



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 07:43 pm BST

PDB ID : 3IRO
Title : Trypanosoma cruzi Dihydrofolate Reductase-Thymidylate Synthase complexed with NADPH and Q-8 antifolate
Authors : Chitnumsub, P.; Yuvaniyama, J.; Yuthavong, Y.
Deposited on : 2009-08-24
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 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

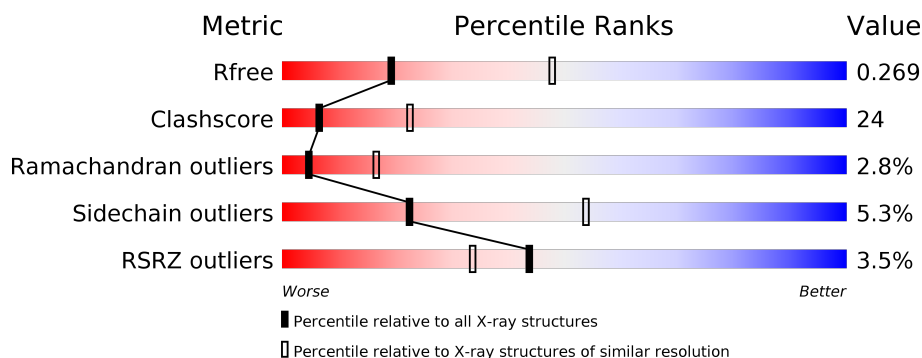
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	A	521	<div> <div>3%</div> <div> <div></div> <div>55%</div> <div>42%</div> <div>..</div> </div> </div>
1	B	521	<div> <div>4%</div> <div> <div></div> <div>51%</div> <div>43%</div> <div>..</div> </div> </div>
1	C	521	<div> <div>3%</div> <div> <div></div> <div>56%</div> <div>38%</div> <div>..</div> </div> </div>
1	D	521	<div> <div>4%</div> <div> <div></div> <div>56%</div> <div>37%</div> <div>5%</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
5	ACT	A	809	-	-	X	-

2 Entry composition [i](#)

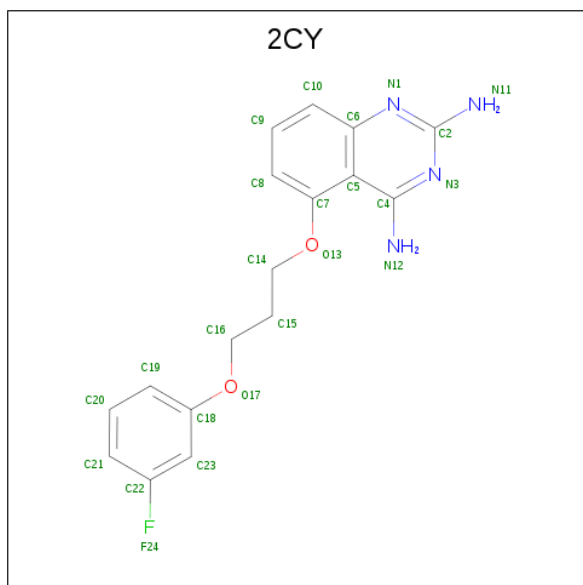
There are 7 unique types of molecules in this entry. The entry contains 16862 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bifunctional dihydrofolate reductase-thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	518	Total	C	N	O	S	0	0	0
			4124	2616	729	759	20			
1	B	515	Total	C	N	O	S	0	0	0
			4101	2602	725	755	19			
1	C	516	Total	C	N	O	S	0	0	0
			4107	2605	726	757	19			
1	D	513	Total	C	N	O	S	0	0	0
			4087	2594	723	752	18			

- Molecule 2 is 5-[3-(3-fluorophenoxy)propoxy]quinazoline-2,4-diamine (three-letter code: 2CY) (formula: C₁₇H₁₇FN₄O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			24	17	1	4	2		
2	B	1	Total	C	F	N	O	0	0
			24	17	1	4	2		

Continued on next page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total 24	C 17	F 1	N 4	O 2	0	0
2	D	1	Total 24	C 17	F 1	N 4	O 2	0	0

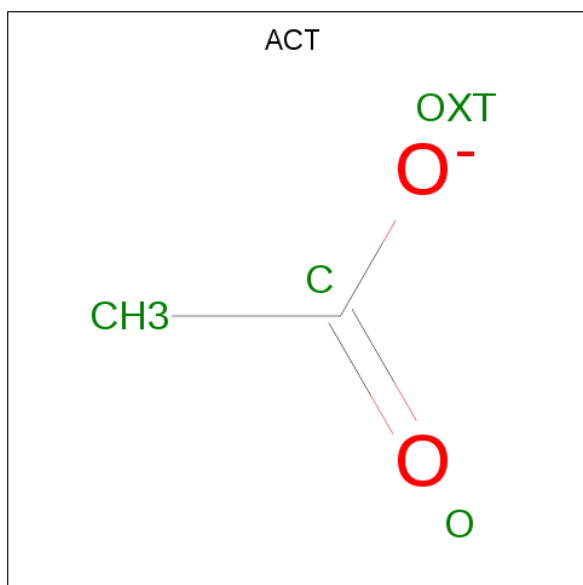
-
- The chemical structure of NDP (NDPase) is shown, consisting of a nucleotide chain and the NDPase subunit. The nucleotide chain is composed of a 5'-phosphate, a 3'-phosphate, a 5'-phosphate, and a 3'-phosphate, with a 5'-phosphate at the end. The NDPase subunit is a protein with a molecular weight of 10.5 kDa, containing 105 amino acids. The structure is shown in a ribbon representation, with the nucleotide chain in red and the NDPase subunit in blue. The NDPase subunit is a monomer, and the nucleotide chain is attached to the 5' position of the NDPase subunit. The NDPase subunit is a protein with a molecular weight of 10.5 kDa, containing 105 amino acids. The structure is shown in a ribbon representation, with the nucleotide chain in red and the NDPase subunit in blue. The NDPase subunit is a monomer, and the nucleotide chain is attached to the 5' position of the NDPase subunit.

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



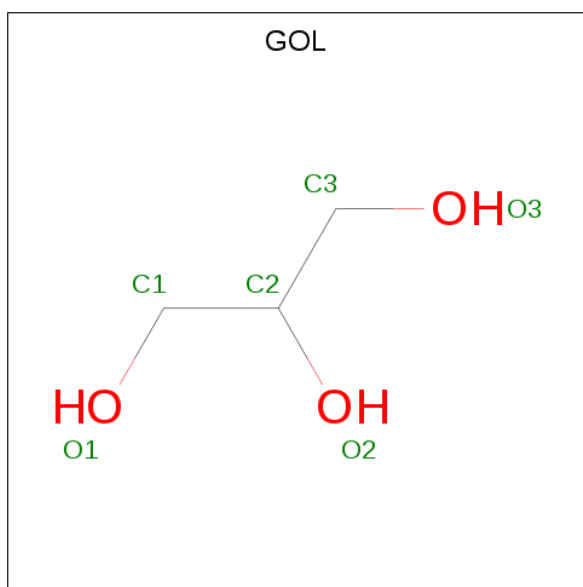
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

