



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 07:28 am BST

PDB ID : 4FJ2  
Title : Crystal structure of the ternary complex between a fungal 17beta-hydroxysteroid dehydrogenase (Holo form) and biochanin A  
Authors : Cassetta, A.; Lamba, D.; Krastanova, I.  
Deposited on : 2012-06-11  
Resolution : 2.50 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

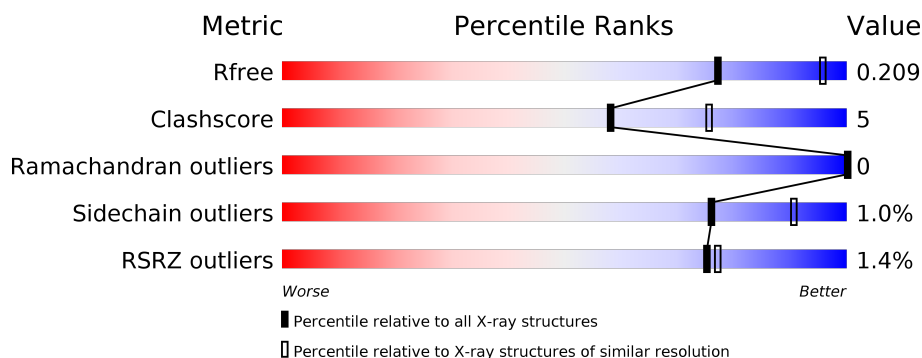
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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  $\geq 3$ , 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	270	<div> <div>2%</div> <div>88%</div> <div>8%</div> <div>.</div> </div>
1	B	270	<div> <div>2%</div> <div>87%</div> <div>9%</div> <div>.</div> </div>
1	C	270	<div> <div>2%</div> <div>86%</div> <div>9%</div> <div>.</div> </div>
1	D	270	<div> <div>87%</div> <div>9%</div> <div>..</div> </div>

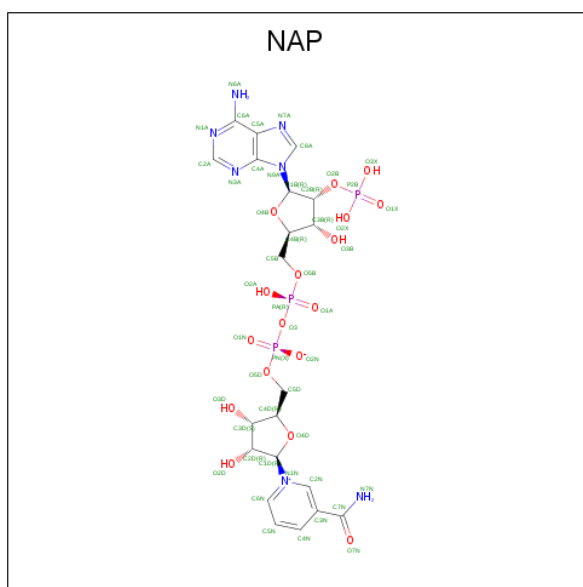


In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 17beta-hydroxysteroid dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total 1964	C 1236	N 353	O 372	S 3	0	0	0
1	B	260	Total 1980	C 1245	N 355	O 376	S 4	0	2	0
1	C	258	Total 1944	C 1221	N 351	O 369	S 3	0	0	0
1	D	261	Total 1971	C 1240	N 354	O 374	S 3	0	0	0

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



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

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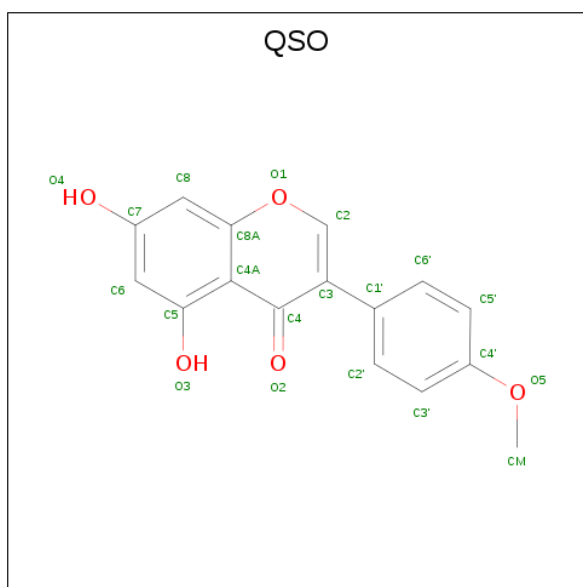
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 4 is 5,7-dihydroxy-3-(4-methoxyphenyl)-4H-chromen-4-one (three-letter code: QSO) (formula: C<sub>16</sub>H<sub>12</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	1
			42	32	10		
4	D	1	Total	C	O	0	0
			21	16	5		

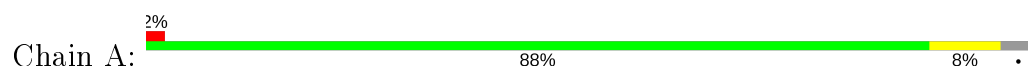
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	29	Total	O	0	0
			29	29		
5	B	51	Total	O	0	0
			51	51		
5	C	54	Total	O	0	0
			54	54		
5	D	63	Total	O	0	0
			63	63		

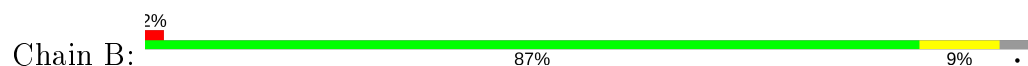
### 3 Residue-property plots [i](#)

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

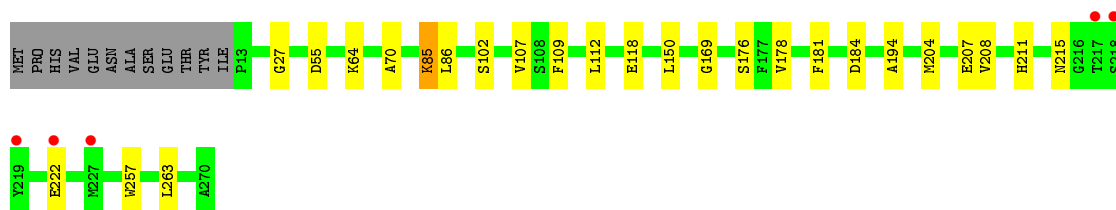
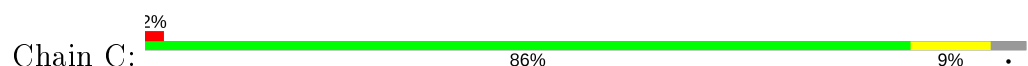
- Molecule 1: 17beta-hydroxysteroid dehydrogenase



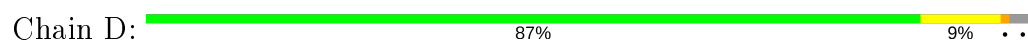
- Molecule 1: 17beta-hydroxysteroid dehydrogenase



- Molecule 1: 17beta-hydroxysteroid dehydrogenase



- Molecule 1: 17beta-hydroxysteroid dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.43 Å 115.28 Å 69.60 Å 90.00° 102.93° 90.00°	Depositor
Resolution (Å)	33.43 – 2.50 33.43 – 2.30	Depositor EDS
% Data completeness (in resolution range)	81.3 (33.43-2.50) 76.7 (33.43-2.30)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.50 (at 2.29 Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.166 , 0.208 0.171 , 0.209	Depositor DCC
$R_{free}$ test set	1635 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.6	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 28.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8331	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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, QSO, 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	0.57	0/2003	0.67	1/2710 (0.0%)
1	B	0.58	0/2019	0.64	0/2731
1	C	0.59	1/1982 (0.1%)	0.66	0/2680
1	D	0.60	0/2010	0.66	0/2720
All	All	0.59	1/8014 (0.0%)	0.66	1/10841 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	257	TRP	CD2-CE2	5.14	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	VAL	CB-CA-C	-5.19	101.53	111.40

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	1964	0	1945	18	0
1	B	1980	0	1957	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1944	0	1926	17	0
1	D	1971	0	1952	26	0
2	A	48	0	25	0	0
2	B	48	0	25	1	0
2	C	48	0	25	0	0
2	D	48	0	25	0	0
3	A	4	0	6	0	0
3	B	4	0	6	0	0
3	C	8	0	12	0	0
3	D	4	0	6	0	0
4	B	42	0	21	4	0
4	D	21	0	11	5	0
5	A	29	0	0	0	0
5	B	51	0	0	1	0
5	C	54	0	0	0	0
5	D	63	0	0	1	0
All	All	8331	0	7942	77	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 5.

