



Full wwPDB X-ray Structure Validation Report

Mar 31, 2014 – 04:17 PM BST

PDB ID : 4A3G
Title : RNA Polymerase II initial transcribing complex with a 2nt DNA-RNA hybrid
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
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

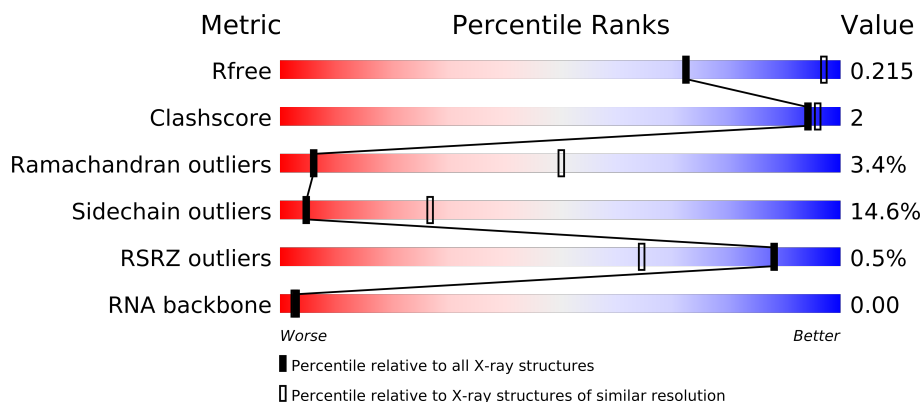
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable23004
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) : stable23004

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 ≥ 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	
2	B	1224	
3	C	318	
4	D	221	
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	

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Mol	Chain	Length	Quality of chain
13	N	14	
14	P	2	
15	T	27	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 31728 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	1422	Total	C	N	O	S	0	0	0
			11174	7037	1954	2121	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 RPABC 1.

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 RPABC 2.

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 RPB7, 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 RPABC 3.

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 RPABC 5.

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 RPABC 4.

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 NON TEMPLATE DNA 5'-D(*GP*GP*CP*AP*CP*AP*AP*CP*TP*GP*CP*GP*CP*TP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	9	Total	C	N	O	P	0	0	0
			181	87	36	50	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	2	Total	C	N	O	P	0	0	0
			42	19	8	13	2			

- Molecule 15 is a DNA chain called TEMPLATE DNA 5'-D(*AP*GP*CP*GP*CP*AP*GP*TP*TP*GP*TP*GP*CP*TP*AP*TP*GP*AP*BRUP*AP*TP*TP*TP*TP*TP*AP*DT)-3'.

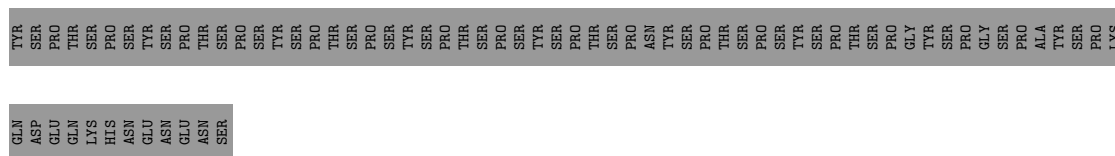
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
15	T	15	Total	Br	C	N	O	P	0	0	0
			309	1	147	53	93	15			

- 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		

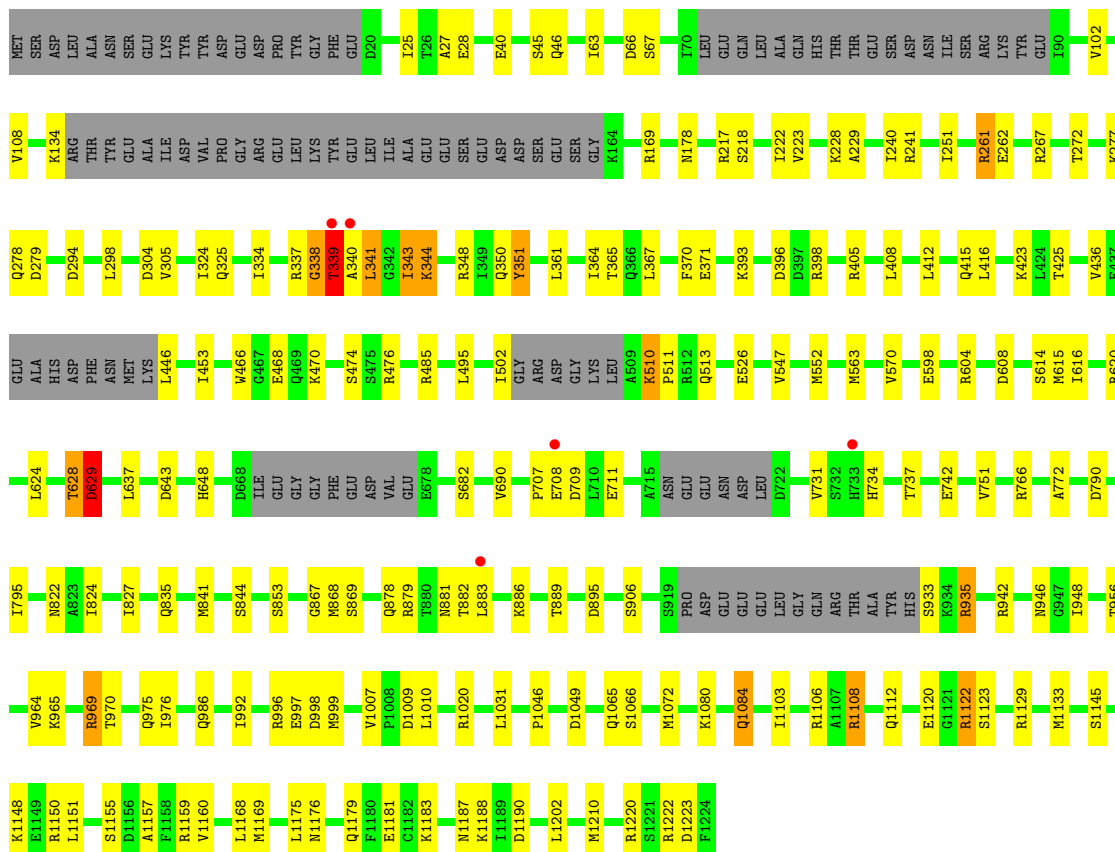
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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



