wwPDB X-ray Structure Validation Summary Report (i)

Mar 3, 2024 – 07:19 AM EST

PDB ID	:	6BM4
Title	:	Pol II elongation complex with an abasic lesion at i-1 position,soaking UMP-NPP
Authors	:	Wang, W.; Wang, D.
Deposited on	:	2017-11-13
Resolution	:	2.95 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:

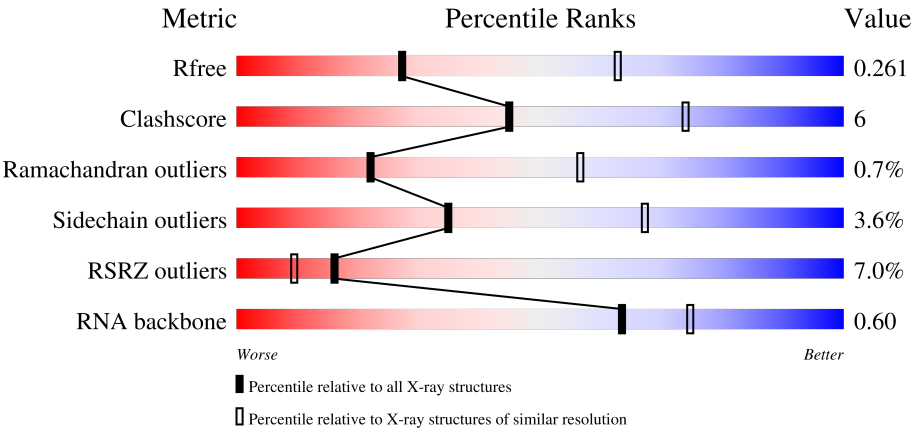
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)
RNA backbone	3102	1065 (3.22-2.70)

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	8% 63% 15% • 21%
2	B	1224	3% 70% 18% • 10%
3	C	318	% 68% 15% • 16%
4	E	215	21% 89% 9% ••

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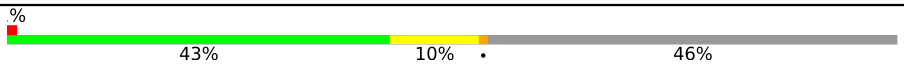
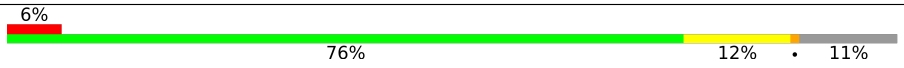
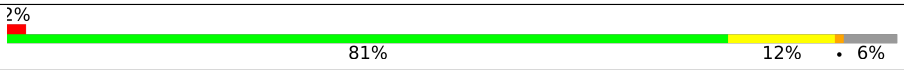
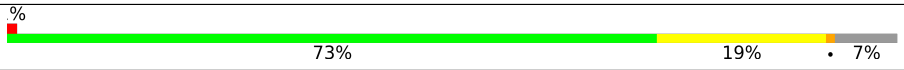
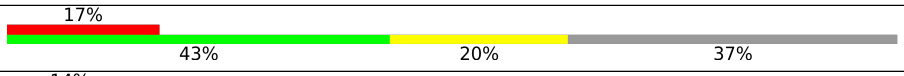
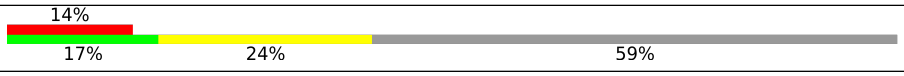
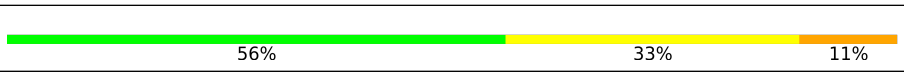
Mol	Chain	Length	Quality of chain
5	F	155	
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	T	29	
12	R	9	

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 28274 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	1372	Total	C	N	O	S	0	0	0
			10784	6802	1887	2034	61			

- 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
			8726	5526	1530	1615	55			

- 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 polymerases I, II, and III subunit RPABC1.

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

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	130	Total	C	N	O	S	0	0	0
			1043	660	173	206	4			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	115	Total	C	N	O	S	0	0	0
			935	575	170	180	10			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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 subunit RPB11.

