



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 07:56 PM EDT

PDB ID : 5G6S  
Title : Imine reductase from *Aspergillus oryzae* in complex with NADP(H) and (R)-rasagiline  
Authors : Man, H.; Aleku, G.; Turner, N.J.; Grogan, G.  
Deposited on : 2016-06-23  
Resolution : 2.35 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.

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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

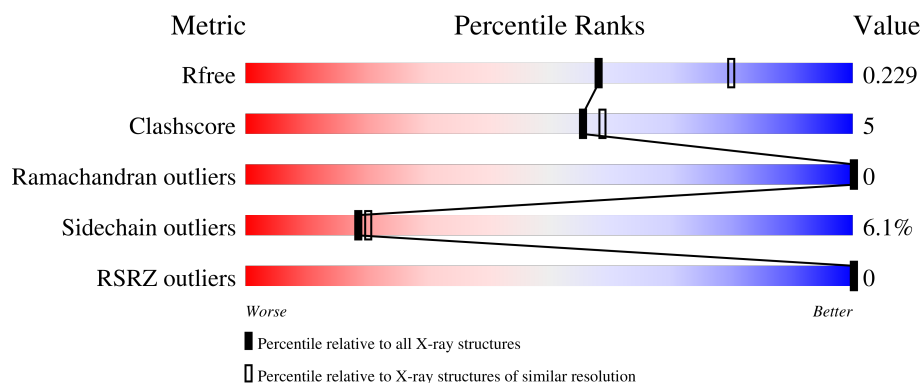
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*






The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	295	 88% 8% ..
1	B	295	 86% 10% ..
1	C	295	 85% 11% ..
1	D	295	 84% 11% ...
1	E	295	 86% 10% ..

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Mol	Chain	Length	Quality of chain
1	F	295	 86% 11% ..
1	G	295	 86% 11% ..
1	H	295	 83% 12% ..

## 2 Entry composition

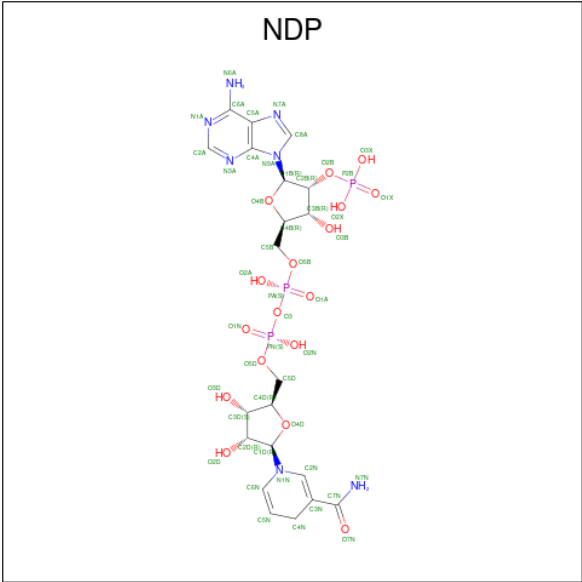
There are 4 unique types of molecules in this entry. The entry contains 17882 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 IMINE REDUCTASE.

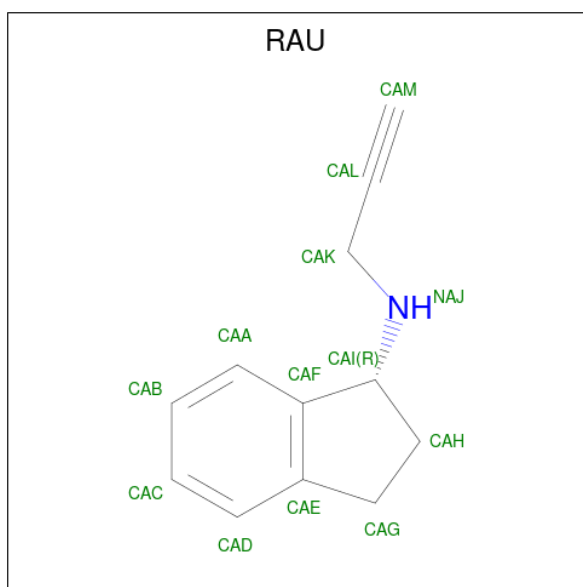
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2114	1342	348	415	9			
1	B	289	Total	C	N	O	S	0	0	0
			2114	1344	348	413	9			
1	C	288	Total	C	N	O	S	0	0	0
			2100	1334	345	412	9			
1	D	288	Total	C	N	O	S	0	0	0
			2104	1337	346	412	9			
1	E	288	Total	C	N	O	S	0	0	0
			2094	1334	340	411	9			
1	F	289	Total	C	N	O	S	0	0	0
			2109	1341	345	414	9			
1	G	289	Total	C	N	O	S	0	0	0
			2115	1344	348	414	9			
1	H	289	Total	C	N	O	S	0	0	0
			2114	1344	349	412	9			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



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

- Molecule 3 is RASAGILINE (three-letter code: RAU) (formula: C<sub>12</sub>H<sub>13</sub>N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			13	12	1		
3	B	1	Total	C	N	0	0
			13	12	1		
3	C	1	Total	C	N	0	0
			13	12	1		
3	D	1	Total	C	N	0	0
			13	12	1		
3	E	1	Total	C	N	0	0
			13	12	1		
3	F	1	Total	C	N	0	0
			13	12	1		
3	G	1	Total	C	N	0	0
			13	12	1		
3	H	1	Total	C	N	0	0
			13	12	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	76	Total	O	0	0
			76	76		
4	B	71	Total	O	0	0
			71	71		
4	C	58	Total	O	0	0
			58	58		
4	D	89	Total	O	0	0
			89	89		

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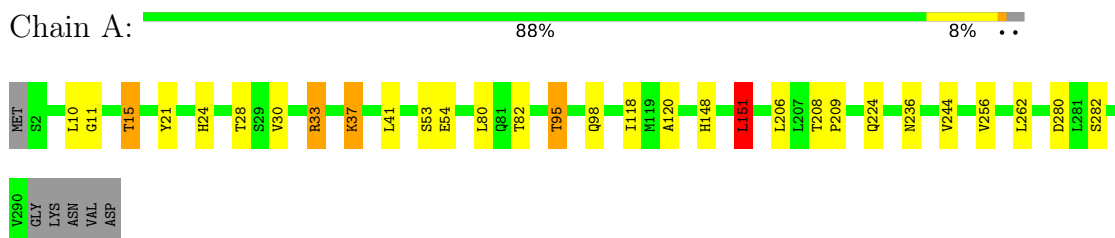
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	92	Total 92	O 92	0	0
4	F	54	Total 54	O 54	0	0
4	G	46	Total 46	O 46	0	0
4	H	44	Total 44	O 44	0	0