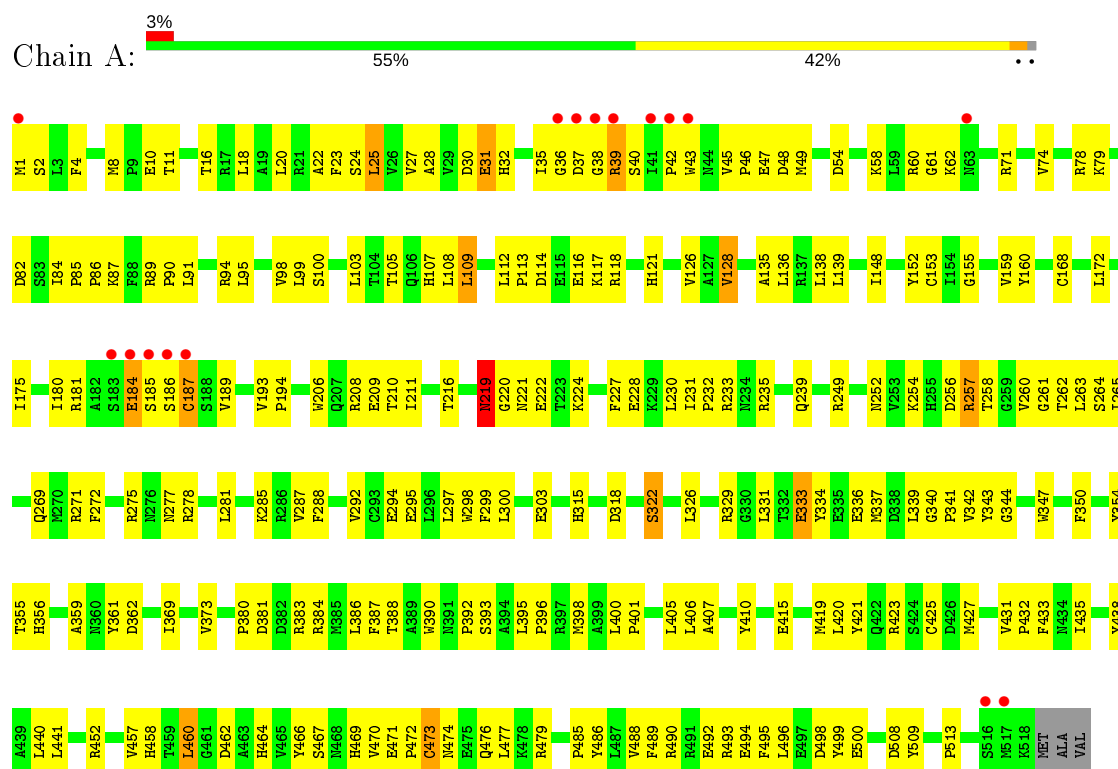
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	23	Total 23	O 23	0	0
7	B	12	Total 12	O 12	0	0
7	C	23	Total 23	O 23	0	0
7	D	25	Total 25	O 25	0	0

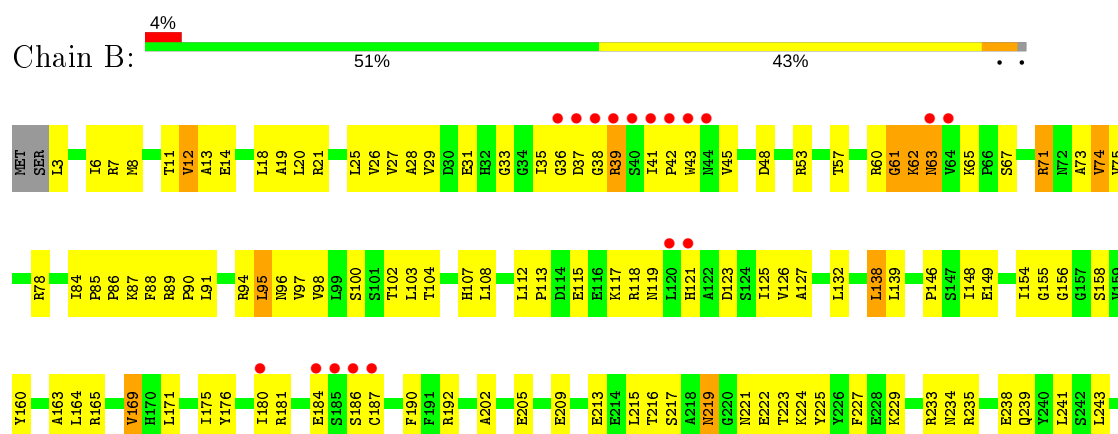
3 Residue-property plots [i](#)

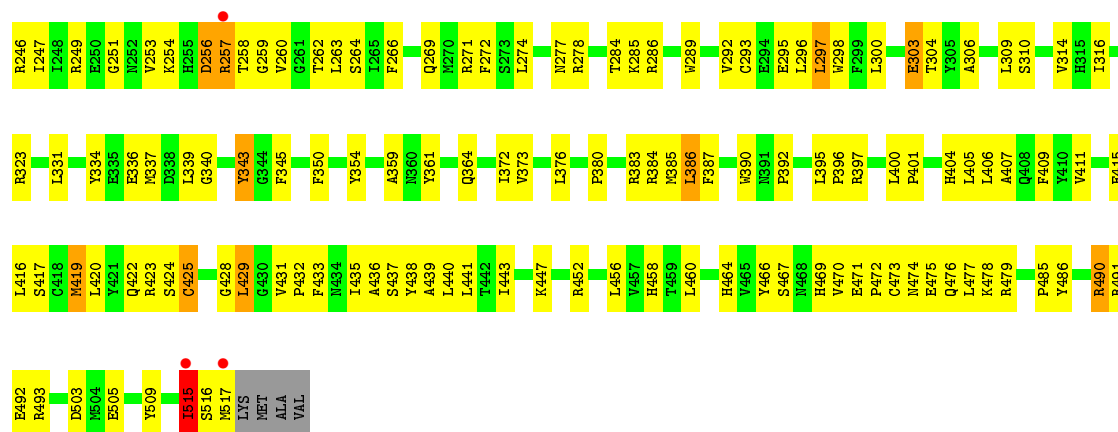
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Bifunctional dihydrofolate reductase-thymidylate synthase