All (77) 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:107:VAL:HB	4:B:302[B]:QSO:HM2	1.46	0.97
1:D:107:VAL:HB	4:D:302:QSO:HM2	1.51	0.92
1:C:207:GLU:HG3	1:C:208:VAL:HG13	1.59	0.84
1:D:107:VAL:HG12	1:D:204:MET:HE2	1.63	0.80
1:A:12:ILE:HG23	1:A:13:PRO:HD2	1.63	0.80
1:B:12:ILE:HG21	1:D:12:ILE:HG23	1.76	0.66
1:A:157:LYS:HE3	1:B:157:LYS:HE3	1.80	0.62
1:D:220:THR:HG22	1:D:222:GLU:N	2.15	0.62
1:A:102:SER:HB3	1:A:150:LEU:HD22	1.84	0.60
1:D:102:SER:HB3	1:D:150:LEU:HD22	1.83	0.59
1:C:204:MET:O	1:C:208:VAL:HG22	2.01	0.59
1:D:131:GLN:HB3	1:D:150:LEU:HD13	1.86	0.58
1:A:157:LYS:HE3	1:B:157:LYS:CE	2.33	0.57
1:B:227:MET:HE3	4:B:302[A]:QSO:HM2	1.86	0.57
1:C:112:LEU:HD13	1:D:181:PHE:CE1	2.40	0.56
1:A:12:ILE:CG2	1:A:13:PRO:HD2	2.35	0.56
1:B:107:VAL:HG11	1:B:208:VAL:HG11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:GLN:HB3	1:A:150:LEU:HD13	1.89	0.55
1:D:205:PHE:HA	4:D:302:QSO:H2'	1.87	0.55
1:A:40:ARG:HA	1:A:66:LEU:HD13	1.88	0.55
1:D:71:ILE:HG12	1:D:93:HIS:CD2	2.43	0.54
1:B:204[A]:MET:O	1:B:208:VAL:HG22	2.07	0.54
1:C:107:VAL:HG11	1:C:208:VAL:HG11	1.90	0.52
1:D:107:VAL:CG1	1:D:204:MET:HE2	2.36	0.50
1:A:157:LYS:CE	1:B:157:LYS:HE3	2.39	0.50
1:B:204[B]:MET:O	1:B:208:VAL:HG22	2.09	0.50
1:C:178:VAL:HG11	1:C:194:ALA:HB2	1.93	0.49
1:B:12:ILE:HG21	1:D:12:ILE:HD12	1.94	0.49
1:C:181:PHE:CE1	1:D:112:LEU:HD13	2.48	0.48
1:D:120:PHE:HA	1:D:166:LEU:HD21	1.95	0.48
1:B:204[B]:MET:CE	1:B:207:GLU:OE2	2.62	0.47
1:B:178:VAL:HG11	1:B:194:ALA:HB2	1.97	0.47
1:A:12:ILE:HB	1:A:15:ARG:HD3	1.96	0.46
1:B:213:ILE:HD13	1:B:227:MET:HE2	1.97	0.46
1:C:263:LEU:HD12	1:C:263:LEU:N	2.30	0.46
1:C:169:GLY:HA2	1:D:176:SER:HB2	1.98	0.46
1:D:220:THR:HG22	1:D:222:GLU:H	1.79	0.45
1:C:102:SER:HB3	1:C:150:LEU:HD22	1.99	0.45
1:B:12:ILE:CG2	1:D:12:ILE:HG23	2.45	0.45
1:B:213:ILE:CG2	1:B:227:MET:HE1	2.47	0.45
1:B:213:ILE:HG23	1:B:227:MET:HE1	1.99	0.45
1:A:120:PHE:HA	1:A:166:LEU:HD21	1.99	0.44
1:B:11:TYR:HA	5:B:442:HOH:O	2.16	0.44
1:C:107:VAL:CG1	1:C:208:VAL:HG11	2.48	0.44
1:B:150:LEU:O	1:B:194:ALA:HA	2.18	0.44
1:A:150:LEU:O	1:A:194:ALA:HA	2.17	0.43
1:B:131:GLN:HB3	1:B:150:LEU:HD13	2.00	0.43
1:D:220:THR:CG2	1:D:221:ALA:N	2.82	0.43
1:A:176:SER:HB2	1:B:169:GLY:HA2	2.00	0.43
1:D:107:VAL:HB	4:D:302:QSO:CM	2.37	0.43
1:C:176:SER:HB2	1:D:169:GLY:HA2	2.01	0.43
1:D:107:VAL:CB	4:D:302:QSO:HM2	2.37	0.43
1:C:150:LEU:O	1:C:194:ALA:HA	2.19	0.43
1:D:27:GLY:O	1:D:55:ASP:HB3	2.19	0.43
1:B:107:VAL:CG1	1:B:208:VAL:HG11	2.48	0.42
1:A:181:PHE:CE1	1:B:112:LEU:HD13	2.55	0.42
1:A:132:PHE:O	1:A:135:ALA:HB3	2.20	0.42
1:B:77:ILE:O	1:B:77:ILE:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:SER:CB	1:D:150:LEU:HD22	2.49	0.41
1:C:64:LYS:NZ	1:C:70:ALA:O	2.53	0.41
1:A:27:GLY:O	1:A:55:ASP:HB3	2.21	0.41
1:C:85:LYS:HG2	1:C:86:LEU:N	2.35	0.41
1:D:235:HIS:CE1	5:D:442:HOH:O	2.73	0.41
1:A:107:VAL:HG21	1:A:208:VAL:HG11	2.02	0.41
1:B:205:PHE:HA	4:B:302[B]:QSO:H2'	2.03	0.41
1:D:77:ILE:O	1:D:77:ILE:HG22	2.20	0.41
1:B:22:LEU:C	1:B:22:LEU:HD23	2.40	0.41
1:C:109:PHE:CE1	1:C:211:HIS:HB3	2.56	0.41
1:C:27:GLY:O	1:C:55:ASP:HB3	2.20	0.41
1:B:27:GLY:O	1:B:55:ASP:HB3	2.21	0.41
1:A:109:PHE:CE1	1:A:211:HIS:HB3	2.57	0.40
1:D:208:VAL:HG23	4:D:302:QSO:H2	2.02	0.40
1:B:40:ARG:HA	1:B:66:LEU:HD13	2.03	0.40
1:A:12:ILE:CG2	1:A:13:PRO:CD	2.99	0.40
1:B:102:SER:HB3	1:B:150:LEU:HD22	2.03	0.40
2:B:301:NAP:H2D	4:B:302[B]:QSO:CM	2.51	0.40
1:C:184:ASP:HB3	1:D:111:HIS:CE1	2.56	0.40

