



# Full wwPDB X-ray Structure Validation Report ⓘ

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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (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

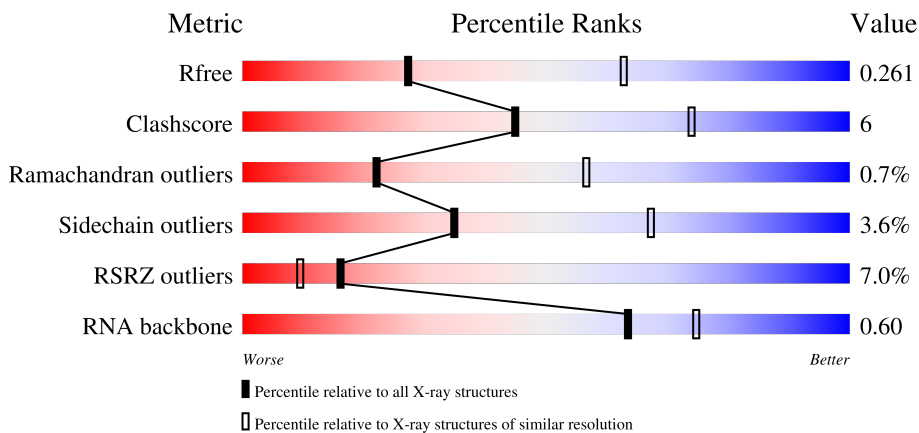
# 1 Overall quality at a glance

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  $\geq 3$ , 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	E	215	

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Mol	Chain	Length	Quality of chain
5	F	155	<p>% 43% 10% 46%</p>
6	H	146	<p>6% 76% 12% 11%</p>
7	I	122	<p>2% 81% 12% 6%</p>
8	J	70	<p>% 73% 19% 7%</p>
9	K	120	<p>80% 15% 5%</p>
10	L	70	<p>17% 43% 20% 37%</p>
11	T	29	<p>14% 17% 24% 59%</p>
12	R	9	<p>56% 33% 11%</p>

## 2 Entry composition

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
			Total	C	N	O	S			
1	A	1372	10784	6802	1887	2034	61	0	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1097	8726	5526	1530	1615	55	0	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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 polymerases I, II, and III subunit RPABC1.

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 polymerases I, II, and III subunit RPABC2.

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 polymerases I, II, and III subunit RPABC3.

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

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

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

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

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

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- 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
			Total	C	N	O	P			
11	T	12	233	111	38	72	12	0	0	0

- 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
			Total	C	N	O	P			
12	R	9	194	88	40	58	8	0	0	0

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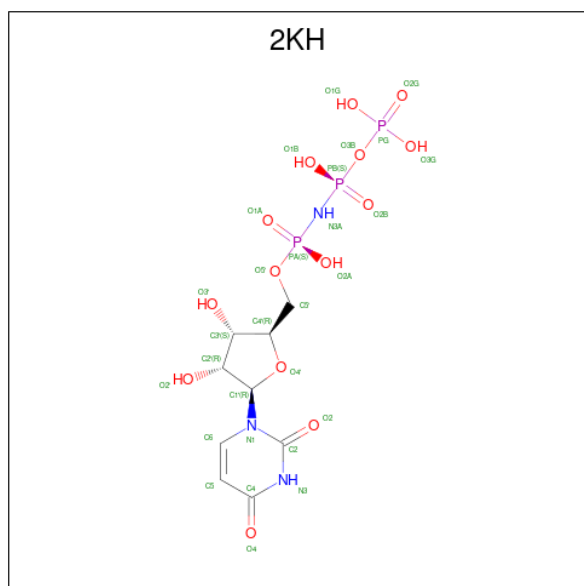
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	1	Total	Zn	0	0
			1	1		
13	C	1	Total	Zn	0	0
			1	1		
13	I	2	Total	Zn	0	0
			2	2		
13	J	1	Total	Zn	0	0
			1	1		
13	L	1	Total	Zn	0	0
			1	1		

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

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

- Molecule 15 is 5'-O-[(S)-hydroxy{[(S)-hydroxy(phosphonoxy)phosphoryl]amino}phosphoryl]uridine (three-letter code: 2KH) (formula: C<sub>9</sub>H<sub>16</sub>N<sub>3</sub>O<sub>14</sub>P<sub>3</sub>).

