



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 10:57 AM UTC

PDB ID : 1N38 / pdb_00001n38
Title : reovirus polymerase lambda3 elongation complex with one phosphodiester bond formed
Authors : Tao, Y.; Farsetta, D.L.; Nibert, M.L.; Harrison, S.C.
Deposited on : 2002-10-25
Resolution : 2.80 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

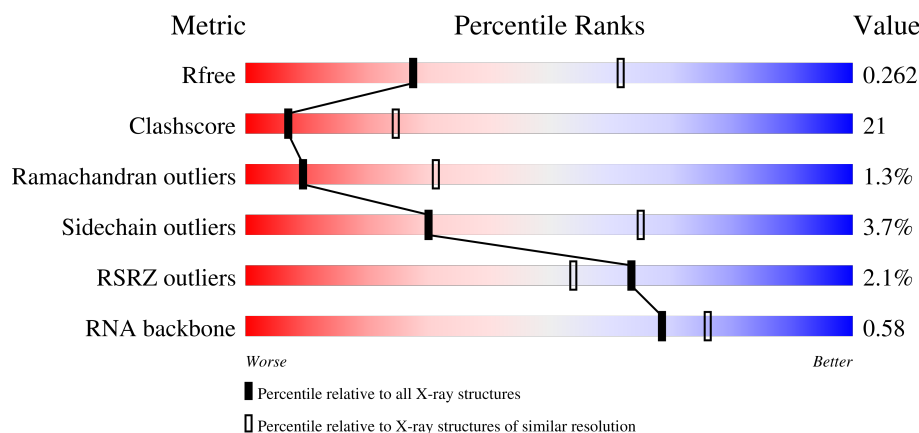
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)
RNA backbone	3983	1114 (3.00-2.60)

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 of 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	2	100% 50% 50%
2	C	6	33% 33% 50% 17%
3	A	1267	2% 60% 36% .

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
5	U3H	A	1291	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10485 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*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	2	Total	C	N	O	P	0	0	0
			43	19	8	14	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	5	Total	C	N	O	P	0	0	0
			105	47	17	36	5			

- 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 (CCD ID: MN) (formula: Mn).

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

- Molecule 5 is 3'-DEOXY-URIDINE 5'-TRIPHOSPHATE (CCD ID: U3H) (formula: C₉H₁₇N₂O₁₄P₃).

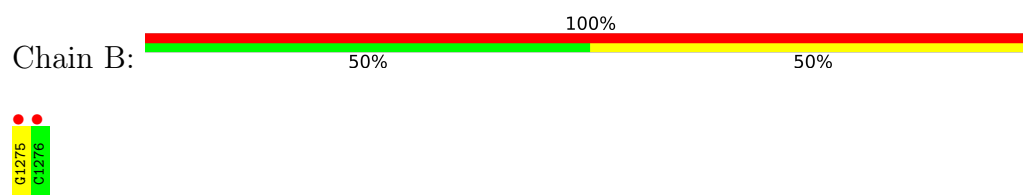
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total 2	O 2	0	0
7	C	2	Total 2	O 2	0	0
7	A	261	Total 261	O 261	0	0

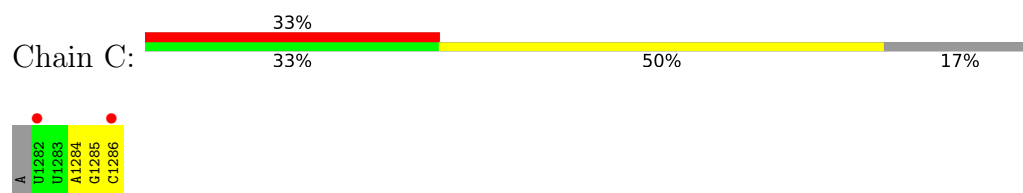
3 Residue-property plots [i](#)

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.

