



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:02 AM GMT

PDB ID : 4A3L  
Title : RNA POLYMERASE II INITIAL TRANSCRIBING COMPLEX WITH A  
7NT DNA-RNA HYBRID AND SOAKED WITH AMPCPP  
Authors : Cheung, A.C.M.; Sainsbury, S.; Cramer, P.  
Deposited on : 2011-09-30  
Resolution : 3.50 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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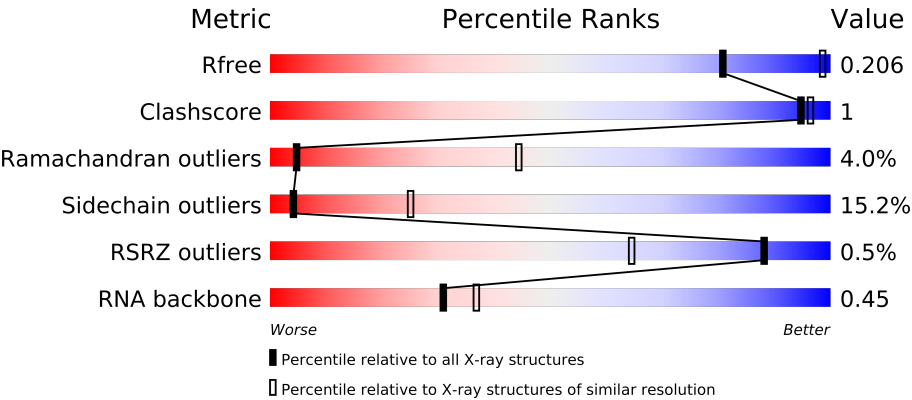
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.50 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))
$R_{free}$	66092	1243 (3.70-3.30)
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)
RNA backbone	1838	1007 (4.22-2.76)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1732	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
2	B	1224	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
3	C	318	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
4	D	221	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
5	E	215	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
6	F	155	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
7	G	171	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
8	H	146	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
9	I	122	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
10	J	70	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
11	K	120	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
12	L	70	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>

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Mol	Chain	Length	Quality of chain
13	N	14	
14	P	7	
15	T	26	

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 31950 atoms, of which 0 are hydrogen and 0 are deuterium.

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	1425	Total	C	N	O	S	0	0	0
			11197	7051	1958	2126	62			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1115	Total	C	N	O	S	0	0	0
			8859	5609	1554	1641	55			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	178	Total	C	N	O	S	0	0	0
			1434	887	257	288	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 13 is a DNA chain called 5'-D(\*AP\*AP\*GP\*TP\*AP\*CP\*TP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	9	Total	C	N	O	P	0	0	0
			183	89	34	52	8			

- Molecule 14 is a RNA chain called 5'-R(\*AP\*CP\*CP\*AP\*GP\*GP\*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	7	Total	C	N	O	P	0	0	0
			152	68	31	46	7			

- Molecule 15 is a DNA chain called 5'-D(\*AP\*GP\*CP\*TP\*CP\*AP\*AP\*GP\*TP\*AP\*CP\*TP\*TP\*TP\*TP\*CP\*CP\*BRU\*GP\*GP\*TP\*CP\*AP\*TP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	18	Total	Br	C	N	O	P	0	0
			365	1	175	58	113	18		

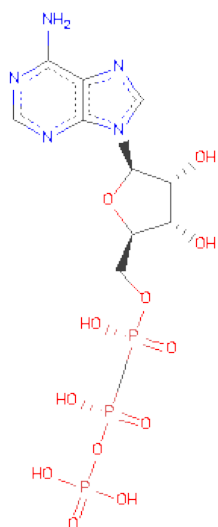
- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 18 is DIPHOSPHOMETHYLPHOSPHONICACID ADENOSYL ESTER (three-letter code: APC) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).

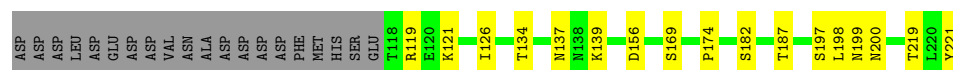


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
18	P	1	31	11	5	12	3	0	0



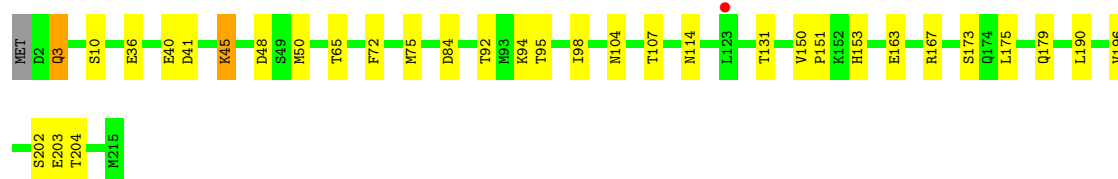






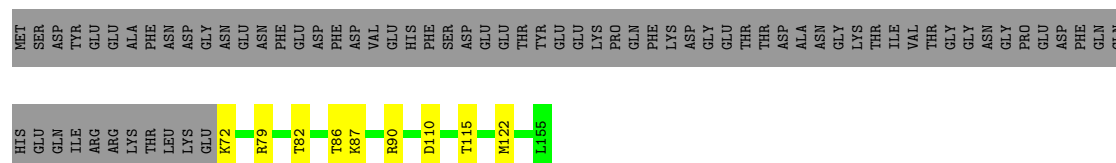
- Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC1