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	258/270 (96%)	247 (96%)	11 (4%)	0	100	100
1	B	260/270 (96%)	252 (97%)	8 (3%)	0	100	100
1	C	256/270 (95%)	248 (97%)	8 (3%)	0	100	100
1	D	259/270 (96%)	251 (97%)	8 (3%)	0	100	100
All	All	1033/1080 (96%)	998 (97%)	35 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	207/216 (96%)	207 (100%)	0	100	100
1	B	209/216 (97%)	208 (100%)	1 (0%)	88	96
1	C	205/216 (95%)	201 (98%)	4 (2%)	55	79
1	D	208/216 (96%)	205 (99%)	3 (1%)	67	86
All	All	829/864 (96%)	821 (99%)	8 (1%)	76	90

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	215	ASN
1	C	85	LYS
1	C	118	GLU
1	C	215	ASN
1	C	222	GLU
1	D	71	ILE
1	D	207	GLU
1	D	220	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	HIS
1	C	96	HIS
1	C	226	GLN
1	D	93	HIS
1	D	226	GLN
1	D	235	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

12 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	NAP	D	301	-	45,52,52	0.87	2 (4%)	56,80,80	1.36	5 (8%)
4	QSO	D	302	-	19,23,23	1.66	3 (15%)	28,33,33	2.05	6 (21%)
3	EDO	A	302	-	3,3,3	0.49	0	2,2,2	0.18	0
3	EDO	B	303	-	3,3,3	0.38	0	2,2,2	0.56	0
2	NAP	C	301	-	45,52,52	0.86	0	56,80,80	1.49	9 (16%)
2	NAP	A	301	-	45,52,52	0.84	1 (2%)	56,80,80	1.38	8 (14%)
2	NAP	B	301	-	45,52,52	0.94	2 (4%)	56,80,80	1.32	5 (8%)
3	EDO	D	303	-	3,3,3	0.54	0	2,2,2	0.42	0
4	QSO	B	302[B]	-	19,23,23	1.75	2 (10%)	28,33,33	1.78	7 (25%)
3	EDO	C	303	-	3,3,3	0.69	0	2,2,2	0.22	0
4	QSO	B	302[A]	-	19,23,23	1.71	2 (10%)	28,33,33	1.57	4 (14%)
3	EDO	C	302	-	3,3,3	0.60	0	2,2,2	0.41	0

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	NAP	D	301	-	-	4/31/67/67	0/5/5/5
4	QSO	D	302	-	-	2/6/6/6	0/3/3/3
3	EDO	A	302	-	-	0/1/1/1	-
3	EDO	B	303	-	-	0/1/1/1	-
2	NAP	C	301	-	-	4/31/67/67	0/5/5/5
2	NAP	A	301	-	-	6/31/67/67	0/5/5/5
2	NAP	B	301	-	-	3/31/67/67	0/5/5/5
3	EDO	D	303	-	-	0/1/1/1	-
4	QSO	B	302[B]	-	-	2/6/6/6	0/3/3/3
3	EDO	C	303	-	-	1/1/1/1	-
4	QSO	B	302[A]	-	-	3/6/6/6	0/3/3/3
3	EDO	C	302	-	-	0/1/1/1	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	302[A]	QSO	C4A-C8A	5.76	1.49	1.41
4	B	302[B]	QSO	C4A-C8A	5.71	1.49	1.41
4	D	302	QSO	C4A-C8A	5.16	1.48	1.41
4	B	302[A]	QSO	C5-C4A	3.63	1.49	1.43
4	B	302[B]	QSO	C5-C4A	3.54	1.49	1.43
4	D	302	QSO	C5-C4A	3.03	1.48	1.43
2	B	301	NAP	O4B-C1B	3.03	1.45	1.41
2	D	301	NAP	C2A-N3A	2.39	1.35	1.32
2	B	301	NAP	C2A-N3A	2.32	1.35	1.32
4	D	302	QSO	C6'-C5'	2.16	1.42	1.38
2	D	301	NAP	C5A-C4A	2.08	1.46	1.40
2	A	301	NAP	C5A-C4A	2.04	1.46	1.40

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	302	QSO	O1-C8A-C8	6.08	123.24	116.07
4	D	302	QSO	C8-C8A-C4A	-4.45	118.12	123.05
2	D	301	NAP	N3A-C2A-N1A	-4.36	121.87	128.68
4	B	302[A]	QSO	O1-C8A-C8	4.27	121.11	116.07
4	B	302[B]	QSO	O1-C8A-C8	4.26	121.10	116.07
2	C	301	NAP	O4D-C1D-C2D	-4.12	100.90	106.93
2	B	301	NAP	C3N-C7N-N7N	3.77	122.28	117.75
2	A	301	NAP	N3A-C2A-N1A	-3.76	122.80	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	302	QSO	C8-C7-C6	3.75	123.97	120.94
2	C	301	NAP	C3N-C7N-N7N	3.56	122.02	117.75
4	B	302[B]	QSO	C6'-C1'-C3	3.50	126.58	120.91
2	B	301	NAP	C4A-C5A-N7A	-3.46	105.79	109.40
4	B	302[B]	QSO	C8-C8A-C4A	-3.44	119.24	123.05
2	B	301	NAP	N3A-C2A-N1A	-3.43	123.32	128.68
4	B	302[A]	QSO	CM-O5-C4'	3.41	124.92	117.51
2	C	301	NAP	N3A-C2A-N1A	-3.41	123.35	128.68
2	C	301	NAP	PN-O3-PA	-3.33	121.40	132.83
2	D	301	NAP	C1B-N9A-C4A	-3.30	120.85	126.64
2	A	301	NAP	C6N-N1N-C2N	-3.27	118.99	121.97
4	B	302[A]	QSO	C8-C8A-C4A	-3.19	119.52	123.05
4	B	302[B]	QSO	C2'-C1'-C3	-3.10	115.88	120.91
2	D	301	NAP	C4A-C5A-N7A	-3.10	106.17	109.40
4	B	302[B]	QSO	CM-O5-C4'	3.07	124.17	117.51
2	A	301	NAP	C4A-C5A-N7A	-2.96	106.31	109.40
4	D	302	QSO	CM-O5-C4'	2.84	123.67	117.51
2	C	301	NAP	C6N-N1N-C2N	-2.81	119.41	121.97
2	C	301	NAP	O7N-C7N-N7N	-2.76	118.65	122.58
2	B	301	NAP	PN-O3-PA	-2.76	123.36	132.83
2	C	301	NAP	C4A-C5A-N7A	-2.66	106.63	109.40
2	C	301	NAP	O2A-PA-O1A	2.56	124.89	112.24
4	D	302	QSO	C6'-C1'-C3	2.53	125.01	120.91
2	A	301	NAP	O2A-PA-O1A	2.51	124.66	112.24
4	D	302	QSO	O1-C8A-C4A	-2.43	118.64	121.03
2	A	301	NAP	C3D-C2D-C1D	2.36	104.53	100.98
2	A	301	NAP	O4D-C1D-C2D	-2.35	103.50	106.93
4	B	302[B]	QSO	C3-C4-C4A	-2.32	116.53	120.60
2	A	301	NAP	O2N-PN-O1N	2.29	123.57	112.24
2	D	301	NAP	O3X-P2B-O2X	2.22	116.12	107.64
4	B	302[B]	QSO	C5-C6-C7	2.19	121.68	119.70
2	B	301	NAP	C1B-N9A-C4A	-2.16	122.84	126.64
4	B	302[A]	QSO	C8-C7-C6	2.12	122.66	120.94
2	C	301	NAP	C3D-C2D-C1D	2.10	104.14	100.98
2	A	301	NAP	PN-O3-PA	-2.09	125.67	132.83
2	D	301	NAP	C6N-N1N-C2N	-2.04	120.11	121.97

