



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:57 pm BST

PDB ID : 3HW3  
Title : The crystal structure of avian influenza virus PA\_N in complex with UMP  
Authors : Zhao, C.; Lou, Z.; Guo, Y.; Ma, M.; Chen, Y.; Rao, Z.  
Deposited on : 2009-06-17  
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

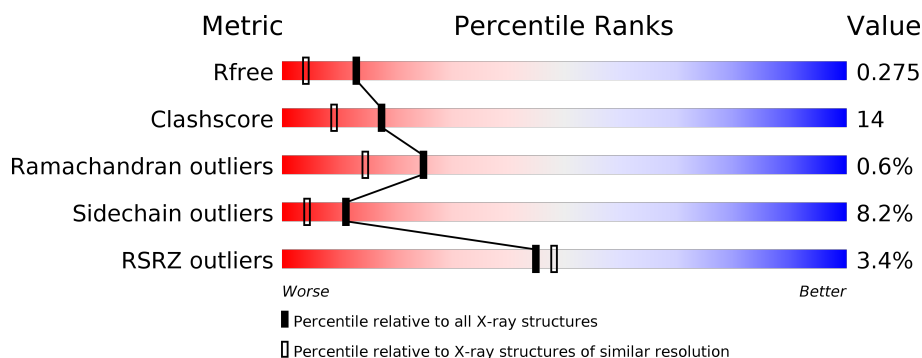
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	261	
1	B	261	
1	C	261	
1	D	261	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	U5P	A	257	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6372 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Polymerase acidic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	177	Total	C	N	O	S	0	0	0
			1462	924	251	276	11			
1	B	180	Total	C	N	O	S	0	0	0
			1496	948	258	279	11			
1	C	177	Total	C	N	O	S	0	0	0
			1463	925	253	274	11			
1	D	176	Total	C	N	O	S	0	0	0
			1453	919	250	273	11			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	EXPRESSION TAG	UNP Q9Q0U9
A	-3	PRO	-	EXPRESSION TAG	UNP Q9Q0U9
A	-2	LEU	-	EXPRESSION TAG	UNP Q9Q0U9
A	-1	GLY	-	EXPRESSION TAG	UNP Q9Q0U9
A	0	SER	-	EXPRESSION TAG	UNP Q9Q0U9
A	201	ILE	VAL	SEE REMARK 999	UNP Q9Q0U9
B	-4	GLY	-	EXPRESSION TAG	UNP Q9Q0U9
B	-3	PRO	-	EXPRESSION TAG	UNP Q9Q0U9
B	-2	LEU	-	EXPRESSION TAG	UNP Q9Q0U9
B	-1	GLY	-	EXPRESSION TAG	UNP Q9Q0U9
B	0	SER	-	EXPRESSION TAG	UNP Q9Q0U9
B	201	ILE	VAL	SEE REMARK 999	UNP Q9Q0U9
C	-4	GLY	-	EXPRESSION TAG	UNP Q9Q0U9
C	-3	PRO	-	EXPRESSION TAG	UNP Q9Q0U9
C	-2	LEU	-	EXPRESSION TAG	UNP Q9Q0U9
C	-1	GLY	-	EXPRESSION TAG	UNP Q9Q0U9
C	0	SER	-	EXPRESSION TAG	UNP Q9Q0U9
C	201	ILE	VAL	SEE REMARK 999	UNP Q9Q0U9
D	-4	GLY	-	EXPRESSION TAG	UNP Q9Q0U9
D	-3	PRO	-	EXPRESSION TAG	UNP Q9Q0U9
D	-2	LEU	-	EXPRESSION TAG	UNP Q9Q0U9

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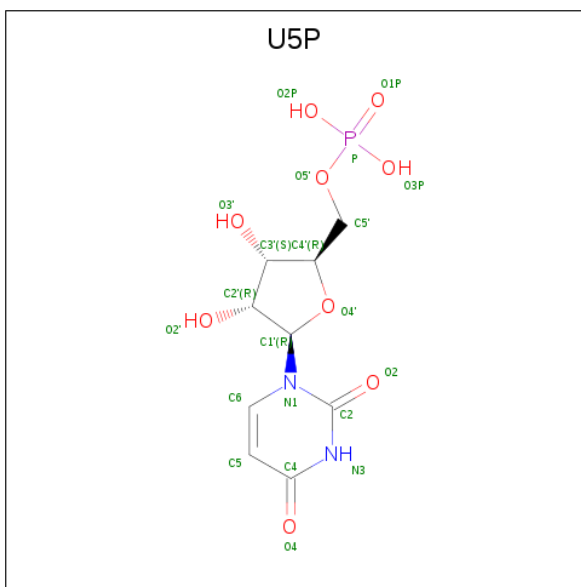
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	EXPRESSION TAG	UNP Q9Q0U9
D	0	SER	-	EXPRESSION TAG	UNP Q9Q0U9
D	201	ILE	VAL	SEE REMARK 999	UNP Q9Q0U9

