



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 29, 2020 – 10:27 PM BST

PDB ID : 6PD2  
Title : PntC-AEPT: fusion protein of phosphonate-specific cytidyltransferase and 2-aminoethylphosphonate (AEP) transaminase from *Treponema denticola* in complex with cytidine monophosphate-AEP  
Authors : Suits, M.D.L.; Whiteside, J.  
Deposited on : 2019-06-18  
Resolution : 1.95 Å(reported)

This is a wwPDB X-ray Structure 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

<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 : 2.13  
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) : 2.13

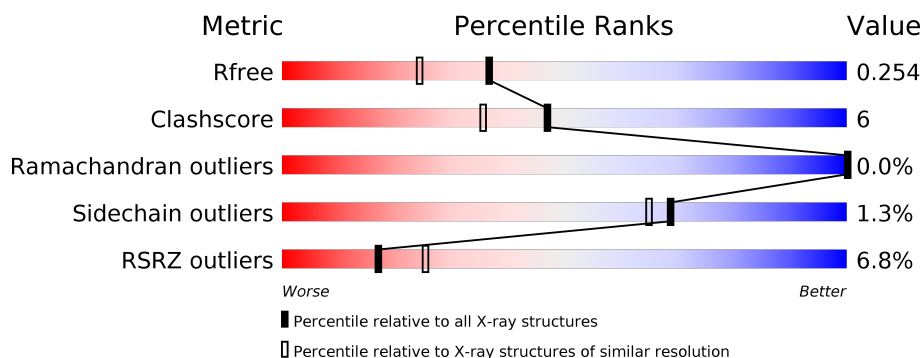
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	624	<div> <div>6%</div> <div> <div></div> <div>86%</div> <div>13%</div> <div></div> </div> </div>
1	B	624	<div> <div>8%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div></div> </div> </div>
1	C	624	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>13%</div> <div></div> </div> </div>
1	D	624	<div> <div>9%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div></div> </div> </div>

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
4	PO4	D	709	-	-	X	-
6	EDO	A	709	-	-	X	-
6	EDO	A	716	-	-	X	-
6	EDO	B	706	-	-	X	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 21090 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 Nucleotidyl transferase/aminotransferase, class V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	615	Total	C	N	O	S	0	0	0
			4831	3084	798	914	35			
1	B	615	Total	C	N	O	S	0	0	0
			4831	3084	798	914	35			
1	C	616	Total	C	N	O	S	0	0	0
			4838	3089	799	915	35			
1	D	608	Total	C	N	O	S	0	0	0
			4776	3051	786	904	35			

There are 32 discrepancies between the modelled and reference sequences:

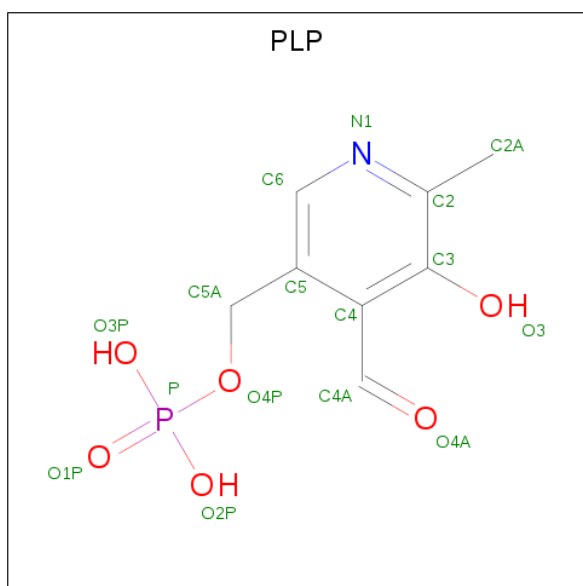
Chain	Residue	Modelled	Actual	Comment	Reference
A	617	LEU	-	expression tag	UNP Q73MU2
A	618	GLU	-	expression tag	UNP Q73MU2
A	619	HIS	-	expression tag	UNP Q73MU2
A	620	HIS	-	expression tag	UNP Q73MU2
A	621	HIS	-	expression tag	UNP Q73MU2
A	622	HIS	-	expression tag	UNP Q73MU2
A	623	HIS	-	expression tag	UNP Q73MU2
A	624	HIS	-	expression tag	UNP Q73MU2
B	617	LEU	-	expression tag	UNP Q73MU2
B	618	GLU	-	expression tag	UNP Q73MU2
B	619	HIS	-	expression tag	UNP Q73MU2
B	620	HIS	-	expression tag	UNP Q73MU2
B	621	HIS	-	expression tag	UNP Q73MU2
B	622	HIS	-	expression tag	UNP Q73MU2
B	623	HIS	-	expression tag	UNP Q73MU2
B	624	HIS	-	expression tag	UNP Q73MU2
C	617	LEU	-	expression tag	UNP Q73MU2
C	618	GLU	-	expression tag	UNP Q73MU2
C	619	HIS	-	expression tag	UNP Q73MU2
C	620	HIS	-	expression tag	UNP Q73MU2
C	621	HIS	-	expression tag	UNP Q73MU2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	622	HIS	-	expression tag	UNP Q73MU2
C	623	HIS	-	expression tag	UNP Q73MU2
C	624	HIS	-	expression tag	UNP Q73MU2
D	617	LEU	-	expression tag	UNP Q73MU2
D	618	GLU	-	expression tag	UNP Q73MU2
D	619	HIS	-	expression tag	UNP Q73MU2
D	620	HIS	-	expression tag	UNP Q73MU2
D	621	HIS	-	expression tag	UNP Q73MU2
D	622	HIS	-	expression tag	UNP Q73MU2
D	623	HIS	-	expression tag	UNP Q73MU2
D	624	HIS	-	expression tag	UNP Q73MU2

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).

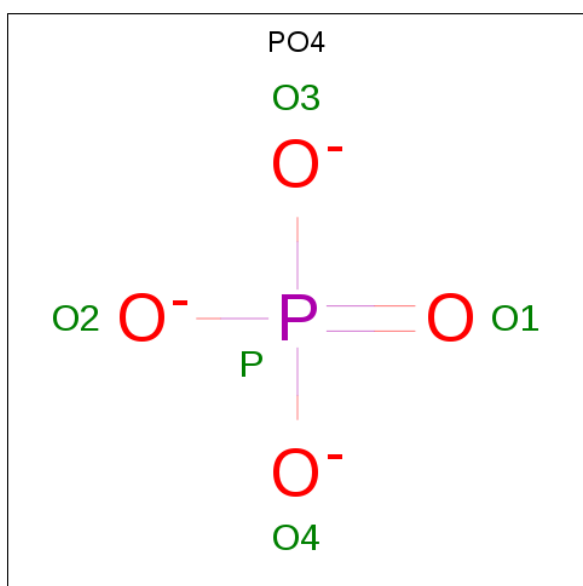


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	B	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	C	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	D	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



