



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:03 AM GMT

PDB ID : 4A3D
Title : RNA POLYMERASE II INITIAL TRANSCRIBING COMPLEX WITH A
6NT DNA-RNA HYBRID
Authors : Cheung, A.C.M.; Sainsbury, S.; Cramer, P.
Deposited on : 2011-09-30
Resolution : 3.40 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>

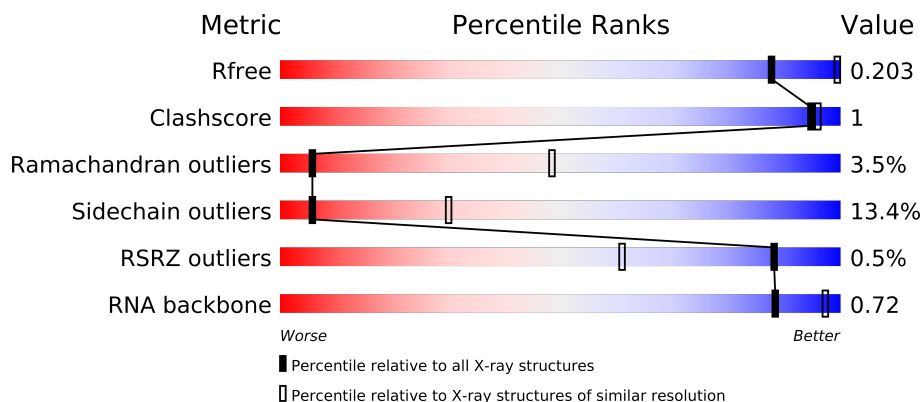
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : 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 3.40 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}	66092	1017 (3.52-3.28)
Clashscore	79885	1214 (3.50-3.30)
Ramachandran outliers	78287	1177 (3.50-3.30)
Sidechain outliers	78261	1177 (3.50-3.30)
RSRZ outliers	66119	1017 (3.52-3.28)
RNA backbone	1838	1002 (4.02-2.76)

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	6	
15	T	26	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 31937 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(*TP*AP*AP*GP*TP*AP*CP*TP*TP*GP*AP*GP*CP*TP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	10	Total	C	N	O	P	0	0	0
			207	99	39	59	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	6	Total	C	N	O	P	0	0	0
			130	58	26	40	6			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
15	T	20	Total	Br	C	N	O	P	0	0	0
			404	1	194	63	126	20			

- 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).

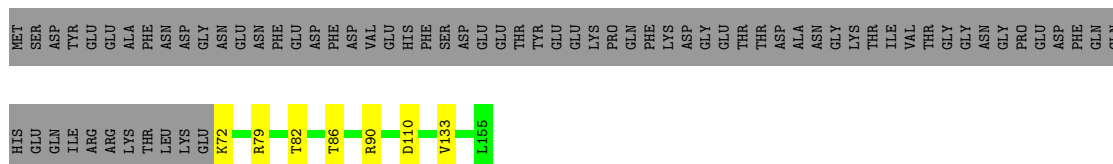
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Mg	0	0
			1	1		

Chain E: 



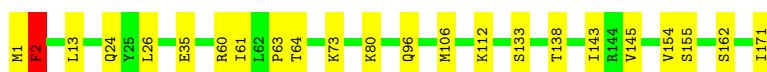
- Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2

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: 



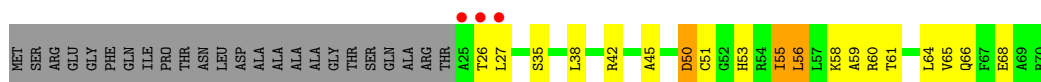
- Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11

Chain K: 



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

Chain L: 



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

Chain N:



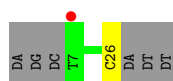
- Molecule 14: TRANSCRIPT RNA 5'-R(*CP*CP*AP*GP*GP*AP)-3'

Chain P:



- Molecule 15: TEMPLATE DNA 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*TP*TP*TP*CP*CP*TP*BRUP*GP*GP*TP*CP*AP*TP*TP)-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	221.91Å 391.36Å 283.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.96 – 3.40 49.96 – 3.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.96-3.40) 100.0 (49.96-3.40)	Depositor EDS
R_{merge}	0.93	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 3.40Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.161 , 0.186 0.180 , 0.203	Depositor DCC
R_{free} test set	3337 reflections (1.98%)	DCC
Wilson B-factor (Å ²)	95.8	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 78.7	EDS
Estimated twinning fraction	0.034 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.037 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 168581 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	31937	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% 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	10/15383 (0.1%)
2	B	0.51	0/9029	0.79	4/12171 (0.0%)
3	C	0.49	0/2133	0.78	2/2891 (0.1%)
4	D	0.51	0/1444	0.83	2/1935 (0.1%)
5	E	0.48	0/1788	0.71	0/2406
6	F	0.62	0/691	0.81	0/933
7	G	0.52	0/1368	0.81	0/1844
8	H	0.50	0/1086	0.80	0/1470
9	I	0.47	0/989	0.78	0/1331
10	J	0.54	0/541	0.88	1/727 (0.1%)
11	K	0.47	0/938	0.71	0/1267
12	L	0.54	0/365	0.95	0/485
13	N	1.07	0/232	1.06	0/356
14	P	1.21	0/145	0.79	0/224
15	T	1.26	1/426 (0.2%)	1.08	0/652
All	All	0.55	1/32549 (0.0%)	0.82	19/44075 (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)
15	T	26	DC	C1'-N1	5.63	1.56	1.49