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is URIDINE-5'-MONOPHOSPHATE (three-letter code: U5P) (formula: C<sub>9</sub>H<sub>13</sub>N<sub>2</sub>O<sub>9</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			21	9	2	9	1		

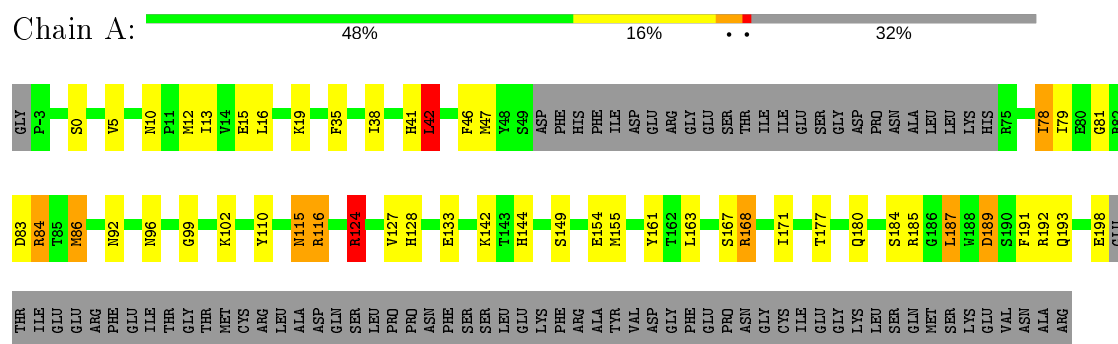
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	144	Total 144	O 144	0	0
4	B	112	Total 112	O 112	0	0
4	C	111	Total 111	O 111	0	0
4	D	106	Total 106	O 106	0	0

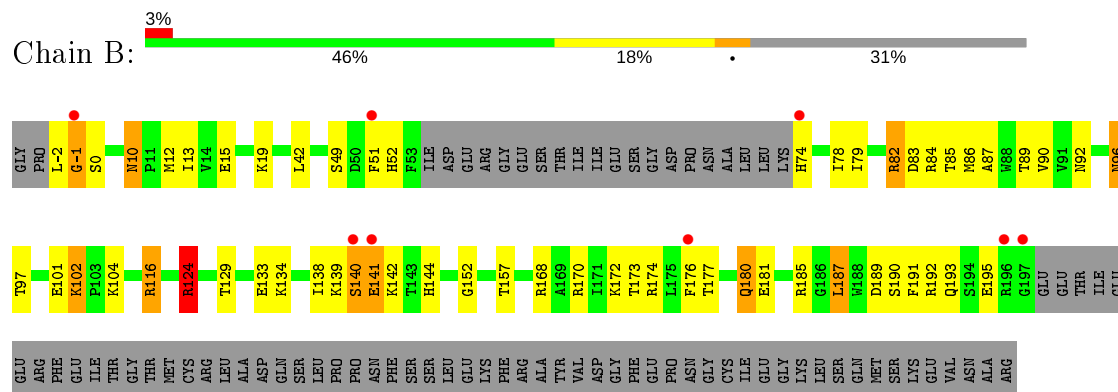
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

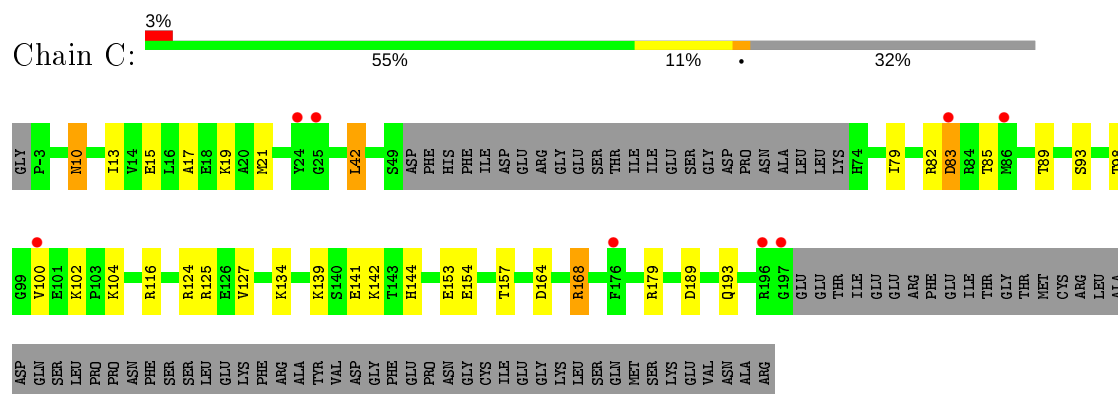
#### • Molecule 1: Polymerase acidic protein