Chain E:



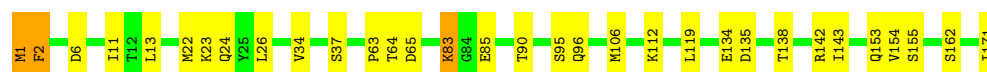
- Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC2

Chain F:



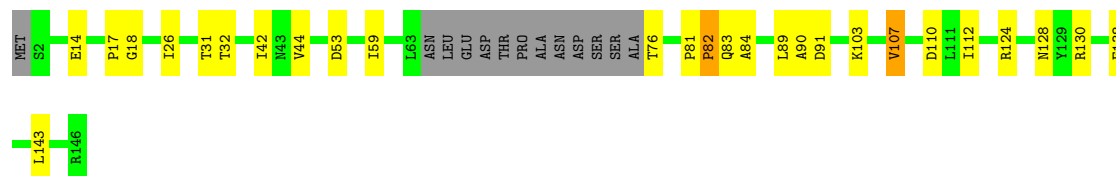
- Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

Chain G:



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

Chain H:



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

Chain I:



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

Chain J:



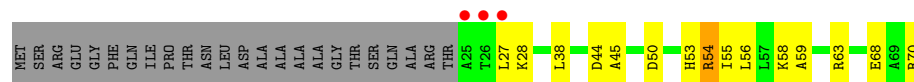
- Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11

Chain K: 



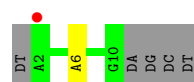
- Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4

Chain L: 



- Molecule 13: 5'-D(\*AP\*AP\*GP\*TP\*AP\*CP\*TP)-3'

Chain N: 



- Molecule 14: 5'-R(\*AP\*CP\*CP\*AP\*GP\*GP\*AP)-3'

Chain P: 



- Molecule 15: 5'-D(\*AP\*GP\*CP\*TP\*CP\*AP\*AP\*GP\*TP\*AP\*CP\*TP\*TP\*TP\*TP\*TP\*CP\*CP\*BRU\*GP\*GP\*TP\*CP\*AP\*TP\*T)-3'

Chain T: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	222.81Å 392.44Å 279.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.82 – 3.50 47.82 – 3.50	Depositor EDS
% Data completeness (in resolution range)	95.4 (47.82-3.50) 95.4 (47.82-3.50)	Depositor EDS
$R_{merge}$	0.77	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 3.48Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, $R_{free}$	0.159 , 0.187 0.180 , 0.206	Depositor DCC
$R_{free}$ test set	2869 reflections (1.96%)	DCC
Wilson B-factor (Å <sup>2</sup> )	107.7	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 97.5	EDS
Estimated twinning fraction	0.039 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.048 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 146430 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	31950	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, APC, ZN, BRU

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	0.54	1/11397 (0.0%)	0.85	8/15415 (0.1%)
2	B	0.51	0/9029	0.81	1/12171 (0.0%)
3	C	0.50	0/2133	0.80	0/2891
4	D	0.54	0/1444	0.88	0/1935
5	E	0.48	0/1788	0.73	0/2406
6	F	0.57	0/691	0.78	0/933
7	G	0.52	0/1368	0.83	0/1844
8	H	0.51	0/1086	0.85	0/1470
9	I	0.46	0/989	0.77	0/1331
10	J	0.52	0/541	0.85	1/727 (0.1%)
11	K	0.51	0/938	0.75	0/1267
12	L	0.53	0/365	0.96	0/485
13	N	1.13	0/205	1.07	0/315
14	P	1.19	0/170	0.86	0/263
15	T	1.33	0/383	1.10	0/586
All	All	0.55	1/32527 (0.0%)	0.83	10/44039 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	867	ILE	CG1-CD1	5.18	1.86	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	LYS	C-N-CA	7.75	141.08	121.70
1	A	399	HIS	N-CA-CB	6.86	122.95	110.60
1	A	56	PRO	C-N-CA	6.39	137.68	121.70
1	A	35	ILE	N-CA-CB	6.21	125.09	110.80
1	A	54	ASN	C-N-CA	5.83	136.28	121.70
1	A	34	LYS	N-CA-C	-5.66	95.71	111.00
1	A	55	ASP	N-CA-CB	5.43	120.37	110.60
1	A	194	ALA	C-N-CA	5.35	135.07	121.70
10	J	5	VAL	N-CA-C	-5.20	96.95	111.00
2	B	1181	GLU	N-CA-C	5.07	124.68	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	34	LYS	Mainchain,Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11197	0	0	16	0
2	B	8859	0	0	15	0
3	C	2095	0	0	5	0
4	D	1434	0	0	2	0
5	E	1752	0	0	2	0
6	F	679	0	0	1	0
7	G	1340	0	0	3	0
8	H	1068	0	0	1	0
9	I	971	0	0	1	0
10	J	532	0	0	4	0
11	K	920	0	0	2	0
12	L	363	0	0	0	0
13	N	183	0	0	1	0
14	P	152	0	0	0	0
15	T	365	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	A	1	0	0	0	0
18	P	31	0	14	0	0
All	All	31950	0	14	45	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 1.