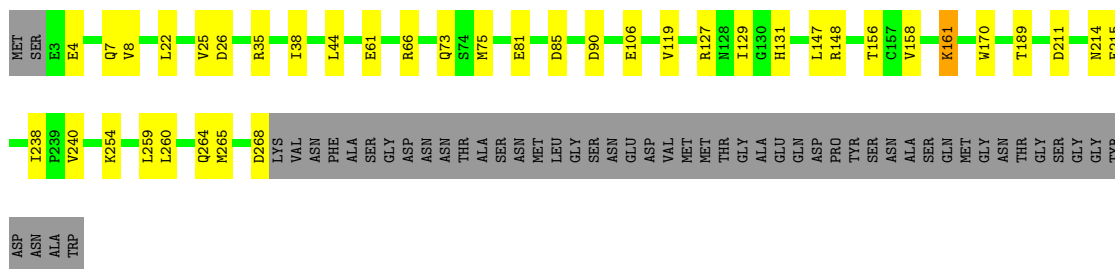
● Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2

Chain B:



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

Chain C:



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

Chain D:

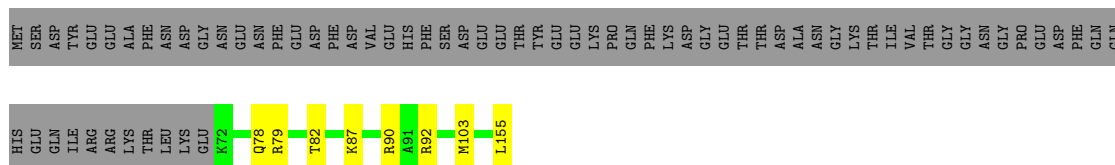
- Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1

Chain E:



- Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2

Chain F:



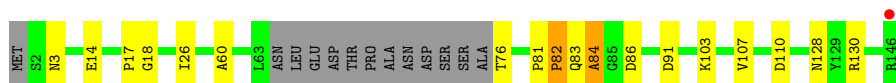
- Molecule 7: RPB7, DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

Chain G:



- Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

Chain H:



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

Chain I: 

- Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

Chain J:



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

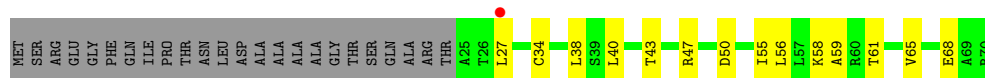
Chain K:





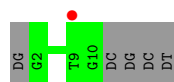
- Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4

Chain L:



- Molecule 13: NON TEMPLATE DNA 5'-D(*GP*GP*CP*AP*CP*AP*AP*CP*TP*GP*C
P*GP*CP*TP)-3'

Chain N:



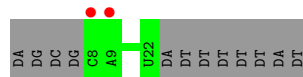
- Molecule 14: TRANSCRIPT RNA 5'-R(*CP*AP)-3'

Chain P:



- Molecule 15: TEMPLATE DNA 5'-D(*AP*GP*CP*GP*CP*AP*GP*TP*TP*GP*TP*GP*C
P*TP*AP*TP*GP*AP*BRUP*AP*TP*TP*TP*TP*TP*AP*DT)-3'

Chain T:



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	220.67Å 394.13Å 282.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.27 – 3.50 49.27 – 3.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.27-3.50) 100.0 (49.27-3.50)	Depositor EDS
R_{merge}	0.96	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 3.48Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.166 , 0.194 0.185 , 0.215	Depositor DCC
R_{free} test set	3037 reflections (1.97%)	DCC
Wilson B-factor (Å ²)	103.7	Xtriage
Anisotropy	0.457	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 95.5	EDS
Estimated twinning fraction	0.036 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.043 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 154255 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	31728	wwPDB-VP
Average B, all atoms (Å ²)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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, 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	0/11374	0.85	14/15383 (0.1%)
2	B	0.52	0/9029	0.81	2/12171 (0.0%)
3	C	0.50	0/2133	0.78	0/2891
4	D	0.52	0/1444	0.85	2/1935 (0.1%)
5	E	0.47	0/1788	0.74	0/2406
6	F	0.61	0/691	0.83	0/933
7	G	0.52	0/1368	0.82	0/1844
8	H	0.50	0/1086	0.79	0/1470
9	I	0.46	0/989	0.76	0/1331
10	J	0.58	0/541	0.92	1/727 (0.1%)
11	K	0.49	0/938	0.73	0/1267
12	L	0.55	0/365	1.01	0/485
13	N	1.24	0/203	1.05	0/311
14	P	1.48	1/46 (2.2%)	0.90	0/69
15	T	1.19	0/323	1.01	0/497
All	All	0.54	1/32318 (0.0%)	0.83	19/43720 (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)
14	P	9	C	C1'-N1	6.17	1.58	1.48

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	LYS	C-N-CA	7.55	140.58	121.70
4	D	25	ALA	C-N-CA	7.43	140.28	121.70
1	A	399	HIS	N-CA-CB	6.90	123.03	110.60
1	A	56	PRO	C-N-CA	6.78	138.65	121.70
1	A	310	GLY	C-N-CA	5.91	136.46	121.70
4	D	26	THR	N-CA-C	-5.81	95.31	111.00
1	A	35	ILE	CB-CA-C	5.76	123.12	111.60
2	B	628	THR	C-N-CA	5.63	135.78	121.70
1	A	57	ARG	C-N-CA	5.63	135.77	121.70
2	B	339	THR	C-N-CA	5.51	135.47	121.70
1	A	47	ARG	C-N-CA	5.32	134.99	121.70
1	A	54	ASN	CB-CA-C	5.28	120.97	110.40
1	A	69	THR	C-N-CA	5.26	134.84	121.70
10	J	5	VAL	N-CA-C	-5.15	97.10	111.00
1	A	1403	GLU	N-CA-C	5.13	124.84	111.00
1	A	194	ALA	C-N-CA	5.11	134.47	121.70
1	A	54	ASN	C-N-CA	5.05	134.34	121.70
1	A	223	GLY	C-N-CA	5.05	134.32	121.70
1	A	331	GLY	N-CA-C	5.03	125.67	113.10

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	11174	0	0	21	0
2	B	8859	0	0	16	0
3	C	2095	0	0	7	0
4	D	1434	0	0	3	0
5	E	1752	0	0	0	0
6	F	679	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	1340	0	0	4	0
8	H	1068	0	0	2	0
9	I	971	0	0	0	0
10	J	532	0	0	4	0
11	K	920	0	0	0	0
12	L	363	0	0	0	0
13	N	181	0	0	0	0
14	P	42	0	22	0	0
15	T	309	0	0	0	0
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
All	All	31728	0	22	47	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 2.