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 polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	44	Total	C	N	O	S	0	0	0
			351	217	70	60	4			

- Molecule 11 is a DNA chain called DNA (5'-D(P*CP*AP*(3DR)P*CP*TP*CP*TP*TP*G P*AP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	T	12	Total	C	N	O	P	0	0	0
			233	111	38	72	12			

- Molecule 12 is a RNA chain called RNA (5'-R(*AP*UP*CP*AP*AP*GP*AP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	R	9	Total	C	N	O	P	0	0	0
			194	88	40	58	8			

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	2	Total	Zn	0	0
			2	2		

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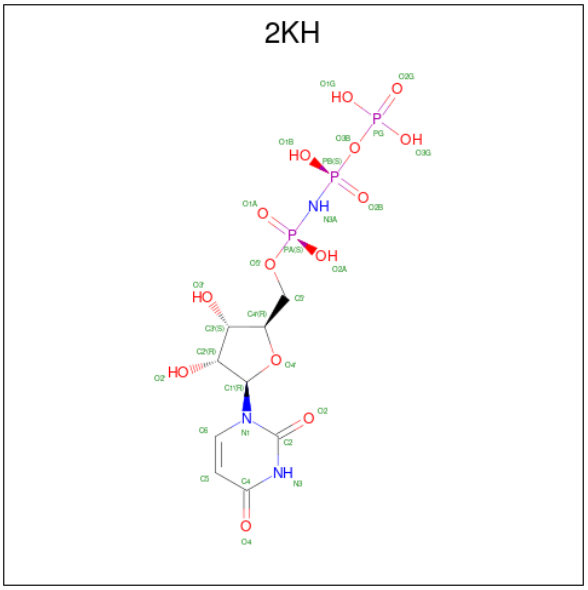
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	B	1	Total Zn 1 1	0	0
13	C	1	Total Zn 1 1	0	0
13	I	2	Total Zn 2 2	0	0
13	J	1	Total Zn 1 1	0	0
13	L	1	Total Zn 1 1	0	0

- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	2	Total Mg 2 2	0	0

- Molecule 15 is 5'-O-[(S)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]amino}phosphoryl]uridine (three-letter code: 2KH) (formula: $C_9H_{16}N_3O_{14}P_3$).



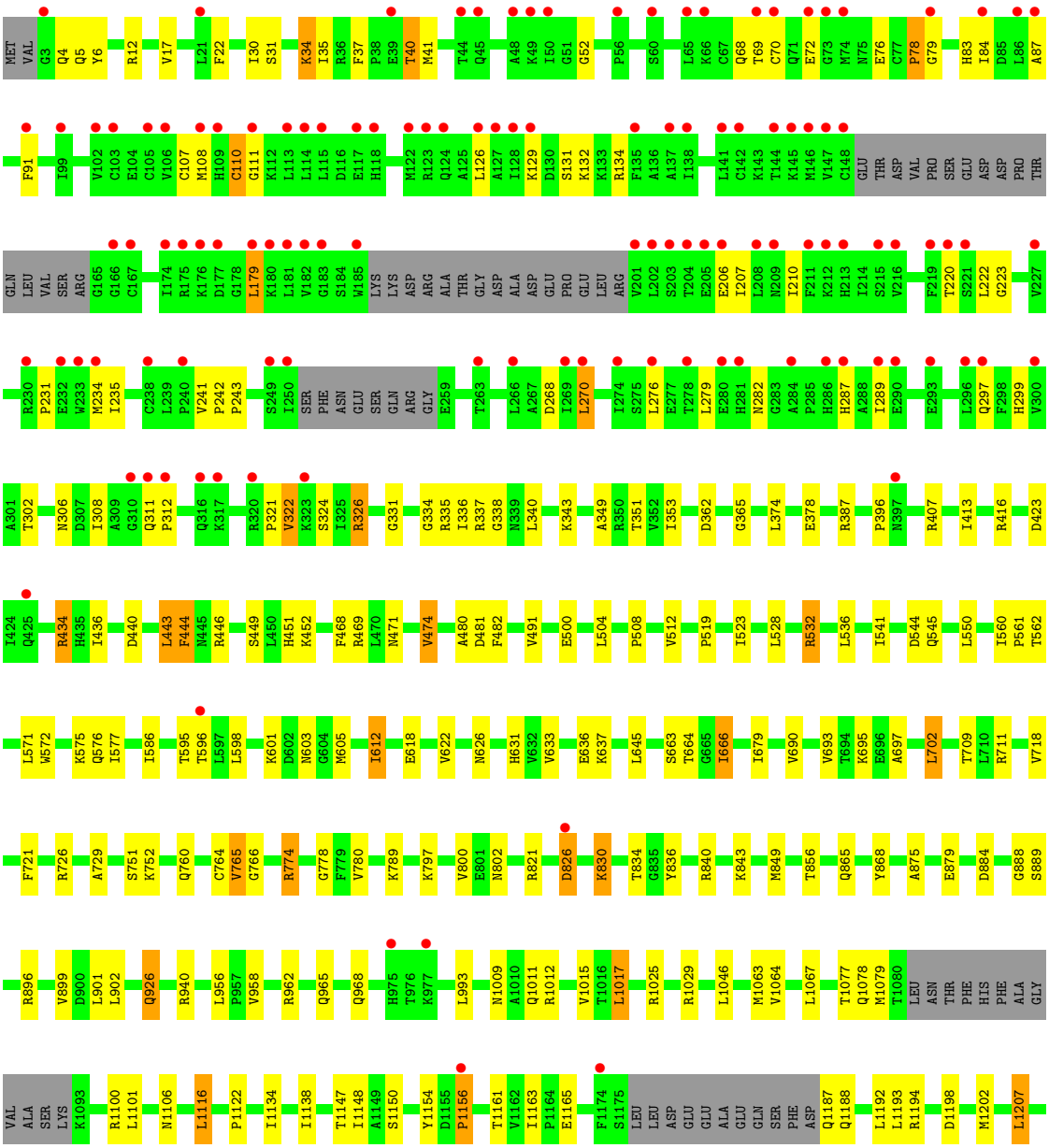
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	B	1	Total C N O P 29 9 3 14 3	0	0