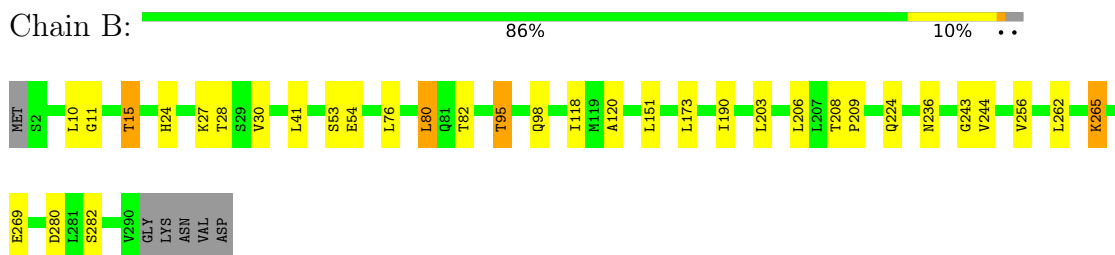
### 3 Residue-property plots

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

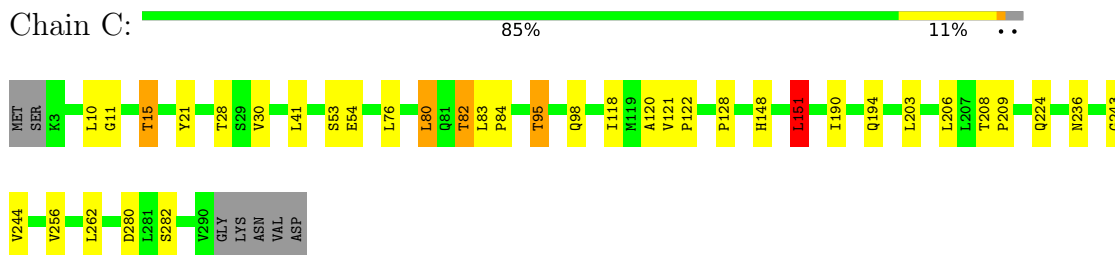
#### • Molecule 1: IMINE REDUCTASE



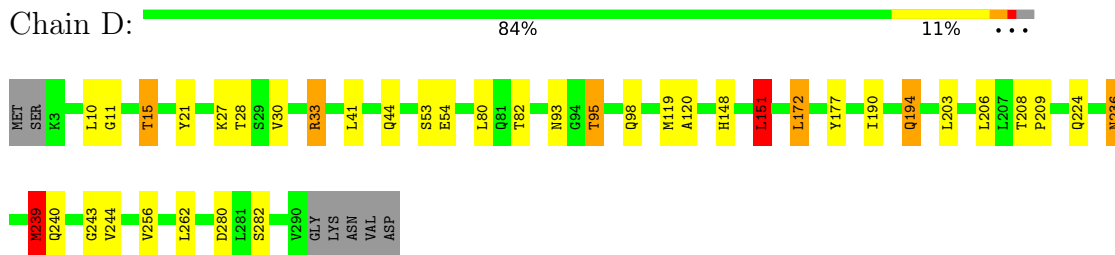
#### • Molecule 1: IMINE REDUCTASE



#### • Molecule 1: IMINE REDUCTASE


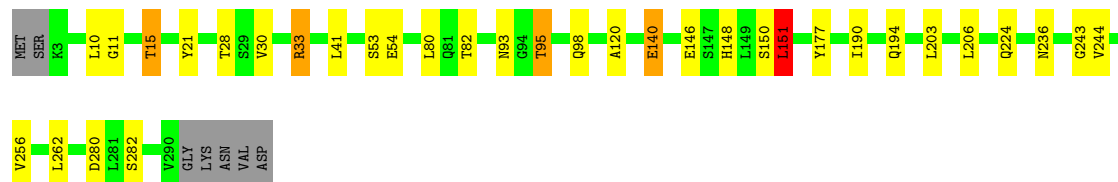


#### • Molecule 1: IMINE REDUCTASE


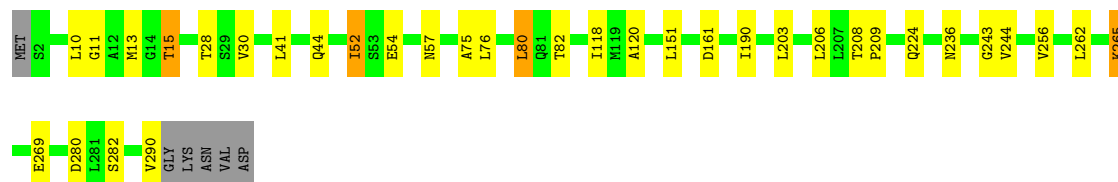





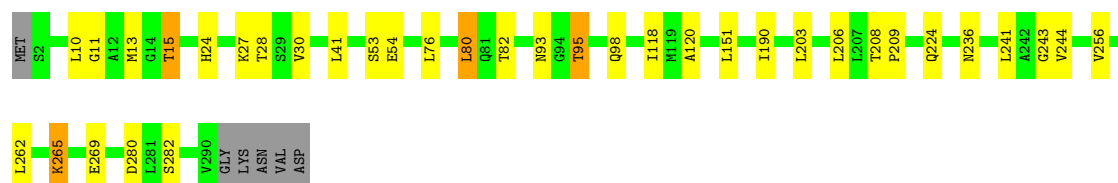
## ● Molecule 1: IMINE REDUCTASE

Chain E:  86% 10% ..


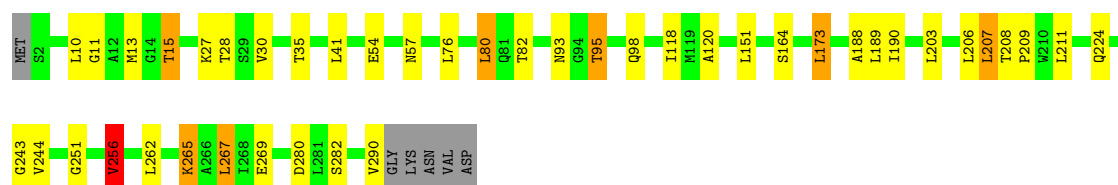
## ● Molecule 1: IMINE REDUCTASE

Chain F:  86% 11% ..

## ● Molecule 1: IMINE REDUCTASE

Chain G:  86% 11% ..

## ● Molecule 1: IMINE REDUCTASE

Chain H:  83% 12% ..

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.82Å 80.25Å 123.89Å 108.75° 108.78° 90.05°	Depositor
Resolution (Å)	110.32 – 2.35 56.62 – 2.35	Depositor EDS
% Data completeness (in resolution range)	97.3 (110.32-2.35) 96.7 (56.62-2.35)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.204 , 0.229 0.208 , 0.229	Depositor DCC
$R_{free}$ test set	5656 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.4	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 10.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.379 for k,-h,h+1 0.379 for -k,h,k+1 0.047 for h,-k,-h-l 0.047 for -h,k,-k-l 0.046 for k,h,-h-k-l 0.046 for -k,-h,-l 0.447 for -h,-k,h+k+1	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	17882	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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

### 5.1 Standard geometry

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

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	0.54	0/2149	0.73	1/2921 (0.0%)
1	B	0.54	0/2149	0.72	0/2920
1	C	0.54	0/2135	0.75	3/2904 (0.1%)
1	D	0.54	0/2139	0.79	4/2908 (0.1%)
1	E	0.58	1/2129 (0.0%)	0.74	2/2897 (0.1%)
1	F	0.54	0/2143	0.74	1/2912 (0.0%)
1	G	0.54	0/2150	0.72	0/2921
1	H	0.55	0/2149	0.80	5/2919 (0.2%)
All	All	0.54	1/17143 (0.0%)	0.75	16/23302 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	140	GLU	CA-CB	5.35	1.65	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	267	LEU	CB-CG-CD2	9.80	127.66	111.00
1	F	151	LEU	CA-CB-CG	9.56	137.28	115.30
1	H	151	LEU	CA-CB-CG	9.51	137.18	115.30
1	D	239	MET	CG-SD-CE	7.41	112.06	100.20
1	D	172	LEU	CB-CG-CD2	6.96	122.83	111.00
1	D	172	LEU	CB-CG-CD1	-6.64	99.70	111.00
1	H	173	LEU	CB-CG-CD2	6.47	122.00	111.00
1	C	82	THR	CA-CB-CG2	5.76	120.47	112.40
1	H	267	LEU	CB-CG-CD1	-5.48	101.68	111.00
1	C	151	LEU	CA-CB-CG	5.48	127.90	115.30
1	E	151	LEU	CA-CB-CG	5.47	127.87	115.30
1	C	82	THR	CB-CA-C	-5.40	97.02	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	140	GLU	CB-CA-C	5.38	121.16	110.40
1	D	151	LEU	CA-CB-CG	5.31	127.51	115.30
1	A	151	LEU	CA-CB-CG	5.19	127.24	115.30
1	H	256	VAL	CA-CB-CG1	5.06	118.49	110.90

There are no chirality outliers.

There are no planarity outliers.