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	399	HIS	N-CA-CB	7.25	123.66	110.60
1	A	34	LYS	C-N-CA	7.21	139.73	121.70
4	D	25	ALA	C-N-CA	6.11	136.98	121.70
1	A	56	PRO	C-N-CA	6.01	136.73	121.70
1	A	35	ILE	N-CA-CB	5.95	124.49	110.80
2	B	340	ALA	C-N-CA	5.70	135.94	121.70
1	A	194	ALA	C-N-CA	5.65	135.83	121.70
1	A	311	GLN	N-CA-C	5.56	126.01	111.00
4	D	26	THR	N-CA-C	-5.52	96.11	111.00
1	A	54	ASN	C-N-CA	5.44	135.31	121.70
3	C	39	ALA	N-CA-C	5.44	125.68	111.00
2	B	628	THR	C-N-CA	5.43	135.29	121.70
3	C	89	GLU	N-CA-C	-5.29	96.73	111.00
1	A	53	LEU	N-CA-CB	5.27	120.94	110.40
1	A	310	GLY	C-N-CA	5.17	134.63	121.70
2	B	1181	GLU	N-CA-C	5.16	124.92	111.00
1	A	1403	GLU	N-CA-C	5.11	124.81	111.00
10	J	5	VAL	N-CA-C	-5.03	97.43	111.00
2	B	1156	ASP	N-CA-C	5.01	124.52	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	11174	0	0	21	0
2	B	8859	0	0	18	0
3	C	2095	0	0	5	0
4	D	1434	0	0	3	0
5	E	1752	0	0	0	0
6	F	679	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	1340	0	0	5	0
8	H	1068	0	0	1	0
9	I	971	0	0	1	0
10	J	532	0	0	1	0
11	K	920	0	0	1	0
12	L	363	0	0	1	0
13	N	207	0	0	0	0
14	P	130	0	0	0	0
15	T	404	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	31937	0	0	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	1.83	1.53
3:C:66:ARG:NH2	10:J:3:VAL:O	2.23	0.72
7:G:1:MET:SD	7:G:2:PHE:N	2.63	0.70
7:G:1:MET:CE	7:G:80:LYS:O	2.45	0.65
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.34	0.60
1:A:590:ARG:NH2	1:A:621:THR:OG1	2.36	0.57
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.39	0.56
1:A:53:LEU:CD2	1:A:54:ASN:N	2.72	0.53
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.42	0.53
2:B:1166:CYS:O	2:B:1168:LEU:N	2.42	0.53
2:B:530:GLY:O	2:B:532:ALA:N	2.44	0.51
7:G:1:MET:CG	7:G:2:PHE:N	2.76	0.49
3:C:165:LYS:O	11:K:6:ARG:NH1	2.46	0.49
2:B:933:SER:O	2:B:935:ARG:N	2.45	0.48
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.46	0.48
1:A:448:PRO:O	1:A:449:SER:CB	2.63	0.47
1:A:399:HIS:O	1:A:401:GLY:N	2.48	0.45
2:B:296:GLU:O	2:B:300:HIS:CD2	2.70	0.45
2:B:1033:LYS:NZ	2:B:1070:GLU:OE1	2.50	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:265:LYS:NZ	1:A:299:HIS:ND1	2.64	0.45
1:A:836:TYR:OH	1:A:1403:GLU:OE2	2.34	0.45
2:B:1167:GLY:O	2:B:1216:LEU:N	2.51	0.44
1:A:1436:ILE:O	1:A:1437:GLY:C	2.56	0.43
1:A:481:ASP:OD1	1:A:485:ASP:OD1	2.37	0.42
4:D:176:GLU:OE2	4:D:201:LYS:NZ	2.52	0.42
3:C:184:ASN:ND2	3:C:189:THR:O	2.52	0.42
8:H:82:PRO:O	8:H:84:ALA:N	2.52	0.42
1:A:562:THR:O	1:A:576:GLN:NE2	2.53	0.42
1:A:497:THR:CG2	2:B:1146:PHE:CD1	3.02	0.42
4:D:66:ARG:NH2	7:G:35:GLU:OE2	2.53	0.42
1:A:469:ARG:NH2	2:B:991:GLY:O	2.52	0.42
2:B:857:ARG:NH1	2:B:945:GLU:OE2	2.52	0.42
1:A:632:VAL:O	1:A:636:GLU:N	2.52	0.42
2:B:635:ARG:NH1	2:B:742:GLU:OE2	2.52	0.42
1:A:867:ILE:CD1	1:A:867:ILE:CB	2.87	0.41
2:B:279:ASP:OD1	2:B:279:ASP:N	2.53	0.41
1:A:626:ASN:O	1:A:631:HIS:ND1	2.53	0.41
1:A:311:GLN:O	1:A:312:PRO:C	2.59	0.41
1:A:7:SER:OG	2:B:1161:HIS:NE2	2.55	0.40
4:D:40:HIS:ND1	7:G:73:LYS:NZ	2.69	0.40
1:A:433:GLU:OE1	2:B:1108:ARG:NH2	2.54	0.40
9:I:8:ARG:O	9:I:9:ASP:CB	2.69	0.40
2:B:904:ARG:NH1	12:L:66:GLN:O	2.55	0.40
1:A:1402:PHE:CE1	1:A:1403:GLU:CG	3.04	0.40
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.55	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%)	1236 (87%)	126 (9%)	52 (4%)	5	46
2	B	1095/1224 (90%)	968 (88%)	85 (8%)	42 (4%)	5	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	264/318 (83%)	242 (92%)	20 (8%)	2 (1%)	27	81
4	D	174/221 (79%)	148 (85%)	17 (10%)	9 (5%)	3	32
5	E	212/215 (99%)	195 (92%)	13 (6%)	4 (2%)	12	64
6	F	82/155 (53%)	75 (92%)	7 (8%)	0	100	100
7	G	169/171 (99%)	158 (94%)	8 (5%)	3 (2%)	13	65
8	H	129/146 (88%)	106 (82%)	14 (11%)	9 (7%)	2	23
9	I	117/122 (96%)	98 (84%)	16 (14%)	3 (3%)	8	56
10	J	63/70 (90%)	51 (81%)	9 (14%)	3 (5%)	4	36
11	K	113/120 (94%)	109 (96%)	4 (4%)	0	100	100
12	L	44/70 (63%)	27 (61%)	9 (20%)	8 (18%)	0	3
All	All	3876/4564 (85%)	3413 (88%)	328 (8%)	135 (4%)	6	48

