



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 25, 2020 – 02:55 PM BST

PDB ID : 4ECK
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 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	:	2.13
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)	:	2.13

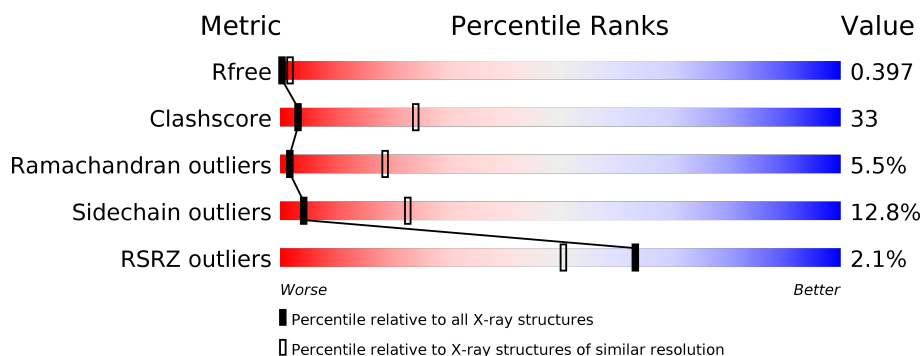
1 Overall quality at a glance ⓘ

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}	130704	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)

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	610	<div> <div> <div></div> <div>37%</div> <div>36%</div> <div>8%</div> <div>18%</div> </div> </div>
1	B	610	<div> <div>2%</div> <div> <div></div> <div>36%</div> <div>37%</div> <div>9%</div> <div>18%</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 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	X
3	CB3	B	702	-	-	X	X
4	FOL	A	703	-	-	X	X
4	FOL	B	703	-	-	X	X

2 Entry composition [i](#)

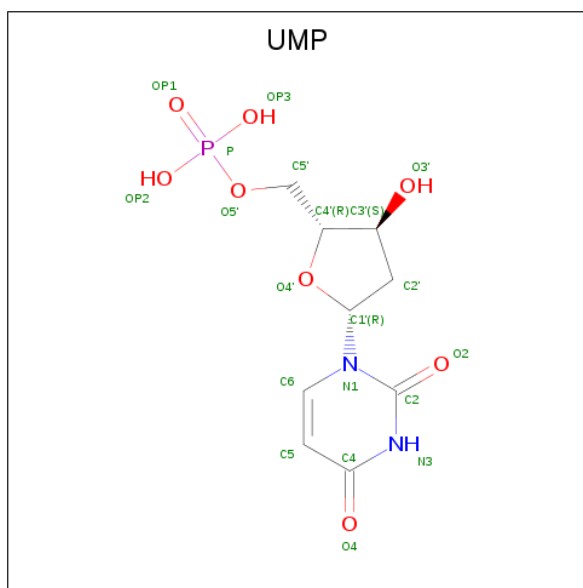
There are 5 unique types of molecules in this entry. The entry contains 8248 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

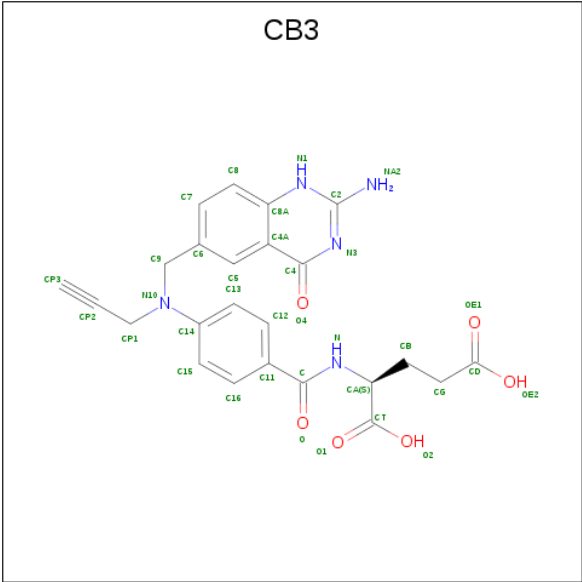
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	0	0
			3989	2550	697	717	25			
1	B	498	Total	C	N	O	S	0	0	0
			3989	2550	697	717	25			

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



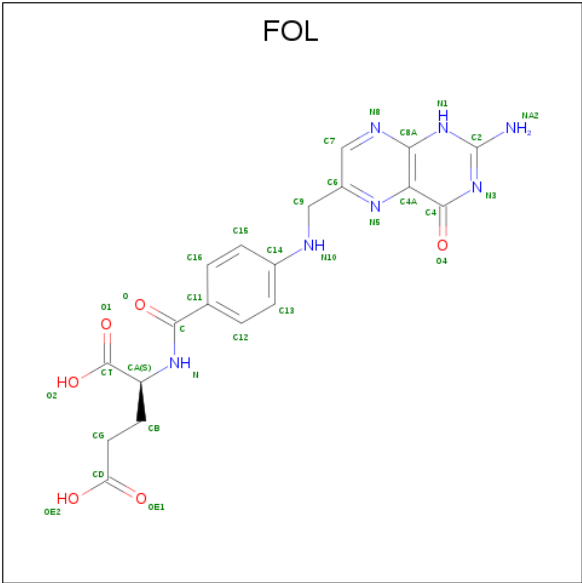
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

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



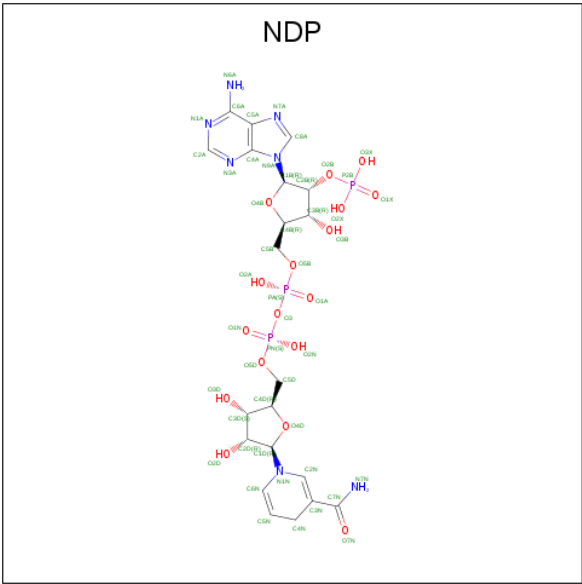
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			35	24	5	6		
3	B	1	Total	C	N	O	0	0
			35	24	5	6		

- Molecule 4 is FOLIC ACID (three-letter code: 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 (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).

