



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 03:43 PM GMT

PDB ID : 3PO3  
Title : Arrested RNA Polymerase II reactivation intermediate  
Authors : Cheung, A.C.M.; Cramer, P.  
Deposited on : 2010-11-21  
Resolution : 3.30 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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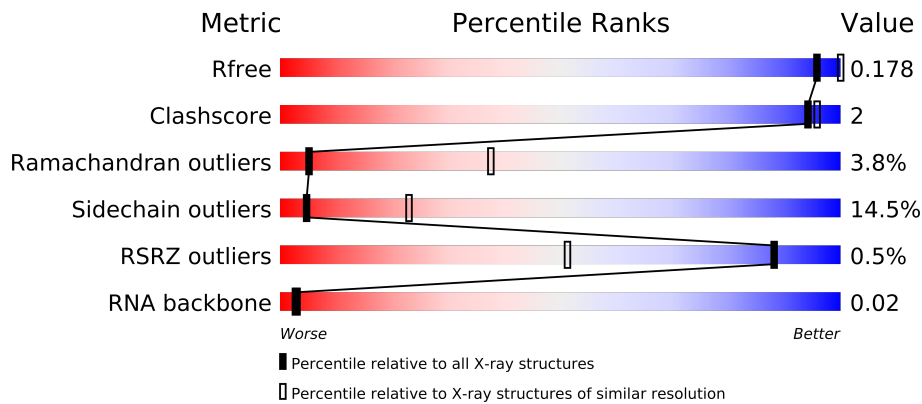
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 3.30 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	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)
RNA backbone	1838	1042 (3.90-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1733	
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	5	
15	S	178	
16	T	27	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
19	ACT	A	1734	-	X

## 2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 33008 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	1426	Total	C	N	O	S	0	0	0
			11214	7069	1959	2124	62			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1108	Total	C	N	O	S	0	0	0
			8810	5580	1541	1634	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	177	Total	C	N	O	S	0	0	0
			1417	876	252	287	2			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			

- Molecule 13 is a DNA chain called DNA non-template strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	7	Total	C	N	O	P	0	0	0
			144	69	30	39	6			

- Molecule 14 is a RNA chain called RNA product strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	5	Total	C	N	O	P	0	0	0
			100	45	15	35	5			

- Molecule 15 is a protein called Transcription elongation factor S-II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	S	164	Total	C	N	O	S	0	0	0
			1294	809	230	247	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	290	ALA	ASP	ENGINEERED MUTATION	UNP P07273
S	291	ALA	GLU	ENGINEERED MUTATION	UNP P07273

- Molecule 16 is a DNA chain called DNA template strand.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
16	T	13	Total	Br	C	N	O	P	0	0	0
			266	1	126	44	82	13			

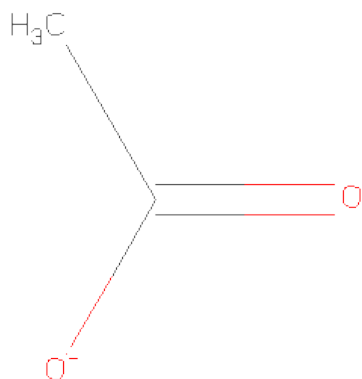
- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

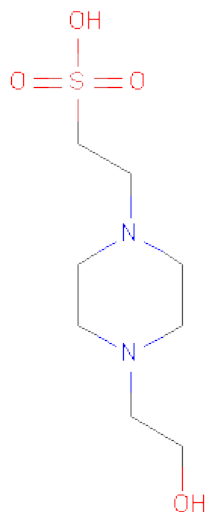
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	1	Total	Mg	0	0
			1	1		

- Molecule 19 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



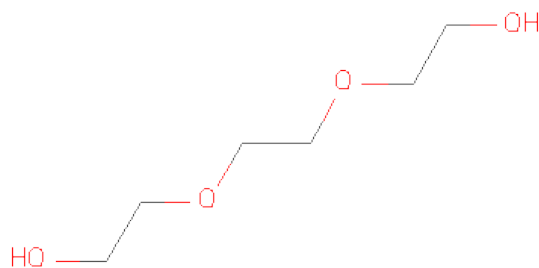
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	B	1	Total	C	O	0	0
			4	2	2		
19	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 20 is 4-(2-HYDROXYETHYL)-1-PIPERAZINEETHANESULFONIC ACID (three-letter code: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
20	A	1	15	8	2	4	1	0	0

