



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 04:07 AM GMT

PDB ID : 4A3E
Title : RNA POLYMERASE II INITIAL TRANSCRIBING COMPLEX WITH A
5NT DNA-RNA HYBRID AND SOAKED WITH AMPCPP
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>

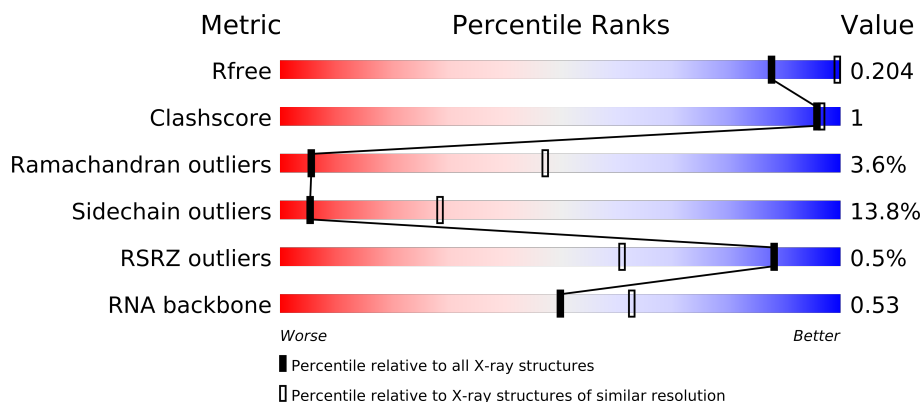
The following versions of software and data (see [references](#)) were used in the production of this report:

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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
13	N	14	
14	P	5	
15	T	26	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 31855 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	1423	Total	C	N	O	S	0	0	0
			11182	7043	1955	2122	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*A P*CP*TP*TP*GP*AP*GP*CP*TP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	8	Total	C	N	O	P	0	0	0
			165	79	29	49	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	4	Total	C	N	O	P	0	0	0
			90	40	20	26	4			

- 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*CP*CP*BRU*GP*GP*TP*CP*AP*TP*TP)-3'.

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

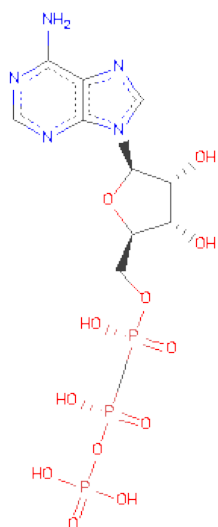
- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

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: C₁₁H₁₈N₅O₁₂P₃).

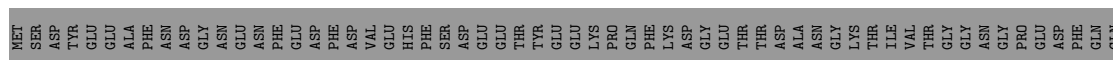


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
18	P	1	31	11	5	12	3	0	0



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

Chain F:



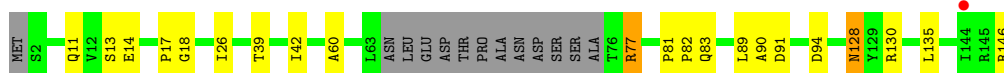
- Molecule 7: RPB7, DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

Chain G:



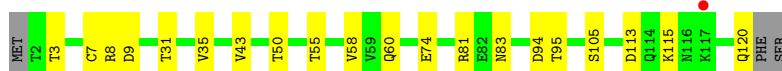
- Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

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:



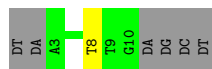
- Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4

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: 



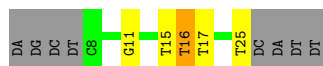
- Molecule 14: TRANSCRIPT RNA 5'-R(*CP*AP*GP*GP*AP)-3'

Chain P: 



