



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 01:42 am BST

PDB ID : 1N35
Title : lambda3 elongation complex with four phosphodiester bond formed
Authors : Tao, Y.; Farsetta, D.L.; Nibert, M.L.; Harrison, S.C.
Deposited on : 2002-10-25
Resolution : 2.50 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

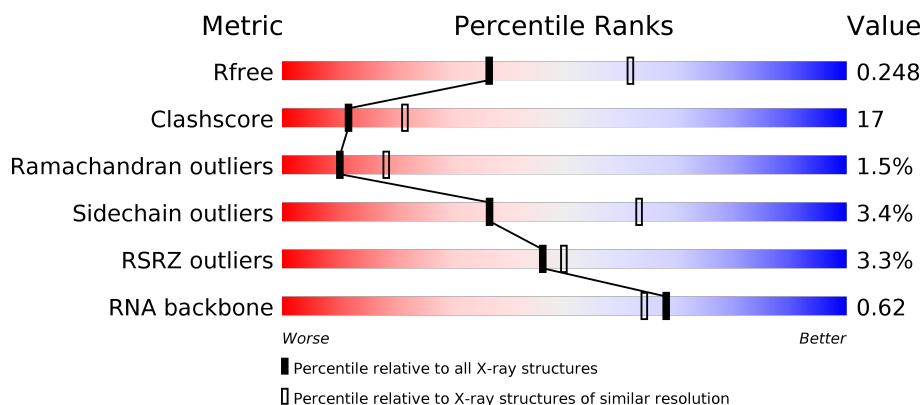
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)
RNA backbone	3102	1008 (2.84-2.16)

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 ≥ 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	B	5	<div> <div>100%</div> <div>20%</div> <div>80%</div> </div>
2	C	10	<div> <div>20%</div> <div>60%</div> <div>20%</div> <div>20%</div> </div>
3	A	1267	<div> <div>3%</div> <div>69%</div> <div>29%</div> <div>.</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10703 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 RNA chain called 5'-R(P*GP*GP*GP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	5	Total	C	N	O	P	0	0	0
			116	50	25	36	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	8	Total	C	N	O	P	0	0	0
			165	74	27	56	8			

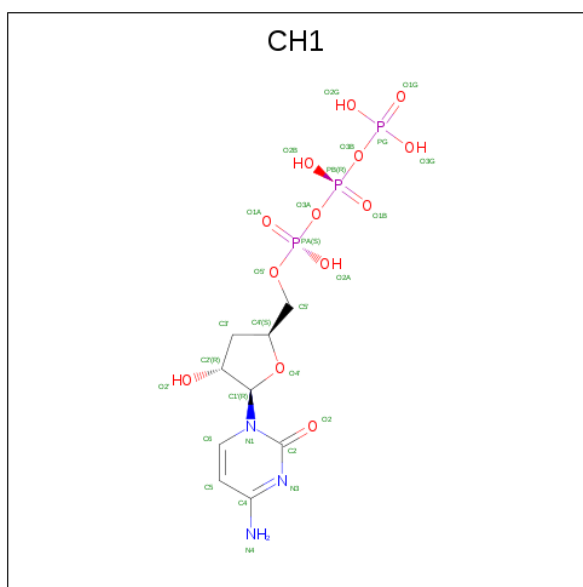
- Molecule 3 is a protein called Minor core protein lambda 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	1264	Total	C	N	O	S	0	0	0
			9986	6369	1712	1841	64			

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mn	0	0
			2	2		

- Molecule 5 is 3'-DEOXY-CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CH1) (formula: C₉H₁₆N₃O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 28	C 9	N 3	O 13	P 3	0	0
5	A	1	Total 28	C 9	N 3	O 13	P 3	0	0
5	A	1	Total 28	C 9	N 3	O 13	P 3	0	0