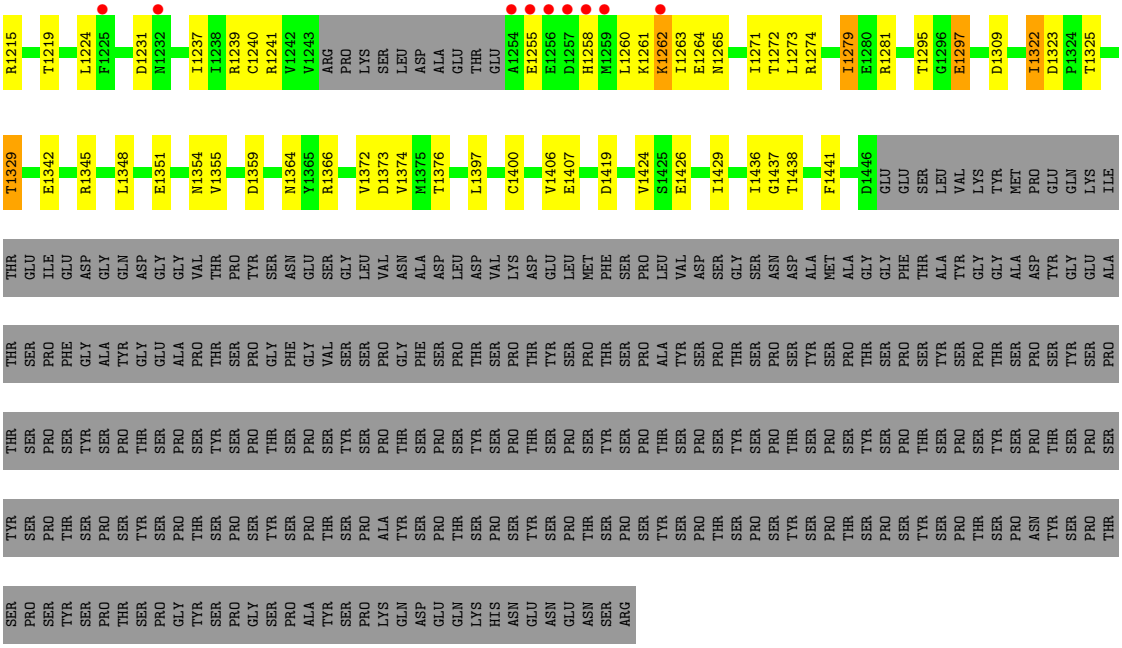
3 Residue-property plots (i)