## 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	2114	0	2104	17	0
1	B	2114	0	2104	19	0
1	C	2100	0	2082	22	0
1	D	2104	0	2093	31	0
1	E	2094	0	2064	23	0
1	F	2109	0	2101	21	0
1	G	2115	0	2108	22	0
1	H	2114	0	2113	23	0
2	A	48	0	26	3	0
2	B	48	0	26	2	0
2	C	48	0	26	3	0
2	D	48	0	26	2	0
2	E	48	0	26	5	0
2	F	48	0	26	3	0
2	G	48	0	26	5	0
2	H	48	0	26	3	0
3	A	13	0	0	1	0
3	B	13	0	0	4	0
3	C	13	0	0	1	0
3	D	13	0	0	4	0
3	E	13	0	0	3	0
3	F	13	0	0	3	0
3	G	13	0	0	0	0
3	H	13	0	0	1	0
4	A	76	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	71	0	0	1	0
4	C	58	0	0	0	0
4	D	89	0	0	1	0
4	E	92	0	0	0	0
4	F	54	0	0	1	0
4	G	46	0	0	0	0
4	H	44	0	0	0	0
All	All	17882	0	16977	176	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 (176) 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)
3:B:400:RAU:CAM	3:B:400:RAU:CAK	2.18	1.21
3:B:400:RAU:CAM	3:B:400:RAU:CAL	0.90	0.90
1:D:239:MET:HE2	1:D:240:GLN:HA	1.57	0.86
1:B:265:LYS:NZ	1:B:269:GLU:OE1	2.16	0.79
1:F:265:LYS:NZ	1:F:269:GLU:OE1	2.16	0.78
1:G:265:LYS:NZ	1:G:269:GLU:OE1	2.16	0.78
1:E:243:GLY:HA3	3:H:400:RAU:CAM	2.14	0.76
1:E:11:GLY:HA3	2:E:300:NDP:H51A	1.69	0.74
3:E:400:RAU:CAM	1:H:243:GLY:HA3	2.17	0.74
1:D:239:MET:HE2	1:D:240:GLN:CA	2.18	0.74
1:B:243:GLY:HA3	3:C:400:RAU:CAM	2.17	0.73
1:D:239:MET:CE	1:D:240:GLN:HA	2.18	0.73
3:D:400:RAU:CAM	1:F:243:GLY:HA3	2.22	0.70
1:F:11:GLY:O	1:F:15:THR:HG23	2.00	0.61
1:B:11:GLY:O	1:B:15:THR:HG23	2.01	0.61
1:H:207:LEU:HD22	1:H:211:LEU:HG	1.81	0.61
1:D:11:GLY:O	1:D:15:THR:HG23	2.01	0.61
1:A:11:GLY:O	1:A:15:THR:HG23	2.01	0.60
1:E:11:GLY:O	1:E:15:THR:HG23	2.01	0.60
1:G:11:GLY:O	1:G:15:THR:HG23	2.00	0.60
1:H:265:LYS:HE2	1:H:269:GLU:OE1	2.01	0.60
1:C:11:GLY:O	1:C:15:THR:HG23	2.01	0.60
1:H:11:GLY:O	1:H:15:THR:HG23	2.00	0.60
1:D:11:GLY:O	1:D:15:THR:CG2	2.51	0.59
1:E:11:GLY:O	1:E:15:THR:CG2	2.51	0.59
1:G:11:GLY:O	1:G:15:THR:CG2	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:11:GLY:O	1:H:15:THR:CG2	2.51	0.58
1:C:11:GLY:O	1:C:15:THR:CG2	2.51	0.58
1:E:15:THR:HB	1:E:41:LEU:HD11	1.85	0.58
1:A:11:GLY:O	1:A:15:THR:CG2	2.51	0.58
1:F:11:GLY:O	1:F:15:THR:CG2	2.51	0.58
1:E:11:GLY:HA3	2:E:300:NDP:C5B	2.33	0.57
1:A:15:THR:HB	1:A:41:LEU:HD11	1.87	0.57
1:D:15:THR:HB	1:D:41:LEU:HD11	1.86	0.57
1:D:224:GLN:HE22	1:D:280:ASP:HB2	1.69	0.57
1:E:224:GLN:HE22	1:E:280:ASP:HB2	1.68	0.57
3:D:400:RAU:CAL	1:F:243:GLY:HA3	2.35	0.57
1:A:224:GLN:HE22	1:A:280:ASP:HB2	1.70	0.57
1:B:11:GLY:O	1:B:15:THR:CG2	2.53	0.57
1:F:224:GLN:HE22	1:F:280:ASP:HB2	1.70	0.56
1:H:224:GLN:HE22	1:H:280:ASP:HB2	1.70	0.56
3:B:400:RAU:CAM	1:C:243:GLY:HA3	2.35	0.56
1:C:224:GLN:HE22	1:C:280:ASP:HB2	1.70	0.56
1:G:224:GLN:HE22	1:G:280:ASP:HB2	1.70	0.56
1:C:15:THR:HB	1:C:41:LEU:HD11	1.87	0.56
1:D:239:MET:HE1	3:F:400:RAU:CAL	2.35	0.56
1:F:52:ILE:HD12	1:F:75:ALA:O	2.06	0.56
1:D:243:GLY:HA3	3:F:400:RAU:CAM	2.36	0.56
1:F:44:GLN:NE2	4:F:2006:HOH:O	2.32	0.56
1:B:224:GLN:HE22	1:B:280:ASP:HB2	1.71	0.55
1:F:15:THR:HB	1:F:41:LEU:HD11	1.88	0.55
1:B:15:THR:HB	1:B:41:LEU:HD11	1.87	0.55
1:D:44:GLN:NE2	4:D:2011:HOH:O	2.34	0.55
1:A:120:ALA:O	2:A:300:NDP:H42N	2.07	0.55
1:G:15:THR:HB	1:G:41:LEU:HD11	1.87	0.55
1:B:118:ILE:O	2:B:300:NDP:H5N	2.07	0.55
3:A:400:RAU:CAM	1:G:243:GLY:HA3	2.37	0.54
1:H:15:THR:HB	1:H:41:LEU:HD11	1.88	0.54
1:D:190:ILE:HG12	1:D:203:LEU:HD22	1.90	0.54
1:C:120:ALA:O	2:C:300:NDP:H42N	2.07	0.54
1:F:190:ILE:HG12	1:F:203:LEU:HD22	1.90	0.54
1:H:251:GLY:HA2	1:H:256:VAL:HG23	1.90	0.54
1:B:190:ILE:HG12	1:B:203:LEU:HD22	1.90	0.53
1:B:24:HIS:CD2	1:B:151:LEU:HD13	2.43	0.53
1:C:190:ILE:HG12	1:C:203:LEU:HD22	1.89	0.53
1:G:24:HIS:CD2	1:G:151:LEU:HD13	2.44	0.53
1:H:190:ILE:HG12	1:H:203:LEU:HD22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:241:LEU:HA	1:G:244:VAL:HG22	1.91	0.52
1:A:224:GLN:NE2	1:A:282:SER:OG	2.43	0.52
1:G:190:ILE:HG12	1:G:203:LEU:HD22	1.91	0.52
1:E:190:ILE:HG12	1:E:203:LEU:HD22	1.89	0.52
1:C:224:GLN:NE2	1:C:282:SER:OG	2.42	0.52
1:F:118:ILE:O	2:F:300:NDP:H5N	2.10	0.52
1:B:24:HIS:CG	1:B:151:LEU:HD13	2.45	0.52
1:B:224:GLN:NE2	1:B:282:SER:OG	2.43	0.52
1:H:188:ALA:O	1:H:256:VAL:HG11	2.09	0.52
1:D:224:GLN:NE2	1:D:282:SER:OG	2.43	0.51
1:H:224:GLN:NE2	1:H:282:SER:OG	2.42	0.51
1:F:120:ALA:O	2:F:300:NDP:H42N	2.09	0.51
1:F:224:GLN:NE2	1:F:282:SER:OG	2.43	0.51
1:G:224:GLN:NE2	1:G:282:SER:OG	2.43	0.51
1:D:120:ALA:O	2:D:300:NDP:H42N	2.10	0.50
1:B:173:LEU:HD13	3:B:400:RAU:CAM	2.42	0.50
1:G:24:HIS:CG	1:G:151:LEU:HD13	2.46	0.50
1:E:224:GLN:NE2	1:E:282:SER:OG	2.43	0.50
1:C:21:TYR:CE1	1:C:151:LEU:HD21	2.47	0.50
1:D:21:TYR:CE1	1:D:151:LEU:HD21	2.47	0.49
1:E:120:ALA:O	2:E:300:NDP:H42N	2.13	0.49
1:D:177:TYR:OH	3:D:400:RAU:CAM	2.61	0.49
1:D:239:MET:HE2	1:D:240:GLN:N	2.27	0.49
1:A:21:TYR:CE1	1:A:151:LEU:HD21	2.47	0.49
1:A:118:ILE:O	2:A:300:NDP:H5N	2.13	0.49
1:G:13:MET:CE	2:G:300:NDP:H42N	2.44	0.48
1:G:118:ILE:O	2:G:300:NDP:H5N	2.14	0.48
1:H:120:ALA:O	2:H:300:NDP:H42N	2.14	0.48
1:H:189:LEU:HD23	1:H:256:VAL:HG21	1.96	0.47
1:B:120:ALA:O	2:B:300:NDP:H42N	2.14	0.47
1:A:24:HIS:CD2	1:C:128:PRO:HB3	2.50	0.47
1:G:93:ASN:HB2	2:G:300:NDP:O2D	2.15	0.46
1:E:21:TYR:CE1	1:E:151:LEU:HD21	2.51	0.46
1:G:13:MET:HE3	2:G:300:NDP:H42N	1.98	0.46
1:D:239:MET:CE	3:F:400:RAU:CAL	2.94	0.45
1:B:190:ILE:CG1	1:B:203:LEU:HD22	2.47	0.45
1:C:118:ILE:O	2:C:300:NDP:H5N	2.16	0.45
1:F:13:MET:CE	2:F:300:NDP:H42N	2.47	0.45
1:E:190:ILE:CG1	1:E:203:LEU:HD22	2.47	0.45
1:A:37:LYS:HE2	1:A:37:LYS:HB3	1.64	0.45
1:A:95:THR:HG22	1:A:98:GLN:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:53:SER:HA	1:G:82:THR:HG21	1.99	0.45
1:C:190:ILE:CG1	1:C:203:LEU:HD22	2.47	0.45
1:H:118:ILE:O	2:H:300:NDP:H5N	2.17	0.45
1:G:190:ILE:CG1	1:G:203:LEU:HD22	2.47	0.45
1:H:190:ILE:CG1	1:H:203:LEU:HD22	2.47	0.45
1:F:190:ILE:CG1	1:F:203:LEU:HD22	2.47	0.44
1:G:208:THR:HB	1:G:209:PRO:HD3	1.99	0.44
1:D:190:ILE:CG1	1:D:203:LEU:HD22	2.47	0.44
1:G:120:ALA:O	2:G:300:NDP:H42N	2.16	0.44
1:B:53:SER:HA	1:B:82:THR:HG21	1.99	0.44
1:A:148:HIS:O	1:A:151:LEU:HD22	2.18	0.44
1:A:33:ARG:HD2	2:A:300:NDP:O3X	2.18	0.44
1:E:53:SER:HA	1:E:82:THR:HG21	2.00	0.44
1:C:53:SER:HA	1:C:82:THR:HG21	1.99	0.43
1:C:148:HIS:O	1:C:151:LEU:HD22	2.18	0.43
1:D:10:LEU:HD11	1:D:30:VAL:HB	2.00	0.43
1:F:57:ASN:HD21	1:F:82:THR:HG22	1.83	0.43
1:F:208:THR:HB	1:F:209:PRO:HD3	2.00	0.43
1:G:95:THR:HG22	1:G:98:GLN:H	1.83	0.43
1:H:13:MET:CE	2:H:300:NDP:H42N	2.48	0.43
1:H:208:THR:HB	1:H:209:PRO:HD3	2.00	0.43
1:E:10:LEU:HD11	1:E:30:VAL:HB	2.01	0.43
1:E:177:TYR:OH	3:E:400:RAU:CAM	2.66	0.43
1:D:53:SER:HA	1:D:82:THR:HG21	1.99	0.43
1:C:95:THR:HG22	1:C:98:GLN:H	1.83	0.43
1:D:93:ASN:ND2	1:F:243:GLY:HA2	2.33	0.43
1:D:33:ARG:HD2	2:D:300:NDP:O1X	2.19	0.43
1:D:95:THR:HG22	1:D:98:GLN:H	1.84	0.43
1:E:95:THR:HG22	1:E:98:GLN:H	1.84	0.43
1:D:119:MET:HG3	1:D:172:LEU:HD23	2.01	0.42
2:E:300:NDP:H41N	3:E:400:RAU:CAG	2.49	0.42
4:B:2053:HOH:O	1:C:121:VAL:HG13	2.19	0.42
1:C:83:LEU:N	1:C:84:PRO:CD	2.82	0.42
1:E:146:GLU:O	1:E:150:SER:OG	2.31	0.42
1:E:148:HIS:O	1:E:151:LEU:HD22	2.18	0.42
1:G:10:LEU:HD11	1:G:30:VAL:HB	2.01	0.42
1:D:148:HIS:O	1:D:151:LEU:HD22	2.18	0.42
1:A:10:LEU:HD11	1:A:30:VAL:HB	2.01	0.42
1:B:208:THR:HB	1:B:209:PRO:HD3	2.00	0.42
1:H:95:THR:HG22	1:H:98:GLN:H	1.84	0.42
1:G:76:LEU:O	1:G:80:LEU:HD13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:LEU:HD11	1:B:30:VAL:HB	2.02	0.42
1:H:76:LEU:O	1:H:80:LEU:HD13	2.20	0.42
1:B:95:THR:HG22	1:B:98:GLN:H	1.85	0.42
1:F:10:LEU:HD11	1:F:30:VAL:HB	2.02	0.42
1:F:76:LEU:O	1:F:80:LEU:HD13	2.19	0.42
1:D:11:GLY:O	1:D:15:THR:HG22	2.20	0.41
1:E:33:ARG:HD2	2:E:300:NDP:O3X	2.21	0.41
1:A:208:THR:HB	1:A:209:PRO:HD3	2.02	0.41
1:B:76:LEU:O	1:B:80:LEU:HD13	2.20	0.41
1:H:10:LEU:HD11	1:H:30:VAL:HB	2.02	0.41
1:H:57:ASN:HD21	1:H:82:THR:HG22	1.84	0.41
1:A:53:SER:HA	1:A:82:THR:HG21	2.01	0.41
1:A:151:LEU:C	1:A:151:LEU:HD23	2.40	0.41
1:D:194:GLN:NE2	1:F:161:ASP:OD2	2.53	0.41
1:C:122:PRO:HD3	2:C:300:NDP:N7N	2.36	0.41
1:C:76:LEU:O	1:C:80:LEU:HD13	2.21	0.41
1:E:93:ASN:ND2	1:H:243:GLY:HA2	2.36	0.41
1:C:10:LEU:HD11	1:C:30:VAL:HB	2.01	0.41
1:D:151:LEU:C	1:D:151:LEU:HD23	2.41	0.41
1:D:236:ASN:O	1:D:239:MET:HG3	2.21	0.41
1:E:151:LEU:C	1:E:151:LEU:HD23	2.42	0.41
1:C:208:THR:HB	1:C:209:PRO:HD3	2.02	0.40
1:E:11:GLY:O	1:E:15:THR:HG22	2.21	0.40
1:D:177:TYR:CE2	3:D:400:RAU:CAM	3.05	0.40
1:C:151:LEU:HD23	1:C:151:LEU:C	2.41	0.40
1:E:243:GLY:HA2	1:H:93:ASN:ND2	2.37	0.40
1:D:208:THR:HB	1:D:209:PRO:HD3	2.03	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	287/295 (97%)	283 (99%)	4 (1%)	0	100	100
1	B	287/295 (97%)	283 (99%)	4 (1%)	0	100	100
1	C	286/295 (97%)	282 (99%)	4 (1%)	0	100	100
1	D	286/295 (97%)	282 (99%)	4 (1%)	0	100	100
1	E	286/295 (97%)	282 (99%)	4 (1%)	0	100	100
1	F	287/295 (97%)	283 (99%)	4 (1%)	0	100	100
1	G	287/295 (97%)	283 (99%)	4 (1%)	0	100	100
1	H	287/295 (97%)	283 (99%)	4 (1%)	0	100	100
All	All	2293/2360 (97%)	2261 (99%)	32 (1%)	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	221/233 (95%)	208 (94%)	13 (6%)	19	22
1	B	219/233 (94%)	207 (94%)	12 (6%)	21	24
1	C	218/233 (94%)	206 (94%)	12 (6%)	21	24
1	D	219/233 (94%)	204 (93%)	15 (7%)	16	16
1	E	214/233 (92%)	200 (94%)	14 (6%)	17	18
1	F	219/233 (94%)	207 (94%)	12 (6%)	21	24
1	G	220/233 (94%)	209 (95%)	11 (5%)	24	28
1	H	220/233 (94%)	203 (92%)	17 (8%)	13	12
All	All	1750/1864 (94%)	1644 (94%)	106 (6%)	18	20