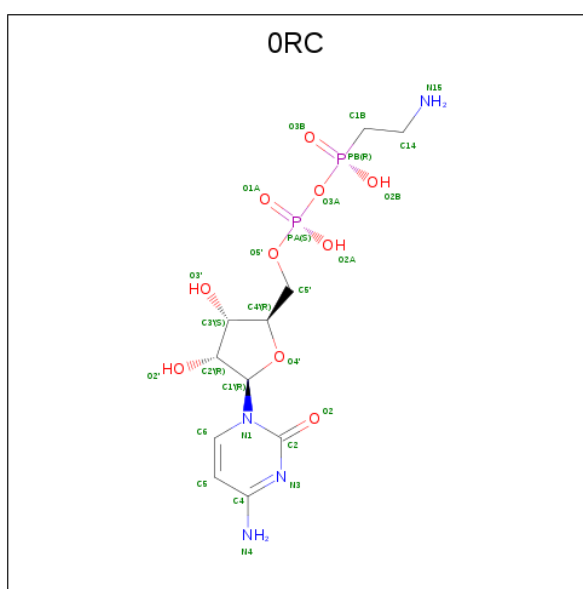
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	A	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
4	C	1	Total O P 5 4 1	0	0
4	C	1	Total O P 5 4 1	0	0
4	C	1	Total O P 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is 5'-O-[(S)-{[(R)-(2-aminoethyl)(hydroxy)phosphoryl]oxy}(hydroxy)phosphoryl]cytidine (three-letter code: 0RC) (formula: C<sub>11</sub>H<sub>20</sub>N<sub>4</sub>O<sub>10</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	11	4	10	2		
5	B	1	Total	C	N	O	P	0	0
			27	11	4	10	2		
5	C	1	Total	C	N	O	P	0	0
			27	11	4	10	2		
5	D	1	Total	C	N	O	P	0	0
			27	11	4	10	2		

- Molecule 6 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
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		

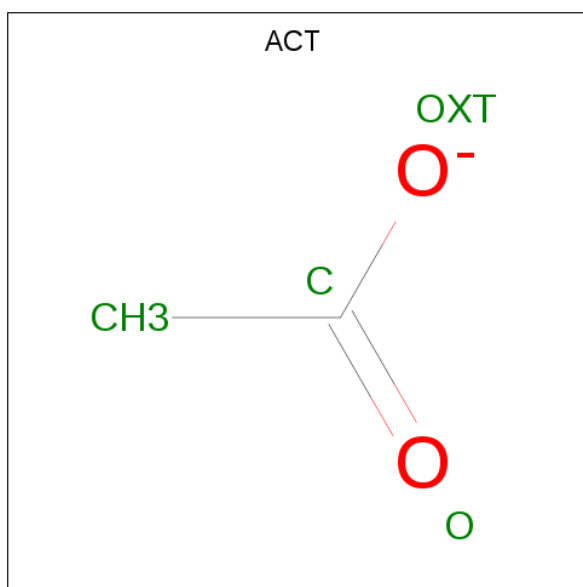
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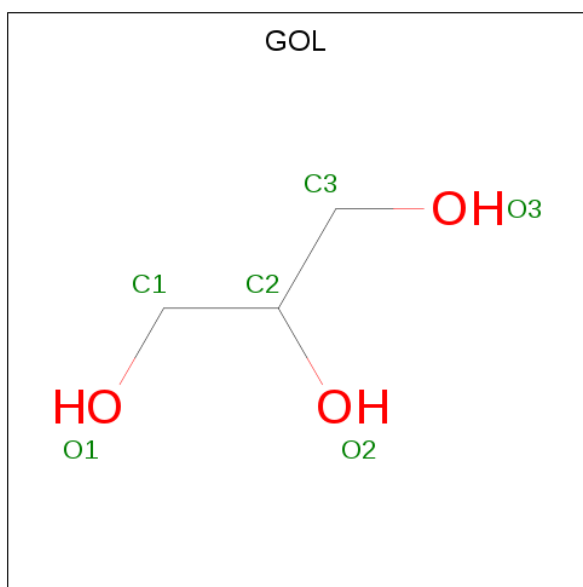
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	D	1	Total 4	C 2	O 2	0	0
6	D	1	Total 4	C 2	O 2	0	0
6	D	1	Total 4	C 2	O 2	0	0
6	D	1	Total 4	C 2	O 2	0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

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			6	3	3		

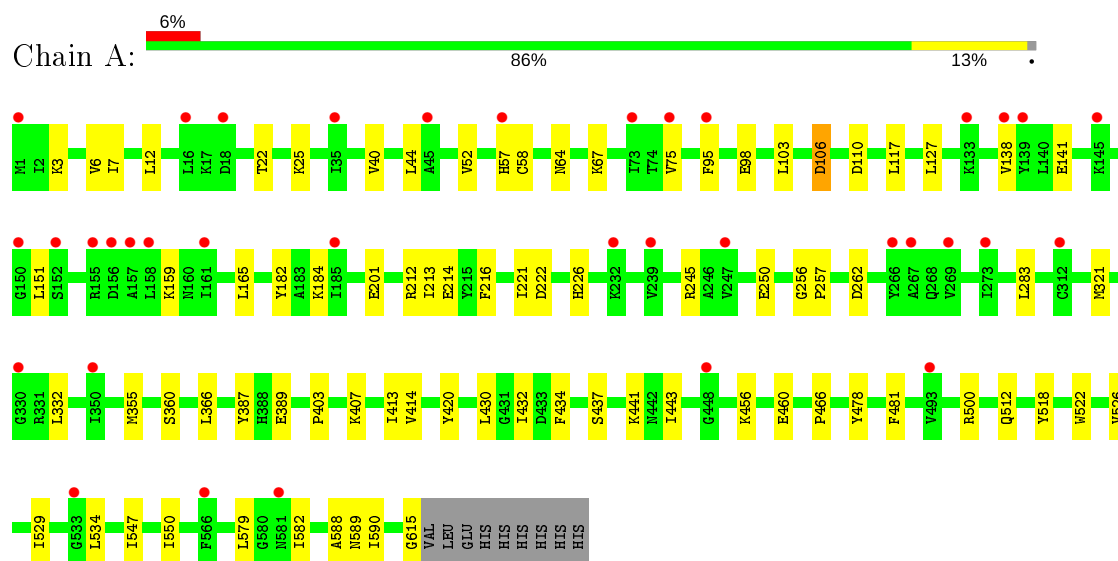
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	354	Total	O	0	0
			354	354		
9	B	352	Total	O	0	0
			352	352		
9	C	411	Total	O	0	0
			411	411		
9	D	330	Total	O	0	0
			330	330		

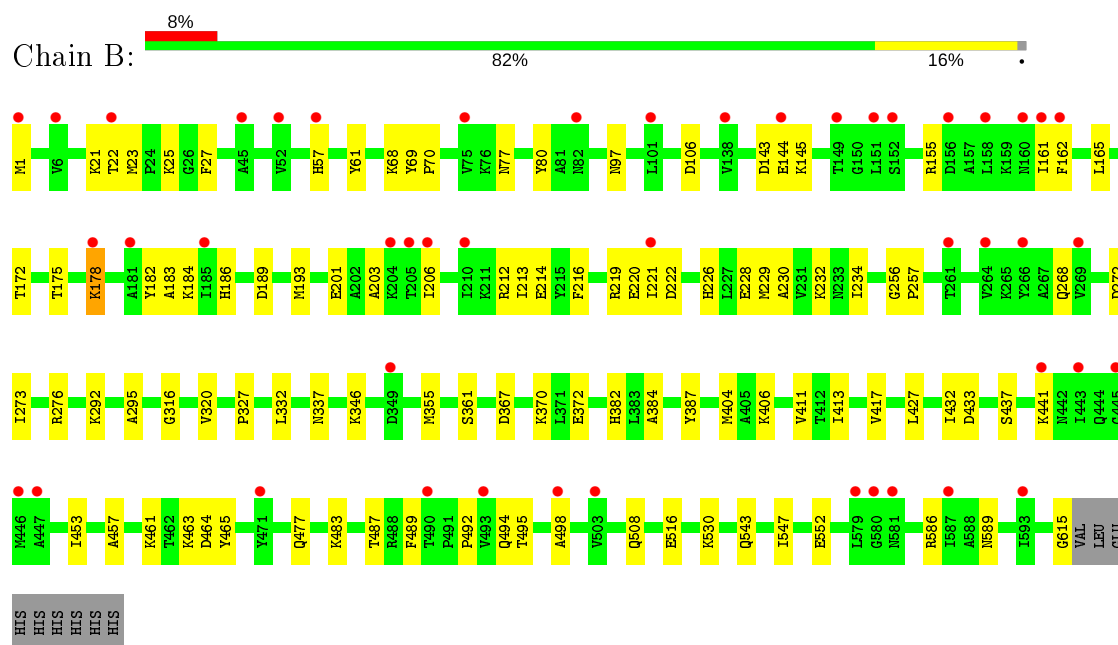
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

