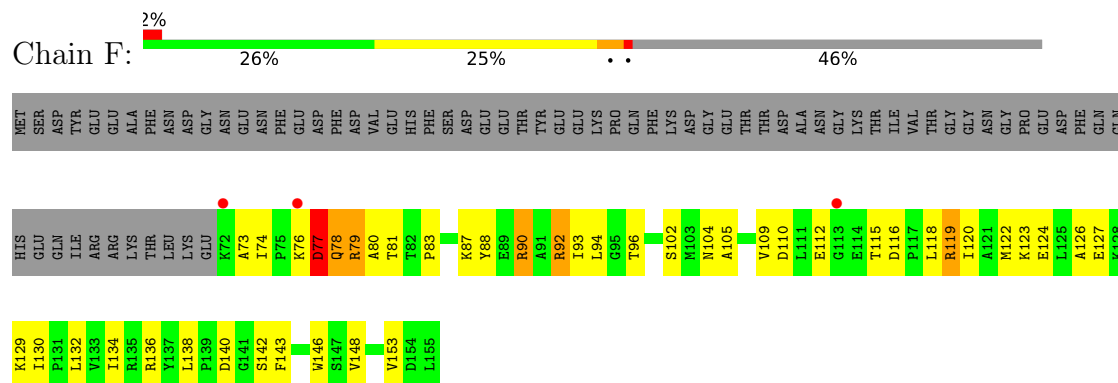
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC1

Chain E: 5% 54% 37% 7%

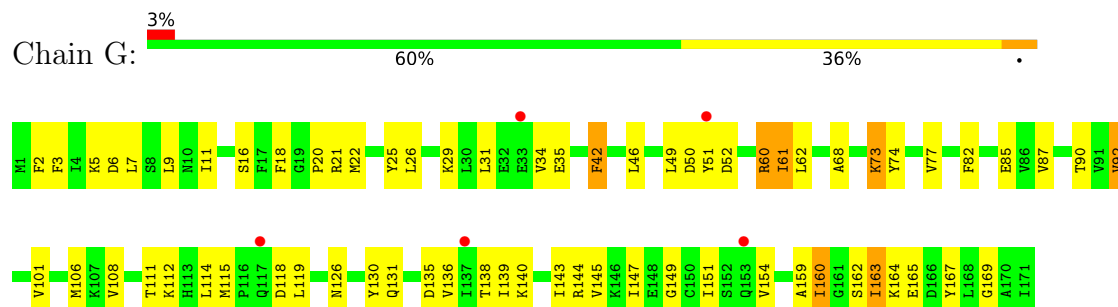




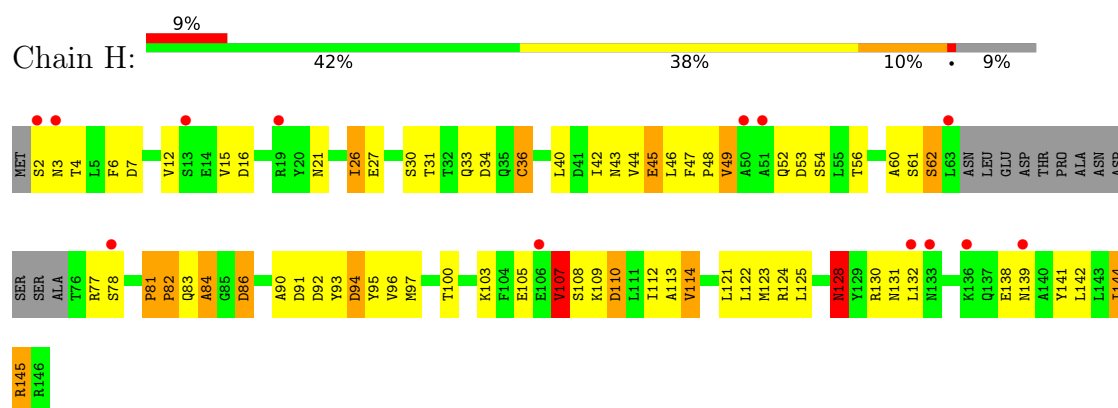
• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC2



• Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

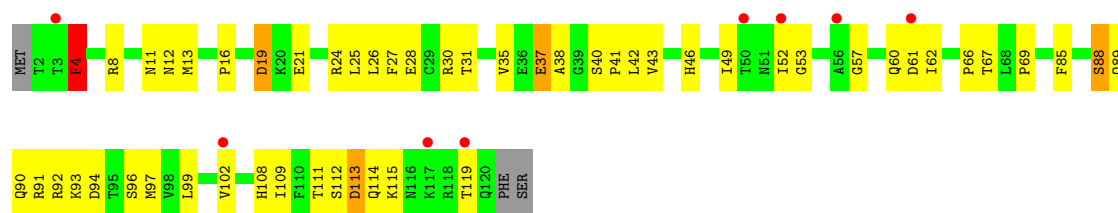


• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC3

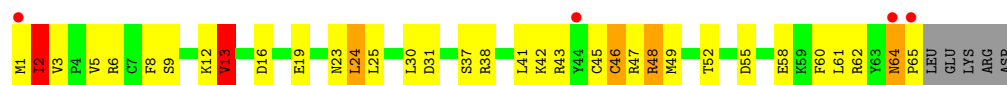
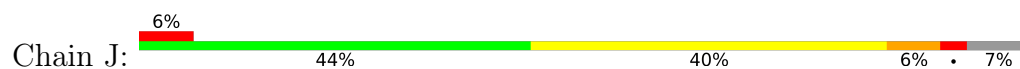


• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9

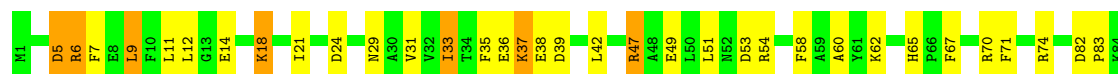




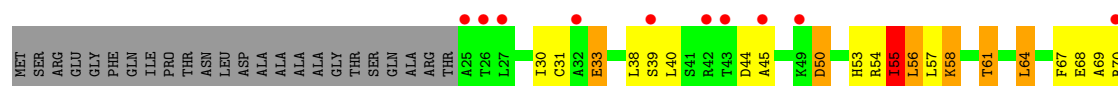
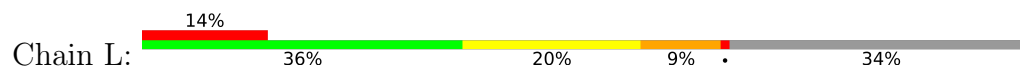
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC5



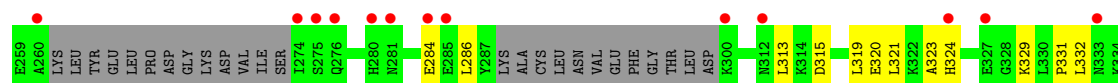
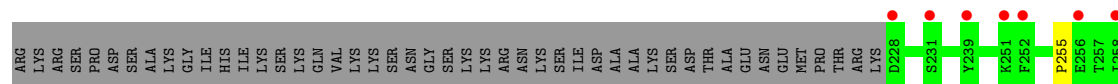
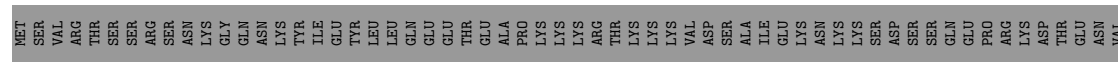
• Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11



• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4



• Molecule 13: TRANSCRIPTION FACTOR BYE1



ILE	ILE	ASP	SER
HIS	PRO	GLY	LVS
	LYS	LYS	ILE
	THR	LEU	GLU
	THR	TVR	GLN
	ARG	VAL	THR
	GLY	VAL	HIS
	TVR	GLU	ALA
	THR	GLY	ALA
	ASP	ARG	ILE
	ASP	LEU	SER
	PHE	PRO	LVS
	TYR	THR	GLU
	ILE	THR	PRO
	VAL	THR	SER
	PRO	ALA	PRO
	SER	ALA	SER
	LYS	PRO	THR
	GLY	TVR	ILE
	GLY	LEU	ASN
	GLU	LYS	ASN
	ILE	GLU	GLY
	PRO	ILE	GLU
	GLU	SER	SER
	ILE	CYS	LEU
	LEU	SER	ASN
	LYS	ARG	LYS
	ASP	ALA	ALA
	ILE	ILE	PHE
	LEU	LEU	LEU
	GLY	VAL	TVR
	SER	TVR	PRO
	HIS	GLN	GLY
	ASN	LEU	LEU
	ASP	PHE	GLY
	GLU	PRO	LEU
	ARG	SER	GLU
	SER	ASN	PHE
	GLU	ASP	THR
	ARG	ASP	GLY
	PHE	GLU	TVR
	SER	SER	LEU
	ARG	LYS	ASN
	MET	THR	TVR
	LYS	THR	ILE
	SER	PHE	GLY
	ASP	ALA	SER
	GLU	ASP	SER
	ARG	VAL	GLN
	THR	VAL	LYS
	LEU	ASP	LEU
	PHE	SER	ARG
	ALA	LEU	ASN
	PHE	GLU	ASP
	VAL	ASN	ILE
	VAL	LYS	PHE
	VAL	GLY	LYS
	LYS	ARG	GLU
	GLN	ILE	ALA
	GLU	ALA	ILE
	PHE	GLY	CYS