- Molecule 21 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



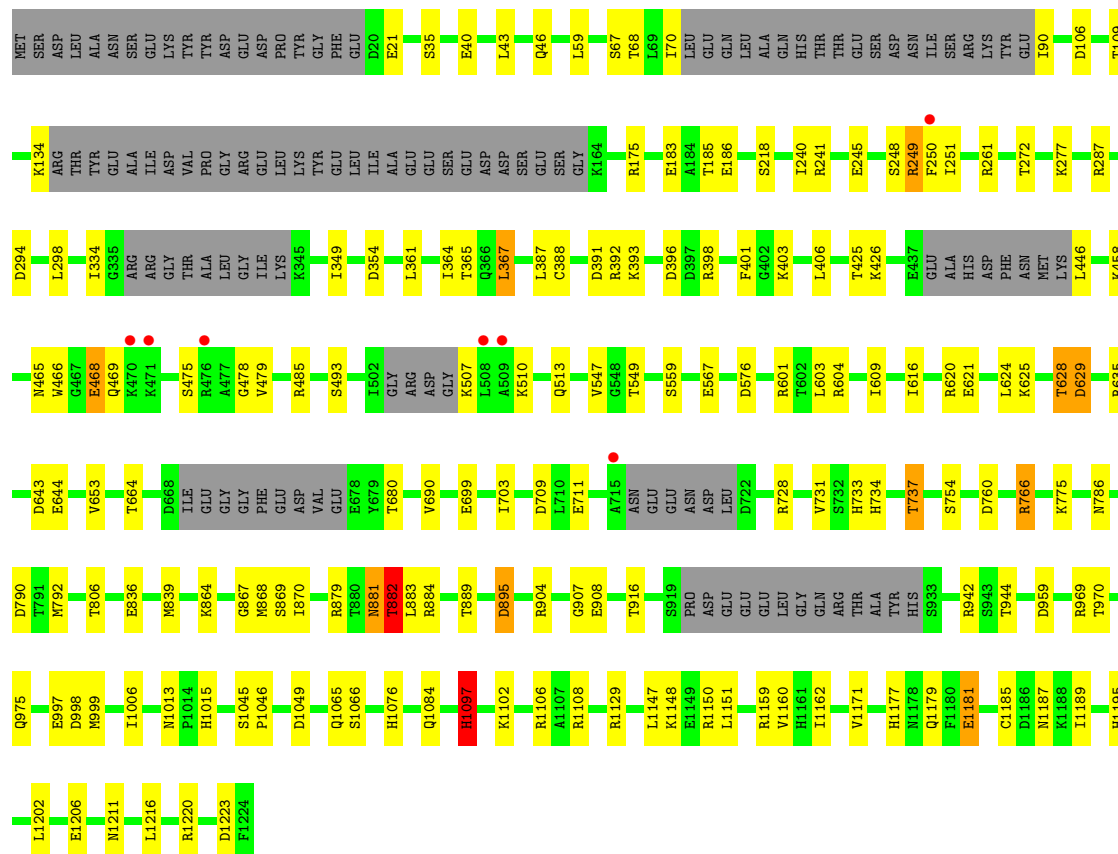
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
21	L	1	10	6	4	0	0



PRO  
ALA  
SER  
TYR  
LEU  
SER  
PRO  
LYS  
GLN  
ASP  
GLU  
GLN  
LYS  
HIS  
ASN  
GLU  
ASN  
GLU  
ASN  
SER  
ARG

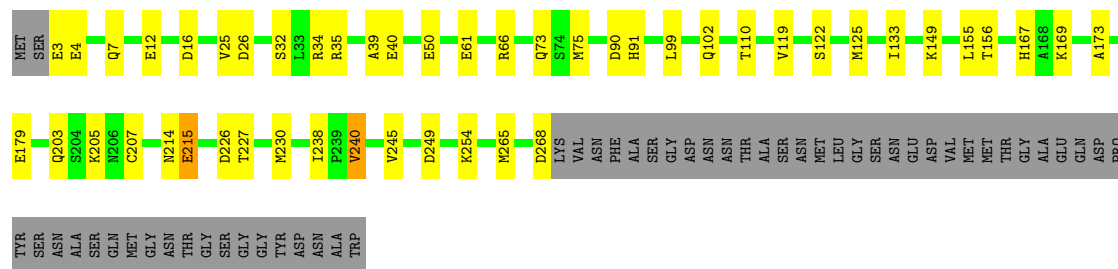
• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

Chain B: 



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

Chain C: 



• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

Chain D: 





Y221

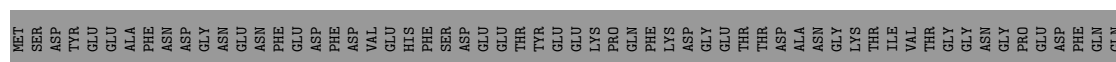
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:



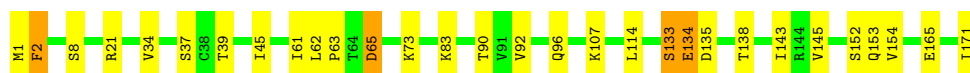
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



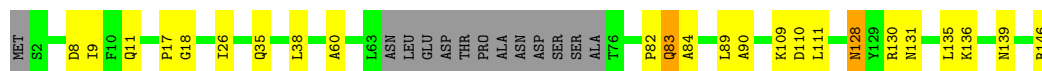
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G:



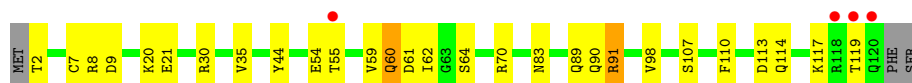
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



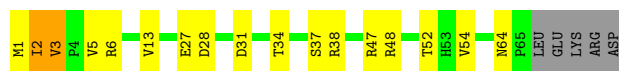
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I:



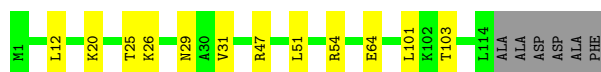
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



- Molecule 11: DNA-directed RNA polymerase II subunit RPB11

Chain K:



- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:



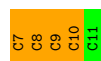
- Molecule 13: DNA non-template strand

Chain N:



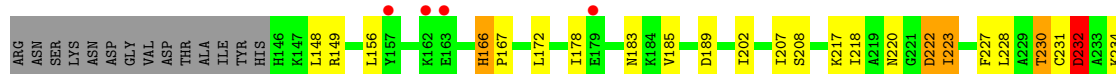
- Molecule 14: RNA product strand

Chain P:



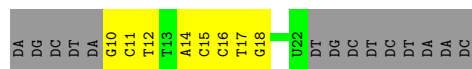
- Molecule 15: Transcription elongation factor S-II

Chain S:



- Molecule 16: DNA template strand

Chain T:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	220.02Å 395.07Å 280.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.97 – 3.30 49.97 – 3.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.97-3.30) 99.7 (49.97-3.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.00 (at 3.33Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, $R_{free}$	0.161 , 0.189 0.179 , 0.178	Depositor DCC
$R_{free}$ test set	3594 reflections (1.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	111.5	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 100.9	EDS
Estimated twinning fraction	0.018 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.026 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 181822 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	33008	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	127.0	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.*

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

## 5 Model quality

### 5.1 Standard geometry

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

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	2/11417 (0.0%)	0.85	7/15442 (0.0%)
2	B	0.51	0/8981	0.79	4/12108 (0.0%)
3	C	0.50	0/2133	0.77	1/2891 (0.0%)
4	D	0.52	0/1427	0.86	2/1914 (0.1%)
5	E	0.44	0/1788	0.71	0/2406
6	F	0.56	0/691	0.77	0/933
7	G	0.55	0/1368	0.82	0/1844
8	H	0.47	0/1086	0.80	0/1470
9	I	0.47	0/989	0.79	0/1331
10	J	0.52	0/541	0.87	1/727 (0.1%)
11	K	0.51	0/937	0.71	0/1265
12	L	0.53	0/366	0.97	1/485 (0.2%)
13	N	0.99	0/162	1.81	6/249 (2.4%)
14	P	1.26	0/109	2.55	10/166 (6.0%)
15	S	0.50	0/1317	0.79	0/1778
16	T	1.16	0/274	1.82	9/421 (2.1%)
All	All	0.53	2/33586 (0.0%)	0.85	41/45430 (0.1%)

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	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	867	ILE	CG1-CD1	5.94	1.91	1.50
1	A	56	PRO	C-N	5.29	1.46	1.34

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	P	8	C	P-O3'-C3'	13.71	136.16	119.70
13	N	6	DA	O4'-C1'-N9	9.07	114.35	108.00
16	T	15	DC	O4'-C1'-N1	8.13	113.69	108.00
14	P	9	C	P-O3'-C3'	7.96	129.25	119.70
16	T	15	DC	O4'-C4'-C3'	-7.65	101.41	106.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	55	ASP	Mainchain

