



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 28, 2025 – 02:15 PM EDT

PDB ID : 3HBB / pdb\_00003hbb  
Title : Structures of dihydrofolate reductase-thymidylate synthase of *Trypanosoma cruzi* in the folate-free state and in complex with two antifolate drugs, trimetrexate and methotrexate  
Authors : Schormann, N.; Senkovich, O.; Chattopadhyay, D.  
Deposited on : 2009-05-04  
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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>.

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

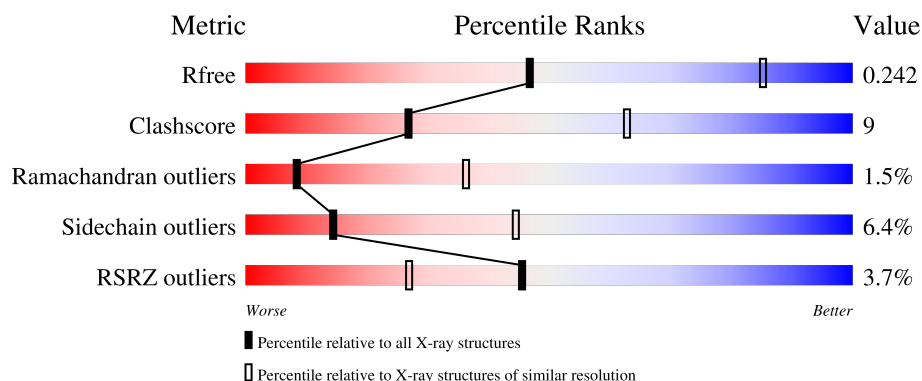
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 3.00 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))
$R_{free}$	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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  $\geq 3$ , 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	
1	B	521	
1	C	521	
1	D	521	

## 2 Entry composition [i](#)

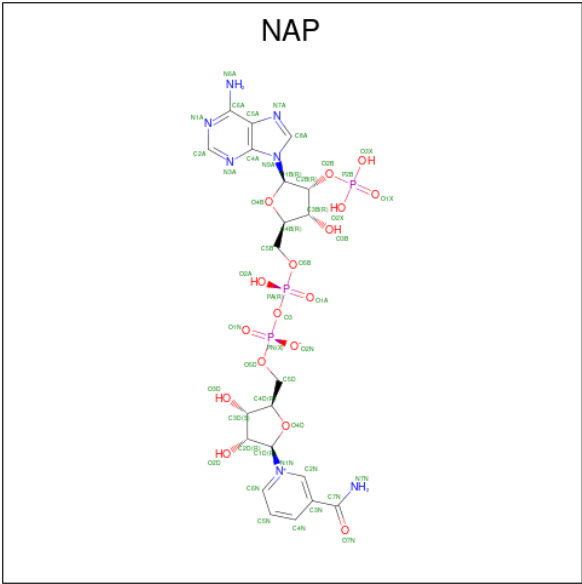
There are 6 unique types of molecules in this entry. The entry contains 16812 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dihydrofolate reductase-thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	0	0
			4052	2571	714	749	18			
1	B	505	Total	C	N	O	S	0	0	0
			4010	2546	707	739	18			
1	C	510	Total	C	N	O	S	0	0	0
			4049	2570	712	748	19			
1	D	507	Total	C	N	O	S	0	0	0
			4023	2553	711	741	18			

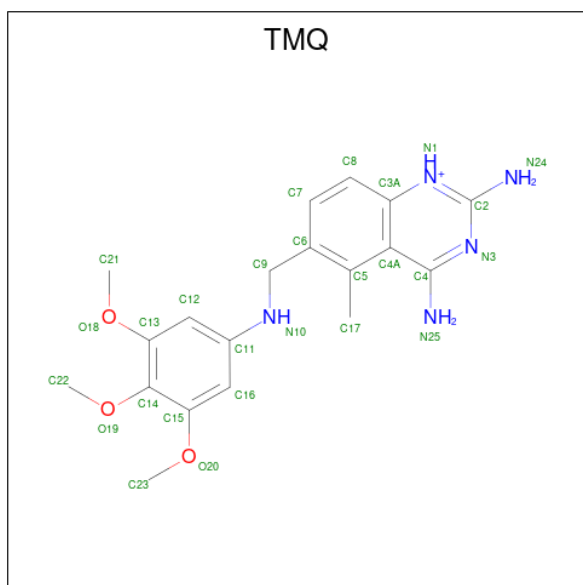
- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			48	21	7	17		
2	D	1	Total	C	N	O	0	0
			48	21	7	17		

- Molecule 3 is TRIMETREXATE (CCD ID: TMQ) (formula:  $C_{19}H_{24}N_5O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			27	19	5	3		
3	B	1	Total	C	N	O	0	0
			27	19	5	3		
3	C	1	Total	C	N	O	0	0
			27	19	5	3		
3	D	1	Total	C	N	O	0	0
			27	19	5	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula:  $O_4S$ ).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 6 is water.

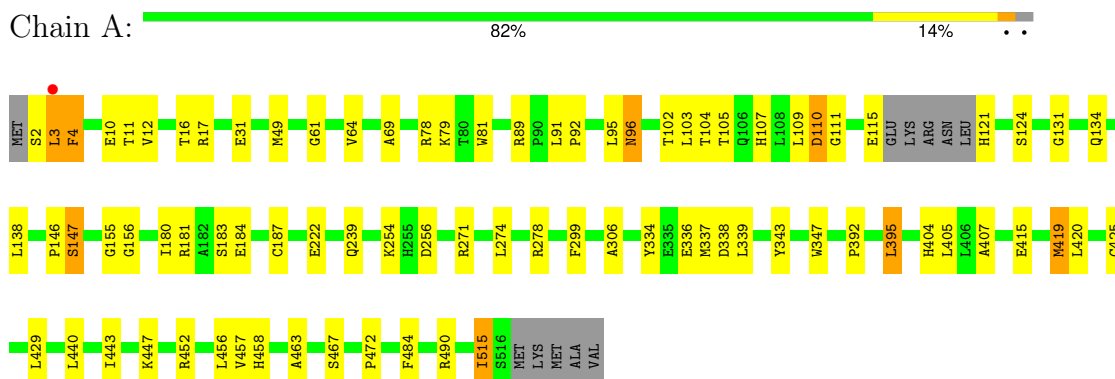
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	43	Total 43	O 43	0	0
6	B	45	Total 45	O 45	0	0
6	C	56	Total 56	O 56	0	0
6	D	46	Total 46	O 46	0	0



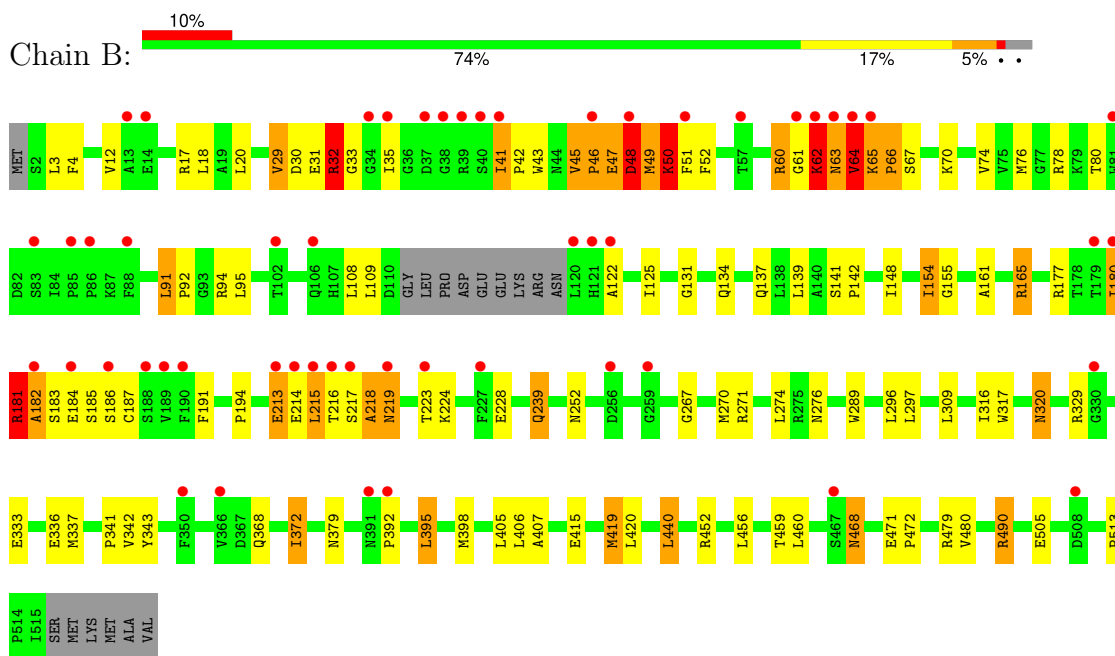
### 3 Residue-property plots [i](#)

