



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 09:28 PM UTC

PDB ID : 4ECK / pdb_00004eck
Title : Crystal Structure of the Toxoplasma gondii TS-DHFR
Authors : Sharma, H.; Anderson, K.S.
Deposited on : 2012-03-26
Resolution : 3.52 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

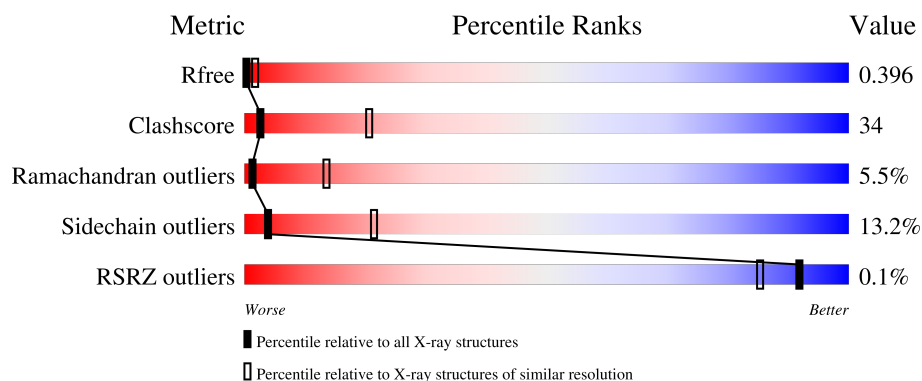
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.52 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	1025 (3.56-3.48)
Clashscore	190562	1079 (3.56-3.48)
Ramachandran outliers	187476	1052 (3.56-3.48)
Sidechain outliers	187428	1053 (3.56-3.48)
RSRZ outliers	180081	1024 (3.56-3.48)

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	A	610	
1	B	610	

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
2	UMP	A	701	-	-	X	-
2	UMP	B	701	-	-	X	-
3	CB3	A	702	-	-	X	-
3	CB3	B	702	-	-	X	-
4	FOL	A	703	-	-	X	-
4	FOL	B	703	-	-	X	-

2 Entry composition [i](#)

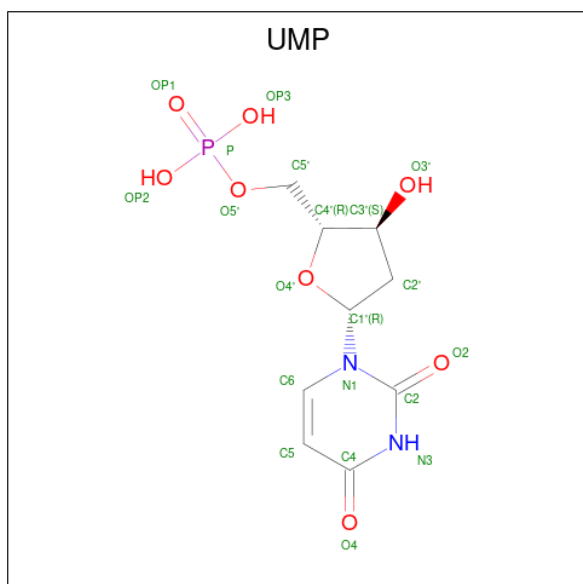
There are 5 unique types of molecules in this entry. The entry contains 8248 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

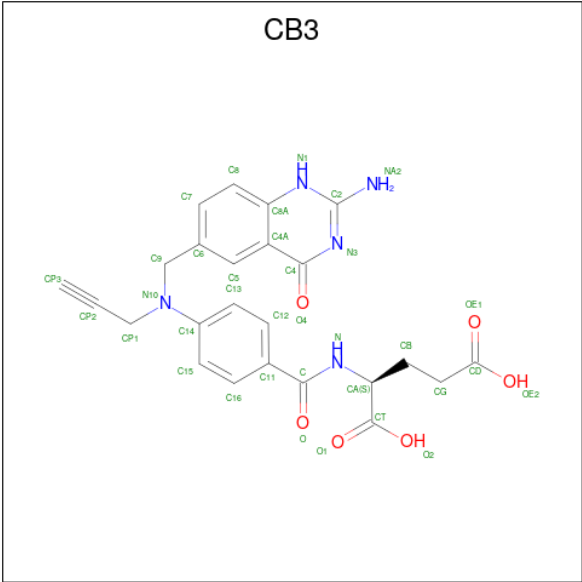
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	0	0
			3989	2550	697	717	25			
1	B	498	Total	C	N	O	S	0	0	0
			3989	2550	697	717	25			

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (CCD ID: UMP) (formula: $C_9H_{13}N_2O_8P$).



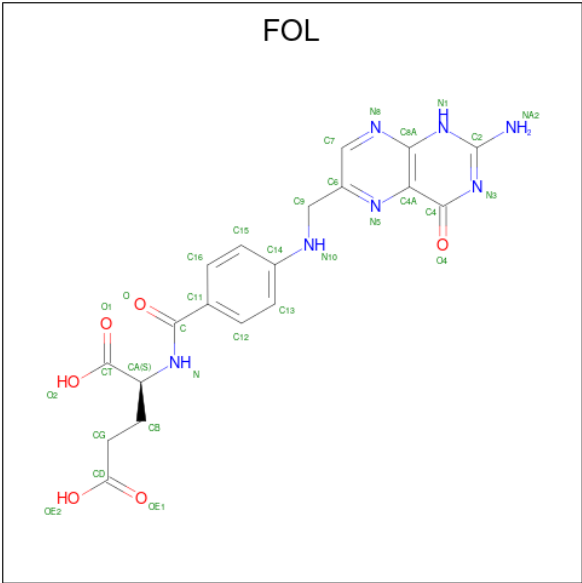
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 3 is 10-PROPARGYL-5,8-DIDEAZAFOLIC ACID (CCD ID: CB3) (formula: $C_{24}H_{23}N_5O_6$).



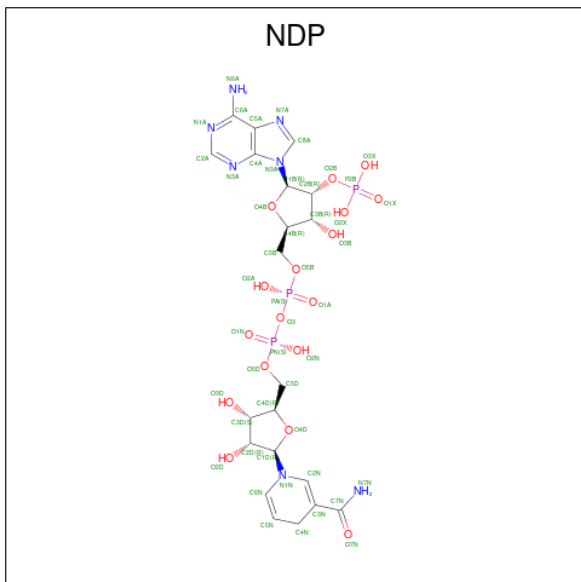
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			35	24	5	6		
3	B	1	Total	C	N	O	0	0
			35	24	5	6		

- Molecule 4 is FOLIC ACID (CCD ID: FOL) (formula: C₁₉H₁₉N₇O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			32	19	7	6		
4	B	1	Total	C	N	O	0	0
			32	19	7	6		

- Molecule 5 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$).