All (135) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ARG
1	A	58	LEU
1	A	76	GLU
1	A	189	ARG
1	A	195	ASP
1	A	257	ARG
1	A	318	SER
1	A	399	HIS
1	A	449	SER
1	A	628	GLY
1	A	1377	THR
1	A	1403	GLU
1	A	1405	THR
2	B	108	VAL
2	B	229	ALA
2	B	307	ASP
2	B	344	LYS
2	B	473	MET
2	B	531	GLN
2	B	772	ALA
2	B	867	GLY
2	B	943	SER
2	B	1046	PRO

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Mol	Chain	Res	Type
2	B	1181	GLU
4	D	18	VAL
4	D	53	SER
4	D	199	ASN
9	I	9	ASP
9	I	95	THR
12	L	50	ASP
12	L	53	HIS
1	A	47	ARG
1	A	54	ASN
1	A	167	CYS
1	A	178	GLY
1	A	193	ASP
1	A	224	PHE
1	A	286	HIS
1	A	332	LYS
1	A	672	ASP
1	A	1175	SER
1	A	1281	ARG
2	B	262	GLU
2	B	282	ILE
2	B	339	THR
2	B	341	LEU
2	B	466	TRP
2	B	707	PRO
2	B	731	VAL
2	B	792	MET
2	B	879	ARG
2	B	1175	LEU
2	B	1176	ASN
4	D	16	LYS
4	D	52	LEU
4	D	169	SER
5	E	36	GLU
7	G	2	PHE
8	H	17	PRO
8	H	81	PRO
8	H	82	PRO
8	H	83	GLN
8	H	90	ALA
10	J	6	ARG
12	L	45	ALA

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Mol	Chain	Res	Type
12	L	56	LEU
1	A	335	ARG
1	A	975	HIS
1	A	1173	HIS
2	B	58	THR
2	B	340	ALA
2	B	343	ILE
2	B	711	GLU
2	B	1156	ASP
2	B	1157	ALA
2	B	1167	GLY
4	D	22	GLU
5	E	45	LYS
5	E	48	ASP
7	G	154	VAL
8	H	18	GLY
12	L	59	ALA
1	A	42	ASP
1	A	52	GLY
1	A	74	MET
1	A	465	TYR
1	A	569	LYS
1	A	846	GLU
1	A	958	VAL
1	A	1255	GLU
1	A	1437	GLY
1	A	1438	THR
2	B	648	HIS
2	B	883	LEU
2	B	942	ARG
2	B	1108	ARG
2	B	1155	SER
3	C	88	CYS
9	I	91	ARG
10	J	29	GLU
12	L	26	THR
12	L	55	ILE
12	L	64	LEU
1	A	156	ASP
1	A	311	GLN
1	A	336	ILE
1	A	567	LYS

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Mol	Chain	Res	Type
1	A	1171	GLN
1	A	1366	ARG
2	B	251	ILE
2	B	469	GLN
2	B	880	THR
2	B	907	GLY
2	B	1223	ASP
4	D	21	GLU
8	H	60	ALA
8	H	128	ASN
10	J	2	ILE
1	A	35	ILE
1	A	55	ASP
1	A	155	GLU
1	A	885	THR
3	C	214	ASN
4	D	15	LEU
1	A	196	GLU
1	A	1388	GLY
5	E	90	VAL
7	G	63	PRO
2	B	364	ILE
1	A	192	GLY
1	A	312	PRO
2	B	1121	GLY
1	A	448	PRO
2	B	1214	PRO
8	H	59	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	1240/1519 (82%)	1062 (86%)	178 (14%)	5	26
2	B	966/1061 (91%)	842 (87%)	124 (13%)	6	32
3	C	234/274 (85%)	206 (88%)	28 (12%)	7	35
4	D	160/200 (80%)	129 (81%)	31 (19%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	196/197 (100%)	175 (89%)	21 (11%)	10	43
6	F	74/137 (54%)	67 (90%)	7 (10%)	12	50
7	G	152/152 (100%)	135 (89%)	17 (11%)	9	39
8	H	117/128 (91%)	103 (88%)	14 (12%)	7	35
9	I	113/116 (97%)	106 (94%)	7 (6%)	26	72
10	J	60/65 (92%)	49 (82%)	11 (18%)	2	13
11	K	99/102 (97%)	87 (88%)	12 (12%)	7	35
12	L	40/57 (70%)	27 (68%)	13 (32%)	0	2
All	All	3451/4008 (86%)	2988 (87%)	463 (13%)	6	30