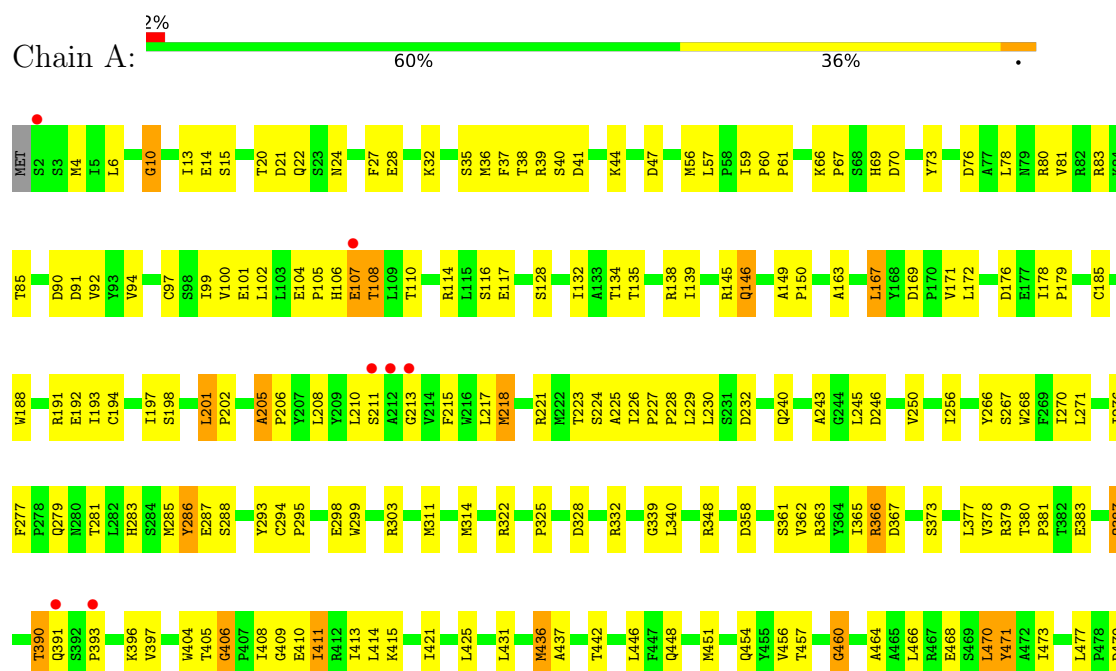
- Molecule 1: 5'-R(P*GP*C)-3'



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



- Molecule 3: Minor core protein lambda 3



W1259	V1148	L1052	R953	W838	G746	Q649	V563	F480
Q1262	G1149	R1062	K957	I839	K747	H650	I564	L483
E1263	L1150	M1063	R957	R840	V748	L651	E565	K486
G1264	Q1151	C1064	R960	L845	S750	L654	K566	I568
R1265	V1167	E1065	R964	C846	E751	P659	V567	A488
SER	N1168	S1070	E965	C847	Q754	P659	P569	T489
ALA	L1172	V1071	V966	R851	N755	R662	S571	K490
	A1173	D1072	R967	T854	D756	N664	V572	I491
	R1174	L1073	E968	M855	L757	D665	S576	Q496
	V1175	R1074	Q969	I856	Y763	P577	P578	P501
	V1176	L1077	Y977	C857	G764	P578	N579	H504
	N1177		Q980	S858	E765	N670	Q580	S581
	P1181	D1082	E983	S859	V860	N671	I582	V507
	D1182	P1083	L984	V868	L863	G683	D585	A508
	T1183	L1084	R987	W867	Q864	S684		I509
	W1184	M1085	R990	W868	Y775	T685	A591	D512
	M1185	S1086	R991	K879	D776	A686	S592	T513
	S1186	P1088	R992	A880	G777	T687	W596	S514
	M1192	F1089	S993	F881	T778	S688	L599	Q516
	F1193	L1090	E994	W886	A779	T689	S600	L517
	K1194	M1098	R995		E780	E690	M603	M515
	H1195	V1093	Q999	W890	Y781	E700	I606	Q520
	H1196	S1094	R1002	Y891	L782	T701		R523
	V1197	V1095	T1003	M892	G789	F702		R524
	K1198	M1098	H1004	P893	R797	W706		P525
	L1199	L1099	P1006	T894	H798	G707		R526
	L1200	Q1100	P1007	R907	P799	V716		S527
	P1201	S1101	V1012	P908	E804	W720		I528
	G1204	T1102	P1013	L909	R805	G621		M529
	R1206	R1103	E1022	M910	S809	P623		P530
	P1212	F1106	A1023	V915		A624		L531
	M1215	T1109	A1024	V920	P813	V627		N532
	G1216	M1112	A1025	R923	W814	E630		V533
	W1217	T1115	A1026	T926	P815	V730		P534
	L1218	V1116	E1029	L940	A816	C731		Q535
	R1219	V1121	M1034	K941	I817	Q732		Q536
	R1223	L1129	D1035	L942	L818	W728		Q537
	M1229	R1130	M1039	Y943	Q820	V729		V538
	T1232	T1133	R1040	Q944	I821	C731		S539
	A1237	L1134	A1041		V829	Q732		P541
	V1238	G1135	R1043	M948	Q834			H542
	E1243	A1136	H1045	L951	W835			N554
	D1244	A1143	L1146	P952	Q836			P557
	I1245	Q1144			T743			T558
	H1246	L1145			T744			S559
	M1257	T1258			A745			G560
								S561
								A562