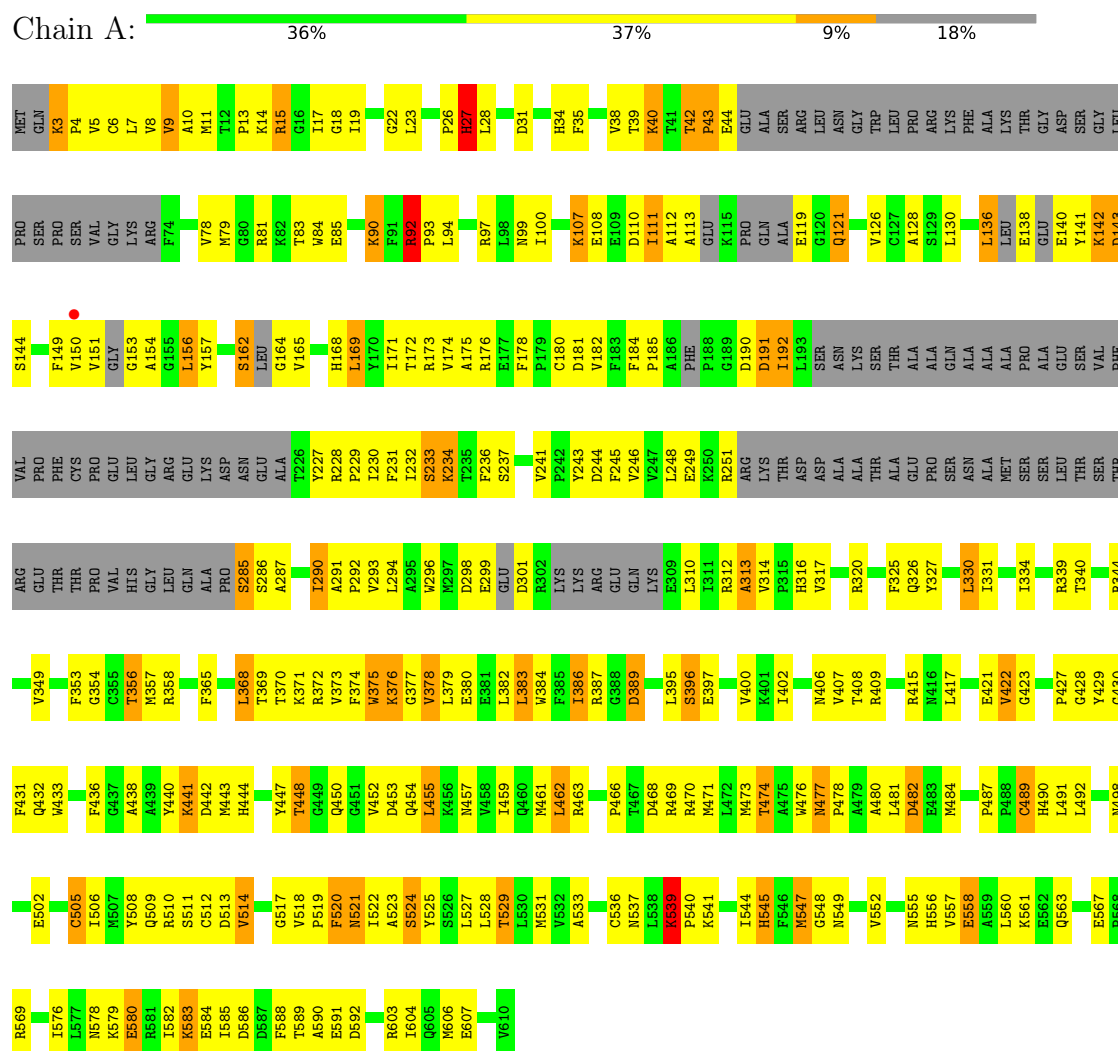


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
5	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

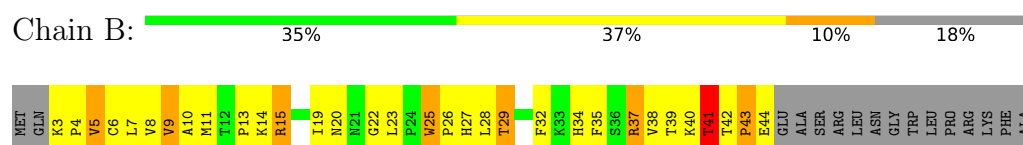
3 Residue-property plots

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: Bifunctional dihydrofolate reductase-thymidylate synthase



- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



P568	Q500	D424	I331	SER	GLN	L134	GLY
R569	C506	P427	I334	ASN	ALA	S135	LEU
P570	I506	W433	I335	ALA	ALA	L136	PRO
I573	M507	F436	R339	MET	PRO	LEU	SER
M578	Q509	Y440	R344	SER	ALA	E138	SER
K579	R510	K441	T345	LEU	GLU	GLU	VAL
E580	S511	D442	I350	THR	SER	E140	GLY
R581	C512	M443	F353	ARG	VAL	Y141	LYS
I582	D513	H444	G354	THR	PHE	K142	ARG
I585	G515	T445	C355	GLU	PRO	D143	F74
D586	L516	Y447	T356	THR	CYS	S144	N75
D587	G517	D453	R357	THR	PRO	V145	A76
F588	V518	Q454	L361	ALA	GLU	I148	V77
T589	P519	L455	P366	PRO	LYS	F149	V78
A590	F520	K456	L367	ASP	GLY	M79	M79
E591	M521	V458	L368	ASN	LEU	V150	G80
D592	I522	M461	T369	GLU	GLY	V151	R81
V599	S524	L462	T370	ALA	ARG	GLY	K82
P600	Y525	M465	K371	GLN	GLU	G153	
H601	S526	N467	F373	ALA	LYS	A154	M87
G602	L527	D468	V374	PRO	ASP	G155	P88
R603	L528	R469	V378	S285	ASN	L156	R89
I604	T529	M470	L379	S286	GLU	Y157	K90
Q605	L530	M471	E380	A287	ALA	E158	F91
M606	M531	L472	E299	I290	T226	S162	R92
E607	V532	M473	E381	V293	Y227	LEU	P93
Y610	C536	T474	L382	W296	R228	GLU	L94
		A475	L383	M297	P229	G164	V95
		W476	W384	D298	I230	V165	D96
		P477	F385	E298	F231	A166	R97
		P478	I386	E299	I232	S167	L98
		A479	D389	GLU	S233	H168	N99
		A480	T390	D301	K234	L169	I100
		L481	N391	R302	T235	Y170	V101
		M484	A392	LYS	F236	I171	V102
		A485	N393	LYS	S237	T172	
		L486	H394	LYS	V241	R173	K107
		P487	L395	ARG	P242	V174	E108
		P488	S396	GLU	Y243		E109
		C489		GLN	D244		D110
		H490	I402	LYS	F245	D181	I111
		L491	W403	ARG	V246	F184	A112
		L492	D404	LYS	V247	P185	A113
		C493	K405	THR	L248	P186	GLU
		Q494	H409	ASP	E249	PHE	K115
		F495	E421	ALA	K250	PRO	PRO
		Y496	G423	ALA	R251	ALA	ALA
		V497		THR	ARG	E119	E119
		N498		ALA	LYS	G120	G120
		E567		THR	THR	I192	Q121
				ALA	ASP	L193	Q122
				ALA	ASP	SER	R123
				ALA	ALA	ASN	
				ALA	ALA	LYS	C127
				ALA	ALA	SER	A128
				ALA	ALA	THR	S129
				ALA	ALA	ALA	L130
				ALA	ALA	ALA	L131

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	185.94Å 143.01Å 59.84Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	46.18 – 3.52 46.18 – 3.52	Depositor EDS
% Data completeness (in resolution range)	95.9 (46.18-3.52) 95.9 (46.18-3.52)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.332 , 0.395 0.328 , 0.396	Depositor DCC
R_{free} test set	982 reflections (5.24%)	wwPDB-VP
Wilson B-factor (Å ²)	70.5	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 150.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.387 for -h,-k,l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	8248	wwPDB-VP
Average B, all atoms (Å ²)	60.0	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 23.87 % 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 4.2797e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: UMP, FOL, NDP, CB3

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	0.79	0/4078	1.03	11/5510 (0.2%)
1	B	0.80	0/4078	1.02	13/5510 (0.2%)
All	All	0.79	0/8156	1.03	24/11020 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	111	ILE	N-CA-C	-9.94	104.27	113.71
1	A	539	LYS	CA-C-N	8.88	130.28	119.98
1	A	539	LYS	C-N-CA	8.88	130.28	119.98
1	B	233	SER	N-CA-C	8.29	120.09	111.14
1	A	365	PHE	CA-C-N	7.01	128.60	119.84

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	42	THR	Peptide
1	A	92	ARG	Peptide

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	3989	0	3939	269	0
1	B	3989	0	3940	304	0
2	A	20	0	11	25	0
2	B	20	0	11	15	0
3	A	35	0	21	15	0
3	B	35	0	21	18	0
4	A	32	0	17	10	0
4	B	32	0	17	24	0
5	A	48	0	26	7	0
5	B	48	0	26	16	0
All	All	8248	0	8029	554	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 34.