All (47) 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	1.75	1.54
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.28	0.66
7:G:1:MET:SD	7:G:2:PHE:N	2.69	0.66
2:B:933:SER:O	2:B:935:ARG:N	2.34	0.60
1:A:42:ASP:O	1:A:44:THR:N	2.35	0.60
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.85	0.60
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.35	0.59
7:G:1:MET:CE	7:G:80:LYS:O	2.51	0.58
1:A:433:GLU:OE1	2:B:1108:ARG:NH2	2.39	0.56
2:B:822:ASN:O	10:J:48:ARG:NH1	2.39	0.55
3:C:161:LYS:O	3:C:170:TRP:NE1	2.40	0.54
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.41	0.54
4:D:8:PHE:CZ	7:G:5:LYS:NZ	2.76	0.54
1:A:31:SER:OG	1:A:33:ALA:O	2.26	0.54
10:J:9:SER:OG	10:J:48:ARG:NH2	2.44	0.51
2:B:824:ILE:O	2:B:1009:ASP:N	2.43	0.51
1:A:200:ARG:NH2	1:A:206:GLU:OE1	2.44	0.51
1:A:879:GLU:OE2	1:A:962:ARG:NH2	2.44	0.51
3:C:66:ARG:NH2	10:J:3:VAL:O	2.44	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:1084:GLN:OE1	3:C:189:THR:CG2	2.59	0.50
2:B:1187:ASN:OD1	2:B:1190:ASP:N	2.45	0.49
1:A:867:ILE:CB	1:A:867:ILE:CD1	2.81	0.49
1:A:503:GLN:OE1	6:F:90:ARG:NH2	2.46	0.48
8:H:82:PRO:O	8:H:84:ALA:N	2.47	0.48
2:B:339:THR:OG1	2:B:351:TYR:CE2	2.67	0.48
4:D:14:ARG:O	4:D:16:LYS:N	2.48	0.47
1:A:1035:TYR:N	1:A:1035:TYR:CD1	2.82	0.46
10:J:37:SER:OG	10:J:47:ARG:NH2	2.49	0.46
2:B:405:ARG:NE	2:B:629:ASP:OD1	2.48	0.46
8:H:82:PRO:C	8:H:84:ALA:N	2.70	0.45
2:B:510:LYS:N	2:B:511:PRO:CD	2.79	0.45
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.50	0.45
1:A:55:ASP:CG	1:A:55:ASP:O	2.54	0.45
1:A:55:ASP:OD2	1:A:55:ASP:O	2.34	0.45
2:B:228:LYS:O	2:B:261:ARG:NH2	2.50	0.44
1:A:626:ASN:O	1:A:631:HIS:ND1	2.51	0.44
1:A:562:THR:O	1:A:576:GLN:NE2	2.51	0.44
1:A:62:ASP:O	1:A:64:ASN:N	2.51	0.44
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.51	0.43
3:C:161:LYS:O	3:C:170:TRP:CD1	2.72	0.43
2:B:338:GLY:CA	2:B:339:THR:CB	2.98	0.42
1:A:590:ARG:NH2	1:A:621:THR:OG1	2.52	0.42
1:A:1033:GLN:O	1:A:1036:ARG:NH1	2.53	0.41
3:C:73:GLN:N	3:C:131:HIS:O	2.53	0.41
1:A:663:SER:OG	2:B:827:ILE:O	2.38	0.41
4:D:32:GLU:OE1	7:G:41:LYS:NZ	2.54	0.40
1:A:1436:ILE:O	1:A:1437:GLY:C	2.59	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	1414/1732 (82%)	1224 (87%)	137 (10%)	53 (4%)	5 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1095/1224 (90%)	956 (87%)	101 (9%)	38 (4%)	6	50
3	C	264/318 (83%)	232 (88%)	28 (11%)	4 (2%)	15	69
4	D	174/221 (79%)	155 (89%)	10 (6%)	9 (5%)	3	35
5	E	212/215 (99%)	192 (91%)	17 (8%)	3 (1%)	16	70
6	F	82/155 (53%)	75 (92%)	7 (8%)	0	100	100
7	G	169/171 (99%)	152 (90%)	12 (7%)	5 (3%)	7	53
8	H	129/146 (88%)	101 (78%)	20 (16%)	8 (6%)	2	30
9	I	117/122 (96%)	94 (80%)	18 (15%)	5 (4%)	4	42
10	J	63/70 (90%)	53 (84%)	4 (6%)	6 (10%)	1	17
11	K	113/120 (94%)	108 (96%)	5 (4%)	0	100	100
12	L	44/70 (63%)	28 (64%)	14 (32%)	2 (4%)	4	40
All	All	3876/4564 (85%)	3370 (87%)	373 (10%)	133 (3%)	6	50

All (133) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	GLU
1	A	48	ALA
1	A	55	ASP
1	A	57	ARG
1	A	58	LEU
1	A	74	MET
1	A	76	GLU
1	A	195	ASP
1	A	257	ARG
1	A	286	HIS
1	A	318	SER
1	A	335	ARG
1	A	449	SER
1	A	775	ILE
1	A	1124	HIS
2	B	340	ALA
2	B	343	ILE
2	B	344	LYS
2	B	510	LYS
2	B	731	VAL
2	B	751	VAL
2	B	881	ASN

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Mol	Chain	Res	Type
2	B	1181	GLU
2	B	1223	ASP
3	C	161	LYS
4	D	18	VAL
4	D	119	ARG
4	D	199	ASN
8	H	81	PRO
9	I	9	ASP
10	J	6	ARG
1	A	70	CYS
1	A	72	GLU
1	A	178	GLY
1	A	189	ARG
1	A	311	GLN
1	A	628	GLY
1	A	1173	HIS
1	A	1206	ASP
1	A	1403	GLU
2	B	27	ALA
2	B	108	VAL
2	B	229	ALA
2	B	341	LEU
2	B	476	ARG
2	B	629	ASP
2	B	643	ASP
2	B	707	PRO
2	B	772	ALA
2	B	879	ARG
2	B	883	LEU
2	B	1046	PRO
2	B	1066	SER
2	B	1176	ASN
3	C	90	ASP
4	D	11	ARG
4	D	53	SER
5	E	45	LYS
5	E	104	ASN
7	G	154	VAL
8	H	17	PRO
8	H	60	ALA
8	H	128	ASN
9	I	95	THR

