



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 05:12 AM BST

PDB ID : 5W51  
Title : Pol II elongation complex with an N6-methyladenine-containing template and a matched UMPNPP  
Authors : Wang, W.; Wang, D.  
Deposited on : 2017-06-13  
Resolution : 3.40 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 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)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

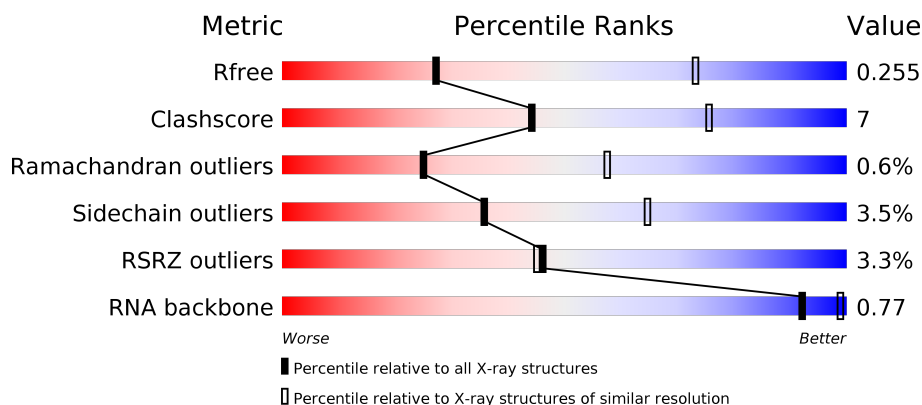
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)
RNA backbone	3102	1006 (3.84-2.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>3%</div> <div> <div></div> <div>63%</div> <div>16%</div> <div>•</div> <div>21%</div> </div> </div>
2	B	1224	<div> <div>0%</div> <div> <div></div> <div>69%</div> <div>19%</div> <div>•</div> <div>11%</div> </div> </div>
3	C	318	<div> <div></div> <div> <div></div> <div>69%</div> <div>14%</div> <div>•</div> <div>16%</div> </div> </div>
4	E	215	<div> <div>11%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div>••</div> </div> </div>

*Continued on next page...*

*Continued from previous page...*

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	N	14	
13	R	9	

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 28880 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	1371	Total	C	N	O	S	0	0	0
			10787	6806	1886	2034	61			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1089	Total	C	N	O	S	0	0	0
			8657	5485	1517	1601	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 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 29mer template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	T	29	Total	C	N	O	P	0	0	0
			588	283	107	170	28			

- Molecule 12 is a DNA chain called 14mer non-template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	N	14	Total	C	N	O	P	0	0	0
			284	137	49	85	13			

- Molecule 13 is a RNA chain called 9mer RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	R	9	Total	C	N	O	P	0	0	0
			198	89	42	59	8			

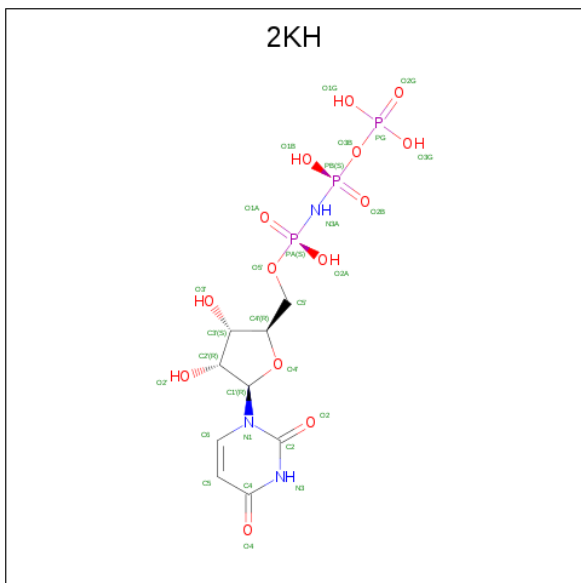
- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

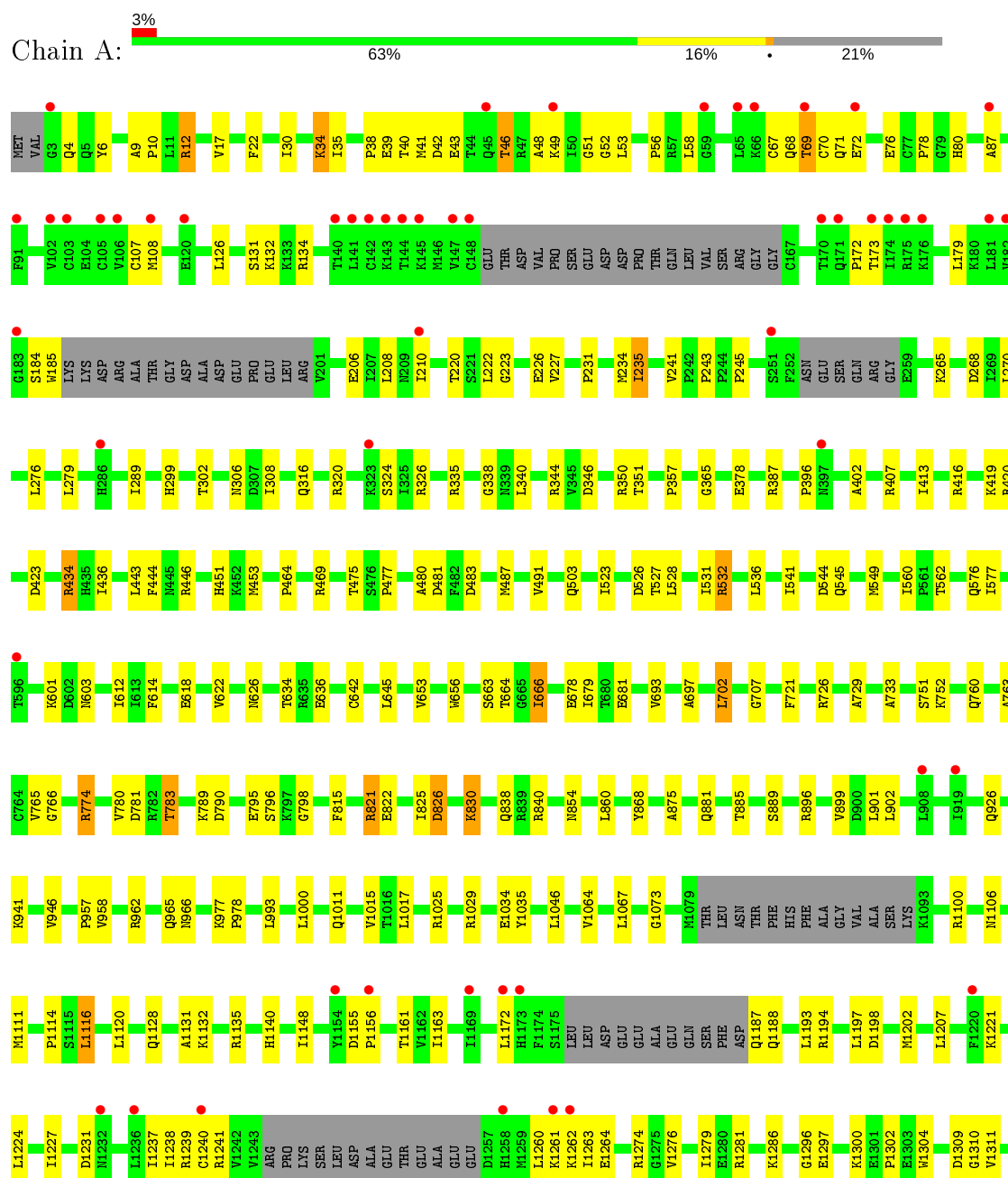


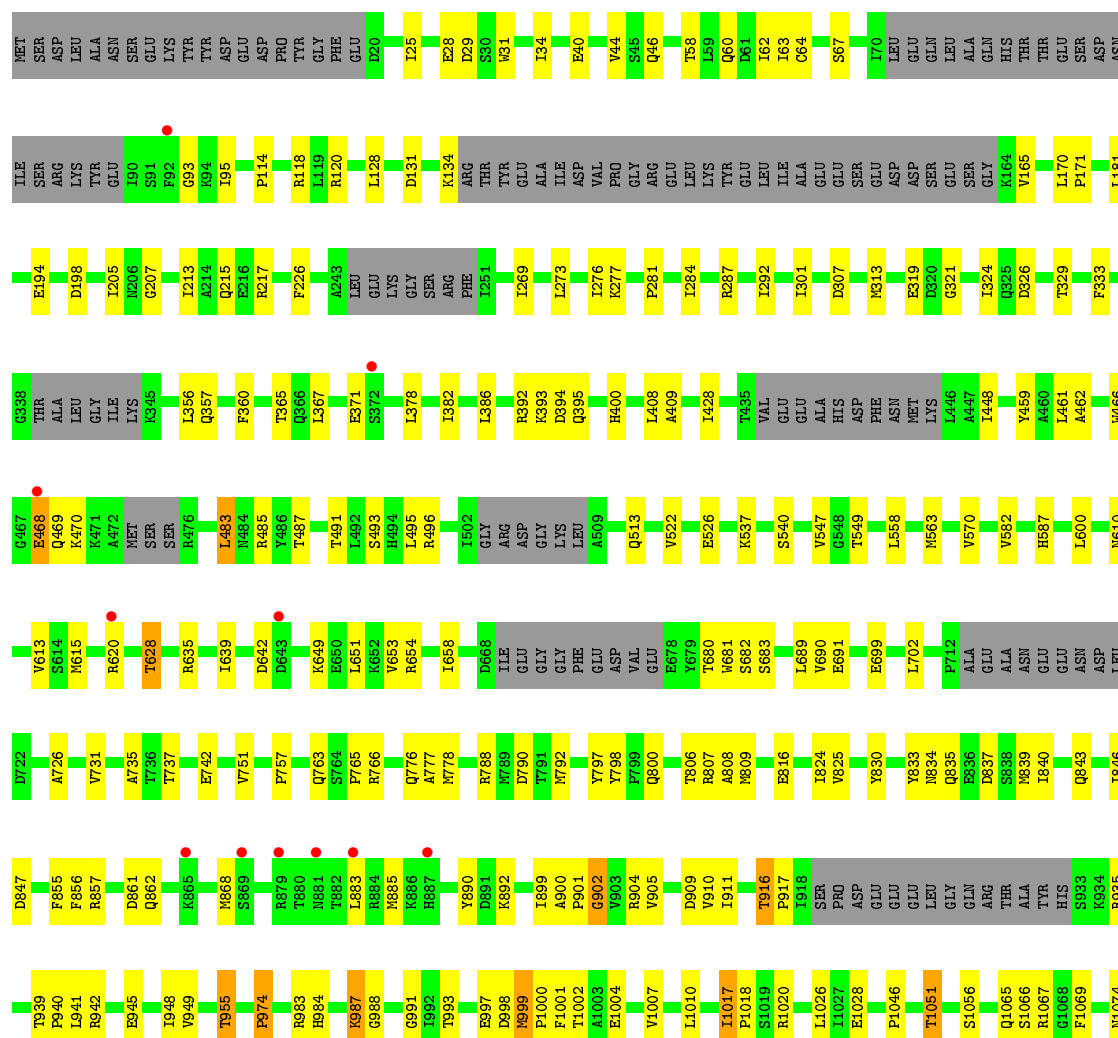
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
16	A	1	Total	C	N	O	P	0	1
			58	18	6	28	6		