The worst 5 of 554 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:B:402:ILE:HG22	3:B:702:CB3:C16	1.09	1.56
1:B:402:ILE:CG2	3:B:702:CB3:C16	1.91	1.46
1:B:510:ARG:HH12	2:B:701:UMP:P	1.40	1.41
1:A:489:CYS:SG	2:A:701:UMP:C6	2.28	1.25
1:A:344:ARG:NH2	2:A:701:UMP:OP3	1.72	1.21

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	474/610 (78%)	379 (80%)	68 (14%)	27 (6%)	1	13
1	B	474/610 (78%)	385 (81%)	64 (14%)	25 (5%)	1	14
All	All	948/1220 (78%)	764 (81%)	132 (14%)	52 (6%)	1	13

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	PRO
1	A	92	ARG
1	A	128	ALA
1	A	165	VAL
1	A	313	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	433/525 (82%)	379 (88%)	54 (12%)	4	22
1	B	433/525 (82%)	373 (86%)	60 (14%)	3	20
All	All	866/1050 (82%)	752 (87%)	114 (13%)	4	21

5 of 114 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	29	THR
1	B	589	THR
1	B	162	SER
1	B	580	GLU
1	B	529	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	509	GLN
1	B	578	ASN
1	A	450	GLN
1	A	465	ASN
1	A	490	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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](#)

8 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	$\# Z > 2$
2	UMP	B	701	-	21,21,21	1.32	4 (19%)	30,31,31	1.90	8 (26%)
4	FOL	A	703	-	34,34,34	1.06	2 (5%)	43,47,47	1.32	2 (4%)
2	UMP	A	701	-	21,21,21	1.26	4 (19%)	30,31,31	1.79	6 (20%)
4	FOL	B	703	-	34,34,34	1.13	3 (8%)	43,47,47	1.44	4 (9%)
3	CB3	A	702	-	37,37,37	1.41	3 (8%)	50,51,51	1.47	7 (14%)
5	NDP	B	704	-	51,52,52	1.82	8 (15%)	71,80,80	2.27	11 (15%)
5	NDP	A	704	-	51,52,52	1.82	8 (15%)	71,80,80	2.26	11 (15%)
3	CB3	B	702	-	37,37,37	1.40	3 (8%)	50,51,51	1.36	6 (12%)

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
2	UMP	B	701	-	-	5/10/22/22	0/2/2/2
4	FOL	A	703	-	-	6/22/22/22	0/3/3/3
2	UMP	A	701	-	-	5/10/22/22	0/2/2/2
4	FOL	B	703	-	-	5/22/22/22	0/3/3/3
3	CB3	A	702	-	-	10/27/28/28	0/3/3/3
5	NDP	B	704	-	-	3/34/77/77	0/5/5/5
5	NDP	A	704	-	-	3/34/77/77	0/5/5/5
3	CB3	B	702	-	-	9/27/28/28	0/3/3/3

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	704	NDP	C6A-N6A	5.45	1.48	1.34
5	A	704	NDP	C6A-N6A	5.25	1.47	1.34
5	A	704	NDP	C2N-C3N	4.93	1.48	1.35
3	A	702	CB3	C4A-C8A	4.91	1.48	1.41
5	B	704	NDP	C6N-C5N	4.90	1.48	1.33

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	704	NDP	C1D-N1N-C2N	10.23	137.99	121.14
5	B	704	NDP	C1D-N1N-C2N	9.73	137.16	121.14
5	A	704	NDP	C1D-N1N-C6N	-8.04	103.77	120.77
5	B	704	NDP	C1D-N1N-C6N	-7.40	105.12	120.77
5	B	704	NDP	O4D-C1D-N1N	6.45	120.39	108.08

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

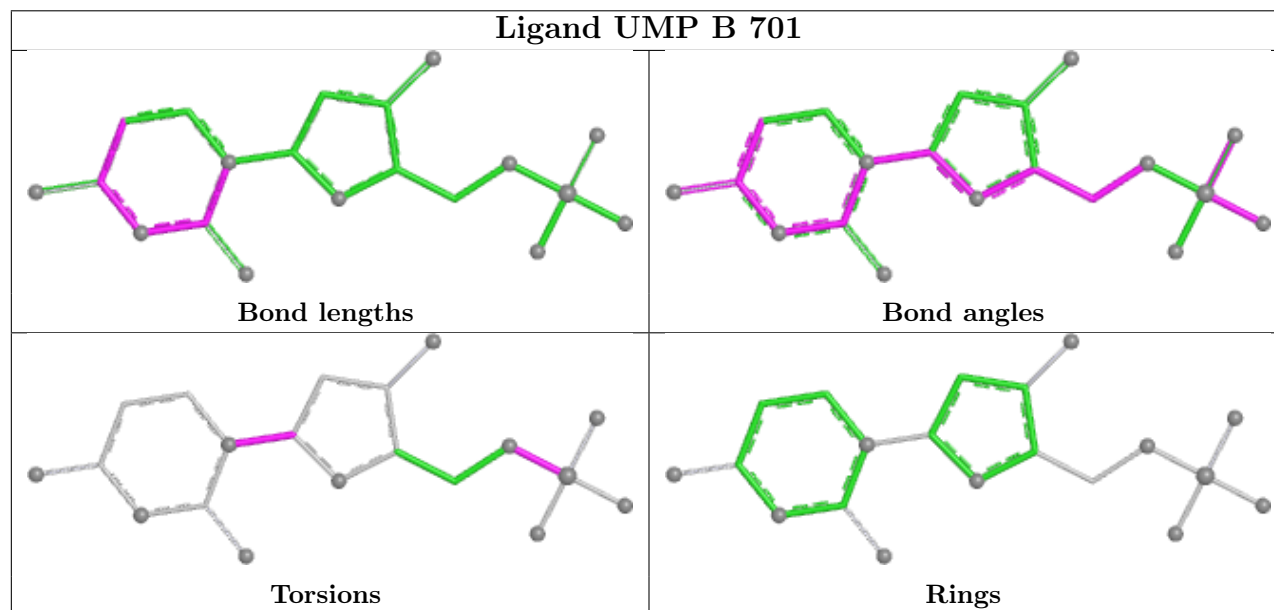
Mol	Chain	Res	Type	Atoms
2	A	701	UMP	C5'-O5'-P-OP1
2	A	701	UMP	C5'-O5'-P-OP2
2	B	701	UMP	C5'-O5'-P-OP1
4	A	703	FOL	N-CA-CB-CG
4	B	703	FOL	N-CA-CB-CG

There are no ring outliers.