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

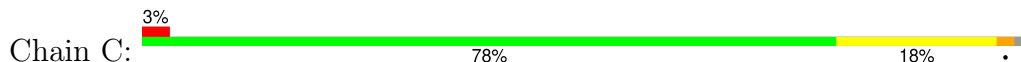
- Molecule 1: Dihydrofolate reductase-thymidylate synthase

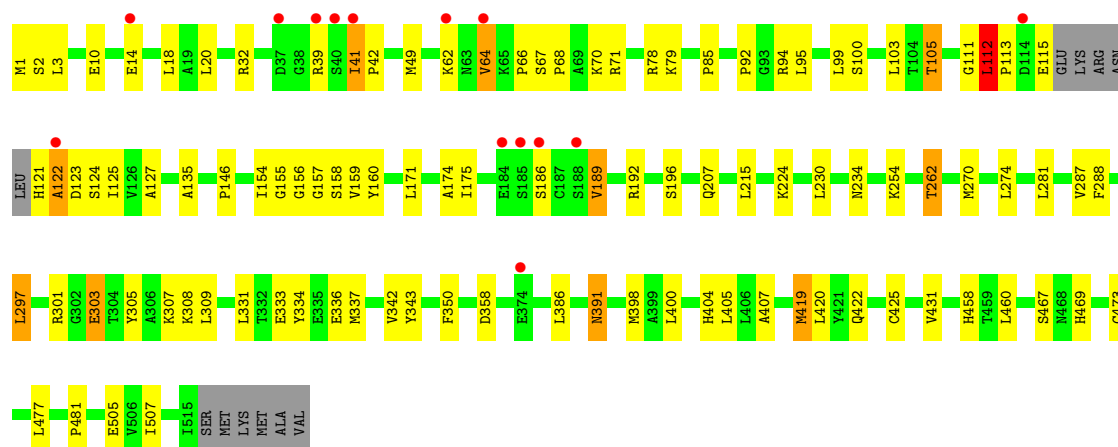


- Molecule 1: Dihydrofolate reductase-thymidylate synthase

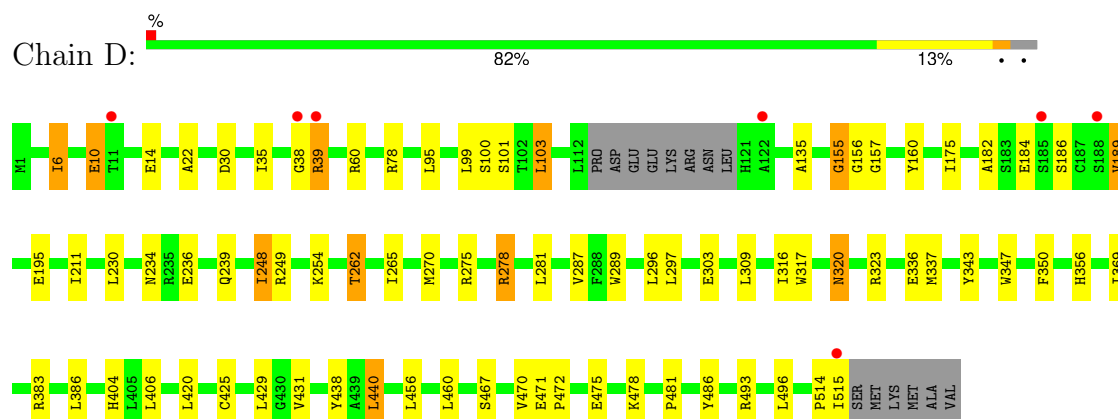


- Molecule 1: Dihydrofolate reductase-thymidylate synthase





• Molecule 1: Dihydrofolate reductase-thymidylate synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	176.57Å 176.57Å 251.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 3.00 19.94 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.1 (19.94-3.00) 96.7 (19.94-3.00)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.16 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.5.0053	Depositor
R, $R_{free}$	0.201 , 0.239 0.204 , 0.242	Depositor DCC
$R_{free}$ test set	3898 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.9	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 56.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	16812	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.99% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, TMQ, SO4, EDO

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	0.47	0/4150	0.83	3/5632 (0.1%)
1	B	0.51	0/4106	0.85	2/5572 (0.0%)
1	C	0.52	0/4146	0.82	6/5626 (0.1%)
1	D	0.48	0/4120	0.78	1/5590 (0.0%)
All	All	0.50	0/16522	0.82	12/22420 (0.1%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	45	VAL	C-N-CD	-15.90	59.82	125.00
1	B	48	ASP	N-CA-C	-7.71	102.81	111.14
1	D	155	GLY	N-CA-C	7.10	121.82	111.24
1	A	155	GLY	N-CA-C	7.00	121.66	111.24
1	A	111	GLY	N-CA-C	-6.06	107.48	114.69

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	4052	0	4000	46	4
1	B	4010	0	3959	126	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4049	0	4002	61	0
1	D	4023	0	3973	47	4
2	A	48	0	25	5	0
2	B	48	0	25	6	0
2	C	48	0	25	9	0
2	D	48	0	25	10	0
3	A	27	0	24	8	0
3	B	27	0	24	4	0
3	C	27	0	24	6	0
3	D	27	0	24	8	0
4	A	30	0	0	0	0
4	B	25	0	0	0	0
4	C	45	0	0	0	0
4	D	40	0	0	0	0
5	A	8	0	12	0	0
5	B	4	0	6	1	0
5	C	16	0	24	2	0
5	D	20	0	30	2	0
6	A	43	0	0	0	0
6	B	45	0	0	5	0
6	C	56	0	0	3	0
6	D	46	0	0	1	0
All	All	16812	0	16202	300	4

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 9.

The worst 5 of 300 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:47:GLU:CG	1:B:217:SER:OG	1.75	1.33
1:B:64:VAL:CG2	1:B:66:PRO:HD3	1.62	1.29
1:B:47:GLU:HG3	1:B:217:SER:OG	1.02	1.19
1:B:180:ILE:HG23	1:B:181:ARG:N	1.54	1.14
1:B:64:VAL:CG2	1:B:65:LYS:N	2.12	1.13

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LEU:CG	1:D:39:ARG:CB[4_555]	1.85	0.35
1:A:3:LEU:CD1	1:D:39:ARG:CB[4_555]	2.05	0.15
1:A:3:LEU:CD2	1:D:39:ARG:CB[4_555]	2.14	0.06
1:A:3:LEU:CD2	1:D:39:ARG:CG[4_555]	2.18	0.02

## 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	506/521 (97%)	490 (97%)	13 (3%)	3 (1%)	22	57
1	B	501/521 (96%)	458 (91%)	24 (5%)	19 (4%)	2	15
1	C	506/521 (97%)	473 (94%)	25 (5%)	8 (2%)	8	34
1	D	503/521 (96%)	484 (96%)	18 (4%)	1 (0%)	44	77
All	All	2016/2084 (97%)	1905 (94%)	80 (4%)	31 (2%)	8	36

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	343	TYR
1	B	46	PRO
1	B	60	ARG
1	B	62	LYS
1	B	65	LYS

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	436/446 (98%)	411 (94%)	25 (6%)	17	49
1	B	430/446 (96%)	391 (91%)	39 (9%)	7	30
1	C	435/446 (98%)	414 (95%)	21 (5%)	21	55
1	D	431/446 (97%)	405 (94%)	26 (6%)	16	47
All	All	1732/1784 (97%)	1621 (94%)	111 (6%)	14	44