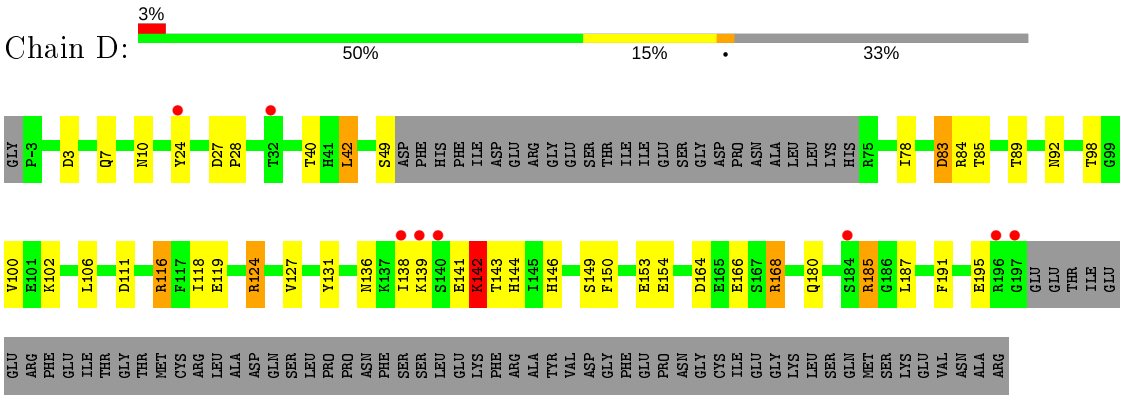
#### • Molecule 1: Polymerase acidic protein



#### • Molecule 1: Polymerase acidic protein



● Molecule 1: Polymerase acidic protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.13Å 59.70Å 66.85Å 96.28° 96.65° 109.44°	Depositor
Resolution (Å)	50.00 – 1.90 47.58 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.9 (50.00-1.90) 95.9 (47.58-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.42 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.218 , 0.276 0.217 , 0.275	Depositor DCC
$R_{free}$ test set	2806 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.7	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 51.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6372	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.63% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, U5P

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	0.78	0/1491	0.89	7/2000 (0.3%)
1	B	0.77	0/1528	0.96	6/2050 (0.3%)
1	C	0.70	0/1493	0.86	6/2003 (0.3%)
1	D	0.74	0/1482	0.92	7/1988 (0.4%)
All	All	0.75	0/5994	0.91	26/8041 (0.3%)

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	B	0	1

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	ARG	NE-CZ-NH1	10.59	125.59	120.30
1	B	168	ARG	NE-CZ-NH2	-10.21	115.19	120.30
1	C	168	ARG	NE-CZ-NH2	-10.01	115.29	120.30
1	D	116	ARG	NE-CZ-NH1	9.74	125.17	120.30
1	D	168	ARG	NE-CZ-NH2	-9.51	115.55	120.30
1	A	116	ARG	NE-CZ-NH2	-9.32	115.64	120.30
1	B	168	ARG	NE-CZ-NH1	8.93	124.77	120.30
1	B	116	ARG	NE-CZ-NH2	-8.72	115.94	120.30
1	C	168	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	D	168	ARG	NE-CZ-NH1	8.29	124.44	120.30
1	D	116	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	B	116	ARG	NE-CZ-NH1	7.29	123.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	ARG	NE-CZ-NH2	-7.11	116.74	120.30
1	C	42	LEU	CB-CG-CD1	6.90	122.73	111.00
1	A	116	ARG	CD-NE-CZ	5.86	131.80	123.60
1	B	124	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	D	164	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	124	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	B	124	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	C	164	ASP	CB-CG-OD2	5.75	123.48	118.30
1	C	124	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	D	42	LEU	CA-CB-CG	5.36	127.62	115.30
1	D	106	LEU	CA-CB-CG	5.34	127.58	115.30
1	A	42	LEU	CB-CG-CD1	5.18	119.81	111.00
1	C	124	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	42	LEU	CA-CB-CG	5.07	126.95	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	-1	GLY	Peptide