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	THR
1	A	28	THR

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Mol	Chain	Res	Type
1	A	33	ARG
1	A	37	LYS
1	A	54	GLU
1	A	80	LEU
1	A	95	THR
1	A	151	LEU
1	A	206	LEU
1	A	236	ASN
1	A	244	VAL
1	A	256	VAL
1	A	262	LEU
1	B	15	THR
1	B	27	LYS
1	B	28	THR
1	B	54	GLU
1	B	80	LEU
1	B	95	THR
1	B	206	LEU
1	B	236	ASN
1	B	244	VAL
1	B	256	VAL
1	B	262	LEU
1	B	265	LYS
1	C	15	THR
1	C	28	THR
1	C	54	GLU
1	C	80	LEU
1	C	95	THR
1	C	151	LEU
1	C	194	GLN
1	C	206	LEU
1	C	236	ASN
1	C	244	VAL
1	C	256	VAL
1	C	262	LEU
1	D	15	THR
1	D	27	LYS
1	D	28	THR
1	D	33	ARG
1	D	54	GLU
1	D	80	LEU
1	D	95	THR

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Mol	Chain	Res	Type
1	D	151	LEU
1	D	194	GLN
1	D	206	LEU
1	D	236	ASN
1	D	239	MET
1	D	244	VAL
1	D	256	VAL
1	D	262	LEU
1	E	15	THR
1	E	28	THR
1	E	33	ARG
1	E	54	GLU
1	E	80	LEU
1	E	95	THR
1	E	140	GLU
1	E	151	LEU
1	E	194	GLN
1	E	206	LEU
1	E	236	ASN
1	E	244	VAL
1	E	256	VAL
1	E	262	LEU
1	F	15	THR
1	F	28	THR
1	F	52	ILE
1	F	54	GLU
1	F	80	LEU
1	F	206	LEU
1	F	236	ASN
1	F	244	VAL
1	F	256	VAL
1	F	262	LEU
1	F	265	LYS
1	F	290	VAL
1	G	15	THR
1	G	27	LYS
1	G	28	THR
1	G	54	GLU
1	G	80	LEU
1	G	95	THR
1	G	206	LEU
1	G	236	ASN

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Mol	Chain	Res	Type
1	G	256	VAL
1	G	262	LEU
1	G	265	LYS
1	H	15	THR
1	H	27	LYS
1	H	28	THR
1	H	35	THR
1	H	54	GLU
1	H	80	LEU
1	H	95	THR
1	H	164	SER
1	H	173	LEU
1	H	206	LEU
1	H	207	LEU
1	H	244	VAL
1	H	256	VAL
1	H	262	LEU
1	H	265	LYS
1	H	267	LEU
1	H	290	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	224	GLN
1	A	236	ASN
1	A	246	ASN
1	B	57	ASN
1	B	81	GLN
1	B	224	GLN
1	B	236	ASN
1	C	57	ASN
1	C	194	GLN
1	C	224	GLN
1	C	236	ASN
1	C	246	ASN
1	D	57	ASN
1	D	93	ASN
1	D	224	GLN
1	D	236	ASN
1	D	246	ASN

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Mol	Chain	Res	Type
1	E	57	ASN
1	E	93	ASN
1	E	224	GLN
1	E	236	ASN
1	E	246	ASN
1	F	57	ASN
1	F	81	GLN
1	F	93	ASN
1	F	224	GLN
1	F	236	ASN
1	F	246	ASN
1	G	57	ASN
1	G	81	GLN
1	G	93	ASN
1	G	143	GLN
1	G	224	GLN
1	G	236	ASN
1	G	246	ASN
1	H	57	ASN
1	H	81	GLN
1	H	93	ASN
1	H	143	GLN
1	H	224	GLN
1	H	246	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

16 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	NDP	G	300	-	45,52,52	1.15	3 (6%)	53,80,80	1.40	7 (13%)
3	RAU	E	400	-	13,14,14	4.86	8 (61%)	15,18,18	1.43	2 (13%)
3	RAU	G	400	-	13,14,14	4.35	7 (53%)	15,18,18	2.09	6 (40%)
2	NDP	D	300	-	45,52,52	1.00	3 (6%)	53,80,80	1.54	11 (20%)
2	NDP	A	300	-	45,52,52	1.02	2 (4%)	53,80,80	1.39	8 (15%)
2	NDP	F	300	-	45,52,52	1.12	3 (6%)	53,80,80	1.29	7 (13%)
3	RAU	A	400	-	13,14,14	4.32	5 (38%)	15,18,18	2.29	3 (20%)
3	RAU	H	400	-	13,14,14	4.30	8 (61%)	15,18,18	2.16	3 (20%)
3	RAU	F	400	-	13,14,14	4.57	7 (53%)	15,18,18	2.67	6 (40%)
2	NDP	B	300	-	45,52,52	1.29	5 (11%)	53,80,80	1.45	7 (13%)
2	NDP	C	300	-	45,52,52	1.04	3 (6%)	53,80,80	1.36	6 (11%)
3	RAU	B	400	-	13,14,14	5.25	7 (53%)	15,18,18	1.98	2 (13%)
3	RAU	D	400	-	13,14,14	4.50	7 (53%)	15,18,18	2.19	3 (20%)
2	NDP	H	300	-	45,52,52	1.16	4 (8%)	53,80,80	1.43	8 (15%)
2	NDP	E	300	-	45,52,52	1.24	6 (13%)	53,80,80	1.75	11 (20%)
3	RAU	C	400	-	13,14,14	4.16	6 (46%)	15,18,18	2.46	3 (20%)

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	NDP	G	300	-	-	7/30/77/77	0/5/5/5
3	RAU	E	400	-	-	0/3/13/13	0/2/2/2
3	RAU	G	400	-	-	1/3/13/13	0/2/2/2
2	NDP	D	300	-	-	6/30/77/77	0/5/5/5
2	NDP	A	300	-	-	5/30/77/77	0/5/5/5
2	NDP	F	300	-	-	8/30/77/77	0/5/5/5
3	RAU	A	400	-	-	1/3/13/13	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	RAU	H	400	-	-	1/3/13/13	0/2/2/2
3	RAU	F	400	-	-	2/3/13/13	0/2/2/2
2	NDP	B	300	-	-	8/30/77/77	0/5/5/5
2	NDP	C	300	-	-	6/30/77/77	0/5/5/5
3	RAU	B	400	-	-	1/3/13/13	0/2/2/2
3	RAU	D	400	-	-	0/3/13/13	0/2/2/2
2	NDP	H	300	-	-	7/30/77/77	0/5/5/5
2	NDP	E	300	-	-	5/30/77/77	0/5/5/5
3	RAU	C	400	-	-	0/3/13/13	0/2/2/2