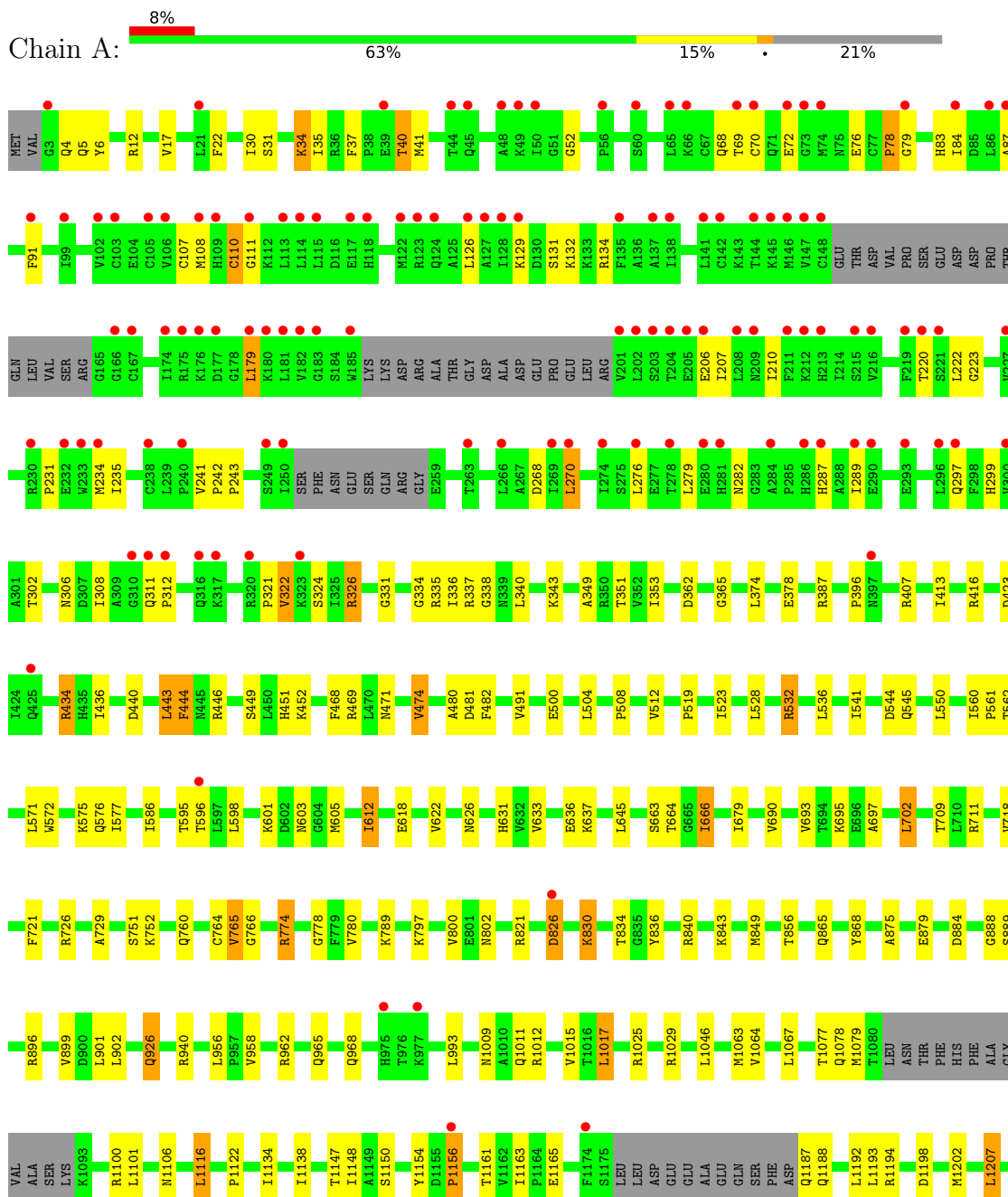


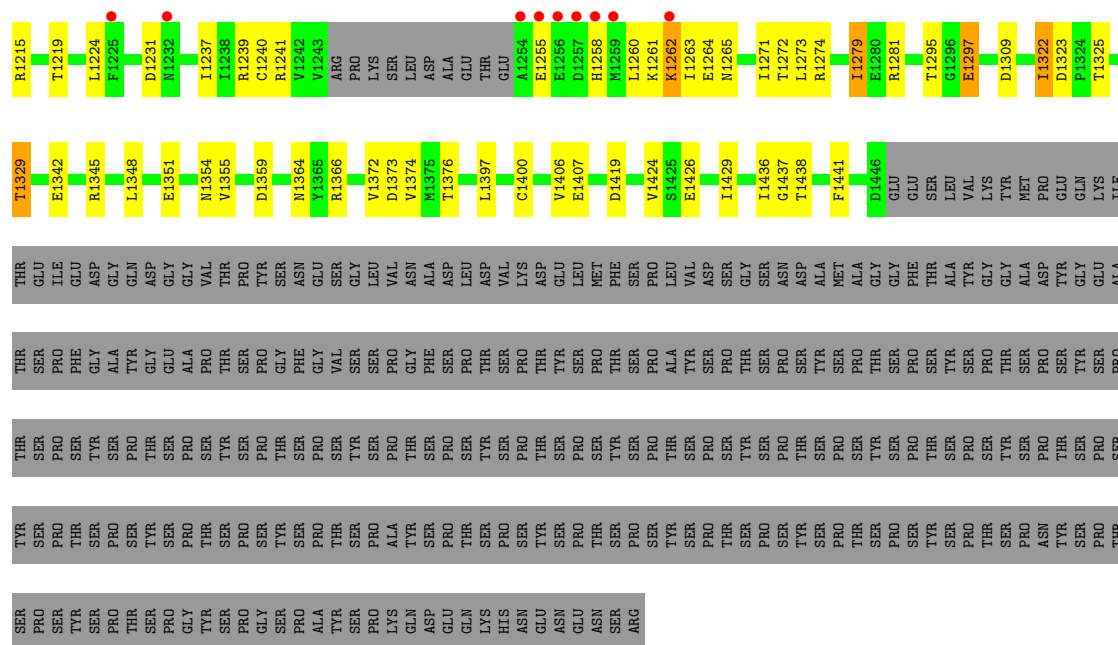
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
15	B	1	29	9	3	14	3	0	0

### 3 Residue-property plots [i](#)

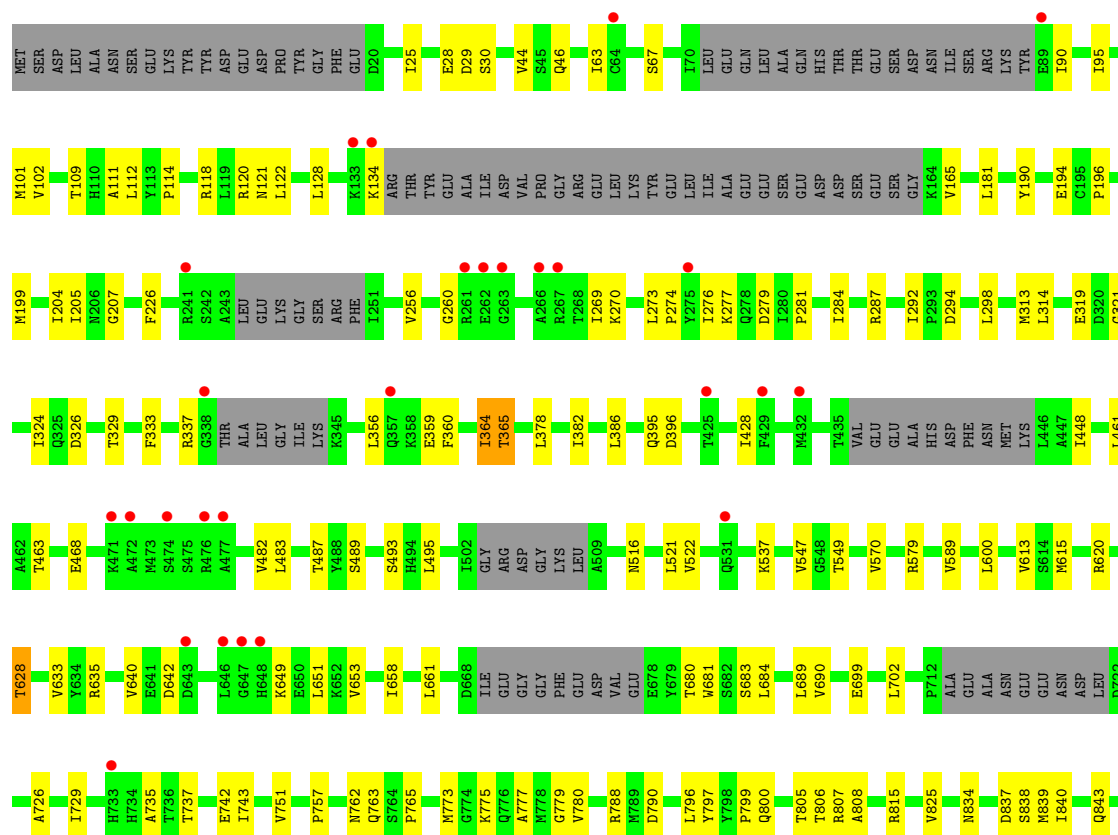
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

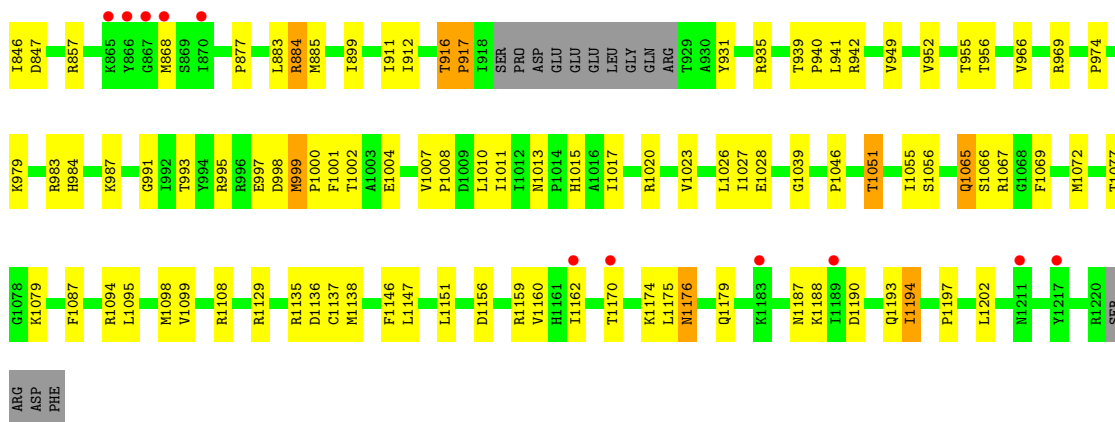




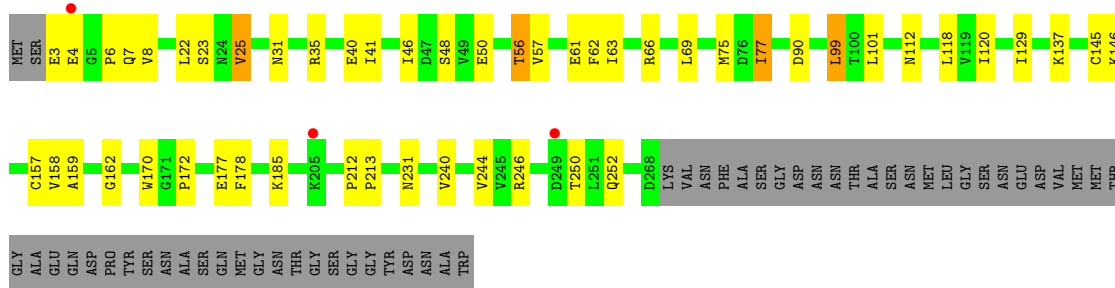
• Molecule 2: DNA-directed RNA polymerase II subunit RPB2



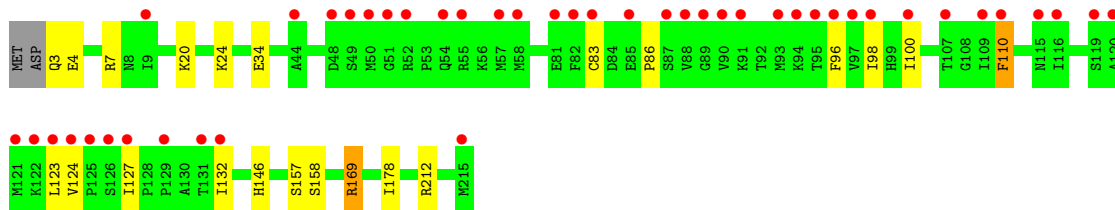
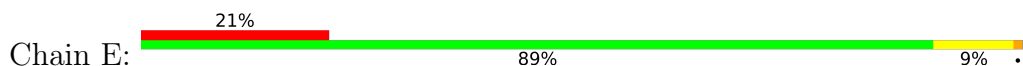




