



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 12:37 am BST

PDB ID : 6OZS  
Title : Crystal structure of Mus musculus (Mm) Endonuclease V in complex with a 23mer RNA oligo containing an inosine after a 90 min soak in 10 mM Mg<sup>2+</sup>  
Authors : Samara, N.L.; Yang, W.  
Deposited on : 2019-05-15  
Resolution : 2.41 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:

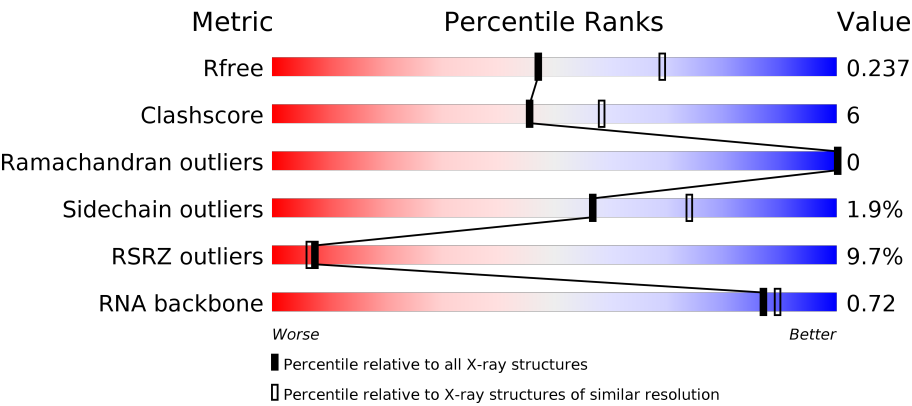
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.41 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 <sub>free</sub>	130704	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)
RNA backbone	3102	1080 (2.80-2.04)

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	247	<div><div>2%</div><div><div></div><div>87%</div><div>12%</div><div>.</div></div></div>
1	B	247	<div><div>17%</div><div><div></div><div>81%</div><div>17%</div><div>..</div></div></div>
2	c	11	<div><div>18%</div><div><div></div><div>36%</div><div>64%</div></div></div>
2	d	11	<div><div>18%</div><div><div></div><div>36%</div><div>64%</div></div></div>

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Mol	Chain	Length	Quality of chain
3	C	12	<div><div></div><div>83%</div><div>8%</div><div>8%</div></div>
3	D	12	<div><div></div><div>83%</div><div>8%</div><div>8%</div></div>

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 4621 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 Endonuclease V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	2	0
			1895	1204	342	341	8			
1	B	244	Total	C	N	O	S	0	3	0
			1919	1218	353	340	8			

- Molecule 2 is DNA/RNA hybrid called DNA/RNA (5'-R(\*CP\*GP\*GP\*UP\*AP\*AP\*CP\*C P\*C)-D(P\*I)-R(P\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	c	4	Total	C	N	O	P	0	0	0
			83	38	15	26	4			
2	d	4	Total	C	N	O	P	0	0	0
			83	38	15	26	4			

- Molecule 3 is a RNA chain called RNA (5'-R(P\*UP\*AP\*UP\*GP\*CP\*AP\*UP\*GP\*CP\*AP \*UP\*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	12	Total	C	N	O	P	0	0	0
			253	113	41	87	12			
3	D	12	Total	C	N	O	P	0	0	0
			253	113	41	87	12			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

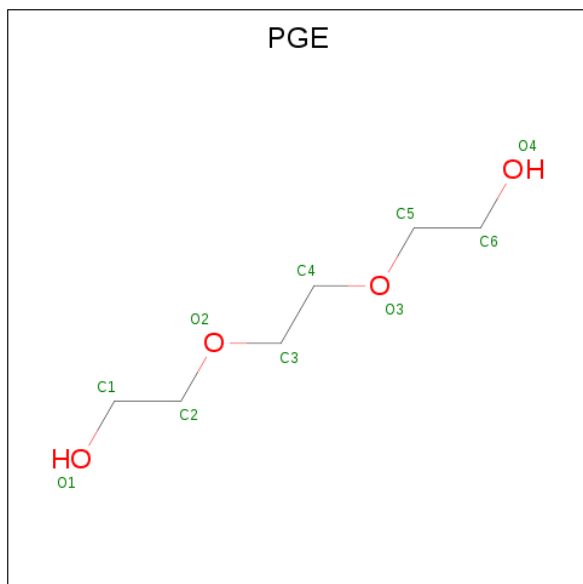
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Mg	0	0
			2	2		
4	A	2	Total	Mg	0	0
			2	2		
4	D	1	Total	Mg	0	0
			1	1		

