



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 13, 2019 – 04:59 PM EST

PDB ID : 5D0A  
Title : Crystal structure of epoxyqueuosine reductase with cleaved RNA stem loop  
Authors : Dowling, D.P.; Miles, Z.D.; Kohrer, C.; Bandarian, V.; Drennan, C.L.  
Deposited on : 2015-08-03  
Resolution : 2.10 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 : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : 2.4  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

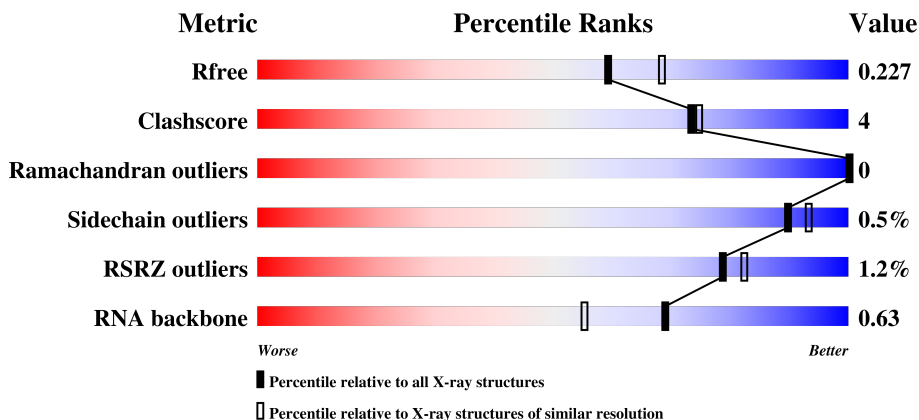
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	111664	4608 (2.10-2.10)
Clashscore	122126	5109 (2.10-2.10)
Ramachandran outliers	120053	5059 (2.10-2.10)
Sidechain outliers	120020	5060 (2.10-2.10)
RSRZ outliers	108989	4497 (2.10-2.10)
RNA backbone	2636	1006 (2.62-1.58)

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. 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	437	<div> <div> <div></div> <div>80%</div> <div>7%</div> <div>13%</div> </div> </div>
1	B	437	<div> <div> <div>2%</div> <div>78%</div> <div>9%</div> <div>13%</div> </div> </div>
1	C	437	<div> <div> <div></div> <div>76%</div> <div>11%</div> <div>14%</div> </div> </div>
1	D	437	<div> <div> <div></div> <div>79%</div> <div>7%</div> <div>14%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	E	17	
2	F	17	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SF4	A	501	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13688 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 Epoxyqueuosine reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	3	0
			2982	1896	504	564	18			
1	B	379	Total	C	N	O	S	0	2	0
			2977	1892	505	562	18			
1	C	376	Total	C	N	O	S	0	4	0
			2984	1894	512	561	17			
1	D	375	Total	C	N	O	S	0	4	0
			2972	1889	506	560	17			

There are 204 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	initiating methionine	UNP P97030
A	-26	ALA	-	expression tag	UNP P97030
A	-25	SER	-	expression tag	UNP P97030
A	-24	ARG	-	expression tag	UNP P97030
A	-23	GLY	-	expression tag	UNP P97030
A	-22	SER	-	expression tag	UNP P97030
A	-21	HIS	-	expression tag	UNP P97030
A	-20	HIS	-	expression tag	UNP P97030
A	-19	HIS	-	expression tag	UNP P97030
A	-18	HIS	-	expression tag	UNP P97030
A	-17	HIS	-	expression tag	UNP P97030
A	-16	HIS	-	expression tag	UNP P97030
A	-15	GLY	-	expression tag	UNP P97030
A	-14	ALA	-	expression tag	UNP P97030
A	-13	GLY	-	expression tag	UNP P97030
A	-12	ASP	-	expression tag	UNP P97030
A	-11	ARG	-	expression tag	UNP P97030
A	-10	GLY	-	expression tag	UNP P97030
A	-9	PRO	-	expression tag	UNP P97030
A	-8	GLU	-	expression tag	UNP P97030
A	-7	PHE	-	expression tag	UNP P97030

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLU	-	expression tag	UNP P97030
A	-5	LEU	-	expression tag	UNP P97030
A	-4	GLY	-	expression tag	UNP P97030
A	-3	THR	-	expression tag	UNP P97030
A	-2	ARG	-	expression tag	UNP P97030
A	-1	GLY	-	expression tag	UNP P97030
A	0	SER	-	expression tag	UNP P97030
A	387	GLY	-	expression tag	UNP P97030
A	388	SER	-	expression tag	UNP P97030
A	389	LEU	-	expression tag	UNP P97030
A	390	GLU	-	expression tag	UNP P97030
A	391	VAL	-	expression tag	UNP P97030
A	392	ASP	-	expression tag	UNP P97030
A	393	LEU	-	expression tag	UNP P97030
A	394	GLN	-	expression tag	UNP P97030
A	395	GLY	-	expression tag	UNP P97030
A	396	ASP	-	expression tag	UNP P97030
A	397	HIS	-	expression tag	UNP P97030
A	398	GLY	-	expression tag	UNP P97030
A	399	LEU	-	expression tag	UNP P97030
A	400	SER	-	expression tag	UNP P97030
A	401	ALA	-	expression tag	UNP P97030
A	402	TRP	-	expression tag	UNP P97030
A	403	SER	-	expression tag	UNP P97030
A	404	HIS	-	expression tag	UNP P97030
A	405	PRO	-	expression tag	UNP P97030
A	406	GLN	-	expression tag	UNP P97030
A	407	PHE	-	expression tag	UNP P97030
A	408	GLU	-	expression tag	UNP P97030
A	409	LYS	-	expression tag	UNP P97030
B	-27	MET	-	initiating methionine	UNP P97030
B	-26	ALA	-	expression tag	UNP P97030
B	-25	SER	-	expression tag	UNP P97030
B	-24	ARG	-	expression tag	UNP P97030
B	-23	GLY	-	expression tag	UNP P97030
B	-22	SER	-	expression tag	UNP P97030
B	-21	HIS	-	expression tag	UNP P97030
B	-20	HIS	-	expression tag	UNP P97030
B	-19	HIS	-	expression tag	UNP P97030
B	-18	HIS	-	expression tag	UNP P97030
B	-17	HIS	-	expression tag	UNP P97030
B	-16	HIS	-	expression tag	UNP P97030