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	400	RAU	CAF-CAI	-10.47	1.38	1.51
3	E	400	RAU	CAF-CAI	-9.88	1.39	1.51
3	C	400	RAU	CAF-CAI	-9.76	1.39	1.51
3	F	400	RAU	CAF-CAI	-9.71	1.39	1.51
3	G	400	RAU	CAG-CAE	-9.69	1.36	1.51
3	B	400	RAU	CAF-CAI	-9.45	1.39	1.51
3	F	400	RAU	CAG-CAE	-9.20	1.37	1.51
3	E	400	RAU	CAG-CAE	-9.18	1.37	1.51
3	B	400	RAU	CAL-CAM	-9.11	0.90	1.18
3	A	400	RAU	CAG-CAE	-9.04	1.37	1.51
3	C	400	RAU	CAG-CAE	-9.04	1.37	1.51
3	D	400	RAU	CAF-CAI	-8.85	1.40	1.51
3	G	400	RAU	CAF-CAI	-8.81	1.40	1.51
3	B	400	RAU	CAK-CAL	-8.48	1.27	1.46
3	H	400	RAU	CAG-CAE	-8.23	1.38	1.51
3	D	400	RAU	CAG-CAE	-8.15	1.38	1.51
3	H	400	RAU	CAF-CAI	-7.66	1.41	1.51
3	B	400	RAU	CAG-CAE	-7.66	1.39	1.51
3	D	400	RAU	CAK-CAL	-7.39	1.30	1.46
3	H	400	RAU	CAL-CAM	-6.26	0.99	1.18
3	F	400	RAU	CAA-CAF	-5.86	1.32	1.39
3	E	400	RAU	CAL-CAM	-5.62	1.01	1.18
3	G	400	RAU	CAA-CAF	-5.42	1.32	1.39
3	H	400	RAU	CAK-CAL	-5.30	1.34	1.46
3	D	400	RAU	CAL-CAM	-5.25	1.02	1.18
3	A	400	RAU	CAA-CAF	-5.18	1.32	1.39
3	E	400	RAU	CAH-CAI	-5.10	1.48	1.54
3	B	400	RAU	CAA-CAF	-5.02	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	400	RAU	CAK-CAL	-4.74	1.36	1.46
3	H	400	RAU	CAA-CAF	-4.45	1.33	1.39
3	F	400	RAU	CAK-CAL	4.37	1.56	1.46
3	E	400	RAU	CAA-CAF	-4.23	1.34	1.39
3	E	400	RAU	CAD-CAE	-4.22	1.32	1.39
3	C	400	RAU	CAA-CAF	-4.14	1.34	1.39
3	F	400	RAU	CAD-CAE	-4.09	1.32	1.39
3	G	400	RAU	CAD-CAE	-3.97	1.32	1.39
3	C	400	RAU	CAD-CAE	-3.96	1.32	1.39
3	D	400	RAU	CAA-CAF	-3.87	1.34	1.39
3	F	400	RAU	CAL-CAM	3.81	1.29	1.18
3	B	400	RAU	CAD-CAE	-3.79	1.33	1.39
2	B	300	NDP	C2A-N3A	3.78	1.38	1.32
3	A	400	RAU	CAD-CAE	-3.69	1.33	1.39
3	H	400	RAU	CAD-CAE	-3.58	1.33	1.39
3	B	400	RAU	CAE-CAF	-3.42	1.33	1.39
2	G	300	NDP	C6N-C5N	3.29	1.39	1.33
3	G	400	RAU	CAL-CAM	-3.24	1.08	1.18
2	H	300	NDP	C6N-C5N	3.18	1.39	1.33
2	B	300	NDP	C6N-C5N	3.06	1.38	1.33
2	E	300	NDP	O4B-C1B	3.03	1.45	1.41
2	F	300	NDP	C6N-C5N	3.03	1.38	1.33
2	B	300	NDP	C5A-C4A	2.97	1.48	1.40
3	D	400	RAU	CAD-CAE	-2.96	1.34	1.39
2	G	300	NDP	C5A-C4A	2.95	1.48	1.40
2	H	300	NDP	C5A-C4A	2.83	1.48	1.40
2	A	300	NDP	C6N-C5N	2.80	1.38	1.33
3	C	400	RAU	CAE-CAF	-2.78	1.34	1.39
3	H	400	RAU	CAE-CAF	-2.76	1.34	1.39
2	H	300	NDP	P2B-O2B	2.75	1.64	1.59
3	G	400	RAU	CAH-CAG	-2.74	1.47	1.53
2	F	300	NDP	C5A-C4A	2.71	1.48	1.40
3	D	400	RAU	CAE-CAF	-2.63	1.34	1.39
2	G	300	NDP	C2A-N3A	2.61	1.36	1.32
2	B	300	NDP	C4A-N3A	2.58	1.39	1.35
3	E	400	RAU	CAE-CAF	-2.56	1.34	1.39
2	E	300	NDP	C6N-C5N	2.56	1.37	1.33
2	D	300	NDP	C5A-C4A	2.51	1.47	1.40
2	E	300	NDP	C2A-N3A	2.50	1.36	1.32
2	E	300	NDP	C5A-C4A	2.47	1.47	1.40
2	B	300	NDP	P2B-O2B	2.46	1.63	1.59
2	F	300	NDP	C2A-N3A	2.46	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	300	NDP	O5B-C5B	-2.45	1.35	1.44
2	C	300	NDP	C5A-C4A	2.44	1.47	1.40
2	D	300	NDP	C6N-C5N	2.42	1.37	1.33
3	A	400	RAU	CAE-CAF	-2.33	1.35	1.39
2	A	300	NDP	C2A-N3A	2.26	1.35	1.32
3	C	400	RAU	CAH-CAI	-2.20	1.51	1.54
2	E	300	NDP	C4N-C5N	-2.20	1.43	1.48
2	D	300	NDP	C4N-C5N	-2.19	1.43	1.48
3	G	400	RAU	CAE-CAF	-2.15	1.35	1.39
2	C	300	NDP	C4N-C5N	-2.08	1.43	1.48
3	F	400	RAU	CAH-CAG	-2.07	1.48	1.53
2	C	300	NDP	O4B-C1B	2.07	1.44	1.41
2	H	300	NDP	C2A-N3A	2.02	1.35	1.32
3	H	400	RAU	CAH-CAI	-2.02	1.51	1.54

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	400	RAU	CAG-CAH-CAI	-7.56	93.41	105.54
3	C	400	RAU	CAG-CAH-CAI	-7.05	94.22	105.54
3	D	400	RAU	CAH-CAG-CAE	6.55	109.68	103.31
3	B	400	RAU	CAH-CAG-CAE	5.95	109.09	103.31
3	F	400	RAU	CAG-CAH-CAI	-5.24	97.13	105.54
3	H	400	RAU	CAH-CAG-CAE	5.20	108.37	103.31
2	D	300	NDP	N3A-C2A-N1A	-4.56	121.55	128.68
3	C	400	RAU	CAL-CAK-NAJ	-4.54	97.43	112.71
2	E	300	NDP	N3A-C2A-N1A	-4.51	121.62	128.68
2	A	300	NDP	N3A-C2A-N1A	-4.49	121.66	128.68
2	G	300	NDP	N3A-C2A-N1A	-4.42	121.77	128.68
2	H	300	NDP	N3A-C2A-N1A	-4.40	121.81	128.68
3	F	400	RAU	CAH-CAI-NAJ	-4.38	106.12	115.26
2	C	300	NDP	N3A-C2A-N1A	-4.36	121.87	128.68
3	H	400	RAU	CAG-CAH-CAI	-4.27	98.68	105.54
2	B	300	NDP	C5A-C6A-N6A	-4.25	113.90	120.35
3	F	400	RAU	CAK-NAJ-CAI	4.22	122.36	113.85
2	F	300	NDP	N3A-C2A-N1A	-4.10	122.28	128.68
2	B	300	NDP	N3A-C2A-N1A	-3.99	122.44	128.68
2	E	300	NDP	C5B-C4B-C3B	-3.86	100.72	115.18
3	B	400	RAU	CAG-CAH-CAI	-3.80	99.44	105.54
2	B	300	NDP	N6A-C6A-N1A	3.79	126.44	118.57
3	G	400	RAU	CAD-CAE-CAF	3.75	124.35	120.00
2	E	300	NDP	O4B-C4B-C5B	3.70	121.55	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	400	RAU	CAG-CAH-CAI	-3.69	99.62	105.54
3	E	400	RAU	CAG-CAH-CAI	-3.49	99.94	105.54
2	E	300	NDP	O2N-PN-O1N	3.41	129.08	112.24
2	E	300	NDP	O4B-C4B-C3B	3.39	111.82	105.11
3	G	400	RAU	CAH-CAI-NAJ	-3.37	108.24	115.26
2	G	300	NDP	C1B-N9A-C4A	-3.33	120.79	126.64
3	H	400	RAU	CAL-CAK-NAJ	-3.24	101.81	112.71
3	F	400	RAU	CAL-CAK-NAJ	-3.24	101.81	112.71
2	H	300	NDP	O2B-P2B-O1X	-3.19	97.06	109.39
3	F	400	RAU	CAD-CAE-CAF	3.16	123.67	120.00
2	A	300	NDP	C5A-C6A-N6A	-3.12	115.61	120.35
3	D	400	RAU	CAL-CAK-NAJ	-3.02	102.54	112.71
2	C	300	NDP	O3X-P2B-O2X	3.00	119.08	107.64
2	C	300	NDP	PN-O3-PA	-2.95	122.69	132.83
3	G	400	RAU	CAH-CAG-CAE	2.94	106.17	103.31
2	F	300	NDP	O2B-P2B-O1X	-2.94	98.05	109.39
3	C	400	RAU	CAK-NAJ-CAI	2.90	119.70	113.85
2	D	300	NDP	PN-O3-PA	-2.88	122.93	132.83
2	B	300	NDP	C3B-C2B-C1B	-2.88	97.48	102.89
2	D	300	NDP	O2N-PN-O1N	2.88	126.47	112.24
2	E	300	NDP	O5B-C5B-C4B	2.84	118.77	108.99
3	G	400	RAU	CAG-CAH-CAI	-2.83	101.00	105.54
2	H	300	NDP	O4D-C1D-N1N	2.81	113.56	108.06
2	E	300	NDP	O4B-C1B-C2B	-2.79	101.75	106.59
2	H	300	NDP	PN-O3-PA	-2.77	123.32	132.83
2	G	300	NDP	C2A-N1A-C6A	2.75	123.46	118.75
2	G	300	NDP	O2B-P2B-O1X	-2.73	98.84	109.39
2	H	300	NDP	C1B-N9A-C4A	-2.71	121.87	126.64
3	F	400	RAU	CAB-CAA-CAF	-2.66	117.63	121.01
2	E	300	NDP	O7N-C7N-C3N	-2.62	115.97	120.90
2	A	300	NDP	PN-O3-PA	-2.59	123.94	132.83
2	D	300	NDP	O2B-P2B-O1X	-2.57	99.47	109.39
2	H	300	NDP	C2A-N1A-C6A	2.55	123.12	118.75
2	D	300	NDP	O3X-P2B-O2X	2.53	117.32	107.64
2	C	300	NDP	C1B-N9A-C4A	-2.53	122.19	126.64
3	E	400	RAU	CAL-CAK-NAJ	-2.51	104.28	112.71
3	A	400	RAU	CAD-CAE-CAF	2.49	122.90	120.00
2	B	300	NDP	O2B-P2B-O1X	-2.44	99.99	109.39
2	H	300	NDP	C3B-C2B-C1B	-2.42	98.35	102.89
2	G	300	NDP	C3B-C2B-C1B	-2.41	98.36	102.89
2	D	300	NDP	O2A-PA-O5B	-2.41	96.57	107.75
2	F	300	NDP	C1B-N9A-C4A	-2.39	122.44	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	300	NDP	N6A-C6A-N1A	2.38	123.52	118.57
2	A	300	NDP	O7N-C7N-C3N	-2.37	116.44	120.90
2	A	300	NDP	N6A-C6A-N1A	2.33	123.42	118.57
2	D	300	NDP	O2X-P2B-O1X	2.33	119.80	110.68
2	D	300	NDP	O4B-C4B-C3B	2.30	109.67	105.11
2	G	300	NDP	PN-O3-PA	-2.30	124.94	132.83
2	E	300	NDP	O3X-P2B-O1X	2.27	119.56	110.68
2	D	300	NDP	C1B-N9A-C4A	-2.23	122.72	126.64
2	C	300	NDP	O2N-PN-O1N	2.22	123.24	112.24
2	E	300	NDP	PN-O3-PA	-2.22	125.21	132.83
2	A	300	NDP	C1B-N9A-C4A	-2.21	122.75	126.64
2	C	300	NDP	O4D-C4D-C3D	2.20	109.46	105.11
2	A	300	NDP	O3X-P2B-O1X	2.18	119.22	110.68
3	G	400	RAU	CAB-CAC-CAD	-2.18	116.88	120.19
2	B	300	NDP	C3N-C2N-N1N	-2.17	120.01	123.10
2	B	300	NDP	C1B-N9A-C4A	-2.15	122.86	126.64
2	F	300	NDP	C2A-N1A-C6A	2.15	122.43	118.75
2	F	300	NDP	C3B-C2B-C1B	-2.14	98.88	102.89
3	A	400	RAU	CAH-CAI-NAJ	-2.13	110.81	115.26
3	G	400	RAU	CAG-CAE-CAD	-2.12	124.17	129.89
2	E	300	NDP	O3B-C3B-C2B	2.09	117.11	111.17
2	A	300	NDP	O2A-PA-O1A	2.09	122.57	112.24
2	G	300	NDP	N6A-C6A-N1A	2.07	122.87	118.57
2	D	300	NDP	N6A-C6A-N1A	2.06	122.84	118.57
2	F	300	NDP	O2N-PN-O1N	2.05	122.37	112.24
2	H	300	NDP	O4D-C4D-C3D	2.03	109.13	105.11
2	D	300	NDP	C2B-C3B-C4B	-2.02	97.61	101.99