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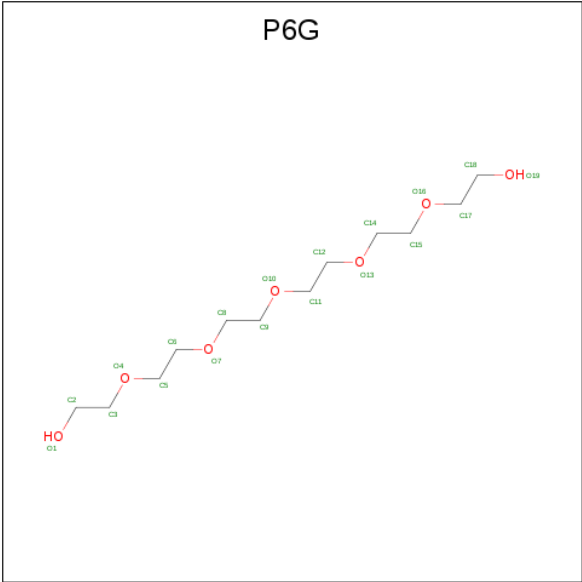
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



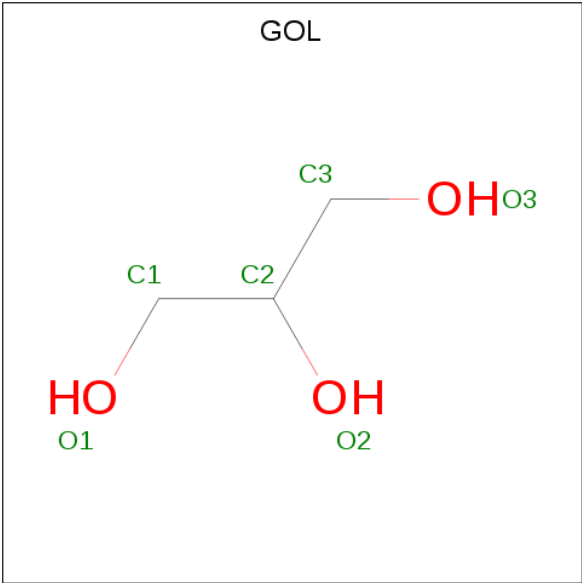
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula:  $C_{12}H_{26}O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			19	12	7		
6	A	1	Total	C	O	0	0
			19	12	7		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).