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	GLY	-	expression tag	UNP P97030
B	-14	ALA	-	expression tag	UNP P97030
B	-13	GLY	-	expression tag	UNP P97030
B	-12	ASP	-	expression tag	UNP P97030
B	-11	ARG	-	expression tag	UNP P97030
B	-10	GLY	-	expression tag	UNP P97030
B	-9	PRO	-	expression tag	UNP P97030
B	-8	GLU	-	expression tag	UNP P97030
B	-7	PHE	-	expression tag	UNP P97030
B	-6	GLU	-	expression tag	UNP P97030
B	-5	LEU	-	expression tag	UNP P97030
B	-4	GLY	-	expression tag	UNP P97030
B	-3	THR	-	expression tag	UNP P97030
B	-2	ARG	-	expression tag	UNP P97030
B	-1	GLY	-	expression tag	UNP P97030
B	0	SER	-	expression tag	UNP P97030
B	387	GLY	-	expression tag	UNP P97030
B	388	SER	-	expression tag	UNP P97030
B	389	LEU	-	expression tag	UNP P97030
B	390	GLU	-	expression tag	UNP P97030
B	391	VAL	-	expression tag	UNP P97030
B	392	ASP	-	expression tag	UNP P97030
B	393	LEU	-	expression tag	UNP P97030
B	394	GLN	-	expression tag	UNP P97030
B	395	GLY	-	expression tag	UNP P97030
B	396	ASP	-	expression tag	UNP P97030
B	397	HIS	-	expression tag	UNP P97030
B	398	GLY	-	expression tag	UNP P97030
B	399	LEU	-	expression tag	UNP P97030
B	400	SER	-	expression tag	UNP P97030
B	401	ALA	-	expression tag	UNP P97030
B	402	TRP	-	expression tag	UNP P97030
B	403	SER	-	expression tag	UNP P97030
B	404	HIS	-	expression tag	UNP P97030
B	405	PRO	-	expression tag	UNP P97030
B	406	GLN	-	expression tag	UNP P97030
B	407	PHE	-	expression tag	UNP P97030
B	408	GLU	-	expression tag	UNP P97030
B	409	LYS	-	expression tag	UNP P97030
C	-27	MET	-	initiating methionine	UNP P97030
C	-26	ALA	-	expression tag	UNP P97030
C	-25	SER	-	expression tag	UNP P97030

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-24	ARG	-	expression tag	UNP P97030
C	-23	GLY	-	expression tag	UNP P97030
C	-22	SER	-	expression tag	UNP P97030
C	-21	HIS	-	expression tag	UNP P97030
C	-20	HIS	-	expression tag	UNP P97030
C	-19	HIS	-	expression tag	UNP P97030
C	-18	HIS	-	expression tag	UNP P97030
C	-17	HIS	-	expression tag	UNP P97030
C	-16	HIS	-	expression tag	UNP P97030
C	-15	GLY	-	expression tag	UNP P97030
C	-14	ALA	-	expression tag	UNP P97030
C	-13	GLY	-	expression tag	UNP P97030
C	-12	ASP	-	expression tag	UNP P97030
C	-11	ARG	-	expression tag	UNP P97030
C	-10	GLY	-	expression tag	UNP P97030
C	-9	PRO	-	expression tag	UNP P97030
C	-8	GLU	-	expression tag	UNP P97030
C	-7	PHE	-	expression tag	UNP P97030
C	-6	GLU	-	expression tag	UNP P97030
C	-5	LEU	-	expression tag	UNP P97030
C	-4	GLY	-	expression tag	UNP P97030
C	-3	THR	-	expression tag	UNP P97030
C	-2	ARG	-	expression tag	UNP P97030
C	-1	GLY	-	expression tag	UNP P97030
C	0	SER	-	expression tag	UNP P97030
C	387	GLY	-	expression tag	UNP P97030
C	388	SER	-	expression tag	UNP P97030
C	389	LEU	-	expression tag	UNP P97030
C	390	GLU	-	expression tag	UNP P97030
C	391	VAL	-	expression tag	UNP P97030
C	392	ASP	-	expression tag	UNP P97030
C	393	LEU	-	expression tag	UNP P97030
C	394	GLN	-	expression tag	UNP P97030
C	395	GLY	-	expression tag	UNP P97030
C	396	ASP	-	expression tag	UNP P97030
C	397	HIS	-	expression tag	UNP P97030
C	398	GLY	-	expression tag	UNP P97030
C	399	LEU	-	expression tag	UNP P97030
C	400	SER	-	expression tag	UNP P97030
C	401	ALA	-	expression tag	UNP P97030
C	402	TRP	-	expression tag	UNP P97030
C	403	SER	-	expression tag	UNP P97030

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Chain	Residue	Modelled	Actual	Comment	Reference
C	404	HIS	-	expression tag	UNP P97030
C	405	PRO	-	expression tag	UNP P97030
C	406	GLN	-	expression tag	UNP P97030
C	407	PHE	-	expression tag	UNP P97030
C	408	GLU	-	expression tag	UNP P97030
C	409	LYS	-	expression tag	UNP P97030
D	-27	MET	-	initiating methionine	UNP P97030
D	-26	ALA	-	expression tag	UNP P97030
D	-25	SER	-	expression tag	UNP P97030
D	-24	ARG	-	expression tag	UNP P97030
D	-23	GLY	-	expression tag	UNP P97030
D	-22	SER	-	expression tag	UNP P97030
D	-21	HIS	-	expression tag	UNP P97030
D	-20	HIS	-	expression tag	UNP P97030
D	-19	HIS	-	expression tag	UNP P97030
D	-18	HIS	-	expression tag	UNP P97030
D	-17	HIS	-	expression tag	UNP P97030
D	-16	HIS	-	expression tag	UNP P97030
D	-15	GLY	-	expression tag	UNP P97030
D	-14	ALA	-	expression tag	UNP P97030
D	-13	GLY	-	expression tag	UNP P97030
D	-12	ASP	-	expression tag	UNP P97030
D	-11	ARG	-	expression tag	UNP P97030
D	-10	GLY	-	expression tag	UNP P97030
D	-9	PRO	-	expression tag	UNP P97030
D	-8	GLU	-	expression tag	UNP P97030
D	-7	PHE	-	expression tag	UNP P97030
D	-6	GLU	-	expression tag	UNP P97030
D	-5	LEU	-	expression tag	UNP P97030
D	-4	GLY	-	expression tag	UNP P97030
D	-3	THR	-	expression tag	UNP P97030
D	-2	ARG	-	expression tag	UNP P97030
D	-1	GLY	-	expression tag	UNP P97030
D	0	SER	-	expression tag	UNP P97030
D	387	GLY	-	expression tag	UNP P97030
D	388	SER	-	expression tag	UNP P97030
D	389	LEU	-	expression tag	UNP P97030
D	390	GLU	-	expression tag	UNP P97030
D	391	VAL	-	expression tag	UNP P97030
D	392	ASP	-	expression tag	UNP P97030
D	393	LEU	-	expression tag	UNP P97030
D	394	GLN	-	expression tag	UNP P97030