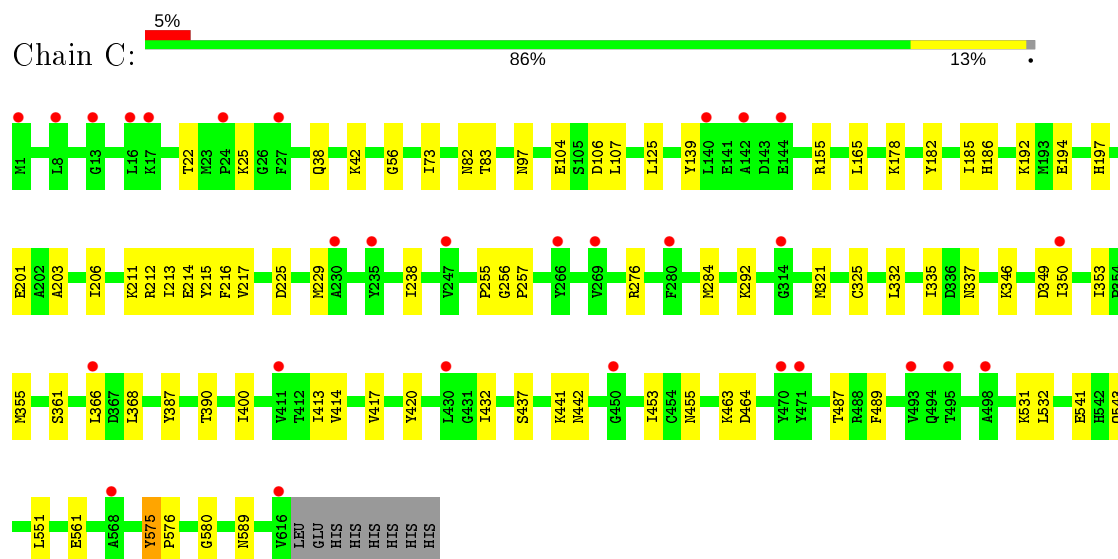
- Molecule 1: Nucleotidyl transferase/aminotransferase, class V



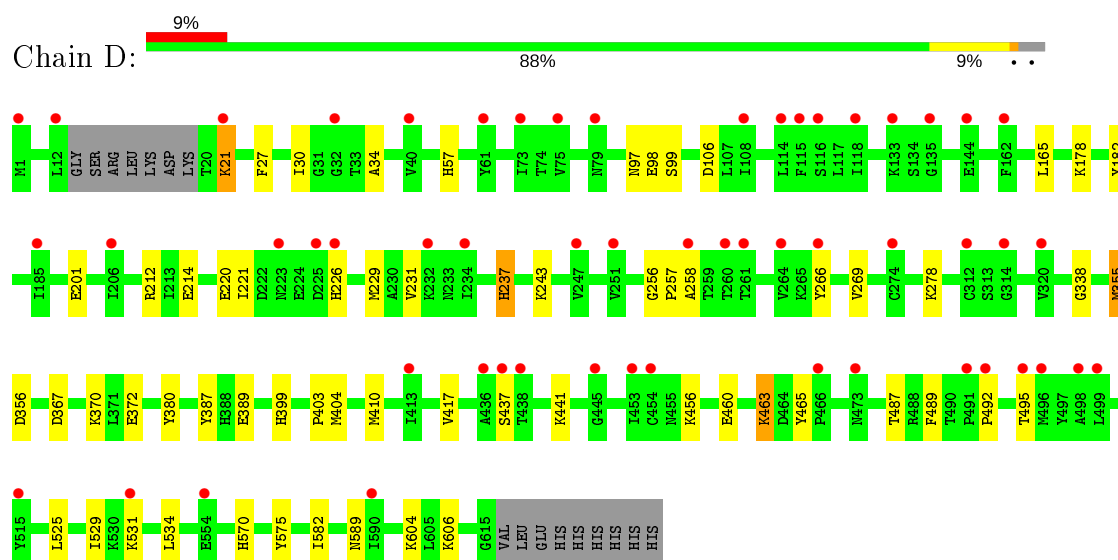
- Molecule 1: Nucleotidyl transferase/aminotransferase, class V



• Molecule 1: Nucleotidyl transferase/aminotransferase, class V



• Molecule 1: Nucleotidyl transferase/aminotransferase, class V



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.45Å 154.05Å 134.58Å 90.00° 90.90° 90.00°	Depositor
Resolution (Å)	47.98 – 1.95 47.98 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.0 (47.98-1.95) 98.1 (47.98-1.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 1.95Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, $R_{free}$	0.220 , 0.254 0.220 , 0.254	Depositor DCC
$R_{free}$ test set	10992 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.1	Xtriage
Anisotropy	0.768	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	21090	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, ORC, PLP, PO4, EDO, ACT

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	0.55	0/4925	0.64	2/6655 (0.0%)
1	B	0.54	0/4925	0.63	0/6655
1	C	0.59	0/4932	0.67	2/6665 (0.0%)
1	D	0.54	0/4869	0.66	0/6581
All	All	0.55	0/19651	0.65	4/26556 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	276	ARG	NE-CZ-NH1	-9.47	115.57	120.30
1	C	276	ARG	NE-CZ-NH2	8.08	124.34	120.30
1	A	151	LEU	CA-CB-CG	5.23	127.34	115.30
1	A	106	ASP	CB-CG-OD1	5.09	122.88	118.30

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	4831	0	4866	62	0
1	B	4831	0	4866	76	0
1	C	4838	0	4875	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4776	0	4803	42	0
2	A	16	0	7	1	0
2	B	16	0	8	0	0
2	C	16	0	7	1	0
2	D	16	0	7	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	10	0	0	0	0
4	B	15	0	0	0	0
4	C	15	0	0	0	0
4	D	15	0	0	3	0
5	A	27	0	0	2	0
5	B	27	0	0	2	0
5	C	27	0	0	0	0
5	D	27	0	0	0	0
6	A	40	0	58	16	0
6	B	12	0	18	9	0
6	C	28	0	42	9	0
6	D	28	0	42	2	0
7	A	8	0	6	0	0
7	C	4	0	3	0	0
8	B	12	0	14	3	0
9	A	354	0	0	7	1
9	B	352	0	0	13	1
9	C	411	0	0	15	0
9	D	330	0	0	9	0
All	All	21090	0	19622	244	1

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.