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.72Å 85.21Å 248.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.67 – 2.80 46.67 – 2.80	Depositor EDS
% Data completeness (in resolution range)	85.6 (46.67-2.80) 86.3 (46.67-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.201 , 0.263 0.200 , 0.262	Depositor DCC
R_{free} test set	2767 reflections (5.28%)	wwPDB-VP
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.2	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	0.92	EDS
Total number of atoms	10485	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, U3H, CH1

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	0.82	0/47	0.71	0/69
2	C	0.65	0/116	0.64	0/178
3	A	0.48	0/10239	0.98	44/13905 (0.3%)
All	All	0.49	0/10402	0.97	44/14152 (0.3%)

There are no bond length outliers.

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	566	LYS	N-CA-C	-12.90	95.64	112.41
3	A	1194	LYS	N-CA-C	8.21	120.01	111.14
3	A	287	GLU	N-CA-C	-7.98	102.65	112.38
3	A	201	LEU	CA-C-N	7.20	127.04	119.05
3	A	201	LEU	C-N-CA	7.20	127.04	119.05

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	43	0	21	6	0
2	C	105	0	54	4	0
3	A	9986	0	9903	422	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	2	0	0	0	0
5	A	28	0	11	0	0
6	A	56	0	24	0	0
7	A	261	0	0	10	0
7	B	2	0	0	0	0
7	C	2	0	0	0	0
All	All	10485	0	10013	424	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 21.

The worst 5 of 424 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:410:GLU:H	3:A:649:GLN:NE2	1.49	1.09
3:A:561:SER:HB3	3:A:566:LYS:HE3	1.34	1.07
3:A:223:THR:HG22	3:A:225:ALA:H	1.21	1.03
3:A:1005:ASN:HD21	3:A:1263:GLU:HB3	1.27	0.99
3:A:410:GLU:H	3:A:649:GLN:HE22	1.07	0.96

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%)	1162 (92%)	84 (7%)	16 (1%)	9	31

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	91	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	108	THR
3	A	561	SER
3	A	563	VAL
3	A	814	TRP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	1081/1083 (100%)	1041 (96%)	40 (4%)	30 65

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	980	GLN
3	A	1077	LEU
3	A	984	LEU
3	A	1052	LEU
3	A	1151	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	536	GLN
3	A	1005	ASN
3	A	671	ASN
3	A	1246	HIS
3	A	917	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	0/2	-	-
2	C	4/6 (66%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	4/8 (50%)	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 oligosaccharides 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	$\# Z > 2$
6	CH1	A	1294	-	27,29,29	3.13	7 (25%)	37,45,45	2.70	16 (43%)
5	U3H	A	1291	4	25,29,29	3.52	9 (36%)	31,45,45	2.94	14 (45%)
6	CH1	A	1295	-	27,29,29	2.89	6 (22%)	37,45,45	2.58	14 (37%)