All (45) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:867:ILE:CD1	1:A:867:ILE:CG1	1.86	1.50
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.30	0.64
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.30	0.64
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.31	0.63
1:A:399:HIS:O	1:A:401:GLY:N	2.33	0.61
3:C:66:ARG:NH2	10:J:3:VAL:O	2.40	0.54
2:B:882:THR:O	2:B:884:ARG:N	2.41	0.53
7:G:1:MET:SD	7:G:2:PHE:N	2.82	0.52
1:A:42:ASP:O	1:A:44:THR:N	2.45	0.50
10:J:9:SER:OG	10:J:48:ARG:NH2	2.44	0.50
1:A:663:SER:OG	2:B:827:ILE:O	2.30	0.49
2:B:296:GLU:O	2:B:300:HIS:CD2	2.65	0.49
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.47	0.48
13:N:6:DA:C2	15:T:13:DA:C2	3.02	0.48
10:J:1:MET:N	10:J:54:VAL:O	2.48	0.47
2:B:996:ARG:NH2	3:C:174:ALA:O	2.48	0.47
1:A:1059:HIS:ND1	6:F:87:LYS:N	2.63	0.47
3:C:165:LYS:O	11:K:6:ARG:NH1	2.48	0.46
8:H:82:PRO:O	8:H:84:ALA:N	2.48	0.46
2:B:412:LEU:O	2:B:466:TRP:NE1	2.49	0.46
7:G:34:VAL:O	7:G:37:SER:OG	2.34	0.45
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.99	0.45
2:B:1166:CYS:SG	2:B:1166:CYS:O	2.75	0.45
10:J:37:SER:OG	10:J:47:ARG:NH2	2.50	0.44
11:K:65:HIS:CE1	11:K:67:PHE:CG	3.06	0.44
5:E:163:GLU:OE2	5:E:167:ARG:NE	2.50	0.44
1:A:434:ARG:NH2	1:A:440:ASP:OD2	2.51	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:1033:LYS:NZ	2:B:1070:GLU:OE1	2.52	0.43
7:G:83:LYS:N	7:G:83:LYS:CD	2.80	0.43
4:D:198:LEU:O	4:D:200:ASN:N	2.52	0.43
1:A:55:ASP:OD2	1:A:55:ASP:O	2.37	0.42
4:D:14:ARG:O	4:D:16:LYS:N	2.52	0.42
1:A:7:SER:OG	2:B:1161:HIS:NE2	2.52	0.42
2:B:1013:ASN:OD1	2:B:1015:HIS:ND1	2.53	0.42
1:A:265:LYS:NZ	1:A:299:HIS:ND1	2.68	0.42
1:A:1035:TYR:N	1:A:1035:TYR:CD1	2.85	0.42
1:A:906:HIS:ND1	1:A:906:HIS:N	2.65	0.42
1:A:409:SER:O	1:A:411:ASP:N	2.53	0.41
9:I:8:ARG:CG	9:I:34:TYR:CE2	3.03	0.41
3:C:145:CYS:SG	3:C:146:LYS:N	2.93	0.41
2:B:882:THR:OG1	2:B:935:ARG:N	2.54	0.41
1:A:870:GLU:OE2	1:A:1365:TYR:OH	2.38	0.41
5:E:151:PRO:O	5:E:153:HIS:ND1	2.54	0.41
2:B:179:CYS:SG	2:B:180:TYR:N	2.95	0.40
2:B:100:PRO:O	2:B:180:TYR:OH	2.40	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	1417/1732 (82%)	1225 (86%)	132 (9%)	60 (4%)	4	43
2	B	1095/1224 (90%)	960 (88%)	86 (8%)	49 (4%)	4	40
3	C	264/318 (83%)	234 (89%)	26 (10%)	4 (2%)	15	69
4	D	174/221 (79%)	151 (87%)	14 (8%)	9 (5%)	3	35
5	E	212/215 (99%)	195 (92%)	12 (6%)	5 (2%)	9	59
6	F	82/155 (53%)	72 (88%)	10 (12%)	0	100	100
7	G	169/171 (99%)	153 (90%)	13 (8%)	3 (2%)	13	65
8	H	129/146 (88%)	103 (80%)	16 (12%)	10 (8%)	1	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	117/122 (96%)	93 (80%)	20 (17%)	4 (3%)	6	50
10	J	63/70 (90%)	54 (86%)	6 (10%)	3 (5%)	4	38
11	K	113/120 (94%)	103 (91%)	9 (8%)	1 (1%)	25	80
12	L	44/70 (63%)	22 (50%)	15 (34%)	7 (16%)	0	5
All	All	3879/4564 (85%)	3365 (87%)	359 (9%)	155 (4%)	5	44