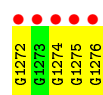
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	4	Total O 4 4	0	0
6	C	6	Total O 6 6	0	0
6	A	340	Total O 340 340	0	0

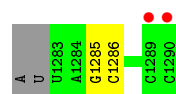
3 Residue-property plots [i](#)

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

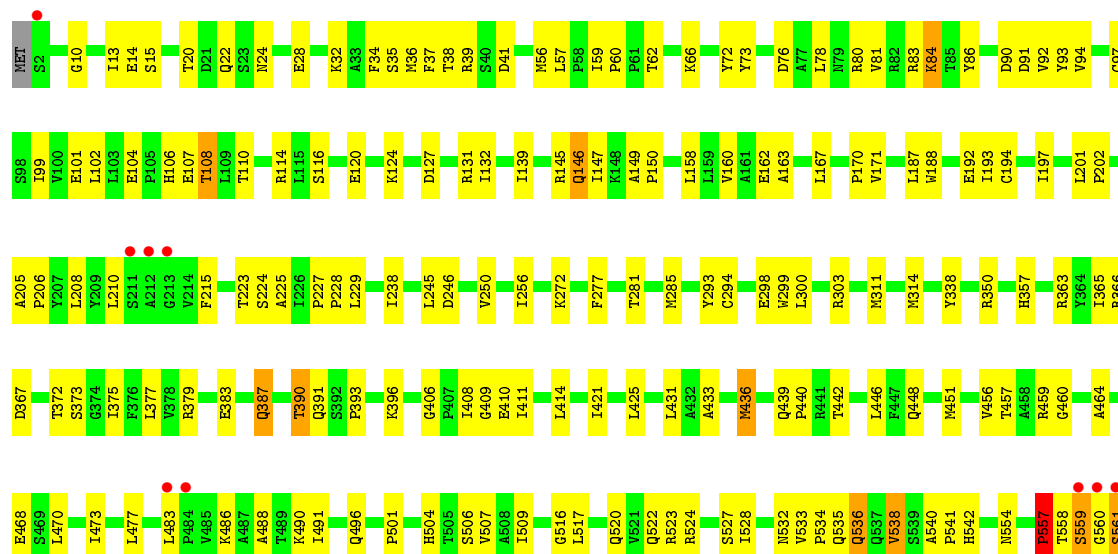
- Molecule 1: 5'-R(P*GP*GP*GP*GP*G)-3'



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



- Molecule 3: Minor core protein lambda 3



SER ALA	W1112	P1006	L877	T778	A562
	D1120	P1007	V878	A779	V663
	V1121	H1014		E780	I564
	R1122		F881	E781	E565
	A1123	Q1018			K566
			W886	L784	V567
	R1130	A1024	I887	V785	I568
		I1025	F888	F786	P569
	L1134	A1026	S889	I787	L570
	G1135		F788	F788	G571
	A1136	E1029	G789	G789	V572
			W890	C790	
	L1146	M1034	T894	R791	P578
	G1149	R1040	R907	N794	I582
	L1150	A1041	P908	L795	
	Q1151	R1042	L909	S796	D585
	E1152	R1043	V920	R797	
		H1044		W798	S592
	L1172	S1045	R923	F799	W595
	A1173			E804	
	R1174	F1049	T926	R805	L599
	V1175				S600
	V1176	L1052	I940	R814	
		L1053	K941	P815	M603
	P1181			A816	
			Q944	I817	I606
	W1184	K1060		L818	H607
	M1185	R1061	M948	D819	
		M1063		Q820	V610
	L1199	C1064	P952	I821	A611
	I1200	E1065	R953		
	P1201			W824	M620
		D1072	R956		
	G1204	L1073	K957	W829	I626
		R1074			V627
	W1217		R960	Q834	
	I1218	L1077	A961	W835	E630
	R1219		A962	Q836	S631
		D1082	S963	R837	V632
	R1223	P1083	R964		V633
				R840	G634
	A1237	S1086	R967	Y841	V635
	V1238	D1087	E968		
		F1089	Y977	L845	A638
	E1243			R851	
		L1090		L759	S642
	H1246		L984		
		V1093			Q645
	F1256	S1094	R987	W855	R646
	M1257	V1095		I856	M647
	T1258		R990	Q857	I648
	W1259	Q1100		E858	Q649
	M1260	S1101	W995	S859	H650
		T1102		W860	L651
	R1261	R1103	I1002	G861	
	Q1262		I1003	I862	L654
	E1263	F1106	H1004	L863	Y655
	G1264				
	R1265		M1005	Q864	K656