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	CH1	A	1294	-	-	6/22/34/34	0/2/2/2
5	U3H	A	1291	4	1/1/9/12	7/22/47/47	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CH1	A	1295	-	-	9/22/34/34	0/2/2/2

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1294	CH1	PA-O3A	9.75	1.70	1.59
5	A	1291	U3H	PA-O3A	9.73	1.70	1.59
5	A	1291	U3H	PB-O3B	8.91	1.69	1.59
6	A	1294	CH1	PB-O3B	8.62	1.68	1.59
6	A	1295	CH1	PB-O3B	8.58	1.68	1.59

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1295	CH1	O3G-PG-O1G	-7.71	80.79	110.83
6	A	1294	CH1	O3G-PG-O1G	-7.43	81.88	110.83
5	A	1291	U3H	O4'-C4'-C5'	7.23	122.37	109.34
6	A	1294	CH1	O3G-PG-O3B	-6.56	82.63	104.64
6	A	1295	CH1	O3G-PG-O3B	-6.39	83.19	104.64

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1291	U3H	C2

5 of 22 torsion outliers are listed below:

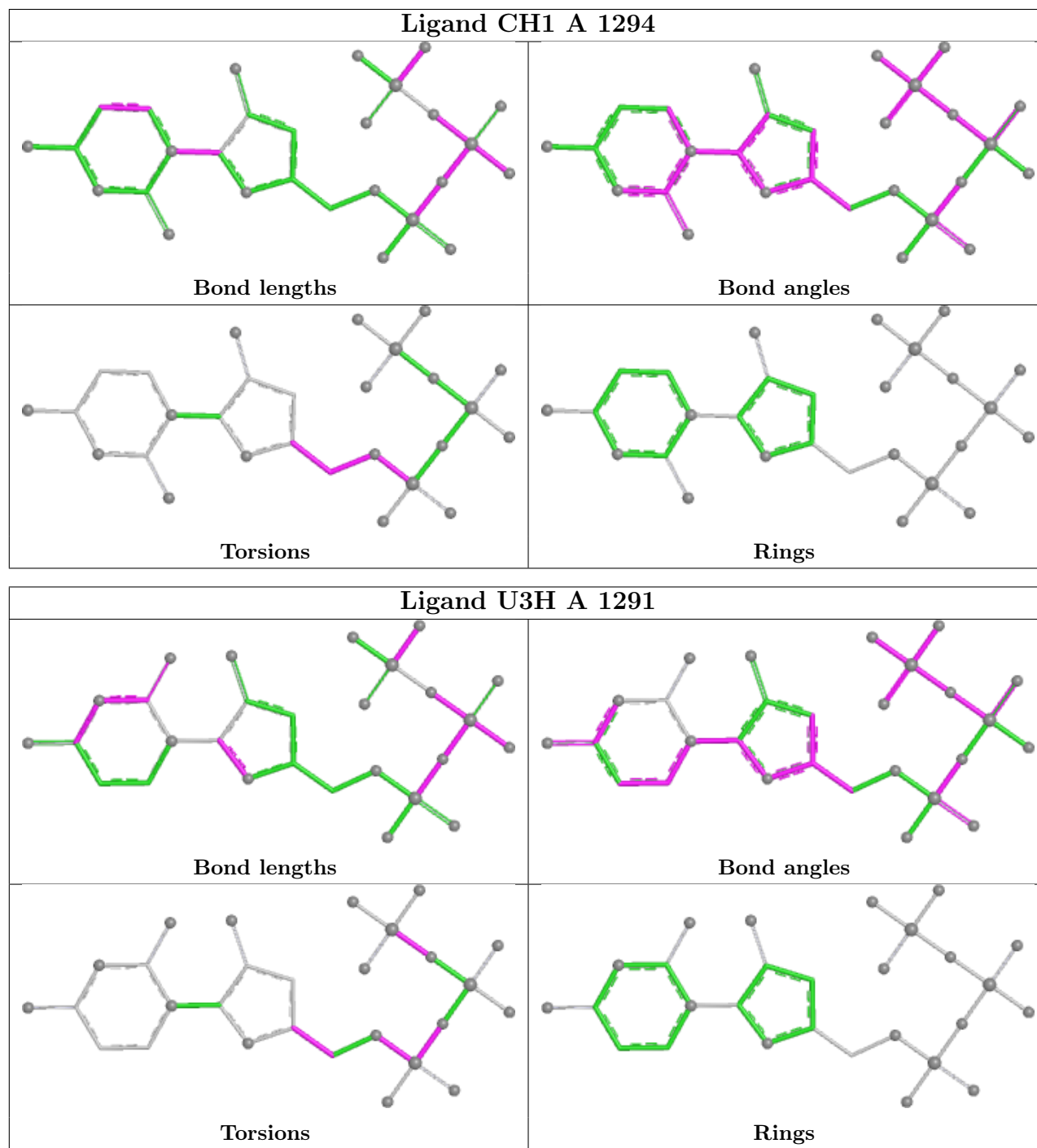
Mol	Chain	Res	Type	Atoms
5	A	1291	U3H	C3'-C4'-C5'-O5'
5	A	1291	U3H	O4'-C4'-C5'-O5'
6	A	1294	CH1	C3'-C4'-C5'-O5'
6	A	1294	CH1	O4'-C4'-C5'-O5'
6	A	1294	CH1	C5'-O5'-PA-O1A