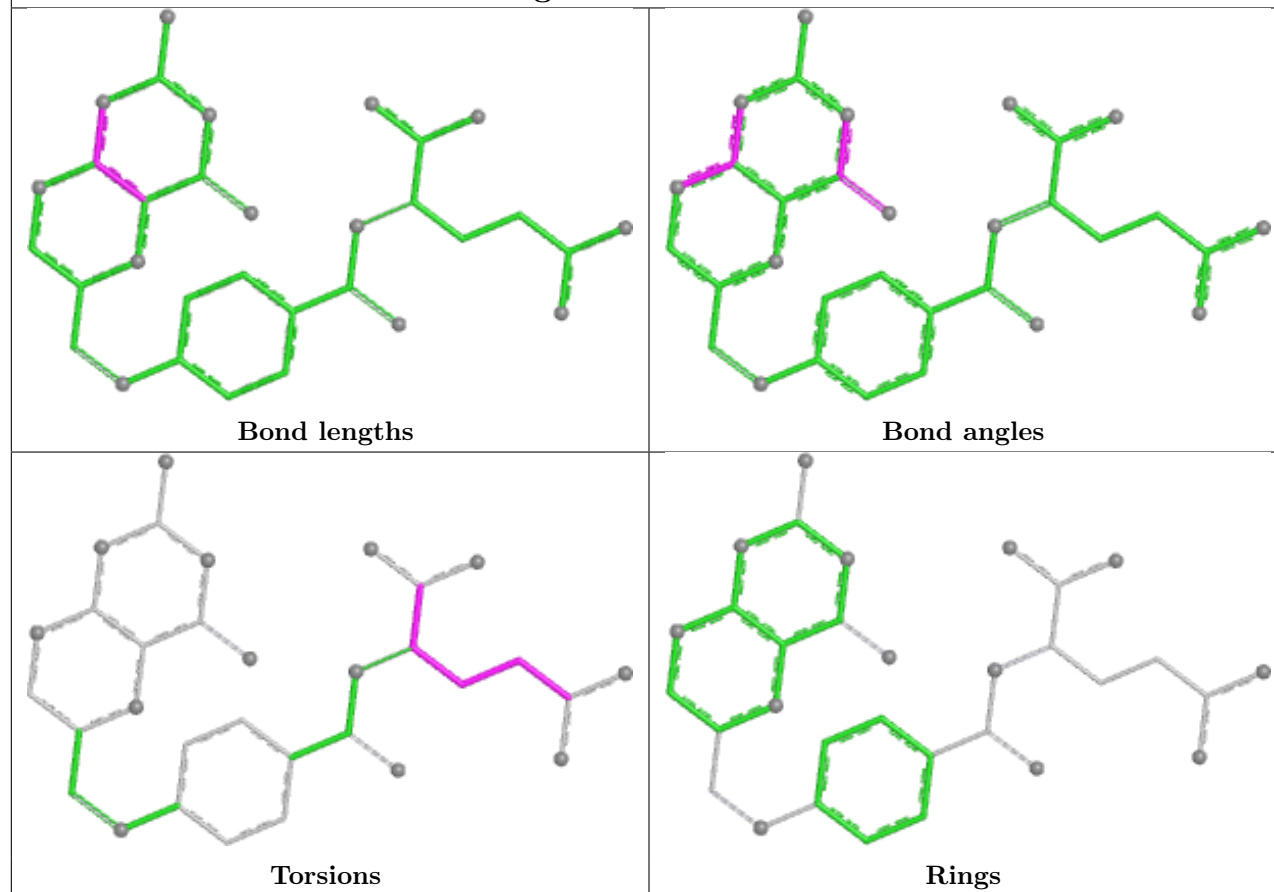
8 monomers are involved in 129 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	UMP	15	0
4	A	703	FOL	10	0
2	A	701	UMP	25	0
4	B	703	FOL	24	0
3	A	702	CB3	15	0
5	B	704	NDP	16	0
5	A	704	NDP	7	0
3	B	702	CB3	18	0

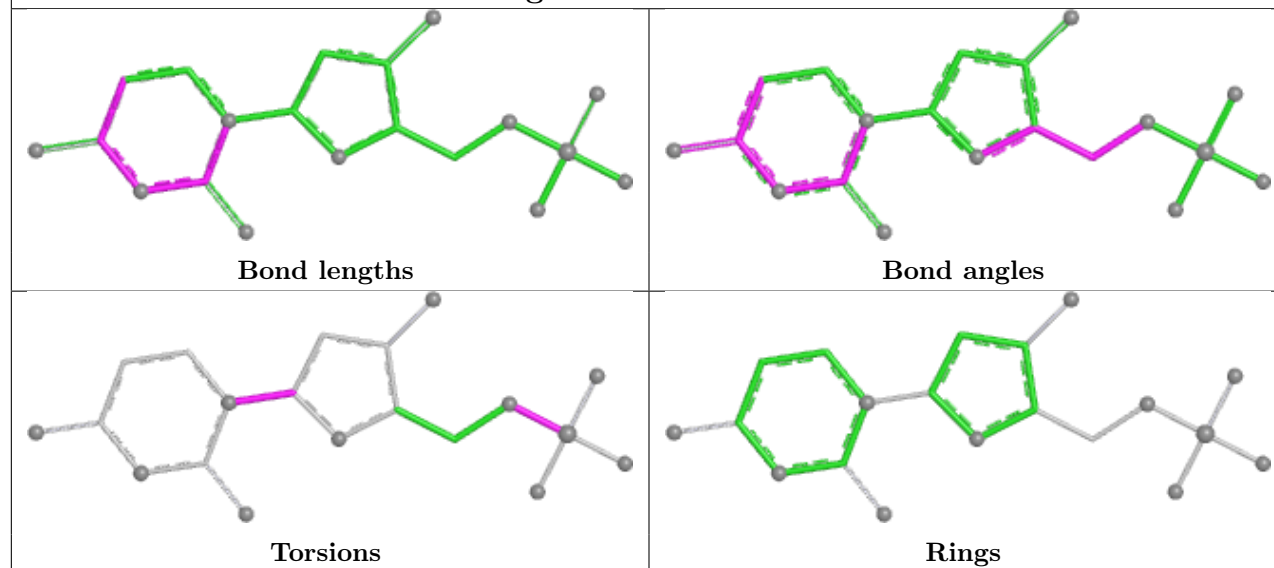
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