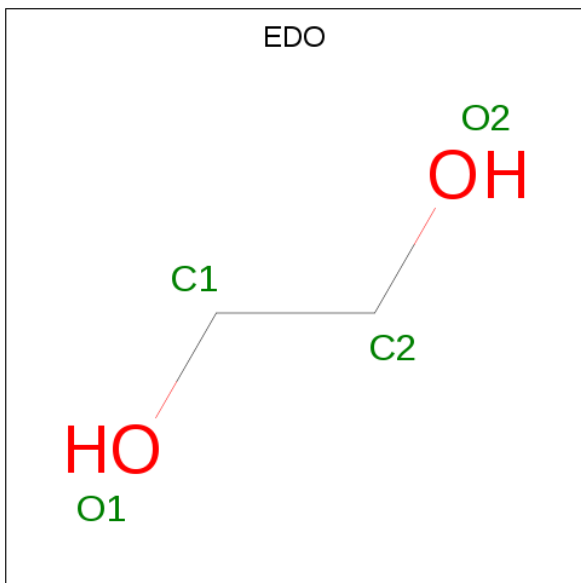


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

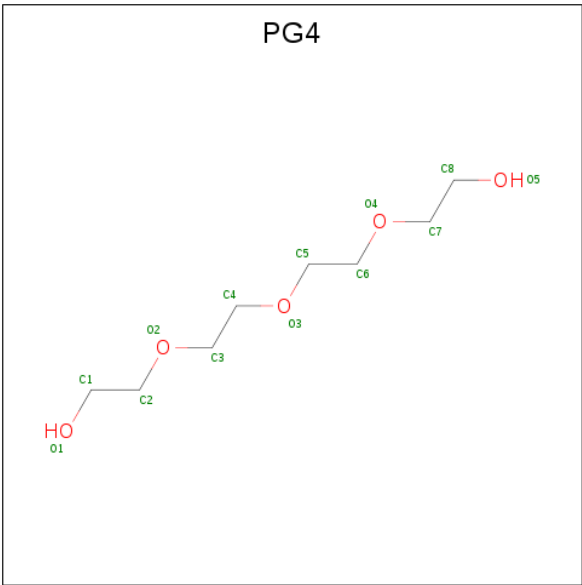
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Na	0	0
			1	1		
8	A	1	Total	Na	0	0
			1	1		

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		
9	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 11 is water.

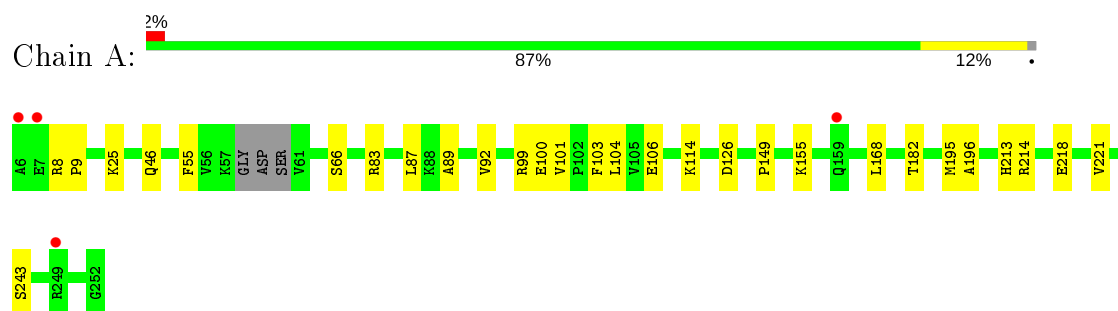
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	25	Total	O	0	0
			25	25		
11	B	5	Total	O	0	0
			5	5		
11	c	2	Total	O	0	0
			2	2		
11	C	3	Total	O	0	0
			3	3		
11	D	1	Total	O	0	0
			1	1		



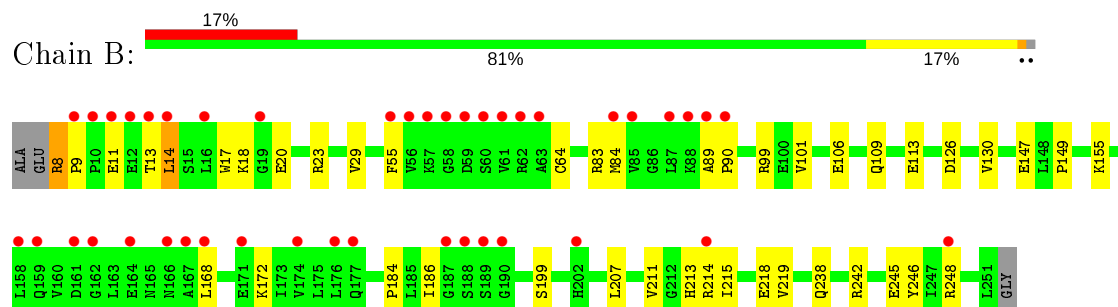
### 3 Residue-property plots [i](#)

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.