All (155) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ARG
1	A	58	LEU
1	A	76	GLU
1	A	169	ASN
1	A	257	ARG
1	A	286	HIS
1	A	311	GLN
1	A	318	SER
1	A	449	SER
1	A	1377	THR
2	B	344	LYS
2	B	473	MET
2	B	731	VAL
2	B	879	ARG
2	B	880	THR
2	B	1046	PRO
2	B	1157	ALA
2	B	1181	GLU
2	B	1190	ASP
3	C	161	LYS
4	D	18	VAL
4	D	53	SER
4	D	199	ASN
8	H	83	GLN
9	I	95	THR
10	J	6	ARG
12	L	28	LYS
1	A	43	GLU
1	A	46	THR
1	A	54	ASN
1	A	156	ASP
1	A	167	CYS

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Mol	Chain	Res	Type
1	A	178	GLY
1	A	189	ARG
1	A	193	ASP
1	A	195	ASP
1	A	332	LYS
1	A	335	ARG
1	A	409	SER
1	A	410	GLY
1	A	465	TYR
1	A	466	SER
1	A	852	TYR
1	A	1124	HIS
2	B	184	ALA
2	B	526	GLU
2	B	711	GLU
2	B	867	GLY
2	B	883	LEU
2	B	907	GLY
2	B	1066	SER
2	B	1156	ASP
2	B	1175	LEU
2	B	1223	ASP
4	D	11	ARG
4	D	21	GLU
5	E	3	GLN
5	E	45	LYS
5	E	48	ASP
5	E	50	MET
7	G	154	VAL
8	H	17	PRO
8	H	18	GLY
9	I	113	ASP
12	L	50	ASP
12	L	53	HIS
12	L	56	LEU
12	L	59	ALA
1	A	74	MET
1	A	331	GLY
1	A	567	LYS
1	A	916	GLY
1	A	1255	GLU
1	A	1366	ARG

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Mol	Chain	Res	Type
2	B	369	GLY
2	B	466	TRP
2	B	707	PRO
2	B	1047	PHE
2	B	1176	ASN
4	D	119	ARG
4	D	169	SER
7	G	2	PHE
8	H	81	PRO
8	H	82	PRO
9	I	3	THR
12	L	45	ALA
12	L	54	ARG
1	A	40	THR
1	A	47	ARG
1	A	48	ALA
1	A	399	HIS
1	A	448	PRO
1	A	525	GLN
1	A	846	GLU
1	A	1281	ARG
2	B	229	ALA
2	B	339	THR
2	B	341	LEU
2	B	469	GLN
2	B	476	ARG
2	B	629	ASP
2	B	792	MET
2	B	868	MET
7	G	63	PRO
8	H	32	THR
8	H	128	ASN
10	J	3	VAL
1	A	55	ASP
1	A	336	ILE
1	A	599	SER
1	A	639	PRO
1	A	958	VAL
1	A	1173	HIS
1	A	1403	GLU
2	B	262	GLU
2	B	282	ILE

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Mol	Chain	Res	Type
2	B	322	PHE
2	B	368	GLU
2	B	648	HIS
2	B	870	ILE
2	B	943	SER
2	B	1069	PHE
2	B	1108	ARG
3	C	227	THR
4	D	16	LYS
8	H	90	ALA
10	J	2	ILE
1	A	35	ILE
1	A	312	PRO
1	A	1257	ASP
2	B	340	ALA
3	C	90	ASP
4	D	174	PRO
5	E	36	GLU
11	K	15	GLY
1	A	283	GLY
1	A	310	GLY
1	A	1123	GLY
1	A	196	GLU
1	A	569	LYS
2	B	338	GLY
2	B	510	LYS
2	B	743	ILE
2	B	1214	PRO
1	A	51	GLY
1	A	1437	GLY
2	B	108	VAL
8	H	59	ILE
8	H	107	VAL
9	I	57	GLY
1	A	1327	ILE
2	B	575	PRO
3	C	5	GLY
1	A	886	ILE
2	B	343	ILE

### 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	1243/1519 (82%)	1046 (84%)	197 (16%)	4	23
2	B	966/1061 (91%)	824 (85%)	142 (15%)	4	26
3	C	234/274 (85%)	203 (87%)	31 (13%)	6	32
4	D	160/200 (80%)	134 (84%)	26 (16%)	3	21
5	E	196/197 (100%)	170 (87%)	26 (13%)	6	31
6	F	74/137 (54%)	66 (89%)	8 (11%)	9	44
7	G	152/152 (100%)	125 (82%)	27 (18%)	2	16
8	H	117/128 (91%)	100 (86%)	17 (14%)	5	27
9	I	113/116 (97%)	98 (87%)	15 (13%)	6	31
10	J	60/65 (92%)	52 (87%)	8 (13%)	6	31
11	K	99/102 (97%)	81 (82%)	18 (18%)	2	14
12	L	40/57 (70%)	31 (78%)	9 (22%)	1	8
All	All	3454/4008 (86%)	2930 (85%)	524 (15%)	4	25