### 3 Residue-property plots

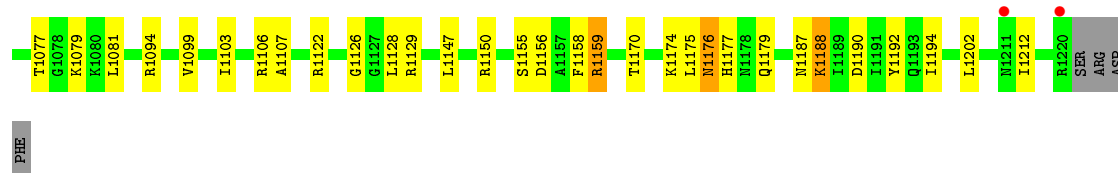
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



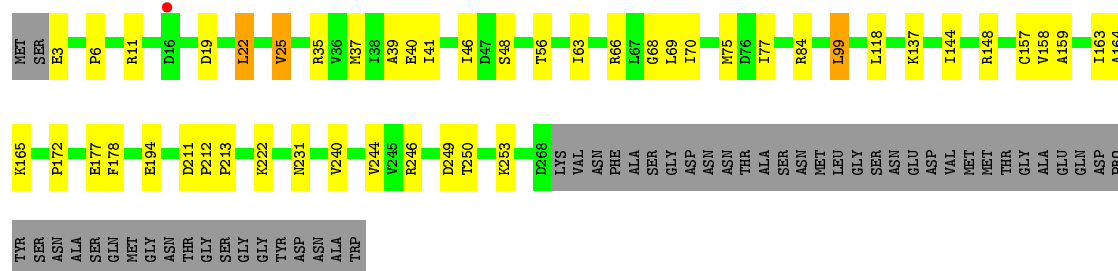






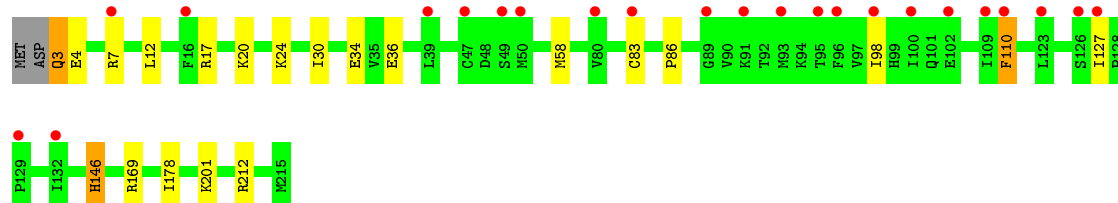
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 69% 14% 16%



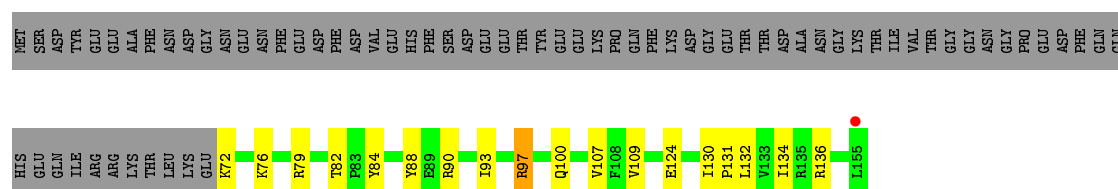
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 11% 89% 8%



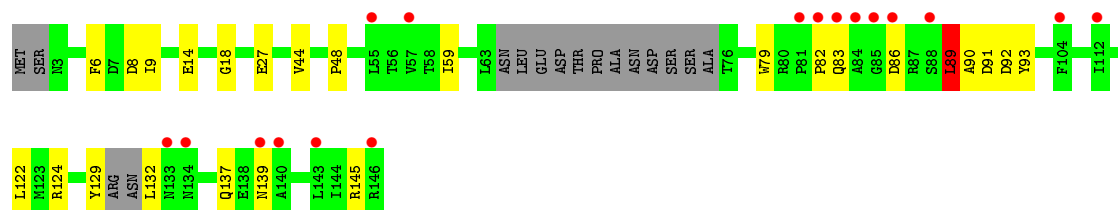
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 43% 11% 46%

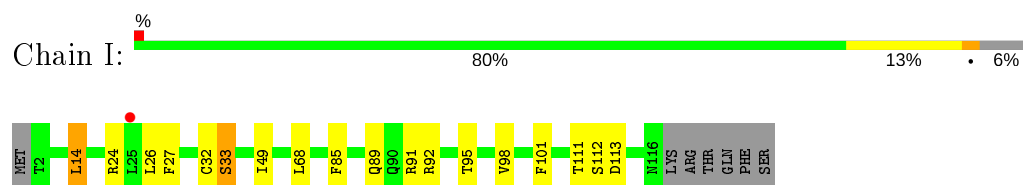


- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

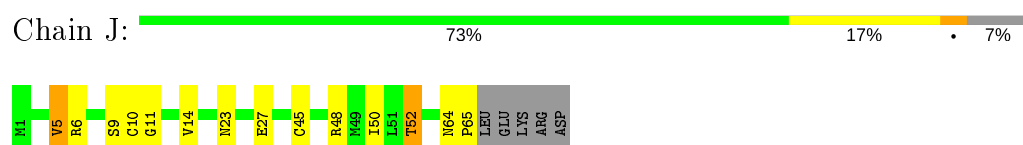
Chain H: 12% 72% 16% 11%



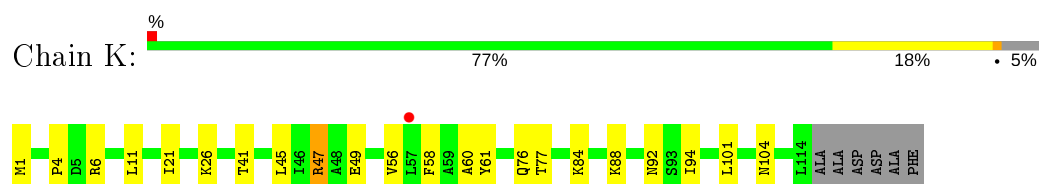
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9



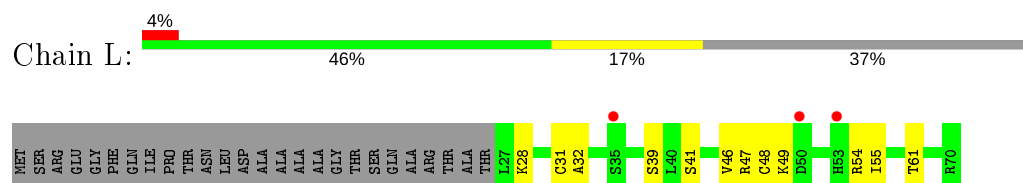
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



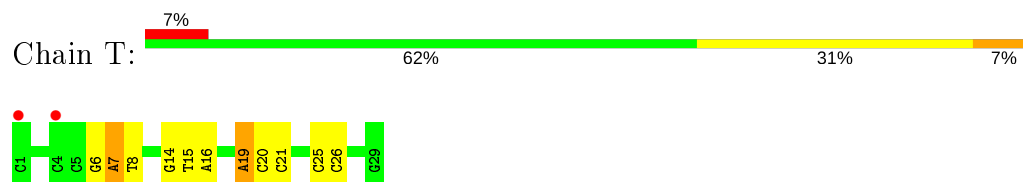
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11



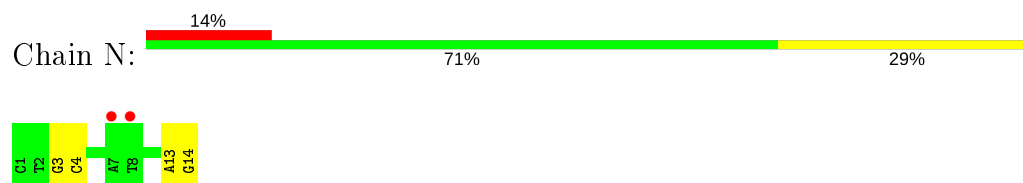
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