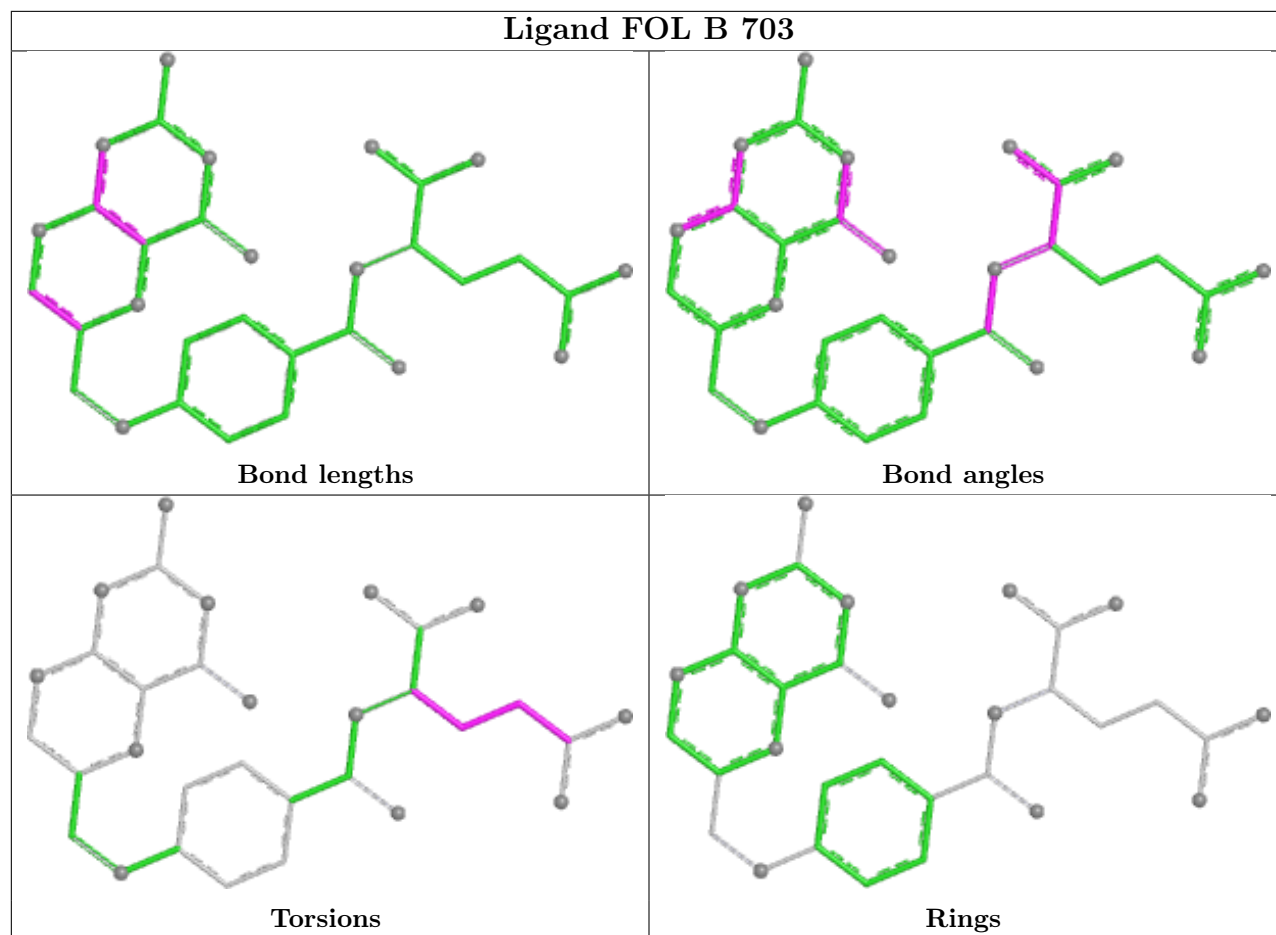


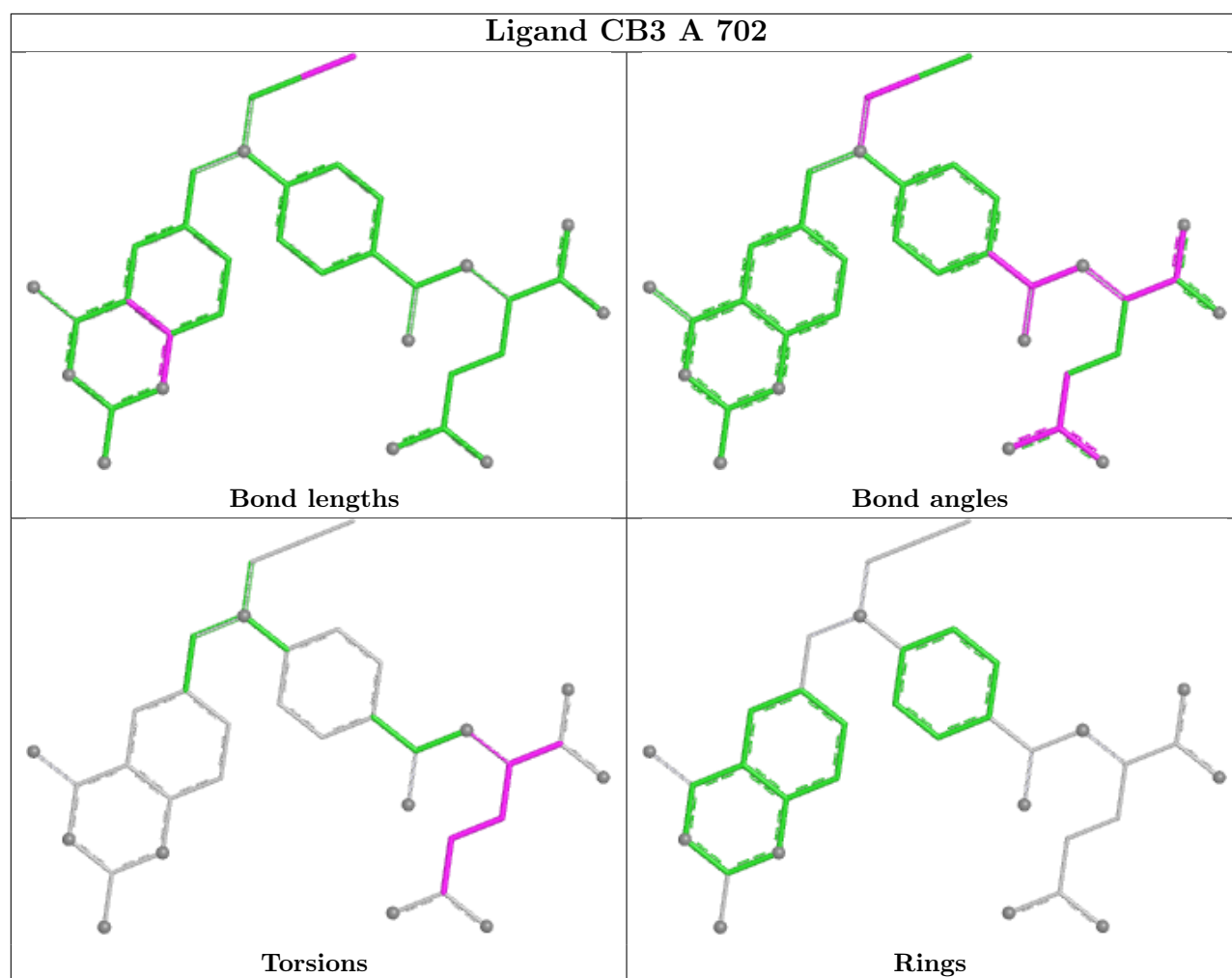
Ligand FOL A 703

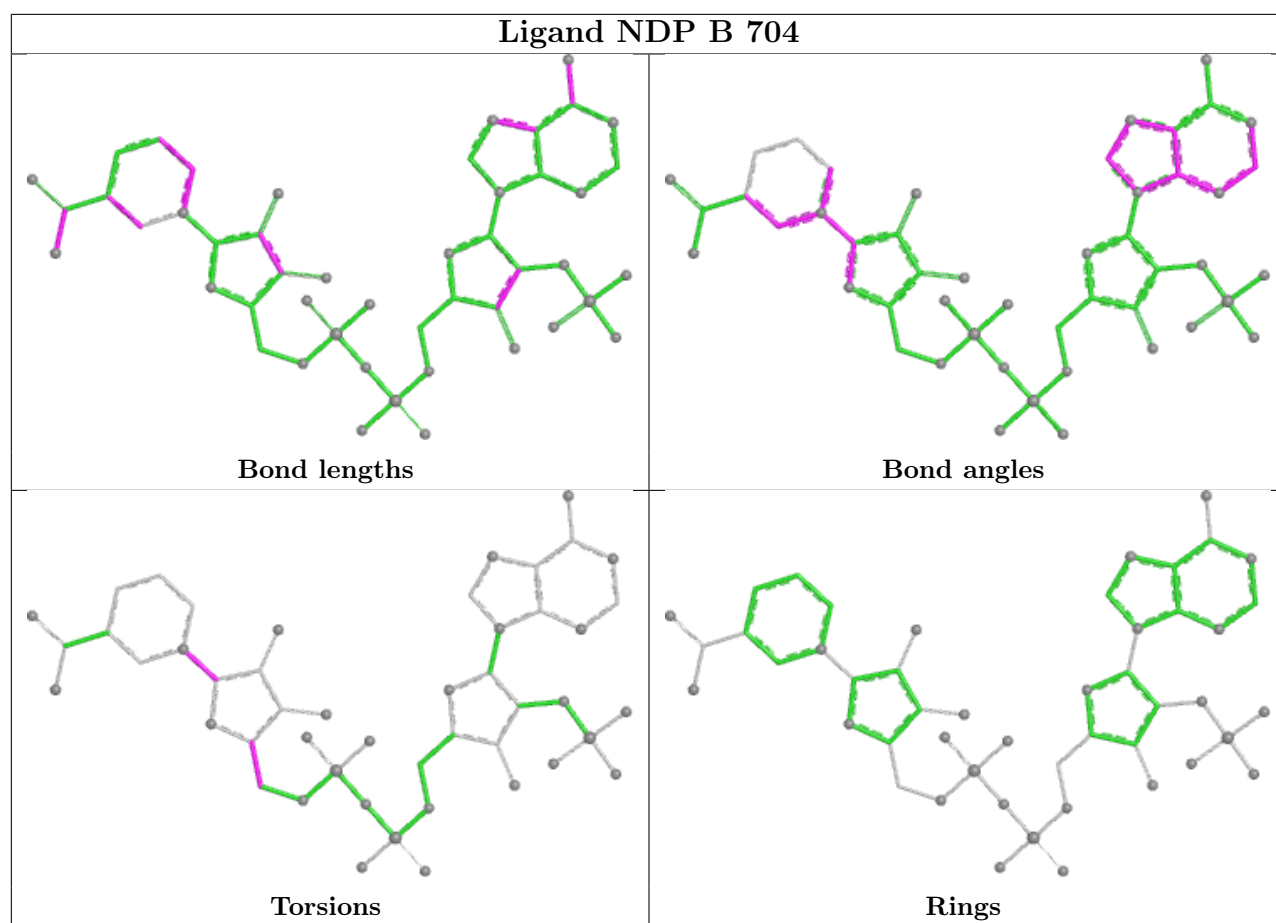


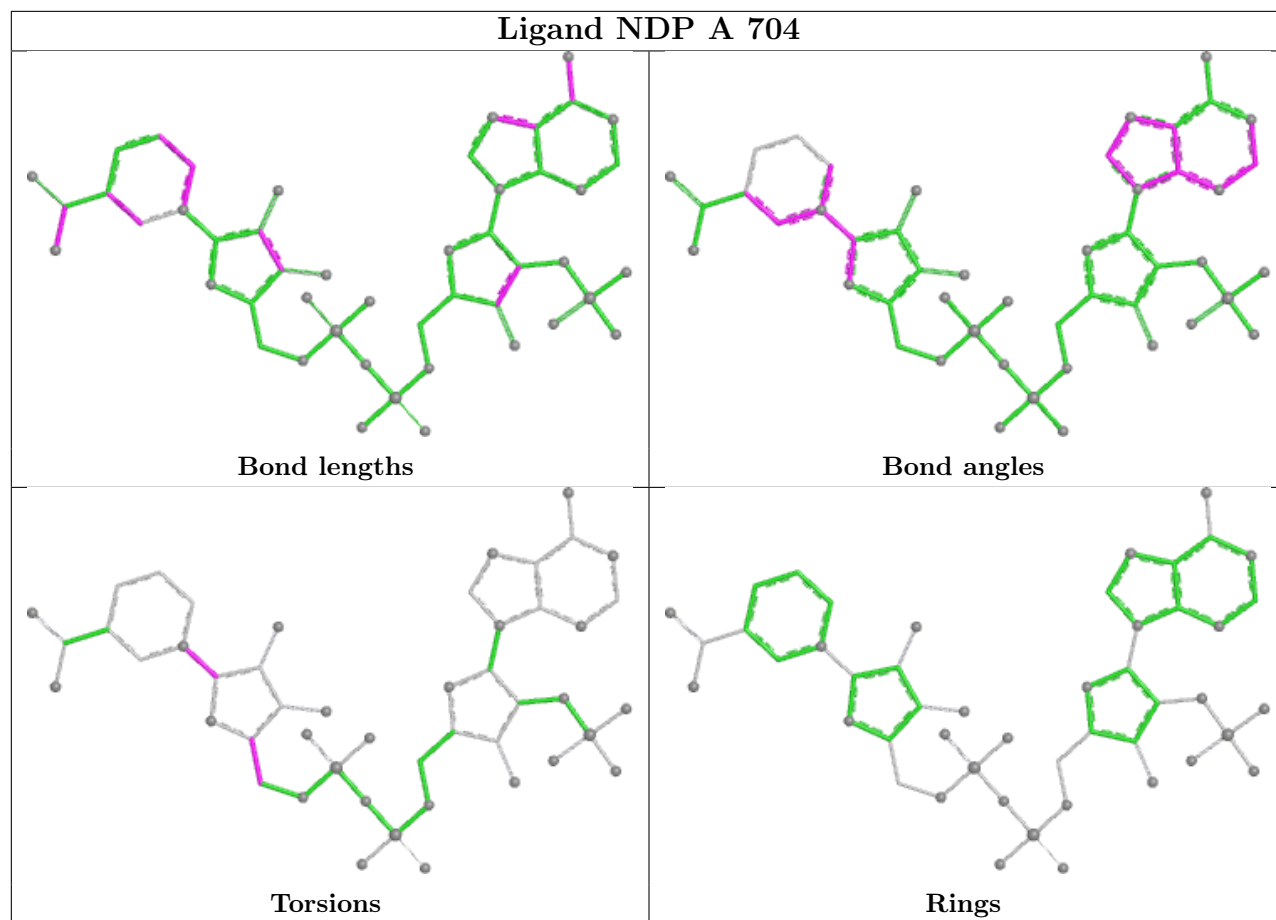
Ligand UMP A 701

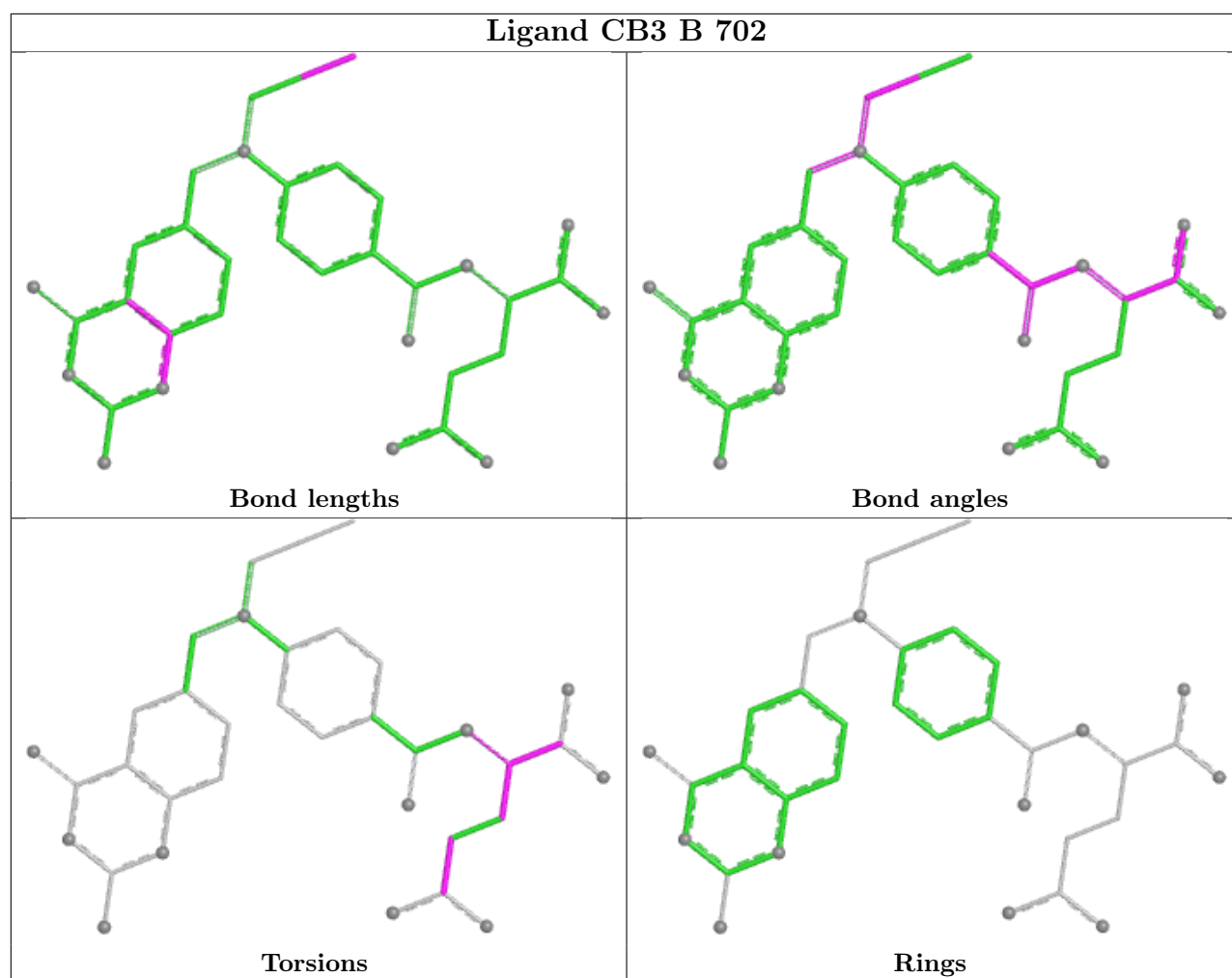












5.7 Other polymers [i](#)

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	A	498/610 (81%)	-0.99	1 (0%) 91 81	16, 57, 83, 115	2 (0%)
1	B	498/610 (81%)	-1.01	0 100 100	26, 57, 79, 103	2 (0%)
All	All	996/1220 (81%)	-1.00	1 (0%) 92 85	16, 57, 81, 115	4 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	150	VAL	2.3