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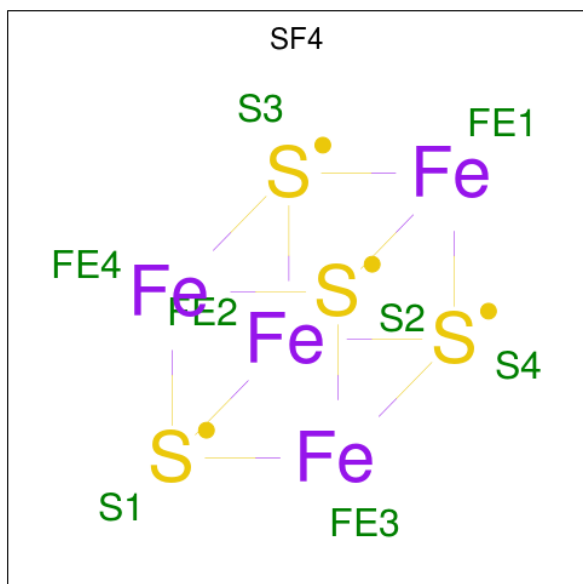
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Chain	Residue	Modelled	Actual	Comment	Reference
D	395	GLY	-	expression tag	UNP P97030
D	396	ASP	-	expression tag	UNP P97030
D	397	HIS	-	expression tag	UNP P97030
D	398	GLY	-	expression tag	UNP P97030
D	399	LEU	-	expression tag	UNP P97030
D	400	SER	-	expression tag	UNP P97030
D	401	ALA	-	expression tag	UNP P97030
D	402	TRP	-	expression tag	UNP P97030
D	403	SER	-	expression tag	UNP P97030
D	404	HIS	-	expression tag	UNP P97030
D	405	PRO	-	expression tag	UNP P97030
D	406	GLN	-	expression tag	UNP P97030
D	407	PHE	-	expression tag	UNP P97030
D	408	GLU	-	expression tag	UNP P97030
D	409	LYS	-	expression tag	UNP P97030

- Molecule 2 is a RNA chain called RNA (5'-R(\*G\*CP\*AP\*GP\*AP\*CP\*UP\*GP\*UP\*AP\*AP\*AP\*UP\*CP\*UP\*GP\*C)-3').

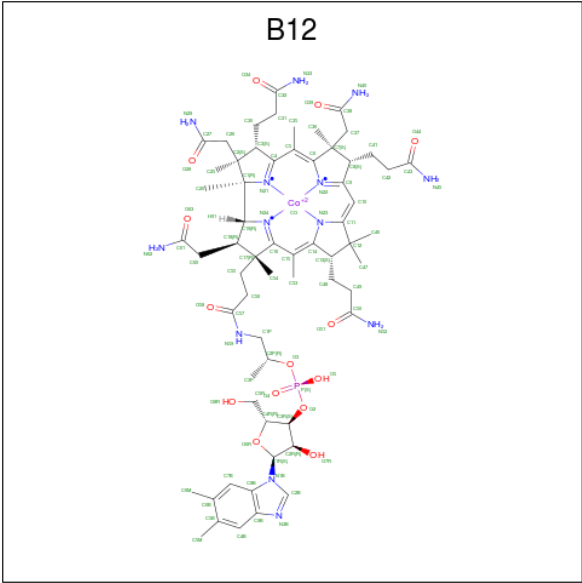
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	12	Total	C	N	O	P	0	0	1
			235	105	42	77	11			
2	F	14	Total	C	N	O	P	0	0	1
			272	123	48	89	12			

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



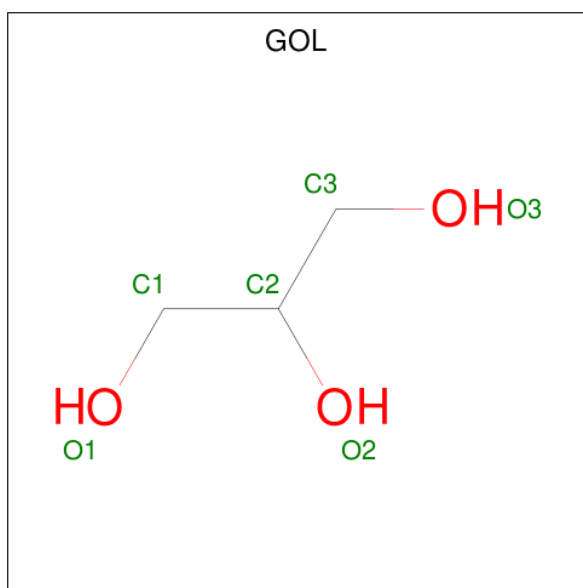
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is COBALAMIN (three-letter code: B12) (formula: C<sub>62</sub>H<sub>89</sub>CoN<sub>13</sub>O<sub>14</sub>P).



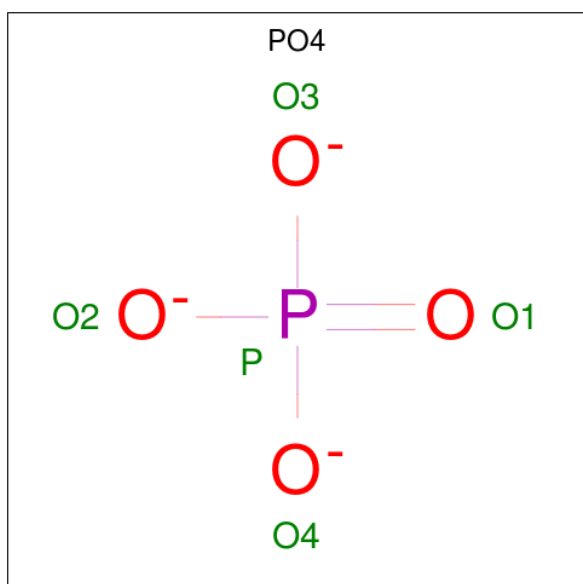
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
4	B	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
4	C	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
4	D	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



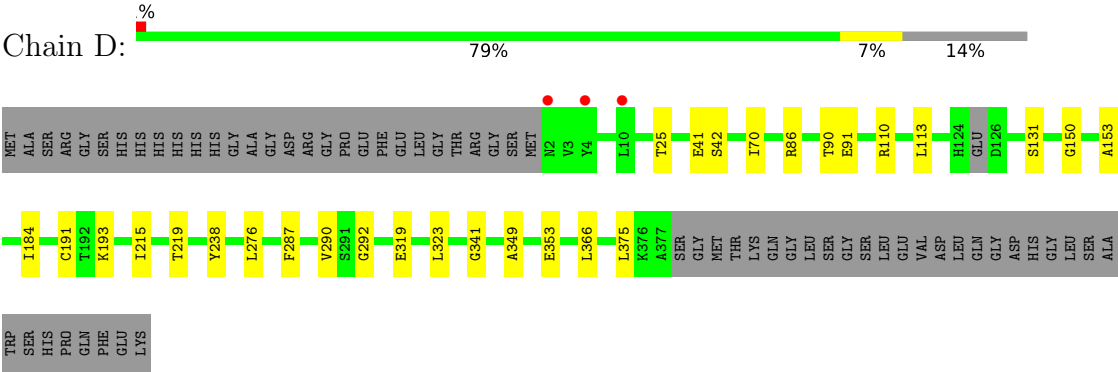
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O P 5 4 1	0	0
6	B	1	Total O P 5 4 1	0	0
6	C	1	Total O P 5 4 1	0	0
6	D	1	Total O P 5 4 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	185	Total O 185 185	0	0
7	B	203	Total O 203 203	0	0
7	C	198	Total O 198 198	0	0
7	D	189	Total O 189 189	0	0
7	E	9	Total O 9 9	0	0
7	F	10	Total O 10 10	0	0