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	301	NAP	C5D-O5D-PN-O1N

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Mol	Chain	Res	Type	Atoms
2	A	301	NAP	C2B-O2B-P2B-O1X
2	A	301	NAP	C5D-O5D-PN-O1N
2	A	301	NAP	C5D-O5D-PN-O2N
2	C	301	NAP	O4D-C4D-C5D-O5D
4	D	302	QSO	C5'-C4'-O5-CM
4	D	302	QSO	C3'-C4'-O5-CM
2	C	301	NAP	C3D-C4D-C5D-O5D
2	B	301	NAP	O4D-C4D-C5D-O5D
2	D	301	NAP	C5D-O5D-PN-O3
2	C	301	NAP	C2B-O2B-P2B-O3X
2	D	301	NAP	C5D-O5D-PN-O2N
3	C	303	EDO	O1-C1-C2-O2
2	A	301	NAP	O4B-C4B-C5B-O5B
4	B	302[A]	QSO	C2'-C1'-C3-C2
2	B	301	NAP	C3D-C4D-C5D-O5D
4	B	302[A]	QSO	C6'-C1'-C3-C4
4	B	302[A]	QSO	C2'-C1'-C3-C4
4	B	302[B]	QSO	C5'-C4'-O5-CM
2	A	301	NAP	C2B-O2B-P2B-O2X
2	A	301	NAP	C5D-O5D-PN-O3
2	D	301	NAP	O4B-C4B-C5B-O5B
2	C	301	NAP	O4B-C4B-C5B-O5B
2	B	301	NAP	O4B-C4B-C5B-O5B
4	B	302[B]	QSO	C3'-C4'-O5-CM

There are no ring outliers.

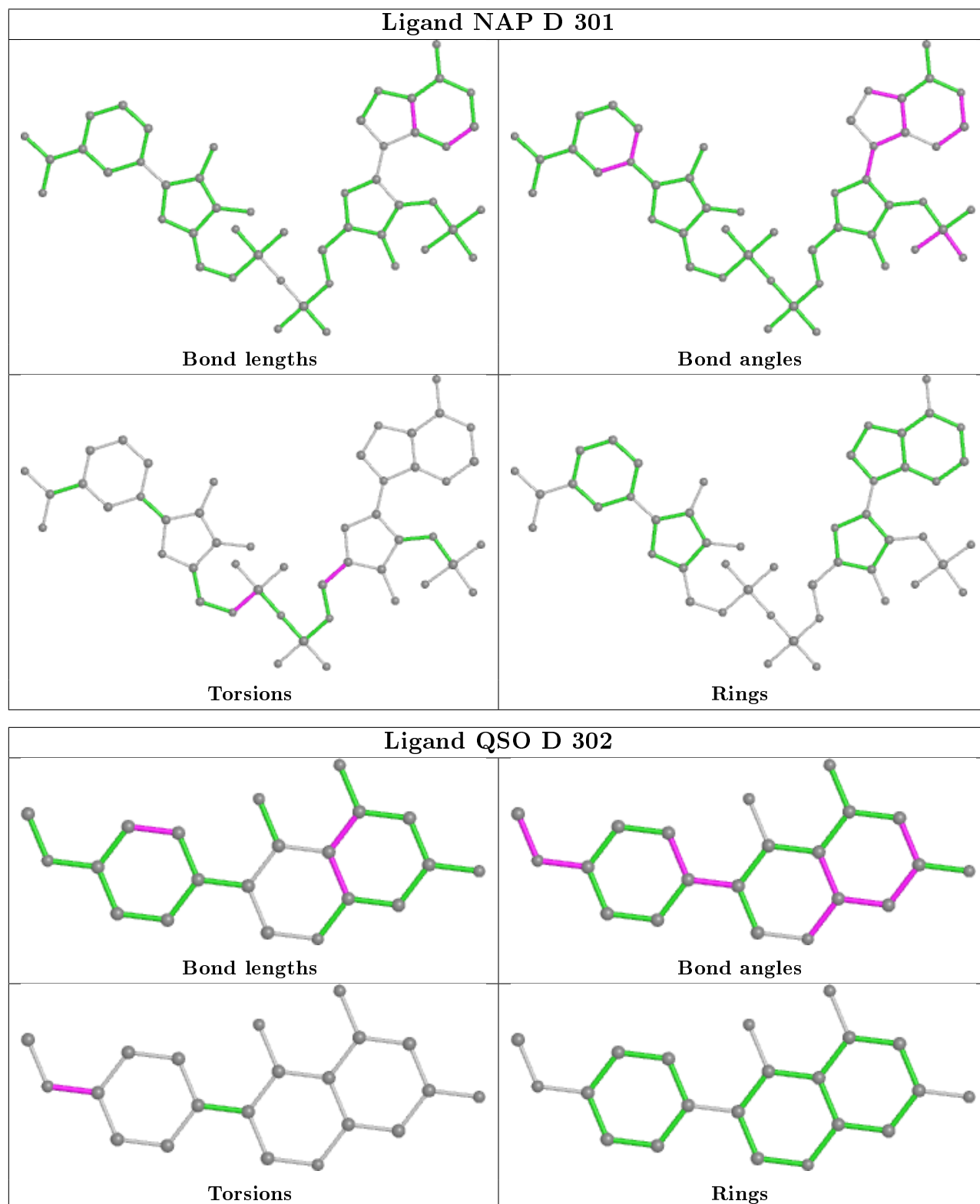
4 monomers are involved in 9 short contacts:

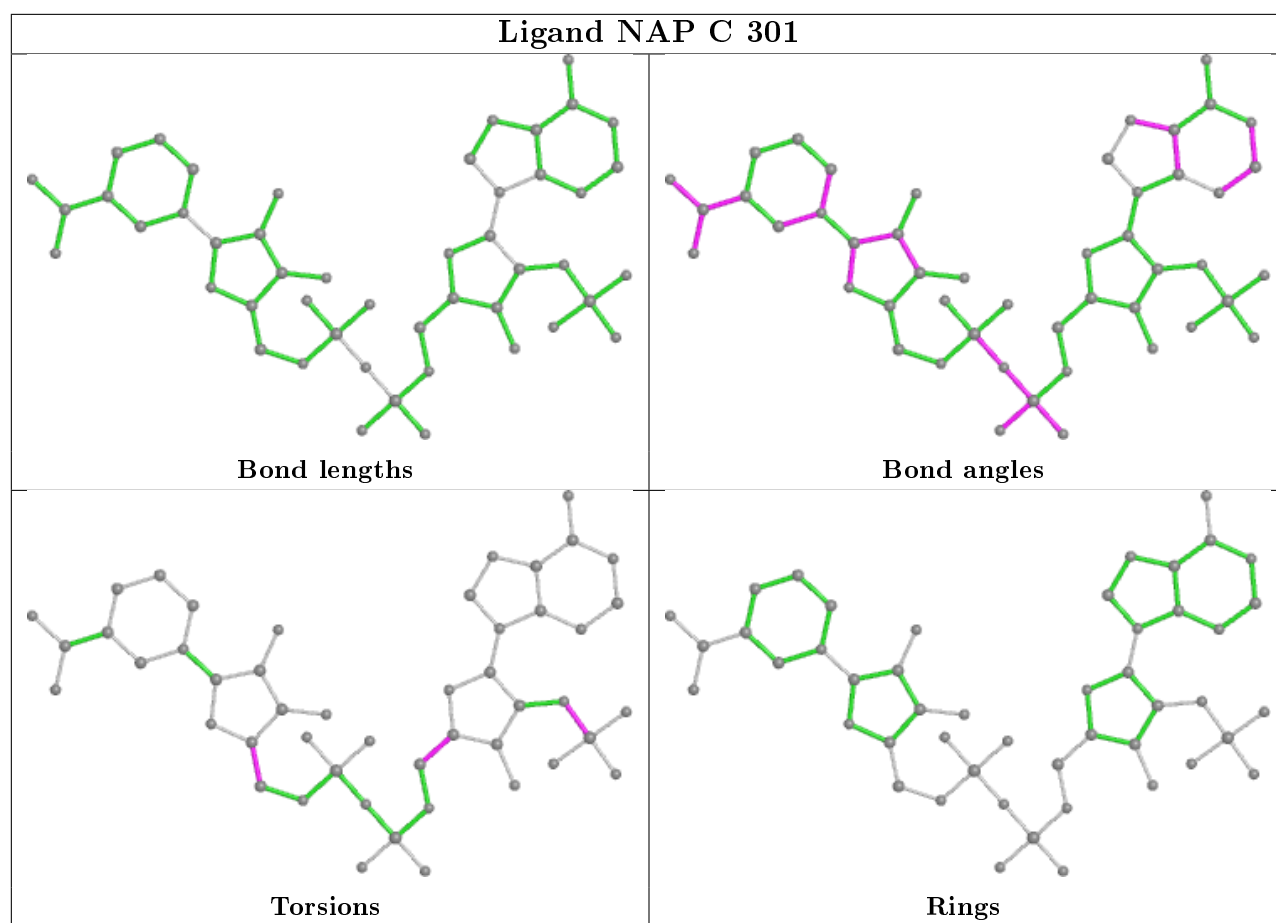
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	302	QSO	5	0
2	B	301	NAP	1	0
4	B	302[B]	QSO	3	0
4	B	302[A]	QSO	1	0

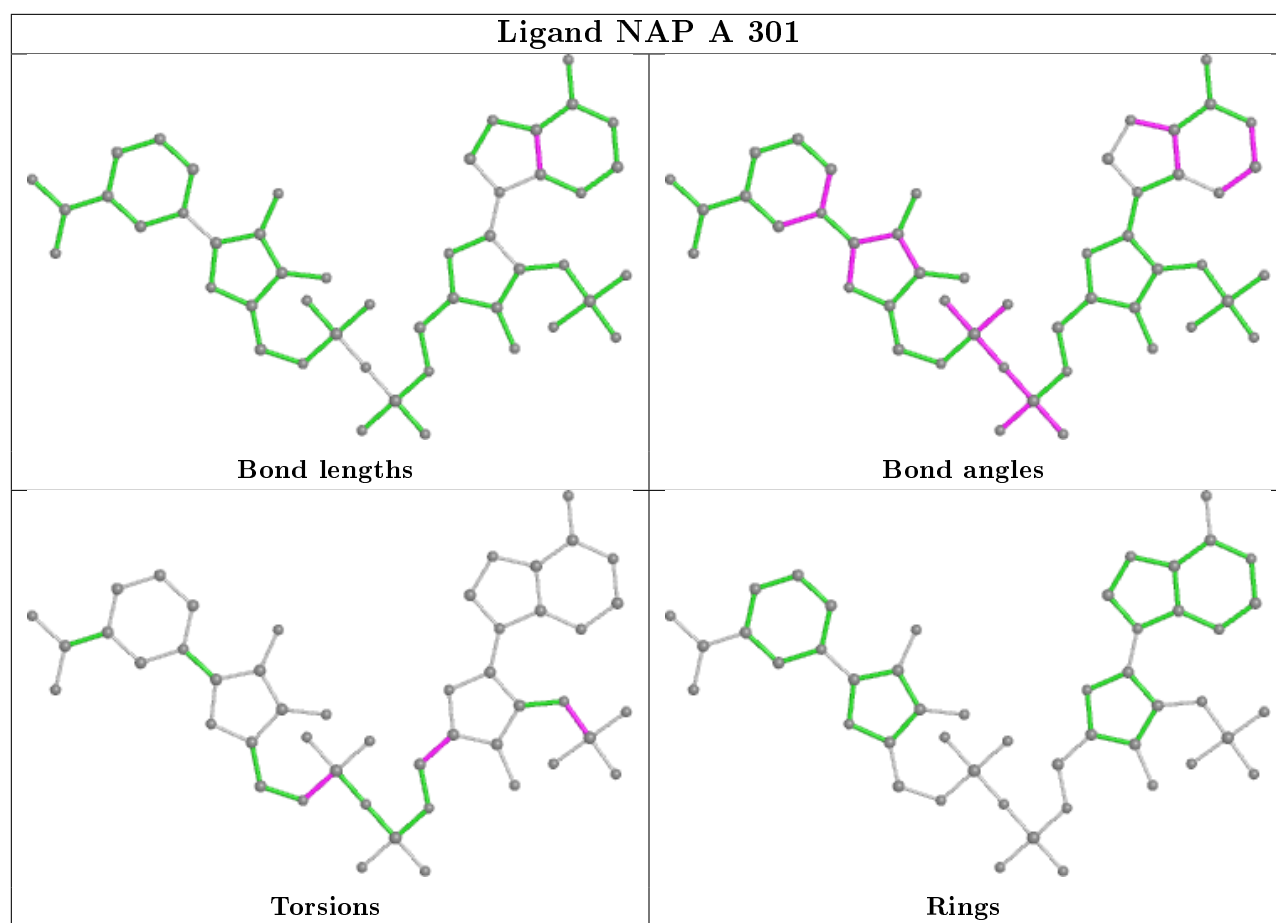
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