## 5.2 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1462	0	1435	49	0
1	B	1496	0	1458	52	0
1	C	1463	0	1436	21	0
1	D	1453	0	1429	39	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	21	0	11	10	0
4	A	144	0	0	3	0
4	B	112	0	0	13	0
4	C	111	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	106	0	0	9	0
All	All	6372	0	5769	160	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (160) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:257:U5P:H3'	3:A:257:U5P:C6	1.67	1.18
1:A:38:ILE:HG12	3:A:257:U5P:H2'	1.23	1.13
3:A:257:U5P:H6	3:A:257:U5P:C3'	1.73	1.13
1:B:170:ARG:O	1:B:173:THR:HG22	1.58	1.04
1:B:173:THR:HB	4:B:400:HOH:O	1.62	0.98
1:B:10:ASN:HD21	1:B:12:MET:HB3	1.28	0.98
1:A:10:ASN:HD21	1:A:12:MET:HB3	1.29	0.96
1:A:92:ASN:HD21	1:A:102:LYS:NZ	1.68	0.92
1:A:92:ASN:HD21	1:A:102:LYS:HZ2	1.06	0.91
1:A:168:ARG:HH11	1:A:168:ARG:CB	1.87	0.88
1:A:127:VAL:HG23	1:A:155:MET:CE	2.04	0.88
1:D:141:GLU:CA	1:D:142:LYS:HB2	2.04	0.87
1:A:38:ILE:CG1	3:A:257:U5P:H2'	2.04	0.87
1:A:127:VAL:HG23	1:A:155:MET:HE3	1.54	0.87
1:C:116:ARG:HD2	1:C:144:HIS:HB2	1.60	0.83
1:B:79:ILE:O	1:B:82:ARG:HG2	1.79	0.83
1:B:85:THR:O	1:B:89:THR:HG23	1.78	0.81
1:A:10:ASN:ND2	1:A:12:MET:HB3	1.95	0.81
1:B:173:THR:CB	4:B:400:HOH:O	2.23	0.81
1:A:124:ARG:HD2	1:A:191:PHE:O	1.82	0.79
1:A:168:ARG:HH11	1:A:168:ARG:HB2	1.47	0.78
1:C:15:GLU:O	1:C:19:LYS:HG2	1.83	0.78
1:A:116:ARG:HD2	1:A:144:HIS:HB2	1.65	0.78
3:A:257:U5P:H6	3:A:257:U5P:H3'	0.82	0.77
1:D:85:THR:O	1:D:89:THR:HG23	1.85	0.77
1:D:142:LYS:HE2	4:D:371:HOH:O	1.84	0.77
1:B:176:PHE:CD1	4:B:1034:HOH:O	2.37	0.76
1:C:116:ARG:NH1	4:C:1021:HOH:O	2.19	0.75
1:C:98:THR:OG1	1:C:100:VAL:HG23	1.86	0.75
1:A:41:HIS:HB3	3:A:257:U5P:H1'	1.69	0.74
1:B:82:ARG:HG3	1:B:87:ALA:HB2	1.70	0.73
1:D:141:GLU:N	1:D:142:LYS:HB2	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ARG:HB2	1:A:168:ARG:NH1	2.03	0.72
1:D:138:ILE:O	4:D:1029:HOH:O	2.08	0.71
1:A:42:LEU:HD13	3:A:257:U5P:HN3	1.55	0.71
1:B:74:HIS:O	4:B:1066:HOH:O	2.08	0.70
1:A:92:ASN:ND2	1:A:102:LYS:NZ	2.38	0.70
1:B:92:ASN:HD21	1:B:102:LYS:HE3	1.56	0.70
1:B:52:HIS:O	1:B:74:HIS:O	2.10	0.70
1:B:185:ARG:HB2	1:B:187:LEU:HD22	1.74	0.69
1:B:116:ARG:NE	4:B:1064:HOH:O	2.04	0.68
1:B:124:ARG:HD2	1:B:191:PHE:O	1.92	0.68
1:B:116:ARG:NH2	4:B:1064:HOH:O	2.20	0.67
1:A:154:GLU:OE1	1:A:168:ARG:NH1	2.27	0.67
1:D:142:LYS:HA	4:D:407:HOH:O	1.95	0.67
1:D:141:GLU:OE1	1:D:141:GLU:HA	1.94	0.66
1:B:49:SER:OG	1:B:78:ILE:HD11	1.96	0.66
1:A:84:ARG:HH11	1:B:84:ARG:HH12	1.44	0.66
1:A:10:ASN:HD22	1:A:13:ILE:H	1.45	0.64