- Molecule 15: TEMPLATE DNA 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*TP*TP*CP*CP*BRU*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	223.68Å 394.17Å 283.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.61 – 3.40 54.61 – 3.40	Depositor EDS
% Data completeness (in resolution range)	97.8 (54.61-3.40) 97.8 (54.61-3.40)	Depositor EDS
R_{merge}	0.63	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 3.40Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.160 , 0.188 0.180 , 0.204	Depositor DCC
R_{free} test set	3323 reflections (1.99%)	DCC
Wilson B-factor (Å ²)	111.9	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 98.7	EDS
Estimated twinning fraction	0.029 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.039 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 167011 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	31855	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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, 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	0/11382	0.84	9/15394 (0.1%)
2	B	0.51	0/9029	0.79	3/12171 (0.0%)
3	C	0.49	0/2133	0.79	2/2891 (0.1%)
4	D	0.51	0/1444	0.82	0/1935
5	E	0.46	0/1788	0.71	0/2406
6	F	0.61	0/691	0.83	0/933
7	G	0.55	0/1368	0.82	0/1844
8	H	0.50	0/1086	0.80	0/1470
9	I	0.47	0/989	0.76	0/1331
10	J	0.55	0/541	0.86	0/727
11	K	0.47	0/938	0.72	0/1267
12	L	0.56	0/365	1.01	0/485
13	N	1.37	0/184	1.03	0/282
14	P	1.09	0/101	0.78	0/156
15	T	1.52	2/383 (0.5%)	1.16	2/586 (0.3%)
All	All	0.55	2/32422 (0.0%)	0.82	16/43878 (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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	25	DT	C1'-N1	7.01	1.58	1.49
15	T	17	DT	C3'-O3'	-5.99	1.36	1.44