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 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(Å ²)	Q<0.9
3	CB3	A	702	35/35	0.98	0.07	80,90,105,105	0
3	CB3	B	702	35/35	0.98	0.08	72,92,110,116	0
2	UMP	A	701	20/20	0.99	0.06	71,78,95,97	0
2	UMP	B	701	20/20	0.99	0.05	68,79,103,105	0

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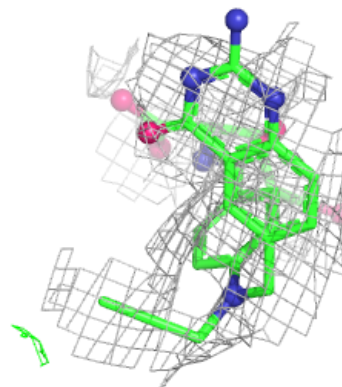
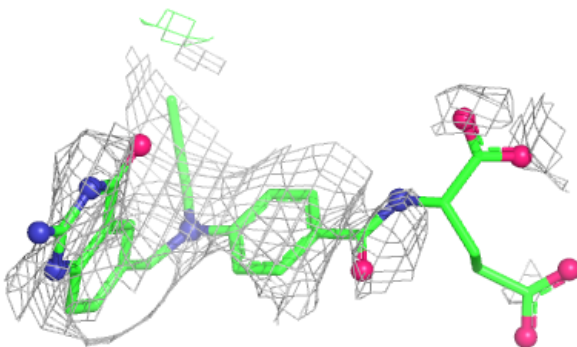
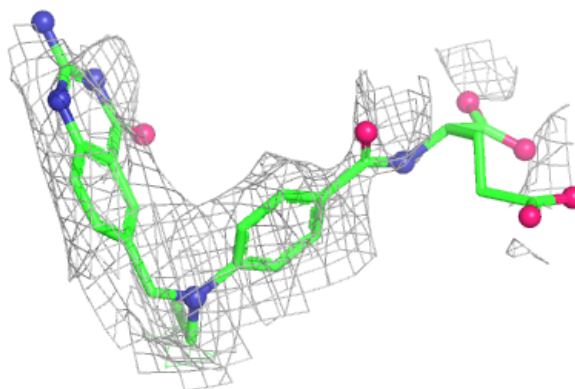
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	FOL	A	703	32/32	0.99	0.05	72,86,94,98	0
4	FOL	B	703	32/32	0.99	0.05	72,82,105,110	0
5	NDP	A	704	48/48	0.99	0.06	75,83,100,104	0
5	NDP	B	704	48/48	0.99	0.06	75,84,99,102	0

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.

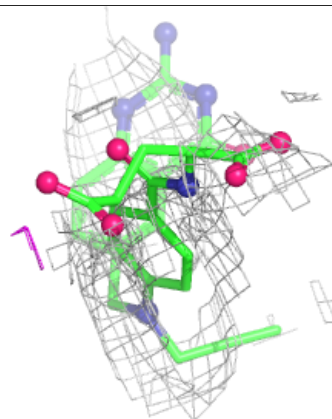
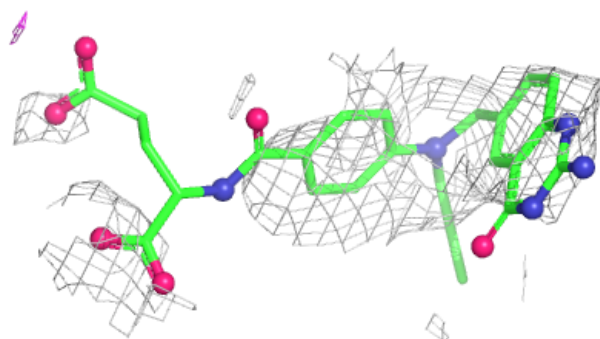
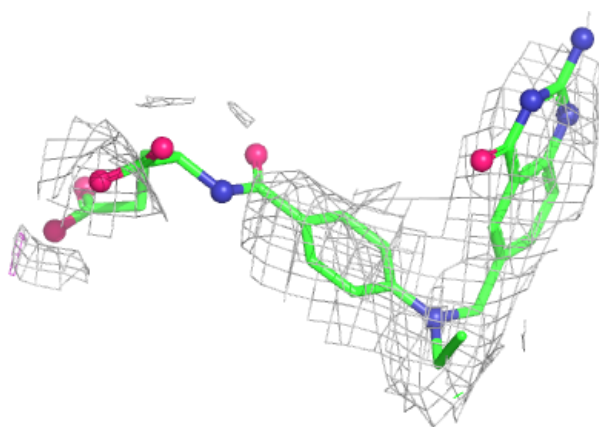
Electron density around CB3 A 702:

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

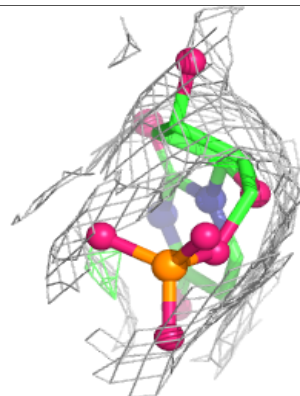
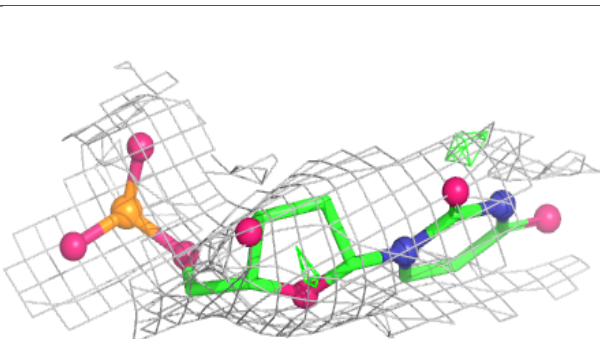
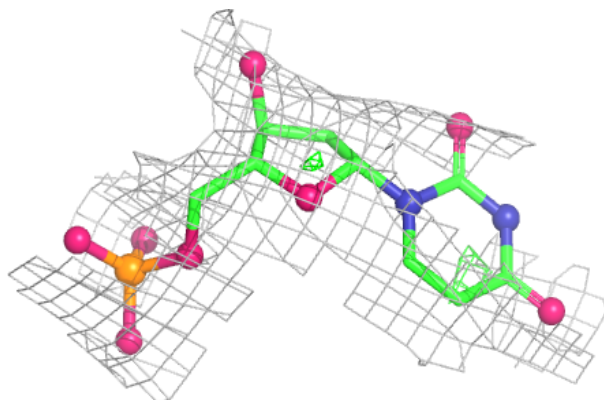


Electron density around CB3 B 702:

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

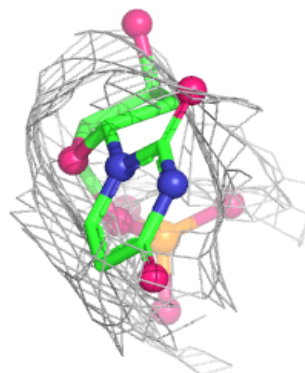
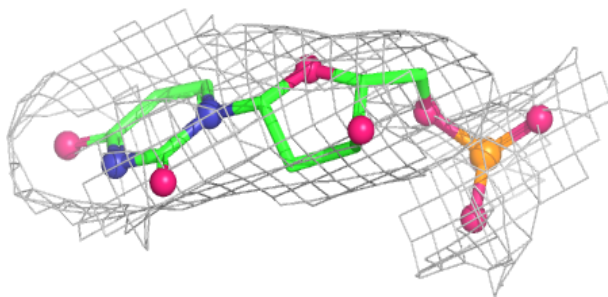
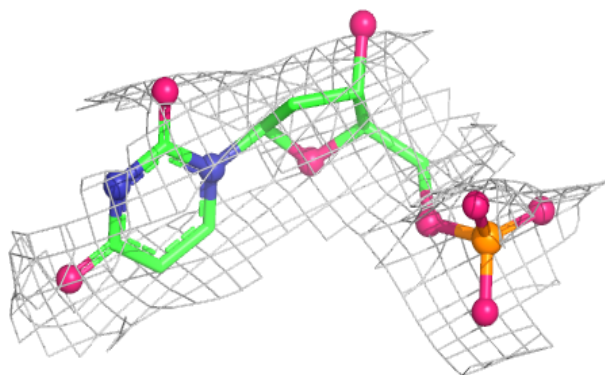
**Electron density around UMP A 701:**