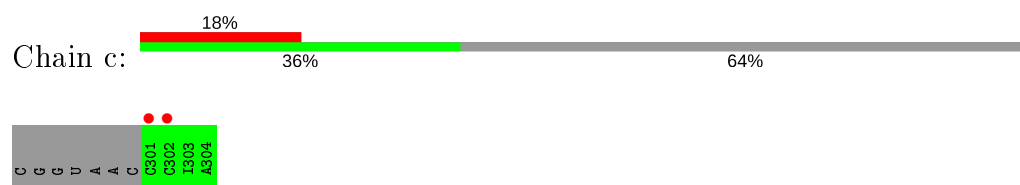
#### • Molecule 1: Endonuclease V



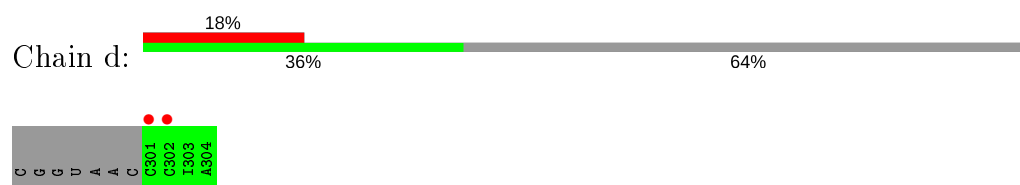
#### • Molecule 1: Endonuclease V




#### • Molecule 2: DNA/RNA (5'-R(\*CP\*GP\*GP\*UP\*AP\*AP\*CP\*CP\*C)-D(P\*I)-R(P\*A)-3')



#### • Molecule 2: DNA/RNA (5'-R(\*CP\*GP\*GP\*UP\*AP\*AP\*CP\*CP\*C)-D(P\*I)-R(P\*A)-3')




#### • Molecule 3: RNA (5'-R(P\*UP\*AP\*UP\*GP\*CP\*AP\*UP\*GP\*CP\*AP\*UP\*U)-3')

Chain C:  83% 8% 8%



- Molecule 3: RNA (5'-R(P\*UP\*AP\*UP\*GP\*CP\*AP\*UP\*GP\*CP\*AP\*UP\*U)-3')

Chain D:  83% 8% 8%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.09 Å 73.26 Å 155.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.25 – 2.41 41.71 – 2.41	Depositor EDS
% Data completeness (in resolution range)	95.2 (36.25-2.41) 95.5 (41.71-2.41)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.32 (at 2.39 Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.191 , 0.236 0.192 , 0.237	Depositor DCC
$R_{free}$ test set	1536 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.7	Xtriage
Anisotropy	0.919	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 60.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4621	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.27 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5943e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, PGE, NA, EDO, PG4, P6G

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	0.44	0/1937	0.61	0/2624
1	B	0.38	0/1966	0.58	0/2662
2	c	0.60	0/67	1.03	0/99
2	d	0.45	0/67	1.11	0/99
3	C	0.79	1/281 (0.4%)	0.92	0/433
3	D	0.81	1/281 (0.4%)	0.97	0/433
All	All	0.48	2/4599 (0.0%)	0.67	0/6350

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	318	U	OP3-P	-11.34	1.47	1.61
3	C	318	U	OP3-P	-10.57	1.48	1.61

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	1895	0	1932	23	0
1	B	1919	0	1967	25	0
2	c	83	0	43	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	d	83	0	43	0	0
3	C	253	0	128	2	0
3	D	253	0	128	3	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	10	0	14	0	0
5	B	10	0	14	0	0
6	A	38	0	52	5	0
7	A	12	0	16	3	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	4	0	6	0	0
9	D	4	0	6	0	0
10	A	13	0	18	0	0
11	A	25	0	0	1	0
11	B	5	0	0	0	0
11	C	3	0	0	0	0
11	D	1	0	0	0	0
11	c	2	0	0	0	0
All	All	4621	0	4367	51	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 6.