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.88Å 85.01Å 249.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.01 – 2.50 43.01 – 2.49	Depositor EDS
% Data completeness (in resolution range)	89.9 (43.01-2.50) 89.4 (43.01-2.49)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.207 , 0.259 0.198 , 0.248	Depositor DCC
R_{free} test set	2767 reflections (5.21%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10703	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CH1, MN

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	B	0.81	1/130 (0.8%)	0.68	0/201
2	C	0.52	0/182	0.71	0/280
3	A	0.38	0/10239	0.61	1/13905 (0.0%)
All	All	0.39	1/10551 (0.0%)	0.61	1/14386 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1272	G	OP3-P	-7.10	1.52	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	408	ILE	N-CA-C	-5.48	96.19	111.00

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	B	116	0	56	8	0
2	C	165	0	88	4	0
3	A	9986	0	9903	354	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	2	0	0	0	0
5	A	84	0	36	3	0
6	A	340	0	0	8	0
6	B	4	0	0	0	0
6	C	6	0	0	0	0
All	All	10703	0	10083	356	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 17.

The worst 5 of 356 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:223:THR:HG22	3:A:225:ALA:H	1.14	1.07
3:A:1112:MET:HE1	3:A:1150:LEU:HD11	1.33	1.05
3:A:410:GLU:H	3:A:649:GLN:NE2	1.58	1.01
1:B:1274:G:H21	3:A:562:ALA:HB2	1.22	1.01
3:A:81:VAL:H	3:A:671:ASN:HD21	1.09	0.99

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
3	A	1262/1267 (100%)	1169 (93%)	74 (6%)	19 (2%)	10 18

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	108	THR
3	A	559	SER

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Mol	Chain	Res	Type
3	A	561	SER
3	A	814	TRP
3	A	564	ILE

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
3	A	1081/1083 (100%)	1044 (97%)	37 (3%)	37 63

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	735	ASP
3	A	804	GLU
3	A	1151	GLN
3	A	778	THR
3	A	784	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	664	ASN
3	A	710	HIS
3	A	1005	ASN
3	A	671	ASN
3	A	296	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	4/5 (80%)	0	0
2	C	7/10 (70%)	0	0
All	All	11/15 (73%)	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 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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
5	CH1	A	1291	4	22,29,29	1.16	1 (4%)	27,45,45	2.98	13 (48%)
5	CH1	A	1294	-	22,29,29	1.19	2 (9%)	27,45,45	2.93	13 (48%)
5	CH1	A	1295	-	22,29,29	1.20	2 (9%)	27,45,45	2.88	13 (48%)

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
5	CH1	A	1291	4	-	5/20/34/34	0/2/2/2
5	CH1	A	1294	-	-	6/20/34/34	0/2/2/2
5	CH1	A	1295	-	-	8/20/34/34	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1295	CH1	C6-N1	2.51	1.38	1.35
5	A	1294	CH1	C6-N1	2.33	1.38	1.35
5	A	1291	CH1	C6-N1	2.16	1.38	1.35
5	A	1294	CH1	PG-O1G	2.15	1.57	1.50
5	A	1295	CH1	PB-O1B	2.01	1.58	1.50