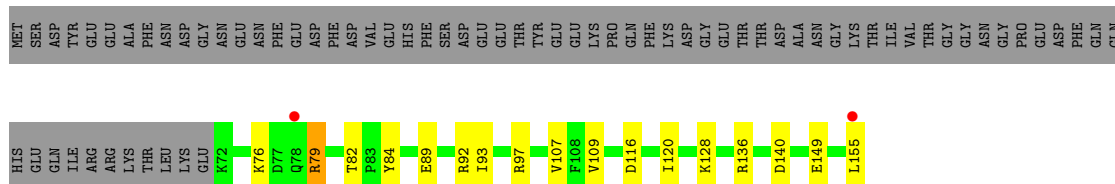
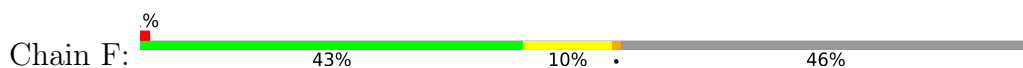
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3



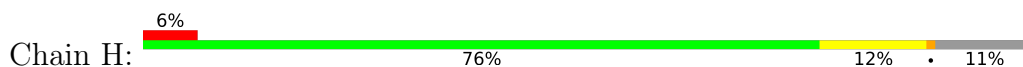
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1



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

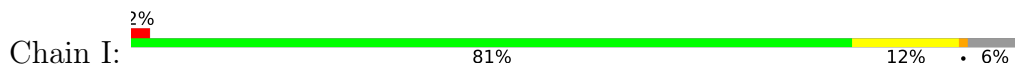


- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3





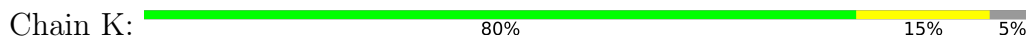
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9



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



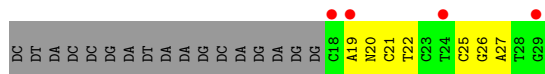
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11



- 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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.10 (at 2.96Å)	Xtrriage
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 <sup>2</sup> )	50.7	Xtrriage
Anisotropy	0.009	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 44.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	28274	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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.