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 subunit RPB1

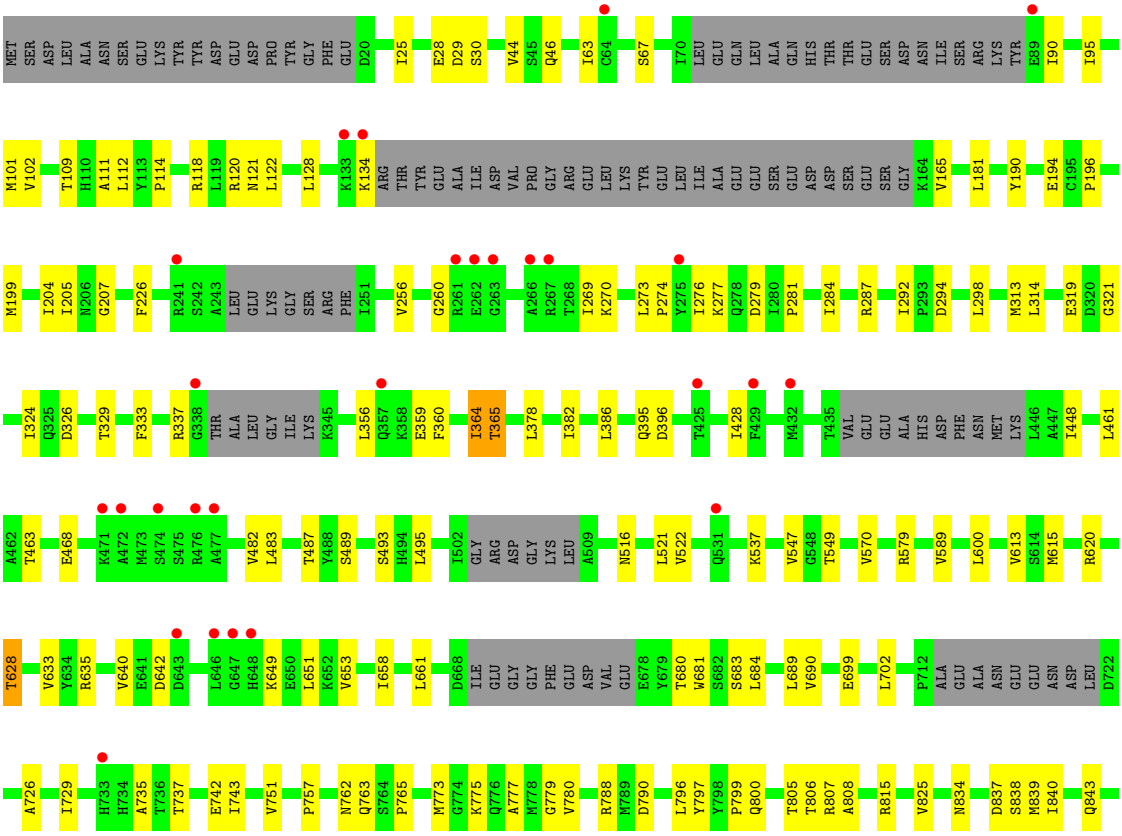
Chain A:

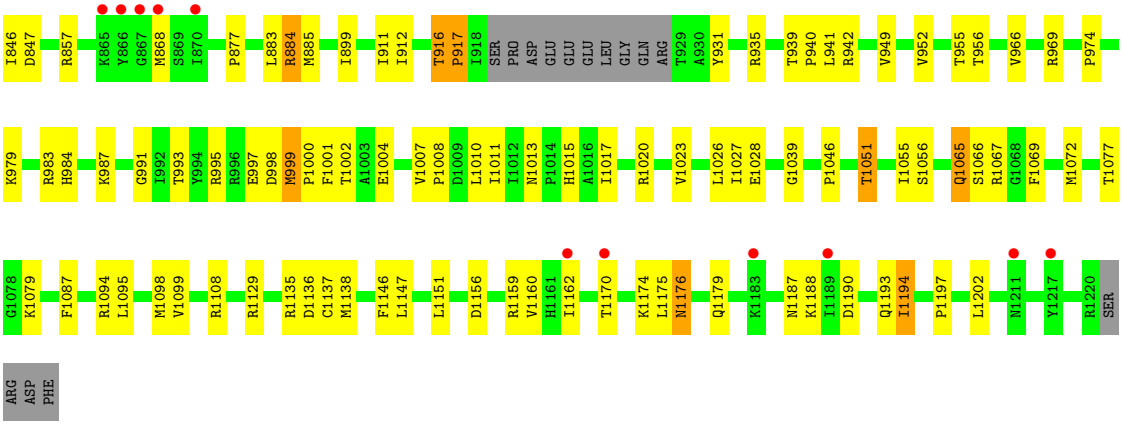




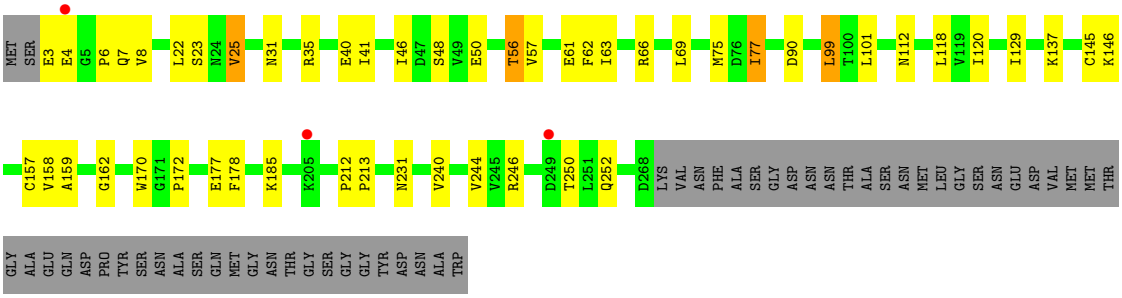
• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

Chain B:

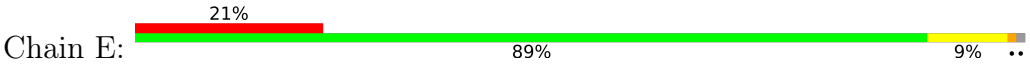


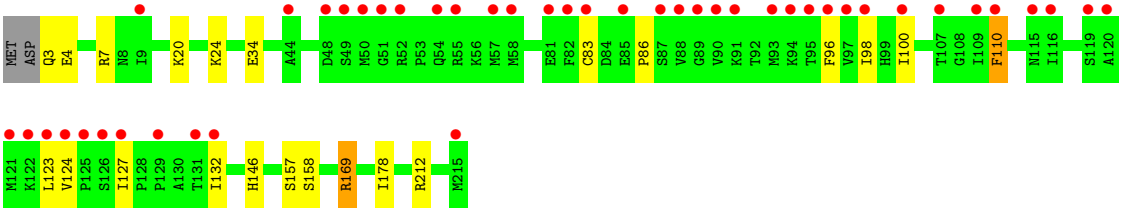


• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

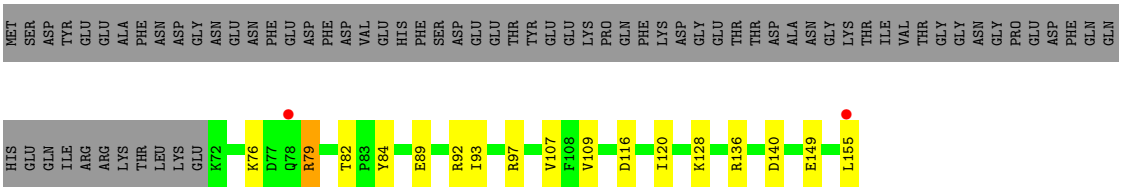


• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

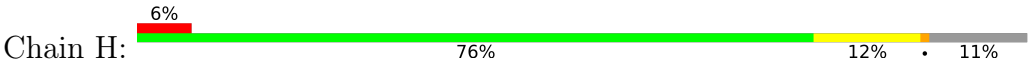


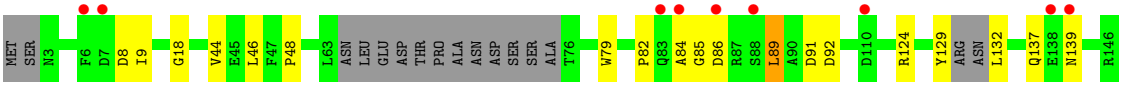


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

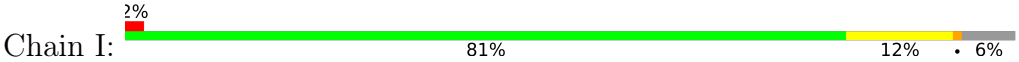


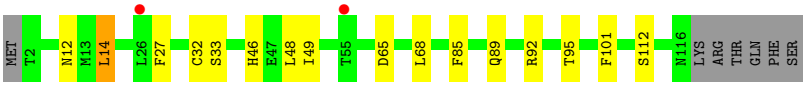
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



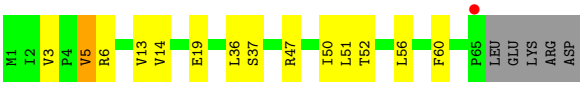


• Molecule 7: DNA-directed RNA polymerase II subunit RPB9

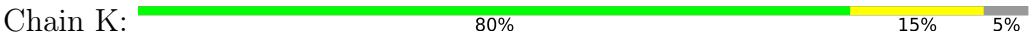


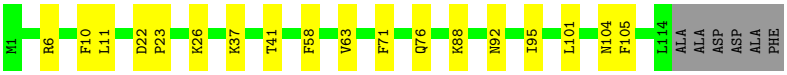


• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

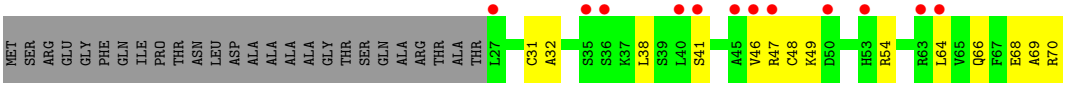


• Molecule 9: DNA-directed RNA polymerase II subunit RPB11

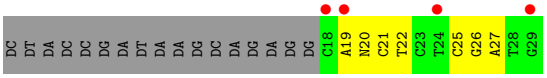




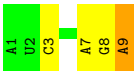
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



• Molecule 11: DNA (5'-D(P*CP*AP*(3DR)P*CP*TP*CP*TP*TP*GP*AP*TP*G)-3')



• Molecule 12: RNA (5'-R(*AP*UP*CP*AP*AP*GP*AP*GP*A)-3')