All (524) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	12	ARG
1	A	15	LYS
1	A	22	PHE
1	A	28	ARG
1	A	41	MET
1	A	42	ASP
1	A	44	THR
1	A	45	GLN
1	A	47	ARG
1	A	58	LEU
1	A	64	ASN
1	A	93	VAL
1	A	106	VAL
1	A	112	LYS

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Mol	Chain	Res	Type
1	A	117	GLU
1	A	129	LYS
1	A	132	LYS
1	A	144	THR
1	A	147	VAL
1	A	151	ASP
1	A	152	VAL
1	A	156	ASP
1	A	157	ASP
1	A	159	THR
1	A	160	GLN
1	A	161	LEU
1	A	164	ARG
1	A	173	THR
1	A	174	ILE
1	A	188	ASP
1	A	195	ASP
1	A	204	THR
1	A	208	LEU
1	A	222	LEU
1	A	225	ASN
1	A	256	GLN
1	A	261	ASP
1	A	270	LEU
1	A	274	ILE
1	A	279	LEU
1	A	289	ILE
1	A	295	LEU
1	A	313	GLN
1	A	315	LEU
1	A	322	VAL
1	A	335	ARG
1	A	337	ARG
1	A	341	MET
1	A	363	GLN
1	A	369	SER
1	A	375	THR
1	A	381	THR
1	A	383	TYR
1	A	385	ILE
1	A	386	ASP
1	A	389	THR

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Mol	Chain	Res	Type
1	A	391	LEU
1	A	393	ARG
1	A	398	GLU
1	A	408	ASP
1	A	425	GLN
1	A	431	LYS
1	A	434	ARG
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	451	HIS
1	A	454	SER
1	A	459	ARG
1	A	461	LYS
1	A	469	ARG
1	A	470	LEU
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	476	SER
1	A	488	ASN
1	A	493	GLN
1	A	496	GLU
1	A	500	GLU
1	A	505	CYS
1	A	512	VAL
1	A	517	ASN
1	A	518	LYS
1	A	524	VAL
1	A	527	THR
1	A	532	ARG
1	A	534	LEU
1	A	538	ASP
1	A	546	VAL
1	A	566	ILE
1	A	567	LYS
1	A	569	LYS
1	A	577	ILE
1	A	588	LEU
1	A	593	GLU
1	A	597	LEU
1	A	598	LEU

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Mol	Chain	Res	Type
1	A	603	ASN
1	A	618	GLU
1	A	629	LEU
1	A	634	THR
1	A	660	ASN
1	A	666	ILE
1	A	672	ASP
1	A	680	THR
1	A	685	GLU
1	A	732	LEU
1	A	738	LYS
1	A	739	ASP
1	A	756	ILE
1	A	762	SER
1	A	764	CYS
1	A	768	GLN
1	A	782	ARG
1	A	788	SER
1	A	811	GLN
1	A	821	ARG
1	A	834	THR
1	A	838	GLN
1	A	839	ARG
1	A	846	GLU
1	A	849	MET
1	A	855	THR
1	A	885	THR
1	A	886	ILE
1	A	901	LEU
1	A	905	ASP
1	A	915	SER
1	A	919	ILE
1	A	920	LEU
1	A	925	LEU
1	A	926	GLN
1	A	929	LEU
1	A	934	LYS
1	A	941	LYS
1	A	948	VAL
1	A	964	ILE
1	A	969	GLN
1	A	973	ILE

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Mol	Chain	Res	Type
1	A	980	ASP
1	A	982	THR
1	A	1024	SER
1	A	1062	GLU
1	A	1064	VAL
1	A	1067	LEU
1	A	1078	GLN
1	A	1116	LEU
1	A	1124	HIS
1	A	1135	ARG
1	A	1142	THR
1	A	1145	SER
1	A	1162	VAL
1	A	1168	GLU
1	A	1170	ILE
1	A	1173	HIS
1	A	1195	LEU
1	A	1208	THR
1	A	1222	ASN
1	A	1233	ASP
1	A	1237	ILE
1	A	1242	VAL
1	A	1255	GLU
1	A	1257	ASP
1	A	1259	MET
1	A	1264	GLU
1	A	1265	ASN
1	A	1271	ILE
1	A	1291	VAL
1	A	1293	SER
1	A	1295	THR
1	A	1297	GLU
1	A	1308	THR
1	A	1309	ASP
1	A	1315	GLU
1	A	1316	VAL
1	A	1325	THR
1	A	1336	MET
1	A	1341	ILE
1	A	1366	ARG
1	A	1370	LEU
1	A	1378	GLN