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	220.55Å 392.09Å 279.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.63 – 4.80 49.63 – 4.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.63-4.80) 99.8 (49.63-4.80)	Depositor EDS
R_{merge}	0.41	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 4.86Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.191 , 0.253 0.218 , 0.282	Depositor DCC
R_{free} test set	1172 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	151.9	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 349.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.017 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.039 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	31509	wwPDB-VP
Average B, all atoms (Å ²)	198.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% 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	0.92	6/11339 (0.1%)	1.57	154/15334 (1.0%)
2	B	0.90	1/8889 (0.0%)	1.52	104/11987 (0.9%)
3	C	0.88	0/2133	1.46	24/2891 (0.8%)
4	D	0.88	0/1365	1.64	17/1837 (0.9%)
5	E	0.85	0/1788	1.51	27/2406 (1.1%)
6	F	0.93	0/691	1.53	9/933 (1.0%)
7	G	0.81	0/1368	1.43	4/1844 (0.2%)
8	H	0.94	0/1086	1.51	18/1470 (1.2%)
9	I	0.85	0/989	1.44	15/1331 (1.1%)
10	J	0.90	0/541	1.44	1/727 (0.1%)
11	K	0.85	0/938	1.50	10/1267 (0.8%)
12	L	0.96	0/365	1.54	2/485 (0.4%)
13	X	1.09	0/561	1.88	11/780 (1.4%)
All	All	0.90	7/32053 (0.0%)	1.54	396/43292 (0.9%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	ARG	CA-C	6.75	1.61	1.52
1	A	274	ILE	CA-C	6.12	1.59	1.52
1	A	858	ASN	CA-C	6.03	1.60	1.52
1	A	244	PRO	CA-C	5.73	1.57	1.52
1	A	491	VAL	CA-C	5.21	1.57	1.53

The worst 5 of 396 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	4	PHE	CA-CB-CG	11.03	124.83	113.80
5	E	5	ASN	N-CA-C	-8.91	102.56	113.97
1	A	517	ASN	CA-CB-CG	8.86	121.46	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	189	ASP	CA-CB-CG	8.50	121.10	112.60
1	A	56	PRO	CA-C-N	8.50	137.77	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11140	0	11218	367	0
2	B	8720	0	8745	231	0
3	C	2095	0	2051	71	0
4	D	1356	0	1319	33	0
5	E	1752	0	1776	48	0
6	F	679	0	701	21	0
7	G	1340	0	1357	30	0
8	H	1068	0	1040	30	0
9	I	971	0	930	26	0
10	J	532	0	543	17	0
11	K	920	0	929	27	0
12	L	363	0	386	13	0
13	X	564	0	239	4	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
All	All	31509	0	31234	807	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 13.

The worst 5 of 807 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:C:83:SER:HA	3:C:95:CYS:HB2	1.36	1.05
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.38	1.04
1:A:567:LYS:HB2	1:A:568:PRO:HD3	1.46	0.97
1:A:821:ARG:HG2	2:B:514:LEU:H	1.31	0.95
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.53	0.89

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	1406/1733 (81%)	1111 (79%)	218 (16%)	77 (6%)	1	15
2	B	1075/1224 (88%)	861 (80%)	155 (14%)	59 (6%)	1	15
3	C	264/318 (83%)	208 (79%)	47 (18%)	9 (3%)	3	20
4	D	173/221 (78%)	144 (83%)	18 (10%)	11 (6%)	1	13
5	E	212/215 (99%)	176 (83%)	30 (14%)	6 (3%)	4	24
6	F	82/155 (53%)	69 (84%)	11 (13%)	2 (2%)	4	27
7	G	169/171 (99%)	143 (85%)	22 (13%)	4 (2%)	4	27
8	H	129/146 (88%)	96 (74%)	17 (13%)	16 (12%)	0	4
9	I	117/122 (96%)	96 (82%)	18 (15%)	3 (3%)	4	25
10	J	63/70 (90%)	46 (73%)	14 (22%)	3 (5%)	2	16
11	K	113/120 (94%)	94 (83%)	18 (16%)	1 (1%)	14	49
12	L	44/70 (63%)	25 (57%)	13 (30%)	6 (14%)	0	3
13	X	107/594 (18%)	83 (78%)	20 (19%)	4 (4%)	2	19
All	All	3954/5159 (77%)	3152 (80%)	601 (15%)	201 (5%)	1	15