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1295	CH1	O3G-PG-O1G	-7.66	80.69	110.68
5	A	1294	CH1	O3G-PG-O1G	-7.38	81.79	110.68
5	A	1291	CH1	O3G-PG-O1G	-7.34	81.95	110.68
5	A	1291	CH1	O3G-PG-O3B	-6.68	82.22	104.64
5	A	1294	CH1	O3G-PG-O3B	-6.61	82.48	104.64

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1291	CH1	C3'-C4'-C5'-O5'
5	A	1291	CH1	O4'-C4'-C5'-O5'
5	A	1291	CH1	C5'-O5'-PA-O1A
5	A	1294	CH1	C3'-C4'-C5'-O5'
5	A	1294	CH1	O4'-C4'-C5'-O5'

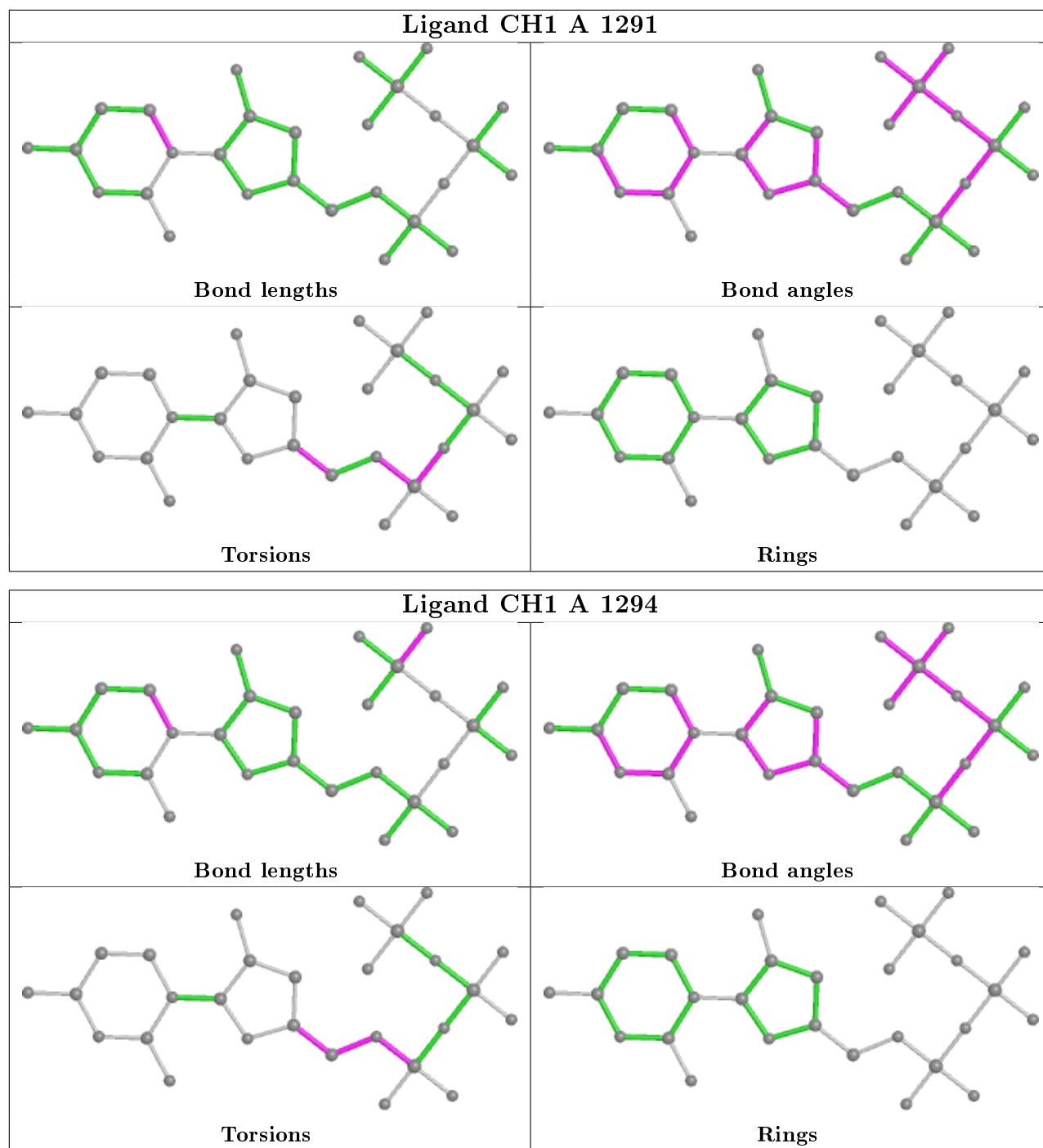
There are no ring outliers.