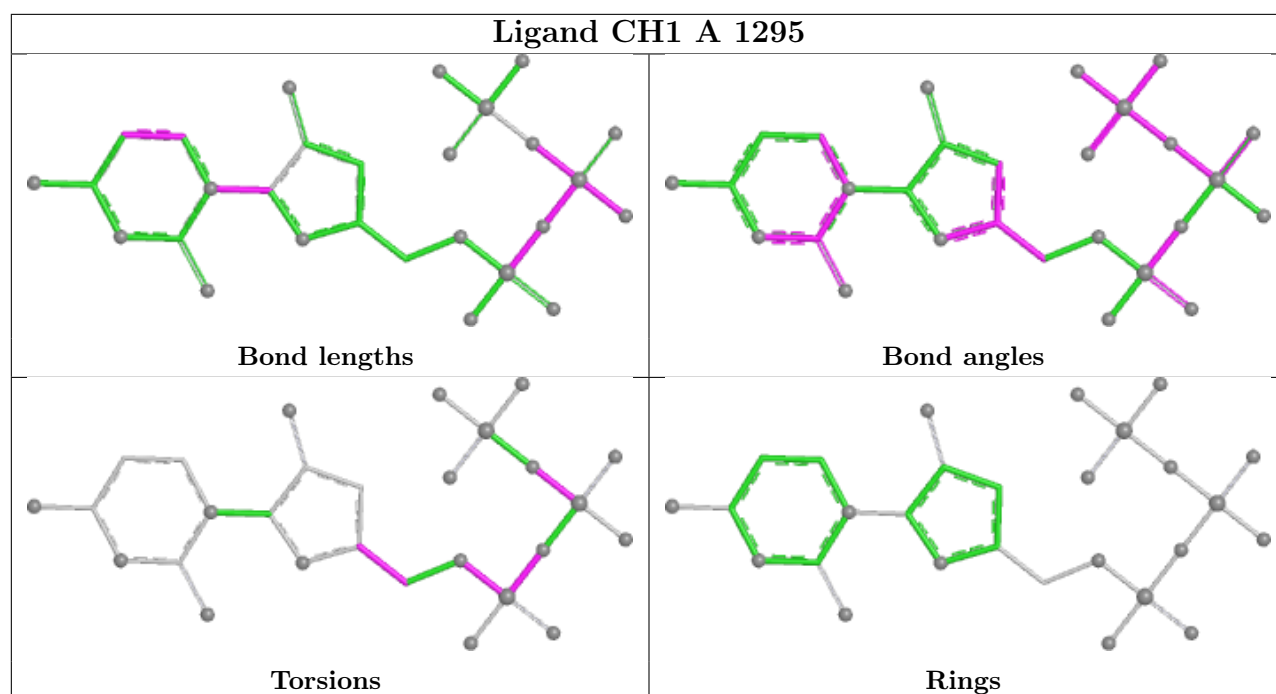
There are no ring outliers.