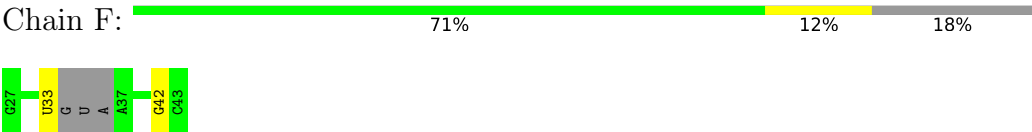
• Molecule 1: Epoxyqueuosine reductase



• Molecule 2: RNA (5'-R(\*G\*CP\*AP\*GP\*AP\*CP\*UP\*GP\*UP\*AP\*AP\*AP\*UP\*CP\*UP\*GP\*C)-3')



• Molecule 2: RNA (5'-R(\*G\*CP\*AP\*GP\*AP\*CP\*UP\*GP\*UP\*AP\*AP\*AP\*UP\*CP\*UP\*GP\*C)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.59Å 111.12Å 96.01Å 90.00° 104.90° 90.00°	Depositor
Resolution (Å)	46.39 – 2.10 47.67 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.1 (46.39-2.10) 97.3 (47.67-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.68 (at 2.10Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.184 , 0.225 0.185 , 0.227	Depositor DCC
$R_{free}$ test set	5114 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.3	Xtriage
Anisotropy	0.886	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 44.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	13688	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	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 64.81 % 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 7.8211e-06. 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, SF4, B12, PO4

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	0/3049	0.52	0/4112
1	B	0.43	0/3041	0.52	0/4100
1	C	0.44	0/3051	0.54	0/4111
1	D	0.44	0/3042	0.52	0/4101
2	E	0.45	0/261	0.85	0/403
2	F	0.44	0/302	0.88	0/468
All	All	0.44	0/12746	0.55	0/17295

There are no bond length outliers.

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	2982	0	3019	19	0
1	B	2977	0	3015	23	0
1	C	2984	0	3027	28	0
1	D	2972	0	3014	19	0
2	E	235	0	120	1	0
2	F	272	0	140	0	0
3	A	16	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	16	0	0	1	0
3	C	16	0	0	1	0
3	D	16	0	0	1	0
4	A	91	0	88	2	0
4	B	91	0	88	3	0
4	C	91	0	88	3	0
4	D	91	0	88	4	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
5	C	6	0	8	0	0
5	D	6	0	8	0	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
6	C	5	0	0	0	0
6	D	5	0	0	0	0
7	A	185	0	0	0	0
7	B	203	0	0	2	0
7	C	198	0	0	2	0
7	D	189	0	0	4	0
7	E	9	0	0	0	0
7	F	10	0	0	0	0
All	All	13688	0	12719	92	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 4.

The worst 5 of 92 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:273:LYS:NZ	1:A:315:SER:OG	2.27	0.68
1:B:90:THR:HG23	1:B:91:GLU:HG2	1.77	0.67
1:D:150:GLY:HA2	1:D:184:ILE:HD11	1.80	0.64
1:B:227:ASP:OD2	1:D:42:SER:HB2	2.00	0.62
1:D:113:LEU:HD13	1:D:131:SER:HB3	1.83	0.60

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	378/437 (86%)	370 (98%)	8 (2%)	0	100	100
1	B	377/437 (86%)	368 (98%)	9 (2%)	0	100	100
1	C	376/437 (86%)	367 (98%)	9 (2%)	0	100	100
1	D	375/437 (86%)	367 (98%)	8 (2%)	0	100	100
All	All	1506/1748 (86%)	1472 (98%)	34 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	325/368 (88%)	325 (100%)	0	100	100
1	B	324/368 (88%)	320 (99%)	4 (1%)	74	80
1	C	325/368 (88%)	323 (99%)	2 (1%)	87	91
1	D	324/368 (88%)	322 (99%)	2 (1%)	87	91
All	All	1298/1472 (88%)	1290 (99%)	8 (1%)	90	91

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	326	LYS
1	D	86[B]	ARG
1	C	350	GLU

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Mol	Chain	Res	Type
1	B	121	LYS
1	C	133	VAL

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

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	E	9/17 (52%)	1 (11%)	0
2	F	11/17 (64%)	2 (18%)	0
All	All	20/34 (58%)	3 (15%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	E	42	G
2	F	33	U
2	F	42	G

There are no RNA pucker outliers to report.

## 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 ⓘ

20 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	SF4	A	501	1	0,12,12	0.00	-	-		
3	SF4	A	502	1	0,12,12	0.00	-	-		
4	B12	A	503	7	81,101,101	0.72	2 (2%)	99,166,166	1.14	11 (11%)
5	GOL	A	504	-	5,5,5	0.44	0	5,5,5	0.50	0
6	PO4	A	505	-	4,4,4	0.93	0	6,6,6	0.50	0
3	SF4	B	501	1	0,12,12	0.00	-	-		
3	SF4	B	502	1	0,12,12	0.00	-	-		
4	B12	B	503	7	81,101,101	0.77	2 (2%)	99,166,166	1.20	9 (9%)
5	GOL	B	504	-	5,5,5	0.42	0	5,5,5	0.92	0
6	PO4	B	505	-	4,4,4	0.94	0	6,6,6	0.59	0
3	SF4	C	501	1	0,12,12	0.00	-	-		
3	SF4	C	502	1	0,12,12	0.00	-	-		
4	B12	C	503	7	81,101,101	0.69	2 (2%)	99,166,166	1.12	11 (11%)
5	GOL	C	504	-	5,5,5	0.30	0	5,5,5	0.75	0
6	PO4	C	505	-	4,4,4	1.29	0	6,6,6	0.78	0
3	SF4	D	501	1	0,12,12	0.00	-	-		
3	SF4	D	502	1	0,12,12	0.00	-	-		
4	B12	D	503	7	81,101,101	0.67	2 (2%)	99,166,166	1.15	11 (11%)
5	GOL	D	504	-	5,5,5	0.39	0	5,5,5	0.45	0
6	PO4	D	505	-	4,4,4	1.16	0	6,6,6	0.71	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
3	SF4	A	501	1	-	-	0/6/5/5
3	SF4	A	502	1	-	-	0/6/5/5
4	B12	A	503	7	-	6/51/223/223	0/3/11/11
5	GOL	A	504	-	-	2/4/4/4	-
3	SF4	B	501	1	-	-	0/6/5/5
3	SF4	B	502	1	-	-	0/6/5/5
4	B12	B	503	7	-	5/51/223/223	0/3/11/11
5	GOL	B	504	-	-	0/4/4/4	-
3	SF4	C	501	1	-	-	0/6/5/5
3	SF4	C	502	1	-	-	0/6/5/5
4	B12	C	503	7	-	7/51/223/223	0/3/11/11