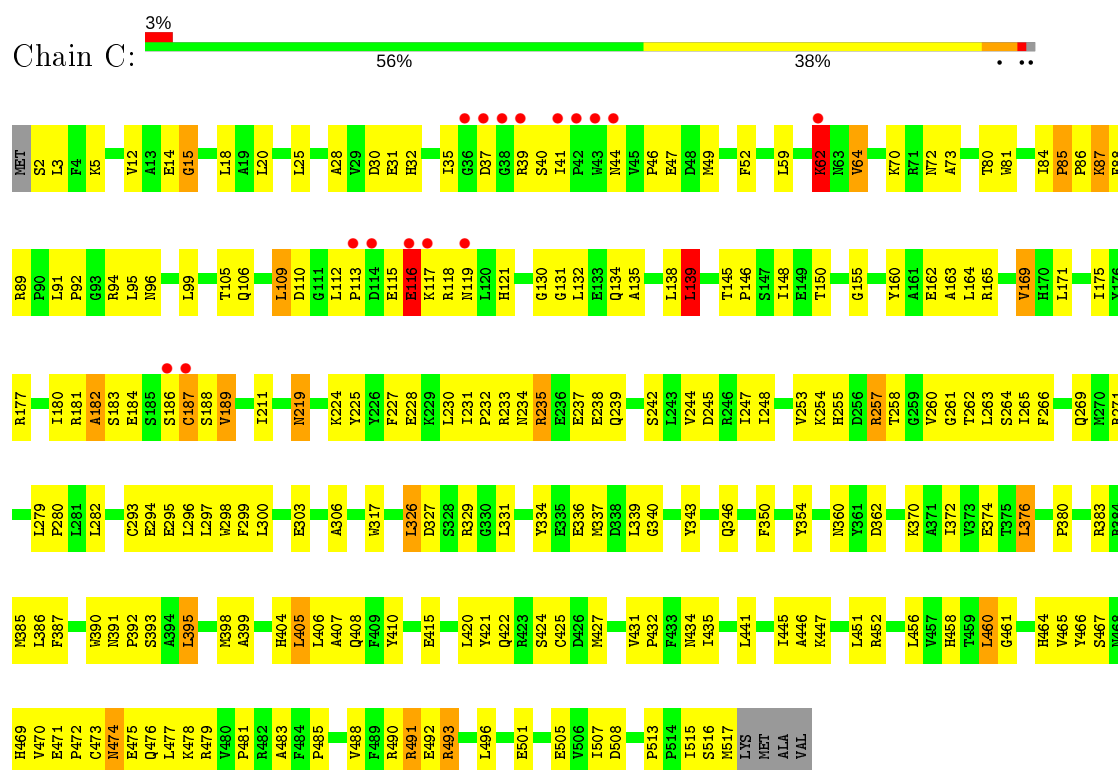


- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

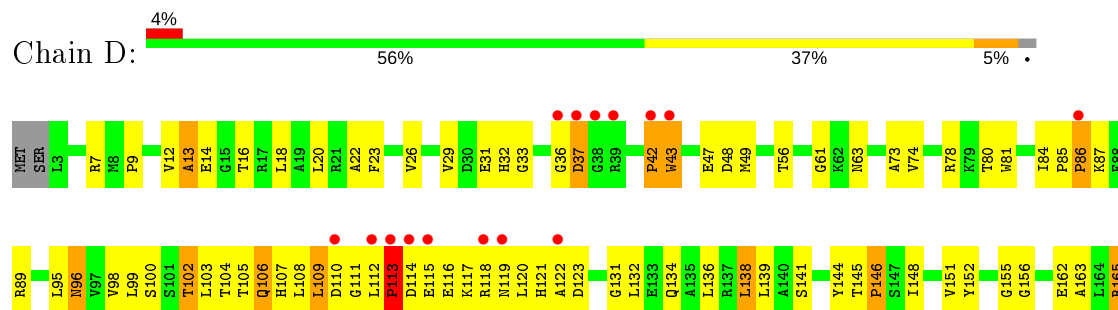




• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.54Å 165.94Å 84.72Å 90.00° 113.41° 90.00°	Depositor
Resolution (Å)	45.07 – 2.80 45.07 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.1 (45.07-2.80) 95.1 (45.07-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.81Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.206 , 0.277 0.199 , 0.269	Depositor DCC
R_{free} test set	2478 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	32.9	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	16862	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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.*

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: GOL, PO4, 2CY, NDP, 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	0.38	0/4224	0.65	0/5729
1	B	0.37	0/4201	0.67	0/5700
1	C	0.37	0/4207	0.66	0/5708
1	D	0.38	0/4187	0.67	0/5682
All	All	0.37	0/16819	0.66	0/22819

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	4124	0	4085	175	0
1	B	4101	0	4055	241	0
1	C	4107	0	4060	203	0
1	D	4087	0	4041	192	0
2	A	24	0	17	1	0
2	B	24	0	17	2	0
2	C	24	0	17	1	0
2	D	24	0	17	3	0
3	A	48	0	26	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	48	0	26	5	0
3	C	48	0	26	4	0
3	D	48	0	26	5	0
4	A	5	0	0	0	0
4	B	5	0	0	1	0
4	C	10	0	0	1	0
5	A	12	0	9	2	0
5	B	4	0	3	0	0
5	C	8	0	6	0	0
5	D	16	0	12	1	0
6	B	6	0	8	0	0
6	C	6	0	8	0	0
7	A	23	0	0	1	0
7	B	12	0	0	0	0
7	C	23	0	0	1	0
7	D	25	0	0	0	0
All	All	16862	0	16459	786	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 24.

The worst 5 of 786 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:C:37:ASP:HB3	1:C:40:SER:HB3	1.40	1.02
1:C:62:LYS:HE2	1:C:64:VAL:HB	1.41	1.00
1:A:329:ARG:HH12	1:A:400:LEU:HA	1.35	0.90
1:C:116:GLU:HA	1:C:119:ASN:ND2	1.87	0.90
1:C:233:ARG:NH1	1:C:235:ARG:HH12	1.70	0.89

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	516/521 (99%)	463 (90%)	39 (8%)	14 (3%)	5	17
1	B	513/521 (98%)	466 (91%)	33 (6%)	14 (3%)	5	17
1	C	514/521 (99%)	453 (88%)	46 (9%)	15 (3%)	4	15
1	D	511/521 (98%)	448 (88%)	49 (10%)	14 (3%)	5	17
All	All	2054/2084 (99%)	1830 (89%)	167 (8%)	57 (3%)	5	17

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	GLY
1	B	12	VAL
1	B	113	PRO
1	B	516	SER
1	C	182	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	444/446 (100%)	429 (97%)	15 (3%)	37	71
1	B	441/446 (99%)	418 (95%)	23 (5%)	23	55
1	C	442/446 (99%)	417 (94%)	25 (6%)	20	50
1	D	439/446 (98%)	409 (93%)	30 (7%)	16	42
All	All	1766/1784 (99%)	1673 (95%)	93 (5%)	22	54

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	95	LEU
1	C	297	LEU
1	D	336	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	106	GLN
1	C	139	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	173	GLN
1	C	320	ASN
1	D	360	ASN
1	C	207	GLN
1	C	219	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

24 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	$\# Z > 2$
5	ACT	A	809	-	1,3,3	2.51	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	B	806	-	5,5,5	0.49	0	5,5,5	0.19	0
2	2CY	B	602	-	26,26,26	2.11	10 (38%)	35,35,35	1.88	8 (22%)
2	2CY	C	603	-	26,26,26	2.07	10 (38%)	35,35,35	1.88	7 (20%)
3	NDP	D	704	-	45,52,52	1.79	10 (22%)	53,80,80	1.51	9 (16%)
5	ACT	A	807	-	1,3,3	2.66	1 (100%)	0,3,3	0.00	-
5	ACT	D	815	-	1,3,3	2.71	1 (100%)	0,3,3	0.00	-
4	PO4	B	801	-	4,4,4	2.30	1 (25%)	6,6,6	0.90	0
6	GOL	C	805	-	5,5,5	0.44	0	5,5,5	0.28	0
5	ACT	C	813	-	1,3,3	2.95	1 (100%)	0,3,3	0.00	-
2	2CY	A	601	-	26,26,26	2.10	10 (38%)	35,35,35	1.92	6 (17%)
5	ACT	B	811	-	1,3,3	3.16	1 (100%)	0,3,3	0.00	-
3	NDP	B	702	-	45,52,52	1.73	10 (22%)	53,80,80	1.62	11 (20%)
5	ACT	D	810	-	1,3,3	1.78	0	0,3,3	0.00	-
5	ACT	C	812	-	1,3,3	2.80	1 (100%)	0,3,3	0.00	-
4	PO4	C	804	-	4,4,4	2.59	1 (25%)	6,6,6	0.83	0
5	ACT	D	816	-	1,3,3	1.71	0	0,3,3	0.00	-
3	NDP	A	701	-	45,52,52	1.87	10 (22%)	53,80,80	1.49	9 (16%)
4	PO4	A	802	-	4,4,4	2.50	1 (25%)	6,6,6	0.87	0
4	PO4	C	803	-	4,4,4	2.56	1 (25%)	6,6,6	0.85	0
5	ACT	A	808	-	1,3,3	2.64	1 (100%)	0,3,3	0.00	-
5	ACT	D	814	-	1,3,3	3.15	1 (100%)	0,3,3	0.00	-
3	NDP	C	703	-	45,52,52	1.81	12 (26%)	53,80,80	1.58	10 (18%)
2	2CY	D	604	-	26,26,26	2.11	9 (34%)	35,35,35	1.90	9 (25%)

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	GOL	B	806	-	-	0/4/4/4	-
3	NDP	B	702	-	-	2/30/77/77	0/5/5/5
2	2CY	B	602	-	-	2/8/8/8	0/3/3/3
6	GOL	C	805	-	-	0/4/4/4	-
3	NDP	C	703	-	-	2/30/77/77	0/5/5/5
2	2CY	C	603	-	-	3/8/8/8	0/3/3/3
3	NDP	D	704	-	-	9/30/77/77	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2CY	D	604	-	-	2/8/8/8	0/3/3/3
3	NDP	A	701	-	-	4/30/77/77	0/5/5/5
2	2CY	A	601	-	-	5/8/8/8	0/3/3/3

The worst 5 of 93 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	2CY	O17-C18	-5.02	1.26	1.37
2	D	604	2CY	O17-C18	-4.99	1.26	1.37
4	C	804	PO4	P-O1	4.92	1.62	1.50
4	C	803	PO4	P-O1	4.84	1.62	1.50
2	C	603	2CY	O17-C18	-4.81	1.26	1.37

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	603	2CY	N1-C2-N3	-5.32	120.12	127.22
2	D	604	2CY	N1-C2-N3	-5.23	120.24	127.22
2	A	601	2CY	N1-C2-N3	-5.17	120.33	127.22
2	B	602	2CY	N1-C2-N3	-5.14	120.36	127.22
2	A	601	2CY	C7-C5-C4	-4.88	124.88	127.36

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	704	NDP	C5D-O5D-PN-O1N
2	C	603	2CY	O13-C14-C15-C16
2	D	604	2CY	O13-C14-C15-C16
2	B	602	2CY	O13-C14-C15-C16
2	A	601	2CY	C15-C14-O13-C7

There are no ring outliers.