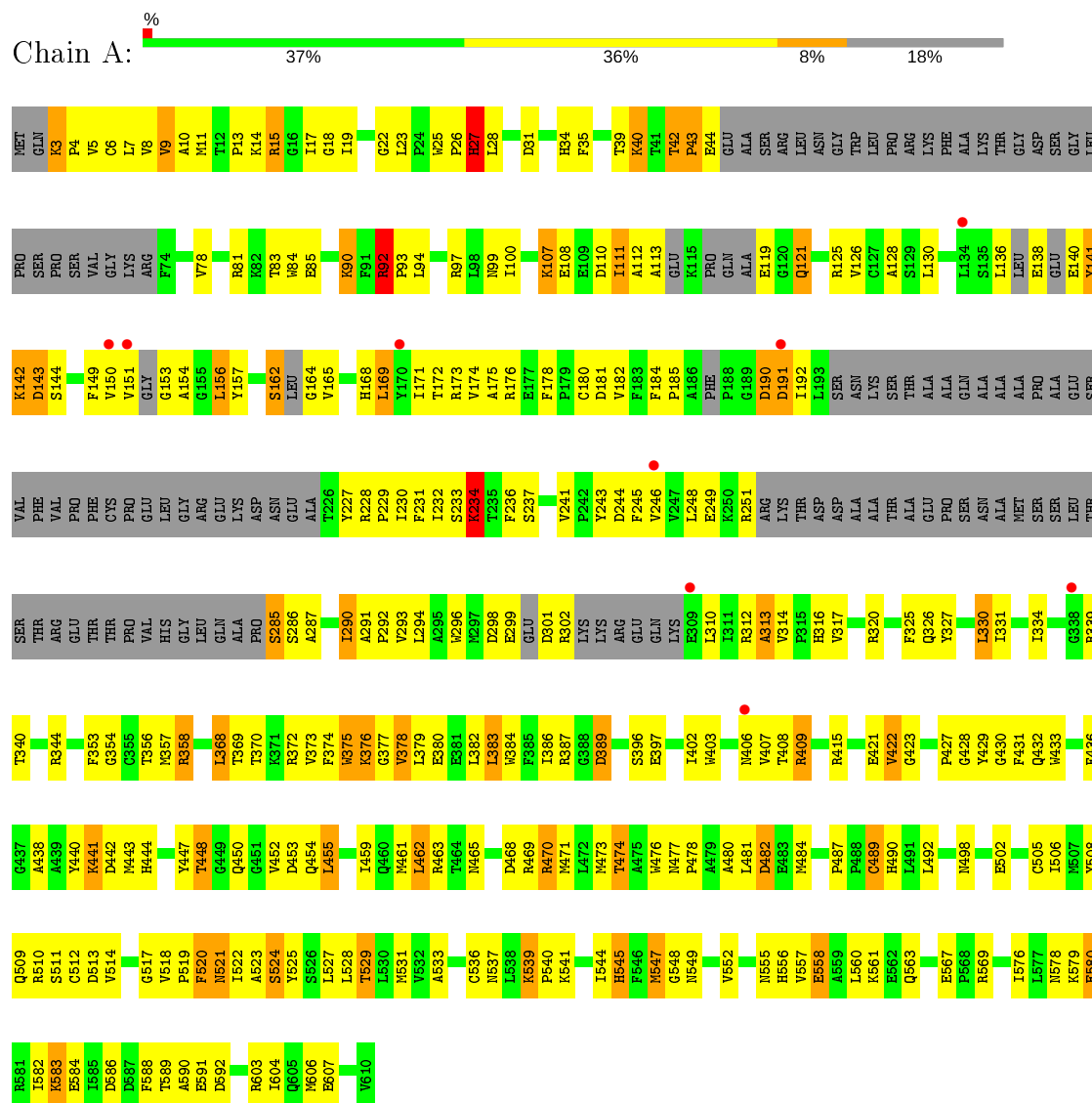


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
5	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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



R569	P570	I573	N578	K579	I582	I585	D586	D587	F588	T589	A590	E591	D592	V596	V599	H601	G602	R603	I604	Q605	M606	A609	V610																																	
M498	D499	Q500	C505	I506	M507	Y508	Q509	R510	S511	C512	D513	V514	G515	S516	L517	S518	S519	S520	S521	S522	A523	S524	S525	S526	L527	L528	T529	L530	M531	V532	A533	H534	V535	C536	K539	P540	F543	I544	H545	F546	M547	H551	V552	H556	A559	L560	K561	E562	C563	L564	F565	R566				
R409	E421	V422	G423	D424	P427	W433	F436	Y440	K441	D442	M443	H444	T445	D446	Y447	D453	Q454	L455	K456	M457	V458	M461	L462	N465	D468	R469	M470	M471	L472	A473	T474	A475	M476	L481	M484	A485	L486	P487	P488	C489	H490	L491	L492	C493	Q494	F495	Y496	V497								
I331	T334	I335	R339	R344	T345	I350	F353	G354	C355	T356	M357	R358	L361	P366	L367	L368	T369	T370	K371	R372	V373	F374	V375	K376	G377	V378	L379	E380	E381	L382	L383	M384	F385	I386	R387	G388	D389	T390	N391	N393	H394	L395	S396	E397	L402	M403	D404	K405	M406							
SER	ASN	ALA	MET	SER	SER	LEU	THR	THR	THR	GLU	THR	THR	GLN	ALA	PRO	PRO	S285	S286	A287	I290	V293	V296	D297	D298	E299	GLU	D301	R302	LYS	LYS	ARG	GLN	LYS	E309	A313	V314	V317	H318	F319	R320	H321	E323	F324	F325	Q326	L330										
GLN	ALA	ALA	PRO	ALA	ALA	GLU	SER	VAL	VAL	PRO	PHE	CYS	PRO	GLU	HIS	LEU	GLY	ARG	GLU	LYS	ASP	ALA	T226	T227	R228	P229	T230	F231	T232	S233	R234	T235	F236	S237	V241	P242	T243	D244	F245	V246	V247	E248	R249	R250	R251	ARG	LYS	THR	ASP	ALA	ALA	THR	ALA	GLU	PRO	
GLY	LEU	PRO	SER	PRO	LEU	VAL	GLY	LYS	ARG	F74	N75	A76	V77	V78	M79	G80	R81	K82	M87	P88	R89	K90	F91	R92	P93	V95	D96	R97	L98	N99	I100	V101	V102	K107	E108	E109	D110	I111	A112	A113	GLU	PRO	ASN	GLN	TRP	LEU	PRO	ARG	LYS	PHE	ALA	LYS	THR	GLY	ASP	SER
MET	GLN	K3	P4	V5	C6	L7	V8	V9	A10	M11	T12	P13	K14	R15	I19	N20	R21	G22	L23	P24	R25	P26	H27	L28	T29	F32	K33	H34	F35	S36	R37	V38	T39	K40	T41	T42	P43	E44	ALA	SER	ARG	LEU	ASN	GLY	ALA	PRO	ARG	LYS	PHE	ALA	LYS	THR	GLY	ASP	SER	

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 , 0.397	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)	0.32 , 30.4	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	0.77	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.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FOL, CB3, UMP, NDP

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	0.58	1/4078 (0.0%)	0.73	0/5510
1	B	0.59	3/4078 (0.1%)	0.73	0/5510
All	All	0.59	4/8156 (0.0%)	0.73	0/11020

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	403	TRP	CD2-CE2	5.34	1.47	1.41
1	B	25	TRP	CD2-CE2	5.26	1.47	1.41
1	B	433	TRP	CD2-CE2	5.02	1.47	1.41
1	A	403	TRP	CD2-CE2	5.01	1.47	1.41

There are no bond angle outliers.

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 ⓘ

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	267	0
1	B	3989	0	3940	295	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	26	0
5	A	48	0	26	8	0
5	B	48	0	26	16	0
All	All	8248	0	8029	543	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 33.

The worst 5 of 543 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 ⓘ

5.3.1 Protein backbone ⓘ

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	18
1	B	474/610 (78%)	385 (81%)	64 (14%)	25 (5%)	2	19
All	All	948/1220 (78%)	764 (81%)	132 (14%)	52 (6%)	2	19

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%)	378 (87%)	55 (13%)	4	23
1	B	433/525 (82%)	377 (87%)	56 (13%)	4	22
All	All	866/1050 (82%)	755 (87%)	111 (13%)	4	23

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	547	MET
1	B	82	LYS
1	B	543	PHE
1	A	558	GLU
1	B	9	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	27	HIS
1	B	99	ASN
1	B	490	HIS
1	A	545	HIS
1	B	444	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
4	FOL	A	703	-	28,34,34	1.38	3 (10%)	36,47,47	2.06	8 (22%)
4	FOL	B	703	-	28,34,34	1.35	4 (14%)	36,47,47	2.25	7 (19%)
3	CB3	A	702	-	30,37,37	1.32	3 (10%)	38,51,51	2.68	8 (21%)
2	UMP	B	701	-	18,21,21	0.79	1 (5%)	21,31,31	1.26	3 (14%)
5	NDP	A	704	-	45,52,52	2.05	8 (17%)	53,80,80	2.28	6 (11%)
5	NDP	B	704	-	45,52,52	2.05	8 (17%)	53,80,80	2.22	7 (13%)
2	UMP	A	701	-	18,21,21	0.77	1 (5%)	21,31,31	1.16	2 (9%)
3	CB3	B	702	-	30,37,37	1.33	3 (10%)	38,51,51	2.59	11 (28%)