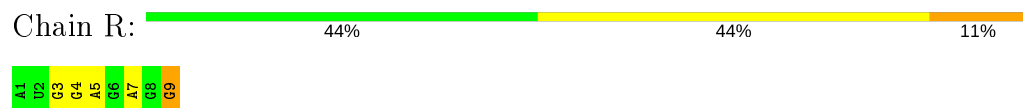
- Molecule 11: 29mer template DNA



- Molecule 12: 14mer non-template DNA



- Molecule 13: 9mer RNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	168.70 Å   224.00 Å   193.06 Å 90.00°   101.04°   90.00°	Depositor
Resolution (Å)	82.79 – 3.40 94.74 – 3.40	Depositor EDS
% Data completeness (in resolution range)	87.1 (82.79-3.40) 87.2 (94.74-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.48 (at 3.41 Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, $R_{free}$	0.227   ,   0.254 0.229   ,   0.255	Depositor DCC
$R_{free}$ test set	4066 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.4	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 40.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	28880	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 2KH, MG, 6MA

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	0/10979	0.38	0/14843
2	B	0.21	0/8824	0.37	0/11898
3	C	0.21	0/2133	0.38	0/2891
4	E	0.21	0/1780	0.36	0/2395
5	F	0.21	0/691	0.38	0/933
6	H	0.21	0/1060	0.39	1/1434 (0.1%)
7	I	0.21	0/953	0.35	0/1284
8	J	0.21	0/541	0.36	0/727
9	K	0.22	0/937	0.35	0/1265
10	L	0.20	0/353	0.35	0/468
11	T	0.46	0/580	0.86	0/884
12	N	0.49	0/317	0.93	0/488
13	R	0.14	0/223	0.61	0/348
All	All	0.22	0/29371	0.40	1/39858 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
6	H	89	LEU	CA-CB-CG	5.38	127.67	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10787	0	10872	164	0
2	B	8657	0	8693	144	0
3	C	2095	0	2051	29	0
4	E	1744	0	1772	10	0
5	F	679	0	701	11	0
6	H	1043	0	1015	14	0
7	I	935	0	887	11	0
8	J	532	0	542	9	0
9	K	919	0	929	16	0
10	L	351	0	375	7	0
11	T	588	0	333	8	0
12	N	284	0	161	2	0
13	R	198	0	99	5	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	2	0	0	0	0
16	A	58	0	32	3	0
All	All	28880	0	28462	376	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 7.