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	LYS	C-N-CA	7.41	140.22	121.70
1	A	399	HIS	N-CA-CB	7.12	123.41	110.60
1	A	56	PRO	C-N-CA	6.21	137.23	121.70
1	A	194	ALA	C-N-CA	5.82	136.26	121.70
1	A	54	ASN	C-N-CA	5.80	136.20	121.70
3	C	39	ALA	N-CA-C	5.79	126.64	111.00
1	A	35	ILE	N-CA-CB	5.66	123.81	110.80
15	T	16	DT	O4'-C4'-C3'	-5.62	102.25	104.50
15	T	15	DT	O4'-C4'-C3'	-5.57	102.27	104.50
2	B	338	GLY	C-N-CA	5.51	135.48	121.70
2	B	1155	SER	C-N-CA	5.32	135.01	121.70
1	A	1403	GLU	N-CA-C	5.31	125.34	111.00
1	A	1403	GLU	C-N-CA	-5.25	108.57	121.70
2	B	628	THR	C-N-CA	5.23	134.77	121.70
1	A	310	GLY	C-N-CA	5.15	134.58	121.70
3	C	89	GLU	N-CA-C	-5.03	97.43	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	11182	0	0	20	0
2	B	8859	0	0	10	0
3	C	2095	0	0	1	0
4	D	1434	0	0	1	0
5	E	1752	0	0	0	0
6	F	679	0	0	1	0
7	G	1340	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	1068	0	0	0	0
9	I	971	0	0	0	0
10	J	532	0	0	7	0
11	K	920	0	0	1	0
12	L	363	0	0	0	0
13	N	165	0	0	1	0
14	P	90	0	44	0	0
15	T	365	0	0	2	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
18	P	31	0	14	0	0
All	All	31855	0	58	38	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 (38) 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	1.78	1.60
7:G:1:MET:SD	7:G:2:PHE:N	2.48	0.87
3:C:66:ARG:NH2	10:J:3:VAL:O	2.19	0.76
2:B:822:ASN:O	10:J:48:ARG:NH1	2.32	0.62
2:B:801:LYS:O	10:J:52:THR:OG1	2.22	0.57
7:G:1:MET:CE	7:G:80:LYS:O	2.52	0.57
15:T:16:DT:C6	15:T:16:DT:C3'	2.88	0.56
1:A:590:ARG:NH2	1:A:621:THR:OG1	2.38	0.56
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.40	0.55
1:A:399:HIS:O	1:A:401:GLY:N	2.43	0.51
1:A:326:ARG:NE	1:A:1407:GLU:OE2	2.43	0.51
1:A:53:LEU:CD2	1:A:54:ASN:N	2.73	0.51
10:J:9:SER:OG	10:J:48:ARG:NH2	2.43	0.50
1:A:469:ARG:NH2	2:B:991:GLY:O	2.44	0.50
1:A:42:ASP:O	1:A:44:THR:N	2.45	0.49
1:A:433:GLU:OE1	2:B:1108:ARG:NH2	2.46	0.49
6:F:77:ASP:O	6:F:78:GLN:CB	2.61	0.49
10:J:48:ARG:O	10:J:52:THR:CG2	2.61	0.48
1:A:335:ARG:NH1	2:B:1206:GLU:OE2	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:562:GLY:O	2:B:590:HIS:ND1	2.47	0.48
1:A:471:ASN:ND2	1:A:650:GLN:OE1	2.47	0.47
11:K:24:ASP:OD2	11:K:74:ARG:NH1	2.48	0.46
1:A:867:ILE:CB	1:A:867:ILE:CD1	2.80	0.46
2:B:635:ARG:NH1	2:B:742:GLU:OE2	2.49	0.46
1:A:55:ASP:CG	1:A:55:ASP:O	2.54	0.45
2:B:1033:LYS:NZ	2:B:1070:GLU:OE1	2.51	0.44
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.49	0.44
1:A:434:ARG:NH2	1:A:440:ASP:OD2	2.51	0.43
1:A:836:TYR:OH	1:A:1403:GLU:OE2	2.36	0.43
10:J:10:CYS:SG	10:J:43:ARG:NH2	2.92	0.42
1:A:378:GLU:OE1	1:A:387:ARG:NH2	2.52	0.42
1:A:879:GLU:OE2	1:A:962:ARG:NH2	2.53	0.42
1:A:951:GLU:O	1:A:954:TRP:NE1	2.53	0.41
10:J:37:SER:OG	10:J:47:ARG:NH2	2.53	0.41
1:A:55:ASP:OD2	1:A:55:ASP:O	2.39	0.41
2:B:1106:ARG:NH1	2:B:1125:ASP:O	2.54	0.41
4:D:66:ARG:NH2	7:G:35:GLU:OE2	2.54	0.41
13:N:8:DT:O2	15:T:11:DG:N2	2.54	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	1415/1732 (82%)	1247 (88%)	113 (8%)	55 (4%)	5	44
2	B	1095/1224 (90%)	963 (88%)	94 (9%)	38 (4%)	6	48
3	C	264/318 (83%)	243 (92%)	19 (7%)	2 (1%)	27	81
4	D	174/221 (79%)	154 (88%)	13 (8%)	7 (4%)	5	43
5	E	212/215 (99%)	198 (93%)	12 (6%)	2 (1%)	25	80
6	F	82/155 (53%)	75 (92%)	5 (6%)	2 (2%)	9	58
7	G	169/171 (99%)	156 (92%)	10 (6%)	3 (2%)	13	65

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	129/146 (88%)	103 (80%)	17 (13%)	9 (7%)	2	23
9	I	117/122 (96%)	94 (80%)	15 (13%)	8 (7%)	2	24
10	J	63/70 (90%)	52 (82%)	7 (11%)	4 (6%)	2	27
11	K	113/120 (94%)	109 (96%)	4 (4%)	0	100	100
12	L	44/70 (63%)	28 (64%)	8 (18%)	8 (18%)	0	3
All	All	3877/4564 (85%)	3422 (88%)	317 (8%)	138 (4%)	5	47