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

Mol	Chain	Res	Type
1	B	419	MET
1	D	493	ARG
1	C	112	LEU
1	D	475	GLU
1	D	297	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	137	GLN
1	C	360	ASN
1	D	422	GLN
1	C	170	HIS
1	C	239	GLN

### 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

48 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	SO4	D	704	-	4,4,4	0.21	0	6,6,6	0.18	0
4	SO4	D	820	-	4,4,4	0.26	0	6,6,6	0.17	0
4	SO4	A	817	-	4,4,4	0.23	0	6,6,6	0.11	0
5	EDO	B	906	-	3,3,3	0.46	0	2,2,2	0.40	0
4	SO4	D	801	-	4,4,4	0.25	0	6,6,6	0.09	0
4	SO4	B	809	-	4,4,4	0.23	0	6,6,6	0.11	0
2	NAP	C	603	-	46,52,52	1.44	8 (17%)	61,80,80	2.73	17 (27%)
4	SO4	C	802	-	4,4,4	0.24	0	6,6,6	0.12	0
4	SO4	C	816	-	4,4,4	0.24	0	6,6,6	0.23	0
4	SO4	B	818	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	C	812	-	4,4,4	0.24	0	6,6,6	0.14	0
5	EDO	C	909	-	3,3,3	0.45	0	2,2,2	0.33	0
3	TMQ	C	613	-	29,29,29	1.50	4 (13%)	39,41,41	2.03	7 (17%)
5	EDO	D	903	-	3,3,3	0.42	0	2,2,2	0.36	0
2	NAP	D	604	-	46,52,52	1.44	9 (19%)	61,80,80	2.75	19 (31%)
4	SO4	B	823	-	4,4,4	0.22	0	6,6,6	0.11	0
4	SO4	C	807	-	4,4,4	0.23	0	6,6,6	0.09	0
4	SO4	D	804	-	4,4,4	0.22	0	6,6,6	0.13	0
4	SO4	A	813	-	4,4,4	0.26	0	6,6,6	0.11	0
4	SO4	A	805	-	4,4,4	0.26	0	6,6,6	0.06	0
4	SO4	D	811	-	4,4,4	0.24	0	6,6,6	0.13	0
5	EDO	C	908	-	3,3,3	0.46	0	2,2,2	0.37	0
4	SO4	D	803	-	4,4,4	0.24	0	6,6,6	0.09	0
2	NAP	B	602	-	46,52,52	1.53	7 (15%)	61,80,80	2.48	14 (22%)
5	EDO	D	901	-	3,3,3	0.41	0	2,2,2	0.38	0
4	SO4	A	814	-	4,4,4	0.24	0	6,6,6	0.12	0
4	SO4	B	821	-	4,4,4	0.24	0	6,6,6	0.08	0
5	EDO	D	911	-	3,3,3	0.39	0	2,2,2	0.47	0
4	SO4	B	806	-	4,4,4	0.25	0	6,6,6	0.19	0
4	SO4	A	701	-	4,4,4	0.23	0	6,6,6	0.28	0
4	SO4	C	822	-	4,4,4	0.23	0	6,6,6	0.14	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	A	904	-	3,3,3	0.40	0	2,2,2	0.41	0
4	SO4	D	810	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	C	824	-	4,4,4	0.23	0	6,6,6	0.17	0
4	SO4	D	819	-	4,4,4	0.22	0	6,6,6	0.15	0
4	SO4	C	703	-	4,4,4	0.26	0	6,6,6	0.26	0
3	TMQ	A	611	-	29,29,29	1.50	4 (13%)	39,41,41	2.02	7 (17%)
2	NAP	A	601	-	46,52,52	1.52	7 (15%)	61,80,80	2.48	14 (22%)
4	SO4	A	815	-	4,4,4	0.24	0	6,6,6	0.09	0
5	EDO	A	902	-	3,3,3	0.49	0	2,2,2	0.26	0
5	EDO	C	912	-	3,3,3	0.52	0	2,2,2	0.17	0
4	SO4	C	808	-	4,4,4	0.24	0	6,6,6	0.11	0
5	EDO	C	910	-	3,3,3	0.44	0	2,2,2	0.39	0
5	EDO	D	905	-	3,3,3	0.45	0	2,2,2	0.29	0
5	EDO	D	907	-	3,3,3	0.38	0	2,2,2	0.56	0
3	TMQ	D	614	-	29,29,29	1.50	4 (13%)	39,41,41	2.02	7 (17%)
4	SO4	C	702	-	4,4,4	0.29	0	6,6,6	0.21	0
3	TMQ	B	612	-	29,29,29	1.50	4 (13%)	39,41,41	2.02	7 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	906	-	-	0/1/1/1	-
5	EDO	C	909	-	-	1/1/1/1	-
2	NAP	C	603	-	-	4/31/67/67	0/5/5/5
5	EDO	D	903	-	-	0/1/1/1	-
3	TMQ	C	613	-	-	2/11/11/11	0/3/3/3
2	NAP	D	604	-	-	6/31/67/67	0/5/5/5
5	EDO	C	908	-	-	1/1/1/1	-
2	NAP	B	602	-	-	4/31/67/67	0/5/5/5
5	EDO	D	901	-	-	0/1/1/1	-
5	EDO	D	911	-	-	1/1/1/1	-
5	EDO	A	904	-	-	1/1/1/1	-
3	TMQ	A	611	-	-	4/11/11/11	0/3/3/3
2	NAP	A	601	-	-	10/31/67/67	0/5/5/5
5	EDO	A	902	-	-	0/1/1/1	-
5	EDO	C	912	-	-	1/1/1/1	-
5	EDO	D	905	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	C	910	-	-	1/1/1/1	-
3	TMQ	D	614	-	-	7/11/11/11	0/3/3/3
5	EDO	D	907	-	-	1/1/1/1	-
3	TMQ	B	612	-	-	4/11/11/11	0/3/3/3

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	NAP	PA-O3	5.60	1.65	1.59
2	B	602	NAP	PA-O3	5.57	1.65	1.59
3	A	611	TMQ	C17-C5	-5.09	1.39	1.51
3	B	612	TMQ	C17-C5	-5.07	1.39	1.51
3	D	614	TMQ	C17-C5	-5.06	1.39	1.51

The worst 5 of 92 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	603	NAP	O2N-PN-O3	-11.07	77.34	107.27
2	D	604	NAP	O2N-PN-O3	-9.58	81.39	107.27
2	A	601	NAP	O3-PN-O1N	-7.85	87.08	110.70
2	B	602	NAP	O3-PN-O1N	-7.84	87.11	110.70
2	C	603	NAP	O5B-PA-O1A	-7.50	79.20	108.94

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	NAP	C5D-O5D-PN-O1N
2	D	604	NAP	C5D-O5D-PN-O1N
2	D	604	NAP	O4D-C1D-N1N-C6N
3	D	614	TMQ	C14-C15-O20-C23
3	B	612	TMQ	C12-C11-N10-C9

There are no ring outliers.