All (51) 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)
1:B:64:CYS:HG	1:B:246:TYR:HD2	0.97	0.93
1:A:83:ARG:HH12	1:A:106:GLU:HG2	1.45	0.81
1:A:83:ARG:NH1	1:A:106:GLU:HG2	2.06	0.70
1:A:89:ALA:O	1:A:99:ARG:NH1	2.26	0.67
1:B:83:ARG:NH1	1:B:106:GLU:OE1	2.27	0.66
1:B:84:MET:HG2	1:B:246:TYR:CE2	2.32	0.64
1:B:55:PHE:CD1	3:D:318:U:H4'	2.35	0.62
1:A:87:LEU:HD23	1:A:103:PHE:CE2	2.38	0.59
1:B:213:HIS:CD2	1:B:214[B]:ARG:HG3	2.38	0.59
1:B:238:GLN:OE1	1:B:242[A]:ARG:NH1	2.37	0.57
3:D:318:U:H2'	3:D:319:A:C8	2.39	0.57
1:A:114:LYS:NZ	7:A:306:GOL:H2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:LEU:HD12	1:B:18:LYS:HE3	1.85	0.57
1:B:20:GLU:OE1	1:B:23:ARG:NH2	2.38	0.56
1:B:147:GLU:O	1:B:214[A]:ARG:NH1	2.38	0.56
1:B:215:ILE:HD11	1:B:219:VAL:HG12	1.88	0.56
1:A:46:GLN:NE2	11:A:401:HOH:O	2.37	0.56
1:B:89:ALA:O	1:B:99:ARG:NH1	2.39	0.51
1:B:55:PHE:HD1	3:D:318:U:H4'	1.75	0.50
3:C:318:U:H2'	3:C:319:A:C8	2.46	0.50
1:A:114:LYS:HD3	7:A:306:GOL:H11	1.94	0.50
1:A:46:GLN:HG2	6:A:303:P6G:H21	1.94	0.49
1:B:109:GLN:O	1:B:113:GLU:HG3	2.13	0.49
1:B:245:GLU:HG3	1:B:248:ARG:NH1	2.28	0.49
1:B:8:ARG:HA	1:B:90:PRO:HG3	1.95	0.49
1:A:114:LYS:HZ2	7:A:306:GOL:H2	1.78	0.48
1:A:182:THR:HA	1:A:196:ALA:O	2.14	0.48
1:B:184:PRO:HB2	1:B:186:ILE:HD11	1.96	0.47
1:A:25:LYS:HE3	6:A:304:P6G:H81	1.95	0.47
1:A:9:PRO:HD2	1:A:92:VAL:HG21	1.97	0.47
1:A:213:HIS:CD2	1:A:214:ARG:HG3	2.51	0.46
1:A:66[B]:SER:HB2	1:A:243:SER:HB3	1.98	0.44
1:B:9:PRO:HD3	1:B:90:PRO:CG	2.47	0.44
1:B:13:THR:HG22	1:B:17:TRP:CE2	2.53	0.43
1:A:55:PHE:CD1	3:C:318:U:H4'	2.53	0.43
1:A:46:GLN:HG2	6:A:303:P6G:C2	2.49	0.43
1:B:126:ASP:OD1	1:B:155:LYS:NZ	2.52	0.43
1:B:199:SER:OG	1:B:207:LEU:HG	2.18	0.43
6:A:303:P6G:H151	6:A:303:P6G:H122	1.84	0.42
1:B:130:VAL:HG13	1:B:211:VAL:O	2.20	0.42
1:A:218:GLU:OE1	1:A:218:GLU:N	2.45	0.42
1:B:149:PRO:HA	1:B:213:HIS:O	2.20	0.42
1:B:168:LEU:O	1:B:172:LYS:HG3	2.20	0.42
1:A:100:GLU:O	1:A:104:LEU:HG	2.20	0.42
1:A:195:MET:HG3	1:A:221:VAL:HG21	2.01	0.42
1:A:149:PRO:HA	1:A:213:HIS:O	2.21	0.41
1:A:55:PHE:CE2	1:A:99:ARG:NH2	2.89	0.41
1:B:90:PRO:HA	1:B:99:ARG:NH1	2.36	0.41
1:A:126:ASP:OD1	1:A:155:LYS:NZ	2.53	0.41
1:A:25:LYS:HZ2	6:A:304:P6G:H52	1.85	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	242/247 (98%)	236 (98%)	6 (2%)	0	100	100
1	B	245/247 (99%)	239 (98%)	6 (2%)	0	100	100
All	All	487/494 (99%)	475 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	207/211 (98%)	204 (99%)	3 (1%)	67	81
1	B	210/211 (100%)	205 (98%)	5 (2%)	49	67
All	All	417/422 (99%)	409 (98%)	8 (2%)	57	74