1:B:74:HIS:N	4:B:1017:HOH:O	2.31	0.64
1:D:119:GLU:OE1	4:D:1003:HOH:O	2.14	0.64
1:D:116:ARG:HD2	4:D:1036:HOH:O	1.97	0.64
1:B:10:ASN:ND2	1:B:12:MET:HB3	2.09	0.64
1:C:10:ASN:ND2	1:C:13:ILE:H	1.96	0.63
1:A:86:MET:HG2	4:A:265:HOH:O	1.98	0.63
1:D:139:LYS:HB3	4:D:1029:HOH:O	1.98	0.63
1:B:176:PHE:CE1	4:B:1034:HOH:O	2.52	0.62
1:A:84:ARG:NH1	1:B:84:ARG:HH12	1.96	0.62
1:A:38:ILE:HG12	3:A:257:U5P:C2'	2.15	0.62
1:A:198:GLU:CD	1:A:198:GLU:H	2.01	0.62
3:A:257:U5P:C3'	3:A:257:U5P:C6	2.39	0.61
1:D:49:SER:OG	1:D:78:ILE:HD11	2.00	0.61
1:B:190:SER:HA	1:B:193:GLN:HG3	1.83	0.61
1:A:163:LEU:HD13	1:A:167:SER:OG	2.01	0.61
1:A:128:HIS:CG	1:A:155:MET:HE1	2.37	0.59
1:B:96:ASN:C	1:B:96:ASN:HD22	2.06	0.59
1:B:116:ARG:HD2	1:B:144:HIS:HB2	1.86	0.58
1:B:96:ASN:HD22	1:B:97:THR:N	2.02	0.58
1:C:127:VAL:CG1	1:C:153:GLU:HG2	2.33	0.58
1:D:141:GLU:HB2	1:D:142:LYS:HD3	1.84	0.58
1:B:92:ASN:ND2	1:B:102:LYS:HE3	2.19	0.57
1:A:161:TYR:HB3	1:A:168:ARG:HE	1.69	0.57
1:A:168:ARG:HH11	1:A:168:ARG:HB3	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:GLU:HG3	1:B:142:LYS:H	1.70	0.56
1:B:152:GLY:O	1:B:172:LYS:HD3	2.06	0.56
1:D:3:ASP:OD2	4:D:1018:HOH:O	2.18	0.56
1:D:92:ASN:ND2	1:D:102:LYS:HE2	2.21	0.56
1:D:141:GLU:HB2	1:D:142:LYS:HB2	1.88	0.55
1:D:141:GLU:CB	1:D:142:LYS:HB2	2.35	0.55
1:A:168:ARG:CB	1:A:168:ARG:NH1	2.61	0.54
1:B:173:THR:CA	4:B:400:HOH:O	2.51	0.54
1:B:124:ARG:HG2	1:B:195:GLU:OE1	2.07	0.54
1:B:124:ARG:HG3	1:B:192:ARG:HA	1.89	0.54
1:D:141:GLU:H	1:D:142:LYS:HB2	1.72	0.53
1:D:111:ASP:HB2	1:D:118:ILE:HD11	1.91	0.53
1:D:141:GLU:N	1:D:142:LYS:CB	2.71	0.53
1:B:92:ASN:HD21	1:B:102:LYS:CE	2.20	0.52
1:B:129:THR:O	1:B:133:GLU:HG3	2.08	0.52
1:C:193:GLN:HG2	4:C:476:HOH:O	2.09	0.51
1:A:13:ILE:HD11	1:A:46:PHE:HD2	1.76	0.51
1:C:154:GLU:OE2	1:C:168:ARG:HD2	2.11	0.51
1:D:116:ARG:HD3	1:D:144:HIS:HB2	1.92	0.50
1:D:84:ARG:NH1	4:D:1006:HOH:O	2.39	0.50
1:D:40:THR:HG21	1:D:150:PHE:CZ	2.47	0.50
1:B:78:ILE:O	1:B:82:ARG:NH1	2.45	0.50
1:B:141:GLU:HB3	4:B:303:HOH:O	2.11	0.49
1:A:83:ASP:OD2	1:B:83:ASP:HB3	2.13	0.49
1:D:124:ARG:HD2	1:D:191:PHE:O	2.13	0.48
1:B:173:THR:CG2	1:B:174:ARG:N	2.77	0.48
1:A:5:VAL:HG11	1:A:35:PHE:CE1	2.48	0.48
1:B:190:SER:HA	1:B:193:GLN:CG	2.44	0.48
1:A:133:GLU:HB3	1:A:198:GLU:OE2	2.14	0.48
1:B:144:HIS:CE1	1:B:157:THR:HB	2.49	0.47
1:B:-1:GLY:O	1:B:187:LEU:HD11	2.14	0.47
1:A:189:ASP:O	1:A:193:GLN:HG3	2.14	0.47
1:A:83:ASP:CG	1:B:85:THR:HB	2.35	0.47
1:B:15:GLU:HG2	4:B:445:HOH:O	2.13	0.47
1:B:173:THR:HG23	1:B:174:ARG:N	2.30	0.47
1:B:138:ILE:HG13	1:B:140:SER:N	2.30	0.47
1:D:92:ASN:HD21	1:D:102:LYS:HE2	1.78	0.47