All (138) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	A	57	ARG
1	A	74	MET
1	A	76	GLU
1	A	189	ARG
1	A	257	ARG
1	A	286	HIS
1	A	311	GLN
1	A	318	SER
1	A	332	LYS
1	A	335	ARG
1	A	448	PRO
1	A	449	SER
1	A	1281	ARG
1	A	1403	GLU
1	A	1405	THR
2	B	229	ALA
2	B	307	ASP
2	B	341	LEU
2	B	344	LYS
2	B	476	ARG
2	B	707	PRO
2	B	731	VAL
2	B	867	GLY
2	B	1066	SER
2	B	1176	ASN
4	D	18	VAL
4	D	199	ASN
10	J	55	ASP
12	L	50	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	L	53	HIS
12	L	56	LEU
1	A	35	ILE
1	A	54	ASN
1	A	58	LEU
1	A	69	THR
1	A	166	GLY
1	A	169	ASN
1	A	178	GLY
1	A	193	ASP
1	A	195	ASP
1	A	331	GLY
1	A	628	GLY
1	A	775	ILE
1	A	1175	SER
1	A	1377	THR
2	B	108	VAL
2	B	340	ALA
2	B	368	GLU
2	B	575	PRO
2	B	629	ASP
2	B	751	VAL
2	B	792	MET
2	B	879	ARG
2	B	1157	ALA
2	B	1175	LEU
2	B	1181	GLU
4	D	119	ARG
4	D	220	LEU
5	E	45	LYS
6	F	78	GLN
9	I	9	ASP
9	I	95	THR
10	J	6	ARG
1	A	43	GLU
1	A	47	ARG
1	A	569	LYS
1	A	1124	HIS
1	A	1173	HIS
1	A	1221	LYS
2	B	282	ILE
2	B	447	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	711	GLU
2	B	881	ASN
2	B	883	LEU
2	B	960	GLY
2	B	1155	SER
6	F	73	ALA
8	H	60	ALA
8	H	82	PRO
8	H	90	ALA
9	I	60	GLN
9	I	113	ASP
10	J	2	ILE
12	L	28	LYS
12	L	45	ALA
1	A	70	CYS
1	A	155	GLU
1	A	167	CYS
1	A	192	GLY
1	A	336	ILE
1	A	399	HIS
1	A	567	LYS
1	A	958	VAL
1	A	1365	TYR
2	B	1046	PRO
4	D	13	ARG
4	D	169	SER
5	E	36	GLU
7	G	63	PRO
7	G	154	VAL
8	H	81	PRO
8	H	83	GLN
8	H	128	ASN
9	I	105	SER
12	L	26	THR
12	L	54	ARG
12	L	59	ALA
1	A	65	LEU
1	A	333	GLU
1	A	1255	GLU
2	B	67	SER
7	G	139	ILE
8	H	17	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	18	GLY
9	I	3	THR
9	I	115	LYS
10	J	17	LYS
1	A	41	MET
1	A	55	ASP
1	A	310	GLY
2	B	249	ARG
2	B	959	ASP
2	B	1017	ILE
2	B	1108	ARG
4	D	16	LYS
8	H	77	ARG
1	A	385	ILE
1	A	312	PRO
2	B	364	ILE
1	A	1437	GLY
2	B	436	VAL
2	B	992	ILE
2	B	247	GLY
3	C	150	GLY
9	I	58	VAL
1	A	910	PRO
3	C	240	VAL

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	1241/1519 (82%)	1053 (85%)	188 (15%)	4	25
2	B	966/1061 (91%)	850 (88%)	116 (12%)	7	35
3	C	234/274 (85%)	204 (87%)	30 (13%)	6	32
4	D	160/200 (80%)	129 (81%)	31 (19%)	2	11
5	E	196/197 (100%)	172 (88%)	24 (12%)	7	34
6	F	74/137 (54%)	66 (89%)	8 (11%)	9	42
7	G	152/152 (100%)	134 (88%)	18 (12%)	8	36

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	117/128 (91%)	103 (88%)	14 (12%)	7	35
9	I	113/116 (97%)	101 (89%)	12 (11%)	10	43
10	J	60/65 (92%)	50 (83%)	10 (17%)	3	19
11	K	99/102 (97%)	85 (86%)	14 (14%)	5	28
12	L	40/57 (70%)	30 (75%)	10 (25%)	1	5
All	All	3452/4008 (86%)	2977 (86%)	475 (14%)	5	28