No monomer is involved in short contacts.

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	2/2 (100%)	5.47	2 (100%) 0 0	96, 96, 96, 122	0
2	C	5/6 (83%)	1.68	2 (40%) 1 0	23, 41, 71, 74	0
3	A	1264/1267 (99%)	-0.17	23 (1%) 67 58	7, 21, 44, 85	0
All	All	1271/1275 (99%)	-0.15	27 (2%) 63 54	7, 21, 45, 122	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1275	G	6.6
3	A	562	ALA	6.4
2	C	1286	C	5.6
3	A	561	SER	5.5
3	A	856	ILE	5.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

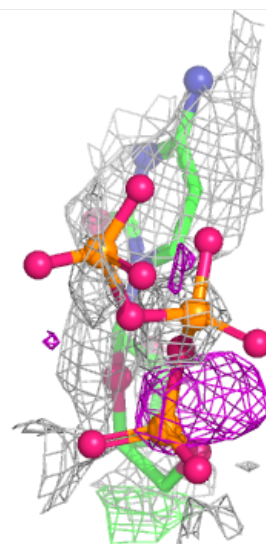
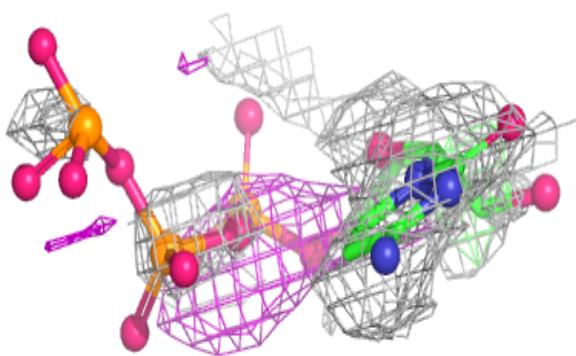
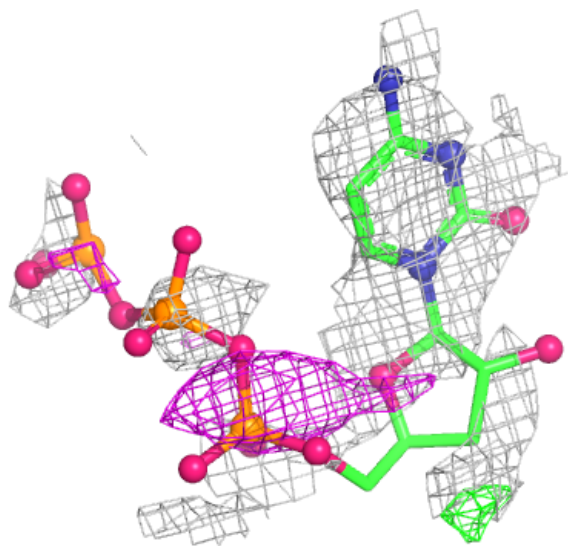
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	CH1	A	1294	28/28	0.48	0.23	98,112,132,132	0
5	U3H	A	1291	28/28	0.74	0.18	82,88,95,95	0
6	CH1	A	1295	28/28	0.80	0.16	48,61,74,75	0
4	MN	A	1301	1/1	0.94	0.10	63,63,63,63	0
4	MN	A	1302	1/1	0.95	0.05	39,39,39,39	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.