All (463) 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	28	ARG
1	A	34	LYS
1	A	41	MET
1	A	45	GLN
1	A	47	ARG
1	A	50	ILE
1	A	53	LEU
1	A	62	ASP
1	A	63	ARG
1	A	67	CYS
1	A	93	VAL
1	A	106	VAL
1	A	131	SER
1	A	134	ARG
1	A	147	VAL
1	A	157	ASP
1	A	173	THR
1	A	174	ILE
1	A	175	ARG
1	A	176	LYS
1	A	199	LEU
1	A	204	THR
1	A	208	LEU

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Mol	Chain	Res	Type
1	A	219	PHE
1	A	220	THR
1	A	222	LEU
1	A	237	THR
1	A	252	PHE
1	A	255	SER
1	A	261	ASP
1	A	270	LEU
1	A	279	LEU
1	A	289	ILE
1	A	307	ASP
1	A	313	GLN
1	A	315	LEU
1	A	322	VAL
1	A	330	LYS
1	A	335	ARG
1	A	337	ARG
1	A	343	LYS
1	A	344	ARG
1	A	353	ILE
1	A	375	THR
1	A	381	THR
1	A	385	ILE
1	A	386	ASP
1	A	393	ARG
1	A	398	GLU
1	A	408	ASP
1	A	411	ASP
1	A	412	ARG
1	A	424	ILE
1	A	425	GLN
1	A	434	ARG
1	A	436	ILE
1	A	438	ASP
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	451	HIS
1	A	454	SER
1	A	469	ARG
1	A	470	LEU
1	A	472	LEU

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Mol	Chain	Res	Type
1	A	474	VAL
1	A	475	THR
1	A	476	SER
1	A	489	LEU
1	A	498	ARG
1	A	500	GLU
1	A	505	CYS
1	A	513	SER
1	A	532	ARG
1	A	544	ASP
1	A	566	ILE
1	A	571	LEU
1	A	582	ILE
1	A	593	GLU
1	A	596	THR
1	A	602	ASP
1	A	603	ASN
1	A	618	GLU
1	A	629	LEU
1	A	634	THR
1	A	664	THR
1	A	666	ILE
1	A	672	ASP
1	A	691	LEU
1	A	702	LEU
1	A	738	LYS
1	A	768	GLN
1	A	769	SER
1	A	773	LYS
1	A	782	ARG
1	A	788	SER
1	A	795	GLU
1	A	797	LYS
1	A	801	GLU
1	A	811	GLN
1	A	821	ARG
1	A	826	ASP
1	A	827	THR
1	A	831	THR
1	A	834	THR
1	A	839	ARG
1	A	849	MET