12 monomers are involved in 27 short contacts:

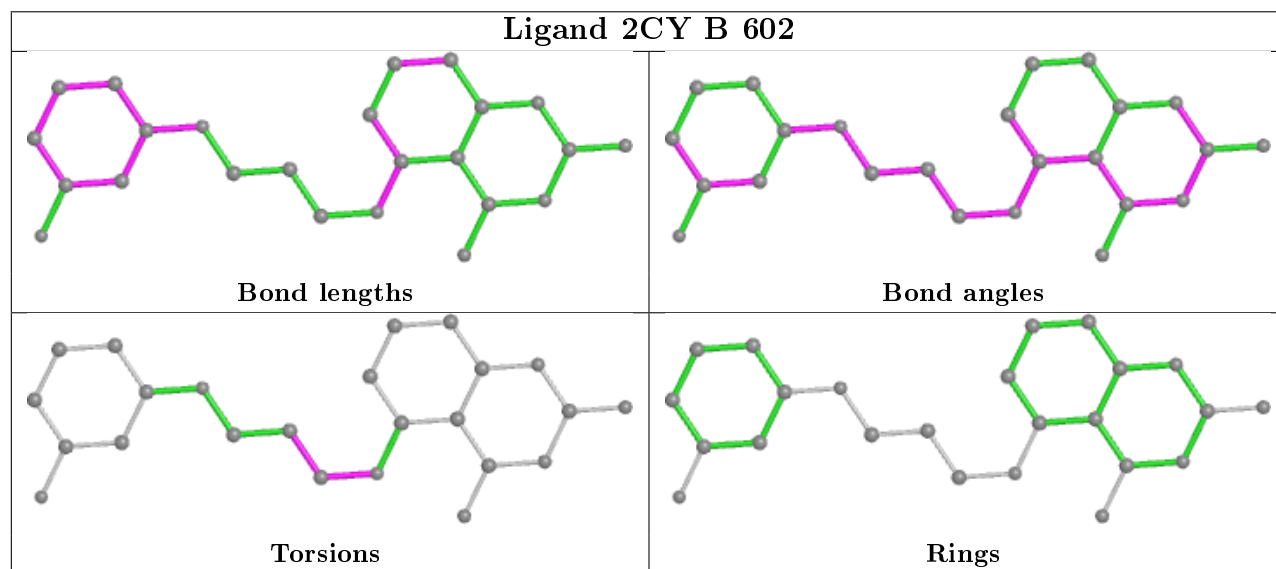
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	809	ACT	2	0
2	B	602	2CY	2	0
2	C	603	2CY	1	0
3	D	704	NDP	5	0

Continued on next page...

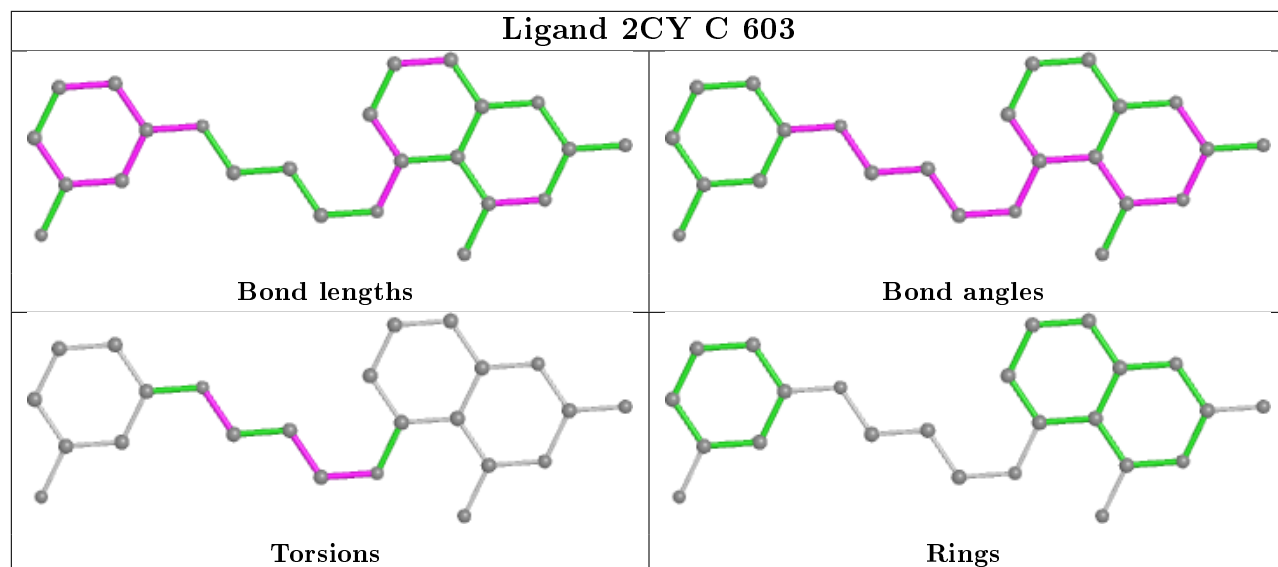
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	801	PO4	1	0
2	A	601	2CY	1	0
3	B	702	NDP	5	0
5	D	810	ACT	1	0
4	C	804	PO4	1	0
3	A	701	NDP	1	0
3	C	703	NDP	4	0
2	D	604	2CY	3	0

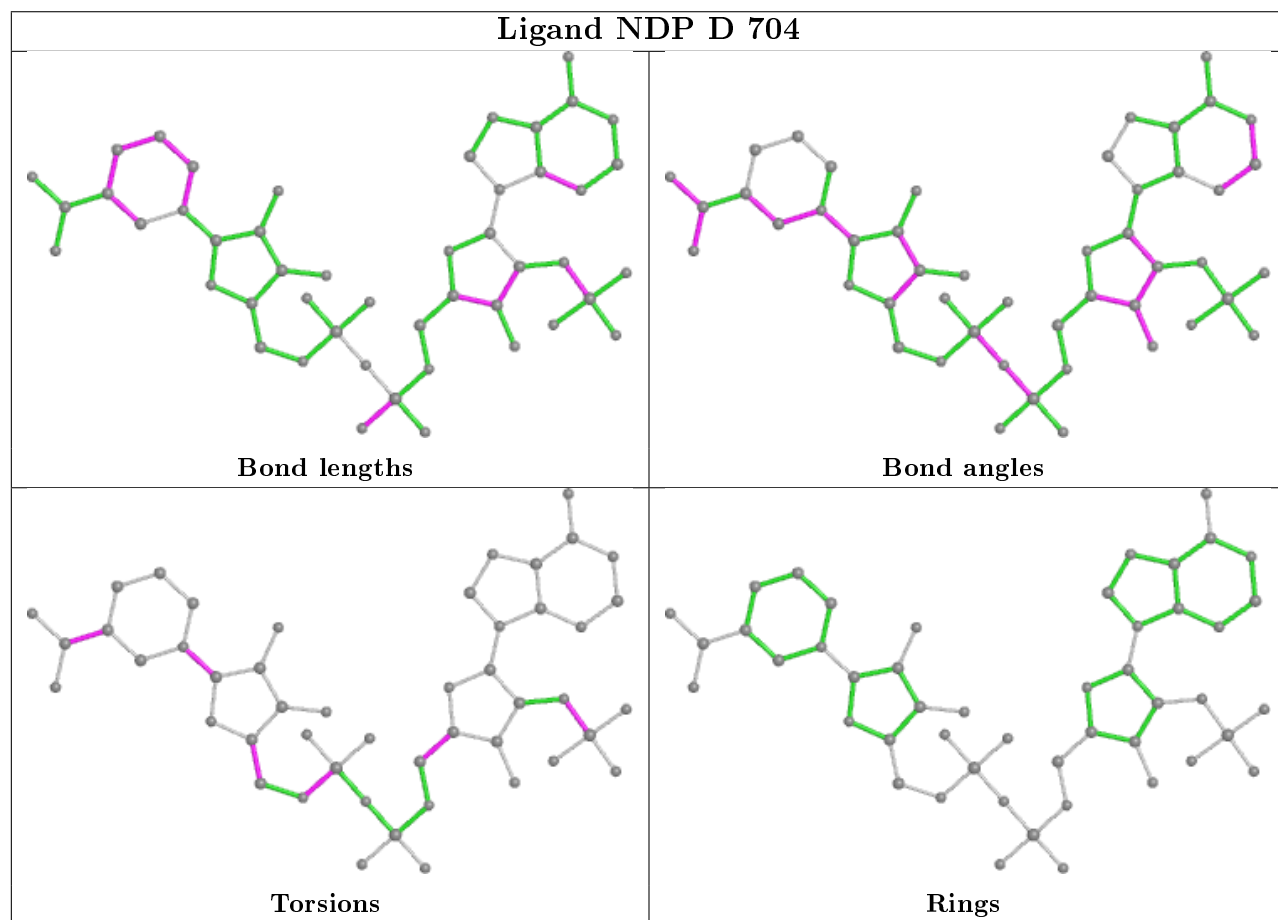
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