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	C	504	-	-	0/4/4/4	-
3	SF4	D	501	1	-	-	0/6/5/5
3	SF4	D	502	1	-	-	0/6/5/5
4	B12	D	503	7	-	6/51/223/223	0/3/11/11
5	GOL	D	504	-	-	1/4/4/4	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	503	B12	C16-C15	3.82	1.55	1.41
4	A	503	B12	C16-C15	3.58	1.54	1.41
4	D	503	B12	C16-C15	3.43	1.54	1.41
4	C	503	B12	C16-C15	2.41	1.50	1.41
4	A	503	B12	C1P-C2P	2.39	1.57	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	503	B12	C20-C1-C19	-3.95	105.55	109.36
4	A	503	B12	C16-C15-C14	-3.71	118.33	124.23
4	B	503	B12	C20-C1-C19	-3.56	105.93	109.36
4	B	503	B12	C16-C15-C14	-3.45	118.74	124.23
4	B	503	B12	C30-C3-C2	-3.31	112.11	119.13

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	B12	C1P-C2P-O3-P
4	C	503	B12	C14-C13-C48-C49
4	C	503	B12	C1P-C2P-O3-P
4	B	503	B12	C1P-C2P-O3-P
4	D	503	B12	C14-C13-C48-C49

There are no ring outliers.

8 monomers are involved in 17 short contacts:

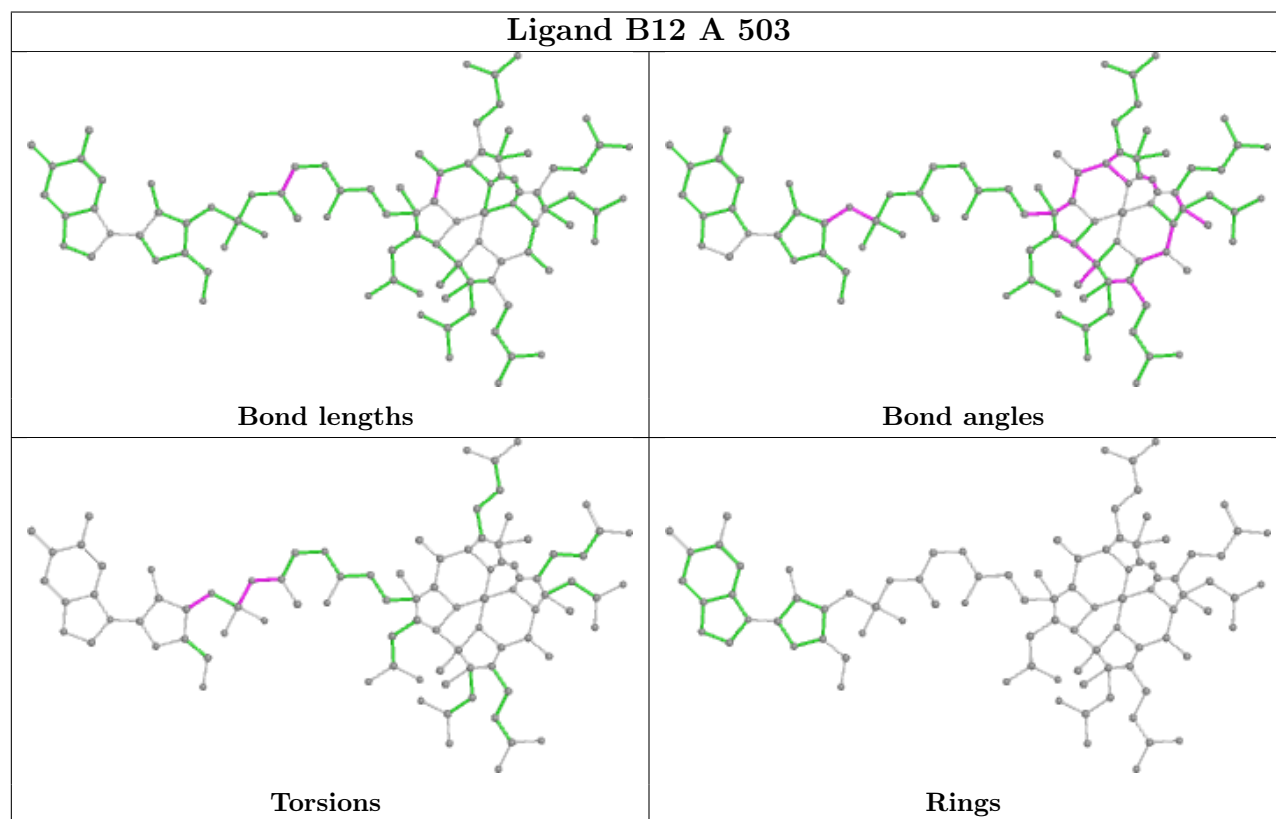
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	SF4	2	0
4	A	503	B12	2	0
3	B	501	SF4	1	0