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	168.72Å 220.43Å 193.15Å 90.00° 100.97° 90.00°	Depositor
Resolution (Å)	55.61 – 2.95 94.81 – 2.95	Depositor EDS
% Data completeness (in resolution range)	87.0 (55.61-2.95) 87.0 (94.81-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.234 , 0.260 0.236 , 0.261	Depositor DCC
R_{free} test set	6426 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	50.7	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 44.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	28274	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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: MG, 3DR, 2KH, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.21	0/10975	0.38	0/14838
2	B	0.21	0/8896	0.38	0/11996
3	C	0.21	0/2133	0.39	0/2891
4	E	0.21	0/1780	0.37	0/2395
5	F	0.20	0/691	0.38	0/933
6	H	0.21	0/1060	0.40	0/1434
7	I	0.22	0/953	0.37	0/1284
8	J	0.22	0/541	0.36	0/727
9	K	0.21	0/937	0.35	0/1265
10	L	0.21	0/353	0.36	0/468
11	T	0.51	0/246	0.89	0/374
12	R	0.14	0/218	0.64	0/339
All	All	0.22	0/28783	0.39	0/38944

There are no bond length outliers.

There are no bond angle outliers.

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	10784	0	10873	166	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	8726	0	8760	131	0
3	C	2095	0	2051	38	0
4	E	1744	0	1772	11	0
5	F	679	0	701	11	0
6	H	1043	0	1015	11	0
7	I	935	0	886	12	0
8	J	532	0	542	12	0
9	K	919	0	929	13	0
10	L	351	0	375	7	0
11	T	233	0	133	6	0
12	R	194	0	99	4	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
14	A	2	0	0	0	0
15	B	29	0	15	1	0
All	All	28274	0	28151	366	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 6.

The worst 5 of 366 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)
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.63	0.80
2:B:25:ILE:HD11	2:B:653:VAL:HB	1.67	0.74
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.70	0.74
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.70	0.73
3:C:66:ARG:NH2	8:J:3:VAL:O	2.21	0.73

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	1358/1733 (78%)	1248 (92%)	100 (7%)	10 (1%)	22	56
2	B	1077/1224 (88%)	1005 (93%)	64 (6%)	8 (1%)	22	56
3	C	264/318 (83%)	246 (93%)	17 (6%)	1 (0%)	34	69
4	E	211/215 (98%)	200 (95%)	10 (5%)	1 (0%)	29	64
5	F	82/155 (53%)	78 (95%)	4 (5%)	0	100	100
6	H	124/146 (85%)	106 (86%)	16 (13%)	2 (2%)	9	36
7	I	113/122 (93%)	101 (89%)	12 (11%)	0	100	100
8	J	63/70 (90%)	60 (95%)	3 (5%)	0	100	100
9	K	112/120 (93%)	108 (96%)	3 (3%)	1 (1%)	17	51
10	L	42/70 (60%)	35 (83%)	5 (12%)	2 (5%)	2	11
All	All	3446/4173 (83%)	3187 (92%)	234 (7%)	25 (1%)	22	56

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	PRO
2	B	1046	PRO
1	A	110	CYS
1	A	322	VAL
1	A	1437	GLY

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%)	1144 (96%)	52 (4%)	29	62
2	B	952/1061 (90%)	916 (96%)	36 (4%)	33	66
3	C	234/274 (85%)	227 (97%)	7 (3%)	41	72
4	E	195/197 (99%)	189 (97%)	6 (3%)	40	71
5	F	74/137 (54%)	71 (96%)	3 (4%)	30	64
6	H	114/128 (89%)	112 (98%)	2 (2%)	59	82
7	I	109/116 (94%)	108 (99%)	1 (1%)	78	91
8	J	60/65 (92%)	58 (97%)	2 (3%)	38	70
9	K	99/102 (97%)	98 (99%)	1 (1%)	76	90
10	L	39/57 (68%)	38 (97%)	1 (3%)	46	75
All	All	3072/3657 (84%)	2961 (96%)	111 (4%)	35	67

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	319	GLU
10	L	64	LEU
2	B	868	MET
9	K	11	LEU
4	E	127	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	650	GLN
2	B	762	ASN
2	B	984	HIS
2	B	1065	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	R	8/9 (88%)	1 (12%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	R	9	A

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is 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	3DR	T	20	11	8,11,12	1.35	1 (12%)	9,14,17	1.27	1 (11%)

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	3DR	T	20	11	-	2/3/15/16	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	T	20	3DR	O4'-C4'	-2.32	1.40	1.44

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	T	20	3DR	O4'-C4'-C3'	2.88	107.96	103.73

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	T	20	3DR	O4'-C4'-C5'-O5'
11	T	20	3DR	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	2KH	B	1302	14	29,30,30	3.49	14 (48%)	42,47,47	1.55	5 (11%)

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
15	2KH	B	1302	14	-	13/19/38/38	0/2/2/2