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	300	NDP	C5D-O5D-PN-O1N
2	B	300	NDP	C2B-O2B-P2B-O1X
2	B	300	NDP	C5D-O5D-PN-O1N
2	C	300	NDP	C5D-O5D-PN-O1N
2	D	300	NDP	C5D-O5D-PN-O2N
2	E	300	NDP	O4B-C4B-C5B-O5B
2	E	300	NDP	C3B-C4B-C5B-O5B
2	F	300	NDP	C5D-O5D-PN-O2N
2	G	300	NDP	C2B-O2B-P2B-O1X
2	H	300	NDP	C2B-O2B-P2B-O1X

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Mol	Chain	Res	Type	Atoms
3	A	400	RAU	CAF-CAI-NAJ-CAK
3	F	400	RAU	CAH-CAI-NAJ-CAK
3	F	400	RAU	CAF-CAI-NAJ-CAK
2	G	300	NDP	PN-O3-PA-O1A
2	F	300	NDP	C2B-O2B-P2B-O1X
2	E	300	NDP	O4D-C1D-N1N-C6N
2	A	300	NDP	C2B-O2B-P2B-O3X
2	A	300	NDP	C5D-O5D-PN-O3
2	B	300	NDP	C2B-O2B-P2B-O3X
2	B	300	NDP	C5D-O5D-PN-O3
2	D	300	NDP	C2B-O2B-P2B-O3X
2	D	300	NDP	C5D-O5D-PN-O3
2	F	300	NDP	C2B-O2B-P2B-O3X
2	F	300	NDP	C5D-O5D-PN-O3
2	G	300	NDP	C2B-O2B-P2B-O3X
2	H	300	NDP	C2B-O2B-P2B-O3X
2	E	300	NDP	PN-O3-PA-O2A
2	D	300	NDP	O4D-C1D-N1N-C6N
2	F	300	NDP	C5D-O5D-PN-O1N
2	A	300	NDP	O4D-C1D-N1N-C6N
2	C	300	NDP	O4D-C1D-N1N-C6N
3	H	400	RAU	CAH-CAI-NAJ-CAK
2	D	300	NDP	PN-O3-PA-O2A
2	G	300	NDP	PN-O3-PA-O2A
2	B	300	NDP	O4D-C1D-N1N-C6N
2	F	300	NDP	O4D-C1D-N1N-C6N
2	H	300	NDP	O4D-C1D-N1N-C6N
2	F	300	NDP	C2D-C1D-N1N-C6N
2	G	300	NDP	C2D-C1D-N1N-C6N
2	G	300	NDP	O4D-C1D-N1N-C6N
2	B	300	NDP	C2D-C1D-N1N-C6N
2	C	300	NDP	C2B-O2B-P2B-O1X
3	B	400	RAU	CAL-CAK-NAJ-CAI
2	C	300	NDP	C2B-O2B-P2B-O2X
2	E	300	NDP	C5B-O5B-PA-O3
2	H	300	NDP	C5D-O5D-PN-O3
2	A	300	NDP	O4B-C4B-C5B-O5B
2	B	300	NDP	O4B-C4B-C5B-O5B
2	C	300	NDP	O4B-C4B-C5B-O5B
2	D	300	NDP	O4B-C4B-C5B-O5B
2	G	300	NDP	O4B-C4B-C5B-O5B
2	H	300	NDP	O4B-C4B-C5B-O5B

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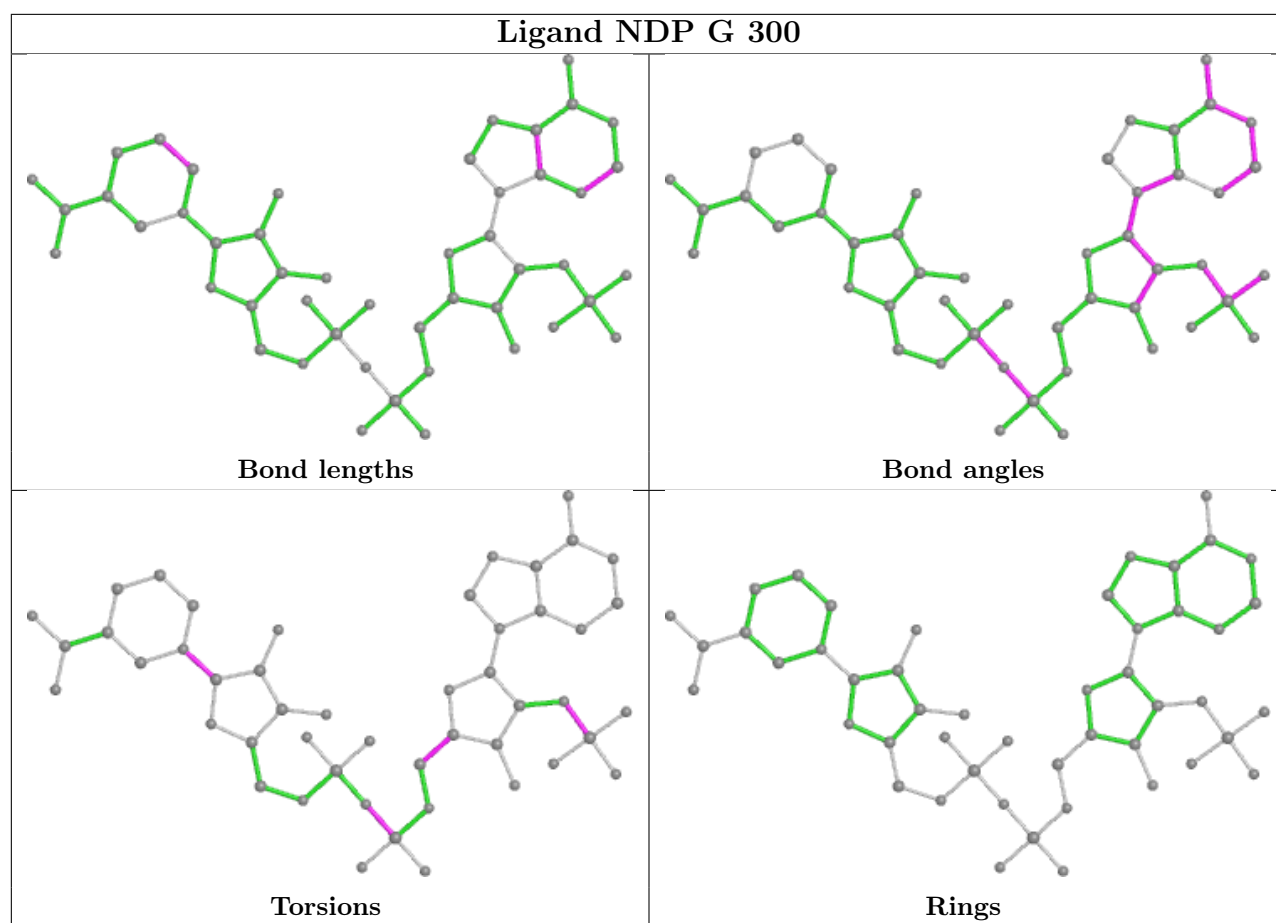
Mol	Chain	Res	Type	Atoms
2	C	300	NDP	PN-O3-PA-O2A
2	B	300	NDP	C5D-O5D-PN-O2N
2	H	300	NDP	C5D-O5D-PN-O1N
2	F	300	NDP	O4B-C4B-C5B-O5B
3	G	400	RAU	CAF-CAI-NAJ-CAK
2	H	300	NDP	C2D-C1D-N1N-C6N