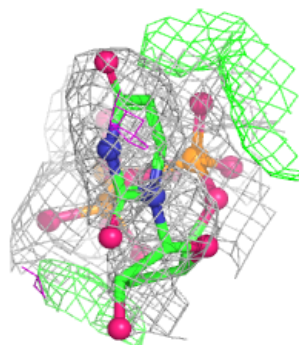
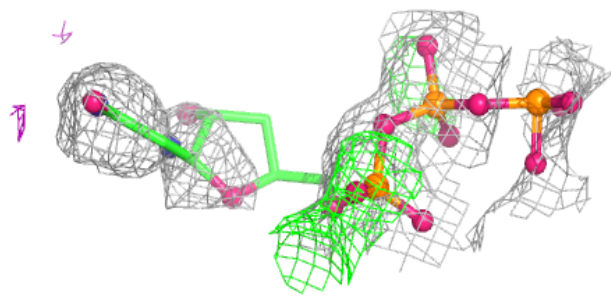
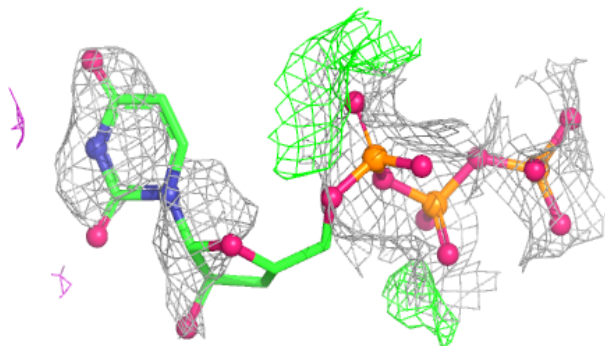
Electron density around CH1 A 1294:

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



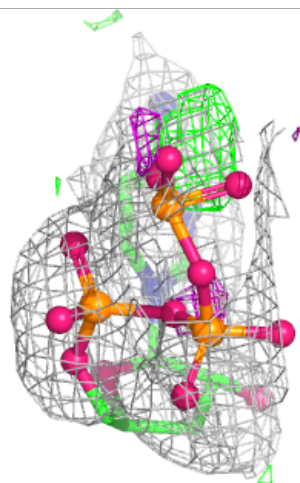
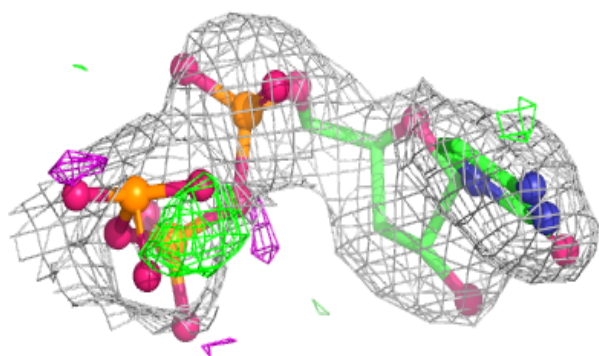
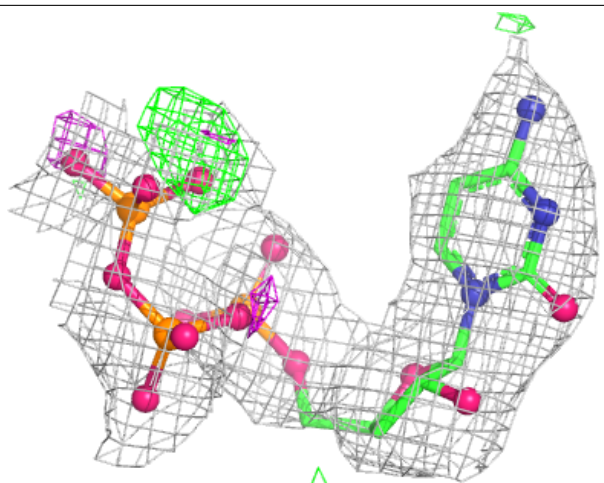
Electron density around U3H A 1291:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.