All (475) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	15	LYS
1	A	34	LYS
1	A	41	MET
1	A	62	ASP
1	A	65	LEU
1	A	70	CYS
1	A	93	VAL
1	A	96	ILE
1	A	123	ARG
1	A	126	LEU
1	A	132	LYS
1	A	147	VAL
1	A	152	VAL
1	A	157	ASP
1	A	163	SER
1	A	174	ILE
1	A	175	ARG
1	A	176	LYS
1	A	188	ASP
1	A	195	ASP
1	A	199	LEU
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	227	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	252	PHE
1	A	253	ASN
1	A	256	GLN
1	A	261	ASP
1	A	265	LYS
1	A	270	LEU
1	A	279	LEU
1	A	291	GLU
1	A	307	ASP
1	A	311	GLN
1	A	315	LEU
1	A	322	VAL
1	A	324	SER
1	A	335	ARG
1	A	337	ARG
1	A	353	ILE
1	A	375	THR
1	A	381	THR
1	A	385	ILE
1	A	386	ASP
1	A	391	LEU
1	A	393	ARG
1	A	397	ASN
1	A	398	GLU
1	A	407	ARG
1	A	408	ASP
1	A	423	ASP
1	A	424	ILE
1	A	425	GLN
1	A	427	GLN
1	A	434	ARG
1	A	436	ILE
1	A	443	LEU
1	A	445	ASN
1	A	448	PRO
1	A	450	LEU
1	A	451	HIS
1	A	454	SER
1	A	461	LYS
1	A	469	ARG
1	A	472	LEU
1	A	474	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	475	THR
1	A	489	LEU
1	A	496	GLU
1	A	500	GLU
1	A	505	CYS
1	A	513	SER
1	A	517	ASN
1	A	532	ARG
1	A	538	ASP
1	A	544	ASP
1	A	571	LEU
1	A	577	ILE
1	A	589	GLN
1	A	593	GLU
1	A	597	LEU
1	A	598	LEU
1	A	602	ASP
1	A	603	ASN
1	A	618	GLU
1	A	622	VAL
1	A	629	LEU
1	A	634	THR
1	A	635	ARG
1	A	640	GLN
1	A	666	ILE
1	A	672	ASP
1	A	685	GLU
1	A	702	LEU
1	A	719	VAL
1	A	738	LYS
1	A	756	ILE
1	A	764	CYS
1	A	768	GLN
1	A	769	SER
1	A	773	LYS
1	A	774	ARG
1	A	782	ARG
1	A	788	SER
1	A	811	GLN
1	A	821	ARG
1	A	826	ASP
1	A	831	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	839	ARG
1	A	846	GLU
1	A	849	MET
1	A	855	THR
1	A	867	ILE
1	A	878	ILE
1	A	885	THR
1	A	886	ILE
1	A	889	SER
1	A	904	THR
1	A	919	ILE
1	A	920	LEU
1	A	926	GLN
1	A	940	ARG
1	A	948	VAL
1	A	960	ILE
1	A	973	ILE
1	A	988	LEU
1	A	991	LYS
1	A	998	LEU
1	A	1001	ARG
1	A	1015	VAL
1	A	1024	SER
1	A	1029	ARG
1	A	1036	ARG
1	A	1040	GLN
1	A	1058	VAL
1	A	1080	THR
1	A	1116	LEU
1	A	1118	VAL
1	A	1124	HIS
1	A	1135	ARG
1	A	1168	GLU
1	A	1173	HIS
1	A	1176	LEU
1	A	1193	LEU
1	A	1195	LEU
1	A	1208	THR
1	A	1218	GLN
1	A	1233	ASP
1	A	1237	ILE
1	A	1242	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1255	GLU
1	A	1257	ASP
1	A	1260	LEU
1	A	1264	GLU
1	A	1274	ARG
1	A	1276	VAL
1	A	1281	ARG
1	A	1289	ARG
1	A	1291	VAL
1	A	1295	THR
1	A	1297	GLU
1	A	1301	GLU
1	A	1309	ASP
1	A	1314	SER
1	A	1325	THR
1	A	1327	ILE
1	A	1341	ILE
1	A	1370	LEU
1	A	1376	THR
1	A	1391	ARG
1	A	1393	ASN
1	A	1400	CYS
1	A	1405	THR
1	A	1420	ASP
1	A	1425	SER
1	A	1426	GLU
1	A	1433	MET
1	A	1442	ASP
1	A	1444	MET
1	A	1445	ILE
1	A	1451	VAL
1	A	1454	MET
2	B	25	ILE
2	B	35	SER
2	B	46	GLN
2	B	109	THR
2	B	110	HIS
2	B	118	ARG
2	B	119	LEU
2	B	134	LYS
2	B	178	ASN
2	B	187	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	225	VAL
2	B	251	ILE
2	B	261	ARG
2	B	272	THR
2	B	278	GLN
2	B	279	ASP
2	B	287	ARG
2	B	294	ASP
2	B	313	MET
2	B	336	ARG
2	B	337	ARG
2	B	339	THR
2	B	341	LEU
2	B	343	ILE
2	B	344	LYS
2	B	346	GLU
2	B	347	LYS
2	B	348	ARG
2	B	351	TYR
2	B	357	GLN
2	B	365	THR
2	B	373	ARG
2	B	387	LEU
2	B	393	LYS
2	B	398	ARG
2	B	401	PHE
2	B	408	LEU
2	B	412	LEU
2	B	416	LEU
2	B	423	LYS
2	B	429	PHE
2	B	446	LEU
2	B	448	ILE
2	B	461	LEU
2	B	466	TRP
2	B	470	LYS
2	B	481	GLN