1:D:141:GLU:CA	1:D:142:LYS:CB	2.87	0.46
1:A:180:GLN:HG2	4:A:1023:HOH:O	2.15	0.46
1:A:198:GLU:HG3	4:A:1060:HOH:O	2.16	0.46
1:D:138:ILE:HD12	1:D:143:THR:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ASN:ND2	1:A:102:LYS:HZ3	2.14	0.46
1:C:10:ASN:ND2	1:C:13:ILE:HG13	2.31	0.46
1:D:127:VAL:HG13	1:D:149:SER:HB3	1.98	0.46
1:D:153:GLU:OE1	4:D:1047:HOH:O	2.21	0.46
1:C:83:ASP:N	1:C:83:ASP:OD2	2.28	0.45
1:C:144:HIS:CE1	1:C:157:THR:HB	2.51	0.45
1:D:98:THR:OG1	1:D:100:VAL:HG12	2.16	0.45
1:D:124:ARG:HG2	1:D:195:GLU:OE1	2.16	0.45
1:A:83:ASP:OD1	1:B:85:THR:HB	2.17	0.45
1:C:100:VAL:HA	1:C:142:LYS:NZ	2.32	0.45
1:C:127:VAL:HG11	1:C:153:GLU:HG2	1.99	0.45
1:C:85:THR:O	1:C:89:THR:HG23	2.18	0.44
1:C:17:ALA:O	1:C:21:MET:HG3	2.18	0.44
1:D:154:GLU:OE2	1:D:168:ARG:HD2	2.18	0.44
1:A:47:MET:HE3	1:A:171:ILE:HG12	2.00	0.44
1:B:82:ARG:HB3	1:B:82:ARG:HE	1.33	0.44
1:D:27:ASP:HA	1:D:28:PRO:HD2	1.87	0.43
1:D:92:ASN:HD21	1:D:102:LYS:CE	2.31	0.43
1:B:10:ASN:ND2	1:B:13:ILE:H	2.17	0.43
1:C:10:ASN:HD21	1:C:13:ILE:H	1.66	0.43
1:A:127:VAL:CG1	1:A:149:SER:HB3	2.48	0.43
1:D:141:GLU:HB2	1:D:142:LYS:CD	2.49	0.43
1:A:16:LEU:HD22	1:A:81:GLY:O	2.19	0.42
1:C:104:LYS:NZ	1:C:139:LYS:HB2	2.34	0.42
1:A:177:THR:O	1:A:180:GLN:HG3	2.19	0.42
1:A:185:ARG:HB2	1:A:187:LEU:HD22	2.00	0.42
1:B:86:MET:HG2	4:B:389:HOH:O	2.19	0.42
1:D:146:HIS:HE1	1:D:168:ARG:HD3	1.84	0.42
1:D:185:ARG:HE	1:D:185:ARG:HB2	1.70	0.42
1:C:125:ARG:NH1	4:C:1042:HOH:O	2.41	0.42
1:B:193:GLN:HG2	4:B:447:HOH:O	2.20	0.42
1:C:79:ILE:O	1:C:82:ARG:HG2	2.20	0.42
1:A:78:ILE:HG13	1:A:79:ILE:N	2.35	0.41
1:B:101:GLU:H	1:B:142:LYS:HZ1	1.66	0.41
1:A:110:TYR:OH	1:A:115:ASN:ND2	2.54	0.41
1:B:177:THR:O	1:B:180:GLN:HG3	2.20	0.41
1:A:46:PHE:CD1	1:A:78:ILE:HD13	2.55	0.41
1:C:82:ARG:NH2	4:C:357:HOH:O	2.48	0.41
1:D:83:ASP:N	1:D:83:ASP:OD2	2.38	0.41
1:A:19:LYS:HA	1:A:19:LYS:HD3	1.66	0.41
1:D:124:ARG:H	1:D:124:ARG:HG2	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ASP:HA	1:A:192:ARG:NH2	2.36	0.40
1:A:41:HIS:HD1	3:A:257:U5P:C2	2.34	0.40
1:B:79:ILE:HD12	1:B:90:VAL:HG22	2.03	0.40
1:D:131:TYR:CD2	1:D:131:TYR:C	2.94	0.40
1:C:127:VAL:HG13	1:C:153:GLU:HG2	2.01	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	173/261 (66%)	168 (97%)	4 (2%)	1 (1%)	25	15
1	B	176/261 (67%)	170 (97%)	4 (2%)	2 (1%)	14	5
1	C	173/261 (66%)	168 (97%)	5 (3%)	0	100	100
1	D	172/261 (66%)	163 (95%)	8 (5%)	1 (1%)	25	15
All	All	694/1044 (66%)	669 (96%)	21 (3%)	4 (1%)	25	15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	142	LYS
1	B	141	GLU
1	B	140	SER
1	A	99	GLY