12 monomers are involved in 58 short contacts:

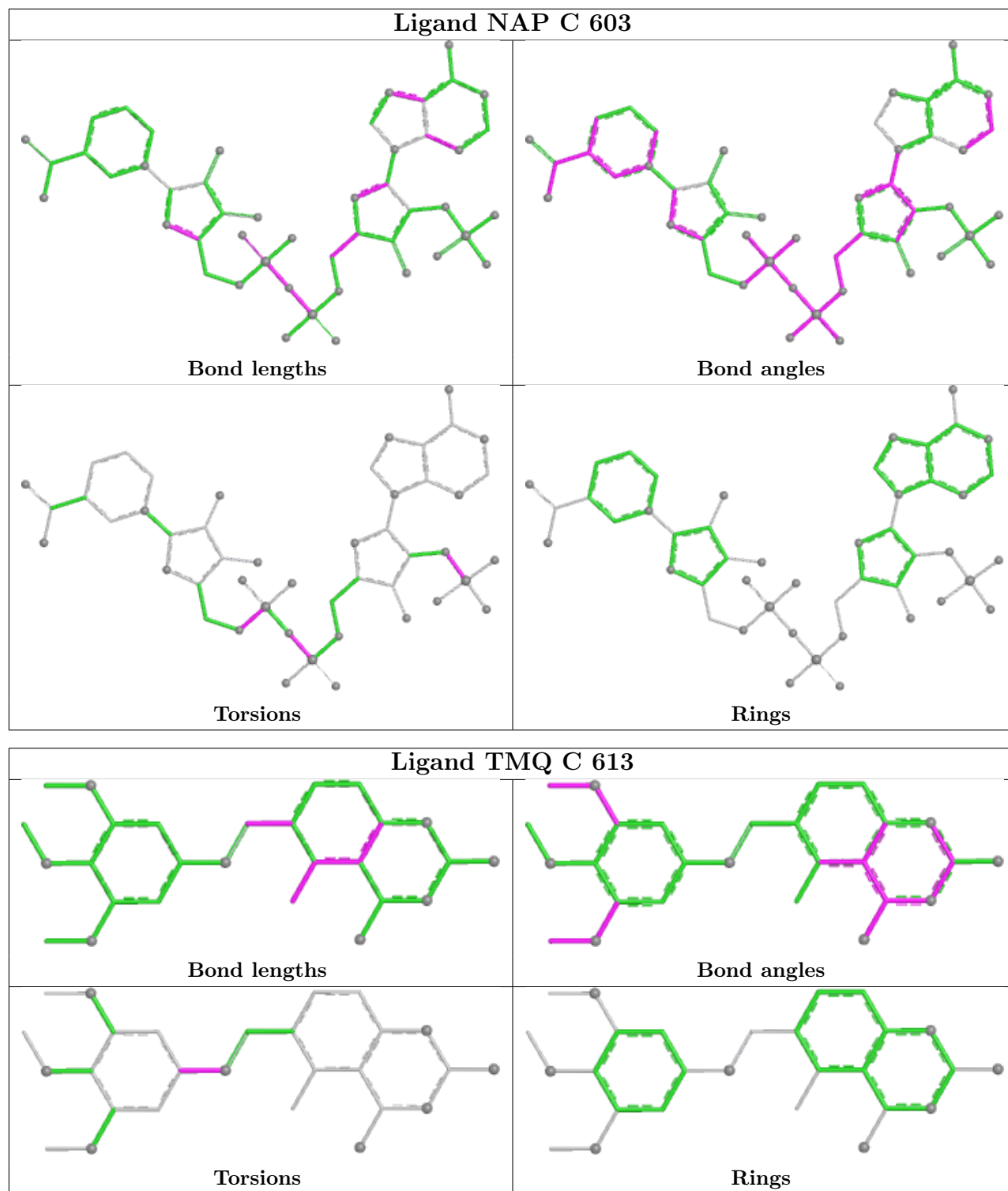
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	906	EDO	1	0
2	C	603	NAP	9	0
5	C	909	EDO	1	0