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1302	2KH	O4'-C1'	8.62	1.62	1.42
15	B	1302	2KH	O4'-C4'	-7.32	1.28	1.45
15	B	1302	2KH	C2'-C1'	-7.23	1.30	1.53
15	B	1302	2KH	C2-N1	5.62	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1302	2KH	C6-C5	5.58	1.48	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1302	2KH	C4-N3-C2	-4.98	120.02	126.58
15	B	1302	2KH	N3-C2-N1	4.06	120.28	114.89
15	B	1302	2KH	C5-C4-N3	3.49	120.05	114.84
15	B	1302	2KH	O4-C4-C5	-2.96	119.96	125.16
15	B	1302	2KH	PB-O3B-PG	-2.35	124.33	132.62

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

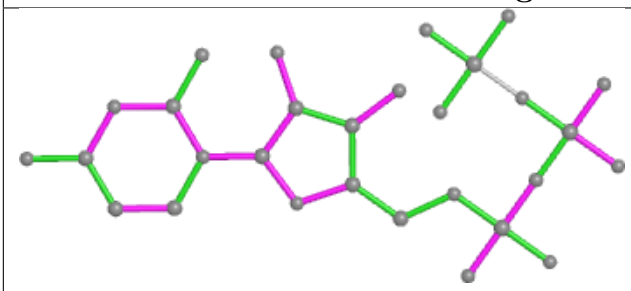
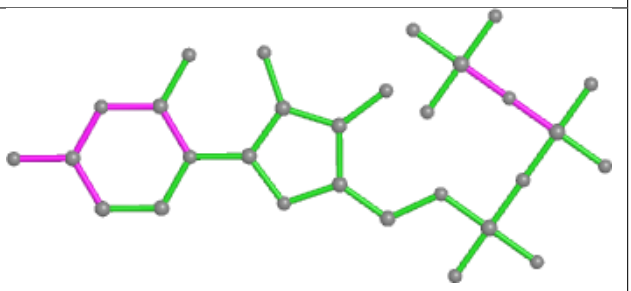
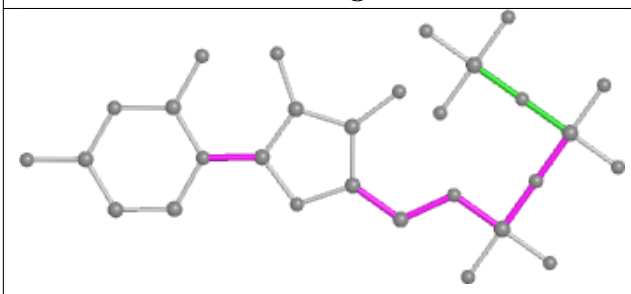
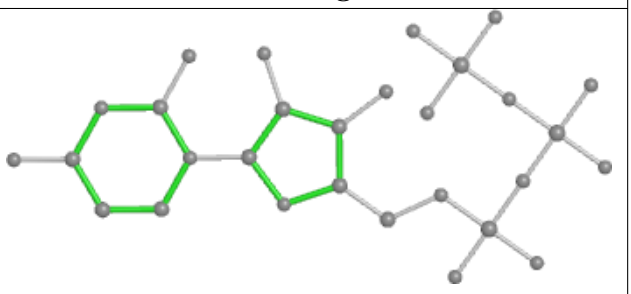
Mol	Chain	Res	Type	Atoms
15	B	1302	2KH	PB-N3A-PA-O1A
15	B	1302	2KH	C5'-O5'-PA-O2A
15	B	1302	2KH	PA-N3A-PB-O2B
15	B	1302	2KH	O4'-C4'-C5'-O5'
15	B	1302	2KH	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B	1302	2KH	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 2KH B 1302	
 Bond lengths	 Bond angles
 Torsions	 Rings

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	1372/1733 (79%)	0.59	131 (9%) 8 5	16, 58, 161, 242	0
2	B	1097/1224 (89%)	0.29	38 (3%) 44 29	13, 46, 119, 225	0
3	C	266/318 (83%)	0.20	3 (1%) 80 65	19, 45, 85, 171	0
4	E	213/215 (99%)	1.06	45 (21%) 1 0	35, 86, 172, 234	0
5	F	84/155 (54%)	0.03	2 (2%) 59 42	35, 58, 109, 179	0
6	H	130/146 (89%)	0.84	9 (6%) 16 10	42, 84, 147, 206	0
7	I	115/122 (94%)	0.33	2 (1%) 70 53	20, 61, 101, 114	0
8	J	65/70 (92%)	0.04	1 (1%) 73 57	22, 36, 82, 159	0
9	K	114/120 (95%)	0.19	0 100 100	20, 49, 90, 108	0
10	L	44/70 (62%)	1.32	12 (27%) 0 0	26, 88, 182, 231	0
11	T	11/29 (37%)	1.39	4 (36%) 0 0	133, 138, 177, 179	0
12	R	9/9 (100%)	0.76	0 100 100	111, 125, 150, 151	0
All	All	3520/4211 (83%)	0.47	247 (7%) 16 9	13, 55, 149, 242	0