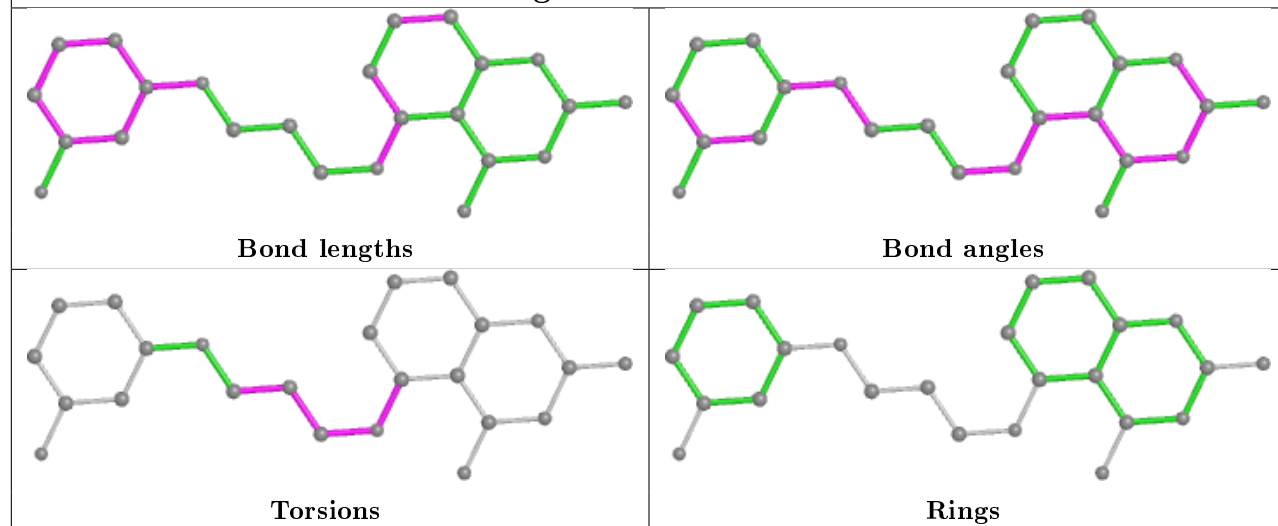
Ligand 2CY C 603



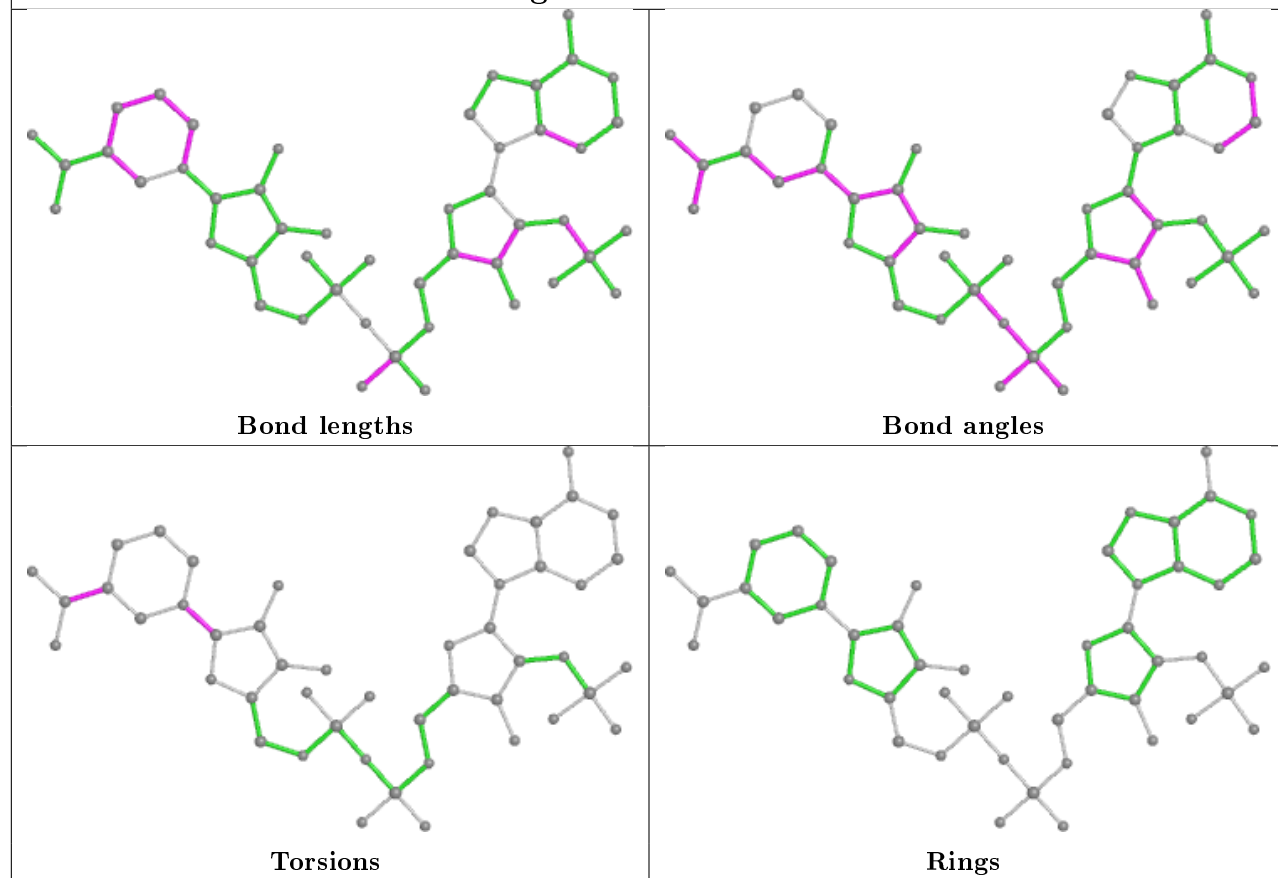
Ligand NDP D 704

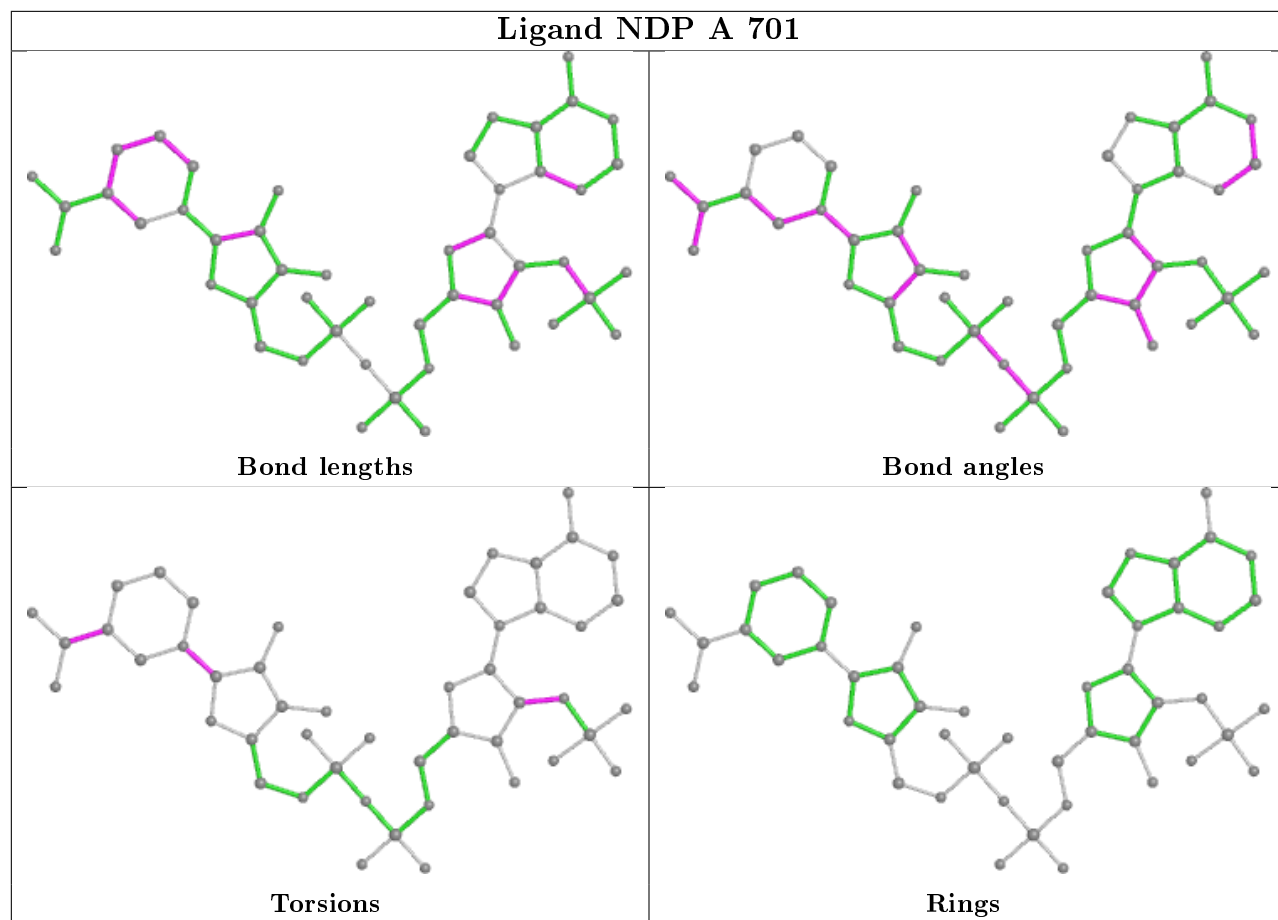


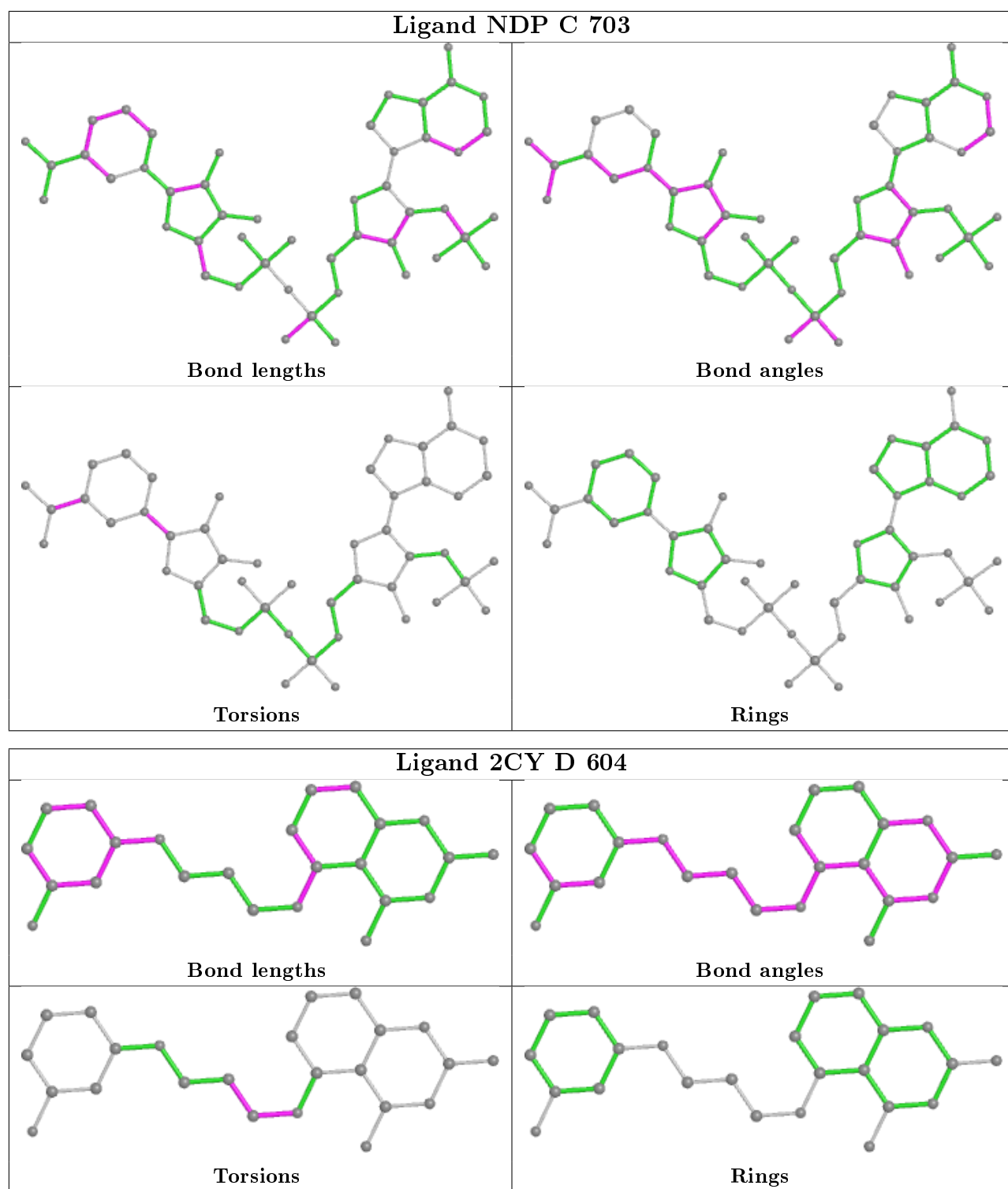
Ligand 2CY A 601



Ligand NDP B 702







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	A	518/521 (99%)	-0.29	16 (3%) 49 39	12, 26, 61, 91	0
1	B	515/521 (98%)	-0.17	21 (4%) 37 27	11, 29, 76, 91	0
1	C	516/521 (99%)	-0.35	16 (3%) 49 39	10, 26, 69, 91	0
1	D	513/521 (98%)	-0.26	19 (3%) 41 31	7, 28, 70, 91	0
All	All	2062/2084 (98%)	-0.27	72 (3%) 44 34	7, 27, 69, 91	0

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	38	GLY	7.9
1	B	186	SER	7.7
1	A	38	GLY	5.9
1	D	39	ARG	5.3
1	B	39	ARG	5.1

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](#)