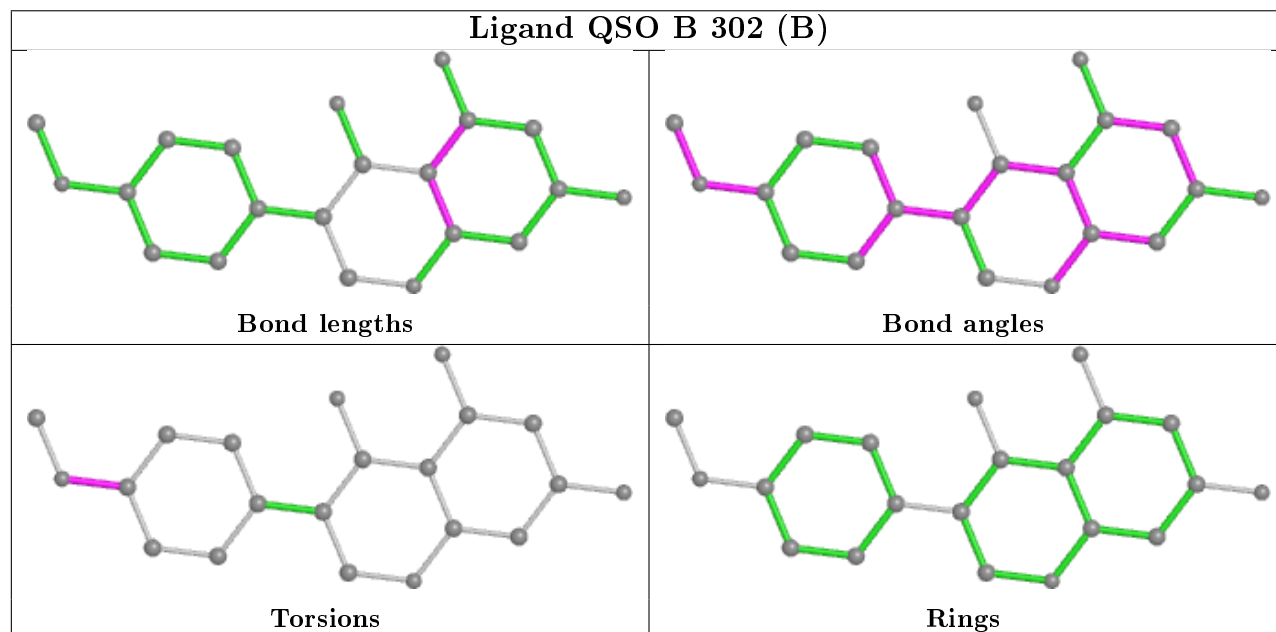
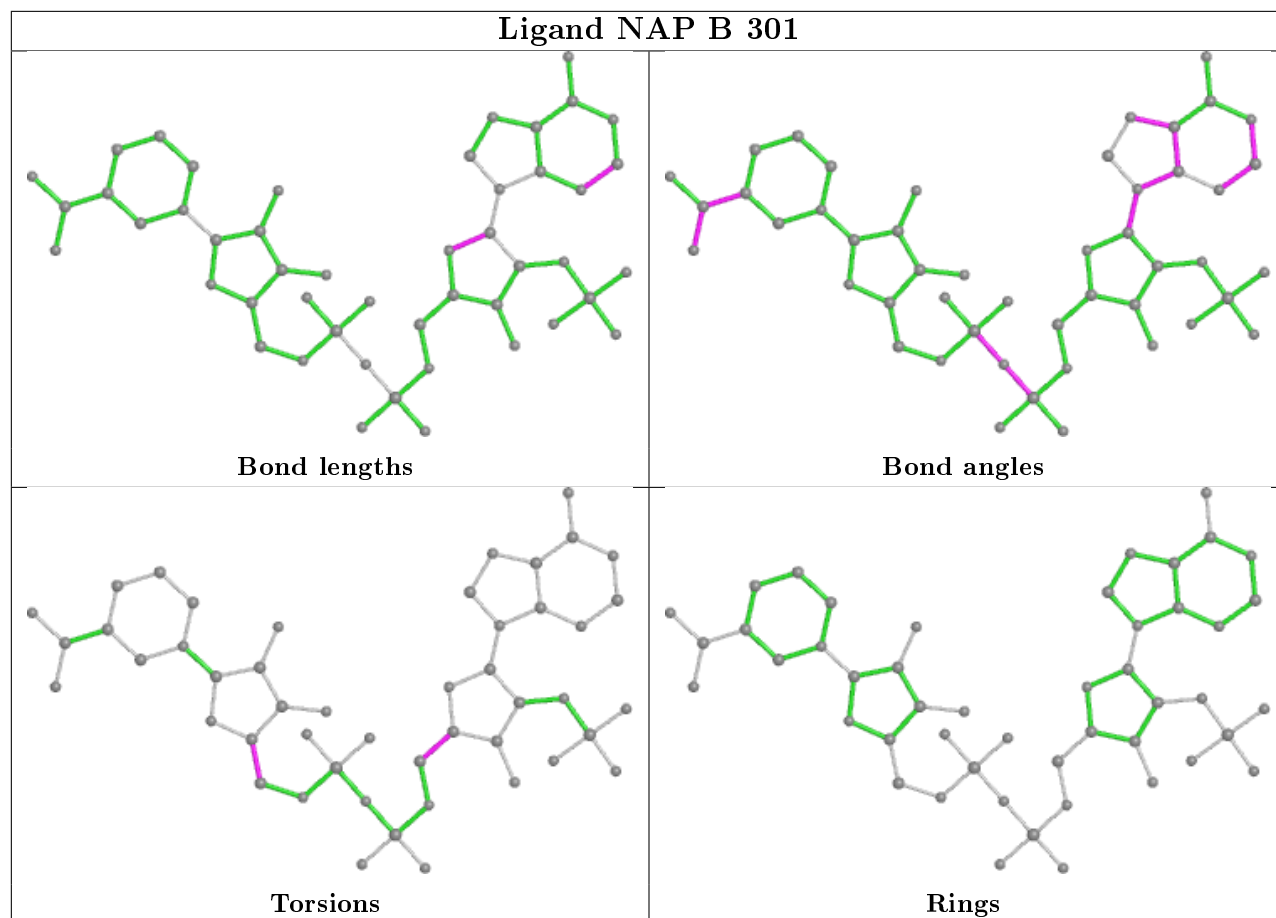


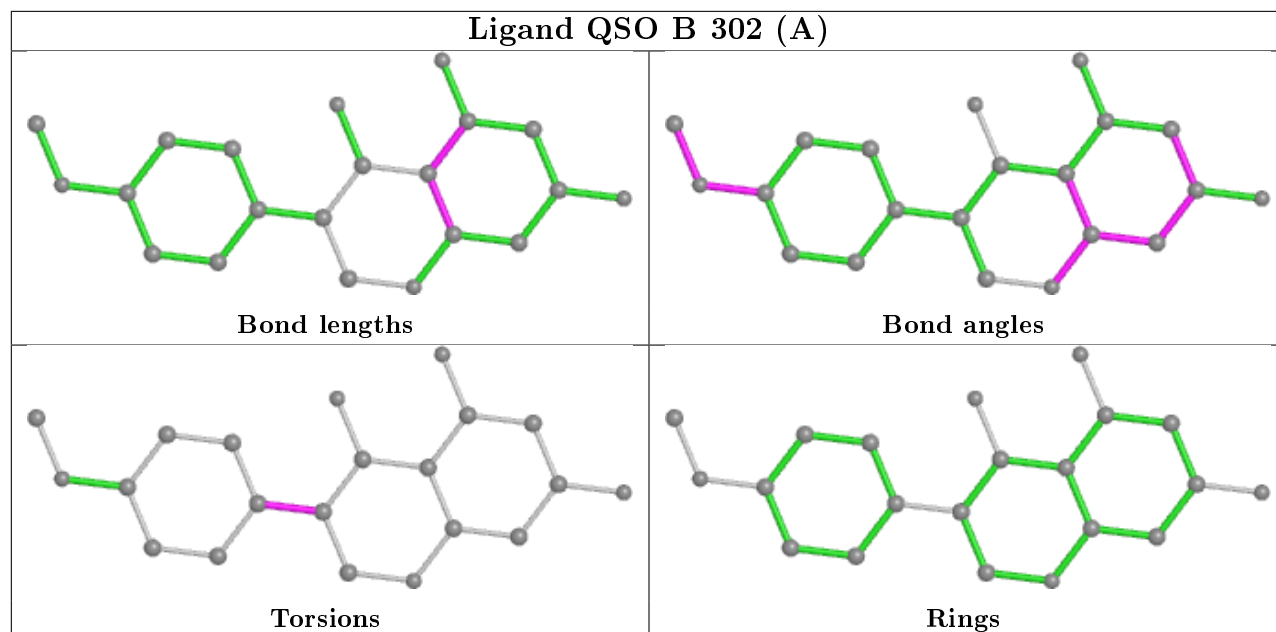
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	260/270 (96%)	-0.45	5 (1%) 66 69	22, 32, 58, 80	0
1	B	260/270 (96%)	-0.48	5 (1%) 66 69	18, 30, 52, 75	0
1	C	258/270 (95%)	-0.40	5 (1%) 66 69	19, 29, 61, 88	0
1	D	261/270 (96%)	-0.52	0 100 100	18, 28, 45, 51	0
All	All	1039/1080 (96%)	-0.46	15 (1%) 75 77	18, 30, 53, 88	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	11	TYR	4.2
1	B	215	ASN	4.1
1	C	218	SER	4.0
1	A	214	PRO	3.5
1	A	12	ILE	3.4
1	C	219	TYR	3.2
1	A	13	PRO	3.1
1	C	217	THR	3.1
1	B	214	PRO	3.0
1	B	11	TYR	2.8
1	B	226	GLN	2.5
1	C	227	MET	2.2
1	A	215	ASN	2.2
1	B	219	TYR	2.1
1	C	222	GLU	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