All (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
1:A:899:VAL:HG22	1:A:1029:ARG:HG2	1.72	0.72
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.23	0.71
1:A:338:GLY:HA2	2:B:1129:ARG:HH21	1.57	0.70
2:B:911:ILE:HD11	2:B:941:LEU:HD23	1.73	0.70
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.74	0.69
1:A:35:ILE:HG13	1:A:241:VAL:HG21	1.73	0.69
8:J:5:VAL:HG22	8:J:6:ARG:HG3	1.73	0.69
3:C:50:GLU:HG2	10:L:66:GLN:HG2	1.75	0.69
2:B:1065:GLN:HG2	2:B:1069:PHE:HB2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:92:ARG:HB3	7:I:95:THR:HG23	1.75	0.69
1:A:40:THR:HG22	1:A:41:MET:HG3	1.76	0.68
4:E:178:ILE:HB	4:E:212:ARG:HD3	1.76	0.68
2:B:635:ARG:NH1	2:B:742:GLU:OE2	2.22	0.67
2:B:1174:LYS:HB2	2:B:1179:GLN:HB2	1.75	0.67
3:C:6:PRO:HB2	9:K:101:LEU:HD23	1.76	0.66
1:A:1009:ASN:OD1	1:A:1012:ARG:NH2	2.28	0.66
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.76	0.66
2:B:205:ILE:HG13	2:B:461:LEU:HB3	1.77	0.66
5:F:82:THR:HG22	5:F:84:TYR:H	1.60	0.66
1:A:134:ARG:NH1	1:A:220:THR:O	2.29	0.65
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.78	0.65
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.79	0.65
2:B:1175:LEU:O	2:B:1176:ASN:ND2	2.30	0.65
1:A:306:ASN:ND2	1:A:321:PRO:O	2.29	0.65
2:B:642:ASP:HB3	2:B:649:LYS:HG2	1.78	0.65
1:A:469:ARG:NH2	2:B:991:GLY:O	2.30	0.64
1:A:693:VAL:HG21	1:A:721:PHE:HE2	1.62	0.64
1:A:4:GLN:OE1	2:B:1159:ARG:NH1	2.29	0.64
2:B:165:VAL:HG21	2:B:448:ILE:HD12	1.80	0.64
3:C:6:PRO:HB3	3:C:25:VAL:HG13	1.80	0.64
2:B:463:THR:HG22	11:T:27:DA:H2'	1.80	0.63
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.80	0.63
7:I:32:CYS:SG	7:I:33:SER:N	2.72	0.63
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.80	0.63
8:J:37:SER:OG	8:J:47:ARG:NH2	2.32	0.63
3:C:7:GLN:HB2	3:C:23:SER:HB2	1.81	0.62
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.81	0.62
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.82	0.62
3:C:48:SER:HB3	3:C:158:VAL:HB	1.81	0.62
3:C:35:ARG:NH1	9:K:41:THR:OG1	2.33	0.61
12:R:7:A:H2'	12:R:8:G:H8	1.64	0.61
3:C:46:ILE:HD13	3:C:159:ALA:HB2	1.82	0.61
1:A:601:LYS:HB2	1:A:603:ASN:HD22	1.67	0.60
2:B:1000:PRO:HB2	2:B:1072:MET:HE3	1.83	0.60
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.83	0.60
1:A:1122:PRO:HD3	1:A:1323:ASP:HB2	1.83	0.60
2:B:995:ARG:NH1	2:B:997:GLU:OE1	2.34	0.60
3:C:145:CYS:SG	3:C:146:LYS:N	2.74	0.60
2:B:522:VAL:HG11	2:B:537:LYS:HD2	1.84	0.60
4:E:4:GLU:OE1	4:E:7:ARG:NH2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.83	0.59
1:A:636:GLU:OE2	1:A:962:ARG:NH1	2.35	0.59
5:F:76:LYS:O	5:F:79:ARG:NH1	2.34	0.59
1:A:68:GLN:O	1:A:70:CYS:N	2.34	0.59
1:A:888:GLY:O	1:A:940:ARG:NH2	2.36	0.59
2:B:702:LEU:HD21	2:B:735:ALA:HB1	1.82	0.59
1:A:1325:THR:OG1	4:E:146:HIS:O	2.20	0.59
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.85	0.59
1:A:1148:ILE:HD13	7:I:49:ILE:HD12	1.84	0.58
2:B:1129:ARG:NH1	11:T:21:DC:OP1	2.36	0.58
1:A:834:THR:HG21	1:A:1077:THR:HA	1.85	0.58
2:B:1077:THR:HG23	2:B:1079:LYS:H	1.69	0.58
6:H:129:TYR:O	6:H:132:LEU:N	2.37	0.58
1:A:1187:GLN:HG3	1:A:1188:GLN:HG3	1.86	0.57
1:A:34:LYS:H	1:A:34:LYS:HD3	1.70	0.57
3:C:77:ILE:HG12	3:C:129:ILE:HD11	1.87	0.56
1:A:331:GLY:HA2	1:A:334:GLY:H	1.70	0.56
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.87	0.56
1:A:1261:LYS:O	1:A:1264:GLU:HG3	2.05	0.56
1:A:1348:LEU:HD23	1:A:1372:VAL:HG13	1.87	0.56
2:B:1002:THR:HG23	2:B:1004:GLU:H	1.69	0.56
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.38	0.56
2:B:780:VAL:HG21	8:J:56:LEU:HD13	1.87	0.56
5:F:82:THR:O	5:F:136:ARG:NH1	2.30	0.56
1:A:110:CYS:SG	1:A:111:GLY:N	2.77	0.56
1:A:532:ARG:HE	1:A:536:LEU:HD21	1.70	0.56
3:C:185:LYS:HG2	3:C:213:PRO:HG3	1.86	0.56
2:B:1135:ARG:NH2	2:B:1136:ASP:OD1	2.39	0.55
6:H:91:ASP:OD1	6:H:92:ASP:N	2.38	0.55
1:A:1138:ILE:HG22	1:A:1279:ILE:HG21	1.88	0.55
1:A:550:LEU:HD21	1:A:561:PRO:HD2	1.89	0.55
1:A:595:THR:OG1	1:A:603:ASN:OD1	2.24	0.55
1:A:697:ALA:HA	1:A:702:LEU:HB2	1.88	0.55
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.46	0.55
6:H:89:LEU:H	6:H:89:LEU:HD13	1.71	0.55
1:A:512:VAL:HA	1:A:519:PRO:HA	1.87	0.55
1:A:765:VAL:HG22	1:A:800:VAL:HB	1.88	0.55
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.88	0.55
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.89	0.55
1:A:868:TYR:CE1	1:A:1064:VAL:HG21	2.42	0.54
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:287:ARG:NH1	2:B:321:GLY:O	2.40	0.54
6:H:137:GLN:HG3	6:H:139:ASN:H	1.71	0.54
1:A:17:VAL:HB	1:A:1419:ASP:HB3	1.90	0.54
1:A:760:GLN:HG2	1:A:765:VAL:HA	1.89	0.54
1:A:1281:ARG:HG2	1:A:1309:ASP:HB2	1.89	0.54
1:A:1397:LEU:HB2	1:A:1426:GLU:HG2	1.90	0.54
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.89	0.54
8:J:36:LEU:HD11	8:J:51:LEU:HB2	1.90	0.54
3:C:252:GLN:HG3	9:K:95:ILE:HG23	1.88	0.54
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.73	0.54
2:B:101:MET:HG2	2:B:111:ALA:HA	1.90	0.54
10:L:38:LEU:HD21	10:L:48:CYS:HA	1.90	0.53
2:B:620:ARG:NH2	7:I:89:GLN:OE1	2.38	0.53
1:A:626:ASN:O	1:A:631:HIS:ND1	2.32	0.53
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.42	0.52
1:A:993:LEU:HD22	1:A:1046:LEU:HG	1.91	0.52
1:A:1079:MET:HE3	1:A:1359:ASP:HB2	1.91	0.52
2:B:28:GLU:OE1	2:B:807:ARG:NH1	2.31	0.52
3:C:99:LEU:HD12	3:C:118:LEU:HB3	1.91	0.52
2:B:837:ASP:OD2	2:B:1020:ARG:NH2	2.43	0.52
3:C:3:GLU:HG3	3:C:4:GLU:HG3	1.90	0.52
6:H:8:ASP:OD1	6:H:9:ILE:N	2.41	0.52
2:B:287:ARG:NH1	2:B:324:ILE:O	2.42	0.52
10:L:68:GLU:O	10:L:70:ARG:N	2.42	0.52
2:B:847:ASP:OD2	9:K:6:ARG:NH2	2.43	0.52
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.92	0.51
1:A:1064:VAL:HG23	1:A:1067:LEU:HD23	1.91	0.51
1:A:1342:GLU:OE2	4:E:212:ARG:NH1	2.43	0.51
1:A:306:ASN:HB2	1:A:324:SER:HB3	1.91	0.51
2:B:487:THR:OG1	2:B:777:ALA:O	2.25	0.51
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.92	0.51
1:A:1193:LEU:HB2	1:A:1260:LEU:HD21	1.93	0.51
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.92	0.51
3:C:46:ILE:HD12	3:C:157:CYS:HB3	1.92	0.51
1:A:544:ASP:OD1	1:A:545:GLN:N	2.42	0.51
3:C:3:GLU:N	9:K:104:ASN:HD21	2.09	0.51
1:A:1116:LEU:HD22	1:A:1329:THR:HB	1.93	0.50
4:E:20:LYS:NZ	4:E:34:GLU:O	2.35	0.50
1:A:562:THR:O	1:A:576:GLN:NE2	2.44	0.50
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.94	0.50
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ILE:HG23	2:B:1170:THR:HG23	1.93	0.50
1:A:868:TYR:OH	1:A:1366:ARG:HD3	2.12	0.50
1:A:378:GLU:OE2	1:A:387:ARG:NH2	2.43	0.50
2:B:877:PRO:HB2	2:B:885:MET:HE1	1.94	0.50
1:A:802:ASN:OD1	2:B:729:ILE:N	2.39	0.50
2:B:118:ARG:NH2	2:B:194:GLU:OE2	2.39	0.50
3:C:57:VAL:HG11	8:J:60:PHE:HB3	1.94	0.50
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.93	0.50
2:B:613:VAL:HG22	2:B:628:THR:HG23	1.93	0.50
3:C:41:ILE:HB	3:C:172:PRO:HG3	1.94	0.50
6:H:85:GLY:HA2	6:H:86:ASP:HB3	1.93	0.49
3:C:69:LEU:HD12	8:J:6:ARG:HD3	1.93	0.49
1:A:774:ARG:HG3	1:A:797:LYS:HZ2	1.77	0.49
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.94	0.49
4:E:83:CYS:HB2	4:E:110:PHE:HE1	1.77	0.49
10:L:48:CYS:SG	10:L:49:LYS:N	2.85	0.49
10:L:47:ARG:HG2	10:L:54:ARG:HG2	1.93	0.49
2:B:779:GLY:HA2	2:B:796:LEU:HB2	1.94	0.49
2:B:916:THR:HG23	2:B:935:ARG:HB2	1.94	0.49
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.95	0.49
1:A:365:GLY:HA3	1:A:469:ARG:HB2	1.94	0.49
1:A:76:GLU:OE2	2:B:1159:ARG:NH1	2.46	0.49
1:A:1134:ILE:HD13	1:A:1322:ILE:HG22	1.94	0.49
6:H:89:LEU:HD23	6:H:91:ASP:H	1.78	0.49
1:A:337:ARG:NH1	11:T:19:DA:OP1	2.34	0.48
1:A:434:ARG:NH2	1:A:440:ASP:OD2	2.46	0.48
2:B:281:PRO:HB2	2:B:284:ILE:HG12	1.94	0.48
1:A:1207:LEU:HD23	1:A:1274:ARG:HD2	1.95	0.48
11:T:26:DG:H1	12:R:3:C:H42	1.60	0.48
2:B:274:PRO:HG2	2:B:359:GLU:HB3	1.94	0.48
1:A:666:ILE:HG23	2:B:1026:LEU:HB2	1.93	0.48
2:B:796:LEU:HB3	2:B:799:PRO:HG3	1.95	0.48
1:A:541:ILE:HD12	1:A:577:ILE:HG12	1.95	0.48
1:A:956:LEU:HD11	1:A:1017:LEU:HD22	1.95	0.48
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.79	0.48
1:A:1194:ARG:HH21	1:A:1237:ILE:HD13	1.79	0.48
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.96	0.48
2:B:294:ASP:HB2	7:I:12:ASN:HA	1.95	0.48
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.95	0.48
3:C:22:LEU:HD22	9:K:101:LEU:HD21	1.95	0.47
1:A:709:THR:HG22	1:A:711:ARG:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:840:ARG:NH2	1:A:1106:ASN:OD1	2.47	0.47
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.96	0.47
3:C:8:VAL:HG11	9:K:105:PHE:HD1	1.79	0.47