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Mol	Chain	Res	Type
10	J	17	LYS
10	J	62	ARG
10	J	64	ASN
12	L	56	LEU
12	L	59	ALA
1	A	332	LYS
1	A	830	LYS
1	A	1255	GLU
1	A	1314	SER
1	A	1378	GLN
1	A	1405	THR
2	B	28	GLU
2	B	67	SER
2	B	339	THR
2	B	526	GLU
2	B	711	GLU
2	B	869	SER
2	B	1157	ALA
4	D	15	LEU
7	G	63	PRO
8	H	84	ALA
9	I	3	THR
1	A	52	GLY
1	A	65	LEU
1	A	167	CYS
1	A	187	LYS
1	A	399	HIS
1	A	569	LYS
1	A	700	ASN
1	A	958	VAL
1	A	1122	PRO
1	A	1123	GLY
2	B	338	GLY
2	B	868	MET
2	B	1108	ARG
2	B	1155	SER
4	D	16	LYS
4	D	218	GLU
7	G	2	PHE
8	H	18	GLY
8	H	82	PRO
8	H	83	GLN

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Mol	Chain	Res	Type
9	I	89	GLN
1	A	336	ILE
1	A	385	ILE
1	A	418	SER
1	A	1437	GLY
2	B	648	HIS
2	B	886	LYS
3	C	214	ASN
4	D	191	ALA
5	E	3	GLN
10	J	2	ILE
1	A	310	GLY
1	A	780	VAL
3	C	38	ILE
7	G	20	PRO
9	I	88	SER
1	A	312	PRO
7	G	139	ILE
1	A	35	ILE
1	A	61	ILE
1	A	196	GLU
1	A	567	LYS
2	B	364	ILE
10	J	3	VAL
1	A	192	GLY
2	B	867	GLY
1	A	448	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	1240/1519 (82%)	1042 (84%)	198 (16%)	3	22
2	B	966/1061 (91%)	822 (85%)	144 (15%)	4	26
3	C	234/274 (85%)	206 (88%)	28 (12%)	7	37
4	D	160/200 (80%)	132 (82%)	28 (18%)	3	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	196/197 (100%)	179 (91%)	17 (9%)	15	57
6	F	74/137 (54%)	67 (90%)	7 (10%)	12	51
7	G	152/152 (100%)	128 (84%)	24 (16%)	4	23
8	H	117/128 (91%)	107 (92%)	10 (8%)	15	58
9	I	113/116 (97%)	103 (91%)	10 (9%)	14	57
10	J	60/65 (92%)	47 (78%)	13 (22%)	1	9
11	K	99/102 (97%)	87 (88%)	12 (12%)	7	36
12	L	40/57 (70%)	28 (70%)	12 (30%)	0	4
All	All	3451/4008 (86%)	2948 (85%)	503 (15%)	5	27

All (503) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	13	THR
1	A	15	LYS
1	A	34	LYS
1	A	37	PHE
1	A	41	MET
1	A	54	ASN
1	A	58	LEU
1	A	63	ARG
1	A	65	LEU
1	A	70	CYS
1	A	84	ILE
1	A	93	VAL
1	A	96	ILE
1	A	106	VAL
1	A	113	LEU
1	A	114	LEU
1	A	129	LYS
1	A	131	SER
1	A	146	MET
1	A	156	ASP
1	A	160	GLN
1	A	170	THR
1	A	182	VAL
1	A	196	GLU
1	A	199	LEU

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Mol	Chain	Res	Type
1	A	204	THR
1	A	208	LEU
1	A	213	HIS
1	A	219	PHE
1	A	220	THR
1	A	222	LEU
1	A	226	GLU
1	A	252	PHE
1	A	253	ASN
1	A	261	ASP
1	A	265	LYS
1	A	270	LEU
1	A	274	ILE
1	A	279	LEU
1	A	289	ILE
1	A	290	GLU
1	A	291	GLU
1	A	295	LEU
1	A	307	ASP
1	A	311	GLN
1	A	315	LEU
1	A	333	GLU
1	A	335	ARG
1	A	337	ARG
1	A	344	ARG
1	A	357	PRO
1	A	367	PRO
1	A	375	THR
1	A	381	THR
1	A	383	TYR
1	A	385	ILE
1	A	386	ASP
1	A	389	THR
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	436	ILE
1	A	438	ASP
1	A	441	PRO

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Mol	Chain	Res	Type
1	A	443	LEU
1	A	445	ASN
1	A	451	HIS
1	A	452	LYS
1	A	454	SER
1	A	459	ARG
1	A	469	ARG
1	A	470	LEU
1	A	472	LEU
1	A	475	THR
1	A	476	SER
1	A	479	ASN
1	A	481	ASP
1	A	489	LEU
1	A	500	GLU
1	A	505	CYS
1	A	516	SER
1	A	517	ASN
1	A	538	ASP
1	A	545	GLN
1	A	566	ILE
1	A	588	LEU
1	A	603	ASN
1	A	618	GLU
1	A	622	VAL
1	A	626	ASN
1	A	629	LEU
1	A	635	ARG
1	A	640	GLN
1	A	652	VAL
1	A	666	ILE
1	A	691	LEU
1	A	738	LYS
1	A	740	LEU
1	A	752	LYS
1	A	754	SER
1	A	755	PHE
1	A	756	ILE
1	A	768	GLN
1	A	769	SER
1	A	773	LYS
1	A	774	ARG