All (376) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1239:ARG:HH22	1:A:1241:ARG:HH21	1.29	0.78
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.67	0.76
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.69	0.73
3:C:6:PRO:HB2	9:K:101:LEU:HD23	1.72	0.72
1:A:42:ASP:HB3	1:A:46:THR:H	1.55	0.71
2:B:25:ILE:HD11	2:B:653:VAL:HB	1.71	0.71
2:B:778:MET:HE1	2:B:1094:ARG:HH11	1.56	0.70
3:C:48:SER:HB3	3:C:158:VAL:HB	1.74	0.69
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.72	0.69
7:I:92:ARG:HB3	7:I:95:THR:HG23	1.74	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:46:ILE:HB	3:C:68:GLY:HA2	1.73	0.68
2:B:911:ILE:HD11	2:B:941:LEU:HD23	1.74	0.68
1:A:1193:LEU:HB2	1:A:1260:LEU:HD21	1.76	0.67
2:B:287:ARG:NH1	2:B:324:ILE:O	2.27	0.67
8:J:5:VAL:HG22	8:J:6:ARG:HG3	1.77	0.67
1:A:338:GLY:HA2	2:B:1129:ARG:HH21	1.60	0.66
1:A:35:ILE:HG13	1:A:241:VAL:HG21	1.78	0.66
2:B:1129:ARG:NH1	11:T:21:DC:OP1	2.28	0.66
3:C:75:MET:O	3:C:246:ARG:NH2	2.29	0.66
2:B:468:GLU:HA	2:B:470:LYS:H	1.60	0.65
7:I:101:PHE:HE1	7:I:112:SER:HB3	1.61	0.65
2:B:1174:LYS:HB2	2:B:1179:GLN:HB2	1.79	0.64
2:B:1065:GLN:HG2	2:B:1069:PHE:HB2	1.78	0.64
1:A:899:VAL:HG22	1:A:1029:ARG:HG2	1.80	0.64
2:B:635:ARG:NH1	2:B:742:GLU:OE2	2.29	0.64
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.80	0.63
1:A:693:VAL:HG21	1:A:721:PHE:HE2	1.64	0.63
4:E:4:GLU:OE1	4:E:7:ARG:NH2	2.30	0.63
1:A:42:ASP:H	1:A:43:GLU:HA	1.64	0.63
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.81	0.63
2:B:1175:LEU:O	2:B:1176:ASN:ND2	2.32	0.62
2:B:468:GLU:HG3	2:B:469:GLN:HA	1.81	0.62
7:I:32:CYS:SG	7:I:33:SER:N	2.72	0.62
1:A:697:ALA:HA	1:A:702:LEU:HB2	1.81	0.62
2:B:496:ARG:NH2	2:B:540:SER:O	2.31	0.61
1:A:1348:LEU:HD23	1:A:1372:VAL:HG13	1.82	0.61
1:A:503:GLN:OE1	5:F:90:ARG:NH2	2.33	0.61
1:A:1397:LEU:HB2	1:A:1426:GLU:HG2	1.83	0.61
1:A:365:GLY:HA3	1:A:469:ARG:HB2	1.82	0.61
1:A:840:ARG:NH2	1:A:1106:ASN:OD1	2.34	0.61
5:F:82:THR:HG22	5:F:84:TYR:H	1.66	0.61
2:B:118:ARG:NH2	2:B:194:GLU:OE1	2.31	0.61
1:A:72:GLU:HG3	2:B:1175:LEU:HB2	1.83	0.61
1:A:822:GLU:HG3	2:B:513:GLN:HE21	1.65	0.61
1:A:483:ASP:HA	2:B:988:GLY:HA2	1.82	0.60
3:C:69:LEU:HD12	8:J:6:ARG:HD3	1.83	0.60
3:C:163:ILE:HG22	3:C:165:LYS:H	1.67	0.60
1:A:1281:ARG:HG2	1:A:1309:ASP:HB2	1.83	0.60
1:A:636:GLU:OE1	1:A:966:ASN:ND2	2.34	0.60
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.81	0.60
2:B:642:ASP:HB3	2:B:649:LYS:HG2	1.84	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:41:ILE:HB	3:C:172:PRO:HG3	1.84	0.59
10:L:48:CYS:SG	10:L:49:LYS:N	2.74	0.59
2:B:522:VAL:HG11	2:B:537:LYS:HD2	1.85	0.59
4:E:20:LYS:NZ	4:E:34:GLU:O	2.33	0.59
1:A:544:ASP:OD1	1:A:545:GLN:N	2.36	0.59
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.83	0.58
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.36	0.58
1:A:993:LEU:HD22	1:A:1046:LEU:HG	1.85	0.58
1:A:562:THR:O	1:A:576:GLN:NE2	2.37	0.58
1:A:491:VAL:O	2:B:1150:ARG:NH2	2.36	0.58
1:A:666:ILE:HG23	2:B:1026:LEU:HB2	1.86	0.58
1:A:469:ARG:NH2	2:B:991:GLY:O	2.31	0.58
6:H:89:LEU:HD13	6:H:89:LEU:H	1.69	0.58
4:E:178:ILE:HB	4:E:212:ARG:HD3	1.86	0.57
1:A:344:ARG:HA	2:B:1129:ARG:HA	1.86	0.57
5:F:97:ARG:NH1	5:F:100:GLN:OE1	2.37	0.57
11:T:14:DG:H2''	11:T:15:DT:H5'	1.86	0.57
2:B:837:ASP:OD2	2:B:1020:ARG:NH2	2.37	0.57
1:A:34:LYS:H	1:A:34:LYS:HD3	1.70	0.57
1:A:40:THR:HB	1:A:41:MET:HA	1.86	0.57
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.84	0.57
2:B:487:THR:OG1	2:B:777:ALA:O	2.22	0.57
9:K:88:LYS:O	9:K:92:ASN:ND2	2.37	0.57
1:A:49:LYS:HB2	1:A:56:PRO:HD3	1.86	0.57
2:B:60:GLN:NE2	2:B:64:CYS:SG	2.77	0.57
2:B:63:ILE:O	2:B:67:SER:OG	2.19	0.56
6:H:129:TYR:O	6:H:132:LEU:N	2.37	0.56
1:A:72:GLU:OE2	2:B:1176:ASN:ND2	2.38	0.56
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.88	0.56
2:B:1187:ASN:ND2	2:B:1190:ASP:O	2.40	0.55
2:B:613:VAL:HG22	2:B:628:THR:HG23	1.88	0.55
6:H:91:ASP:OD1	6:H:92:ASP:N	2.40	0.55
6:H:14:GLU:HB3	6:H:27:GLU:HB3	1.86	0.55
2:B:165:VAL:HG21	2:B:448:ILE:HD12	1.89	0.55
2:B:205:ILE:HG13	2:B:461:LEU:HB3	1.89	0.54
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.71	0.54
2:B:680:THR:O	2:B:683:SER:OG	2.22	0.54
6:H:93:TYR:HD1	6:H:145:ARG:HB3	1.73	0.54
1:A:378:GLU:OE2	1:A:387:ARG:NH2	2.37	0.54
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.89	0.53
2:B:493:SER:OG	2:B:526:GLU:OE2	2.27	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:99:LEU:HD12	3:C:118:LEU:HB3	1.90	0.53
1:A:601:LYS:HB2	1:A:603:ASN:HD22	1.72	0.53
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.91	0.53
3:C:35:ARG:NH1	9:K:41:THR:OG1	2.42	0.53
1:A:946:VAL:HG22	4:E:201:LYS:HD3	1.91	0.52
5:F:82:THR:O	5:F:136:ARG:NH1	2.28	0.52
1:A:42:ASP:O	1:A:48:ALA:N	2.41	0.51
2:B:857:ARG:NH2	11:T:25:DC:OP1	2.43	0.51
2:B:899:ILE:HG21	2:B:949:VAL:HG21	1.92	0.51
1:A:350:ARG:HB2	2:B:1128:LEU:HD11	1.91	0.51
9:K:58:PHE:HB3	9:K:76:GLN:HB3	1.91	0.51
1:A:131:SER:HB3	1:A:223:GLY:HA2	1.93	0.51
12:N:3:DG:H2''	12:N:4:DC:H5''	1.91	0.51
2:B:357:GLN:NE2	2:B:371:GLU:OE1	2.43	0.51
1:A:1325:THR:OG1	4:E:146:HIS:O	2.24	0.51
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.92	0.51
8:J:9:SER:OG	8:J:48:ARG:NH2	2.43	0.51
1:A:475:THR:OG1	1:A:480:ALA:O	2.28	0.51
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.92	0.51
2:B:1077:THR:HG23	2:B:1079:LYS:H	1.76	0.51
13:R:4:G:H2'	13:R:5:A:H8	1.75	0.51
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.93	0.51
1:A:39:GLU:HB3	1:A:41:MET:HB2	1.93	0.51
11:T:26:DC:H42	13:R:3:G:H1	1.59	0.51
1:A:4:GLN:NE2	1:A:76:GLU:OE1	2.43	0.51
10:L:47:ARG:HG2	10:L:54:ARG:HG2	1.93	0.50
1:A:134:ARG:NH1	1:A:220:THR:O	2.44	0.50
2:B:806:THR:HG22	2:B:808:ALA:H	1.76	0.50
1:A:67:CYS:H	1:A:71:GLN:HA	1.77	0.50
2:B:118:ARG:HA	2:B:207:GLY:HA2	1.93	0.50
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.94	0.50
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.93	0.50
1:A:1116:LEU:HD23	1:A:1311:VAL:HA	1.94	0.50
1:A:528:LEU:HD23	1:A:751:SER:HA	1.94	0.50
1:A:760:GLN:HG2	1:A:765:VAL:HA	1.93	0.50
2:B:284:ILE:HG21	2:B:333:PHE:HD2	1.76	0.50
9:K:49:GLU:HG3	9:K:94:ILE:HG12	1.94	0.50
16:A:1805[A]:2KH:O4	11:T:19:6MA:N6	2.35	0.49
1:A:868:TYR:CE1	1:A:1064:VAL:HG21	2.48	0.49
1:A:70:CYS:HA	2:B:1174:LYS:HG2	1.94	0.49
2:B:839:MET:HG3	2:B:1010:LEU:HD11	1.94	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:6:PRO:HB3	3:C:25:VAL:HG13	1.94	0.49
2:B:400:HIS:NE2	2:B:699:GLU:OE1	2.38	0.49
2:B:198:ASP:OD1	2:B:485:ARG:NH2	2.43	0.49
8:J:14:VAL:HB	8:J:50:ILE:HD11	1.93	0.49
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.95	0.49
2:B:114:PRO:HG2	2:B:181:LEU:HD11	1.95	0.49
1:A:1410:PHE:HD2	2:B:1212:ILE:HD11	1.77	0.49
2:B:287:ARG:NH1	2:B:321:GLY:O	2.46	0.49
6:H:8:ASP:OD1	6:H:9:ILE:N	2.45	0.49
12:N:13:DA:H2''	12:N:14:DG:H5'	1.95	0.49
1:A:1194:ARG:HH21	1:A:1237:ILE:HD13	1.77	0.49
3:C:3:GLU:N	9:K:104:ASN:HD21	2.11	0.49
1:A:868:TYR:OH	1:A:1366:ARG:HD3	2.13	0.48
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.95	0.48
1:A:1011:GLN:O	1:A:1015:VAL:HG23	2.13	0.48
2:B:651:LEU:O	2:B:654:ARG:NE	2.44	0.48
1:A:419:LYS:HG3	1:A:420:ARG:HG3	1.95	0.48
7:I:14:LEU:HD13	7:I:27:PHE:HB3	1.95	0.48
1:A:1120:LEU:HD21	1:A:1131:ALA:HB2	1.95	0.48
1:A:173:THR:HB	1:A:184:SER:HB3	1.96	0.48
2:B:95:ILE:HD11	2:B:128:LEU:HB3	1.94	0.48
1:A:752:LYS:NZ	16:A:1805[B]:2KH:O2G	2.39	0.48
2:B:25:ILE:HG23	2:B:29:ASP:HB2	1.96	0.48
1:A:544:ASP:HB2	9:K:47:ARG:HH21	1.79	0.48
2:B:776:GLN:NE2	13:R:7:A:O3'	2.47	0.48
2:B:213:ILE:O	2:B:215:GLN:NE2	2.47	0.48
6:H:137:GLN:HG3	6:H:139:ASN:H	1.79	0.48
2:B:1074:ASN:HB2	2:B:1081:LEU:HD21	1.96	0.47
4:E:12:LEU:HD21	4:E:58:MET:HE1	1.96	0.47
1:A:265:LYS:NZ	1:A:302:THR:HG23	2.29	0.47
1:A:541:ILE:HD12	1:A:577:ILE:HG12	1.95	0.47
3:C:46:ILE:HD12	3:C:157:CYS:HB3	1.95	0.47
1:A:302:THR:OG1	1:A:306:ASN:OD1	2.32	0.47
2:B:892:LYS:NZ	2:B:909:ASP:OD2	2.39	0.47
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.50	0.47
2:B:394:ASP:H	7:I:91:ARG:HG3	1.80	0.47
1:A:1373:ASP:HA	1:A:1376:THR:HG22	1.95	0.47
2:B:1001:PHE:HE2	3:C:178:PHE:HB3	1.79	0.47
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.96	0.47
13:R:4:G:H2'	13:R:5:A:C8	2.50	0.47
1:A:854:ASN:HB2	1:A:1000:LEU:HD21	1.96	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:639:ILE:HD11	2:B:691:GLU:HG3	1.96	0.47
1:A:560:ILE:HB	6:H:79:TRP:H	1.80	0.47
10:L:31:CYS:SG	10:L:32:ALA:N	2.88	0.47
1:A:826:ASP:O	1:A:830:LYS:HB2	2.15	0.47
1:A:962:ARG:O	1:A:966:ASN:HB2	2.14	0.47
2:B:620:ARG:HH21	7:I:89:GLN:HE22	1.62	0.47
5:F:107:VAL:HG12	5:F:109:VAL:H	1.79	0.47
1:A:532:ARG:HE	1:A:536:LEU:HD21	1.79	0.47
1:A:780:VAL:HG23	1:A:789:LYS:HE2	1.97	0.47
2:B:1106:ARG:HH11	2:B:1126:GLY:HA2	1.80	0.47
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.96	0.47
1:A:1148:ILE:HD13	7:I:49:ILE:HD12	1.96	0.46
2:B:378:LEU:O	2:B:382:ILE:HG12	2.15	0.46
3:C:70:ILE:HD11	3:C:144:ILE:HD11	1.97	0.46
1:A:396:PRO:HG3	1:A:416:ARG:HB3	1.97	0.46
1:A:446:ARG:HB2	1:A:487:MET:HG2	1.98	0.46
1:A:523:ILE:HD13	1:A:622:VAL:HG22	1.97	0.46