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	101	VAL
1	A	168	LEU
1	B	8	ARG
1	B	11	GLU
1	B	14	LEU
1	B	101	VAL
1	B	218	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	c	2/11 (18%)	0	0
2	d	2/11 (18%)	0	0
3	C	11/12 (91%)	0	0
3	D	11/12 (91%)	0	0
All	All	26/46 (56%)	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 [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 8 are monoatomic - leaving 9 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	$\# Z  > 2$
10	PG4	A	309	-	12,12,12	0.55	0	11,11,11	0.59	0
9	EDO	D	402	-	3,3,3	0.51	0	2,2,2	0.75	0
5	PGE	B	302	-	9,9,9	0.41	0	8,8,8	0.38	0
6	P6G	A	303	-	18,18,18	0.54	0	17,17,17	0.38	0
6	P6G	A	304	-	18,18,18	0.55	0	17,17,17	0.43	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	GOL	A	306	-	5,5,5	0.37	0	5,5,5	0.19	0
7	GOL	A	305	-	5,5,5	0.39	0	5,5,5	0.26	0
9	EDO	A	308	-	3,3,3	0.55	0	2,2,2	0.10	0
5	PGE	A	302	-	9,9,9	0.35	0	8,8,8	0.42	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
10	PG4	A	309	-	-	7/10/10/10	-
9	EDO	D	402	-	-	1/1/1/1	-
5	PGE	B	302	-	-	5/7/7/7	-
6	P6G	A	303	-	-	8/16/16/16	-
6	P6G	A	304	-	-	10/16/16/16	-
7	GOL	A	306	-	-	2/4/4/4	-
7	GOL	A	305	-	-	0/4/4/4	-
9	EDO	A	308	-	-	0/1/1/1	-
5	PGE	A	302	-	-	5/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	306	GOL	O2-C2-C3-O3
10	A	309	PG4	C4-C3-O2-C2
6	A	304	P6G	O7-C8-C9-O10
6	A	303	P6G	O10-C11-C12-O13
6	A	304	P6G	O4-C5-C6-O7
6	A	304	P6G	O10-C11-C12-O13
6	A	303	P6G	O4-C5-C6-O7
6	A	303	P6G	O13-C14-C15-O16
10	A	309	PG4	O3-C5-C6-O4
6	A	304	P6G	O13-C14-C15-O16
10	A	309	PG4	O4-C7-C8-O5
5	B	302	PGE	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	A	302	PGE	O3-C5-C6-O4
7	A	306	GOL	C1-C2-C3-O3
5	A	302	PGE	O2-C3-C4-O3
10	A	309	PG4	O1-C1-C2-O2
6	A	304	P6G	O16-C17-C18-O19
6	A	303	P6G	C15-C14-O13-C12
6	A	303	P6G	O1-C2-C3-O4
5	A	302	PGE	C6-C5-O3-C4
10	A	309	PG4	C6-C5-O3-C4
6	A	303	P6G	C6-C5-O4-C3
6	A	304	P6G	C18-C17-O16-C15
5	B	302	PGE	C4-C3-O2-C2
5	B	302	PGE	C1-C2-O2-C3
5	B	302	PGE	C3-C4-O3-C5
10	A	309	PG4	C5-C6-O4-C7
6	A	303	P6G	C5-C6-O7-C8
6	A	304	P6G	C2-C3-O4-C5
6	A	304	P6G	O1-C2-C3-O4
9	D	402	EDO	O1-C1-C2-O2
6	A	304	P6G	C14-C15-O16-C17
5	A	302	PGE	O1-C1-C2-O2
5	A	302	PGE	C4-C3-O2-C2
6	A	304	P6G	C5-C6-O7-C8
10	A	309	PG4	O2-C3-C4-O3
6	A	303	P6G	C11-C12-O13-C14
5	B	302	PGE	O3-C5-C6-O4