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Mol	Chain	Res	Type
1	A	782	ARG
1	A	788	SER
1	A	806	ARG
1	A	821	ARG
1	A	824	LEU
1	A	831	THR
1	A	834	THR
1	A	838	GLN
1	A	839	ARG
1	A	848	ILE
1	A	873	MET
1	A	878	ILE
1	A	885	THR
1	A	886	ILE
1	A	906	HIS
1	A	915	SER
1	A	917	SER
1	A	918	GLU
1	A	919	ILE
1	A	920	LEU
1	A	929	LEU
1	A	932	GLU
1	A	934	LYS
1	A	941	LYS
1	A	948	VAL
1	A	973	ILE
1	A	983	ILE
1	A	998	LEU
1	A	1001	ARG
1	A	1015	VAL
1	A	1029	ARG
1	A	1047	SER
1	A	1050	GLU
1	A	1052	GLN
1	A	1062	GLU
1	A	1067	LEU
1	A	1117	THR
1	A	1118	VAL
1	A	1124	HIS
1	A	1128	GLN
1	A	1134	ILE
1	A	1135	ARG

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Mol	Chain	Res	Type
1	A	1142	THR
1	A	1146	VAL
1	A	1171	GLN
1	A	1173	HIS
1	A	1174	PHE
1	A	1175	SER
1	A	1176	LEU
1	A	1195	LEU
1	A	1196	GLU
1	A	1218	GLN
1	A	1223	ASP
1	A	1242	VAL
1	A	1259	MET
1	A	1260	LEU
1	A	1263	ILE
1	A	1265	ASN
1	A	1274	ARG
1	A	1277	GLU
1	A	1288	ASP
1	A	1289	ARG
1	A	1291	VAL
1	A	1293	SER
1	A	1295	THR
1	A	1297	GLU
1	A	1307	GLU
1	A	1308	THR
1	A	1315	GLU
1	A	1317	MET
1	A	1327	ILE
1	A	1341	ILE
1	A	1366	ARG
1	A	1376	THR
1	A	1391	ARG
1	A	1393	ASN
1	A	1394	THR
1	A	1400	CYS
1	A	1403	GLU
1	A	1411	GLU
1	A	1426	GLU
1	A	1438	THR
1	A	1442	ASP
1	A	1444	MET

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Mol	Chain	Res	Type
1	A	1445	ILE
1	A	1451	VAL
1	A	1453	TYR
1	A	1454	MET
2	B	25	ILE
2	B	40	GLU
2	B	45	SER
2	B	46	GLN
2	B	63	ILE
2	B	66	ASP
2	B	102	VAL
2	B	134	LYS
2	B	169	ARG
2	B	178	ASN
2	B	217	ARG
2	B	218	SER
2	B	222	ILE
2	B	223	VAL
2	B	240	ILE
2	B	241	ARG
2	B	251	ILE
2	B	261	ARG
2	B	262	GLU
2	B	267	ARG
2	B	272	THR
2	B	277	LYS
2	B	278	GLN
2	B	279	ASP
2	B	294	ASP
2	B	298	LEU
2	B	304	ASP
2	B	305	VAL
2	B	324	ILE
2	B	325	GLN
2	B	334	ILE
2	B	337	ARG
2	B	341	LEU
2	B	343	ILE
2	B	344	LYS
2	B	348	ARG
2	B	350	GLN
2	B	351	TYR

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Mol	Chain	Res	Type
2	B	361	LEU
2	B	365	THR
2	B	367	LEU
2	B	370	PHE
2	B	371	GLU
2	B	393	LYS
2	B	396	ASP
2	B	398	ARG
2	B	408	LEU
2	B	412	LEU
2	B	415	GLN
2	B	416	LEU
2	B	423	LYS
2	B	425	THR
2	B	436	VAL
2	B	446	LEU
2	B	453	ILE
2	B	466	TRP
2	B	468	GLU
2	B	470	LYS
2	B	474	SER
2	B	485	ARG
2	B	495	LEU
2	B	502	ILE
2	B	513	GLN
2	B	547	VAL
2	B	552	MET
2	B	563	MET
2	B	570	VAL
2	B	598	GLU
2	B	604	ARG
2	B	608	ASP
2	B	614	SER
2	B	615	MET
2	B	616	ILE
2	B	620	ARG
2	B	624	LEU
2	B	628	THR
2	B	629	ASP
2	B	637	LEU
2	B	682	SER
2	B	690	VAL