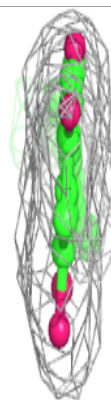
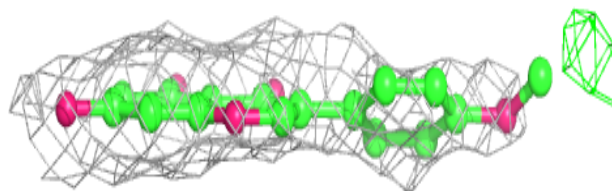
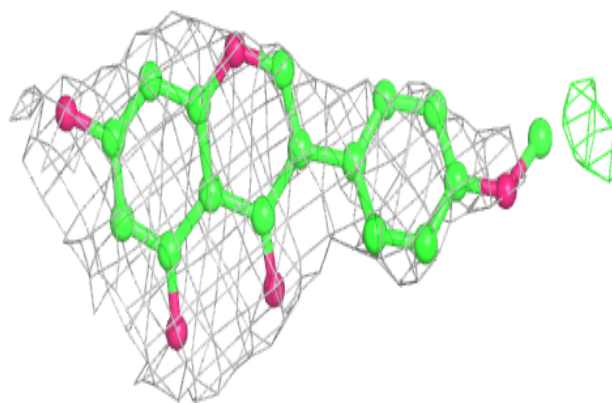
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	EDO	C	303	4/4	0.85	0.17	31,32,34,36	0
3	EDO	B	303	4/4	0.86	0.26	48,48,49,50	0
3	EDO	A	302	4/4	0.88	0.20	52,53,54,59	0
3	EDO	C	302	4/4	0.89	0.23	32,32,34,35	0
3	EDO	D	303	4/4	0.91	0.28	47,48,49,49	0
4	QSO	B	302[A]	21/21	0.93	0.19	32,35,40,42	21
4	QSO	B	302[B]	21/21	0.93	0.19	23,27,30,31	21
4	QSO	D	302	21/21	0.95	0.12	29,31,32,34	0
2	NAP	A	301	48/48	0.97	0.09	23,31,36,38	0
2	NAP	B	301	48/48	0.98	0.10	23,25,28,29	0
2	NAP	C	301	48/48	0.98	0.10	25,27,29,31	0
2	NAP	D	301	48/48	0.98	0.09	20,23,31,33	0

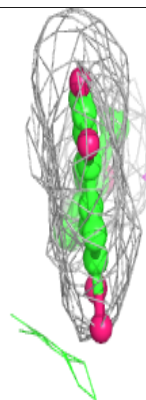
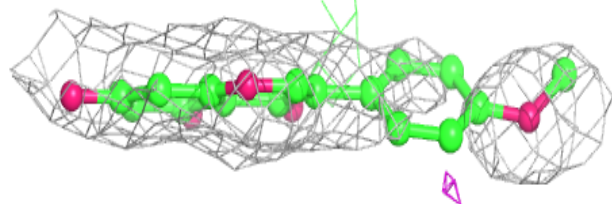
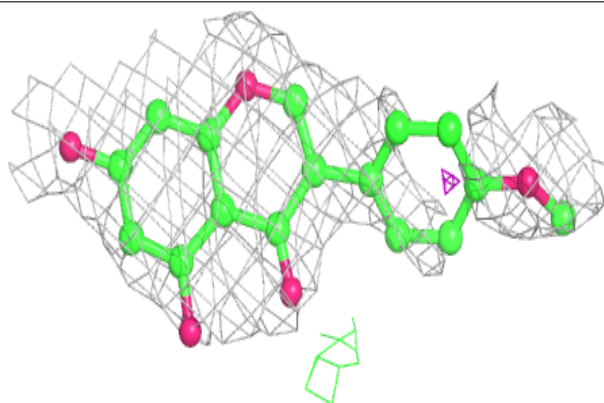
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around QSO B 302 (A):**

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

**Electron density around QSO B 302 (B):**

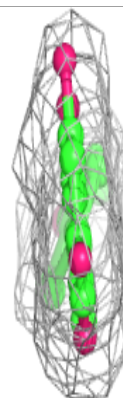
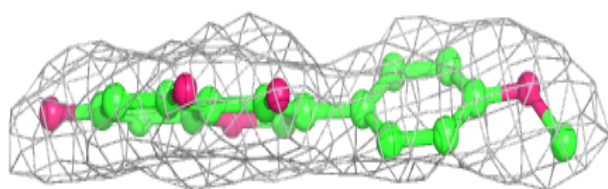
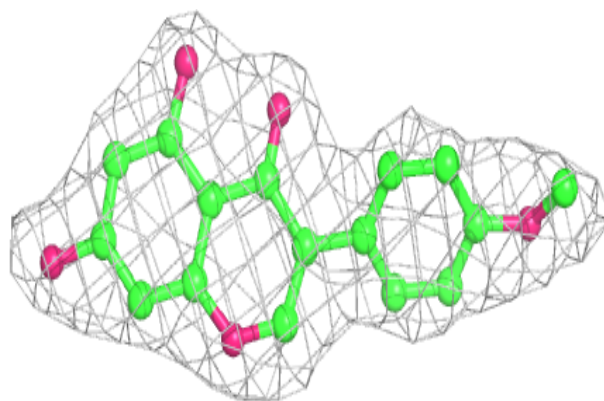
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



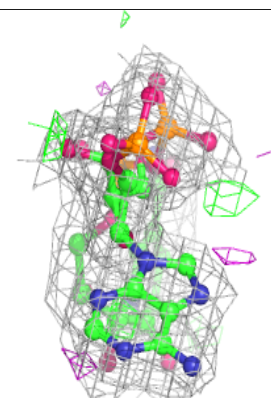
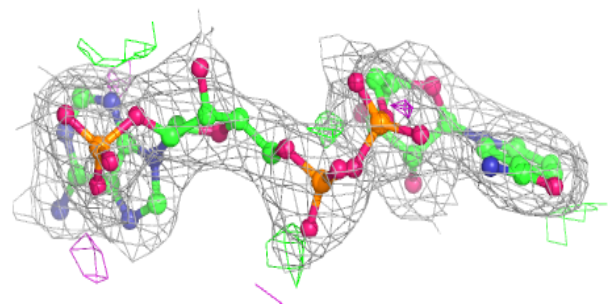
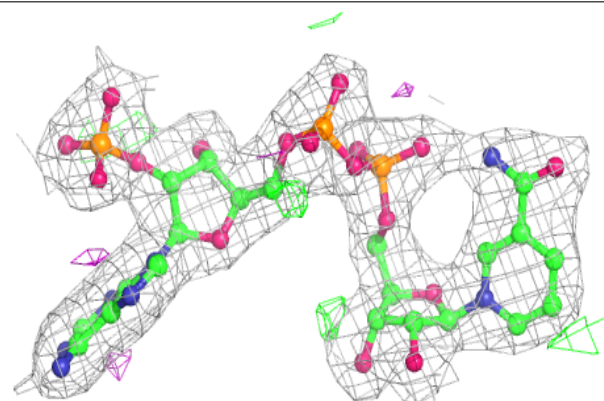