The worst 5 of 244 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:A:321:MET:HE2	1:A:413:ILE:HG23	1.34	1.09
1:C:337:ASN:ND2	1:C:366:LEU:HD11	1.77	0.99
1:B:1:MET:SD	9:B:1144:HOH:O	2.30	0.89
1:C:83:THR:O	1:C:192:LYS:NZ	2.05	0.88
1:D:417:VAL:HG12	1:D:441:LYS:HD2	1.54	0.88



All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:813:HOH:O	9:B:832:HOH:O[1_554]	2.18	0.02

## 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	613/624 (98%)	589 (96%)	24 (4%)	0	100	100
1	B	613/624 (98%)	594 (97%)	19 (3%)	0	100	100
1	C	614/624 (98%)	594 (97%)	19 (3%)	1 (0%)	47	38
1	D	604/624 (97%)	584 (97%)	20 (3%)	0	100	100
All	All	2444/2496 (98%)	2361 (97%)	82 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	56	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	524/533 (98%)	519 (99%)	5 (1%)	76	74
1	B	524/533 (98%)	518 (99%)	6 (1%)	73	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	525/533 (98%)	519 (99%)	6 (1%)	73	71
1	D	518/533 (97%)	507 (98%)	11 (2%)	53	46
All	All	2091/2132 (98%)	2063 (99%)	28 (1%)	69	65

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	165	LEU
1	C	575	TYR
1	D	463	LYS
1	C	387	TYR
1	C	531	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	64	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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 59 ligands modelled in this entry, 8 are monoatomic - leaving 51 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
6	EDO	C	2210	-	3,3,3	0.58	0	2,2,2	0.51	0
4	PO4	A	704	-	4,4,4	0.88	0	6,6,6	1.04	0
6	EDO	A	710	-	3,3,3	0.34	0	2,2,2	0.94	0
6	EDO	C	2206	-	3,3,3	0.42	0	2,2,2	0.67	0
2	PLP	D	702	-	16,16,16	1.20	2 (12%)	20,23,23	1.21	2 (10%)
6	EDO	A	711	-	3,3,3	0.64	0	2,2,2	1.24	0
6	EDO	A	714	-	3,3,3	0.43	0	2,2,2	0.42	0
7	ACT	A	707	-	1,3,3	11.14	1 (100%)	0,3,3	0.00	-
4	PO4	D	714	-	4,4,4	0.41	0	6,6,6	0.70	0
4	PO4	C	2215	-	4,4,4	0.94	0	6,6,6	0.83	0
5	ORC	D	705	3	24,28,28	4.65	13 (54%)	27,42,42	1.98	7 (25%)
4	PO4	C	2204	-	4,4,4	0.64	0	6,6,6	1.24	0
6	EDO	C	2209	-	3,3,3	0.79	0	2,2,2	0.16	0
6	EDO	B	707	-	3,3,3	0.40	0	2,2,2	0.43	0
2	PLP	A	701	-	16,16,16	1.16	2 (12%)	20,23,23	1.46	4 (20%)
2	PLP	C	2202	-	16,16,16	1.08	1 (6%)	20,23,23	1.09	1 (5%)
4	PO4	B	712	-	4,4,4	0.32	0	6,6,6	0.79	0
7	ACT	A	715	-	1,3,3	6.28	1 (100%)	0,3,3	0.00	-
6	EDO	D	711	-	3,3,3	0.31	0	2,2,2	0.82	0
6	EDO	C	2213	-	3,3,3	0.63	0	2,2,2	0.25	0
6	EDO	A	708	-	3,3,3	0.56	0	2,2,2	0.25	0
4	PO4	A	718	-	4,4,4	1.04	0	6,6,6	0.62	0
4	PO4	D	704	-	4,4,4	0.63	0	6,6,6	0.70	0
6	EDO	A	713	-	3,3,3	0.43	0	2,2,2	0.31	0
6	EDO	D	713	-	3,3,3	0.61	0	2,2,2	0.39	0
6	EDO	D	708	-	3,3,3	0.58	0	2,2,2	0.43	0
6	EDO	D	710	-	3,3,3	0.62	0	2,2,2	0.06	0
2	PLP	B	701	-	16,16,16	1.24	1 (6%)	20,23,23	1.23	3 (15%)
6	EDO	A	709	-	3,3,3	0.52	0	2,2,2	0.76	0
8	GOL	B	709	-	5,5,5	0.53	0	5,5,5	1.05	0
6	EDO	B	706	-	3,3,3	0.25	0	2,2,2	0.37	0
6	EDO	D	707	-	3,3,3	0.52	0	2,2,2	0.54	0
8	GOL	B	711	-	5,5,5	1.81	3 (60%)	5,5,5	1.10	0
4	PO4	D	709	-	4,4,4	1.05	0	6,6,6	0.79	0
6	EDO	B	710	-	3,3,3	0.64	0	2,2,2	0.53	0
5	ORC	C	2205	3	24,28,28	4.63	14 (58%)	27,42,42	1.96	9 (33%)
6	EDO	A	706	-	3,3,3	0.74	0	2,2,2	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	ACT	C	2201	-	1,3,3	4.68	1 (100%)	0,3,3	0.00	-
6	EDO	C	2214	-	3,3,3	0.53	0	2,2,2	0.59	0
6	EDO	C	2208	-	3,3,3	0.37	0	2,2,2	0.96	0
4	PO4	B	708	-	4,4,4	0.84	0	6,6,6	0.64	0
6	EDO	A	717	-	3,3,3	0.26	0	2,2,2	0.31	0
6	EDO	D	712	-	3,3,3	0.59	0	2,2,2	0.56	0
5	ORC	A	705	3	24,28,28	4.74	11 (45%)	27,42,42	2.60	8 (29%)
6	EDO	D	706	-	3,3,3	0.46	0	2,2,2	0.76	0
6	EDO	C	2212	-	3,3,3	0.57	0	2,2,2	0.09	0
6	EDO	A	712	-	3,3,3	0.31	0	2,2,2	0.92	0
4	PO4	B	704	-	4,4,4	0.86	0	6,6,6	0.84	0
5	ORC	B	705	3	24,28,28	4.71	13 (54%)	27,42,42	2.53	8 (29%)
6	EDO	A	716	-	3,3,3	0.43	0	2,2,2	0.95	0
4	PO4	C	2207	-	4,4,4	0.72	0	6,6,6	0.68	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
6	EDO	C	2210	-	-	0/1/1/1	-
6	EDO	A	710	-	-	0/1/1/1	-
6	EDO	C	2206	-	-	1/1/1/1	-
2	PLP	D	702	-	-	1/8/8/8	0/1/1/1
6	EDO	A	711	-	-	0/1/1/1	-
6	EDO	A	714	-	-	1/1/1/1	-
5	ORC	D	705	3	-	5/15/36/36	0/2/2/2
6	EDO	C	2209	-	-	0/1/1/1	-
6	EDO	B	707	-	-	1/1/1/1	-
2	PLP	A	701	-	-	1/8/8/8	0/1/1/1
2	PLP	C	2202	-	-	2/8/8/8	0/1/1/1
6	EDO	D	711	-	-	0/1/1/1	-
6	EDO	C	2213	-	-	0/1/1/1	-
6	EDO	A	708	-	-	0/1/1/1	-
6	EDO	A	713	-	-	1/1/1/1	-
6	EDO	D	713	-	-	0/1/1/1	-
6	EDO	D	708	-	-	0/1/1/1	-
2	PLP	B	701	-	-	1/8/8/8	0/1/1/1
6	EDO	A	709	-	-	1/1/1/1	-
8	GOL	B	709	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	B	706	-	-	1/1/1/1	-
6	EDO	D	707	-	-	0/1/1/1	-
6	EDO	B	710	-	-	1/1/1/1	-
5	0RC	C	2205	3	-	4/15/36/36	0/2/2/2
6	EDO	A	706	-	-	0/1/1/1	-
8	GOL	B	711	-	-	2/4/4/4	-
6	EDO	C	2214	-	-	0/1/1/1	-
6	EDO	C	2208	-	-	0/1/1/1	-
6	EDO	A	717	-	-	0/1/1/1	-
6	EDO	D	712	-	-	0/1/1/1	-
5	0RC	A	705	3	-	6/15/36/36	0/2/2/2
6	EDO	D	706	-	-	1/1/1/1	-
6	EDO	C	2212	-	-	1/1/1/1	-
6	EDO	A	712	-	-	1/1/1/1	-
6	EDO	D	710	-	-	0/1/1/1	-
5	0RC	B	705	3	-	4/15/36/36	0/2/2/2
6	EDO	A	716	-	-	0/1/1/1	-