2	B	485	ARG
2	B	537	LYS
2	B	543	SER
2	B	547	VAL
2	B	552	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	570	VAL
2	B	574	SER
2	B	602	THR
2	B	614	SER
2	B	615	MET
2	B	616	ILE
2	B	620	ARG
2	B	628	THR
2	B	642	ASP
2	B	658	ILE
2	B	668	ASP
2	B	678	GLU
2	B	690	VAL
2	B	708	GLU
2	B	709	ASP
2	B	723	VAL
2	B	729	ILE
2	B	731	VAL
2	B	766	ARG
2	B	786	ASN
2	B	790	ASP
2	B	795	ILE
2	B	835	GLN
2	B	839	MET
2	B	853	SER
2	B	857	ARG
2	B	873	THR
2	B	878	GLN
2	B	881	ASN
2	B	882	THR
2	B	889	THR
2	B	904	ARG
2	B	918	ILE
2	B	933	SER
2	B	934	LYS
2	B	953	LEU
2	B	972	LYS
2	B	975	GLN
2	B	982	SER
2	B	983	ARG
2	B	997	GLU
2	B	999	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1010	LEU
2	B	1017	ILE
2	B	1020	ARG
2	B	1028	GLU
2	B	1045	SER
2	B	1050	ILE
2	B	1060	ARG
2	B	1065	GLN
2	B	1072	MET
2	B	1106	ARG
2	B	1133	MET
2	B	1138	MET
2	B	1147	LEU
2	B	1148	LYS
2	B	1151	LEU
2	B	1156	ASP
2	B	1160	VAL
2	B	1183	LYS
2	B	1188	LYS
2	B	1189	ILE
2	B	1201	LYS
2	B	1202	LEU
3	C	11	ARG
3	C	12	GLU
3	C	16	ASP
3	C	22	LEU
3	C	23	SER
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	70	ILE
3	C	84	ARG
3	C	100	THR
3	C	101	LEU
3	C	106	GLU
3	C	108	GLU
3	C	119	VAL
3	C	125	MET
3	C	127	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	129	ILE
3	C	133	ILE
3	C	145	CYS
3	C	148	ARG
3	C	155	LEU
3	C	224	GLN
3	C	226	ASP
3	C	240	VAL
3	C	259	LEU
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	17	LYS
4	D	18	VAL
4	D	22	GLU
4	D	23	ASN
4	D	27	LEU
4	D	28	GLN
4	D	41	GLN
4	D	47	LEU
4	D	53	SER
4	D	67	ARG
4	D	118	THR
4	D	119	ARG
4	D	126	ILE
4	D	127	ASP
4	D	137	ASN
4	D	139	LYS
4	D	153	ARG
4	D	155	ARG
4	D	158	GLU
4	D	177	VAL
4	D	187	THR
4	D	197	SER
4	D	205	ASP
4	D	206	GLU
4	D	213	GLU
4	D	221	TYR
5	E	2	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	8	ASN
5	E	31	THR
5	E	41	ASP
5	E	45	LYS
5	E	57	MET
5	E	67	GLU
5	E	69	ILE
5	E	81	GLU
5	E	92	THR
5	E	96	PHE
5	E	98	ILE
5	E	99	HIS
5	E	157	SER
5	E	166	LYS
5	E	173	SER
5	E	177	ARG
5	E	190	LEU
5	E	191	LYS
5	E	192	ARG
5	E	196	VAL
5	E	202	SER
5	E	204	THR
5	E	210	SER
6	F	82	THR
6	F	87	LYS
6	F	109	VAL
6	F	110	ASP
6	F	111	LEU
6	F	115	THR
6	F	122	MET
6	F	127	GLU
7	G	2	PHE
7	G	13	LEU
7	G	24	GLN
7	G	26	LEU
7	G	29	LYS
7	G	34	VAL
7	G	83	LYS
7	G	90	THR
7	G	92	VAL
7	G	93	SER
7	G	96	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	106	MET
7	G	119	LEU
7	G	134	GLU
7	G	138	THR
7	G	143	ILE
7	G	150	CYS
7	G	151	ILE
8	H	11	GLN
8	H	13	SER
8	H	14	GLU
8	H	26	ILE
8	H	39	THR
8	H	42	ILE
8	H	77	ARG
8	H	89	LEU
8	H	91	ASP
8	H	94	ASP
8	H	128	ASN
8	H	130	ARG
8	H	135	LEU
8	H	146	ARG
9	I	7	CYS
9	I	8	ARG
9	I	31	THR
9	I	35	VAL
9	I	43	VAL
9	I	50	THR
9	I	55	THR
9	I	74	GLU
9	I	81	ARG
9	I	83	ASN
9	I	94	ASP
9	I	120	GLN
10	J	12	LYS
10	J	13	VAL
10	J	20	SER
10	J	24	LEU
10	J	27	GLU
10	J	29	GLU
10	J	36	LEU
10	J	37	SER
10	J	42	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	J	48	ARG
11	K	1	MET
11	K	11	LEU
11	K	18	LYS
11	K	20	LYS
11	K	25	THR
11	K	29	ASN
11	K	34	THR
11	K	37	LYS
11	K	42	LEU
11	K	47	ARG
11	K	76	GLN
11	K	79	GLU
11	K	101	LEU
11	K	114	LEU
12	L	27	LEU
12	L	38	LEU
12	L	40	LEU
12	L	42	ARG
12	L	54	ARG
12	L	55	ILE
12	L	58	LYS
12	L	61	THR
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	3/5 (60%)	0	0