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.97	0.46
2:B:916:THR:HG23	2:B:935:ARG:HB2	1.97	0.46
1:A:663:SER:OG	1:A:664:THR:N	2.47	0.46
2:B:170:LEU:HD12	2:B:171:PRO:HD2	1.97	0.46
2:B:788:ARG:NH1	2:B:790:ASP:OD2	2.48	0.46
2:B:806:THR:HB	2:B:809:MET:HG3	1.97	0.46
1:A:279:LEU:HB3	1:A:289:ILE:HG22	1.98	0.46
1:A:51:GLY:HA2	1:A:52:GLY:HA2	1.51	0.46
2:B:28:GLU:OE1	2:B:807:ARG:NH1	2.48	0.46
2:B:900:ALA:O	2:B:902:GLY:N	2.48	0.46
5:F:130:ILE:HA	5:F:131:PRO:HD3	1.79	0.46
1:A:1064:VAL:HA	1:A:1067:LEU:HB3	1.98	0.46
1:A:208:LEU:HD23	1:A:235:ILE:HD13	1.97	0.46
1:A:1279:ILE:HA	1:A:1310:GLY:HA3	1.98	0.46
2:B:40:GLU:OE2	2:B:682:SER:OG	2.33	0.46
3:C:84:ARG:HD2	9:K:11:LEU:HD21	1.98	0.46
9:K:47:ARG:HD2	9:K:60:ALA:HA	1.98	0.46
1:A:798:GLY:HA2	1:A:815:PHE:CD2	2.51	0.45
9:K:21:ILE:HD13	9:K:84:LYS:HE2	1.98	0.45
1:A:346:ASP:O	2:B:1150:ARG:NH1	2.44	0.45
6:H:44:VAL:HG13	6:H:48:PRO:HA	1.98	0.45
1:A:821:ARG:O	1:A:825:ILE:HG12	2.16	0.45
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.48	0.45
2:B:428:ILE:HD11	2:B:448:ILE:HG23	1.97	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:46:ILE:HD13	3:C:159:ALA:HB2	1.97	0.45
6:H:93:TYR:CD1	6:H:145:ARG:HB3	2.51	0.45
1:A:545:GLN:HG2	1:A:549:MET:HE3	1.99	0.45
2:B:792:MET:HA	2:B:856:PHE:O	2.17	0.45
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.99	0.45
1:A:1261:LYS:O	1:A:1264:GLU:HG3	2.17	0.45
16:A:1805[A]:2KH:PG	2:B:766:ARG:HH12	2.40	0.45
1:A:231:PRO:HA	1:A:234:MET:HG3	1.99	0.45
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.97	0.45
1:A:783:THR:HG21	1:A:796:SER:O	2.16	0.45
2:B:892:LYS:HZ3	2:B:905:VAL:HA	1.81	0.45
2:B:301:ILE:HD13	2:B:382:ILE:HG21	1.99	0.45
2:B:798:TYR:HE2	3:C:66:ARG:HH21	1.64	0.45
4:E:24:LYS:HB3	4:E:30:ILE:HB	1.99	0.45
1:A:107:CYS:SG	1:A:108:MET:N	2.90	0.45
1:A:17:VAL:HB	1:A:1419:ASP:HB3	1.99	0.45
1:A:58:LEU:HA	1:A:80:HIS:HB2	1.98	0.45
1:A:1410:PHE:CD2	2:B:1212:ILE:HD11	2.52	0.44
2:B:610:ASN:HB3	2:B:613:VAL:HG23	1.99	0.44
2:B:855:PHE:HZ	2:B:857:ARG:HH11	1.65	0.44
2:B:1067:ARG:NE	3:C:194:GLU:OE1	2.46	0.44
1:A:346:ASP:HB3	2:B:1107:ALA:O	2.16	0.44
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.98	0.44
1:A:977:LYS:HG3	1:A:978:PRO:HD2	1.99	0.44
2:B:757:PRO:HG2	2:B:984:HIS:NE2	2.32	0.44
1:A:1281:ARG:NE	1:A:1309:ASP:OD2	2.51	0.44
1:A:1386:ARG:HB3	1:A:1403:GLU:HG3	1.98	0.44
3:C:56:THR:HG21	3:C:63:ILE:HD11	2.00	0.44
6:H:6:PHE:HB3	6:H:59:ILE:HB	2.00	0.44
8:J:10:CYS:SG	8:J:11:GLY:N	2.90	0.44
9:K:45:LEU:HG	9:K:94:ILE:HD13	2.00	0.44
1:A:707:GLY:O	1:A:1281:ARG:NH1	2.45	0.44
2:B:459:TYR:HE1	2:B:468:GLU:HB3	1.82	0.44
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.99	0.44
1:A:483:ASP:HB2	2:B:987:LYS:HG2	2.00	0.44
2:B:987:LYS:NZ	13:R:9:G:OP1	2.51	0.44
1:A:402:ALA:HA	1:A:434:ARG:HA	1.99	0.44
2:B:326:ASP:OD1	2:B:329:THR:OG1	2.21	0.44
2:B:902:GLY:HA3	10:L:61:THR:HG22	1.99	0.44
2:B:558:LEU:HB3	2:B:563:MET:SD	2.58	0.43
2:B:916:THR:HA	2:B:917:PRO:HD3	1.88	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:64:ASN:N	8:J:65:PRO:HD2	2.33	0.43
1:A:464:PRO:HB2	9:K:4:PRO:HD3	2.00	0.43
1:A:316:GLN:NE2	1:A:320:ARG:HH12	2.16	0.43
7:I:85:PHE:HB3	7:I:101:PHE:CD2	2.52	0.43
1:A:306:ASN:HB2	1:A:324:SER:HB3	1.99	0.43
1:A:30:ILE:HG23	2:B:1170:THR:HG23	2.00	0.43
6:H:83:GLN:HB3	6:H:86:ASP:HB3	2.01	0.43
1:A:206:GLU:O	1:A:210:ILE:HG12	2.18	0.43
1:A:423:ASP:N	1:A:423:ASP:OD1	2.50	0.43
1:A:679:ILE:HG23	1:A:729:ALA:HB1	2.00	0.43
1:A:881:GLN:NE2	1:A:958:VAL:O	2.46	0.43
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.99	0.43
3:C:22:LEU:HD21	9:K:101:LEU:HD21	2.00	0.43
1:A:42:ASP:N	1:A:43:GLU:HA	2.29	0.43
7:I:24:ARG:NH1	7:I:26:LEU:HD21	2.32	0.43
11:T:19:6MA:H2"	11:T:20:DC:C6	2.53	0.43
1:A:1224:LEU:HD11	1:A:1240:CYS:HB3	2.01	0.43
2:B:1188:LYS:HB2	2:B:1188:LYS:HE3	1.92	0.43
1:A:1132:LYS:HG3	1:A:1135:ARG:HH12	1.83	0.43
1:A:860:LEU:HD21	1:A:1394:THR:HA	2.00	0.43
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.99	0.43
4:E:83:CYS:HB2	4:E:110:PHE:HE1	1.83	0.43
1:A:868:TYR:CZ	1:A:1064:VAL:HG21	2.54	0.43
1:A:1198:ASP:O	1:A:1202:MET:HG2	2.19	0.43
1:A:1323:ASP:OD1	1:A:1325:THR:HG22	2.19	0.43
1:A:68:GLN:HA	1:A:69:THR:HA	1.46	0.43
2:B:702:LEU:HD21	2:B:735:ALA:HB1	2.00	0.43
1:A:526:ASP:HB2	2:B:835:GLN:NE2	2.34	0.43
2:B:861:ASP:OD1	2:B:862:GLN:N	2.50	0.43
5:F:76:LYS:O	5:F:79:ARG:NH1	2.43	0.43
9:K:56:VAL:HG22	9:K:77:THR:HG22	1.99	0.43
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.54	0.42
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.53	0.42
2:B:904:ARG:HG2	2:B:948:ILE:HG12	2.00	0.42
3:C:211:ASP:HA	3:C:212:PRO:HD3	1.91	0.42
1:A:614:PHE:HB3	6:H:122:LEU:HD21	2.01	0.42
8:J:23:ASN:O	8:J:27:GLU:HB3	2.19	0.42
1:A:38:PRO:HA	1:A:270:LEU:HD13	2.00	0.42
3:C:40:GLU:O	3:C:250:THR:HG21	2.19	0.42
1:A:838:GLN:HG2	1:A:1073:GLY:HA3	2.01	0.42
2:B:955:THR:HG23	10:L:55:ILE:HA	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:45:CYS:HB2	8:J:48:ARG:HH21	1.84	0.42
9:K:47:ARG:HD3	9:K:61:TYR:HD1	1.84	0.42
1:A:1395:GLY:HA3	1:A:1426:GLU:OE2	2.19	0.42
1:A:531:ILE:HG21	1:A:622:VAL:HG11	2.01	0.42
2:B:681:TRP:CH2	2:B:690:VAL:HG11	2.55	0.42
1:A:774:ARG:H	1:A:774:ARG:HG2	1.63	0.42
4:E:17:ARG:HH12	4:E:36:GLU:HA	1.85	0.42
5:F:93:ILE:HD11	5:F:134:ILE:HD11	2.01	0.42
1:A:1276:VAL:HG11	1:A:1316:VAL:HG22	2.01	0.42
1:A:4:GLN:NE2	2:B:1159:ARG:HB3	2.35	0.42
2:B:766:ARG:HA	2:B:766:ARG:HD3	1.87	0.42
2:B:468:GLU:CG	2:B:469:GLN:HA	2.47	0.42
2:B:620:ARG:HD2	7:I:68:LEU:HD11	2.02	0.42
2:B:939:THR:HA	2:B:940:PRO:HD3	1.87	0.42
3:C:37:MET:SD	3:C:244:VAL:HG12	2.59	0.42
6:H:89:LEU:HD22	6:H:90:ALA:N	2.34	0.42
2:B:1017:ILE:H	2:B:1018:PRO:HD2	1.84	0.42
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	2.02	0.42
2:B:31:TRP:CE3	2:B:34:ILE:HD12	2.55	0.42
1:A:795:GLU:HG3	2:B:731:VAL:HG21	2.02	0.42
1:A:12:ARG:HH11	2:B:1192:TYR:HE1	1.68	0.41
3:C:249:ASP:O	3:C:253:LYS:HB2	2.20	0.41
4:E:3:GLN:HB2	4:E:4:GLU:H	1.59	0.41
1:A:1187:GLN:HG3	1:A:1188:GLN:HG3	2.03	0.41
1:A:527:THR:O	1:A:653:VAL:HG11	2.20	0.41
2:B:281:PRO:HB2	2:B:284:ILE:HG12	2.02	0.41
1:A:1207:LEU:HB3	1:A:1274:ARG:HH11	1.85	0.41
2:B:816:GLU:OE1	2:B:816:GLU:N	2.54	0.41
1:A:634:THR:HG1	1:A:642:CYS:HG	1.60	0.41
1:A:642:CYS:O	1:A:645:LEU:HB3	2.20	0.41
2:B:58:THR:O	2:B:62:ILE:HG12	2.20	0.41
2:B:942:ARG:HB2	2:B:945:GLU:HB2	2.03	0.41
1:A:1155:ASP:OD2	1:A:1241:ARG:NH2	2.53	0.41
1:A:453:MET:HB3	1:A:477:PRO:HB2	2.02	0.41
1:A:941:LYS:HB3	1:A:941:LYS:HE3	1.91	0.41
1:A:87:ALA:HB3	1:A:276:LEU:HD23	2.02	0.41
2:B:600:LEU:HB3	2:B:615:MET:SD	2.60	0.41
11:T:7:6MA:H2'	11:T:8:DT:H5'	2.02	0.41
1:A:1371:LEU:O	1:A:1374:VAL:HG12	2.21	0.41
1:A:1438:THR:HA	5:F:88:TYR:HB3	2.02	0.41
1:A:781:ASP:O	1:A:790:ASP:N	2.45	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:889:SER:HA	1:A:1296:GLY:HA3	2.02	0.41
2:B:1175:LEU:C	2:B:1177:HIS:H	2.23	0.41
2:B:205:ILE:HG21	2:B:462:ALA:HB2	2.02	0.41
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.86	0.41
1:A:1227:ILE:HD12	1:A:1239:ARG:HH11	1.86	0.41
1:A:1260:LEU:HD12	1:A:1263:ILE:HD12	2.03	0.41
1:A:962:ARG:HA	1:A:965:GLN:HG2	2.02	0.41
2:B:830:TYR:CZ	2:B:1000:PRO:HD3	2.55	0.41
2:B:1002:THR:HG23	2:B:1004:GLU:H	1.86	0.41
10:L:28:LYS:HA	10:L:39:SER:HA	2.03	0.41
1:A:1140:HIS:HB2	1:A:1276:VAL:O	2.21	0.41
1:A:549:MET:HE2	1:A:656:TRP:HD1	1.85	0.41
1:A:733:ALA:HB2	1:A:763:ALA:HB2	2.03	0.41
2:B:93:GLY:N	2:B:131:ASP:O	2.53	0.41
1:A:9:ALA:HA	1:A:10:PRO:HD3	1.89	0.40
2:B:44:VAL:HG11	2:B:495:LEU:HD13	2.02	0.40
7:I:98:VAL:HG11	7:I:113:ASP:HB2	2.03	0.40
11:T:6:DG:H2"	11:T:7:6MA:H8	2.02	0.40
2:B:408:LEU:HB3	2:B:409:ALA:H	1.75	0.40
2:B:843:GLN:HB2	2:B:993:THR:HB	2.04	0.40
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	2.03	0.40
1:A:52:GLY:HA3	1:A:53:LEU:HA	1.89	0.40
2:B:1155:SER:OG	2:B:1156:ASP:N	2.54	0.40
2:B:582:VAL:HB	2:B:587:HIS:CE1	2.56	0.40
5:F:109:VAL:HG11	5:F:124:GLU:HA	2.02	0.40
1:A:1128:GLN:HB3	1:A:1304:TRP:NE1	2.36	0.40
1:A:226:GLU:HG3	1:A:227:VAL:HG13	2.02	0.40
1:A:35:ILE:HG23	1:A:52:GLY:HA3	2.04	0.40
1:A:678:GLU:HA	1:A:681:GLU:HG2	2.03	0.40
2:B:307:ASP:OD1	2:B:392:ARG:NH1	2.46	0.40
2:B:847:ASP:OD2	9:K:6:ARG:NH2	2.52	0.40
3:C:11:ARG:NH2	3:C:19:ASP:OD1	2.55	0.40
1:A:1445:ILE:HG22	5:F:132:LEU:HD23	2.04	0.40
1:A:1286:LYS:HE2	1:A:1302:PRO:HB2	2.03	0.40
2:B:483:LEU:HD21	2:B:491:THR:HG23	2.03	0.40
2:B:890:TYR:CZ	2:B:910:VAL:HG21	2.57	0.40
3:C:212:PRO:HA	3:C:213:PRO:HD3	1.81	0.40
10:L:46:VAL:HA	10:L:47:ARG:HA	1.90	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	1357/1733 (78%)	1258 (93%)	95 (7%)	4 (0%)	41	72
2	B	1067/1224 (87%)	987 (92%)	71 (7%)	9 (1%)	19	51
3	C	264/318 (83%)	245 (93%)	18 (7%)	1 (0%)	34	67
4	E	211/215 (98%)	201 (95%)	9 (4%)	1 (0%)	29	61
5	F	82/155 (53%)	77 (94%)	5 (6%)	0	100	100
6	H	124/146 (85%)	113 (91%)	9 (7%)	2 (2%)	9	34
7	I	113/122 (93%)	101 (89%)	11 (10%)	1 (1%)	17	49
8	J	63/70 (90%)	58 (92%)	5 (8%)	0	100	100
9	K	112/120 (93%)	107 (96%)	4 (4%)	1 (1%)	17	49
10	L	42/70 (60%)	34 (81%)	7 (17%)	1 (2%)	6	28
All	All	3435/4173 (82%)	3181 (93%)	234 (7%)	20 (1%)	25	57