The worst 5 of 63 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	705	0RC	O4'-C1'	13.96	1.60	1.41
5	D	705	0RC	O4'-C1'	13.53	1.60	1.41
5	B	705	0RC	O4'-C1'	13.46	1.59	1.41
5	C	2205	0RC	O4'-C1'	12.84	1.59	1.41
7	A	707	ACT	CH3-C	11.14	1.62	1.48

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	705	0RC	PB-C1B-C14	-7.59	97.86	114.06
5	A	705	0RC	C2-N3-C4	6.04	122.47	116.34
5	B	705	0RC	O4'-C1'-C2'	-5.93	98.26	106.93
5	B	705	0RC	C2-N3-C4	5.73	122.14	116.34
5	D	705	0RC	C2-N3-C4	5.44	121.85	116.34

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	705	0RC	C5'-O5'-PA-O1A

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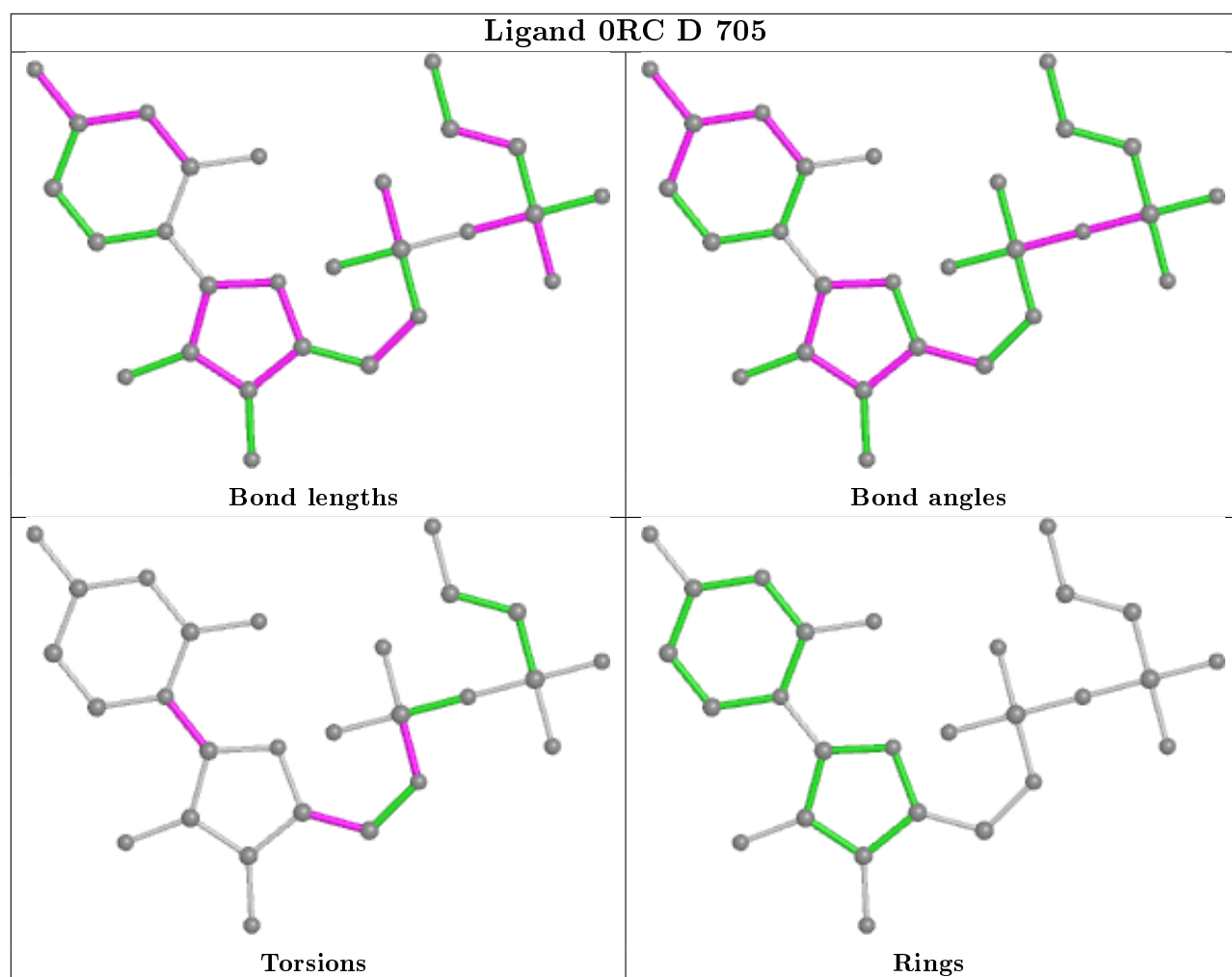
Mol	Chain	Res	Type	Atoms
5	D	705	0RC	C2'-C1'-N1-C6
8	B	709	GOL	O1-C1-C2-C3
8	B	711	GOL	O1-C1-C2-O2
8	B	711	GOL	O1-C1-C2-C3

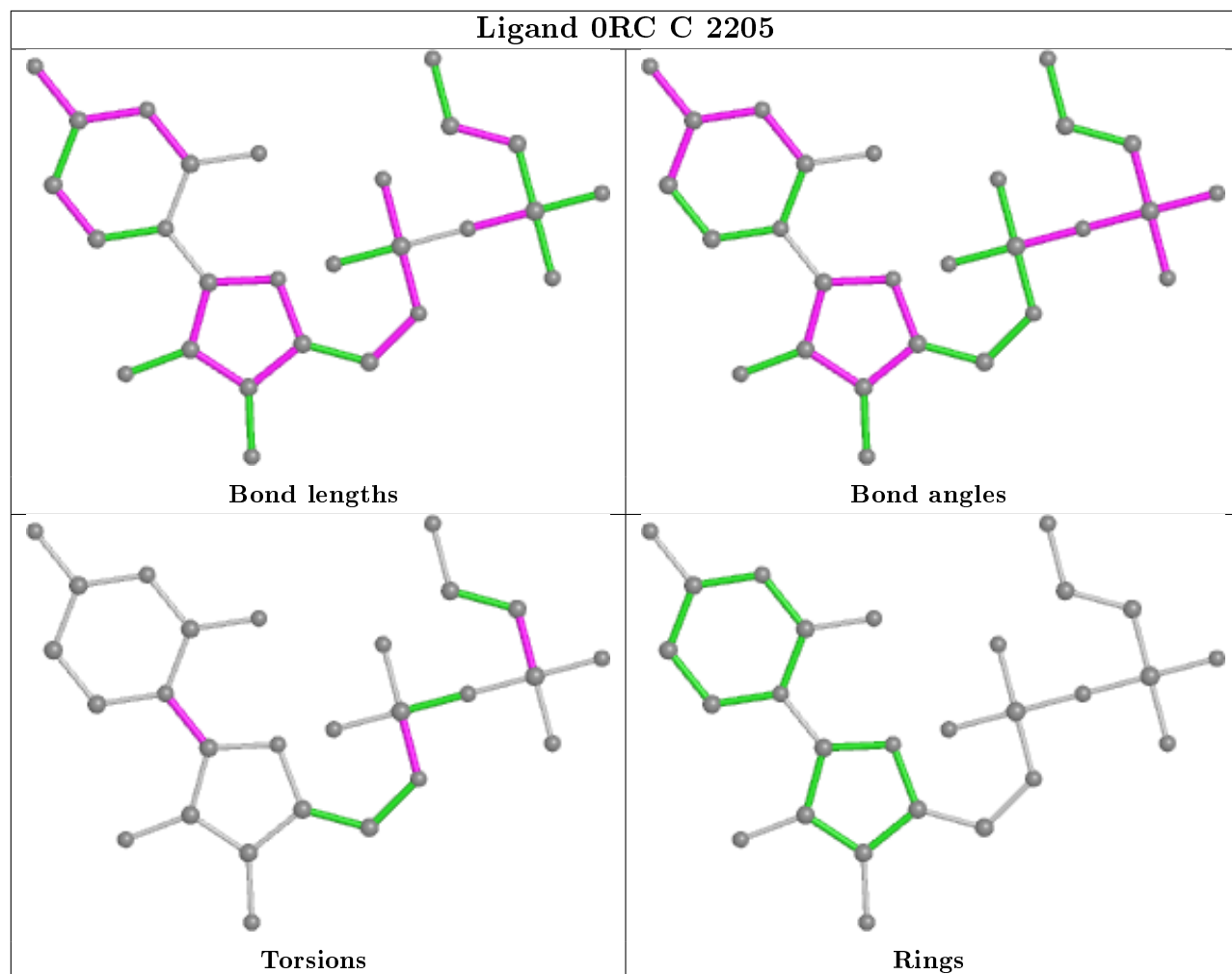
There are no ring outliers.