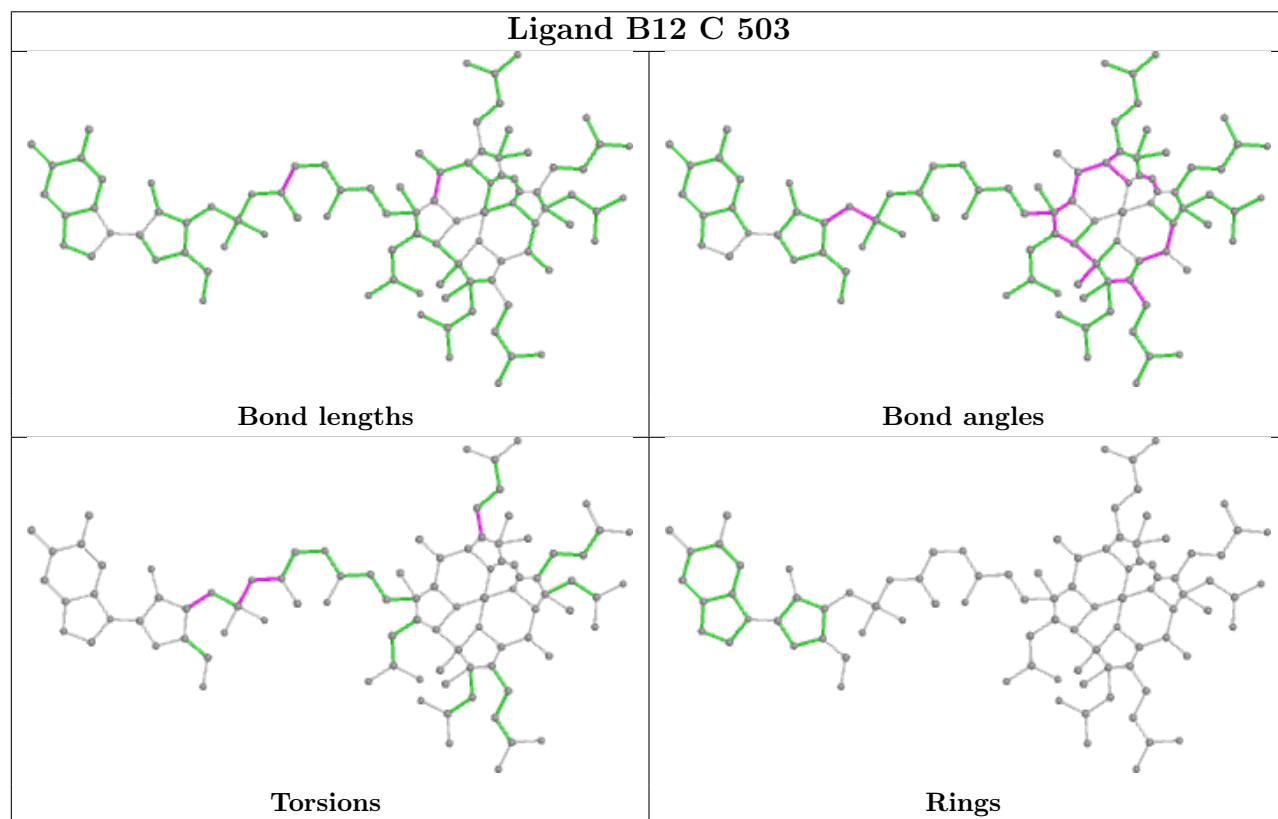
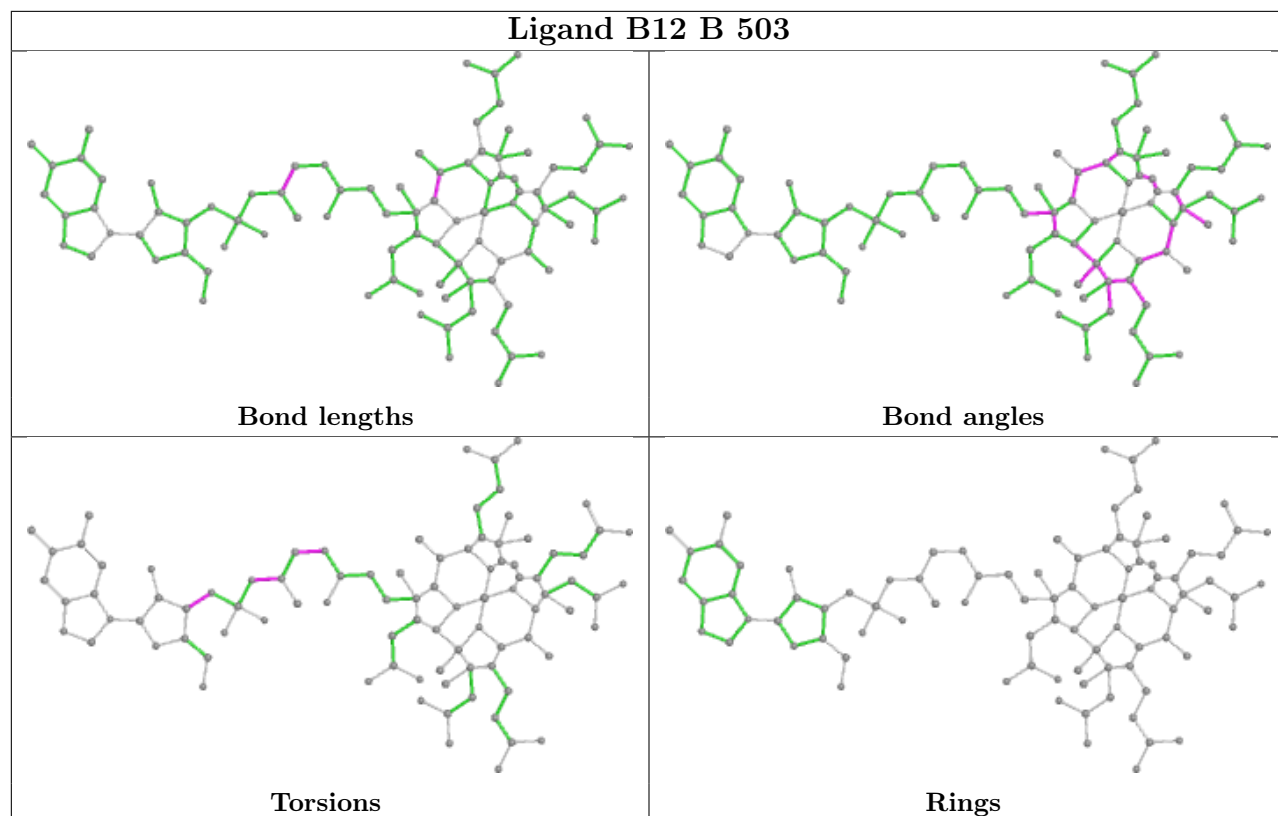
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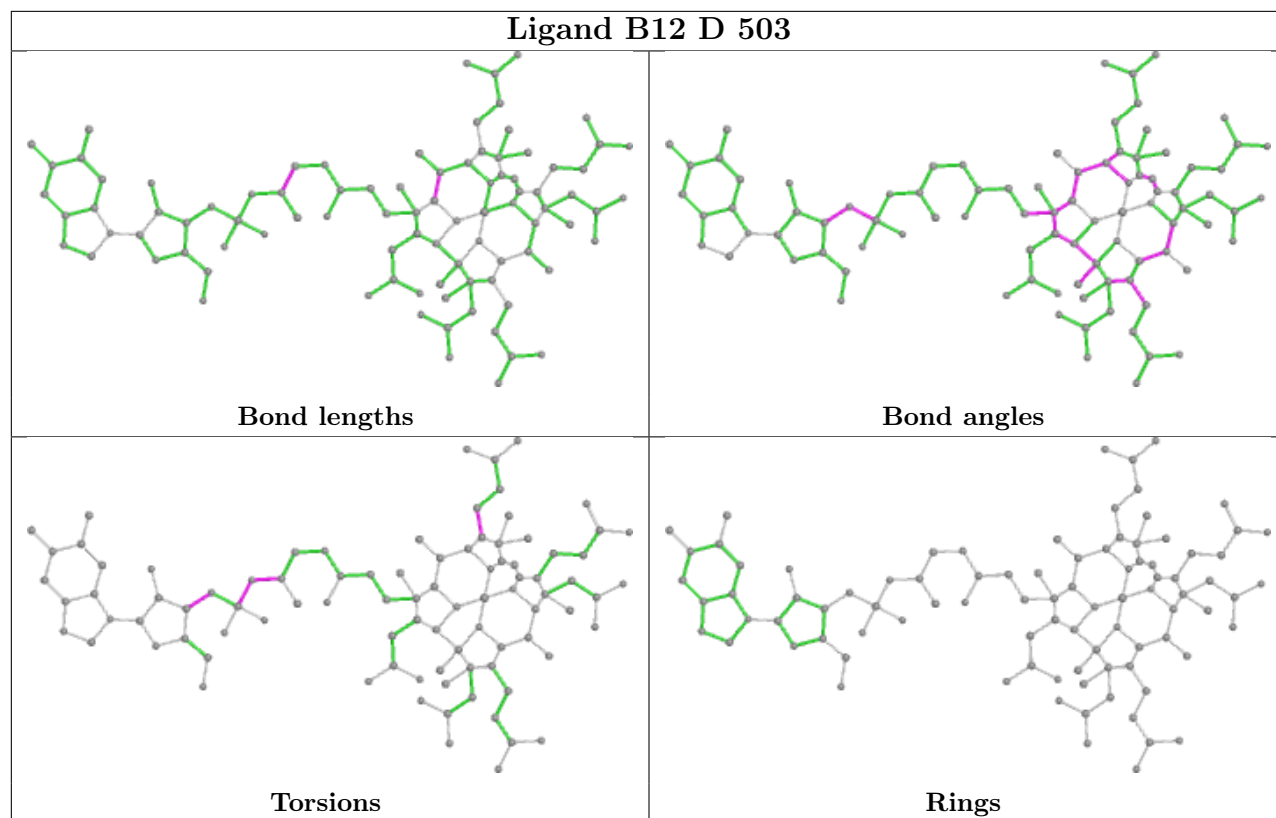
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	503	B12	3	0
3	C	501	SF4	1	0
4	C	503	B12	3	0
3	D	501	SF4	1	0
4	D	503	B12	4	0