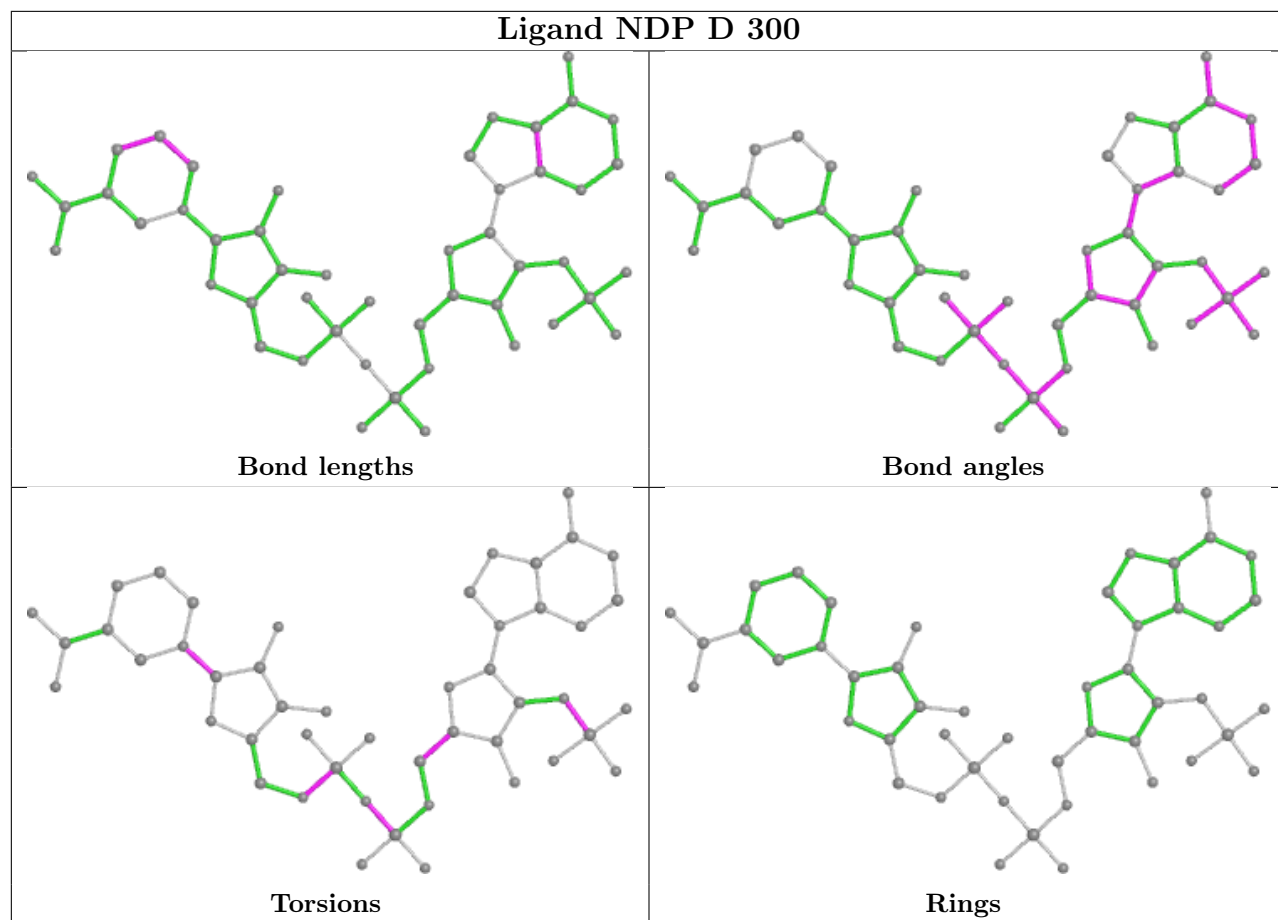
There are no ring outliers.

15 monomers are involved in 42 short contacts:

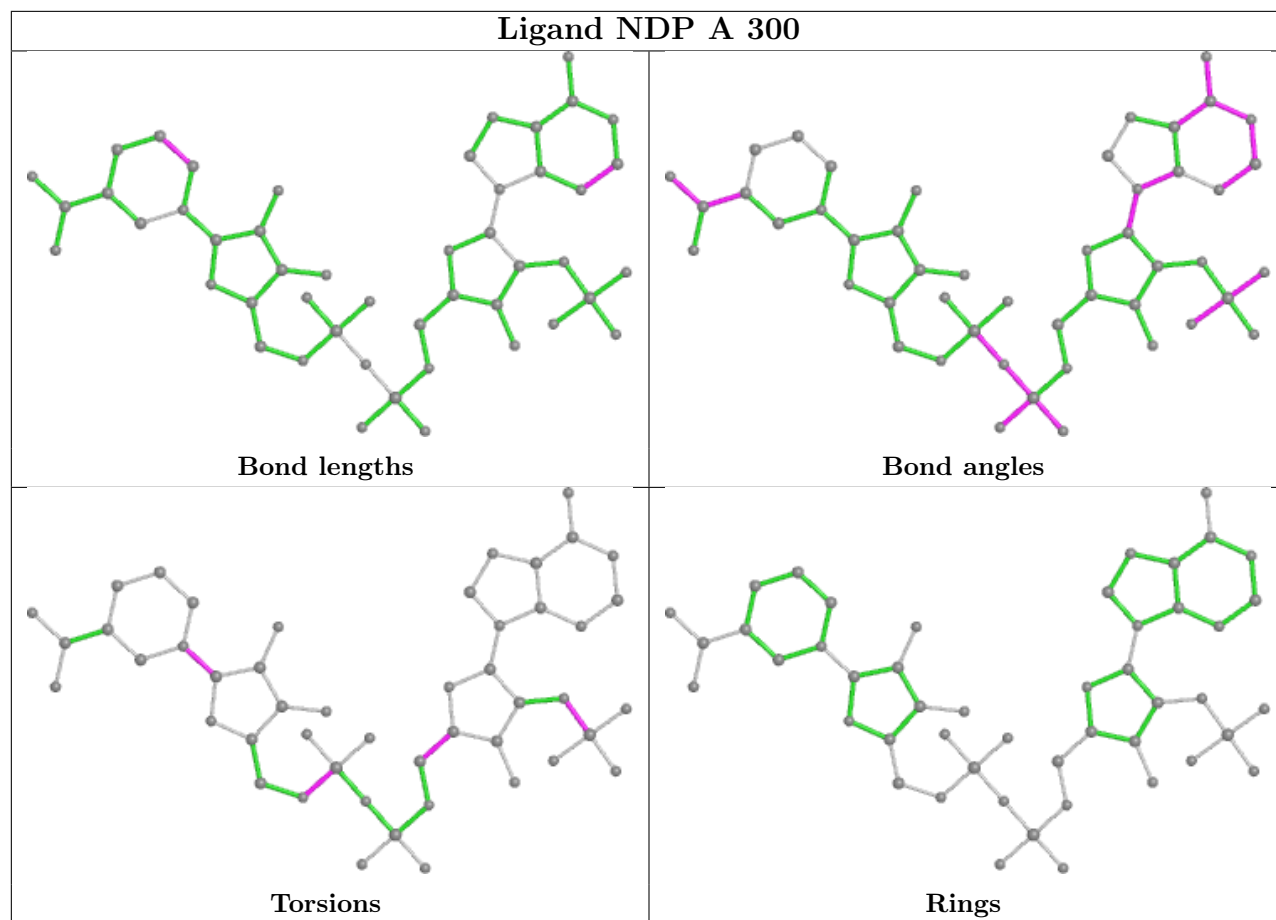
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	300	NDP	5	0
3	E	400	RAU	3	0
2	D	300	NDP	2	0
2	A	300	NDP	3	0
2	F	300	NDP	3	0
3	A	400	RAU	1	0
3	H	400	RAU	1	0
3	F	400	RAU	3	0
2	B	300	NDP	2	0
2	C	300	NDP	3	0
3	B	400	RAU	4	0
3	D	400	RAU	4	0
2	H	300	NDP	3	0
2	E	300	NDP	5	0
3	C	400	RAU	1	0