### 5.3.2 Protein sidechains [i](#)

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	159/232 (68%)	145 (91%)	14 (9%)	10	4
1	B	162/232 (70%)	145 (90%)	17 (10%)	7	2
1	C	159/232 (68%)	150 (94%)	9 (6%)	20	11
1	D	158/232 (68%)	146 (92%)	12 (8%)	13	5
All	All	638/928 (69%)	586 (92%)	52 (8%)	11	4

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	SER
1	A	15	GLU
1	A	42	LEU
1	A	78	ILE
1	A	84	ARG
1	A	86	MET
1	A	96	ASN
1	A	115	ASN
1	A	124	ARG
1	A	142	LYS
1	A	168	ARG
1	A	184	SER
1	A	187	LEU
1	A	189	ASP
1	B	-2	LEU
1	B	0	SER
1	B	10	ASN
1	B	19	LYS
1	B	42	LEU
1	B	51	PHE
1	B	82	ARG
1	B	96	ASN
1	B	102	LYS
1	B	104	LYS
1	B	124	ARG
1	B	134	LYS
1	B	139	LYS
1	B	180	GLN
1	B	181	GLU
1	B	187	LEU

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Mol	Chain	Res	Type
1	B	189	ASP
1	C	10	ASN
1	C	42	LEU
1	C	83	ASP
1	C	93	SER
1	C	102	LYS
1	C	134	LYS
1	C	141	GLU
1	C	179	ARG
1	C	189	ASP
1	D	7	GLN
1	D	10	ASN
1	D	24	TYR
1	D	42	LEU
1	D	83	ASP
1	D	124	ARG
1	D	136	ASN
1	D	142	LYS
1	D	166	GLU
1	D	180	GLN
1	D	185	ARG
1	D	187	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	92	ASN
1	A	96	ASN
1	A	115	ASN
1	A	136	ASN
1	B	10	ASN
1	B	52	HIS
1	B	92	ASN
1	B	96	ASN
1	B	193	GLN
1	C	10	ASN
1	C	33	ASN
1	C	74	HIS
1	C	92	ASN
1	D	92	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 4 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
3	U5P	A	257	2	18,22,22	1.69	5 (27%)	21,33,33	2.79	10 (47%)

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
3	U5P	A	257	2	-	4/8/26/26	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	257	U5P	C2-N3	-3.01	1.32	1.38
3	A	257	U5P	O4'-C4'	-2.59	1.39	1.45
3	A	257	U5P	C3'-C4'	-2.26	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	257	U5P	O5'-C5'	-2.20	1.36	1.44
3	A	257	U5P	P-O3P	-2.10	1.46	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	257	U5P	C2'-C3'-C4'	-7.64	87.80	102.64
3	A	257	U5P	C3'-C2'-C1'	-5.01	93.43	100.98
3	A	257	U5P	O3P-P-O5'	-4.13	95.73	106.73
3	A	257	U5P	O4'-C4'-C3'	-3.24	98.70	105.11
3	A	257	U5P	O2P-P-O5'	-3.18	98.26	106.73
3	A	257	U5P	O4'-C1'-C2'	-2.86	102.75	106.93
3	A	257	U5P	C6-N1-C2	-2.78	116.78	121.20
3	A	257	U5P	P-O5'-C5'	-2.78	110.64	118.30
3	A	257	U5P	O3P-P-O1P	2.33	119.82	110.68
3	A	257	U5P	O3P-P-O2P	2.31	116.48	107.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	257	U5P	C2'-C1'-N1-C6
3	A	257	U5P	O4'-C1'-N1-C6
3	A	257	U5P	O4'-C4'-C5'-O5'
3	A	257	U5P	C3'-C4'-C5'-O5'