1:A:868:TYR:CZ	1:A:1064:VAL:HG21	2.49	0.47
2:B:95:ILE:HD11	2:B:128:LEU:HB3	1.95	0.47
1:A:889:SER:HB3	1:A:1297:GLU:HG3	1.95	0.47
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.49	0.47
2:B:579:ARG:HA	2:B:589:VAL:HA	1.96	0.47
2:B:840:ILE:HB	2:B:1011:ILE:HB	1.96	0.47
2:B:857:ARG:NH2	11:T:25:DC:OP1	2.47	0.47
1:A:1364:ASN:OD1	1:A:1366:ARG:NH1	2.47	0.47
1:A:528:LEU:HD23	1:A:751:SER:HA	1.97	0.47
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.96	0.47
1:A:1064:VAL:HA	1:A:1067:LEU:HB3	1.96	0.46
1:A:107:CYS:SG	1:A:108:MET:N	2.89	0.46
1:A:826:ASP:O	1:A:830:LYS:HB2	2.15	0.46
1:A:1163:ILE:HG22	1:A:1165:GLU:H	1.80	0.46
2:B:378:LEU:O	2:B:382:ILE:HG12	2.15	0.46
2:B:680:THR:O	2:B:683:SER:OG	2.27	0.46
3:C:40:GLU:O	3:C:250:THR:HG21	2.15	0.46
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.97	0.46
2:B:843:GLN:HB2	2:B:993:THR:HB	1.96	0.46
2:B:428:ILE:HD11	2:B:448:ILE:HG23	1.97	0.46
3:C:101:LEU:HB2	3:C:118:LEU:HD23	1.97	0.46
2:B:120:ARG:HB2	2:B:122:LEU:HG	1.98	0.46
2:B:956:THR:HG22	10:L:46:VAL:HG11	1.98	0.46
1:A:856:THR:HB	1:A:865:GLN:HB2	1.97	0.46
2:B:899:ILE:HG21	2:B:949:VAL:HG21	1.97	0.46
1:A:690:VAL:HG13	1:A:718:VAL:HG22	1.97	0.46
1:A:780:VAL:HG23	1:A:789:LYS:HE2	1.97	0.46
2:B:681:TRP:CH2	2:B:690:VAL:HG11	2.51	0.46
7:I:14:LEU:HD13	7:I:27:PHE:HB3	1.98	0.46
2:B:839:MET:HG3	2:B:1010:LEU:HD11	1.98	0.45
1:A:78:PRO:HB2	1:A:79:GLY:H	1.56	0.45
1:A:1239:ARG:HH22	1:A:1241:ARG:HH21	1.64	0.45
2:B:1065:GLN:HG3	2:B:1067:ARG:H	1.81	0.45
6:H:44:VAL:HG13	6:H:48:PRO:HA	1.98	0.45
7:I:101:PHE:HE1	7:I:112:SER:HB3	1.81	0.45
5:F:107:VAL:HG12	5:F:109:VAL:H	1.80	0.45
1:A:242:PRO:HA	1:A:243:PRO:HD3	1.78	0.45
1:A:962:ARG:HA	1:A:965:GLN:HG2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:31:ASN:O	3:C:35:ARG:HG3	2.17	0.45
2:B:640:VAL:HG22	2:B:651:LEU:HD23	1.99	0.45
1:A:1224:LEU:HD11	1:A:1240:CYS:HB3	1.98	0.45
15:B:1302:2KH:H10	15:B:1302:2KH:H14	1.60	0.45
2:B:30:SER:OG	2:B:743:ILE:O	2.27	0.45
2:B:1156:ASP:O	2:B:1197:PRO:HA	2.17	0.45
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.98	0.45
3:C:56:THR:HG21	3:C:63:ILE:HD11	1.99	0.45
1:A:695:LYS:HE3	1:A:695:LYS:HB2	1.81	0.45
1:A:235:ILE:H	1:A:235:ILE:HG13	1.55	0.44
1:A:1154:TYR:CE1	1:A:1156:PRO:HG3	2.52	0.44
1:A:596:THR:C	1:A:598:LEU:H	2.19	0.44
1:A:711:ARG:NH2	7:I:95:THR:OG1	2.49	0.44
2:B:1001:PHE:HE2	3:C:178:PHE:HB3	1.82	0.44
1:A:633:VAL:HG11	1:A:645:LEU:HD22	1.98	0.44
2:B:757:PRO:HG2	2:B:984:HIS:NE2	2.32	0.44
1:A:663:SER:OG	1:A:664:THR:N	2.51	0.44
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.82	0.44
1:A:179:LEU:HD22	1:A:297:GLN:HG3	2.00	0.44
1:A:443:LEU:HD12	2:B:1146:PHE:CE1	2.51	0.44
1:A:1260:LEU:HD12	1:A:1263:ILE:HD12	2.00	0.44
3:C:62:PHE:O	3:C:66:ARG:HG3	2.18	0.44
4:E:157:SER:OG	4:E:158:SER:N	2.50	0.44
9:K:10:PHE:HA	9:K:37:LYS:HB3	1.99	0.44
2:B:1039:GLY:HA2	8:J:51:LEU:HD22	2.00	0.44
1:A:336:ILE:HA	1:A:340:LEU:HD12	2.00	0.44
1:A:343:LYS:HE2	2:B:1151:LEU:HA	1.98	0.44
1:A:446:ARG:NH2	12:R:9:A:O2'	2.51	0.44
1:A:482:PHE:HB2	2:B:838:SER:HB3	1.99	0.44
11:T:22:DT:H3	12:R:7:A:H2	1.66	0.44
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.53	0.44
1:A:1438:THR:HG23	5:F:92:ARG:HB2	1.99	0.44
2:B:979:LYS:HG2	2:B:1095:LEU:HD12	2.00	0.44
8:J:14:VAL:HB	8:J:50:ILE:HD11	1.98	0.44
9:K:58:PHE:HB3	9:K:76:GLN:HB3	1.99	0.44
1:A:279:LEU:HB3	1:A:289:ILE:HG22	1.99	0.44
1:A:879:GLU:OE1	1:A:962:ARG:NH2	2.51	0.44
3:C:99:LEU:HB3	3:C:120:ILE:HD13	2.00	0.44
6:H:84:ALA:HB3	6:H:86:ASP:HB3	2.00	0.44
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.99	0.43
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:VAL:HG11	2:B:495:LEU:HD13	2.00	0.43
2:B:846:ILE:HG23	2:B:974:PRO:HG2	2.00	0.43
3:C:112:ASN:ND2	8:J:19:GLU:OE2	2.51	0.43
9:K:88:LYS:O	9:K:92:ASN:ND2	2.47	0.43
1:A:1364:ASN:OD1	1:A:1366:ARG:HG2	2.18	0.43
2:B:256:VAL:HG11	2:B:382:ILE:HD13	2.00	0.43
7:I:85:PHE:HB3	7:I:101:PHE:CD2	2.54	0.43
9:K:63:VAL:HG22	9:K:71:PHE:HB3	2.01	0.43
1:A:91:PHE:HZ	1:A:207:ILE:HD12	1.84	0.43
2:B:118:ARG:HG3	2:B:204:ILE:HD13	2.00	0.43
2:B:199:MET:SD	2:B:199:MET:N	2.78	0.43
2:B:883:LEU:O	2:B:885:MET:N	2.52	0.43
1:A:471:ASN:O	1:A:474:VAL:HG12	2.18	0.43
2:B:493:SER:OG	2:B:775:LYS:HE2	2.18	0.43
2:B:1051:THR:O	2:B:1055:ILE:HG12	2.19	0.43
10:L:31:CYS:SG	10:L:32:ALA:N	2.92	0.43
2:B:806:THR:HG22	2:B:808:ALA:H	1.84	0.43
1:A:31:SER:HB2	1:A:83:HIS:HB3	2.00	0.43
1:A:541:ILE:N	1:A:572:TRP:O	2.43	0.43
1:A:1255:GLU:HB3	1:A:1258:HIS:CE1	2.54	0.43
2:B:326:ASP:OD1	2:B:329:THR:OG1	2.23	0.43
1:A:378:GLU:OE1	1:A:434:ARG:HD3	2.19	0.43
3:C:22:LEU:HB3	3:C:25:VAL:HG21	2.01	0.43
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	2.01	0.42
1:A:1219:THR:HG21	1:A:1271:ILE:HD11	1.99	0.42
3:C:69:LEU:O	8:J:6:ARG:HD2	2.19	0.42
1:A:560:ILE:HB	6:H:79:TRP:H	1.84	0.42
2:B:805:THR:HG21	2:B:815:ARG:HD3	2.01	0.42
2:B:1187:ASN:ND2	2:B:1190:ASP:O	2.52	0.42
1:A:1215:ARG:HD3	1:A:1272:THR:O	2.19	0.42
1:A:326:ARG:HG2	1:A:1406:VAL:HG11	2.02	0.42
1:A:1011:GLN:O	1:A:1015:VAL:HG23	2.19	0.42
1:A:1373:ASP:HA	1:A:1376:THR:HG22	2.00	0.42
3:C:8:VAL:HG11	9:K:105:PHE:CD1	2.55	0.42
2:B:1162:ILE:HG12	2:B:1194:ILE:HD12	2.02	0.42
3:C:212:PRO:HA	3:C:213:PRO:HD3	1.87	0.42
4:E:124:VAL:HG13	4:E:132:ILE:HB	2.02	0.42
1:A:108:MET:O	1:A:110:CYS:N	2.50	0.42
1:A:443:LEU:HD11	2:B:1138:MET:SD	2.60	0.42
1:A:129:LYS:HA	1:A:134:ARG:HH21	1.85	0.42
1:A:206:GLU:O	1:A:210:ILE:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:284:ILE:HG21	2:B:333:PHE:HD2	1.85	0.42
2:B:884:ARG:HD3	2:B:884:ARG:HA	1.88	0.42
1:A:84:ILE:HD12	1:A:270:LEU:HG	2.02	0.42
1:A:1262:LYS:O	1:A:1265:ASN:HB3	2.20	0.42
2:B:114:PRO:HG2	2:B:181:LEU:HD11	2.01	0.42
2:B:190:TYR:CZ	2:B:196:PRO:HG3	2.55	0.42
1:A:87:ALA:HB3	1:A:276:LEU:HD23	2.01	0.41
1:A:231:PRO:HA	1:A:234:MET:HG3	2.02	0.41
2:B:1094:ARG:NH2	2:B:1098:MET:SD	2.93	0.41
1:A:349:ALA:HB2	1:A:374:LEU:HD11	2.02	0.41
1:A:449:SER:HB3	2:B:1137:CYS:SG	2.61	0.41
2:B:857:ARG:HH21	2:B:942:ARG:NH2	2.18	0.41
1:A:523:ILE:HD13	1:A:622:VAL:HG22	2.03	0.41
2:B:487:THR:HG22	2:B:489:SER:H	1.85	0.41
1:A:131:SER:HB3	1:A:223:GLY:HA2	2.02	0.41
1:A:396:PRO:HG3	1:A:416:ARG:HB3	2.02	0.41
1:A:586:ILE:HD11	1:A:637:LYS:HG2	2.02	0.41
1:A:778:GLY:HA3	2:B:516:ASN:HB2	2.01	0.41
1:A:1436:ILE:O	1:A:1438:THR:N	2.53	0.41
5:F:76:LYS:O	5:F:79:ARG:HD3	2.20	0.41
1:A:70:CYS:O	1:A:72:GLU:HG2	2.20	0.41
2:B:1156:ASP:OD1	2:B:1156:ASP:N	2.53	0.41
4:E:169:ARG:HG3	5:F:140:ASP:HB3	2.03	0.41
7:I:65:ASP:HB3	7:I:68:LEU:HD12	2.03	0.41
1:A:780:VAL:HG22	2:B:699:GLU:OE2	2.20	0.41
1:A:1147:THR:HB	7:I:48:LEU:HD12	2.03	0.41
2:B:364:ILE:HG13	2:B:365:THR:OG1	2.20	0.41
1:A:362:ASP:HB3	1:A:508:PRO:HD3	2.02	0.41
1:A:575:LYS:HB3	1:A:612:ILE:HD13	2.03	0.41
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	2.02	0.41
1:A:1150:SER:OG	7:I:46:HIS:HB3	2.20	0.41
2:B:939:THR:HA	2:B:940:PRO:HD3	1.85	0.41
5:F:93:ILE:HD13	5:F:93:ILE:HA	1.93	0.41
1:A:444:PHE:HD1	1:A:444:PHE:HA	1.72	0.41
1:A:1207:LEU:HD22	1:A:1273:LEU:HD23	2.03	0.41
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.55	0.41
2:B:25:ILE:HG23	2:B:29:ASP:HB2	2.03	0.41
9:K:22:ASP:HA	9:K:23:PRO:HD3	1.90	0.41
1:A:500:GLU:O	1:A:504:LEU:HB2	2.21	0.41
2:B:1023:VAL:O	2:B:1027:ILE:HG13	2.21	0.41
3:C:75:MET:O	3:C:246:ARG:NH2	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:LEU:HD12	6:H:46:LEU:HD11	2.03	0.40
1:A:843:LYS:HD3	1:A:843:LYS:HA	1.94	0.40
1:A:849:MET:HB3	1:A:1063:MET:SD	2.61	0.40
1:A:1198:ASP:O	1:A:1202:MET:HG2	2.21	0.40
2:B:63:ILE:O	2:B:67:SER:OG	2.36	0.40
2:B:762:ASN:HD22	2:B:762:ASN:HA	1.73	0.40
5:F:128:LYS:HD2	5:F:149:GLU:HA	2.03	0.40
1:A:311:GLN:N	1:A:312:PRO:HD2	2.36	0.40
2:B:102:VAL:HG23	2:B:112:LEU:HB2	2.03	0.40
2:B:298:LEU:HD22	2:B:314:LEU:HD13	2.03	0.40
4:E:24:LYS:HE3	4:E:24:LYS:HB2	1.89	0.40
4:E:96:PHE:CZ	4:E:100:ILE:HD11	2.56	0.40
1:A:423:ASP:OD1	1:A:423:ASP:N	2.54	0.40
1:A:752:LYS:HG2	2:B:1015:HIS:O	2.22	0.40
1:A:1261:LYS:HB2	1:A:1261:LYS:HE3	1.88	0.40
2:B:270:LYS:HB3	2:B:279:ASP:HB3	2.03	0.40
2:B:916:THR:HA	2:B:917:PRO:HD3	1.84	0.40
1:A:302:THR:OG1	1:A:306:ASN:OD1	2.39	0.40
1:A:353:ILE:HG22	1:A:468:PHE:HB2	2.03	0.40
1:A:965:GLN:HA	1:A:968:GLN:HG2	2.04	0.40
2:B:600:LEU:HB3	2:B:615:MET:SD	2.61	0.40
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.21	0.40
5:F:116:ASP:O	5:F:120:ILE:HG13	2.22	0.40
2:B:773:MET:SD	2:B:987:LYS:HB3	2.62	0.40