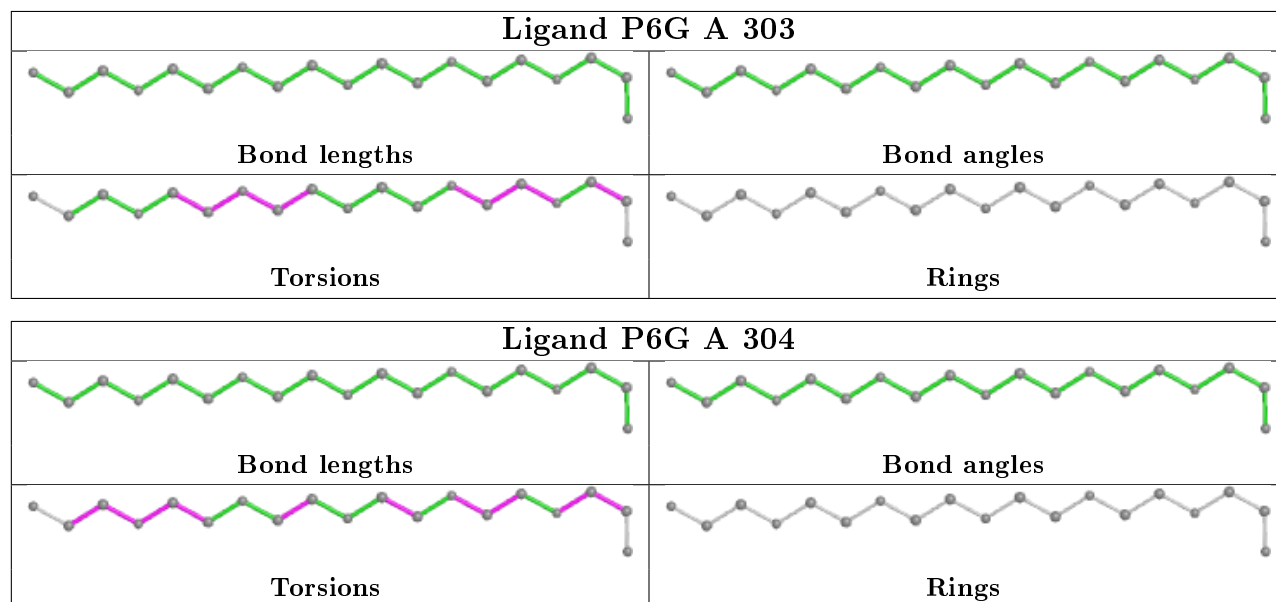
There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	303	P6G	3	0
6	A	304	P6G	2	0
7	A	306	GOL	3	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	244/247 (98%)	0.01	4 (1%) 72 69	39, 53, 81, 115	1 (0%)
1	B	244/247 (98%)	0.80	42 (17%) 1 1	48, 76, 126, 144	1 (0%)
2	c	3/11 (27%)	2.50	2 (66%) 0 0	57, 57, 106, 138	0
2	d	3/11 (27%)	2.57	2 (66%) 0 0	95, 95, 152, 180	0
3	C	12/12 (100%)	-0.36	0 100 100	61, 78, 114, 131	0
3	D	12/12 (100%)	-0.53	0 100 100	55, 82, 104, 109	0
All	All	518/540 (95%)	0.39	50 (9%) 7 6	39, 62, 115, 180	2 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	61	VAL	10.0
1	B	56	VAL	7.1
1	B	60	SER	6.4
1	B	58	GLY	5.9
1	B	87	LEU	5.5
2	c	301	C	5.2
1	B	62	ARG	5.2
1	B	59	ASP	4.8
1	B	164	GLU	4.6
2	d	301	C	4.6
1	A	6	ALA	4.2
1	B	10	PRO	4.0
2	d	302	C	3.9
1	B	189	SER	3.8
1	B	188	SER	3.8
1	B	168	LEU	3.8
1	B	187	GLY	3.7
1	B	159	GLN	3.7
1	B	174	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	176	LEU	3.5
1	B	57	LYS	3.4
2	c	302	C	3.1
1	B	158	LEU	3.0
1	B	84	MET	3.0
1	B	88	LYS	3.0
1	B	13	THR	2.9
1	B	63	ALA	2.9
1	B	55	PHE	2.9
1	B	167	ALA	2.8
1	A	159	GLN	2.7
1	B	9	PRO	2.7
1	B	202	HIS	2.7
1	B	90	PRO	2.7
1	A	249	ARG	2.6
1	B	12	GLU	2.6
1	B	177	GLN	2.6
1	B	214[A]	ARG	2.5
1	B	16	LEU	2.4
1	B	85	VAL	2.3
1	B	19	GLY	2.3
1	B	11	GLU	2.2
1	B	14	LEU	2.2
1	B	248	ARG	2.2
1	A	7	GLU	2.2
1	B	162	GLY	2.1
1	B	161	ASP	2.1
1	B	166	ASN	2.1
1	B	171	GLU	2.1
1	B	190	GLY	2.0
1	B	89	ALA	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