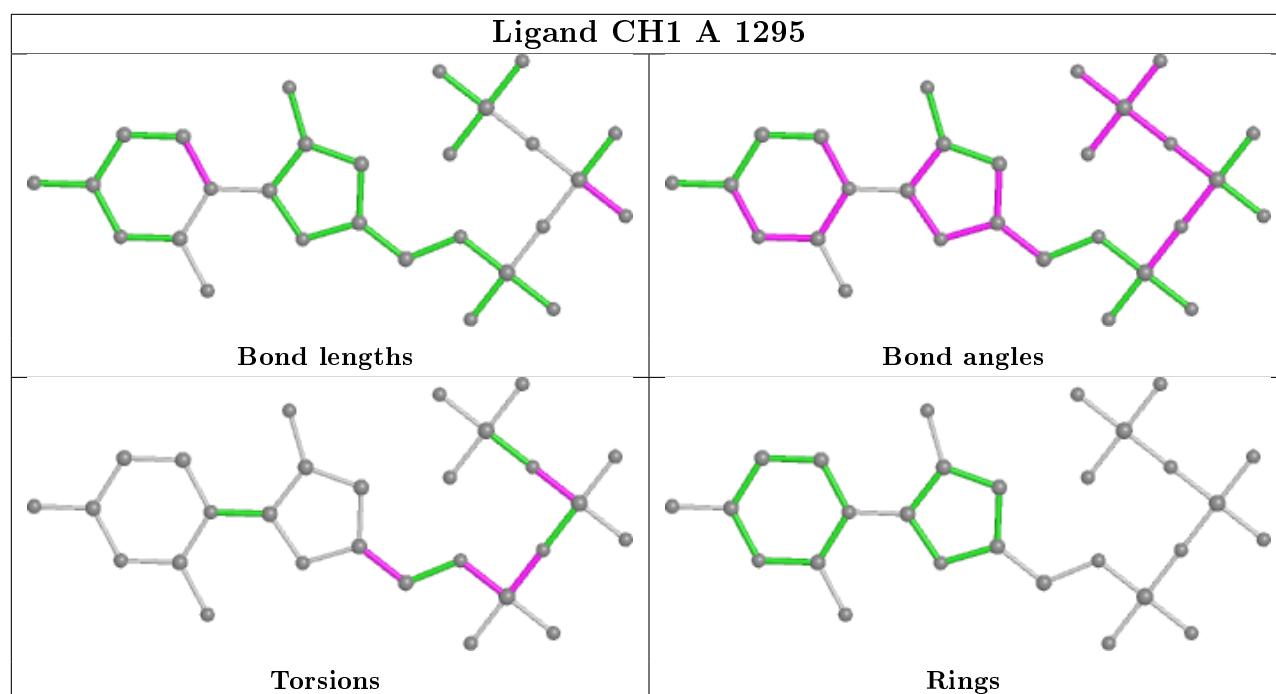
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1291	CH1	2	0
5	A	1294	CH1	1	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, 95th 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 ²)	Q<0.9
1	B	5/5 (100%)	4.45	5 (100%) 0 0	108, 119, 124, 124	0
2	C	8/10 (80%)	2.28	2 (25%) 0 0	35, 69, 127, 133	0
3	A	1264/1267 (99%)	-0.04	35 (2%) 53 56	17, 32, 53, 98	0
All	All	1277/1282 (99%)	-0.00	42 (3%) 46 50	17, 32, 54, 133	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	1290	C	10.1
3	A	2	SER	8.1
3	A	211	SER	6.7
3	A	561	SER	6.6
2	C	1289	C	6.5