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%)	<span style="border: 1px solid red; padding: 2px;">22</span> <span style="border: 1px solid gray; padding: 2px;">56</span>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (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
2	B	337	ARG
2	B	468	GLU
4	E	86	PRO
10	L	69	ALA
1	A	282	ASN
2	B	277	LYS
2	B	884	ARG
2	B	1108	ARG
3	C	90	ASP
10	L	41	SER
1	A	40	THR
1	A	958	VAL
2	B	1017	ILE
9	K	26	LYS
1	A	69	THR
1	A	1156	PRO
1	A	1279	ILE
6	H	18	GLY
6	H	82	PRO
2	B	260	GLY

### 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	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

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	TYR
1	A	12	ARG
1	A	22	PHE
1	A	34	LYS
1	A	126	LEU
1	A	132	LYS
1	A	179	LEU
1	A	222	LEU
1	A	270	LEU
1	A	287	HIS
1	A	308	ILE
1	A	322	VAL
1	A	326	ARG
1	A	335	ARG
1	A	351	THR
1	A	434	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	443	LEU
1	A	444	PHE
1	A	451	HIS
1	A	452	LYS
1	A	474	VAL
1	A	481	ASP
1	A	532	ARG
1	A	605	MET
1	A	612	ILE
1	A	618	GLU
1	A	666	ILE
1	A	702	LEU
1	A	764	CYS
1	A	765	VAL
1	A	774	ARG
1	A	821	ARG
1	A	826	ASP
1	A	830	LYS
1	A	884	ASP
1	A	896	ARG
1	A	926	GLN
1	A	1017	LEU
1	A	1025	ARG
1	A	1078	GLN
1	A	1116	LEU
1	A	1207	LEU
1	A	1231	ASP
1	A	1262	LYS
1	A	1295	THR
1	A	1297	GLU
1	A	1322	ILE
1	A	1329	THR
1	A	1354	ASN
1	A	1374	VAL
1	A	1400	CYS
1	A	1407	GLU
2	B	46	GLN
2	B	90	ILE
2	B	109	THR
2	B	134	LYS
2	B	313	MET
2	B	319	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	364	ILE
2	B	365	THR
2	B	396	ASP
2	B	482	VAL
2	B	483	LEU
2	B	547	VAL
2	B	549	THR
2	B	570	VAL
2	B	628	THR
2	B	737	THR
2	B	751	VAL
2	B	797	TYR
2	B	825	VAL
2	B	868	MET
2	B	916	THR
2	B	917	PRO
2	B	931	TYR
2	B	983	ARG
2	B	999	MET
2	B	1007	VAL
2	B	1028	GLU
2	B	1051	THR
2	B	1065	GLN
2	B	1099	VAL
2	B	1147	LEU
2	B	1160	VAL
2	B	1176	ASN
2	B	1188	LYS
2	B	1194	ILE
2	B	1202	LEU
3	C	25	VAL
3	C	56	THR
3	C	77	ILE
3	C	99	LEU
3	C	137	LYS
3	C	240	VAL
3	C	244	VAL
4	E	3	GLN
4	E	98	ILE
4	E	110	PHE
4	E	123	LEU
4	E	127	ILE

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Mol	Chain	Res	Type
4	E	169	ARG
5	F	79	ARG
5	F	97	ARG
5	F	155	LEU
6	H	89	LEU
6	H	124	ARG
7	I	14	LEU
8	J	5	VAL
8	J	13	VAL
9	K	11	LEU
10	L	64	LEU

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 ⓘ

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 ⓘ

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(°)	Ideal(°)
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

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

All (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
15	B	1302	2KH	C6-C5	5.58	1.48	1.35
15	B	1302	2KH	C2-N3	5.57	1.47	1.38
15	B	1302	2KH	PA-O1A	3.86	1.52	1.46
15	B	1302	2KH	PB-O2B	3.37	1.51	1.46
15	B	1302	2KH	O2'-C2'	2.81	1.49	1.43
15	B	1302	2KH	O3'-C3'	-2.69	1.36	1.43
15	B	1302	2KH	C4-N3	2.17	1.42	1.38
15	B	1302	2KH	PB-O1B	-2.03	1.51	1.56
15	B	1302	2KH	PA-N3A	2.02	1.68	1.63
15	B	1302	2KH	C1'-N1	-2.00	1.41	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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.