There are no RNA backbone outliers to report.

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	1.07	3 (15%)	22,30,33	2.53	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	-	1/5/21/22	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	22	BRU	C6-N1	2.55	1.40	1.34
15	T	22	BRU	C4-C5	2.51	1.44	1.39
15	T	22	BRU	P-OP1	2.23	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	-9.62	119.67	122.41
15	T	22	BRU	N3-C2-N1	4.74	119.93	115.97
15	T	22	BRU	O4'-C1'-N1	3.64	114.52	107.68
15	T	22	BRU	BR-C5-C6	2.12	122.17	117.98

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	T	22	BRU	OP2-P-O5'-C5'

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	2.38	10 (30%)	52,52,52	2.12	14 (26%)

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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	P	1011	APC	PA-C3A	6.64	1.85	1.79
18	P	1011	APC	PB-C3A	5.62	1.84	1.79
18	P	1011	APC	PG-O3B	4.58	1.68	1.60
18	P	1011	APC	PA-O1A	3.97	1.61	1.51
18	P	1011	APC	PG-O1G	3.68	1.63	1.51
18	P	1011	APC	PB-O3B	3.53	1.68	1.59
18	P	1011	APC	O4'-C1'	2.90	1.45	1.41
18	P	1011	APC	PB-O2B	2.62	1.62	1.56
18	P	1011	APC	PG-O2G	2.49	1.63	1.54
18	P	1011	APC	PA-O2A	-2.26	1.50	1.56