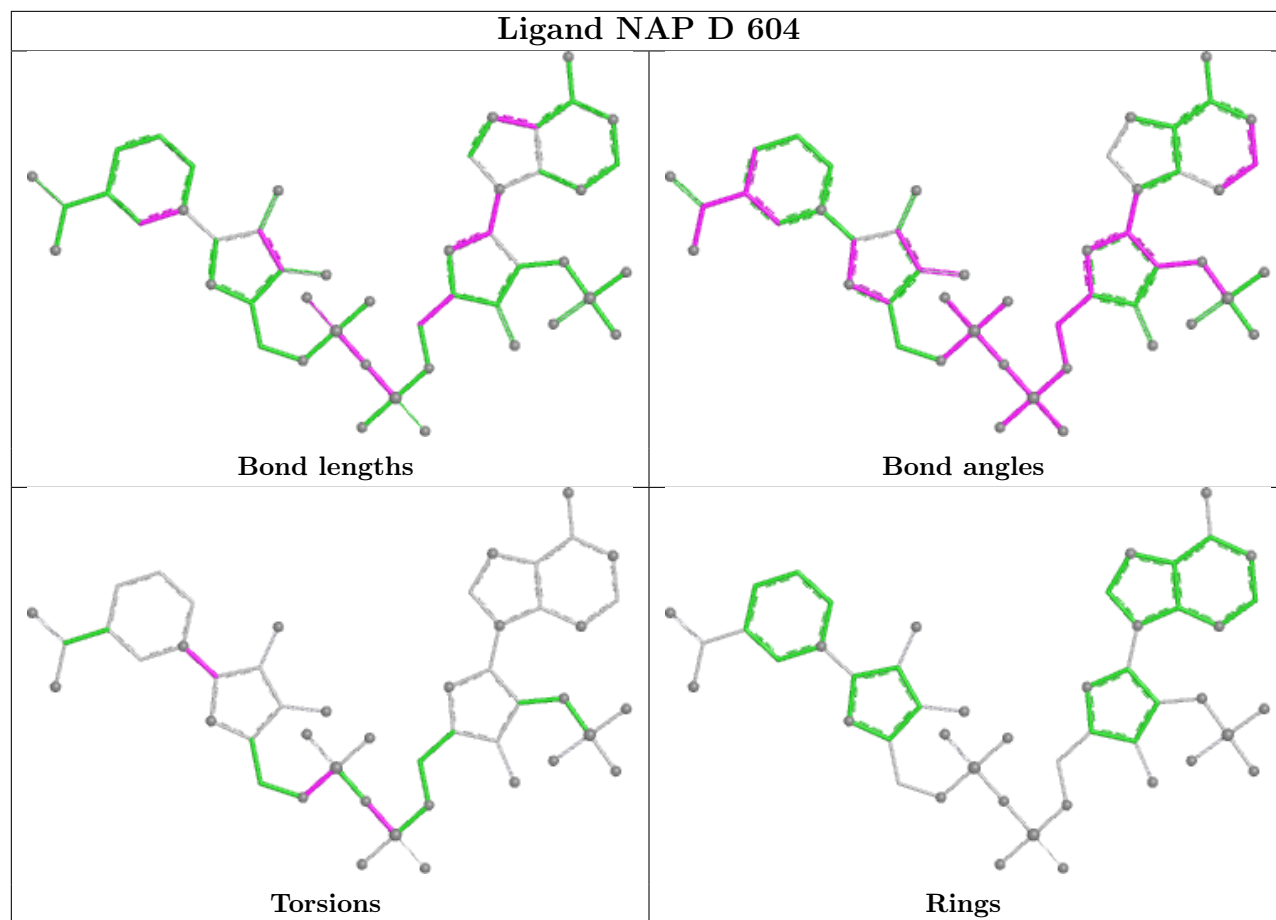
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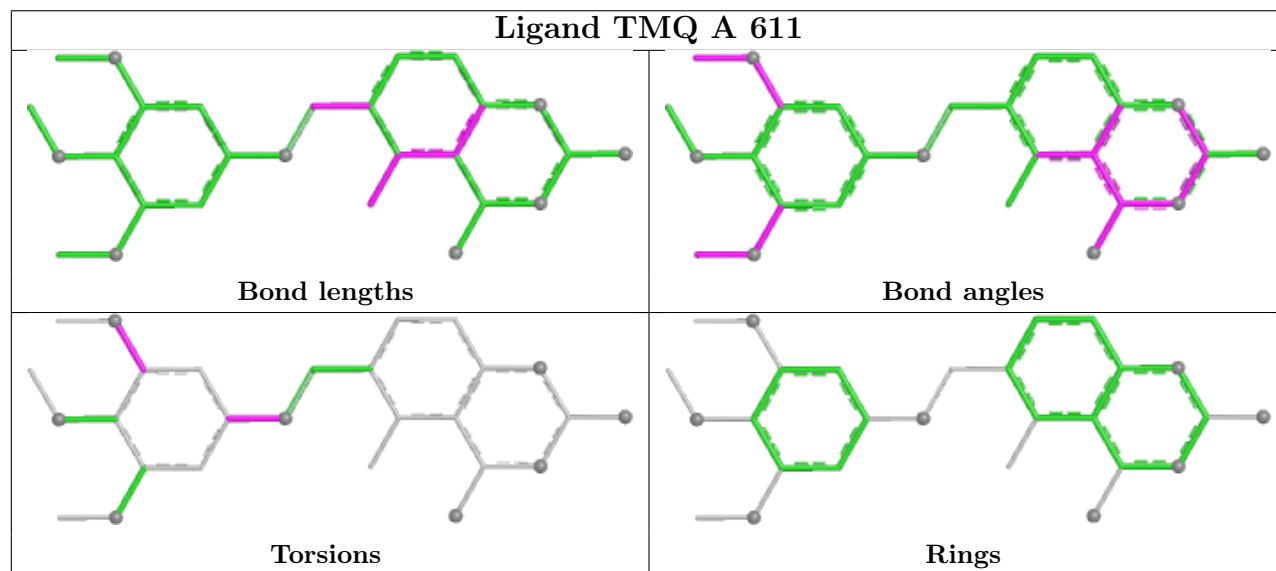
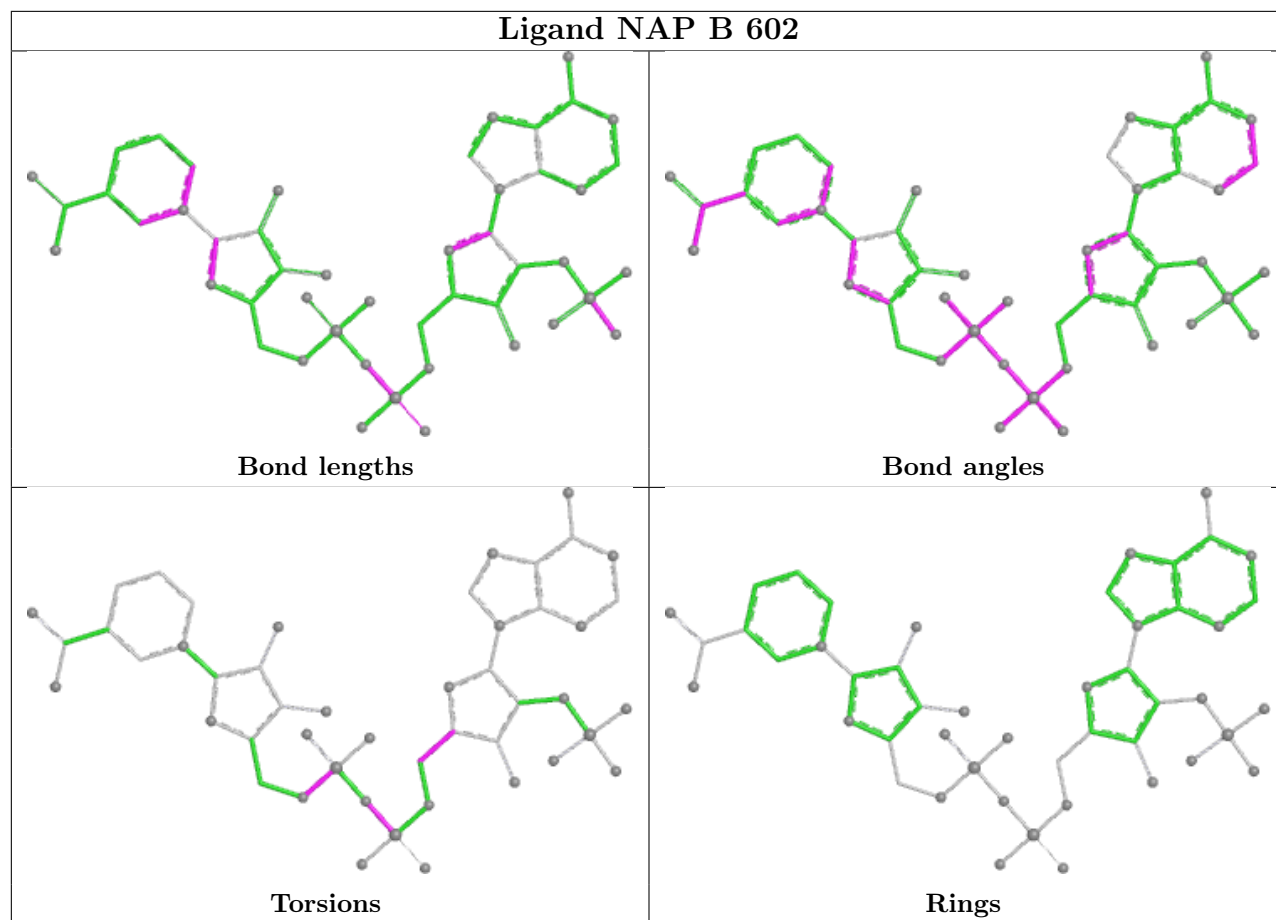
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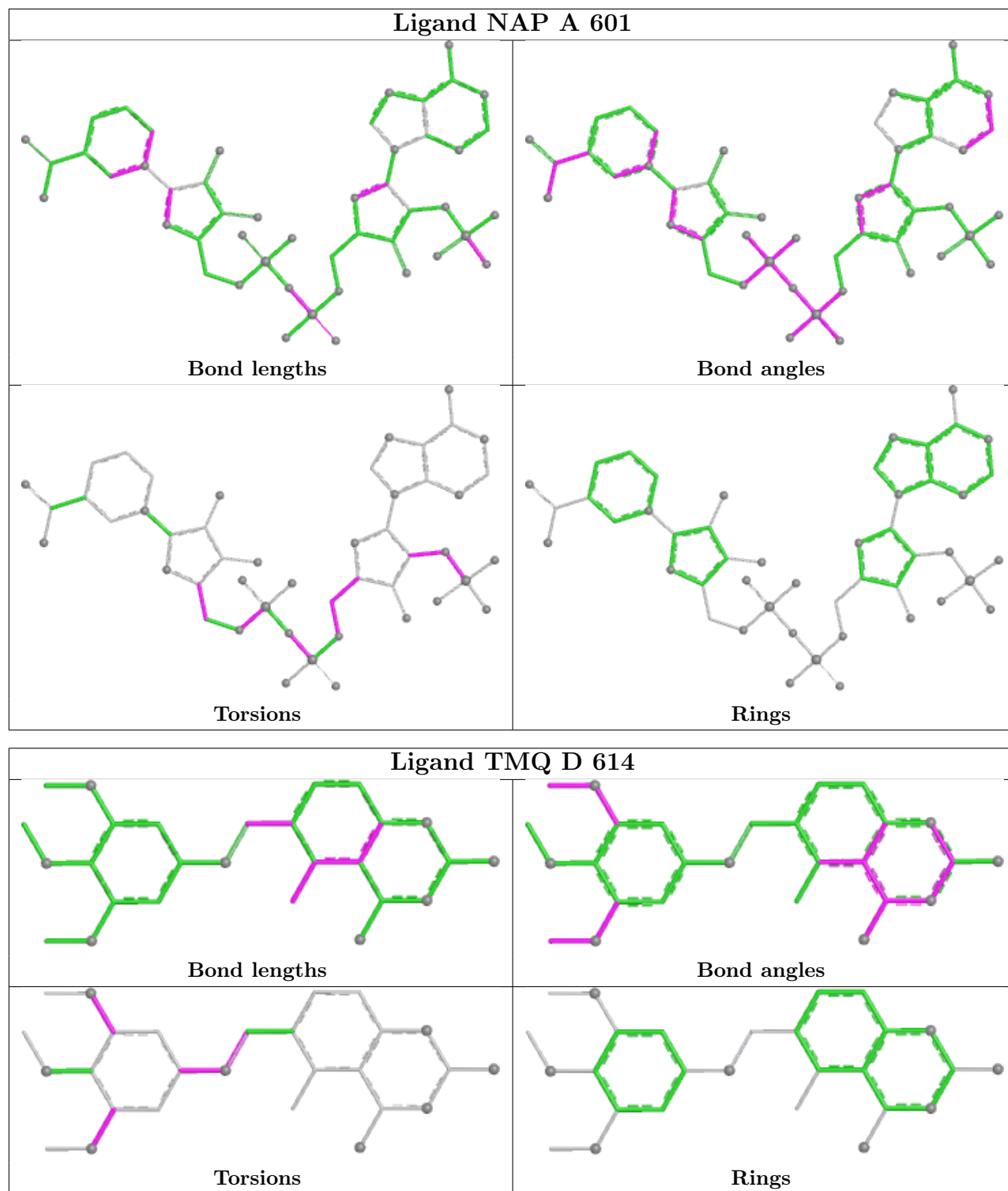
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	613	TMQ	6	0
2	D	604	NAP	10	0
2	B	602	NAP	6	0
5	D	901	EDO	2	0
3	A	611	TMQ	8	0
2	A	601	NAP	5	0
5	C	910	EDO	1	0
3	D	614	TMQ	8	0
3	B	612	TMQ	4	0