All (13) torsion outliers are listed below:

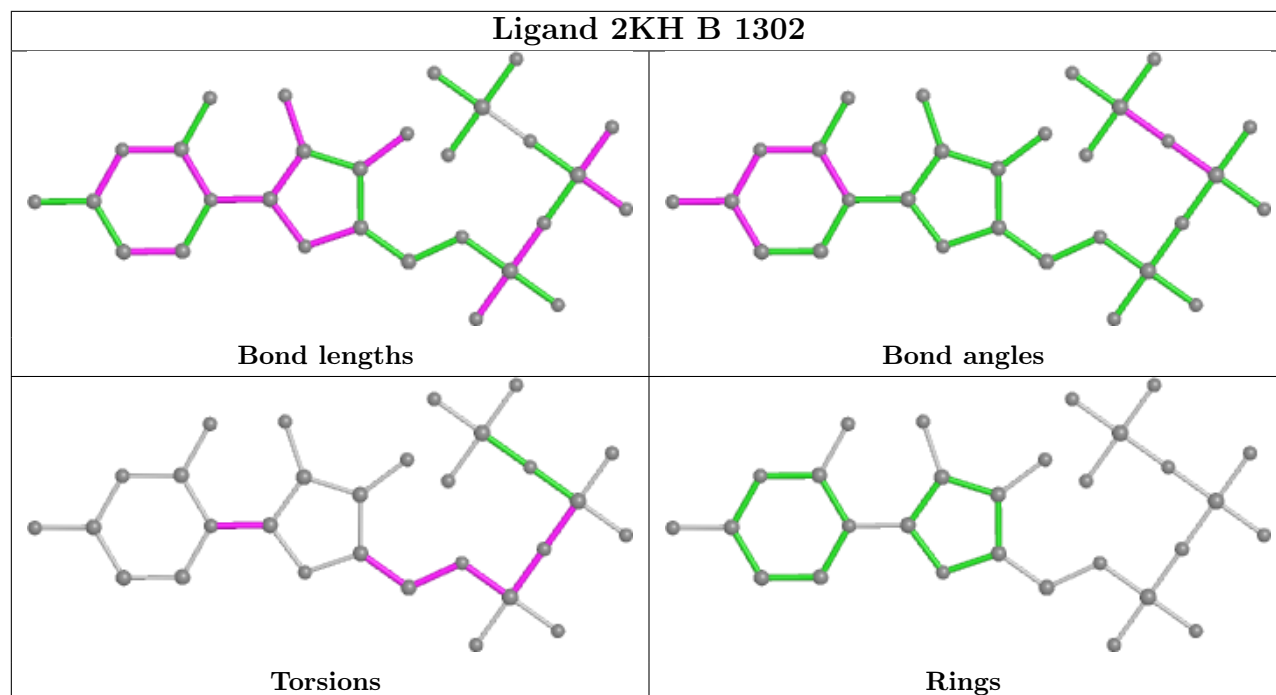
Mol	Chain	Res	Type	Atoms
15	B	1302	2KH	PB-N3A-PA-O1A
15	B	1302	2KH	C5'-O5'-PA-O2A
15	B	1302	2KH	PA-N3A-PB-O2B
15	B	1302	2KH	O4'-C4'-C5'-O5'
15	B	1302	2KH	C3'-C4'-C5'-O5'
15	B	1302	2KH	O4'-C1'-N1-C6
15	B	1302	2KH	O4'-C1'-N1-C2
15	B	1302	2KH	C2'-C1'-N1-C6
15	B	1302	2KH	C2'-C1'-N1-C2
15	B	1302	2KH	C5'-O5'-PA-O1A
15	B	1302	2KH	C5'-O5'-PA-N3A
15	B	1302	2KH	C4'-C5'-O5'-PA
15	B	1302	2KH	PA-N3A-PB-O3B

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 than 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.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	1372/1733 (79%)	0.59	131 (9%) <span style="border: 1px solid red; padding: 0 2px;">8</span> <span style="border: 1px solid red; padding: 0 2px;">5</span>	16, 58, 161, 242	0
2	B	1097/1224 (89%)	0.29	38 (3%) <span style="border: 1px solid red; padding: 0 2px;">44</span> <span style="border: 1px solid red; padding: 0 2px;">29</span>	13, 46, 119, 225	0
3	C	266/318 (83%)	0.20	3 (1%) <span style="border: 1px solid blue; padding: 0 2px;">80</span> <span style="border: 1px solid blue; padding: 0 2px;">65</span>	19, 45, 85, 171	0
4	E	213/215 (99%)	1.06	45 (21%) <span style="border: 1px solid red; padding: 0 2px;">1</span> <span style="border: 1px solid red; padding: 0 2px;">0</span>	35, 86, 172, 234	0
5	F	84/155 (54%)	0.03	2 (2%) <span style="border: 1px solid blue; padding: 0 2px;">59</span> <span style="border: 1px solid blue; padding: 0 2px;">42</span>	35, 58, 109, 179	0
6	H	130/146 (89%)	0.84	9 (6%) <span style="border: 1px solid red; padding: 0 2px;">16</span> <span style="border: 1px solid red; padding: 0 2px;">10</span>	42, 84, 147, 206	0
7	I	115/122 (94%)	0.33	2 (1%) <span style="border: 1px solid blue; padding: 0 2px;">70</span> <span style="border: 1px solid blue; padding: 0 2px;">53</span>	20, 61, 101, 114	0
8	J	65/70 (92%)	0.04	1 (1%) <span style="border: 1px solid blue; padding: 0 2px;">73</span> <span style="border: 1px solid blue; padding: 0 2px;">57</span>	22, 36, 82, 159	0
9	K	114/120 (95%)	0.19	0 <span style="border: 1px solid blue; padding: 0 2px;">100</span> <span style="border: 1px solid blue; padding: 0 2px;">100</span>	20, 49, 90, 108	0
10	L	44/70 (62%)	1.32	12 (27%) <span style="border: 1px solid red; padding: 0 2px;">0</span> <span style="border: 1px solid red; padding: 0 2px;">0</span>	26, 88, 182, 231	0
11	T	11/29 (37%)	1.39	4 (36%) <span style="border: 1px solid red; padding: 0 2px;">0</span> <span style="border: 1px solid red; padding: 0 2px;">0</span>	133, 138, 177, 179	0
12	R	9/9 (100%)	0.76	0 <span style="border: 1px solid blue; padding: 0 2px;">100</span> <span style="border: 1px solid blue; padding: 0 2px;">100</span>	111, 125, 150, 151	0
All	All	3520/4211 (83%)	0.47	247 (7%) <span style="border: 1px solid red; padding: 0 2px;">16</span> <span style="border: 1px solid red; padding: 0 2px;">9</span>	13, 55, 149, 242	0