## 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	11214	0	15	30	0
2	B	8810	0	0	11	0
3	C	2095	0	0	4	0
4	D	1417	0	0	1	0
5	E	1752	0	0	1	0
6	F	679	0	0	2	0
7	G	1340	0	0	2	0
8	H	1068	0	0	1	0
9	I	971	0	0	2	0
10	J	532	0	0	2	0
11	K	919	0	11	0	0
12	L	364	0	0	2	0
13	N	144	0	0	0	0
14	P	100	0	0	0	0
15	S	1294	0	0	4	0
16	T	266	0	0	0	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
17	S	1	0	0	0	0
18	A	1	0	0	0	0
19	A	4	0	3	1	0
19	B	4	0	3	0	0
20	A	15	0	17	2	0
21	L	10	0	14	0	0
All	All	33008	0	63	50	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.

The worst 5 of 50 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	1.91	1.49
7:G:1:MET:SD	7:G:2:PHE:N	2.44	0.91
1:A:567:LYS:O	1:A:569:LYS:N	2.14	0.80
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.26	0.69
9:I:7:CYS:SG	9:I:8:ARG:O	2.53	0.66

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	1418/1733 (82%)	1255 (88%)	105 (7%)	58 (4%)	4	35
2	B	1090/1224 (89%)	963 (88%)	92 (8%)	35 (3%)	6	43
3	C	264/318 (83%)	238 (90%)	17 (6%)	9 (3%)	6	42
4	D	173/221 (78%)	153 (88%)	14 (8%)	6 (4%)	6	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	212/215 (99%)	202 (95%)	8 (4%)	2 (1%)	25	76
6	F	82/155 (53%)	77 (94%)	4 (5%)	1 (1%)	19	71
7	G	169/171 (99%)	154 (91%)	12 (7%)	3 (2%)	13	61
8	H	129/146 (88%)	101 (78%)	18 (14%)	10 (8%)	1	14
9	I	117/122 (96%)	98 (84%)	16 (14%)	3 (3%)	8	50
10	J	63/70 (90%)	54 (86%)	6 (10%)	3 (5%)	4	30
11	K	112/120 (93%)	107 (96%)	5 (4%)	0	100	100
12	L	44/70 (63%)	27 (61%)	8 (18%)	9 (20%)	0	1
15	S	162/178 (91%)	129 (80%)	20 (12%)	13 (8%)	1	13
All	All	4035/4743 (85%)	3558 (88%)	325 (8%)	152 (4%)	5	37

5 of 152 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	42	ASP
1	A	65	LEU
1	A	66	LYS
1	A	68	GLN

### 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	1246/1520 (82%)	1073 (86%)	173 (14%)	5	25
2	B	962/1061 (91%)	832 (86%)	130 (14%)	6	27
3	C	234/274 (85%)	199 (85%)	35 (15%)	4	21
4	D	157/200 (78%)	120 (76%)	37 (24%)	1	4
5	E	196/197 (100%)	178 (91%)	18 (9%)	13	48
6	F	74/137 (54%)	69 (93%)	5 (7%)	22	67
7	G	152/152 (100%)	125 (82%)	27 (18%)	2	13
8	H	117/128 (91%)	103 (88%)	14 (12%)	7	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	113/116 (97%)	90 (80%)	23 (20%)	2	8
10	J	60/65 (92%)	48 (80%)	12 (20%)	2	9
11	K	99/102 (97%)	87 (88%)	12 (12%)	7	33
12	L	40/57 (70%)	30 (75%)	10 (25%)	1	3
15	S	141/153 (92%)	117 (83%)	24 (17%)	3	15
All	All	3591/4162 (86%)	3071 (86%)	520 (14%)	5	23

5 of 520 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	601	ARG
2	B	1150	ARG
11	K	47	ARG
2	B	624	LEU
2	B	868	MET

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	5/5 (100%)	3 (60%)	2 (40%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	8	C
14	P	9	C
14	P	10	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
14	P	7	C
14	P	8	C

## 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	$\# Z  > 2$
16	BRU	T	22	14,16	19,21,22	0.95	1 (5%)	22,30,33	2.92	5 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BRU	T	22	14,16	-	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)
16	T	22	BRU	C4-C5	2.22	1.43	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	T	22	BRU	C6-N1-C2	-11.18	119.23	122.41
16	T	22	BRU	N3-C2-N1	6.01	120.99	115.97
16	T	22	BRU	O4'-C1'-N1	3.10	113.51	107.68
16	T	22	BRU	C5-C6-N1	2.23	121.14	119.67
16	T	22	BRU	C4-N3-C2	-2.01	121.27	125.39