**Electron density around QSO D 302:**

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

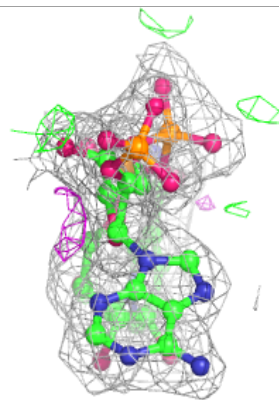
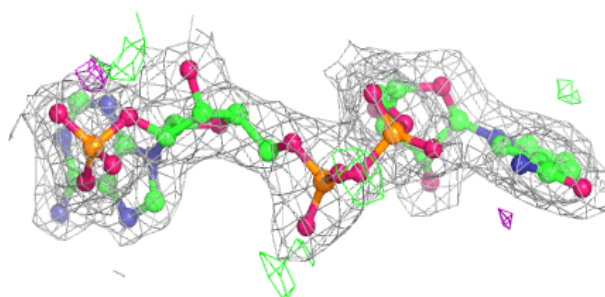
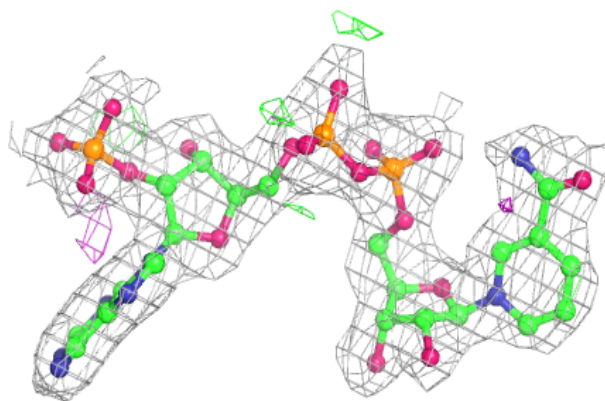
**Electron density around NAP A 301:**

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

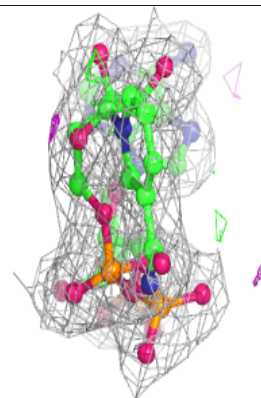
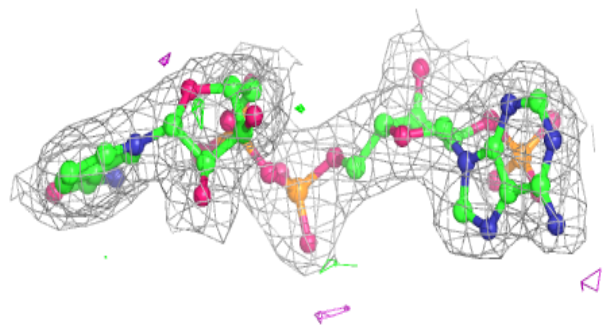
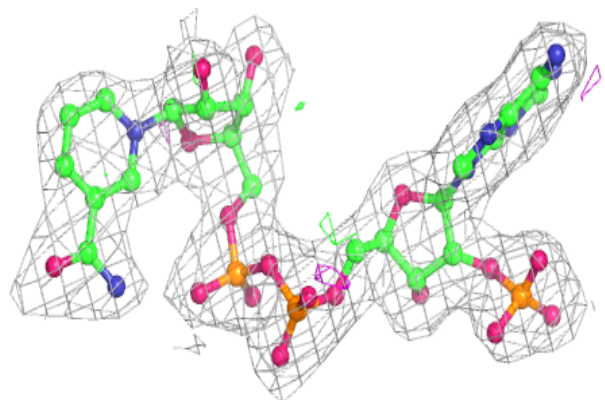


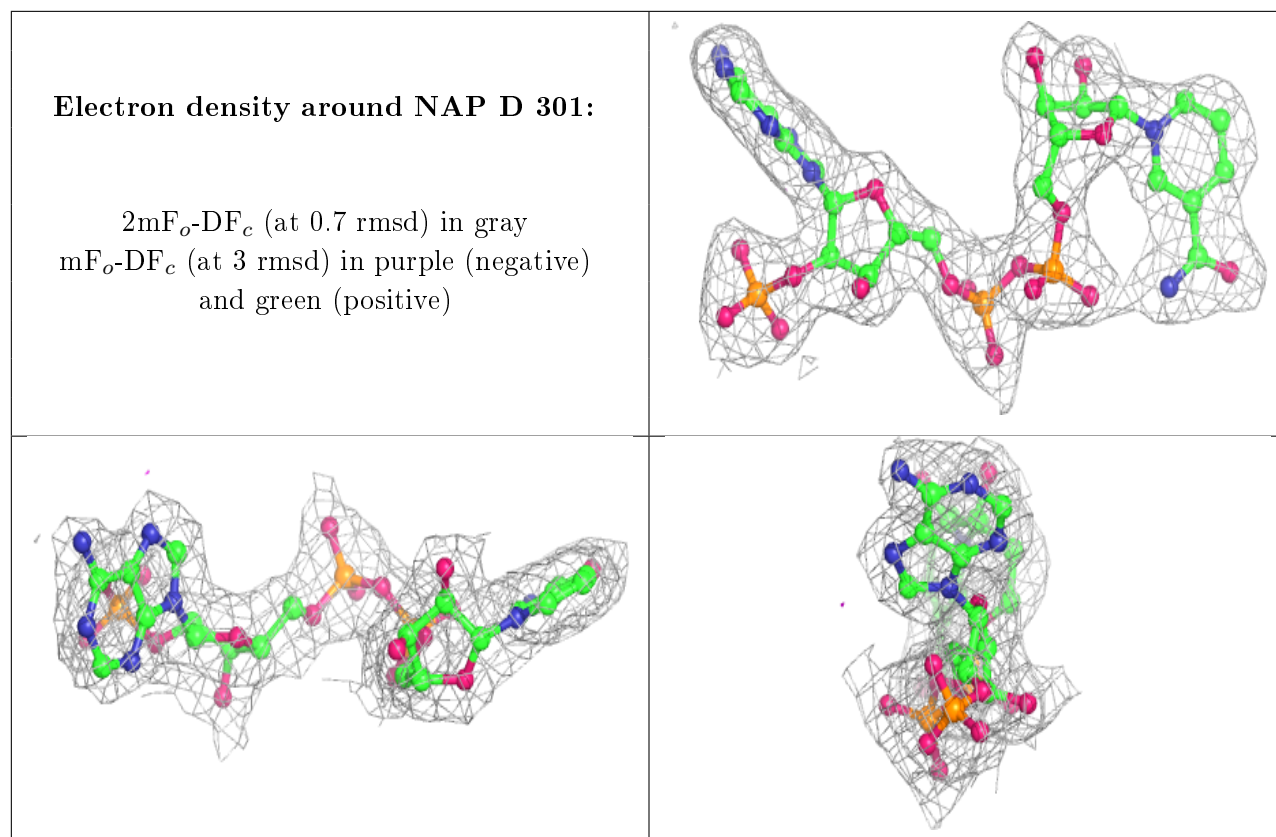
**Electron density around NAP B 301:**

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

**Electron density around NAP C 301:**

$2mF_o-DF_c$  (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.