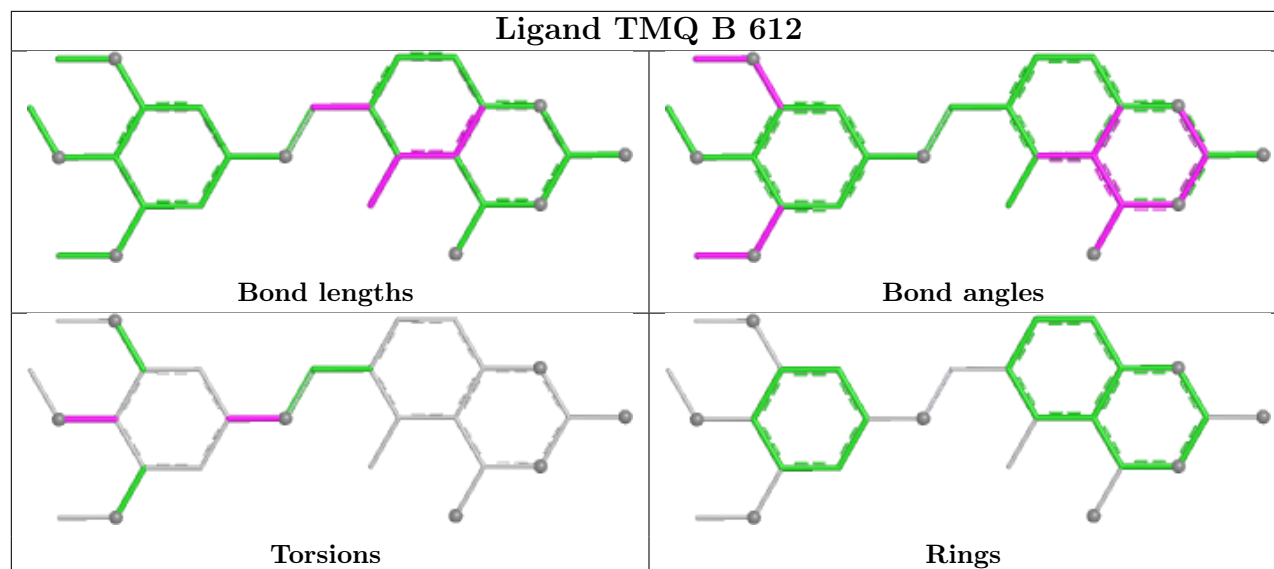
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	510/521 (97%)	-0.32	1 (0%) 92 84	25, 38, 50, 57	0
1	B	505/521 (96%)	0.58	53 (10%) 13 7	27, 37, 54, 62	0
1	C	510/521 (97%)	-0.13	14 (2%) 56 34	22, 35, 49, 61	0
1	D	507/521 (97%)	-0.30	7 (1%) 73 52	25, 37, 51, 56	0
All	All	2032/2084 (97%)	-0.04	75 (3%) 45 27	22, 37, 51, 62	0

The worst 5 of 75 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	40	SER	5.7
1	B	41	ILE	4.6
1	B	180	ILE	4.1
1	B	102	THR	4.0
1	B	83	SER	4.0

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

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

### 6.3 Carbohydrates [i](#)

There are no 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

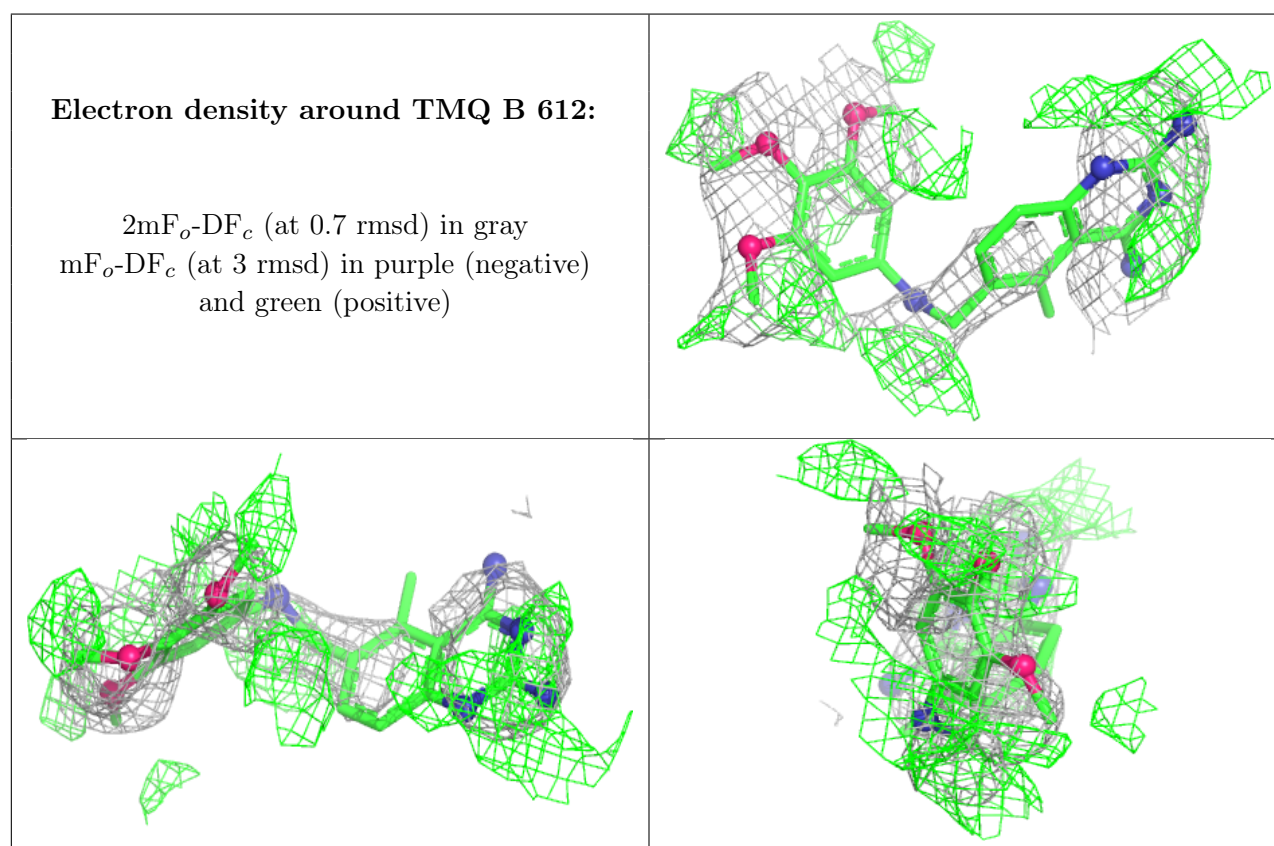
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	D	820	5/5	0.65	0.14	106,106,107,107	0
4	SO4	C	816	5/5	0.69	0.17	106,106,107,107	0
4	SO4	C	807	5/5	0.69	0.13	149,149,149,149	0
4	SO4	B	823	5/5	0.70	0.19	111,111,111,111	0
3	TMQ	B	612	27/27	0.70	0.34	60,61,61,62	27
4	SO4	B	821	5/5	0.71	0.15	121,121,121,121	0
4	SO4	D	810	5/5	0.74	0.12	134,134,134,134	0
4	SO4	C	824	5/5	0.74	0.22	107,107,107,107	0
2	NAP	B	602	48/48	0.75	0.22	74,75,76,76	48
4	SO4	C	812	5/5	0.75	0.14	131,131,131,131	0
4	SO4	D	803	5/5	0.76	0.15	119,119,119,120	0
4	SO4	C	822	5/5	0.76	0.20	139,139,140,140	0
4	SO4	A	805	5/5	0.76	0.13	106,106,106,106	0
4	SO4	A	814	5/5	0.77	0.20	122,122,122,123	0
3	TMQ	D	614	27/27	0.79	0.17	68,70,75,76	0
4	SO4	D	811	5/5	0.80	0.15	137,137,137,137	0
4	SO4	D	801	5/5	0.80	0.16	109,109,109,109	0
5	EDO	C	912	4/4	0.80	0.18	65,66,67,67	0
5	EDO	C	909	4/4	0.81	0.17	74,75,75,75	0
4	SO4	B	806	5/5	0.81	0.18	108,109,109,109	0
4	SO4	D	819	5/5	0.82	0.12	125,125,125,125	0
4	SO4	A	815	5/5	0.82	0.13	128,128,128,128	0
5	EDO	B	906	4/4	0.83	0.16	67,67,68,68	0
2	NAP	A	601	48/48	0.84	0.14	69,71,74,74	0
4	SO4	B	809	5/5	0.84	0.19	123,123,124,124	0
4	SO4	A	817	5/5	0.84	0.11	100,100,100,100	0
2	NAP	C	603	48/48	0.87	0.14	73,79,84,84	0
2	NAP	D	604	48/48	0.88	0.13	89,91,96,97	0
4	SO4	B	818	5/5	0.88	0.15	121,121,121,121	0
3	TMQ	C	613	27/27	0.88	0.13	53,57,62,64	0
5	EDO	C	910	4/4	0.89	0.16	46,48,49,52	0
3	TMQ	A	611	27/27	0.89	0.12	53,56,62,63	0
5	EDO	D	907	4/4	0.90	0.16	57,58,58,60	0
4	SO4	D	804	5/5	0.91	0.17	92,92,92,92	0
4	SO4	C	802	5/5	0.91	0.11	88,89,89,89	0
4	SO4	C	808	5/5	0.91	0.24	106,106,106,106	0
5	EDO	D	905	4/4	0.91	0.11	68,68,68,68	0
5	EDO	C	908	4/4	0.91	0.12	55,56,56,57	0
4	SO4	A	813	5/5	0.92	0.14	104,104,104,104	0
5	EDO	D	903	4/4	0.93	0.14	51,51,52,53	0
5	EDO	A	902	4/4	0.93	0.18	63,64,65,65	0
5	EDO	D	901	4/4	0.93	0.12	45,46,46,48	0
4	SO4	D	704	5/5	0.94	0.08	71,72,72,72	0