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
4	FOL	A	703	-	-	3/16/22/22	0/3/3/3
4	FOL	B	703	-	-	4/16/22/22	0/3/3/3
3	CB3	A	702	-	-	6/21/28/28	0/3/3/3
2	UMP	B	701	-	-	3/7/22/22	0/2/2/2
5	NDP	A	704	-	-	3/30/77/77	0/5/5/5
5	NDP	B	704	-	-	3/30/77/77	0/5/5/5
2	UMP	A	701	-	-	3/7/22/22	0/2/2/2
3	CB3	B	702	-	-	5/21/28/28	0/3/3/3

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	704	NDP	C6N-C5N	8.29	1.48	1.33
5	A	704	NDP	C6N-C5N	8.15	1.47	1.33
5	A	704	NDP	C2N-C3N	4.93	1.48	1.34
5	B	704	NDP	C2N-C3N	4.89	1.48	1.34
4	A	703	FOL	C4A-C8A	4.69	1.49	1.40

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	CB3	C4A-C4-N3	-10.43	117.13	124.40
3	A	702	CB3	C4A-C4-N3	-10.34	117.19	124.40
5	A	704	NDP	C1D-N1N-C2N	10.13	137.99	121.11
5	B	704	NDP	C1D-N1N-C2N	9.64	137.16	121.11
3	A	702	CB3	C4A-C8A-N1	-9.58	118.40	123.60

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	703	FOL	N-CA-CB-CG
4	A	703	FOL	CT-CA-CB-CG
4	A	703	FOL	CA-CB-CG-CD
4	B	703	FOL	N-CA-CB-CG
4	B	703	FOL	CT-CA-CB-CG

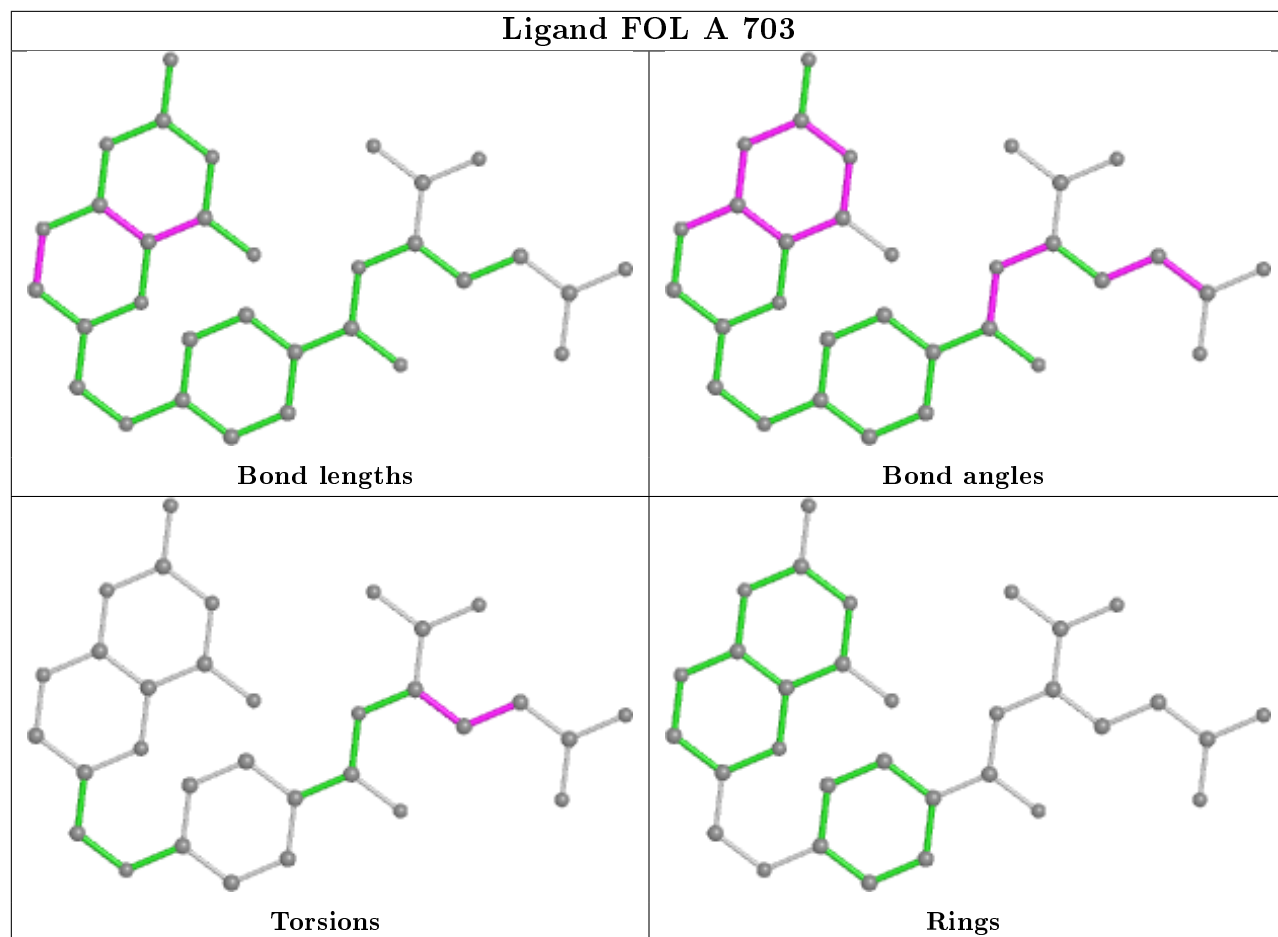
There are no ring outliers.