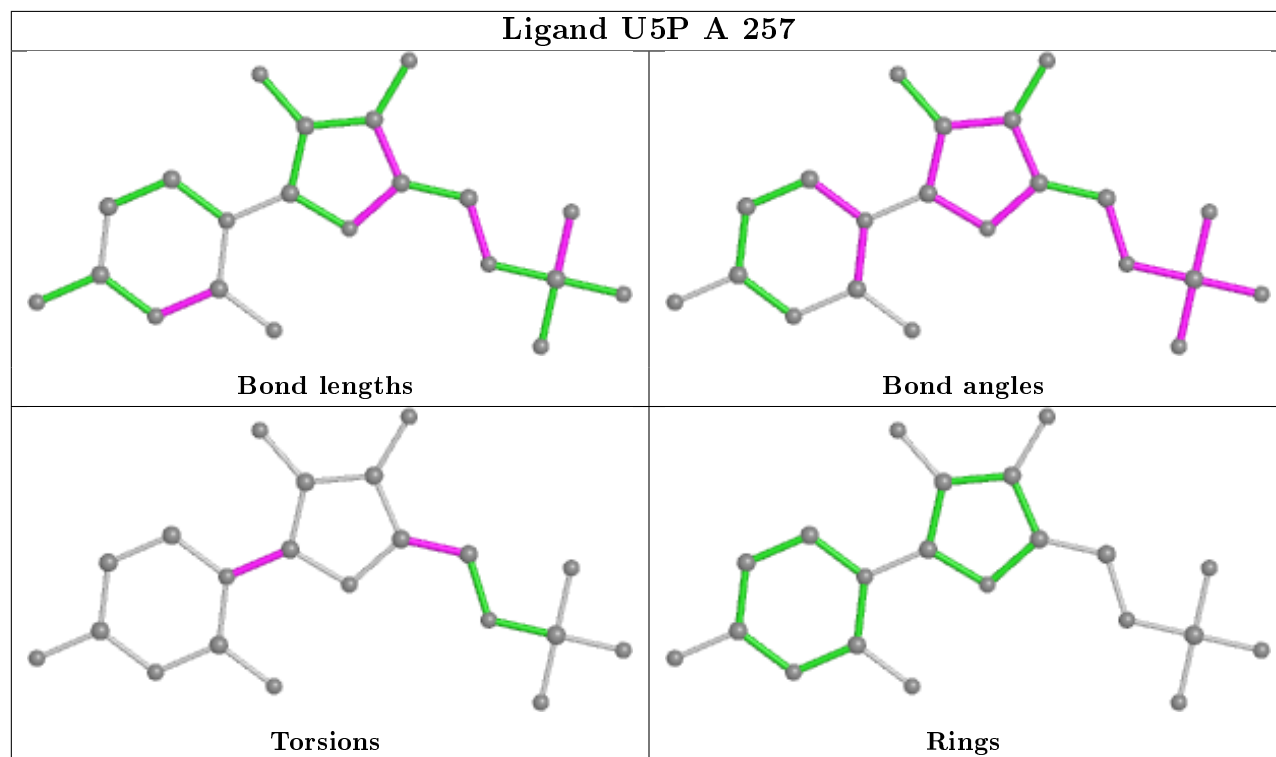
There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	257	U5P	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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	177/261 (67%)	0.07	0 100 100	14, 23, 38, 42	0
1	B	180/261 (68%)	0.27	8 (4%) 34 37	14, 25, 42, 52	0
1	C	177/261 (67%)	0.20	8 (4%) 33 36	18, 29, 43, 55	0
1	D	176/261 (67%)	0.35	8 (4%) 33 36	16, 28, 49, 60	0
All	All	710/1044 (68%)	0.22	24 (3%) 45 48	14, 26, 43, 60	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	196	ARG	7.4
1	D	197	GLY	7.1
1	D	196	ARG	5.3
1	B	140	SER	4.4
1	B	176	PHE	4.4
1	B	197	GLY	4.1
1	B	74	HIS	4.1
1	D	138	ILE	3.9
1	D	24	TYR	3.6
1	D	140	SER	3.5
1	C	197	GLY	3.5
1	C	25	GLY	3.1
1	C	24	TYR	3.1
1	C	196	ARG	2.9
1	D	184	SER	2.8
1	D	139	LYS	2.7
1	C	100	VAL	2.6
1	B	51	PHE	2.6
1	B	-1	GLY	2.4
1	C	83	ASP	2.3
1	D	32	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	86	MET	2.3
1	B	141	GLU	2.1
1	C	176	PHE	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

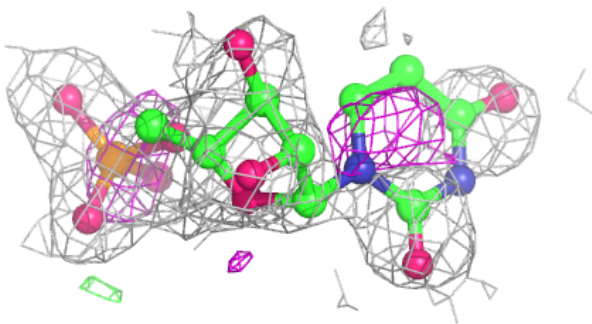
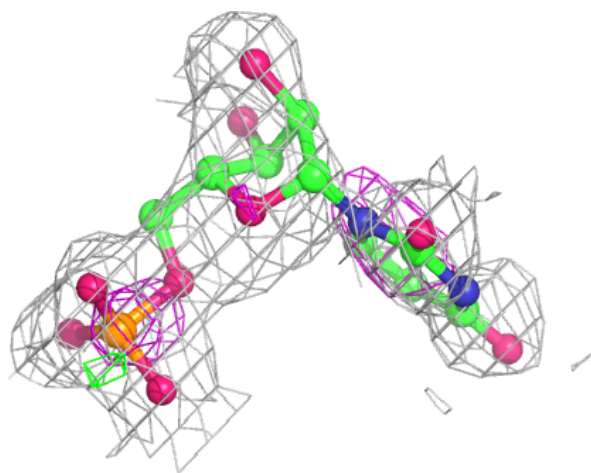
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	U5P	A	257	21/21	0.80	0.24	26,47,51,52	0
2	MG	B	999	1/1	0.93	0.05	23,23,23,23	0
2	MG	D	999	1/1	0.95	0.06	35,35,35,35	0
2	MG	C	999	1/1	0.97	0.04	23,23,23,23	0
2	MG	A	999	1/1	0.97	0.06	24,24,24,24	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around U5P A 257:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.