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Mol	Chain	Res	Type
2	B	708	GLU
2	B	709	ASP
2	B	734	HIS
2	B	737	THR
2	B	742	GLU
2	B	766	ARG
2	B	790	ASP
2	B	795	ILE
2	B	835	GLN
2	B	841	MET
2	B	844	SER
2	B	853	SER
2	B	878	GLN
2	B	882	THR
2	B	889	THR
2	B	895	ASP
2	B	906	SER
2	B	935	ARG
2	B	942	ARG
2	B	946	ASN
2	B	948	ILE
2	B	956	THR
2	B	964	VAL
2	B	965	LYS
2	B	969	ARG
2	B	970	THR
2	B	975	GLN
2	B	976	ILE
2	B	986	GLN
2	B	992	ILE
2	B	996	ARG
2	B	997	GLU
2	B	999	MET
2	B	1007	VAL
2	B	1010	LEU
2	B	1020	ARG
2	B	1031	LEU
2	B	1049	ASP
2	B	1065	GLN
2	B	1072	MET
2	B	1080	LYS
2	B	1084	GLN

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Mol	Chain	Res	Type
2	B	1106	ARG
2	B	1112	GLN
2	B	1120	GLU
2	B	1122	ARG
2	B	1123	SER
2	B	1129	ARG
2	B	1133	MET
2	B	1145	SER
2	B	1148	LYS
2	B	1150	ARG
2	B	1151	LEU
2	B	1160	VAL
2	B	1168	LEU
2	B	1169	MET
2	B	1175	LEU
2	B	1179	GLN
2	B	1183	LYS
2	B	1188	LYS
2	B	1202	LEU
2	B	1210	MET
2	B	1220	ARG
2	B	1222	ARG
3	C	4	GLU
3	C	7	GLN
3	C	8	VAL
3	C	22	LEU
3	C	25	VAL
3	C	26	ASP
3	C	44	LEU
3	C	75	MET
3	C	81	GLU
3	C	85	ASP
3	C	106	GLU
3	C	119	VAL
3	C	127	ARG
3	C	129	ILE
3	C	147	LEU
3	C	148	ARG
3	C	156	THR
3	C	158	VAL
3	C	211	ASP
3	C	215	GLU

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Mol	Chain	Res	Type
3	C	238	ILE
3	C	240	VAL
3	C	254	LYS
3	C	259	LEU
3	C	260	LEU
3	C	264	GLN
3	C	265	MET
3	C	268	ASP
4	D	5	THR
4	D	7	THR
4	D	8	PHE
4	D	9	GLN
4	D	11	ARG
4	D	12	ARG
4	D	17	LYS
4	D	18	VAL
4	D	35	LEU
4	D	41	GLN
4	D	47	LEU
4	D	52	LEU
4	D	67	ARG
4	D	75	LYS
4	D	119	ARG
4	D	123	LEU
4	D	134	THR
4	D	137	ASN
4	D	139	LYS
4	D	156	ASP
4	D	158	GLU
4	D	177	VAL
4	D	187	THR
4	D	197	SER
4	D	206	GLU
4	D	213	GLU
4	D	214	LEU
4	D	219	THR
5	E	14	ARG
5	E	31	THR
5	E	45	LYS
5	E	72	PHE
5	E	83	CYS
5	E	84	ASP

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Mol	Chain	Res	Type
5	E	90	VAL
5	E	95	THR
5	E	121	MET
5	E	140	LEU
5	E	166	LYS
5	E	177	ARG
5	E	191	LYS
5	E	192	ARG
5	E	204	THR
5	E	207	ARG
5	E	214	CYS
6	F	78	GLN
6	F	79	ARG
6	F	82	THR
6	F	87	LYS
6	F	92	ARG
6	F	103	MET
6	F	155	LEU
7	G	2	PHE
7	G	11	ILE
7	G	13	LEU
7	G	22	MET
7	G	26	LEU
7	G	29	LYS
7	G	58	ARG
7	G	64	THR
7	G	90	THR
7	G	95	SER
7	G	96	GLN
7	G	100	GLU
7	G	112	LYS
7	G	114	LEU
7	G	118	ASP
7	G	134	GLU
7	G	138	THR
7	G	141	SER
7	G	143	ILE
7	G	145	VAL
7	G	151	ILE
7	G	152	SER
7	G	162	SER
7	G	171	ILE

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Mol	Chain	Res	Type
8	H	3	ASN
8	H	14	GLU
8	H	26	ILE
8	H	76	THR
8	H	86	ASP
8	H	91	ASP
8	H	103	LYS
8	H	107	VAL
8	H	110	ASP
8	H	130	ARG
9	I	7	CYS
9	I	8	ARG
9	I	17	ARG
9	I	30	ARG
9	I	31	THR
9	I	50	THR
9	I	55	THR
9	I	62	ILE
9	I	83	ASN
9	I	94	ASP
10	J	2	ILE
10	J	12	LYS
10	J	13	VAL
10	J	14	VAL
10	J	16	ASP
10	J	22	LEU
10	J	25	LEU
10	J	28	ASP
10	J	31	ASP
10	J	34	THR
10	J	42	LYS
10	J	48	ARG
10	J	52	THR
11	K	6	ARG
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	37	LYS
11	K	47	ARG