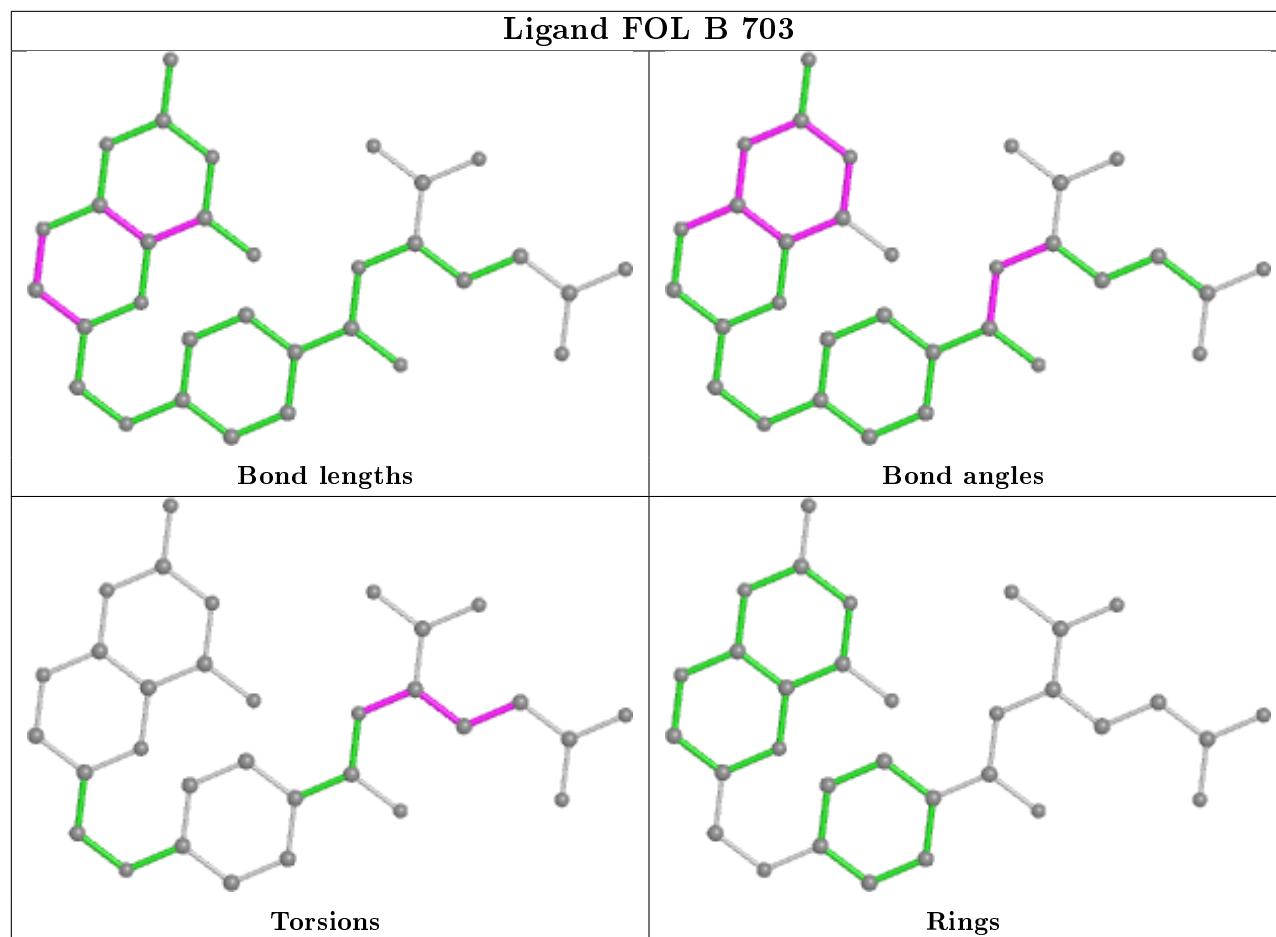
8 monomers are involved in 132 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	703	FOL	10	0
4	B	703	FOL	26	0
3	A	702	CB3	15	0
2	B	701	UMP	15	0
5	A	704	NDP	8	0
5	B	704	NDP	16	0
2	A	701	UMP	25	0
3	B	702	CB3	18	0

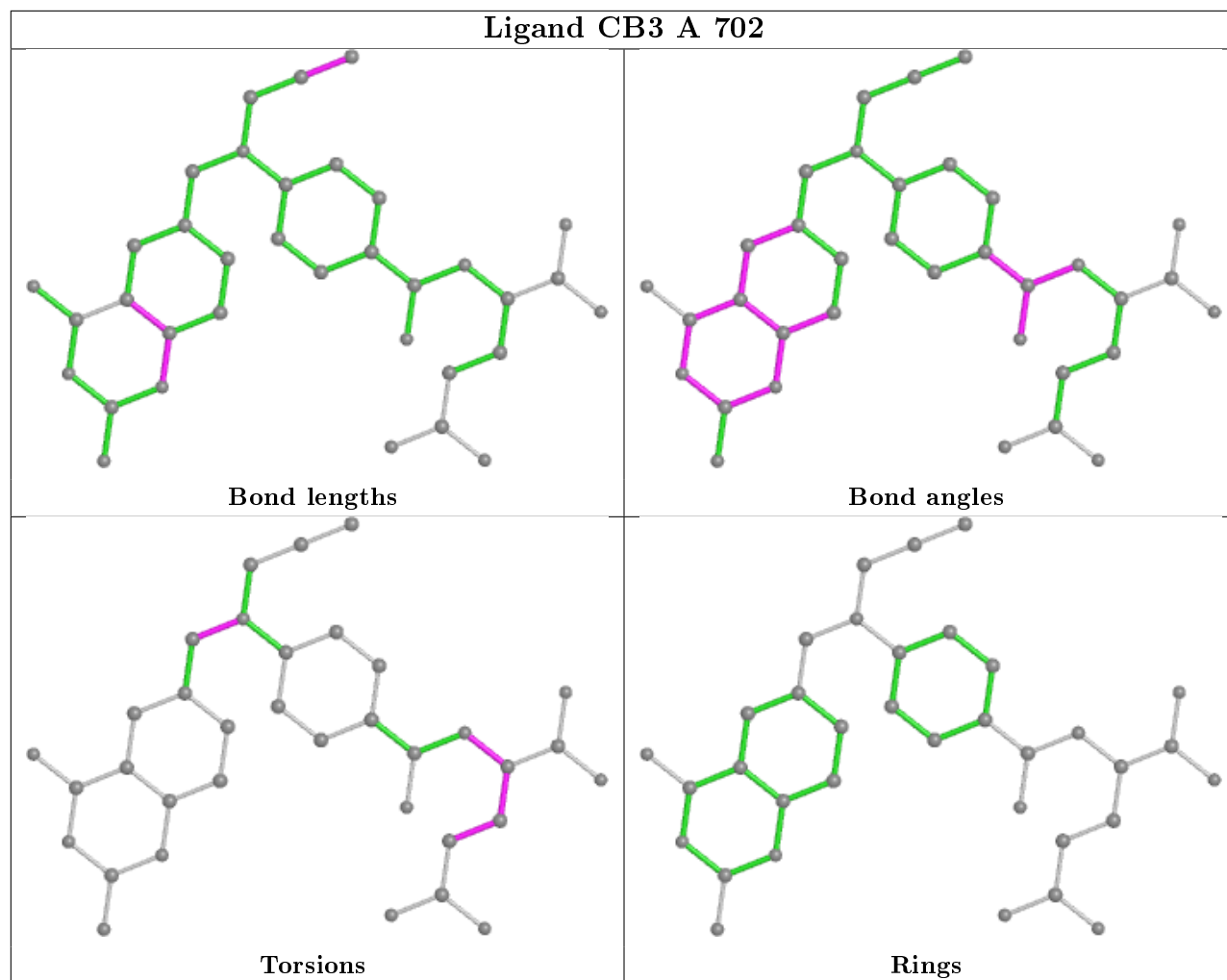
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