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	379/437 (86%)	-0.16	5 (1%) 77 80	24, 34, 56, 91	0
1	B	379/437 (86%)	-0.12	7 (1%) 68 72	25, 35, 55, 84	0
1	C	376/437 (86%)	-0.15	3 (0%) 86 88	24, 33, 50, 73	0
1	D	375/437 (85%)	-0.20	3 (0%) 86 88	25, 34, 51, 63	0
2	E	12/17 (70%)	-0.18	0 100 100	66, 83, 101, 102	0
2	F	14/17 (82%)	-0.21	0 100 100	55, 69, 88, 100	0
All	All	1535/1782 (86%)	-0.16	18 (1%) 79 82	24, 34, 56, 102	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	380	MET	5.5
1	C	378	SER	4.8
1	A	381	THR	4.3
1	C	377	ALA	4.1
1	B	381	THR	3.3

### 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

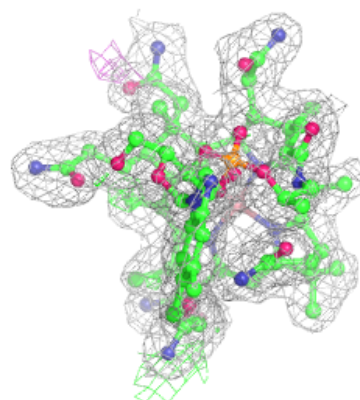
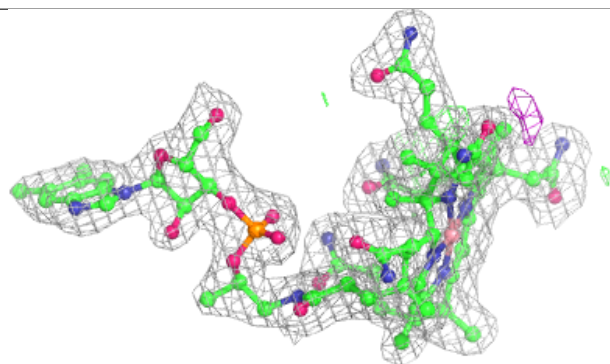
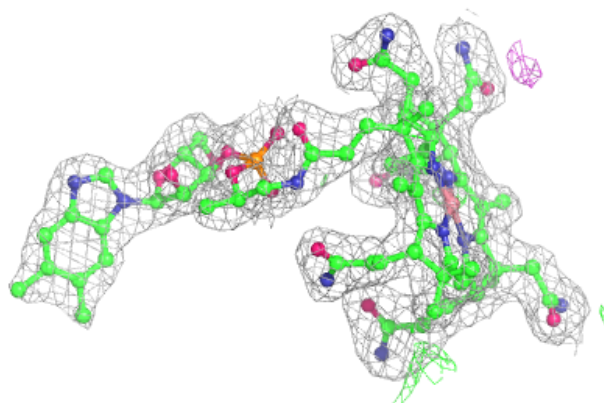
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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
5	GOL	B	504	6/6	0.94	0.15	29,30,37,37	0
5	GOL	C	504	6/6	0.95	0.11	29,30,31,33	0
3	SF4	B	501	8/8	0.96	0.13	39,41,46,47	0
4	B12	A	503	91/91	0.97	0.12	20,27,38,44	0
3	SF4	C	502	8/8	0.97	0.14	27,28,29,30	0
3	SF4	B	502	8/8	0.97	0.12	28,29,31,31	0
4	B12	C	503	91/91	0.97	0.12	21,26,35,40	0
4	B12	B	503	91/91	0.97	0.12	20,27,38,43	0
4	B12	D	503	91/91	0.97	0.11	21,27,38,42	0
6	PO4	A	505	5/5	0.98	0.11	26,28,31,31	0
6	PO4	D	505	5/5	0.98	0.12	24,27,30,31	0
3	SF4	A	501	8/8	0.98	0.15	37,39,45,45	0
3	SF4	D	501	8/8	0.98	0.14	33,38,39,40	0
3	SF4	A	502	8/8	0.98	0.12	30,30,31,31	0
5	GOL	D	504	6/6	0.98	0.09	27,32,34,35	0
3	SF4	D	502	8/8	0.98	0.12	26,27,29,30	0
6	PO4	B	505	5/5	0.98	0.11	28,30,32,37	0
5	GOL	A	504	6/6	0.98	0.08	25,32,34,38	0
6	PO4	C	505	5/5	0.99	0.12	29,29,30,32	0
3	SF4	C	501	8/8	0.99	0.13	34,38,40,41	0