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

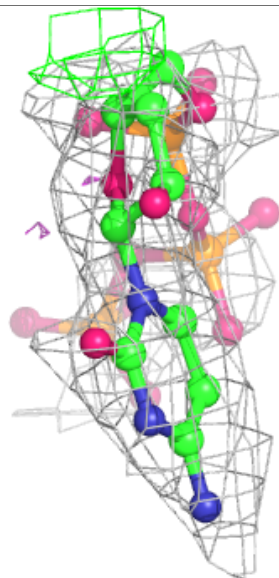
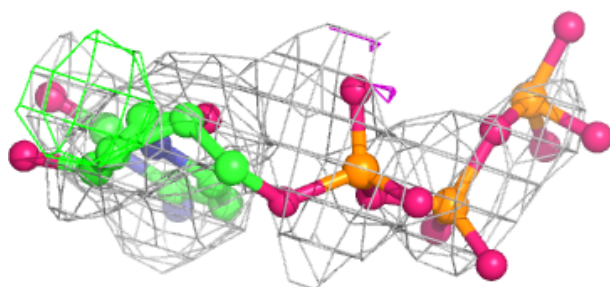
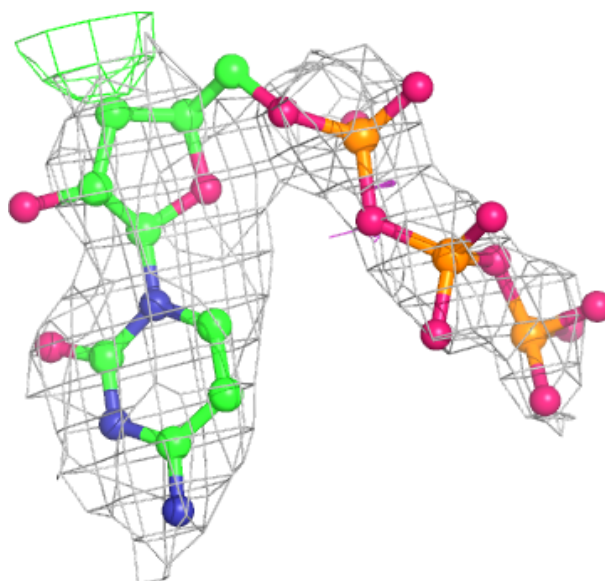
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	CH1	A	1294	28/28	0.65	0.33	86,99,118,119	0
5	CH1	A	1291	28/28	0.83	0.21	83,93,100,100	0
5	CH1	A	1295	28/28	0.88	0.20	44,59,81,81	0
4	MN	A	1301	1/1	0.90	0.06	63,63,63,63	0
4	MN	A	1302	1/1	0.98	0.11	60,60,60,60	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.