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	PRO
2	B	902	GLY
2	B	277	LYS
2	B	883	LEU
2	B	1046	PRO
6	H	82	PRO
9	K	26	LYS
1	A	1156	PRO
2	B	1017	ILE
3	C	148	ARG
4	E	86	PRO
1	A	957	PRO
1	A	1221	LYS
2	B	367	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	824	ILE
7	I	33	SER
10	L	41	SER
2	B	901	PRO
6	H	18	GLY
2	B	974	PRO

### 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	1198/1520 (79%)	1150 (96%)	48 (4%)	31	60
2	B	944/1061 (89%)	908 (96%)	36 (4%)	33	61
3	C	234/274 (85%)	227 (97%)	7 (3%)	41	68
4	E	195/197 (99%)	189 (97%)	6 (3%)	40	68
5	F	74/137 (54%)	72 (97%)	2 (3%)	44	70
6	H	114/128 (89%)	112 (98%)	2 (2%)	59	79
7	I	109/116 (94%)	107 (98%)	2 (2%)	59	79
8	J	60/65 (92%)	58 (97%)	2 (3%)	38	66
9	K	99/102 (97%)	97 (98%)	2 (2%)	55	77
10	L	39/57 (68%)	39 (100%)	0	100	100
All	All	3066/3657 (84%)	2959 (96%)	107 (4%)	36	65

All (107) 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	46	THR
1	A	69	THR
1	A	126	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	132	LYS
1	A	179	LEU
1	A	222	LEU
1	A	235	ILE
1	A	308	ILE
1	A	326	ARG
1	A	335	ARG
1	A	351	THR
1	A	434	ARG
1	A	443	LEU
1	A	444	PHE
1	A	451	HIS
1	A	481	ASP
1	A	532	ARG
1	A	612	ILE
1	A	618	GLU
1	A	626	ASN
1	A	666	ILE
1	A	702	LEU
1	A	774	ARG
1	A	783	THR
1	A	821	ARG
1	A	826	ASP
1	A	830	LYS
1	A	885	THR
1	A	896	ARG
1	A	1017	LEU
1	A	1025	ARG
1	A	1034	GLU
1	A	1035	TYR
1	A	1116	LEU
1	A	1172	LEU
1	A	1231	ASP
1	A	1262	LYS
1	A	1297	GLU
1	A	1300	LYS
1	A	1322	ILE
1	A	1333	ILE
1	A	1374	VAL
1	A	1400	CYS
1	A	1407	GLU
2	B	46	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	134	LYS
2	B	217	ARG
2	B	319	GLU
2	B	365	THR
2	B	393	LYS
2	B	466	TRP
2	B	468	GLU
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	885	MET
2	B	916	THR
2	B	955	THR
2	B	983	ARG
2	B	987	LYS
2	B	997	GLU
2	B	999	MET
2	B	1007	VAL
2	B	1028	GLU
2	B	1051	THR
2	B	1099	VAL
2	B	1147	LEU
2	B	1158	PHE
2	B	1159	ARG
2	B	1176	ASN
2	B	1188	LYS
2	B	1194	ILE
2	B	1202	LEU
3	C	22	LEU
3	C	25	VAL
3	C	77	ILE
3	C	99	LEU
3	C	137	LYS
3	C	222	LYS
3	C	240	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	E	3	GLN
4	E	98	ILE
4	E	110	PHE
4	E	127	ILE
4	E	146	HIS
4	E	169	ARG
5	F	72	LYS
5	F	97	ARG
6	H	89	LEU
6	H	124	ARG
7	I	14	LEU
7	I	111	THR
8	J	5	VAL
8	J	52	THR
9	K	1	MET
9	K	47	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	742	ASN
2	B	762	ASN
2	B	984	HIS

### 5.3.3 RNA ⓘ

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

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	R	9	G

There are no RNA pucker outliers to report.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
11	6MA	T	16	11	18,24,25	1.77	4 (22%)	15,34,37	1.42	2 (13%)
11	6MA	T	7	11,12	18,24,25	1.85	4 (22%)	15,34,37	1.30	2 (13%)
11	6MA	T	19	11	18,24,25	1.85	4 (22%)	15,34,37	1.19	1 (6%)

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	6MA	T	16	11	-	1/5/23/24	0/3/3/3
11	6MA	T	7	11,12	-	3/5/23/24	0/3/3/3
11	6MA	T	19	11	-	0/5/23/24	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	T	19	6MA	C6-N6	4.87	1.43	1.35
11	T	7	6MA	C6-N6	4.85	1.43	1.35
11	T	16	6MA	C6-N6	4.38	1.42	1.35
11	T	7	6MA	C1'-N9	-3.44	1.39	1.49
11	T	19	6MA	C1'-N9	-3.39	1.39	1.49
11	T	16	6MA	C1'-N9	-3.36	1.39	1.49
11	T	16	6MA	C2-N3	2.55	1.36	1.32
11	T	7	6MA	C2-N3	2.45	1.36	1.32
11	T	19	6MA	C2-N3	2.43	1.36	1.32
11	T	7	6MA	C5-N7	2.22	1.47	1.39
11	T	19	6MA	C5-N7	2.18	1.47	1.39
11	T	16	6MA	C5-N7	2.09	1.47	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	T	16	6MA	C1-N6-C6	-3.52	119.84	122.87
11	T	7	6MA	C2-N1-C6	3.22	119.35	116.59
11	T	19	6MA	C2-N1-C6	2.99	119.15	116.59
11	T	16	6MA	C2'-C3'-C4'	2.53	108.04	102.76
11	T	7	6MA	C1-N6-C6	2.09	124.67	122.87