18 monomers are involved in 47 short contacts:

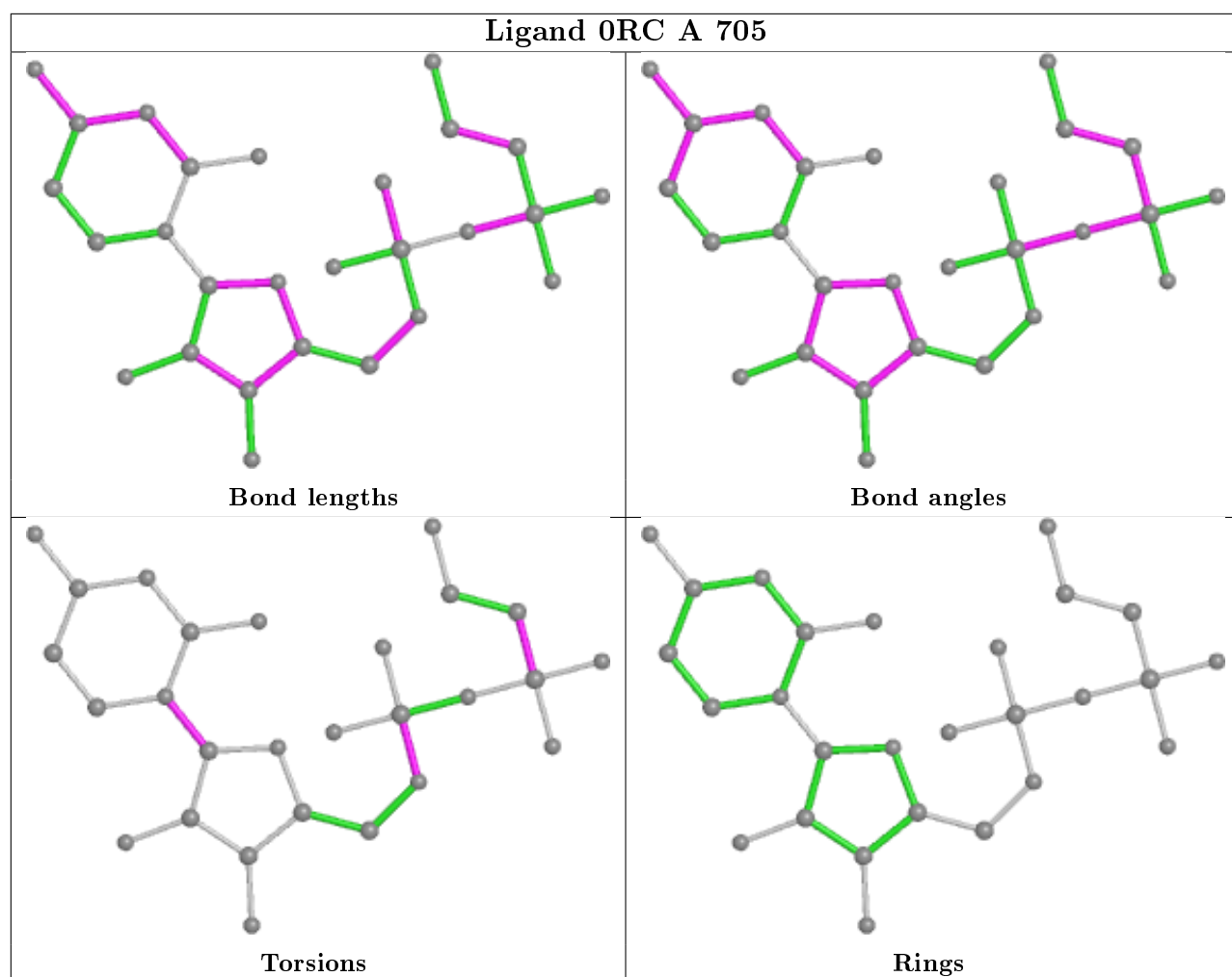
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	2210	EDO	3	0
6	C	2206	EDO	1	0
6	A	714	EDO	1	0
4	D	714	PO4	1	0
6	C	2209	EDO	3	0
2	A	701	PLP	1	0
2	C	2202	PLP	1	0
6	A	709	EDO	5	0
6	B	706	EDO	9	0
8	B	711	GOL	3	0
4	D	709	PO4	2	0
6	C	2208	EDO	2	0
6	A	717	EDO	3	0
5	A	705	0RC	2	0
6	D	706	EDO	2	0
6	A	712	EDO	1	0
5	B	705	0RC	2	0
6	A	716	EDO	6	0

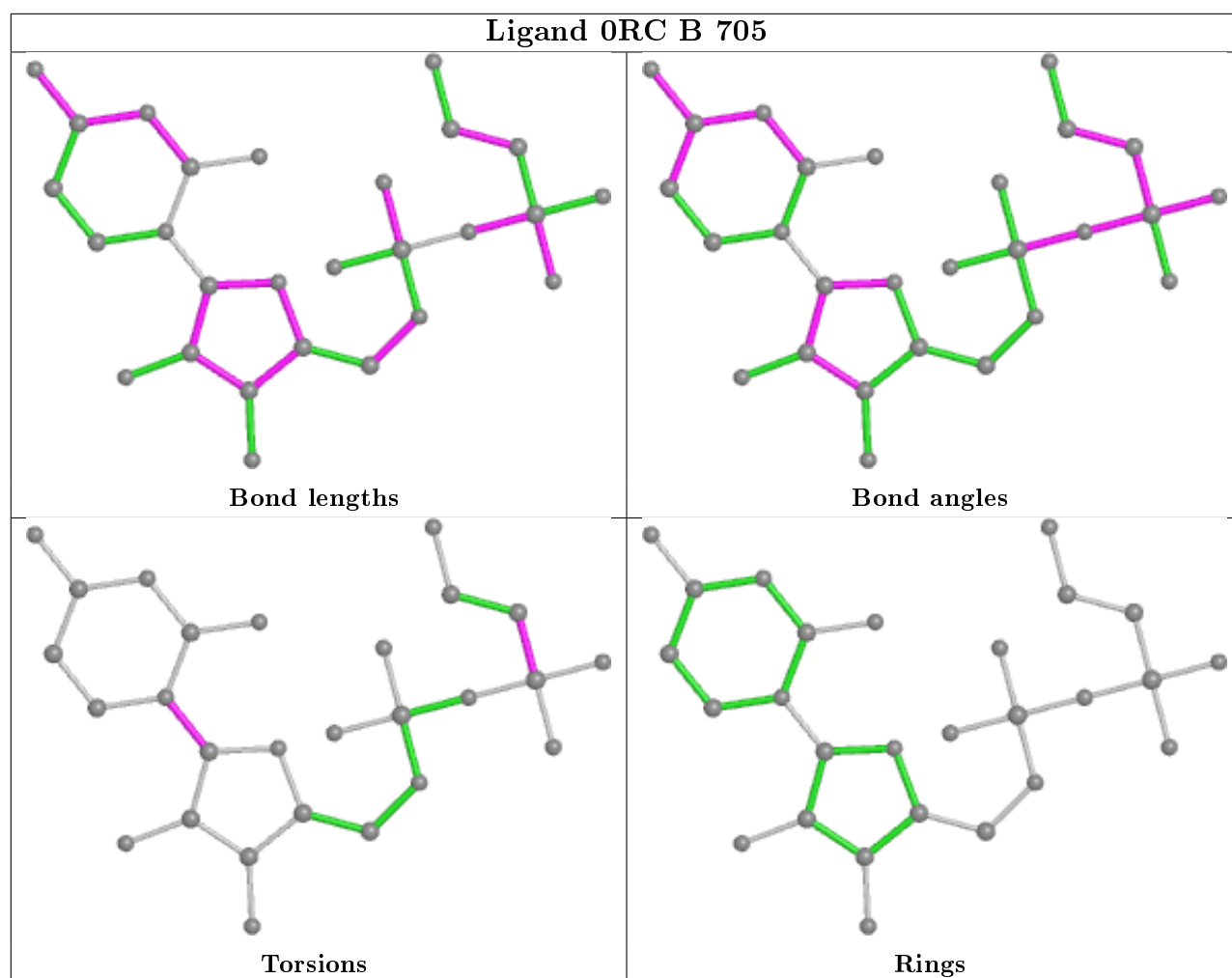
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	615/624 (98%)	0.78	36 (5%) 22 30	15, 25, 37, 51	0
1	B	615/624 (98%)	0.88	47 (7%) 13 21	15, 26, 42, 60	0
1	C	616/624 (98%)	0.77	29 (4%) 31 41	13, 23, 36, 54	0
1	D	608/624 (97%)	0.87	55 (9%) 9 15	15, 25, 42, 51	0
All	All	2454/2496 (98%)	0.83	167 (6%) 17 25	13, 25, 40, 60	0