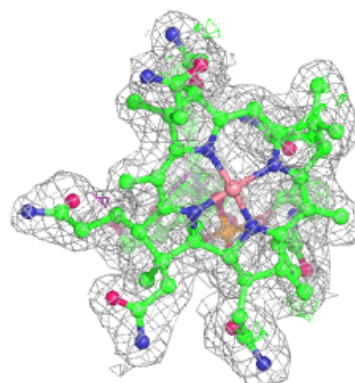
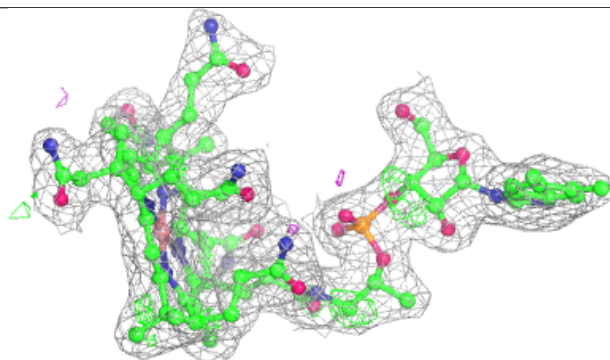
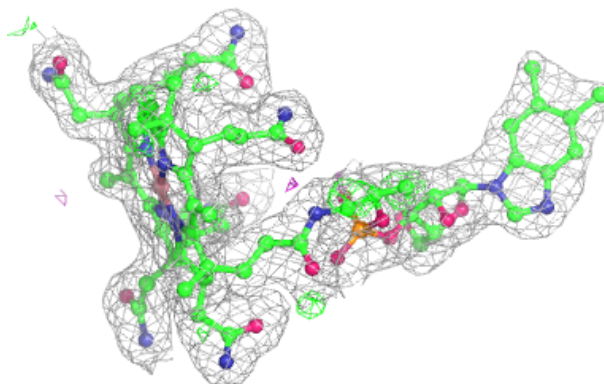
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around B12 A 503:**

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

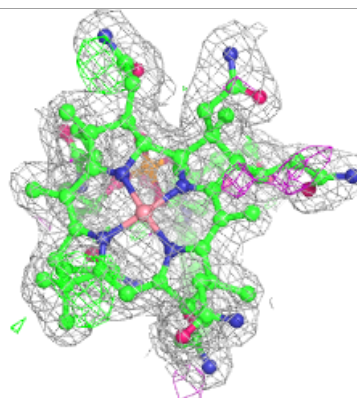
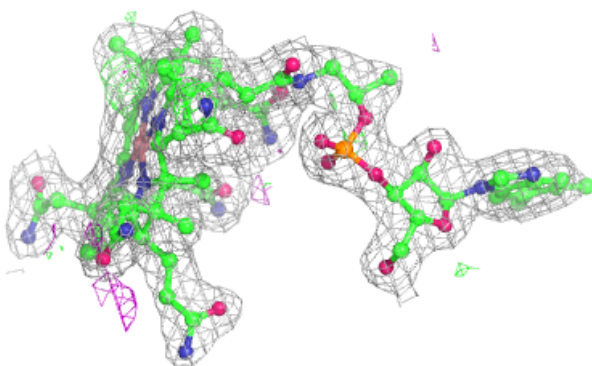
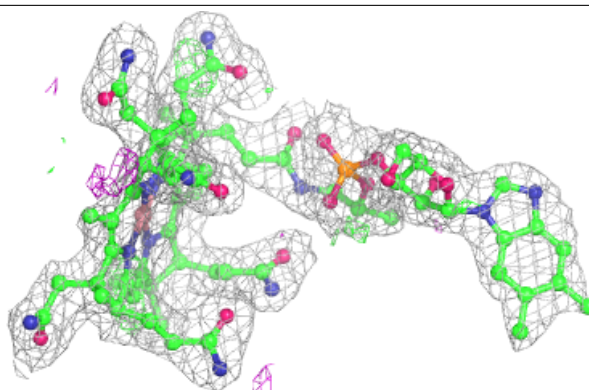
**Electron density around B12 C 503:**

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

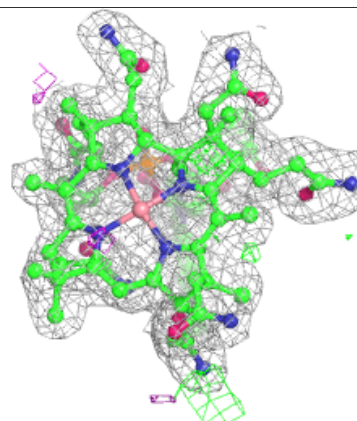
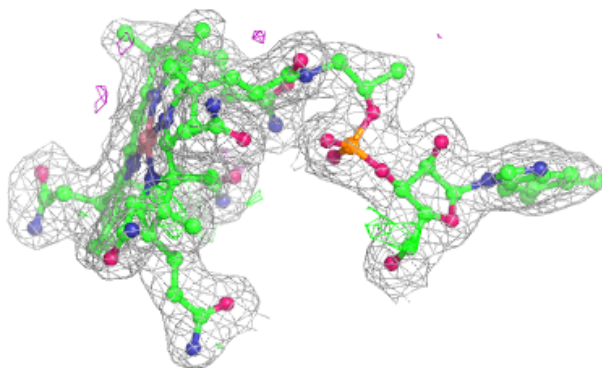
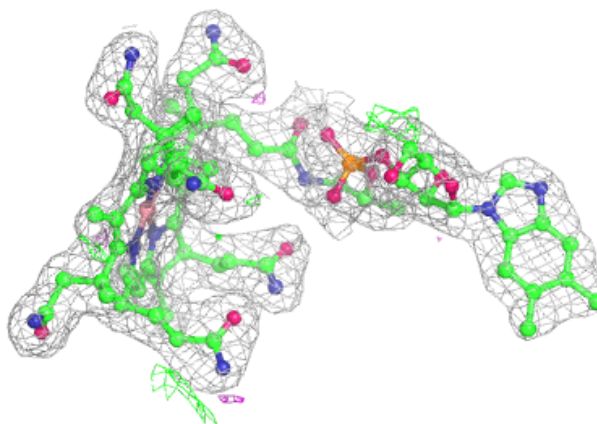


**Electron density around B12 B 503:**

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

**Electron density around B12 D 503:**

$2mF_o-DF_c$  (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.