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	T	7	6MA	C3'-C4'-C5'-O5'
11	T	7	6MA	O4'-C4'-C5'-O5'
11	T	16	6MA	C4'-C5'-O5'-P
11	T	7	6MA	C4'-C5'-O5'-P

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	T	7	6MA	2	0
11	T	19	6MA	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 10 are monoatomic - leaving 2 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
16	2KH	A	1805[B]	15	25,30,30	2.50	9 (36%)	30,47,47	1.93	8 (26%)
16	2KH	A	1805[A]	15	25,30,30	2.45	10 (40%)	30,47,47	1.96	7 (23%)

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
16	2KH	A	1805[B]	15	-	5/17/38/38	0/2/2/2
16	2KH	A	1805[A]	15	-	6/17/38/38	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	1805[A]	2KH	C4-N3	5.19	1.42	1.33
16	A	1805[B]	2KH	C4-N3	5.17	1.42	1.33
16	A	1805[A]	2KH	C6-N1	4.54	1.41	1.35
16	A	1805[B]	2KH	PB-O2B	4.48	1.53	1.46
16	A	1805[B]	2KH	C6-N1	4.48	1.41	1.35
16	A	1805[A]	2KH	PB-O2B	4.42	1.53	1.46
16	A	1805[B]	2KH	PB-N3A	4.16	1.74	1.63
16	A	1805[B]	2KH	PB-O3B	4.03	1.64	1.59
16	A	1805[A]	2KH	PB-O3B	3.91	1.64	1.59
16	A	1805[A]	2KH	PB-N3A	3.91	1.73	1.63
16	A	1805[B]	2KH	PA-N3A	3.78	1.73	1.63
16	A	1805[A]	2KH	PA-N3A	3.53	1.72	1.63
16	A	1805[B]	2KH	PA-O1A	3.11	1.51	1.46
16	A	1805[A]	2KH	PA-O1A	2.98	1.50	1.46
16	A	1805[B]	2KH	PB-O1B	-2.55	1.49	1.56
16	A	1805[A]	2KH	PB-O1B	-2.43	1.50	1.56
16	A	1805[B]	2KH	PA-O5'	2.33	1.66	1.57
16	A	1805[A]	2KH	PA-O5'	2.27	1.66	1.57
16	A	1805[A]	2KH	C5'-C4'	2.02	1.57	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	1805[A]	2KH	O1G-PG-O3B	5.55	123.24	104.64
16	A	1805[B]	2KH	O1G-PG-O3B	5.51	123.10	104.64
16	A	1805[B]	2KH	O3B-PB-N3A	3.82	117.20	106.59
16	A	1805[B]	2KH	O3G-PG-O2G	-3.71	96.14	110.68
16	A	1805[A]	2KH	O3B-PB-N3A	3.65	116.72	106.59
16	A	1805[A]	2KH	O3G-PG-O2G	-3.62	96.49	110.68
16	A	1805[B]	2KH	C5-C4-N3	-3.50	115.60	123.31
16	A	1805[A]	2KH	C5-C4-N3	-3.49	115.63	123.31
16	A	1805[A]	2KH	O2B-PB-N3A	-3.44	106.70	111.77

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	1805[B]	2KH	O2B-PB-N3A	-3.25	106.98	111.77
16	A	1805[A]	2KH	C3'-C2'-C1'	2.84	105.26	100.98
16	A	1805[B]	2KH	C3'-C2'-C1'	2.57	104.85	100.98
16	A	1805[A]	2KH	O2A-PA-O1A	-2.19	105.33	109.92
16	A	1805[B]	2KH	O2A-PA-O1A	-2.17	105.38	109.92
16	A	1805[B]	2KH	O3G-PG-O3B	2.01	111.39	104.64

There are no chirality outliers.

All (11) torsion outliers are listed below:

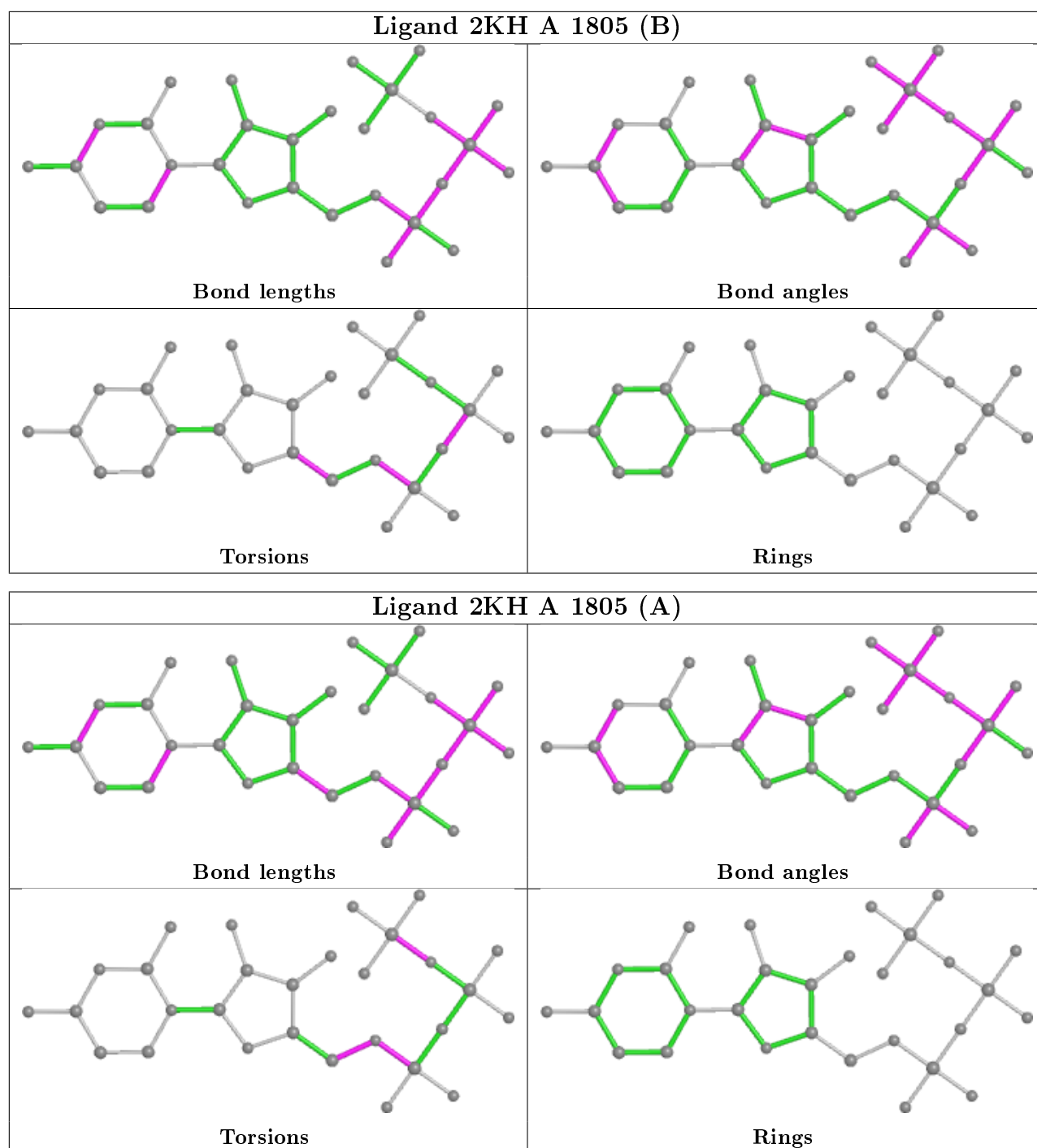
Mol	Chain	Res	Type	Atoms
16	A	1805[A]	2KH	C5'-O5'-PA-O1A
16	A	1805[A]	2KH	C5'-O5'-PA-O2A
16	A	1805[A]	2KH	C4'-C5'-O5'-PA
16	A	1805[A]	2KH	PB-O3B-PG-O1G
16	A	1805[B]	2KH	C5'-O5'-PA-O2A
16	A	1805[B]	2KH	PA-N3A-PB-O2B
16	A	1805[B]	2KH	C3'-C4'-C5'-O5'
16	A	1805[B]	2KH	O4'-C4'-C5'-O5'
16	A	1805[B]	2KH	C5'-O5'-PA-O1A
16	A	1805[A]	2KH	C5'-O5'-PA-N3A
16	A	1805[A]	2KH	PB-O3B-PG-O2G

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	1805[B]	2KH	1	0
16	A	1805[A]	2KH	2	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 ⓘ