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 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 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$
19	ACT	A	1734	-	1,3,3	0.83	0	0,3,3	0.00	-
20	EPE	A	1735	-	15,15,15	0.52	0	20,20,20	2.15	8 (40%)
19	ACT	B	1225	-	1,3,3	3.32	1 (100%)	0,3,3	0.00	-
21	PGE	L	71	-	9,9,9	0.48	0	8,8,8	0.32	0

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
19	ACT	A	1734	-	-	0/0/0/0	0/0/0/0
20	EPE	A	1735	-	-	0/9/19/19	0/1/1/1
19	ACT	B	1225	-	-	0/0/0/0	0/0/0/0
21	PGE	L	71	-	-	0/7/7/7	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1225	ACT	CH3-C	3.32	1.53	1.48

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1735	EPE	C5-N4-C3	4.30	119.54	108.86
20	A	1735	EPE	C7-N4-C3	3.61	120.64	111.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1735	EPE	C9-C10-S	-3.54	100.39	113.01
20	A	1735	EPE	C7-N4-C5	3.24	119.68	111.32
20	A	1735	EPE	O3S-S-C10	2.85	109.54	105.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1426/1733 (82%)	-0.08	3 (0%) 93 70	67, 109, 163, 215	0
2	B	1108/1224 (90%)	0.01	7 (0%) 86 46	69, 126, 191, 217	0
3	C	266/318 (83%)	-0.15	0 100 100	86, 116, 160, 193	0
4	D	177/221 (80%)	-0.12	1 (0%) 86 46	81, 118, 183, 202	0
5	E	214/215 (99%)	-0.09	0 100 100	88, 141, 188, 203	0
6	F	84/155 (54%)	-0.22	0 100 100	70, 90, 123, 136	0
7	G	171/171 (100%)	-0.06	0 100 100	82, 105, 148, 171	0
8	H	133/146 (91%)	0.15	0 100 100	121, 158, 197, 205	0
9	I	119/122 (97%)	0.07	4 (3%) 43 10	123, 156, 197, 216	0
10	J	65/70 (92%)	-0.09	0 100 100	95, 117, 159, 177	0
11	K	114/120 (95%)	-0.12	0 100 100	85, 112, 157, 173	0
12	L	46/70 (65%)	-0.10	1 (2%) 59 16	93, 158, 183, 202	0
13	N	7/14 (50%)	0.74	1 (14%) 3 1	217, 222, 231, 234	0
14	P	5/5 (100%)	0.00	0 100 100	238, 239, 244, 247	0
15	S	164/178 (92%)	0.28	4 (2%) 56 15	116, 181, 240, 254	0
16	T	13/27 (48%)	0.18	0 100 100	162, 195, 247, 252	0
All	All	4112/4789 (85%)	-0.04	21 (0%) 88 51	67, 119, 191, 254	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	S	157	TYR	4.5
9	I	118	ARG	3.5
2	B	470	LYS	3.3
1	A	69	THR	3.1
2	B	476	ARG	3.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
16	BRU	T	22	20/21	0.23	1.71	138,213,293,294	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
19	ACT	A	1734	4/4	0.42	5.45	72,95,126,151	0
21	PGE	L	71	10/10	0.26	1.75	116,149,279,292	0
17	ZN	I	1121	1/1	0.14	0.92	130,130,130,130	0
17	ZN	A	2457	1/1	0.19	0.38	87,87,87,87	0
17	ZN	B	2225	1/1	0.22	0.32	94,94,94,94	0
20	EPE	A	1735	15/15	0.21	0.26	25,77,245,245	0
19	ACT	B	1225	4/4	0.18	-0.19	46,51,87,298	0
17	ZN	C	1269	1/1	0.14	-0.45	94,94,94,94	0
17	ZN	L	1071	1/1	0.10	-0.48	158,158,158,158	0
18	MG	A	2458	1/1	0.19	-0.64	83,83,83,83	0
17	ZN	J	1066	1/1	0.24	-0.79	103,103,103,103	0
17	ZN	S	999	1/1	0.06	-1.02	215,215,215,215	0
17	ZN	A	2456	1/1	0.07	-1.79	145,145,145,145	0
17	ZN	I	1122	1/1	0.05	-2.39	186,186,186,186	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.