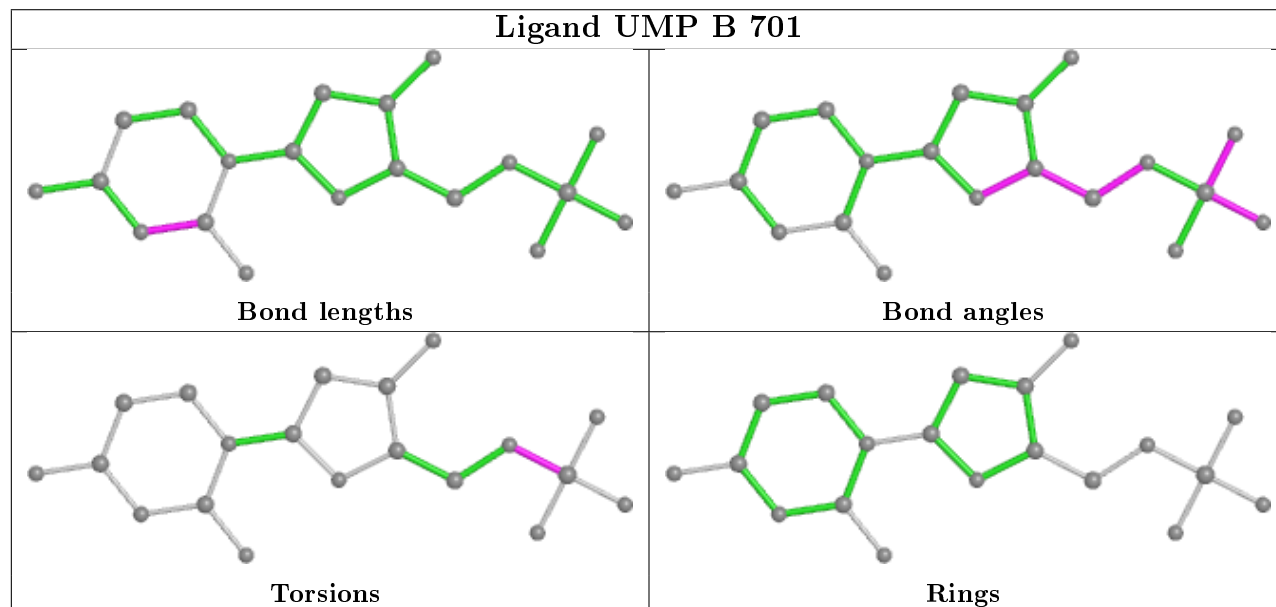


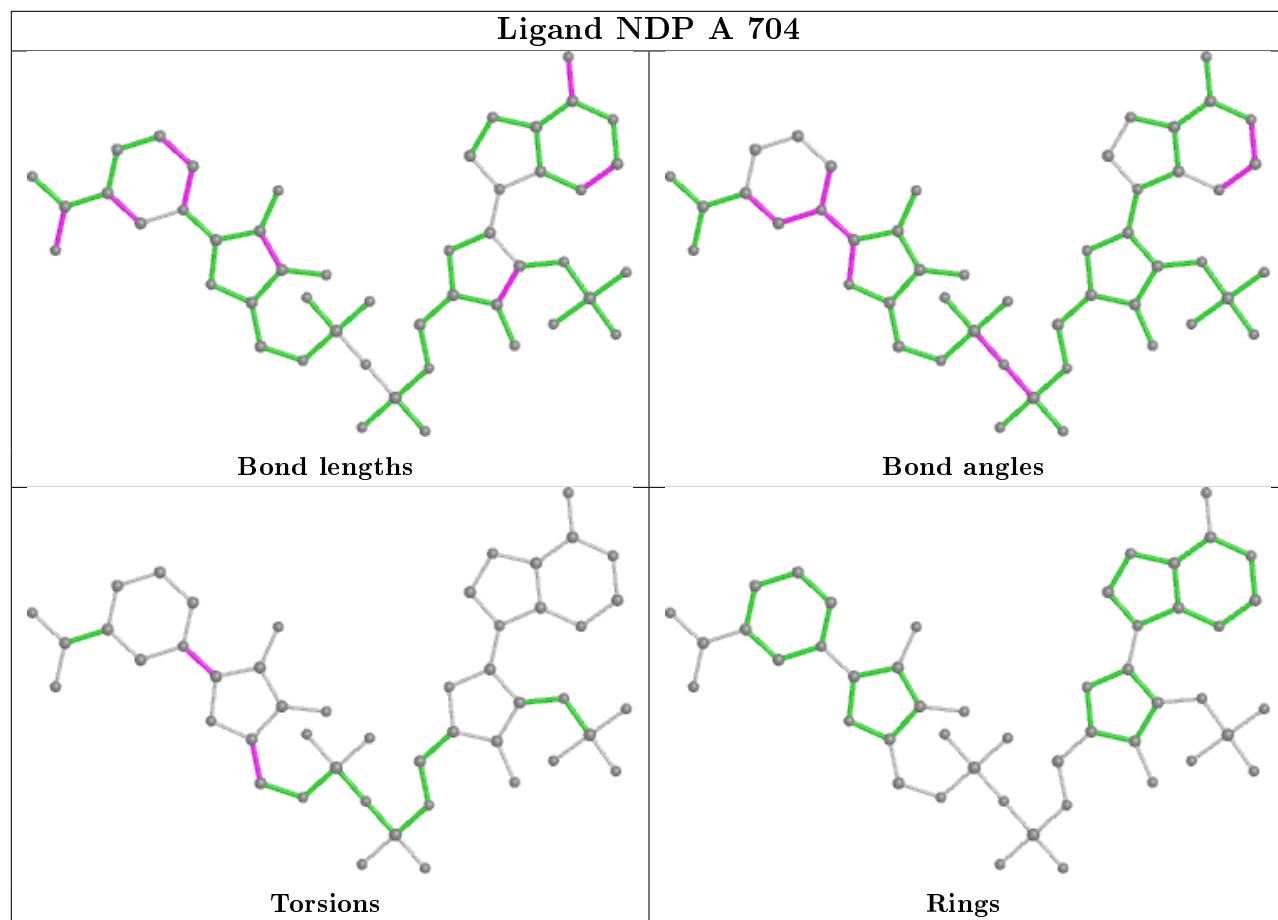


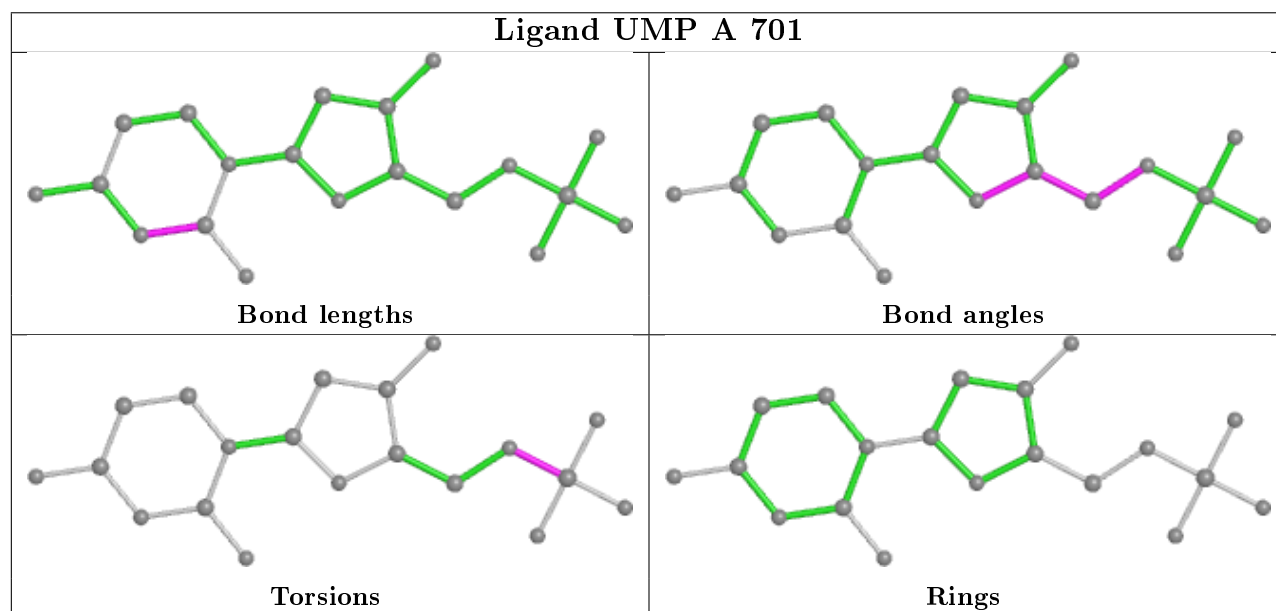
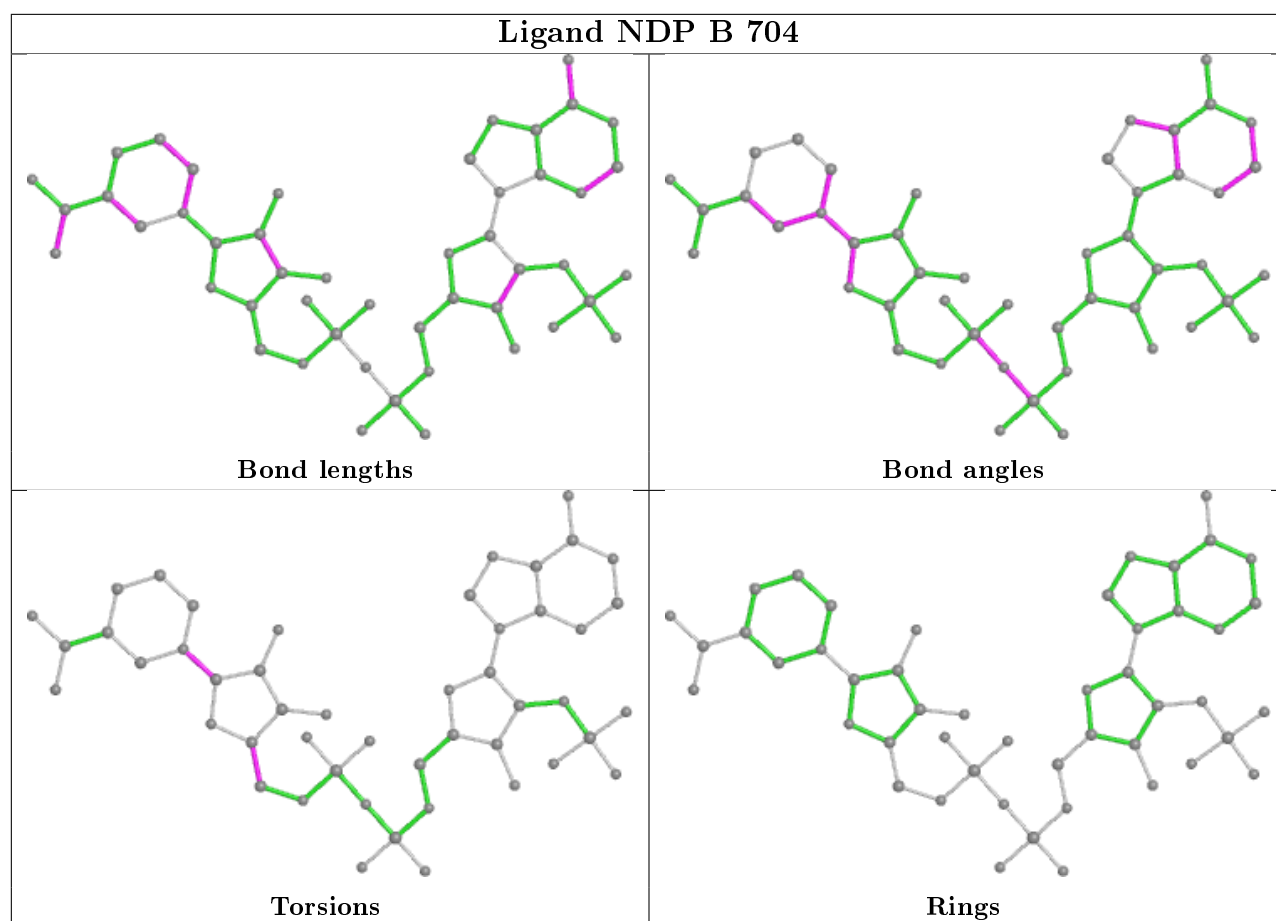
Ligand CB3 A 702

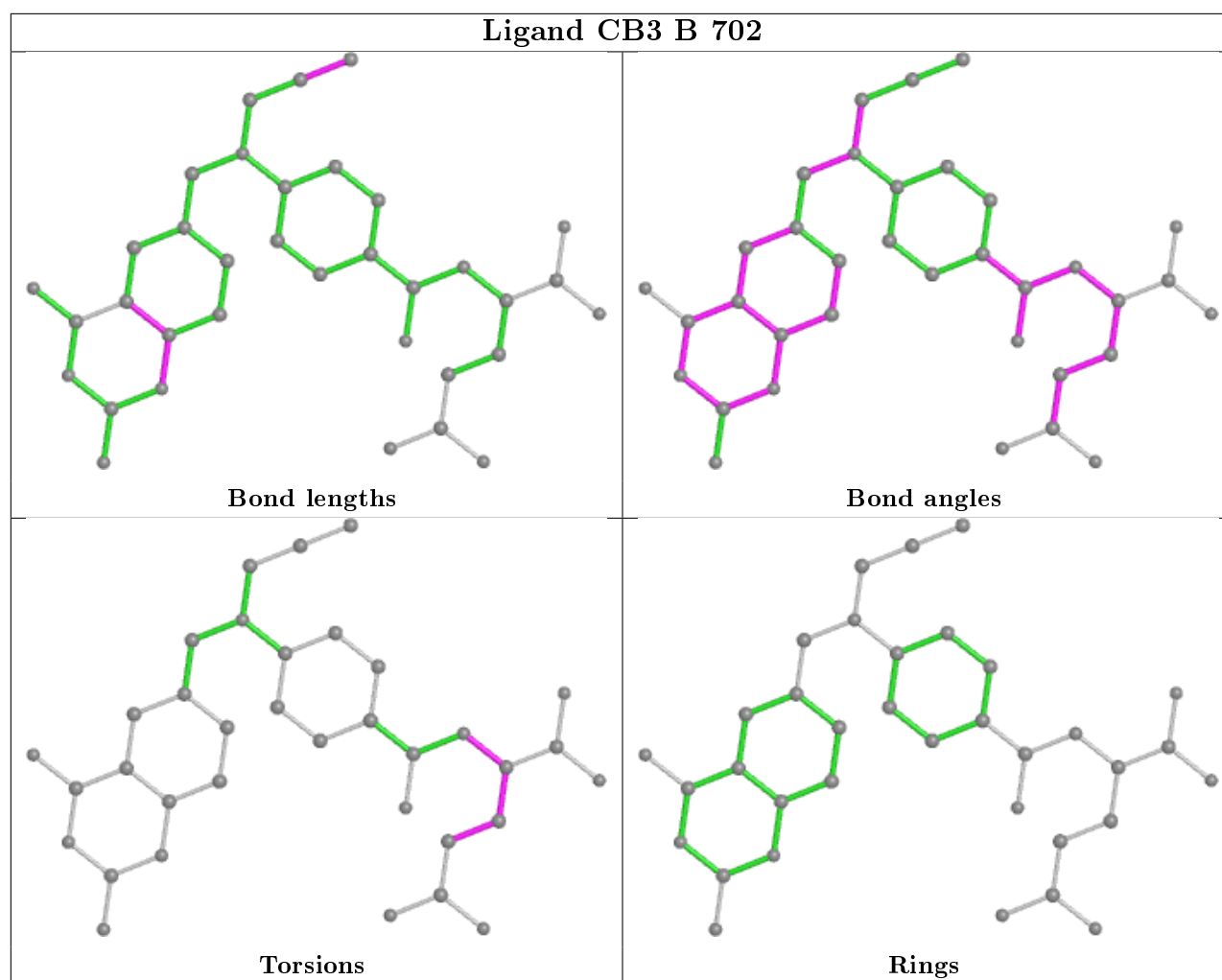


Ligand UMP B 701









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%)	0.08	9 (1%) 68 55	39, 57, 83, 115	2 (0%)
1	B	498/610 (81%)	0.05	12 (2%) 59 45	39, 58, 79, 103	2 (0%)
All	All	996/1220 (81%)	0.07	21 (2%) 63 50	39, 57, 81, 115	4 (0%)

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	150	VAL	3.7
1	A	151	VAL	3.0
1	A	338	GLY	3.0
1	A	309	GLU	2.9
1	A	406	ASN	2.9

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 monosaccharides in this entry.