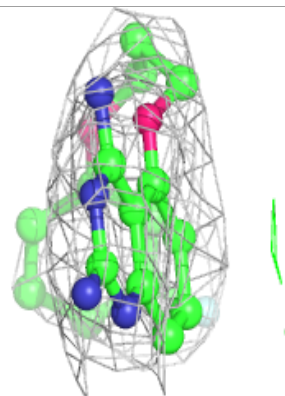
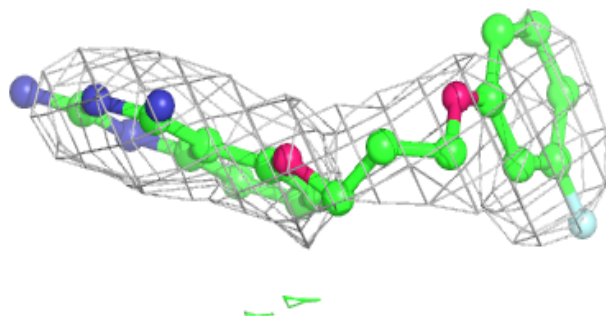
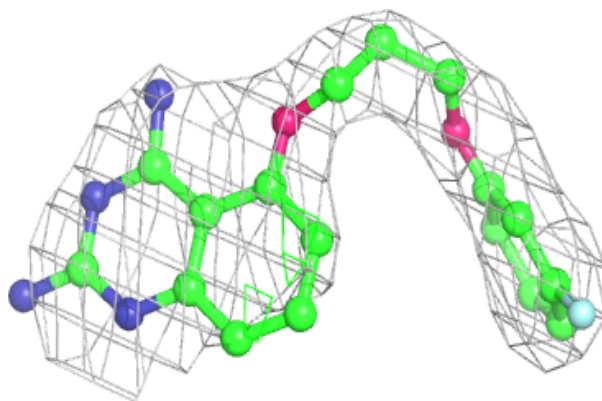
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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	ACT	B	811	4/4	0.72	0.34	42,45,45,46	0
5	ACT	C	812	4/4	0.81	0.27	32,33,33,35	0
4	PO4	A	802	5/5	0.85	0.22	87,87,88,89	0
6	GOL	C	805	6/6	0.87	0.26	42,47,47,48	0
5	ACT	C	813	4/4	0.88	0.26	56,57,57,58	0
4	PO4	C	804	5/5	0.88	0.19	84,84,85,85	0
2	2CY	B	602	24/24	0.88	0.31	46,51,55,58	0
4	PO4	C	803	5/5	0.88	0.22	76,76,78,78	0
5	ACT	A	808	4/4	0.89	0.23	35,36,36,36	0
5	ACT	D	814	4/4	0.89	0.26	31,34,35,37	0
6	GOL	B	806	6/6	0.90	0.23	40,42,43,44	0
2	2CY	A	601	24/24	0.92	0.26	44,49,60,61	0
2	2CY	C	603	24/24	0.92	0.25	44,47,51,52	0
3	NDP	B	702	48/48	0.92	0.19	44,52,89,90	0
2	2CY	D	604	24/24	0.92	0.28	47,53,58,60	0
5	ACT	A	809	4/4	0.93	0.26	38,39,39,41	0
3	NDP	D	704	48/48	0.93	0.22	41,50,88,90	0
3	NDP	A	701	48/48	0.94	0.20	37,45,78,79	0
5	ACT	D	810	4/4	0.94	0.18	32,32,32,33	0
3	NDP	C	703	48/48	0.94	0.22	32,42,80,80	0
5	ACT	D	816	4/4	0.94	0.21	29,29,30,30	0
5	ACT	A	807	4/4	0.95	0.20	35,37,37,37	0
5	ACT	D	815	4/4	0.96	0.16	45,45,45,46	0
4	PO4	B	801	5/5	0.96	0.17	64,65,66,67	0

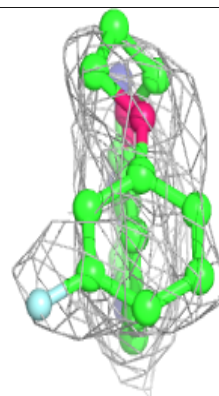
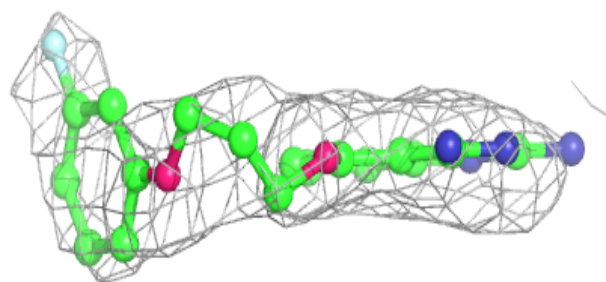
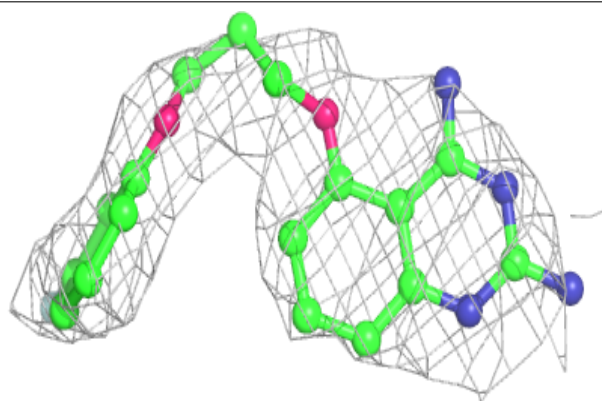
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 2CY B 602:

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

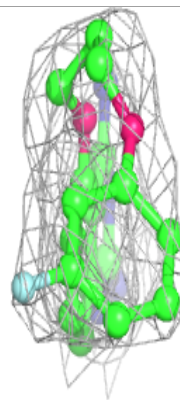
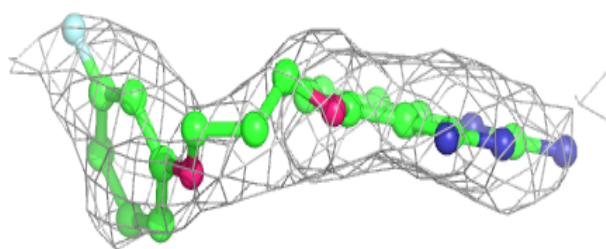
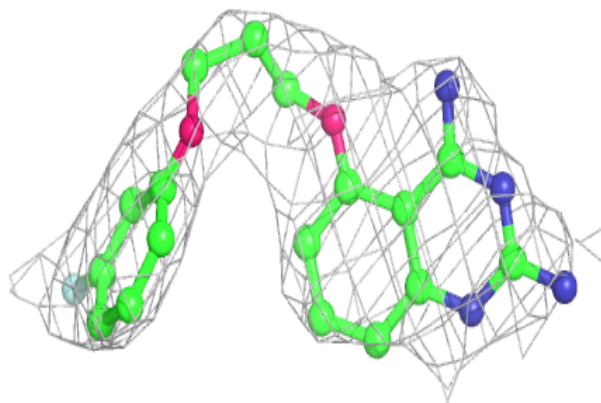
**Electron density around 2CY A 601:**

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

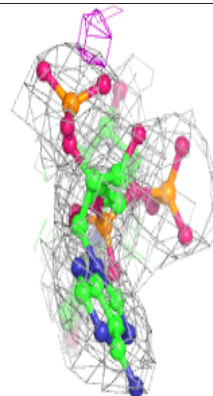
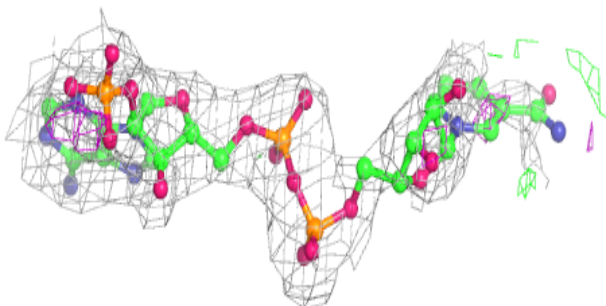
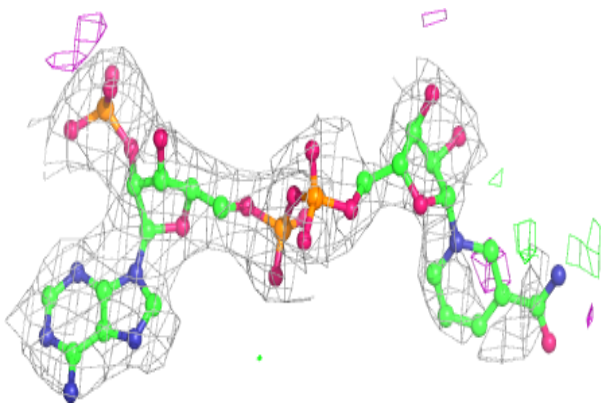