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Mol	Chain	Res	Type
1	A	867	ILE
1	A	886	ILE
1	A	896	ARG
1	A	919	ILE
1	A	920	LEU
1	A	948	VAL
1	A	949	ASP
1	A	964	ILE
1	A	973	ILE
1	A	976	THR
1	A	998	LEU
1	A	1009	ASN
1	A	1015	VAL
1	A	1029	ARG
1	A	1030	ARG
1	A	1047	SER
1	A	1058	VAL
1	A	1062	GLU
1	A	1067	LEU
1	A	1078	GLN
1	A	1116	LEU
1	A	1118	VAL
1	A	1120	LEU
1	A	1121	GLU
1	A	1124	HIS
1	A	1135	ARG
1	A	1142	THR
1	A	1173	HIS
1	A	1176	LEU
1	A	1195	LEU
1	A	1208	THR
1	A	1218	GLN
1	A	1223	ASP
1	A	1237	ILE
1	A	1242	VAL
1	A	1255	GLU
1	A	1257	ASP
1	A	1260	LEU
1	A	1264	GLU
1	A	1265	ASN
1	A	1273	LEU
1	A	1274	ARG

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Mol	Chain	Res	Type
1	A	1291	VAL
1	A	1295	THR
1	A	1297	GLU
1	A	1309	ASP
1	A	1315	GLU
1	A	1317	MET
1	A	1325	THR
1	A	1327	ILE
1	A	1336	MET
1	A	1341	ILE
1	A	1355	VAL
1	A	1366	ARG
1	A	1376	THR
1	A	1382	THR
1	A	1386	ARG
1	A	1391	ARG
1	A	1393	ASN
1	A	1400	CYS
1	A	1403	GLU
1	A	1426	GLU
1	A	1438	THR
1	A	1442	ASP
1	A	1444	MET
1	A	1445	ILE
1	A	1453	TYR
1	A	1454	MET
2	B	25	ILE
2	B	46	GLN
2	B	63	ILE
2	B	118	ARG
2	B	134	LYS
2	B	169	ARG
2	B	183	GLU
2	B	185	THR
2	B	217	ARG
2	B	218	SER
2	B	240	ILE
2	B	251	ILE
2	B	261	ARG
2	B	272	THR
2	B	278	GLN
2	B	279	ASP

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Mol	Chain	Res	Type
2	B	287	ARG
2	B	294	ASP
2	B	313	MET
2	B	337	ARG
2	B	341	LEU
2	B	343	ILE
2	B	344	LYS
2	B	348	ARG
2	B	357	GLN
2	B	365	THR
2	B	393	LYS
2	B	412	LEU
2	B	416	LEU
2	B	423	LYS
2	B	429	PHE
2	B	436	VAL
2	B	446	LEU
2	B	448	ILE
2	B	470	LYS
2	B	476	ARG
2	B	482	VAL
2	B	485	ARG
2	B	487	THR
2	B	529	GLU
2	B	531	GLN
2	B	547	VAL
2	B	552	MET
2	B	563	MET
2	B	570	VAL
2	B	574	SER
2	B	595	ARG
2	B	596	LEU
2	B	601	ARG
2	B	603	LEU
2	B	609	ILE
2	B	612	GLU
2	B	615	MET
2	B	616	ILE
2	B	620	ARG
2	B	646	LEU
2	B	651	LEU
2	B	653	VAL

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Mol	Chain	Res	Type
2	B	658	ILE
2	B	680	THR
2	B	696	GLU
2	B	708	GLU
2	B	734	HIS
2	B	737	THR
2	B	766	ARG
2	B	771	SER
2	B	776	GLN
2	B	786	ASN
2	B	790	ASP
2	B	791	THR
2	B	801	LYS
2	B	839	MET
2	B	841	MET
2	B	844	SER
2	B	868	MET
2	B	871	THR
2	B	878	GLN
2	B	879	ARG
2	B	882	THR
2	B	889	THR
2	B	904	ARG
2	B	906	SER
2	B	909	ASP
2	B	934	LYS
2	B	939	THR
2	B	942	ARG
2	B	944	THR
2	B	951	GLN
2	B	953	LEU
2	B	964	VAL
2	B	970	THR
2	B	973	ILE
2	B	975	GLN
2	B	986	GLN
2	B	997	GLU
2	B	999	MET
2	B	1007	VAL
2	B	1028	GLU
2	B	1045	SER
2	B	1060	ARG