All (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
1	A	182	VAL	8.0
10	L	45	ALA	7.9
6	H	86	ASP	7.5
2	B	643	ASP	7.4
1	A	181	LEU	7.3
2	B	474	SER	7.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	69	THR	7.0
4	E	52	ARG	6.9
1	A	174	ILE	6.7
10	L	35	SER	6.4
1	A	49	LYS	5.9
4	E	123	LEU	5.6
4	E	125	PRO	5.6
2	B	477	ALA	5.5
4	E	126	SER	5.5
1	A	177	ASP	5.5
1	A	179	LEU	5.4
2	B	472	ALA	5.4
6	H	139	ASN	5.4
1	A	185	TRP	5.4
2	B	471	LYS	5.3
1	A	312	PRO	5.2
1	A	102	VAL	5.2
1	A	250	ILE	5.2
1	A	105	CYS	5.2
1	A	147	VAL	5.1
1	A	113	LEU	5.1
4	E	85	GLU	5.1
4	E	110	PHE	4.9
1	A	213	HIS	4.9
1	A	111	GLY	4.8
4	E	98	ILE	4.8
1	A	1256	GLU	4.6
2	B	476	ARG	4.6
1	A	220	THR	4.5
1	A	180	LYS	4.5
1	A	209	ASN	4.5
1	A	73	GLY	4.5
4	E	96	PHE	4.3
1	A	87	ALA	4.3
1	A	65	LEU	4.3
1	A	126	LEU	4.3
3	C	4	GLU	4.3
2	B	266	ALA	4.2
1	A	167	CYS	4.1
1	A	317	LYS	4.1
1	A	176	LYS	4.0
1	A	216	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	274	ILE	4.0
1	A	289	ILE	4.0
4	E	132	ILE	4.0
4	E	83	CYS	3.9
1	A	141	LEU	3.9
1	A	109	HIS	3.9
1	A	215	SER	3.9
6	H	84	ALA	3.9
2	B	865	LYS	3.8
4	E	89	GLY	3.8
1	A	91	PHE	3.8
2	B	1189	ILE	3.8
1	A	270	LEU	3.8
1	A	205	GLU	3.8
1	A	127	ALA	3.8
2	B	647	GLY	3.8
4	E	50	MET	3.7
1	A	1262	LYS	3.7
1	A	146	MET	3.7
1	A	1258	HIS	3.7
1	A	397	ASN	3.7
1	A	175	ARG	3.7
1	A	323	LYS	3.7
1	A	287	HIS	3.6
1	A	975	HIS	3.6
1	A	66	LYS	3.6
2	B	733	HIS	3.6
1	A	166	GLY	3.6
1	A	123	ARG	3.6
2	B	1211	ASN	3.6
1	A	106	VAL	3.6
1	A	39	GLU	3.5
1	A	1255	GLU	3.5
1	A	266	LEU	3.5
2	B	867	GLY	3.5
1	A	122	MET	3.5
4	E	94	LYS	3.4
1	A	137	ALA	3.4
4	E	9	ILE	3.4
1	A	128	ILE	3.4
1	A	227	VAL	3.4
1	A	233	TRP	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	E	127	ILE	3.4
1	A	142	CYS	3.4
4	E	100	ILE	3.3
1	A	21	LEU	3.3
2	B	646	LEU	3.3
7	I	26	LEU	3.3
4	E	97	VAL	3.3
1	A	290	GLU	3.3
1	A	238	CYS	3.3
1	A	212	LYS	3.2
1	A	129	LYS	3.2
2	B	432	MET	3.2
2	B	133	LYS	3.2
1	A	138	ILE	3.2
1	A	293	GLU	3.2
4	E	95	THR	3.1
4	E	90	VAL	3.1
2	B	1183	LYS	3.1
1	A	202	LEU	3.1
4	E	119	SER	3.0
10	L	27	LEU	3.0
2	B	870	ILE	3.0
10	L	40	LEU	3.0
4	E	122	LYS	3.0
1	A	297	GLN	3.0
4	E	82	PHE	3.0
6	H	6	PHE	2.9
1	A	1225	PHE	2.9
11	T	19	DA	2.9
1	A	135	PHE	2.9
1	A	60	SER	2.9
1	A	211	PHE	2.9
4	E	44	ALA	2.9
2	B	263	GLY	2.9
1	A	201	VAL	2.9
4	E	121	MET	2.8
1	A	118	HIS	2.8
1	A	230	ARG	2.8
1	A	1257	ASP	2.8
6	H	83	GLN	2.8
1	A	310	GLY	2.8
6	H	7	ASP	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	148	CYS	2.8
1	A	108	MET	2.8
1	A	70	CYS	2.8
1	A	249	SER	2.8
2	B	262	GLU	2.8
1	A	45	GLN	2.8
1	A	1232	ASN	2.7
1	A	280	GLU	2.7
5	F	155	LEU	2.7
1	A	203	SER	2.7
4	E	57	MET	2.7
4	E	49	SER	2.6
1	A	103	CYS	2.6
1	A	276	LEU	2.6
4	E	131	THR	2.6
1	A	124	GLN	2.6
1	A	84	ILE	2.6
2	B	357	GLN	2.6
1	A	144	THR	2.6
1	A	269	ILE	2.6
2	B	1217	TYR	2.6
8	J	65	PRO	2.6
1	A	240	PRO	2.6
1	A	219	PHE	2.6
1	A	114	LEU	2.6
10	L	50	ASP	2.6
1	A	117	GLU	2.6
1	A	1156	PRO	2.6
1	A	1174	PHE	2.6
1	A	204	THR	2.6
4	E	87	SER	2.5
1	A	1254	ALA	2.5
2	B	1162	ILE	2.5
3	C	205	LYS	2.5
2	B	241	ARG	2.5
4	E	91	LYS	2.5
1	A	206	GLU	2.5
1	A	232	GLU	2.5
2	B	1170	THR	2.5
10	L	41	SER	2.5
6	H	110	ASP	2.5
6	H	88	SER	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
10	L	47	ARG	2.5
4	E	88	VAL	2.4
4	E	55	ARG	2.4
11	T	18	DC	2.4
4	E	116	ILE	2.4
2	B	429	PHE	2.4
1	A	221	SER	2.4
1	A	281	HIS	2.4
1	A	596	THR	2.4
1	A	316	GLN	2.4
10	L	64	LEU	2.4
10	L	53	HIS	2.3
4	E	115	ASN	2.3
10	L	36	SER	2.3
2	B	866	TYR	2.3
1	A	56	PRO	2.3
1	A	99	ILE	2.3
1	A	320	ARG	2.3
2	B	261	ARG	2.3
1	A	145	LYS	2.3
1	A	50	ILE	2.3
4	E	109	ILE	2.3
1	A	3	GLY	2.3
11	T	29	DG	2.3
5	F	78	GLN	2.3
1	A	72	GLU	2.2
1	A	296	LEU	2.2
4	E	215	MET	2.2
1	A	1259	MET	2.2
1	A	826	ASP	2.2
2	B	425	THR	2.2
2	B	648	HIS	2.2
2	B	275	TYR	2.2
6	H	138	GLU	2.2
1	A	115	LEU	2.2
1	A	48	ALA	2.2
1	A	284	ALA	2.2
1	A	234	MET	2.2
1	A	300	VAL	2.2
1	A	79	GLY	2.2
10	L	63	ARG	2.2
4	E	48	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	531	GLN	2.1
1	A	977	LYS	2.1
7	I	55	THR	2.1
4	E	81	GLU	2.1
4	E	120	ALA	2.1
1	A	74	MET	2.1
2	B	134	LYS	2.1
4	E	51	GLY	2.1
10	L	46	VAL	2.1
1	A	311	GLN	2.1
11	T	24	DT	2.1
1	A	263	THR	2.1
3	C	249	ASP	2.1
4	E	129	PRO	2.1
2	B	64	CYS	2.1
1	A	278	THR	2.1
4	E	54	GLN	2.1
2	B	89	GLU	2.1
2	B	267	ARG	2.1
4	E	124	VAL	2.1
1	A	86	LEU	2.0
4	E	107	THR	2.0
1	A	425	GLN	2.0
2	B	338	GLY	2.0
4	E	58	MET	2.0
1	A	208	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
11	3DR	T	20	11/12	0.73	0.31	149,156,161,183	0

## 6.3 Carbohydrates [i](#)

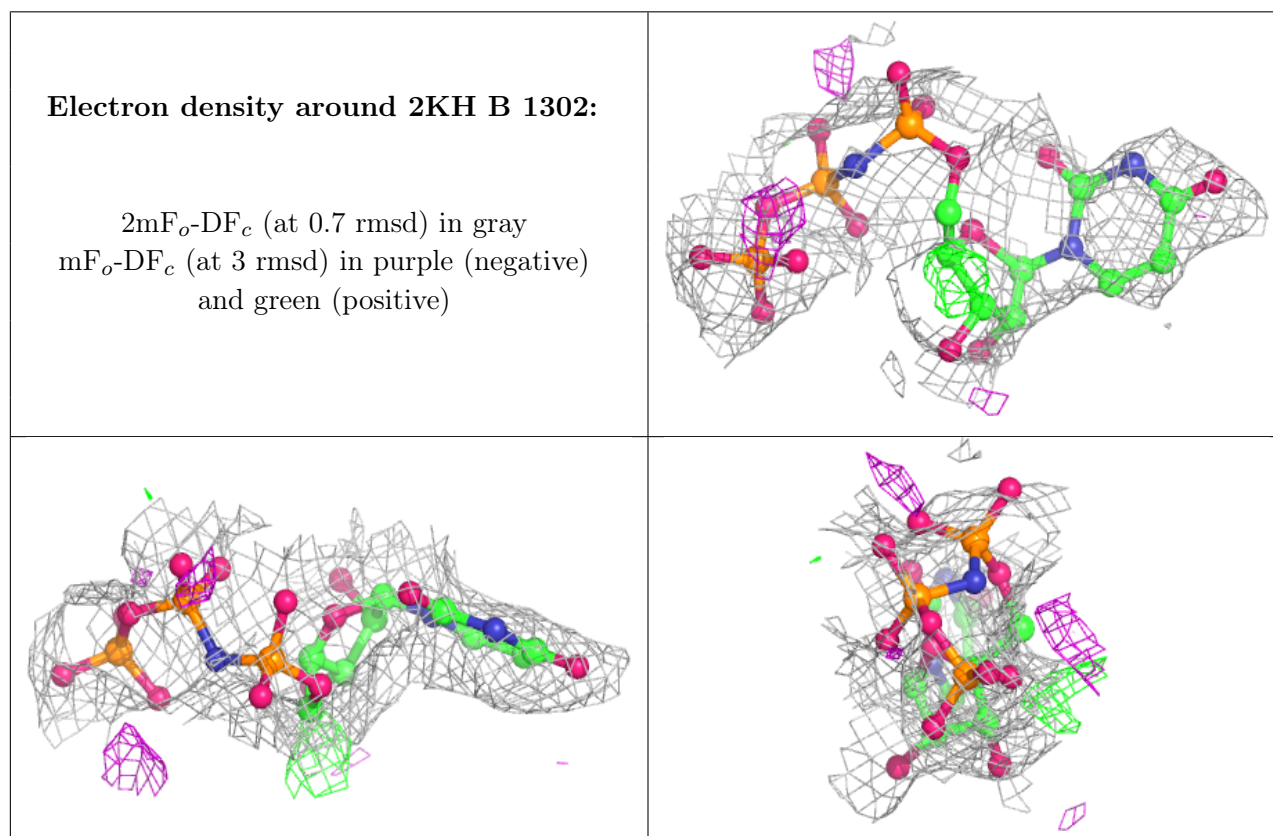
There are no monosaccharides in this entry.

## 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<sup>th</sup> 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 <sup>2</sup> )	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.