Electron density around 2CY C 603:

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

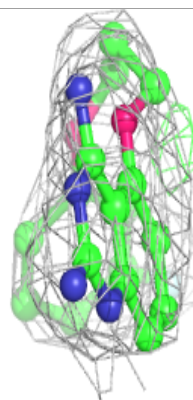
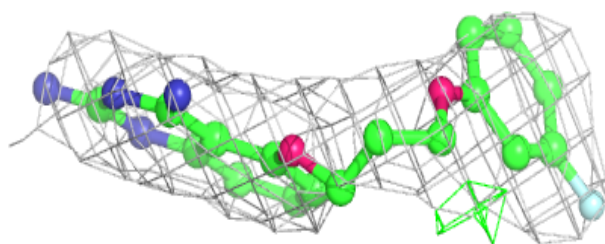
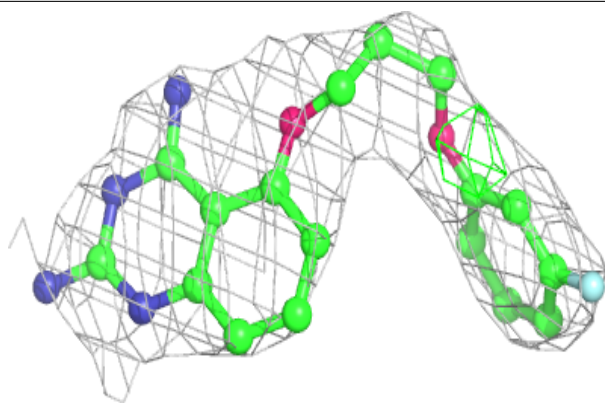
**Electron density around NDP B 702:**

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

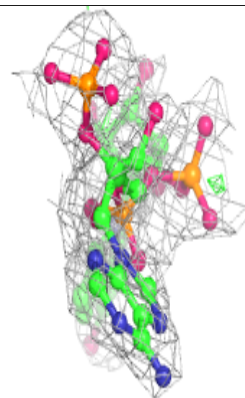
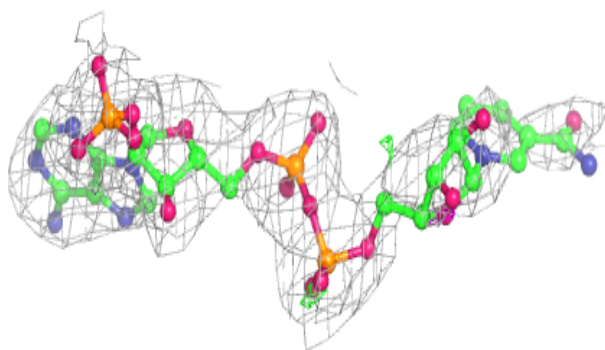
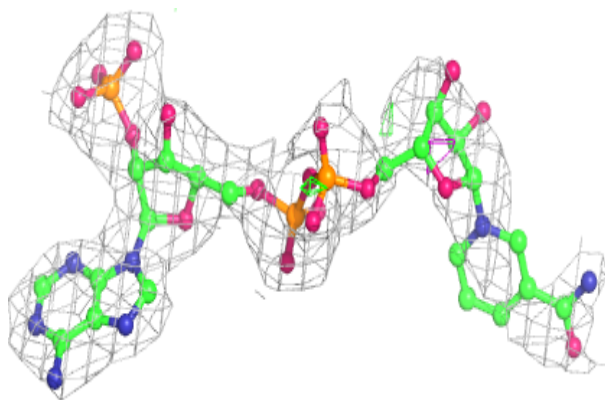


Electron density around 2CY D 604:

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

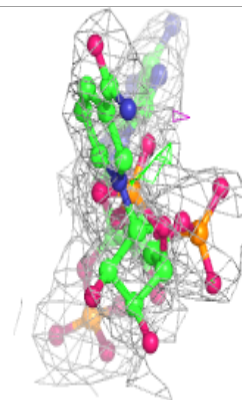
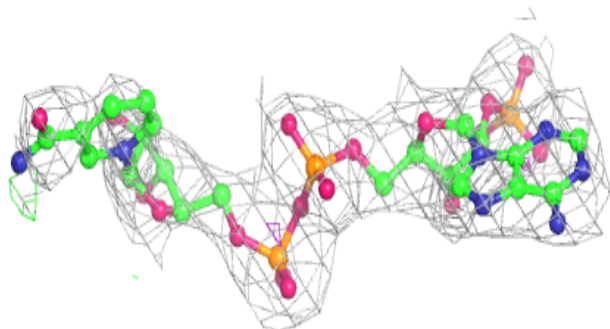
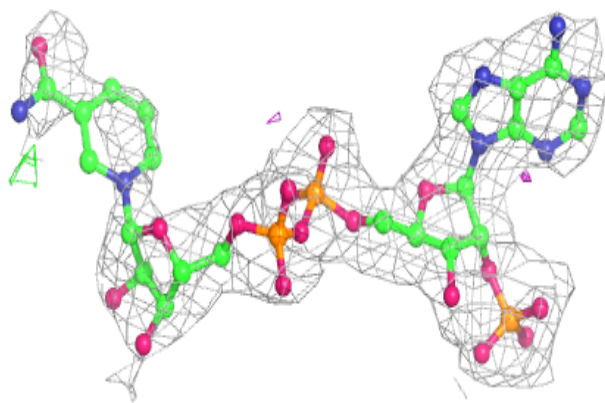
**Electron density around NDP D 704:**

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

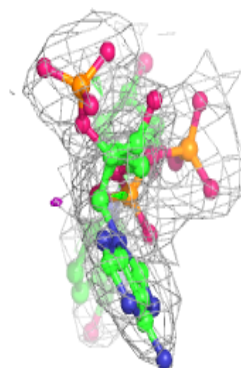
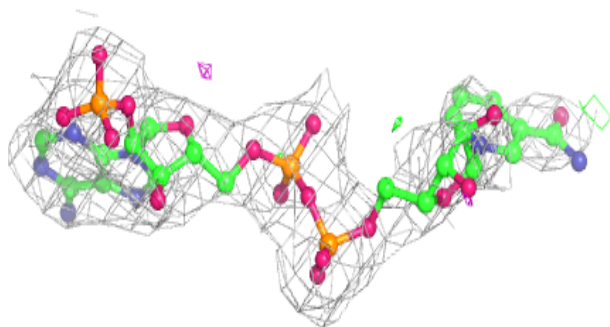
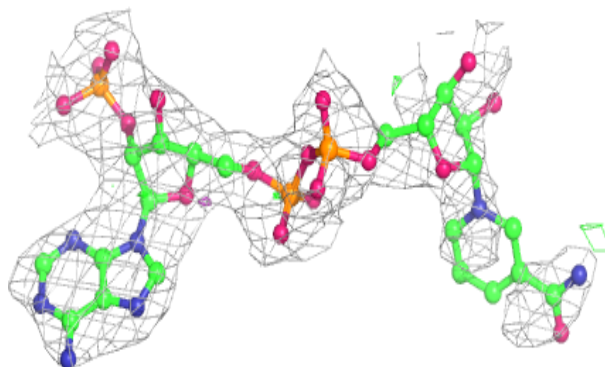


Electron density around NDP A 701:

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

**Electron density around NDP C 703:**

$2mF_o-DF_c$ (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.