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Mol	Chain	Res	Type
2	B	1065	GLN
2	B	1072	MET
2	B	1084	GLN
2	B	1094	ARG
2	B	1106	ARG
2	B	1123	SER
2	B	1129	ARG
2	B	1138	MET
2	B	1145	SER
2	B	1147	LEU
2	B	1151	LEU
2	B	1156	ASP
2	B	1159	ARG
2	B	1160	VAL
2	B	1175	LEU
2	B	1179	GLN
2	B	1183	LYS
2	B	1188	LYS
2	B	1193	GLN
2	B	1201	LYS
2	B	1202	LEU
2	B	1210	MET
2	B	1220	ARG
2	B	1223	ASP
3	C	3	GLU
3	C	12	GLU
3	C	25	VAL
3	C	26	ASP
3	C	52	GLU
3	C	53	THR
3	C	55	THR
3	C	56	THR
3	C	81	GLU
3	C	84	ARG
3	C	100	THR
3	C	101	LEU
3	C	119	VAL
3	C	121	VAL
3	C	124	LEU
3	C	125	MET
3	C	127	ARG
3	C	129	ILE

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Mol	Chain	Res	Type
3	C	133	ILE
3	C	147	LEU
3	C	148	ARG
3	C	215	GLU
3	C	224	GLN
3	C	238	ILE
3	C	240	VAL
3	C	259	LEU
3	C	265	MET
3	C	268	ASP
4	D	5	THR
4	D	7	THR
4	D	9	GLN
4	D	10	THR
4	D	12	ARG
4	D	13	ARG
4	D	17	LYS
4	D	18	VAL
4	D	27	LEU
4	D	32	GLU
4	D	34	GLN
4	D	35	LEU
4	D	40	HIS
4	D	47	LEU
4	D	52	LEU
4	D	53	SER
4	D	65	GLU
4	D	118	THR
4	D	126	ILE
4	D	134	THR
4	D	137	ASN
4	D	139	LYS
4	D	153	ARG
4	D	156	ASP
4	D	177	VAL
4	D	187	THR
4	D	197	SER
4	D	201	LYS
4	D	215	SER
4	D	219	THR
4	D	221	TYR
5	E	3	GLN

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Mol	Chain	Res	Type
5	E	31	THR
5	E	37	LEU
5	E	45	LYS
5	E	57	MET
5	E	67	GLU
5	E	84	ASP
5	E	92	THR
5	E	104	ASN
5	E	131	THR
5	E	140	LEU
5	E	146	HIS
5	E	166	LYS
5	E	173	SER
5	E	177	ARG
5	E	178	ILE
5	E	191	LYS
5	E	192	ARG
5	E	196	VAL
5	E	202	SER
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	133	VAL
7	G	2	PHE
7	G	13	LEU
7	G	24	GLN
7	G	26	LEU
7	G	60	ARG
7	G	61	ILE
7	G	64	THR
7	G	96	GLN
7	G	106	MET
7	G	112	LYS
7	G	133	SER
7	G	138	THR
7	G	143	ILE
7	G	145	VAL
7	G	155	SER

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Mol	Chain	Res	Type
7	G	162	SER
7	G	171	ILE
8	H	14	GLU
8	H	26	ILE
8	H	31	THR
8	H	34	ASP
8	H	76	THR
8	H	77	ARG
8	H	83	GLN
8	H	89	LEU
8	H	91	ASP
8	H	92	ASP
8	H	103	LYS
8	H	130	ARG
8	H	135	LEU
8	H	138	GLU
9	I	8	ARG
9	I	31	THR
9	I	35	VAL
9	I	74	GLU
9	I	94	ASP
9	I	106	CYS
9	I	111	THR
10	J	1	MET
10	J	2	ILE
10	J	3	VAL
10	J	7	CYS
10	J	12	LYS
10	J	13	VAL
10	J	22	LEU
10	J	29	GLU
10	J	42	LYS
10	J	48	ARG
10	J	52	THR
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	42	LEU
11	K	47	ARG