The worst 5 of 167 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	366	LEU	4.5
1	A	350	ILE	4.4
1	B	151	LEU	4.2
1	B	158	LEU	4.1
1	B	266	TYR	3.8

### 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 monosaccharides 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( $\text{\AA}^2$ )	Q<0.9
3	MG	D	703	1/1	0.46	0.21	46,46,46,46	0
6	EDO	A	711	4/4	0.57	0.34	35,40,42,42	0
3	MG	A	702	1/1	0.63	0.22	31,31,31,31	0
3	MG	C	2203	1/1	0.64	0.14	28,28,28,28	0
4	PO4	B	712	5/5	0.66	0.24	30,31,43,51	0
4	PO4	D	704	5/5	0.69	0.19	54,60,67,78	0
4	PO4	C	2215	5/5	0.73	0.24	30,36,40,48	0
3	MG	B	702	1/1	0.73	0.14	34,34,34,34	0
6	EDO	C	2209	4/4	0.74	0.23	22,29,31,32	0
6	EDO	A	716	4/4	0.75	0.37	21,22,23,29	0
3	MG	A	703	1/1	0.77	0.07	27,27,27,27	0
6	EDO	C	2210	4/4	0.77	0.19	23,33,33,37	0
7	ACT	C	2201	4/4	0.79	0.21	21,22,29,34	0
6	EDO	D	707	4/4	0.81	0.27	30,32,38,39	0
7	ACT	A	715	4/4	0.81	0.18	27,34,37,46	0
4	PO4	A	718	5/5	0.81	0.23	30,32,43,51	0
8	GOL	B	709	6/6	0.81	0.19	24,36,38,41	0
6	EDO	B	710	4/4	0.82	0.20	23,24,24,29	0
6	EDO	D	708	4/4	0.83	0.27	30,31,32,40	0
4	PO4	D	714	5/5	0.85	0.24	28,33,38,46	0
6	EDO	A	709	4/4	0.86	0.21	20,22,25,26	0
7	ACT	A	707	4/4	0.87	0.19	25,29,31,33	0
3	MG	B	703	1/1	0.87	0.08	33,33,33,33	0
4	PO4	C	2207	5/5	0.87	0.20	30,37,41,43	0
6	EDO	B	707	4/4	0.88	0.22	22,22,25,26	0
4	PO4	B	708	5/5	0.88	0.16	36,37,48,50	0
6	EDO	D	710	4/4	0.89	0.13	21,24,26,29	0
6	EDO	A	714	4/4	0.89	0.17	26,27,36,38	0
6	EDO	A	717	4/4	0.89	0.34	26,27,30,34	0
5	ORC	A	705	27/27	0.89	0.14	25,27,32,37	0
6	EDO	B	706	4/4	0.89	0.28	20,21,22,24	0
6	EDO	A	706	4/4	0.89	0.18	14,18,18,20	0
6	EDO	A	712	4/4	0.90	0.18	17,20,26,27	0
6	EDO	D	706	4/4	0.90	0.26	19,21,24,30	0
2	PLP	D	702	16/16	0.90	0.18	17,20,31,32	0
6	EDO	D	713	4/4	0.90	0.14	23,25,25,27	0
8	GOL	B	711	6/6	0.91	0.24	15,20,27,27	0
6	EDO	C	2212	4/4	0.91	0.18	16,17,17,22	0
5	ORC	D	705	27/27	0.92	0.14	31,35,37,40	0
5	ORC	B	705	27/27	0.92	0.13	27,33,41,43	0
6	EDO	A	713	4/4	0.93	0.14	24,27,28,28	0
3	MG	D	701	1/1	0.93	0.10	41,41,41,41	0
6	EDO	D	712	4/4	0.93	0.18	15,15,17,18	0

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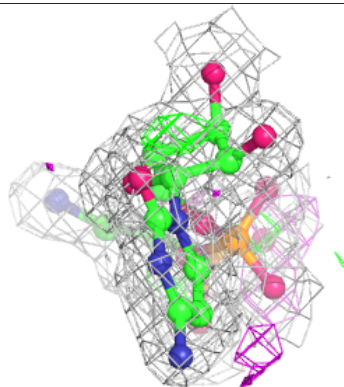
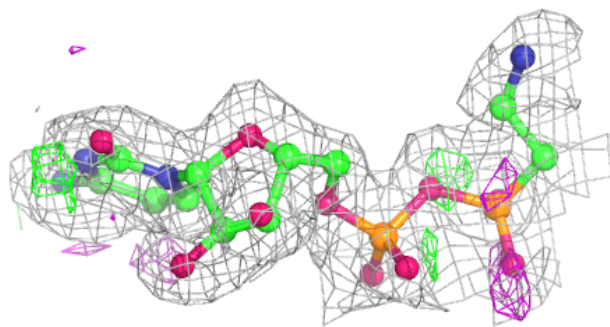
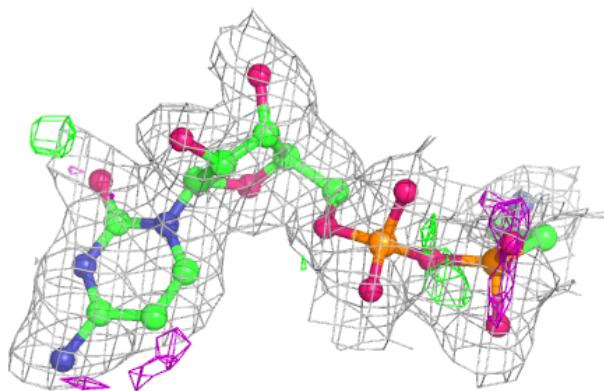
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	0RC	C	2205	27/27	0.93	0.11	22,26,31,34	0
2	PLP	C	2202	16/16	0.93	0.17	14,19,23,30	0
6	EDO	C	2206	4/4	0.94	0.19	24,25,28,33	0
6	EDO	D	711	4/4	0.94	0.13	20,24,25,26	0
4	PO4	C	2204	5/5	0.94	0.13	24,25,26,29	0
6	EDO	C	2214	4/4	0.94	0.14	19,23,24,26	0
6	EDO	A	710	4/4	0.94	0.14	21,21,22,25	0
2	PLP	B	701	16/16	0.94	0.17	18,23,29,36	0
4	PO4	D	709	5/5	0.94	0.12	22,24,29,31	0
3	MG	C	2211	1/1	0.95	0.08	26,26,26,26	0
6	EDO	C	2208	4/4	0.95	0.14	19,24,24,25	0
4	PO4	A	704	5/5	0.95	0.12	23,24,25,35	0
4	PO4	B	704	5/5	0.95	0.13	24,27,30,33	0
6	EDO	C	2213	4/4	0.95	0.15	17,20,21,23	0
2	PLP	A	701	16/16	0.95	0.14	16,20,25,32	0
6	EDO	A	708	4/4	0.95	0.11	21,21,23,29	0