### 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<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	1371/1733 (79%)	0.23	54 (3%) 39 38	13, 68, 150, 221	0
2	B	1089/1224 (88%)	0.06	13 (1%) 79 77	13, 48, 115, 201	0
3	C	266/318 (83%)	0.04	1 (0%) 92 92	21, 50, 93, 148	0
4	E	213/215 (99%)	0.66	23 (10%) 5 7	44, 95, 174, 201	0
5	F	84/155 (54%)	0.06	1 (1%) 79 77	38, 66, 115, 154	0
6	H	130/146 (89%)	1.03	17 (13%) 3 4	41, 88, 155, 215	0
7	I	115/122 (94%)	0.24	1 (0%) 84 83	35, 70, 119, 149	0
8	J	65/70 (92%)	-0.17	0 100 100	17, 40, 78, 138	0
9	K	114/120 (95%)	0.01	1 (0%) 84 83	16, 50, 91, 105	0
10	L	44/70 (62%)	0.94	3 (6%) 17 19	37, 119, 176, 195	0
11	T	26/29 (89%)	0.85	2 (7%) 13 15	45, 185, 246, 273	0
12	N	14/14 (100%)	1.19	2 (14%) 2 3	157, 216, 265, 267	0
13	R	9/9 (100%)	0.13	0 100 100	30, 43, 91, 92	0
All	All	3540/4225 (83%)	0.22	118 (3%) 46 45	13, 62, 145, 273	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	H	84	ALA	7.7
1	A	105	CYS	6.2
2	B	643	ASP	5.1
10	L	50	ASP	5.1
6	H	83	GLN	5.0
4	E	126	SER	4.7
6	H	139	ASN	4.6
6	H	85	GLY	4.5
1	A	49	LYS	4.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	1173	HIS	4.5
1	A	183	GLY	4.4
4	E	93	MET	4.4
1	A	141	LEU	4.3
1	A	147	VAL	4.3
6	H	82	PRO	4.1
1	A	3	GLY	3.8
4	E	100	ILE	3.7
4	E	49	SER	3.7
1	A	1261	LYS	3.6
1	A	59	GLY	3.6
4	E	95	THR	3.5
4	E	39	LEU	3.5
1	A	91	PHE	3.5
11	T	1	DC	3.4
1	A	1449	SER	3.3
11	T	4	DC	3.3
6	H	134	ASN	3.3
1	A	65	LEU	3.3
1	A	175	ARG	3.3
1	A	171	GLN	3.3
4	E	123	LEU	3.2
12	N	8	DT	3.2
1	A	176	LYS	3.2
1	A	145	LYS	3.2
6	H	133	ASN	3.2
1	A	251	SER	3.2
1	A	108	MET	3.1
4	E	110	PHE	3.1
2	B	468	GLU	3.1
1	A	66	LYS	3.1
2	B	1211	ASN	3.0
10	L	35	SER	3.0
4	E	50	MET	3.0
5	F	155	LEU	3.0
1	A	182	VAL	2.9
1	A	1172	LEU	2.9
4	E	102	GLU	2.9
1	A	210	ILE	2.8
2	B	881	ASN	2.8
1	A	174	ILE	2.7
1	A	919	ILE	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	140	THR	2.7
1	A	148	CYS	2.7
1	A	1258	HIS	2.7
4	E	83	CYS	2.7
1	A	173	THR	2.7
4	E	16	PHE	2.6
6	H	86	ASP	2.6
1	A	87	ALA	2.6
6	H	55	LEU	2.6
1	A	286	HIS	2.6
3	C	16	ASP	2.6
4	E	98	ILE	2.6
12	N	7	DA	2.5
1	A	106	VAL	2.5
9	K	57	LEU	2.5
6	H	88	SER	2.5
4	E	109	ILE	2.5
6	H	81	PRO	2.4
6	H	140	ALA	2.4
1	A	181	LEU	2.4
6	H	143	LEU	2.4
2	B	372	SER	2.4
7	I	25	LEU	2.3
4	E	96	PHE	2.3
2	B	1220	ARG	2.3
1	A	1240	CYS	2.3
1	A	170	THR	2.3
1	A	908	LEU	2.3
1	A	1156	PRO	2.3
1	A	69	THR	2.3
2	B	879	ARG	2.3
6	H	112	ILE	2.3
4	E	80	VAL	2.3
1	A	143	LYS	2.3
1	A	142	CYS	2.3
2	B	887	HIS	2.3
4	E	47	CYS	2.2
1	A	323	LYS	2.2
1	A	397	ASN	2.2
4	E	127	ILE	2.2
2	B	620	ARG	2.2
1	A	45	GLN	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
10	L	53	HIS	2.2
4	E	89	GLY	2.2
4	E	129	PRO	2.2
4	E	132	ILE	2.2
6	H	57	VAL	2.2
6	H	146	ARG	2.2
4	E	91	LYS	2.2
6	H	104	PHE	2.1
1	A	72	GLU	2.1
1	A	1262	LYS	2.1
2	B	883	LEU	2.1
1	A	1154	TYR	2.1
1	A	102	VAL	2.1
1	A	103	CYS	2.1
1	A	120	GLU	2.1
1	A	596	THR	2.1
1	A	1236	LEU	2.1
1	A	1220	PHE	2.1
2	B	865	LYS	2.0
4	E	7	ARG	2.0
2	B	869	SER	2.0
1	A	1169	ILE	2.0
2	B	92	PHE	2.0
1	A	144	THR	2.0
1	A	1232	ASN	2.0

## 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<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	6MA	T	7	22/23	0.76	0.24	227,229,235,237	0
11	6MA	T	16	22/23	0.79	0.24	138,145,158,168	0
11	6MA	T	19	22/23	0.93	0.23	63,79,96,101	0

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands

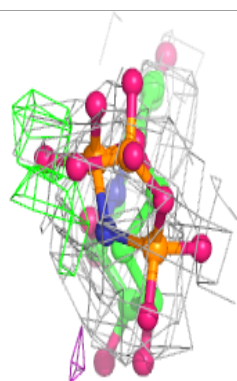
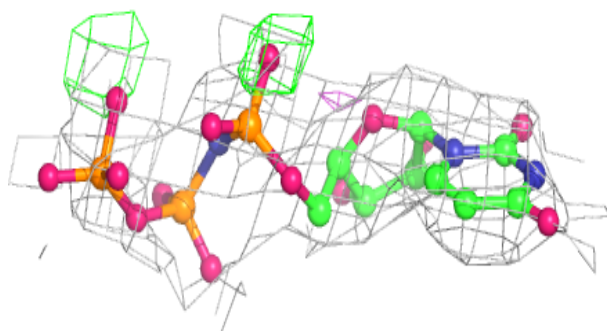
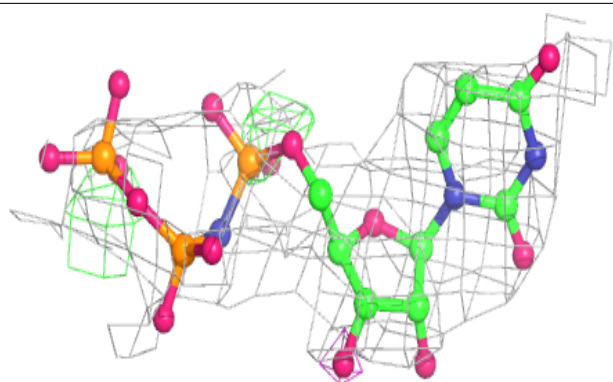
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
16	2KH	A	1805[A]	29/29	0.84	0.32	79,110,128,143	29
16	2KH	A	1805[B]	29/29	0.84	0.32	113,115,127,136	29
14	ZN	L	101	1/1	0.91	0.07	120,120,120,120	0
14	ZN	A	1801	1/1	0.92	0.08	150,150,150,150	0
15	MG	A	1804	1/1	0.93	0.15	31,31,31,31	0
14	ZN	B	1301	1/1	0.94	0.10	83,83,83,83	0
14	ZN	A	1802	1/1	0.96	0.15	77,77,77,77	0
15	MG	A	1803	1/1	0.97	0.19	11,11,11,11	0
14	ZN	I	202	1/1	0.97	0.13	53,53,53,53	0
14	ZN	J	101	1/1	0.97	0.13	33,33,33,33	0
14	ZN	I	201	1/1	0.98	0.12	71,71,71,71	0
14	ZN	C	401	1/1	0.99	0.18	51,51,51,51	0

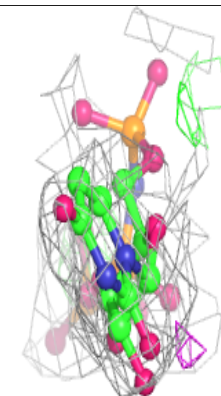
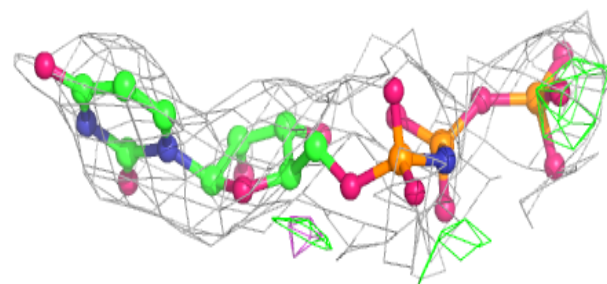
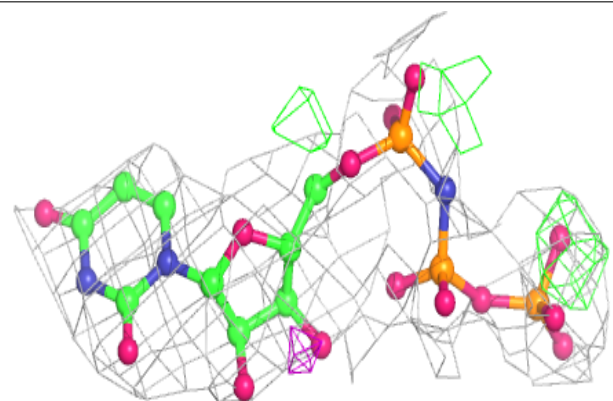
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 2KH A 1805 (A):**

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

**Electron density around 2KH A 1805 (B):**

$2mF_o-DF_c$  (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.