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Mol	Chain	Res	Type
1	A	1382	THR
1	A	1386	ARG
1	A	1391	ARG
1	A	1400	CYS
1	A	1403	GLU
1	A	1404	GLU
1	A	1410	PHE
1	A	1420	ASP
1	A	1426	GLU
1	A	1442	ASP
1	A	1444	MET
1	A	1445	ILE
1	A	1452	LYS
1	A	1454	MET
2	B	22	SER
2	B	46	GLN
2	B	56	ASP
2	B	63	ILE
2	B	90	ILE
2	B	119	LEU
2	B	131	ASP
2	B	134	LYS
2	B	167	ILE
2	B	175	ARG
2	B	194	GLU
2	B	205	ILE
2	B	218	SER
2	B	222	ILE
2	B	261	ARG
2	B	267	ARG
2	B	272	THR
2	B	278	GLN
2	B	279	ASP
2	B	294	ASP
2	B	298	LEU
2	B	305	VAL
2	B	312	GLU
2	B	313	MET
2	B	324	ILE
2	B	337	ARG
2	B	339	THR
2	B	343	ILE

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Mol	Chain	Res	Type
2	B	344	LYS
2	B	346	GLU
2	B	348	ARG
2	B	350	GLN
2	B	361	LEU
2	B	364	ILE
2	B	365	THR
2	B	371	GLU
2	B	393	LYS
2	B	395	GLN
2	B	396	ASP
2	B	412	LEU
2	B	416	LEU
2	B	418	LYS
2	B	423	LYS
2	B	426	LYS
2	B	429	PHE
2	B	434	ARG
2	B	436	VAL
2	B	446	LEU
2	B	448	ILE
2	B	458	LYS
2	B	466	TRP
2	B	470	LYS
2	B	480	SER
2	B	485	ARG
2	B	487	THR
2	B	502	ILE
2	B	513	GLN
2	B	531	GLN
2	B	533	CYS
2	B	537	LYS
2	B	547	VAL
2	B	552	MET
2	B	560	GLU
2	B	567	GLU
2	B	574	SER
2	B	595	ARG
2	B	602	THR
2	B	604	ARG
2	B	616	ILE
2	B	620	ARG

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Mol	Chain	Res	Type
2	B	635	ARG
2	B	644	GLU
2	B	653	VAL
2	B	658	ILE
2	B	664	THR
2	B	668	ASP
2	B	678	GLU
2	B	690	VAL
2	B	694	ASP
2	B	696	GLU
2	B	708	GLU
2	B	734	HIS
2	B	736	THR
2	B	755	ILE
2	B	766	ARG
2	B	780	VAL
2	B	786	ASN
2	B	790	ASP
2	B	791	THR
2	B	795	ILE
2	B	815	ARG
2	B	837	ASP
2	B	841	MET
2	B	844	SER
2	B	868	MET
2	B	871	THR
2	B	878	GLN
2	B	882	THR
2	B	891	ASP
2	B	909	ASP
2	B	934	LYS
2	B	939	THR
2	B	942	ARG
2	B	944	THR
2	B	946	ASN
2	B	948	ILE
2	B	956	THR
2	B	970	THR
2	B	972	LYS
2	B	975	GLN
2	B	976	ILE
2	B	983	ARG

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Mol	Chain	Res	Type
2	B	986	GLN
2	B	997	GLU
2	B	999	MET
2	B	1007	VAL
2	B	1019	SER
2	B	1045	SER
2	B	1048	THR
2	B	1050	ILE
2	B	1065	GLN
2	B	1072	MET
2	B	1122	ARG
2	B	1128	LEU
2	B	1132	GLU
2	B	1133	MET
2	B	1138	MET
2	B	1145	SER
2	B	1147	LEU
2	B	1151	LEU
2	B	1156	ASP
2	B	1168	LEU
2	B	1170	THR
2	B	1175	LEU
2	B	1176	ASN
2	B	1178	ASN
2	B	1179	GLN
2	B	1183	LYS
2	B	1188	LYS
2	B	1189	ILE
2	B	1202	LEU
2	B	1221	SER
3	C	7	GLN
3	C	16	ASP
3	C	25	VAL
3	C	26	ASP
3	C	27	LEU
3	C	34	ARG
3	C	44	LEU
3	C	55	THR
3	C	57	VAL
3	C	78	GLU
3	C	79	GLN
3	C	100	THR

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Mol	Chain	Res	Type
3	C	101	LEU
3	C	108	GLU
3	C	119	VAL
3	C	125	MET
3	C	127	ARG
3	C	129	ILE
3	C	148	ARG
3	C	149	LYS
3	C	155	LEU
3	C	197	SER
3	C	215	GLU
3	C	226	ASP
3	C	235	VAL
3	C	237	SER
3	C	240	VAL
3	C	259	LEU
3	C	260	LEU
3	C	262	LEU
3	C	265	MET
4	D	6	SER
4	D	7	THR
4	D	9	GLN
4	D	13	ARG
4	D	18	VAL
4	D	27	LEU
4	D	28	GLN
4	D	29	LEU
4	D	32	GLU
4	D	38	ILE
4	D	45	GLU
4	D	52	LEU
4	D	65	GLU
4	D	67	ARG
4	D	75	LYS
4	D	121	LYS
4	D	126	ILE
4	D	134	THR
4	D	137	ASN
4	D	139	LYS
4	D	156	ASP
4	D	182	SER
4	D	187	THR