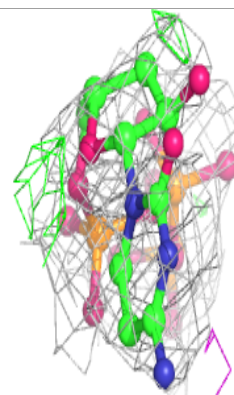
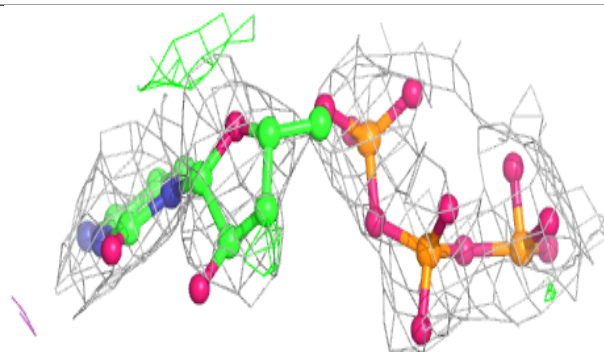
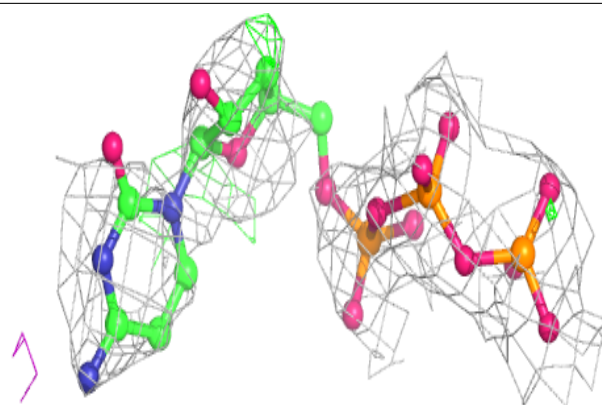
Electron density around CH1 A 1294:

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



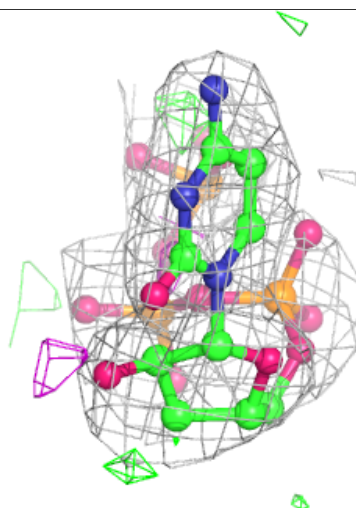
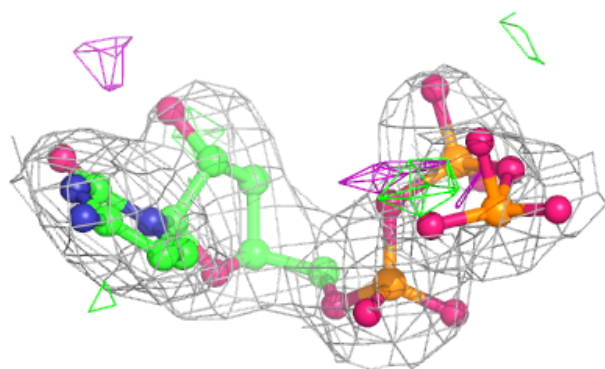
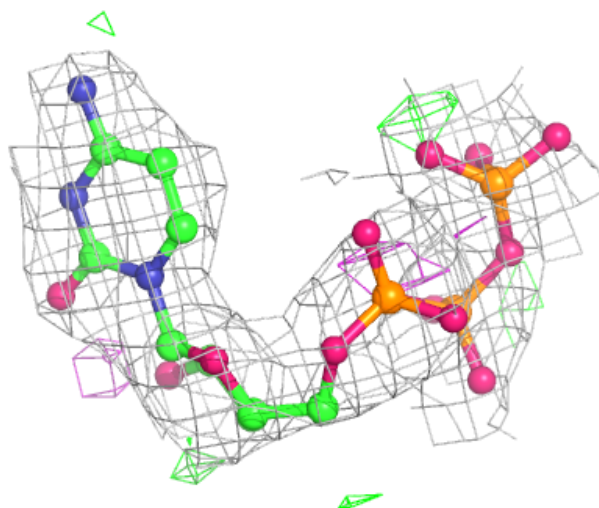
Electron density around CH1 A 1291:

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



Electron density around CH1 A 1295:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.