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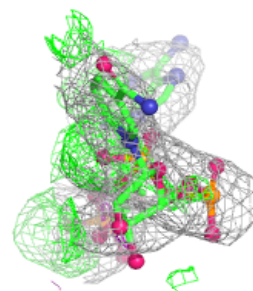
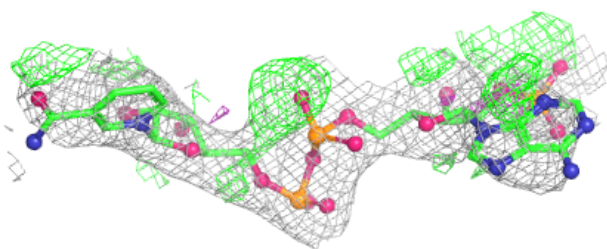
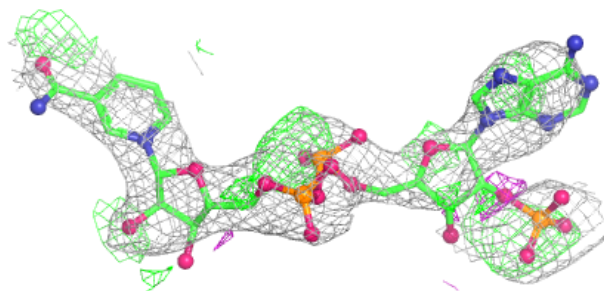
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	D	911	4/4	0.94	0.14	64,64,64,64	0
4	SO4	C	703	5/5	0.95	0.07	62,63,63,63	0
5	EDO	A	904	4/4	0.96	0.10	50,50,50,51	0
4	SO4	A	701	5/5	0.97	0.07	64,64,64,65	0
4	SO4	C	702	5/5	0.98	0.06	58,59,60,60	0

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

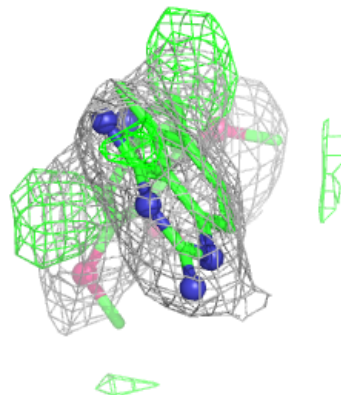
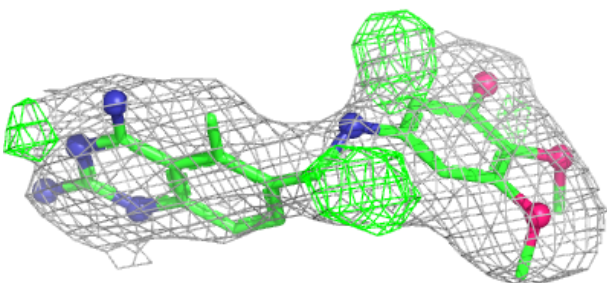
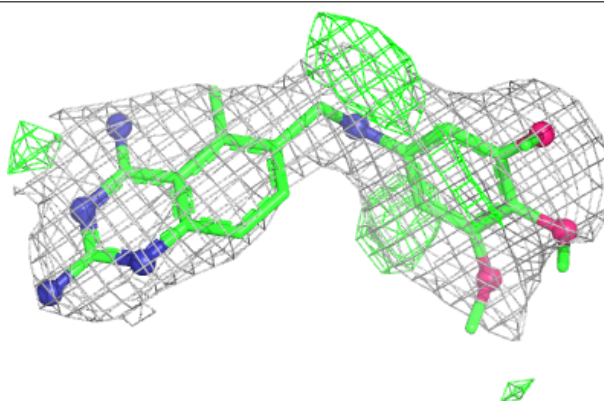


**Electron density around NAP B 602:**

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

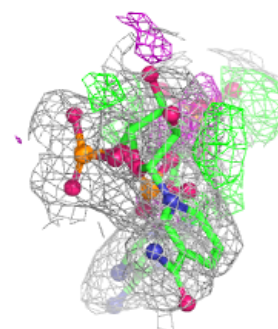
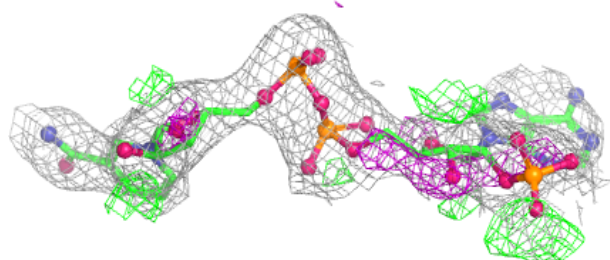
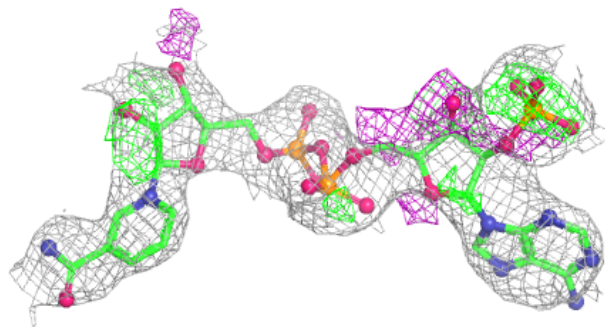
**Electron density around TMQ D 614:**