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Mol	Chain	Res	Type
4	D	197	SER
4	D	219	THR
4	D	221	TYR
5	E	3	GLN
5	E	10	SER
5	E	40	GLU
5	E	41	ASP
5	E	45	LYS
5	E	65	THR
5	E	72	PHE
5	E	75	MET
5	E	84	ASP
5	E	92	THR
5	E	94	LYS
5	E	95	THR
5	E	98	ILE
5	E	104	ASN
5	E	107	THR
5	E	114	ASN
5	E	131	THR
5	E	150	VAL
5	E	173	SER
5	E	175	LEU
5	E	179	GLN
5	E	190	LEU
5	E	196	VAL
5	E	202	SER
5	E	203	GLU
5	E	204	THR
6	F	72	LYS
6	F	79	ARG
6	F	82	THR
6	F	86	THR
6	F	90	ARG
6	F	110	ASP
6	F	115	THR
6	F	122	MET
7	G	1	MET
7	G	6	ASP
7	G	11	ILE
7	G	13	LEU
7	G	22	MET

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Mol	Chain	Res	Type
7	G	23	LYS
7	G	24	GLN
7	G	26	LEU
7	G	64	THR
7	G	65	ASP
7	G	83	LYS
7	G	85	GLU
7	G	90	THR
7	G	95	SER
7	G	96	GLN
7	G	106	MET
7	G	112	LYS
7	G	119	LEU
7	G	134	GLU
7	G	135	ASP
7	G	138	THR
7	G	142	ARG
7	G	143	ILE
7	G	153	GLN
7	G	155	SER
7	G	162	SER
7	G	171	ILE
8	H	14	GLU
8	H	26	ILE
8	H	31	THR
8	H	42	ILE
8	H	44	VAL
8	H	53	ASP
8	H	76	THR
8	H	89	LEU
8	H	91	ASP
8	H	103	LYS
8	H	107	VAL
8	H	110	ASP
8	H	112	ILE
8	H	124	ARG
8	H	130	ARG
8	H	138	GLU
8	H	143	LEU
9	I	8	ARG
9	I	24	ARG
9	I	30	ARG

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Mol	Chain	Res	Type
9	I	31	THR
9	I	43	VAL
9	I	55	THR
9	I	74	GLU
9	I	81	ARG
9	I	83	ASN
9	I	87	GLN
9	I	94	ASP
9	I	95	THR
9	I	109	ILE
9	I	114	GLN
9	I	120	GLN
10	J	2	ILE
10	J	7	CYS
10	J	13	VAL
10	J	14	VAL
10	J	19	GLU
10	J	42	LYS
10	J	48	ARG
10	J	55	ASP
11	K	11	LEU
11	K	18	LYS
11	K	20	LYS
11	K	25	THR
11	K	29	ASN
11	K	31	VAL
11	K	33	ILE
11	K	34	THR
11	K	37	LYS
11	K	47	ARG
11	K	51	LEU
11	K	66	PRO
11	K	74	ARG
11	K	84	LYS
11	K	87	LEU
11	K	91	CYS
11	K	101	LEU
11	K	114	LEU
12	L	27	LEU
12	L	38	LEU
12	L	44	ASP
12	L	54	ARG

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Mol	Chain	Res	Type
12	L	55	ILE
12	L	58	LYS
12	L	63	ARG
12	L	68	GLU
12	L	70	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	6/7 (85%)	1 (16%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	8	G

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	$\# Z  > 2$
15	BRU	T	22	15,14	19,21,22	1.36	4 (21%)	22,30,33	2.18	6 (27%)

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	BRU	T	22	15,14	-	0/5/21/22	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	22	BRU	BR-C5	-2.77	1.83	1.90
15	T	22	BRU	P-OP1	2.67	1.49	1.46
15	T	22	BRU	C4-N3	-2.64	1.32	1.37
15	T	22	BRU	C2-N3	-2.24	1.33	1.37

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	22	BRU	C6-N1-C2	-6.02	120.70	122.41
15	T	22	BRU	N3-C2-N1	4.22	119.49	115.97
15	T	22	BRU	C5-C6-N1	-4.01	117.04	119.67
15	T	22	BRU	O4'-C1'-N1	3.75	114.73	107.68
15	T	22	BRU	C2'-C1'-N1	-2.72	107.01	114.08
15	T	22	BRU	BR-C5-C4	-2.39	115.77	120.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 10 ligands modelled in this entry, 9 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
18	APC	P	1011	-	33,33,33	3.40	13 (39%)	52,52,52	2.13	16 (30%)