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Mol	Chain	Res	Type
11	K	51	LEU
11	K	91	CYS
11	K	101	LEU
12	L	27	LEU
12	L	34	CYS
12	L	38	LEU
12	L	40	LEU
12	L	43	THR
12	L	47	ARG
12	L	50	ASP
12	L	55	ILE
12	L	58	LYS
12	L	61	THR
12	L	65	VAL
12	L	68	GLU

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	1/2 (50%)	1 (100%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	10	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	$\# Z > 2$
15	BRU	T	22	15	19,21,22	1.92	5 (26%)	22,30,33	4.97	7 (31%)

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	-	0/5/21/22	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	22	BRU	C4-C5	4.96	1.48	1.39
15	T	22	BRU	C6-N1	4.04	1.44	1.34
15	T	22	BRU	BR-C5	3.61	1.99	1.90
15	T	22	BRU	P-OP1	2.25	1.49	1.46
15	T	22	BRU	C6-C5	2.12	1.44	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	22	BRU	C6-N1-C2	-19.26	116.94	122.41
15	T	22	BRU	O4'-C1'-N1	7.98	122.67	107.68
15	T	22	BRU	N3-C2-N1	7.00	121.82	115.97
15	T	22	BRU	C5-C6-N1	5.73	123.45	119.67
15	T	22	BRU	C2'-C1'-N1	3.39	122.89	114.08
15	T	22	BRU	C6-N1-C1'	2.30	125.04	119.33
15	T	22	BRU	BR-C5-C6	2.24	122.41	117.98

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 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1422/1732 (82%)	-0.01	4 (0%) 91 76	57, 107, 167, 228	0
2	B	1115/1224 (91%)	0.08	5 (0%) 90 71	62, 118, 181, 206	0
3	C	266/318 (83%)	-0.04	0 100 100	78, 111, 152, 186	0
4	D	178/221 (80%)	-0.02	1 (0%) 86 59	78, 118, 174, 194	0
5	E	214/215 (99%)	-0.01	0 100 100	81, 139, 190, 203	0
6	F	84/155 (54%)	-0.17	0 100 100	58, 83, 118, 131	0
7	G	171/171 (100%)	0.02	0 100 100	81, 102, 144, 164	0
8	H	133/146 (91%)	0.36	1 (0%) 83 53	123, 155, 187, 211	0
9	I	119/122 (97%)	0.12	3 (2%) 54 25	111, 149, 190, 205	0
10	J	65/70 (92%)	-0.07	0 100 100	88, 107, 144, 156	0
11	K	115/120 (95%)	-0.07	1 (0%) 81 51	72, 105, 141, 157	0
12	L	46/70 (65%)	0.08	1 (2%) 59 28	91, 138, 166, 184	0
13	N	9/14 (64%)	1.14	1 (11%) 6 4	216, 225, 263, 270	0
14	P	2/2 (100%)	0.43	0 100 100	185, 185, 185, 193	0
15	T	15/27 (55%)	0.78	2 (13%) 4 3	141, 173, 267, 268	0
All	All	3954/4607 (85%)	0.03	19 (0%) 88 64	57, 114, 180, 270	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	883	LEU	4.1
11	K	115	ALA	3.6
15	T	8	DC	3.2
1	A	194	ALA	3.1
9	I	120	GLN	2.8
2	B	340	ALA	2.7
13	N	9	DT	2.7

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Mol	Chain	Res	Type	RSRZ
15	T	9	DA	2.6
2	B	339	THR	2.6
12	L	27	LEU	2.6
1	A	257	ARG	2.6
8	H	146	ARG	2.2
1	A	1455	PRO	2.2
2	B	708	GLU	2.2
2	B	733	HIS	2.2
9	I	119	THR	2.1
4	D	13	ARG	2.1
1	A	195	ASP	2.0
9	I	117	LYS	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
15	BRU	T	22	20/21	0.20	-0.20	174,184,191,192	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
17	MG	A	2458	1/1	0.24	1.24	287,287,287,287	0
16	ZN	B	2225	1/1	0.22	1.06	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
16	ZN	I	1121	1/1	0.12	-0.22	123,123,123,123	0
16	ZN	C	1269	1/1	0.12	-0.84	84,84,84,84	0
16	ZN	A	2457	1/1	0.15	-0.84	72,72,72,72	0
16	ZN	J	1066	1/1	0.24	-0.97	93,93,93,93	0
16	ZN	L	1071	1/1	0.09	-1.41	144,144,144,144	0
16	ZN	A	2456	1/1	0.08	-1.87	137,137,137,137	0
16	ZN	I	1122	1/1	0.04	-2.08	184,184,184,184	0

6.5 Other polymers ⓘ

There are no such residues in this entry.