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Mol	Chain	Res	Type
11	K	51	LEU
11	K	70	ARG
11	K	101	LEU
11	K	107	THR
12	L	27	LEU
12	L	35	SER
12	L	38	LEU
12	L	42	ARG
12	L	50	ASP
12	L	51	CYS
12	L	55	ILE
12	L	56	LEU
12	L	58	LYS
12	L	60	ARG
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	5/6 (83%)	1 (20%)	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	0.99	1 (5%)	22,30,33	2.42	4 (18%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	22	BRU	P-OP1	2.31	1.49	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	22	BRU	C6-N1-C2	-9.58	119.69	122.41
15	T	22	BRU	O4'-C1'-N1	4.08	115.35	107.68
15	T	22	BRU	N3-C2-N1	3.00	118.48	115.97
15	T	22	BRU	C2'-C1'-N1	-2.25	108.25	114.08

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%)	-0.07	6 (0%) 90 68	52, 96, 155, 215	0
2	B	1115/1224 (91%)	-0.01	6 (0%) 88 61	56, 111, 174, 201	0
3	C	266/318 (83%)	-0.14	0 100 100	68, 97, 135, 165	0
4	D	178/221 (80%)	-0.04	0 100 100	77, 110, 162, 182	0
5	E	214/215 (99%)	-0.02	0 100 100	72, 129, 170, 191	0
6	F	84/155 (54%)	-0.18	0 100 100	55, 76, 106, 122	0
7	G	171/171 (100%)	-0.03	0 100 100	65, 96, 135, 153	0
8	H	133/146 (91%)	0.40	0 100 100	110, 136, 175, 195	0
9	I	119/122 (97%)	-0.04	2 (1%) 67 31	107, 137, 173, 189	0
10	J	65/70 (92%)	-0.24	0 100 100	73, 94, 129, 142	0
11	K	115/120 (95%)	-0.14	1 (0%) 81 47	63, 95, 135, 151	0
12	L	46/70 (65%)	0.37	3 (6%) 18 7	92, 161, 182, 184	0
13	N	10/14 (71%)	0.09	0 100 100	158, 184, 239, 246	0
14	P	6/6 (100%)	-0.34	0 100 100	75, 90, 111, 138	0
15	T	20/26 (76%)	-0.04	1 (5%) 28 10	105, 152, 246, 248	0
All	All	3964/4610 (85%)	-0.04	19 (0%) 88 61	52, 105, 168, 248	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1176	LEU	4.3
12	L	25	ALA	3.3
1	A	257	ARG	3.3
12	L	26	THR	3.2
1	A	251	SER	3.0
2	B	883	LEU	2.7
1	A	194	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
12	L	27	LEU	2.7
1	A	1455	PRO	2.6
1	A	256	GLN	2.6
9	I	119	THR	2.5
2	B	715	ALA	2.5
2	B	918	ILE	2.3
11	K	115	ALA	2.2
2	B	709	ASP	2.1
9	I	118	ARG	2.1
2	B	865	LYS	2.1
15	T	7	DT	2.1
2	B	708	GLU	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	0.13	-1.26	107,109,114,121	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
16	ZN	I	1121	1/1	0.13	0.28	121,121,121,121	0
16	ZN	B	2225	1/1	0.19	0.02	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
16	ZN	J	1066	1/1	0.22	-0.09	91,91,91,91	0
16	ZN	A	2457	1/1	0.14	-0.80	67,67,67,67	0
17	MG	A	2458	1/1	0.16	-0.86	64,64,64,64	0
16	ZN	C	1269	1/1	0.10	-1.07	88,88,88,88	0
16	ZN	A	2456	1/1	0.08	-1.96	133,133,133,133	0
16	ZN	I	1122	1/1	0.04	-2.08	182,182,182,182	0
16	ZN	L	1071	1/1	0.05	-2.86	163,163,163,163	0

6.5 Other polymers

There are no such residues in this entry.