6.4 Ligands [i](#)

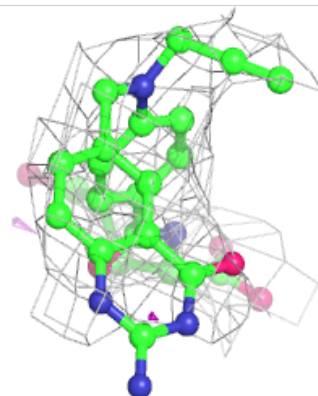
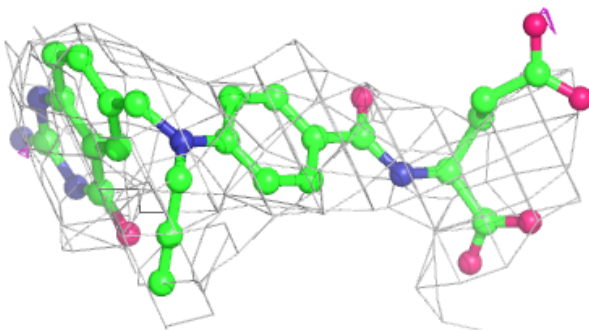
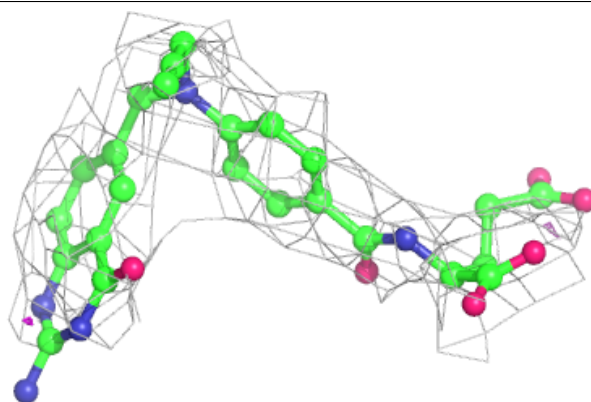
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CB3	A	702	35/35	0.74	0.48	80,90,105,105	0
3	CB3	B	702	35/35	0.74	0.53	72,92,110,116	0
4	FOL	A	703	32/32	0.77	0.47	72,86,94,98	0
4	FOL	B	703	32/32	0.78	0.49	72,82,105,110	0
5	NDP	B	704	48/48	0.86	0.32	75,84,99,102	0
5	NDP	A	704	48/48	0.88	0.31	75,83,100,104	0
2	UMP	B	701	20/20	0.93	0.28	68,79,103,105	0
2	UMP	A	701	20/20	0.94	0.25	71,78,95,97	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.

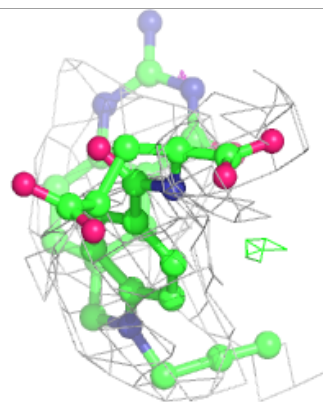
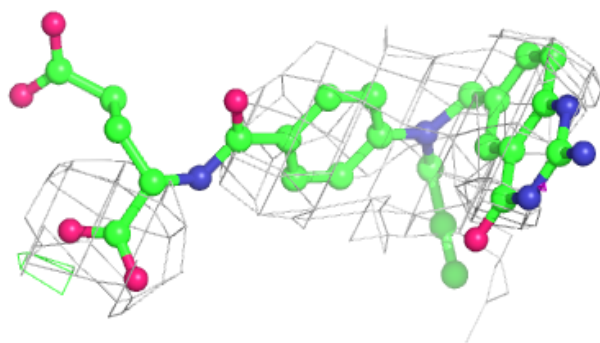
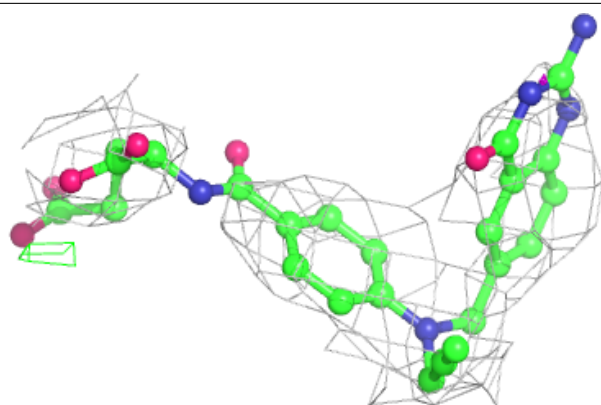
Electron density around CB3 A 702:

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

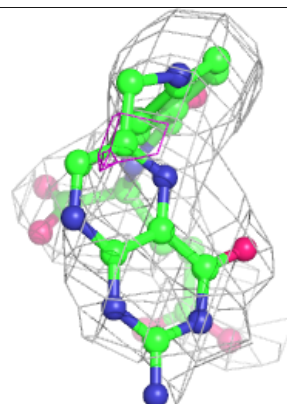
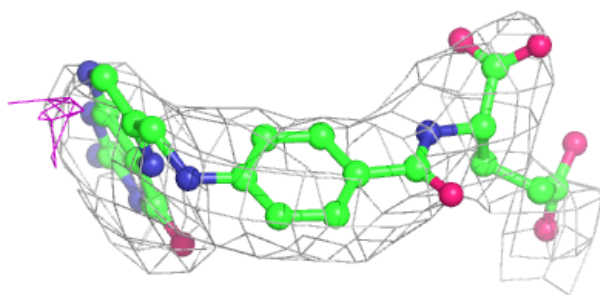
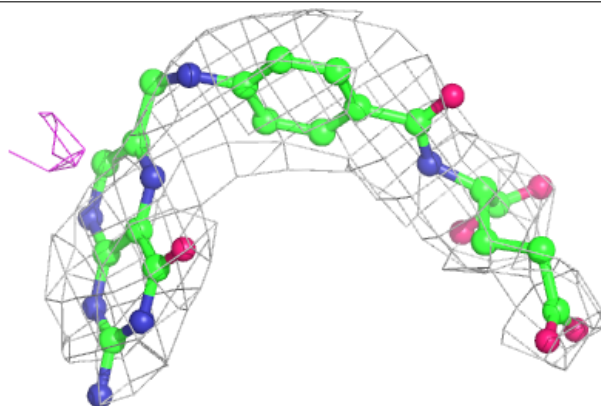


Electron density around CB3 B 702:

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

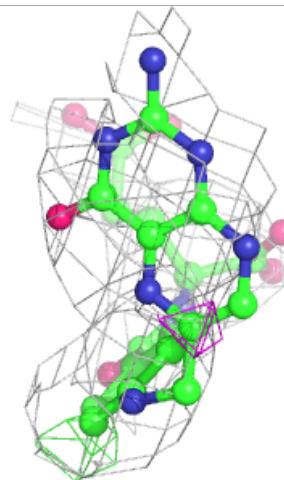
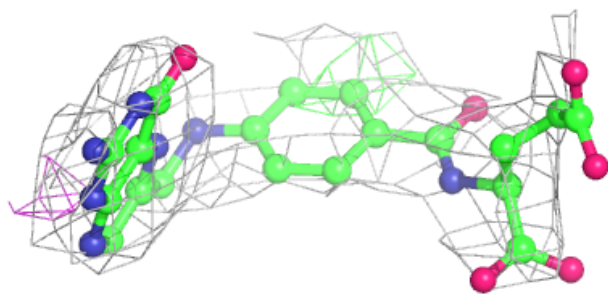
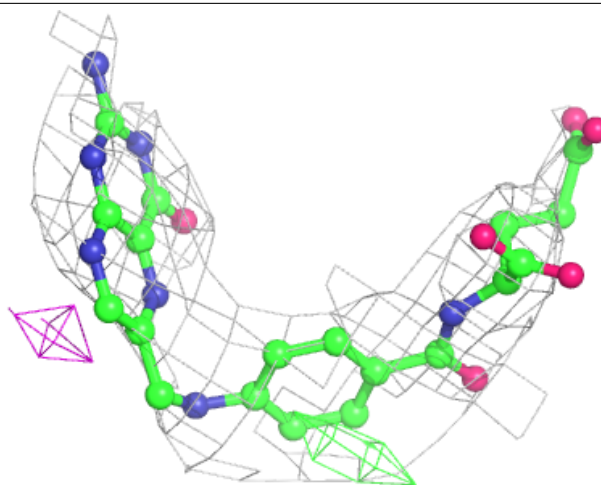
**Electron density around FOL A 703:**