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	P	1011	APC	N3-C2-N1	-7.05	122.81	128.71
18	P	1011	APC	N3-C4-N9	5.30	135.01	125.43
18	P	1011	APC	O4'-C1'-N9	4.30	112.44	108.44
18	P	1011	APC	C4-C5-N7	-4.21	105.92	109.52
18	P	1011	APC	PA-O5'-C5'	-3.92	111.14	122.43
18	P	1011	APC	C5-C4-N3	-3.46	118.17	125.70
18	P	1011	APC	O5'-PA-C3A	3.34	112.26	103.97
18	P	1011	APC	O3B-PB-C3A	3.00	116.06	106.62
18	P	1011	APC	PA-C3A-PB	-2.95	113.37	117.62
18	P	1011	APC	O5'-PA-O1A	-2.68	107.51	114.21
18	P	1011	APC	C2-N3-C4	2.44	120.96	114.01
18	P	1011	APC	PG-O3B-PB	-2.17	124.38	131.81
18	P	1011	APC	O2'-C2'-C3'	2.13	118.76	111.83
18	P	1011	APC	C8-N7-C5	2.01	109.81	103.58

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	1423/1732 (82%)	-0.03	4 (0%) 91 73	65, 110, 174, 230	0
2	B	1115/1224 (91%)	0.05	8 (0%) 84 52	66, 124, 185, 221	0
3	C	266/318 (83%)	-0.15	0 100 100	81, 107, 150, 180	0
4	D	178/221 (80%)	-0.04	1 (0%) 86 55	86, 123, 174, 194	0
5	E	214/215 (99%)	-0.01	2 (0%) 81 47	88, 150, 192, 202	0
6	F	84/155 (54%)	-0.25	0 100 100	64, 92, 119, 142	0
7	G	171/171 (100%)	-0.06	0 100 100	84, 107, 145, 165	0
8	H	133/146 (91%)	0.32	1 (0%) 83 49	123, 155, 192, 207	0
9	I	119/122 (97%)	-0.09	1 (0%) 83 49	114, 156, 190, 213	0
10	J	65/70 (92%)	-0.05	0 100 100	88, 108, 145, 161	0
11	K	115/120 (95%)	-0.12	0 100 100	80, 110, 147, 166	0
12	L	46/70 (65%)	0.45	2 (4%) 34 13	93, 184, 198, 207	0
13	N	8/14 (57%)	-0.42	0 100 100	214, 229, 237, 240	0
14	P	4/5 (80%)	-0.01	0 100 100	146, 154, 170, 189	0
15	T	18/26 (69%)	-0.04	0 100 100	156, 210, 225, 227	0
All	All	3959/4609 (85%)	-0.01	19 (0%) 88 61	64, 119, 185, 240	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	L	27	LEU	4.7
2	B	715	ALA	3.4
1	A	257	ARG	3.2
2	B	470	LYS	2.9
2	B	250	PHE	2.7
1	A	1176	LEU	2.7
1	A	194	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	343	ILE	2.5
2	B	340	ALA	2.4
4	D	13	ARG	2.4
2	B	167	ILE	2.3
2	B	339	THR	2.3
12	L	26	THR	2.2
1	A	1092	LYS	2.2
9	I	117	LYS	2.2
2	B	883	LEU	2.1
8	H	144	ILE	2.1
5	E	110	PHE	2.0
5	E	93	MET	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	0.10	-2.61	170,185,187,190	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
18	APC	P	1011	31/31	0.33	1.27	195,198,211,212	0
16	ZN	I	1121	1/1	0.15	0.70	130,130,130,130	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
16	ZN	B	2225	1/1	0.23	0.65	95,95,95,95	0
16	ZN	J	1066	1/1	0.24	0.47	98,98,98,98	0
16	ZN	C	1269	1/1	0.16	0.42	96,96,96,96	0
16	ZN	A	2457	1/1	0.19	0.32	85,85,85,85	0
16	ZN	I	1122	1/1	0.06	-1.36	191,191,191,191	0
17	MG	A	2458	1/1	0.16	-1.71	110,110,110,110	0
16	ZN	L	1071	1/1	0.05	-2.01	198,198,198,198	0
16	ZN	A	2456	1/1	0.06	-2.86	138,138,138,138	0

6.5 Other polymers ⓘ

There are no such residues in this entry.