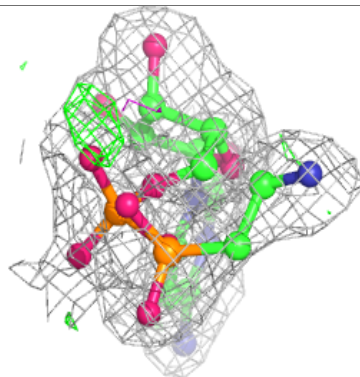
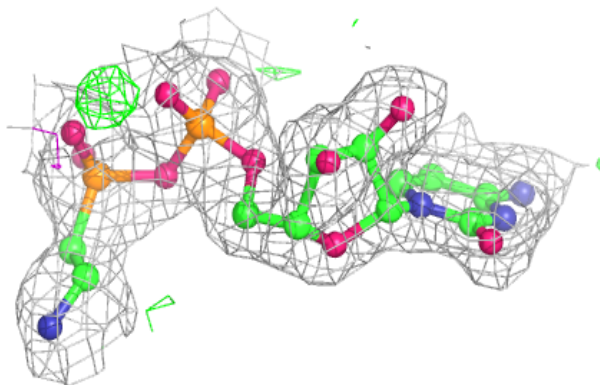
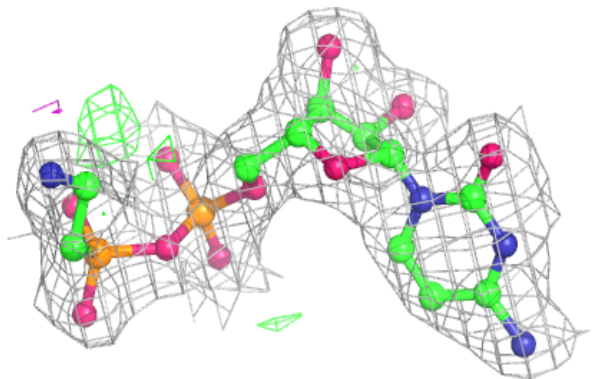
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 0RC A 705:**

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

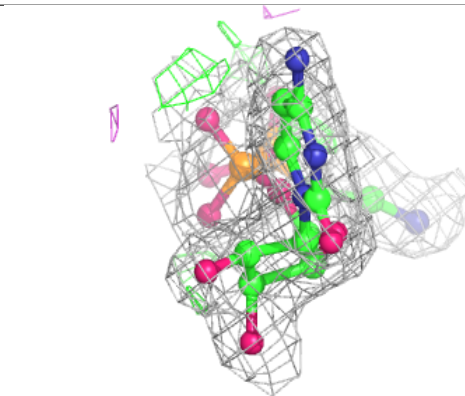
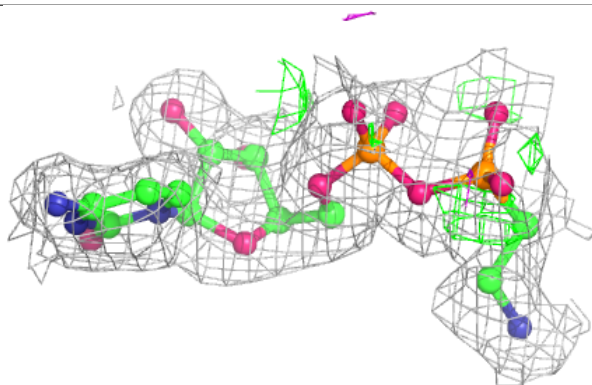
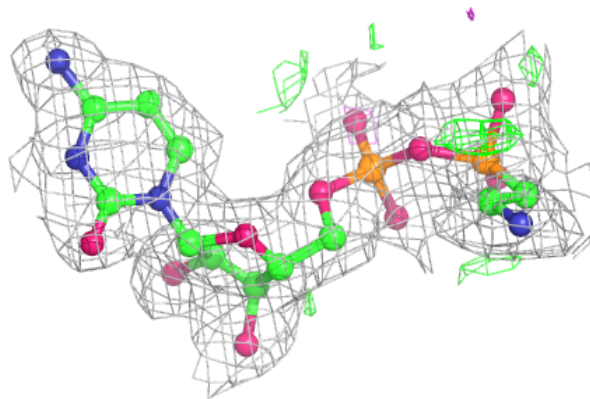
**Electron density around 0RC D 705:**

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

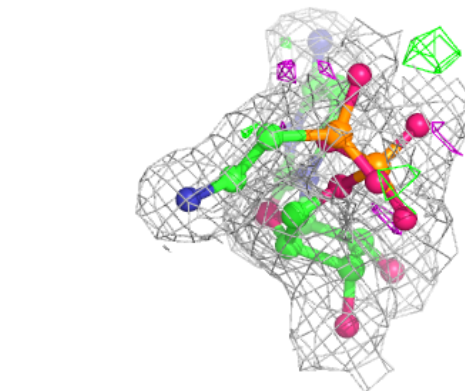
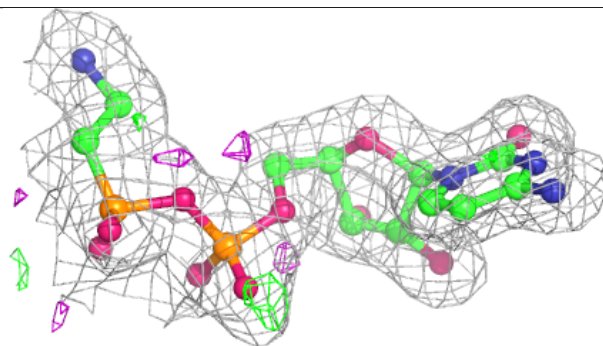
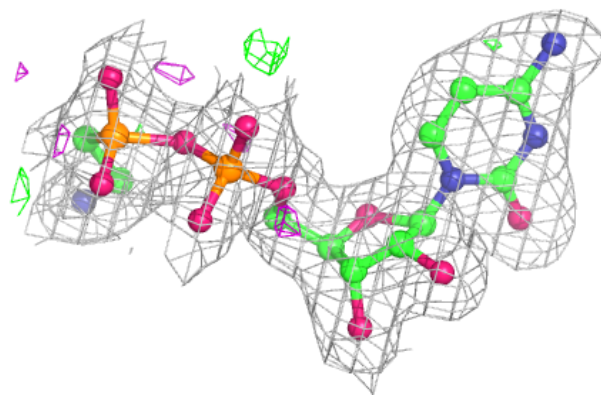


**Electron density around 0RC B 705:**

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

**Electron density around 0RC C 2205:**

$2mF_o-DF_c$  (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.