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



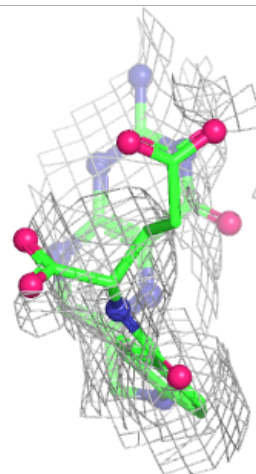
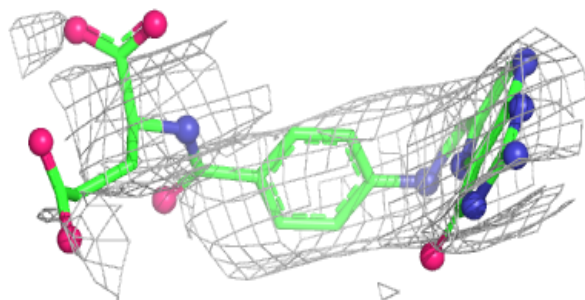
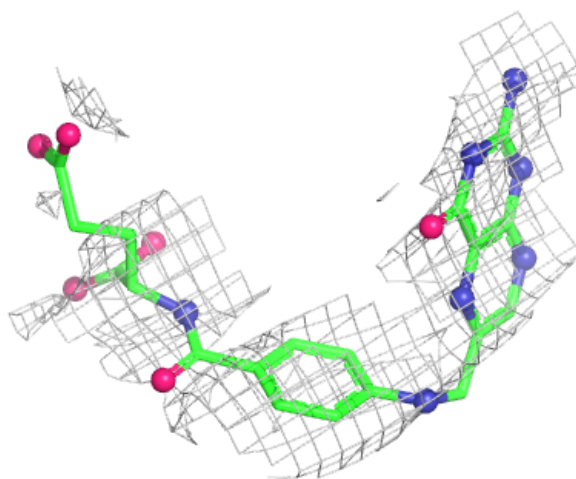
Electron density around UMP B 701:

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



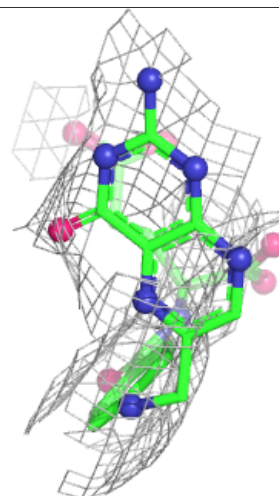
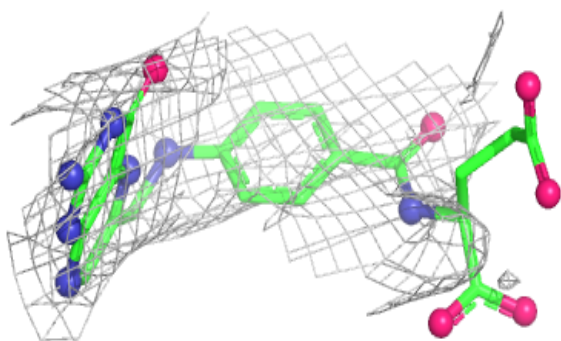
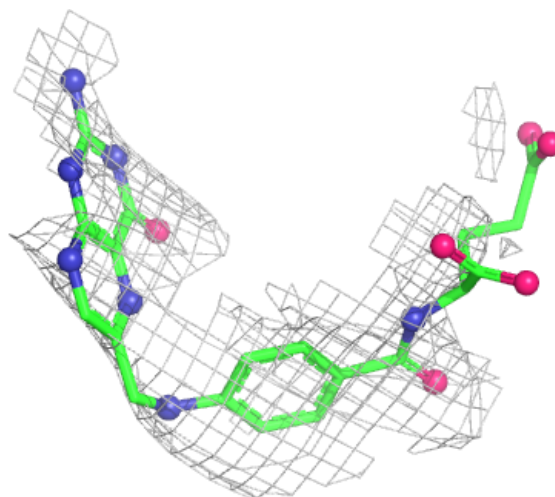
Electron density around FOL A 703:

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



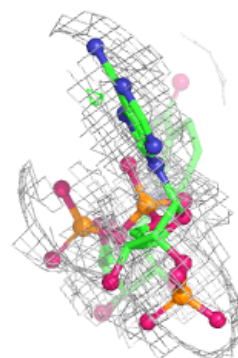
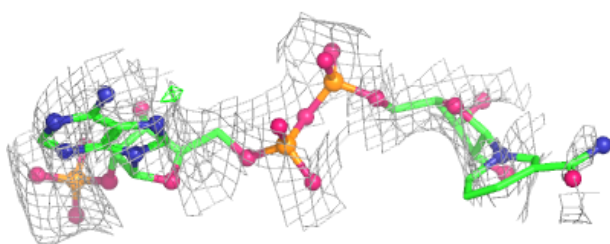
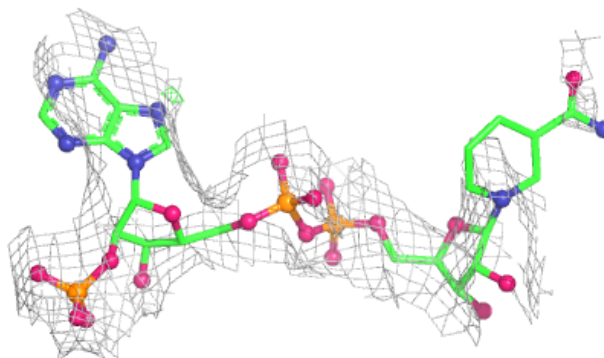
Electron density around FOL B 703:

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

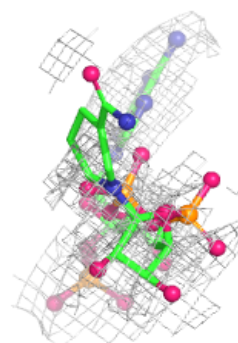
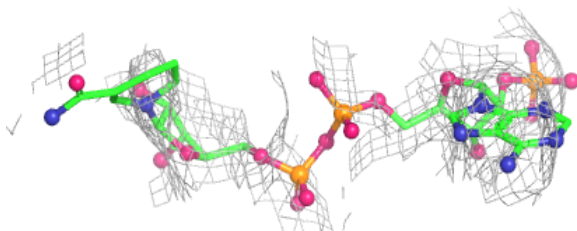
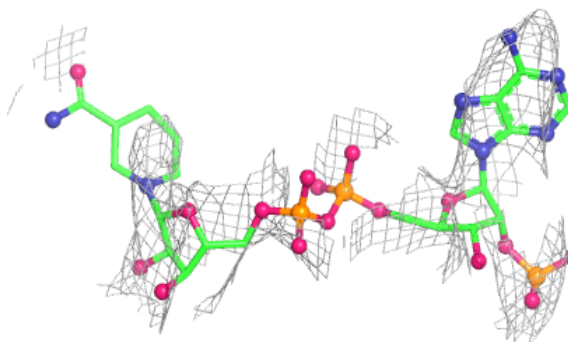


Electron density around NDP A 704:

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

**Electron density around NDP B 704:**

$2mF_o-DF_c$ (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.