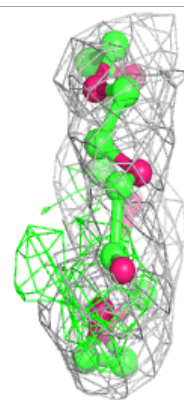
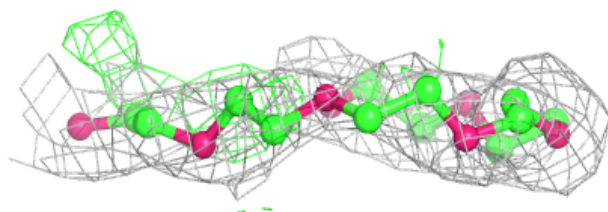
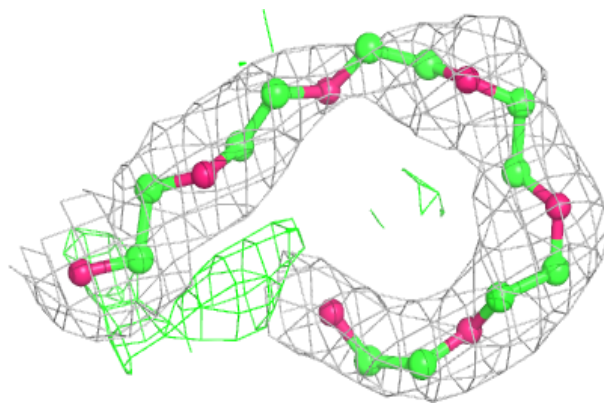
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
8	NA	A	307	1/1	0.66	0.15	67,67,67,67	0
6	P6G	A	304	19/19	0.72	0.27	68,80,91,95	0
4	MG	C	401	1/1	0.74	0.08	71,71,71,71	0
6	P6G	A	303	19/19	0.76	0.25	75,81,88,88	0
7	GOL	A	306	6/6	0.77	0.21	72,76,79,81	0
9	EDO	A	308	4/4	0.80	0.15	77,77,78,78	0
8	NA	B	303	1/1	0.80	0.17	76,76,76,76	0
5	PGE	B	302	10/10	0.81	0.19	80,83,92,92	0
9	EDO	D	402	4/4	0.83	0.30	80,81,82,85	0
4	MG	D	401	1/1	0.84	0.26	91,91,91,91	0
4	MG	A	310	1/1	0.84	0.16	65,65,65,65	0
10	PG4	A	309	13/13	0.89	0.27	62,71,81,82	0
7	GOL	A	305	6/6	0.90	0.10	62,71,74,76	0
5	PGE	A	302	10/10	0.91	0.26	69,75,78,83	0
4	MG	B	304	1/1	0.95	0.25	81,81,81,81	0
4	MG	B	301	1/1	0.97	0.08	79,79,79,79	0
4	MG	A	301	1/1	0.99	0.09	55,55,55,55	0

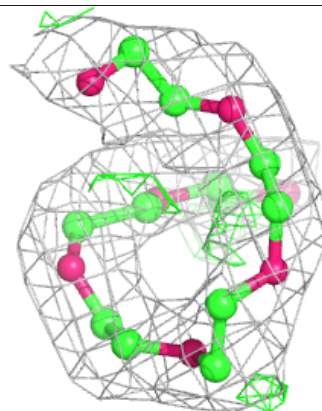
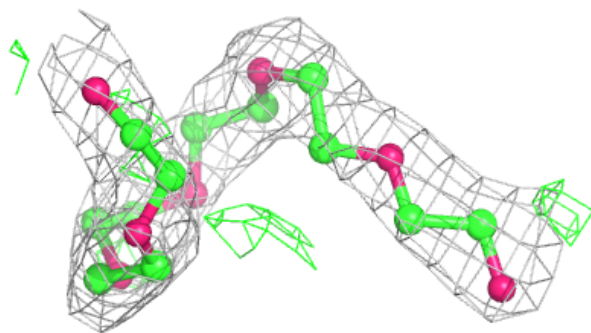
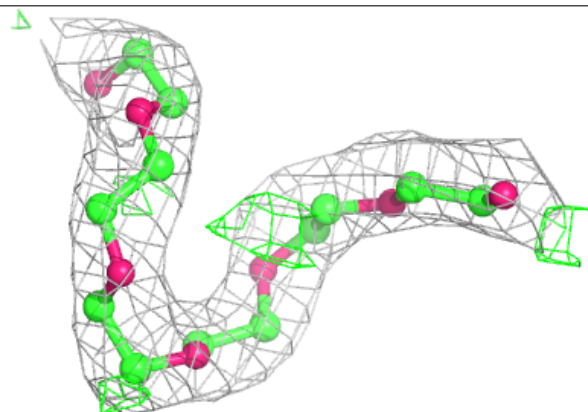
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around P6G A 304:**

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

**Electron density around P6G A 303:**

$2mF_o-DF_c$  (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.