The worst 5 of 247 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	183	GLY	12.7
2	B	868	MET	9.9
1	A	44	THR	9.5
4	E	93	MET	8.9
1	A	286	HIS	8.3

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	3DR	T	20	11/12	0.73	0.31	149,156,161,183	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

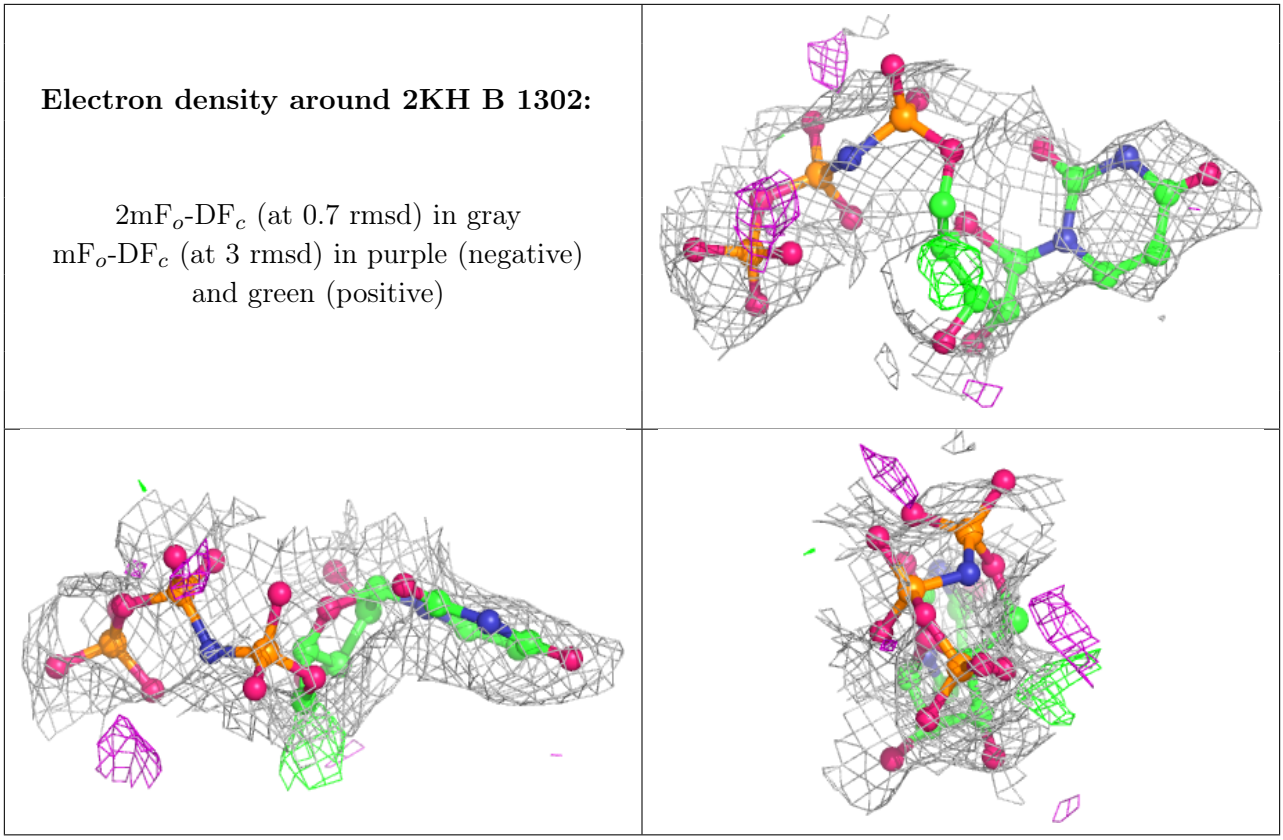
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
15	2KH	B	1302	29/29	0.72	0.29	101,150,192,196	0
13	ZN	A	1802	1/1	0.91	0.16	80,80,80,80	0
13	ZN	A	1801	1/1	0.92	0.09	136,136,136,136	0
13	ZN	B	1301	1/1	0.95	0.09	93,93,93,93	0
14	MG	A	1804	1/1	0.96	0.22	36,36,36,36	0
13	ZN	J	101	1/1	0.98	0.14	34,34,34,34	0
14	MG	A	1803	1/1	0.98	0.18	9,9,9,9	0
13	ZN	L	101	1/1	0.99	0.10	70,70,70,70	0
13	ZN	I	201	1/1	0.99	0.14	49,49,49,49	0
13	ZN	I	202	1/1	0.99	0.17	34,34,34,34	0
13	ZN	C	401	1/1	0.99	0.20	41,41,41,41	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 2KH B 1302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.