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
18	APC	P	1011	-	-	0/20/38/38	0/1/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	P	1011	APC	PB-C3A	9.99	1.88	1.79
18	P	1011	APC	PA-C3A	9.08	1.87	1.79
18	P	1011	APC	PG-O3B	7.01	1.72	1.60
18	P	1011	APC	PB-O3B	4.84	1.71	1.59
18	P	1011	APC	PA-O1A	4.57	1.63	1.51
18	P	1011	APC	PG-O1G	4.32	1.65	1.51
18	P	1011	APC	PB-O2B	4.20	1.66	1.56
18	P	1011	APC	O4'-C1'	3.22	1.46	1.41
18	P	1011	APC	PG-O2G	3.15	1.66	1.54
18	P	1011	APC	C4-N3	-2.70	1.31	1.35
18	P	1011	APC	C8-N7	-2.43	1.29	1.34
18	P	1011	APC	PA-O5'	2.10	1.68	1.53
18	P	1011	APC	C5-N7	-2.02	1.32	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	P	1011	APC	N3-C2-N1	-6.71	123.10	128.71
18	P	1011	APC	C4-C5-N7	-5.30	104.99	109.52
18	P	1011	APC	N3-C4-N9	4.81	134.11	125.43
18	P	1011	APC	C4'-O4'-C1'	3.87	113.95	109.75
18	P	1011	APC	C5-C4-N3	-3.73	117.59	125.70
18	P	1011	APC	C2'-C3'-C4'	3.14	108.91	102.65
18	P	1011	APC	O2A-PA-O5'	2.94	115.21	105.82
18	P	1011	APC	O2'-C2'-C3'	2.92	121.32	111.83
18	P	1011	APC	O5'-PA-C3A	2.72	110.72	103.97
18	P	1011	APC	O3'-C3'-C2'	2.68	120.55	111.83
18	P	1011	APC	O1A-PA-C3A	-2.56	103.06	109.49
18	P	1011	APC	C2-N3-C4	2.54	121.25	114.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	P	1011	APC	C8-N7-C5	2.15	110.26	103.58
18	P	1011	APC	C2'-C1'-N9	-2.10	107.87	113.27
18	P	1011	APC	O5'-PA-O1A	-2.04	109.11	114.21
18	P	1011	APC	PG-O3B-PB	-2.02	124.89	131.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	1425/1732 (82%)	-0.05	5 (0%) 90 71	58, 109, 170, 229	0
2	B	1115/1224 (91%)	0.03	5 (0%) 90 71	60, 125, 185, 220	0
3	C	266/318 (83%)	-0.08	0 100 100	79, 108, 151, 176	0
4	D	178/221 (80%)	-0.02	1 (0%) 86 59	80, 120, 168, 185	0
5	E	214/215 (99%)	-0.02	1 (0%) 88 64	84, 146, 186, 199	0
6	F	84/155 (54%)	-0.15	0 100 100	66, 90, 120, 142	0
7	G	171/171 (100%)	-0.08	0 100 100	84, 106, 146, 169	0
8	H	133/146 (91%)	0.29	0 100 100	125, 153, 187, 208	0
9	I	119/122 (97%)	0.12	2 (1%) 67 34	116, 161, 191, 203	0
10	J	65/70 (92%)	-0.08	0 100 100	85, 104, 151, 156	0
11	K	115/120 (95%)	-0.08	1 (0%) 81 51	74, 107, 143, 161	0
12	L	46/70 (65%)	0.37	3 (6%) 18 8	88, 166, 186, 202	0
13	N	9/14 (64%)	0.48	1 (11%) 6 4	202, 213, 240, 250	0
14	P	7/7 (100%)	-0.57	0 100 100	100, 112, 162, 182	0
15	T	18/26 (69%)	-0.13	0 100 100	92, 153, 246, 250	0
All	All	3965/4611 (85%)	-0.01	19 (0%) 88 64	58, 117, 181, 250	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1176	LEU	4.9
12	L	27	LEU	4.0
12	L	26	THR	3.9
9	I	119	THR	3.3
11	K	115	ALA	3.3
1	A	257	ARG	3.2
1	A	1455	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
12	L	25	ALA	3.0
1	A	194	ALA	2.9
13	N	2	DA	2.8
2	B	883	LEU	2.8
5	E	123	LEU	2.8
1	A	256	GLN	2.6
2	B	865	LYS	2.3
9	I	118	ARG	2.2
2	B	870	ILE	2.1
4	D	13	ARG	2.1
2	B	340	ALA	2.0
2	B	435	THR	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
15	BRU	T	22	20/21	0.12	-1.34	100,112,119,124	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
16	ZN	I	1121	1/1	0.13	0.54	137,137,137,137	0
18	APC	P	1011	31/31	0.26	0.33	148,151,173,174	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
16	ZN	B	2225	1/1	0.19	0.09	85,85,85,85	0
16	ZN	A	2456	1/1	0.10	-0.70	146,146,146,146	0
16	ZN	A	2457	1/1	0.15	-0.73	76,76,76,76	0
16	ZN	C	1269	1/1	0.11	-1.06	91,91,91,91	0
16	ZN	J	1066	1/1	0.25	-1.52	98,98,98,98	0
16	ZN	I	1122	1/1	0.03	-1.86	202,202,202,202	0
16	ZN	L	1071	1/1	0.04	-2.35	203,203,203,203	0
17	MG	A	2458	1/1	0.10	-4.17	95,95,95,95	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.