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

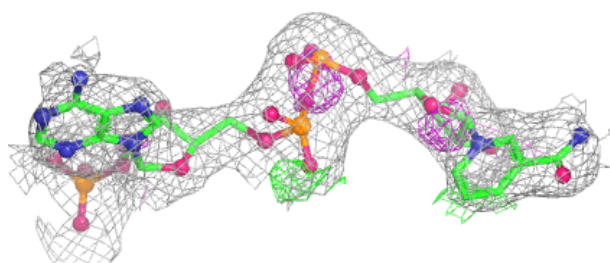
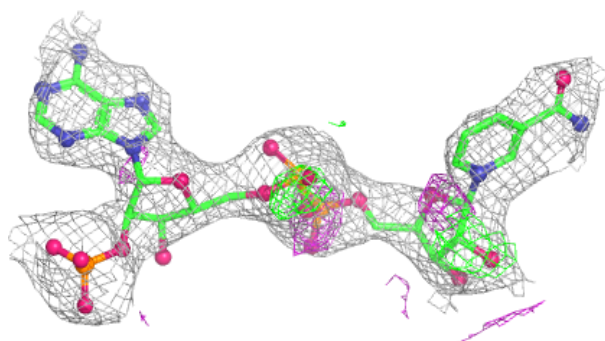


**Electron density around NAP A 601:**

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

**Electron density around NAP C 603:**

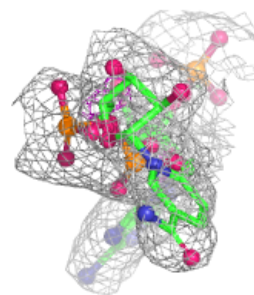
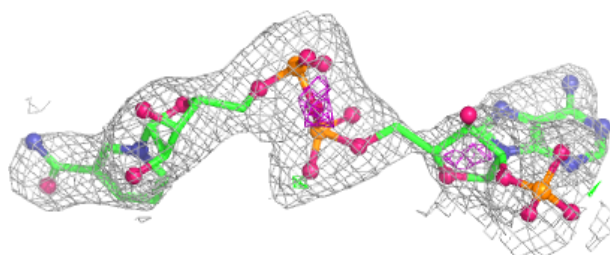
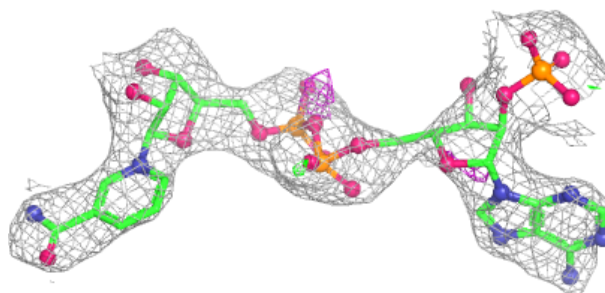
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



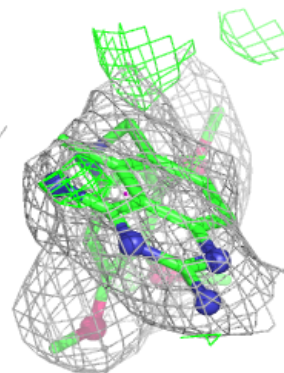
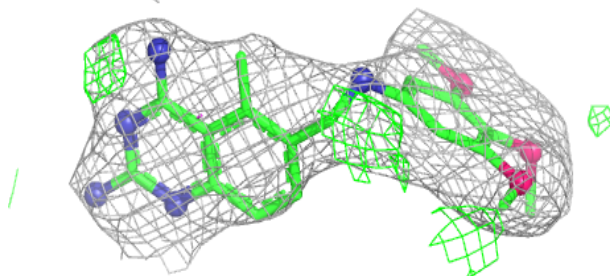
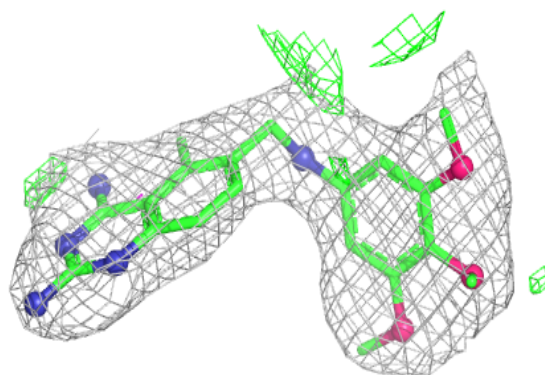


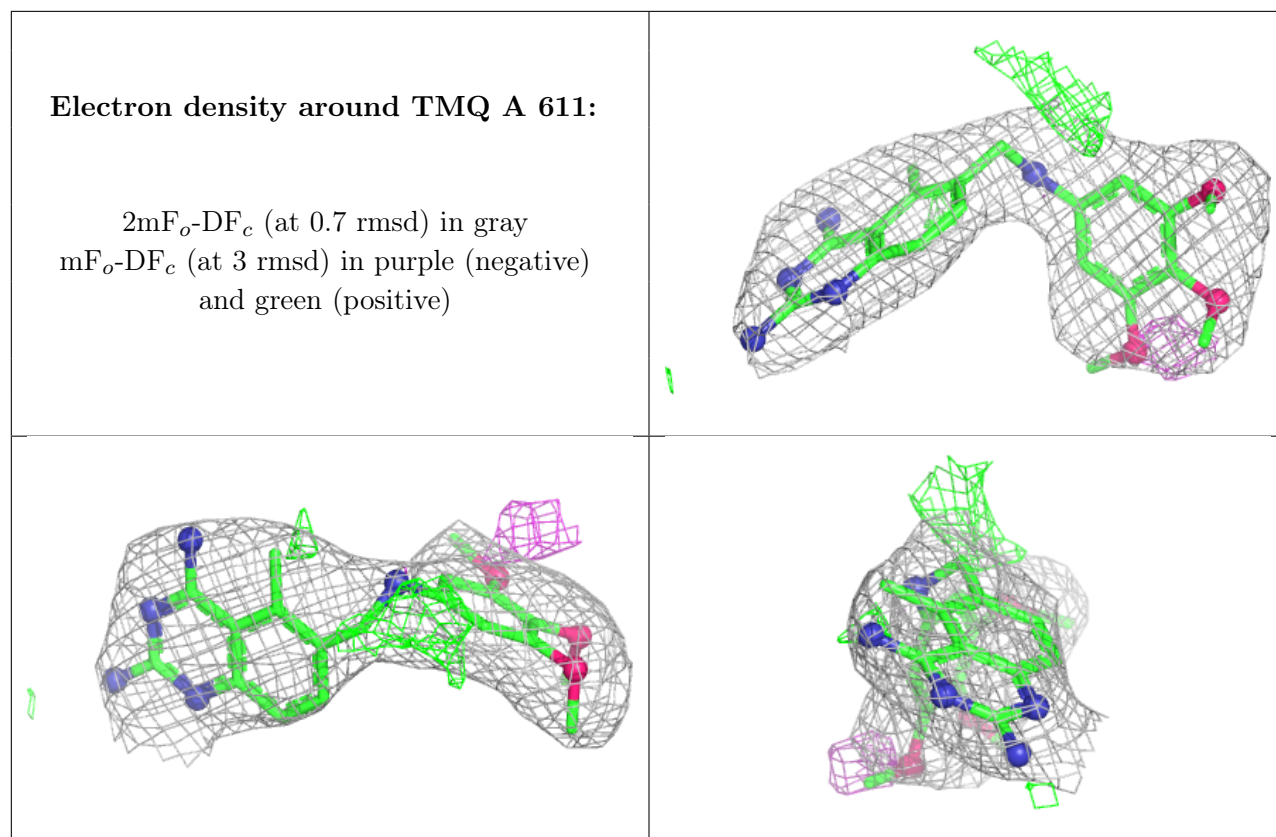
**Electron density around NAP D 604:**

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

**Electron density around TMQ C 613:**

$2mF_o-DF_c$  (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.