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



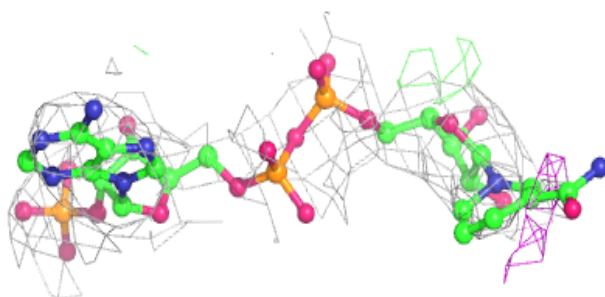
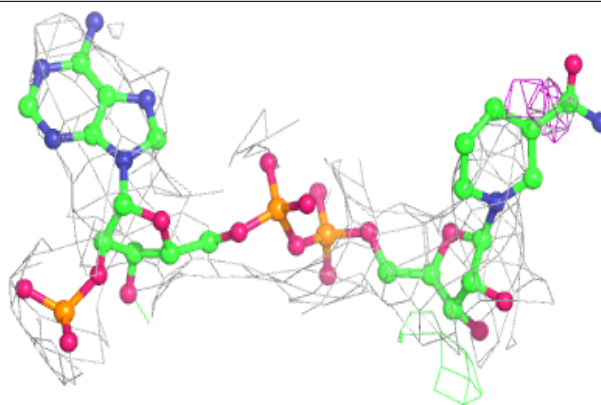
Electron density around FOL B 703:

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

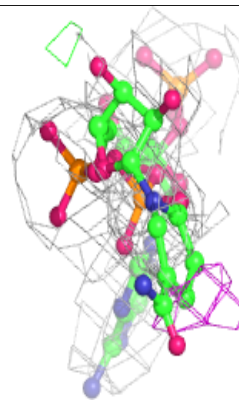
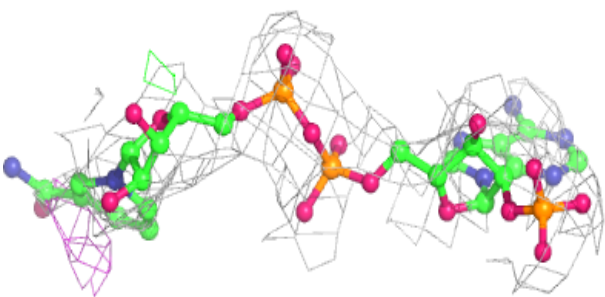
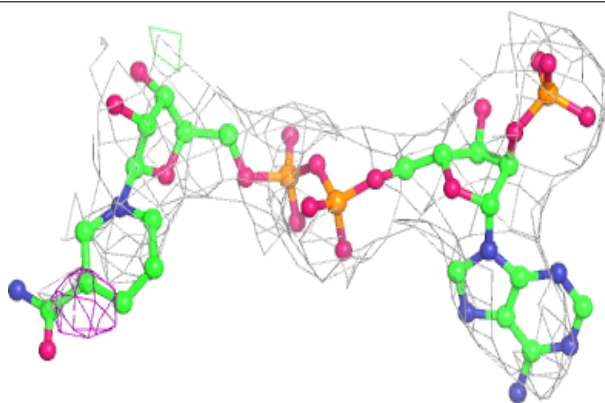


Electron density around NDP B 704:

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

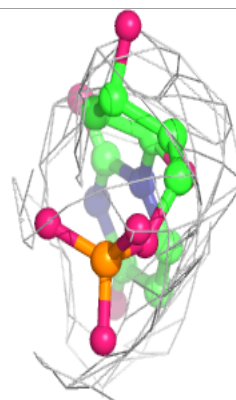
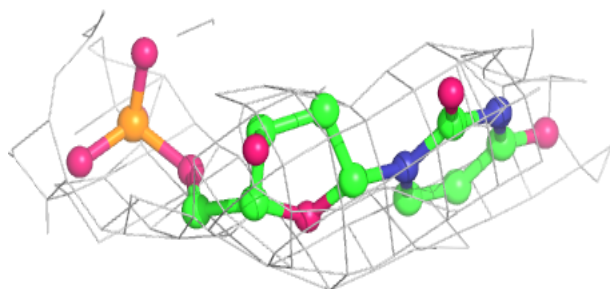
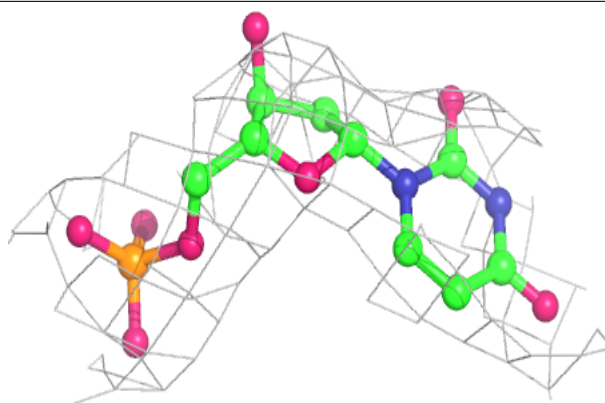
**Electron density around NDP A 704:**

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

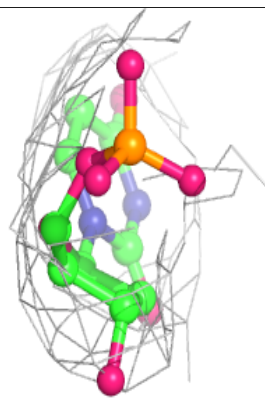
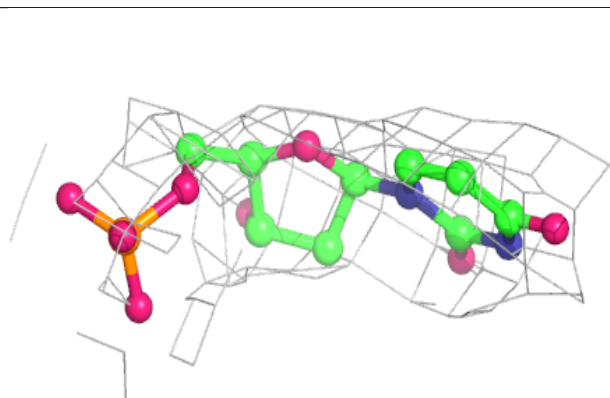
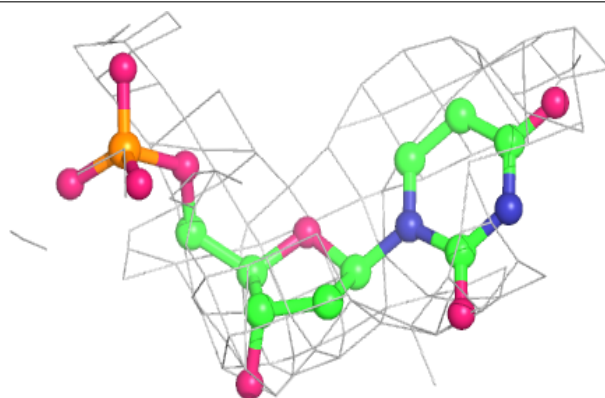


Electron density around UMP B 701:

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

**Electron density around 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.