5 of 201 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	ILE
1	A	47	ARG
1	A	57	ARG
1	A	65	LEU
1	A	71	GLN

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	1239/1520 (82%)	974 (79%)	265 (21%)	1	6
2	B	952/1061 (90%)	770 (81%)	182 (19%)	1	8
3	C	234/274 (85%)	190 (81%)	44 (19%)	1	9
4	D	140/200 (70%)	112 (80%)	28 (20%)	1	8
5	E	196/197 (100%)	164 (84%)	32 (16%)	2	12
6	F	74/137 (54%)	62 (84%)	12 (16%)	2	12
7	G	152/152 (100%)	126 (83%)	26 (17%)	2	11
8	H	117/128 (91%)	95 (81%)	22 (19%)	1	9
9	I	113/116 (97%)	99 (88%)	14 (12%)	4	18
10	J	60/65 (92%)	44 (73%)	16 (27%)	0	3
11	K	99/102 (97%)	83 (84%)	16 (16%)	2	12
12	L	40/57 (70%)	30 (75%)	10 (25%)	0	4
All	All	3416/4009 (85%)	2749 (80%)	667 (20%)	1	8

5 of 667 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	80	LEU
7	G	85	GLU
3	C	186	LEU
3	C	72	LEU
5	E	8	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 110 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	481	GLN
2	B	843	GLN
11	K	112	GLN
9	I	11	ASN
2	B	499	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	934:LYS	C	935:ARG	N	3.44

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	1416/1733 (81%)	0.35	52 (3%) 45 38	118, 185, 242, 274	0
2	B	1097/1224 (89%)	0.45	57 (5%) 33 31	111, 200, 254, 282	0
3	C	266/318 (83%)	0.24	1 (0%) 88 77	139, 193, 237, 271	0
4	D	177/221 (80%)	0.63	11 (6%) 26 28	149, 199, 250, 261	0
5	E	214/215 (99%)	0.49	11 (5%) 33 32	153, 223, 267, 279	0
6	F	84/155 (54%)	0.32	3 (3%) 46 39	113, 165, 217, 239	0
7	G	171/171 (100%)	0.26	5 (2%) 53 43	157, 188, 230, 261	0
8	H	133/146 (91%)	0.65	13 (9%) 13 17	185, 229, 254, 261	0
9	I	119/122 (97%)	0.60	8 (6%) 24 26	185, 233, 264, 271	0
10	J	65/70 (92%)	0.31	4 (6%) 26 28	148, 173, 225, 245	0
11	K	115/120 (95%)	0.33	2 (1%) 69 55	140, 182, 230, 246	0
12	L	46/70 (65%)	1.02	10 (21%) 2 6	153, 242, 260, 266	0
13	X	113/594 (19%)	1.25	25 (22%) 2 6	232, 271, 294, 295	0
All	All	4016/5159 (77%)	0.43	202 (5%) 34 32	111, 196, 260, 295	0

The worst 5 of 202 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	335	GLY	6.9
4	D	4	SER	6.6
7	G	51	TYR	4.6
13	X	260	ALA	4.6
13	X	228	ASP	4.4

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
15	MG	A	2458	1/1	0.69	0.19	130,130,130,130	0
14	ZN	L	1071	1/1	0.94	0.07	266,266,266,266	0
14	ZN	I	1121	1/1	0.98	0.09	230,230,230,230	0
14	ZN	A	2456	1/1	0.99	0.06	181,181,181,181	0
14	ZN	I	1122	1/1	0.99	0.02	245,245,245,245	0
14	ZN	B	2225	1/1	1.00	0.04	96,96,96,96	0
14	ZN	J	1066	1/1	1.00	0.06	192,192,192,192	0
14	ZN	C	1269	1/1	1.00	0.07	140,140,140,140	0
14	ZN	A	2457	1/1	1.00	0.06	105,105,105,105	0

6.5 Other polymers [i](#)

There are no such residues in this entry.