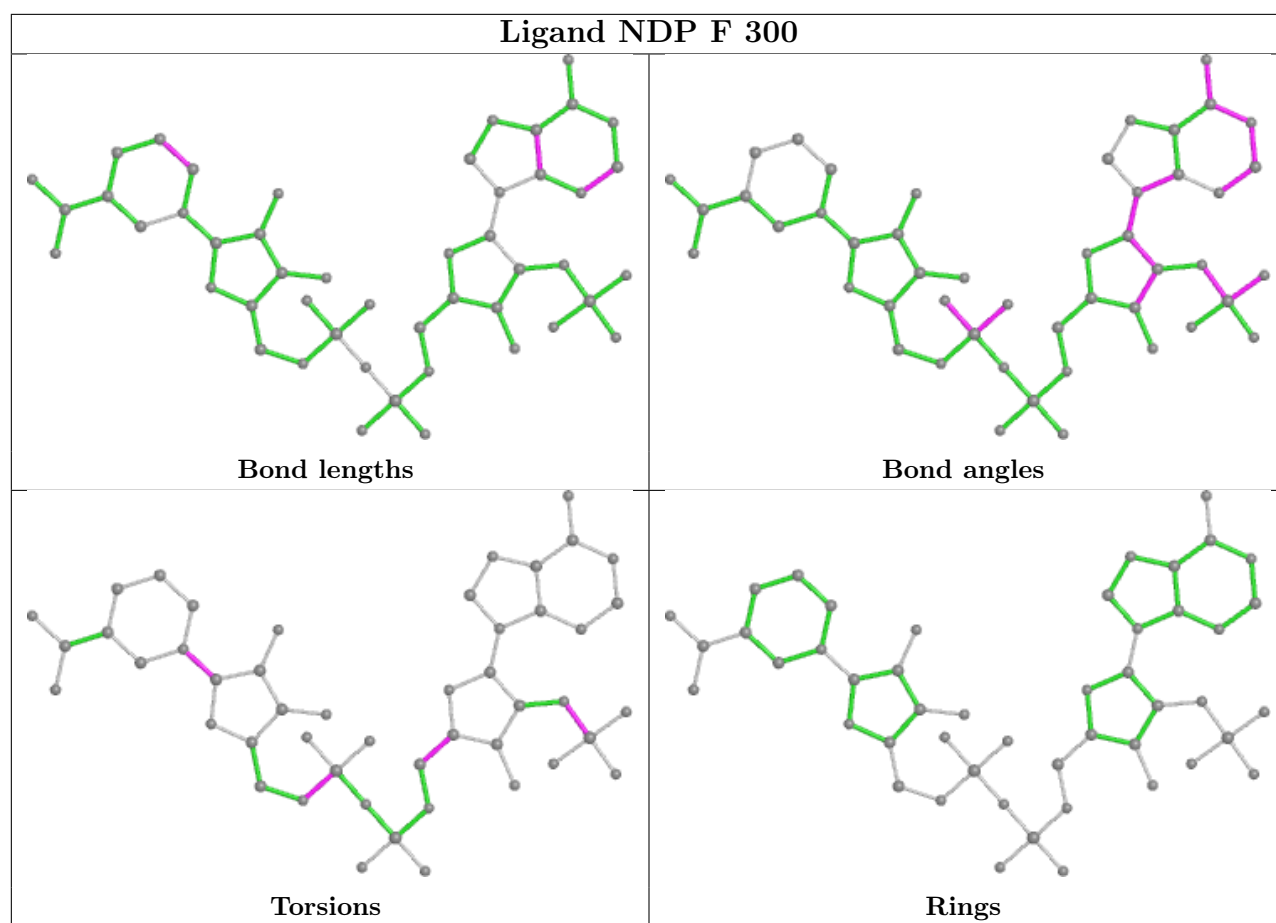
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

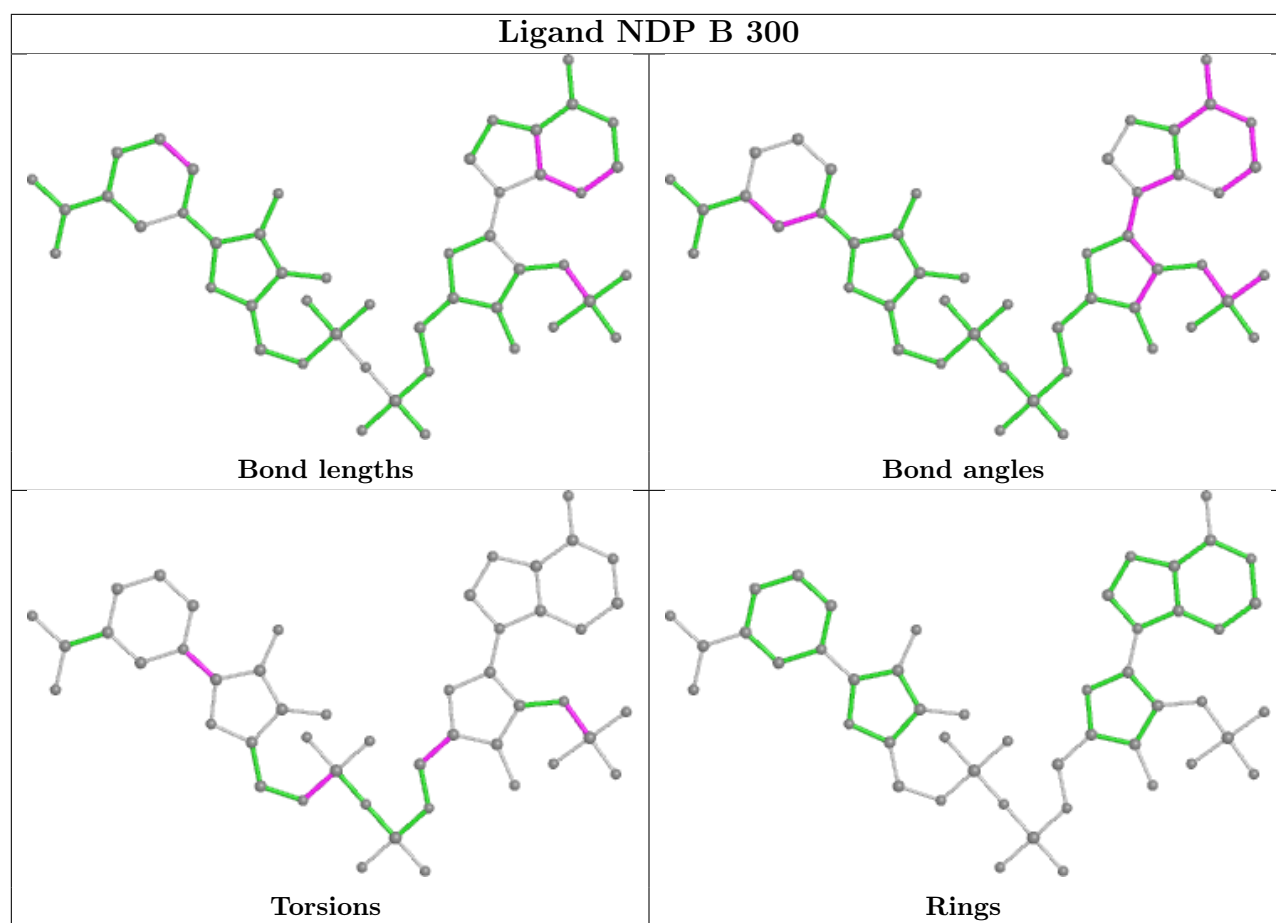


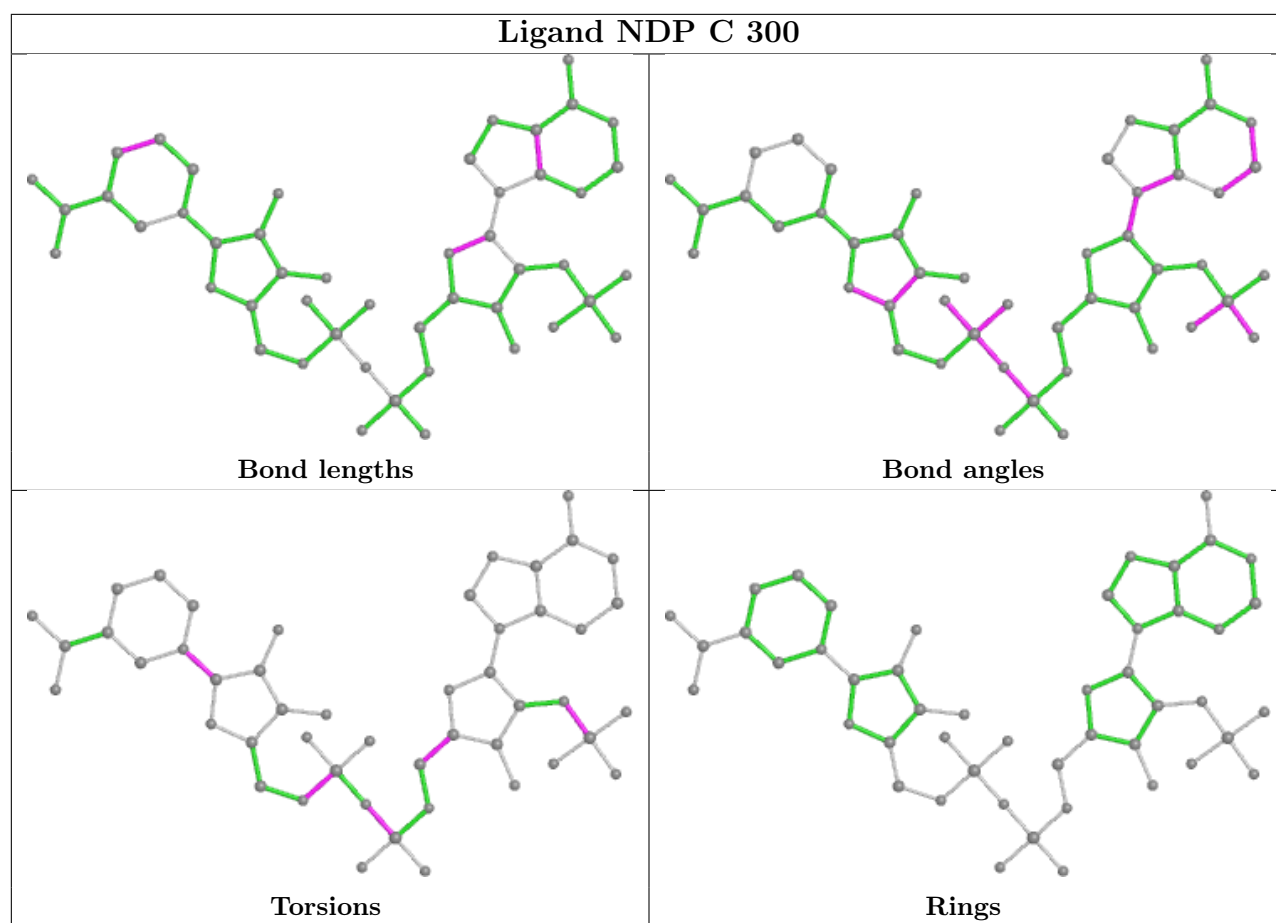


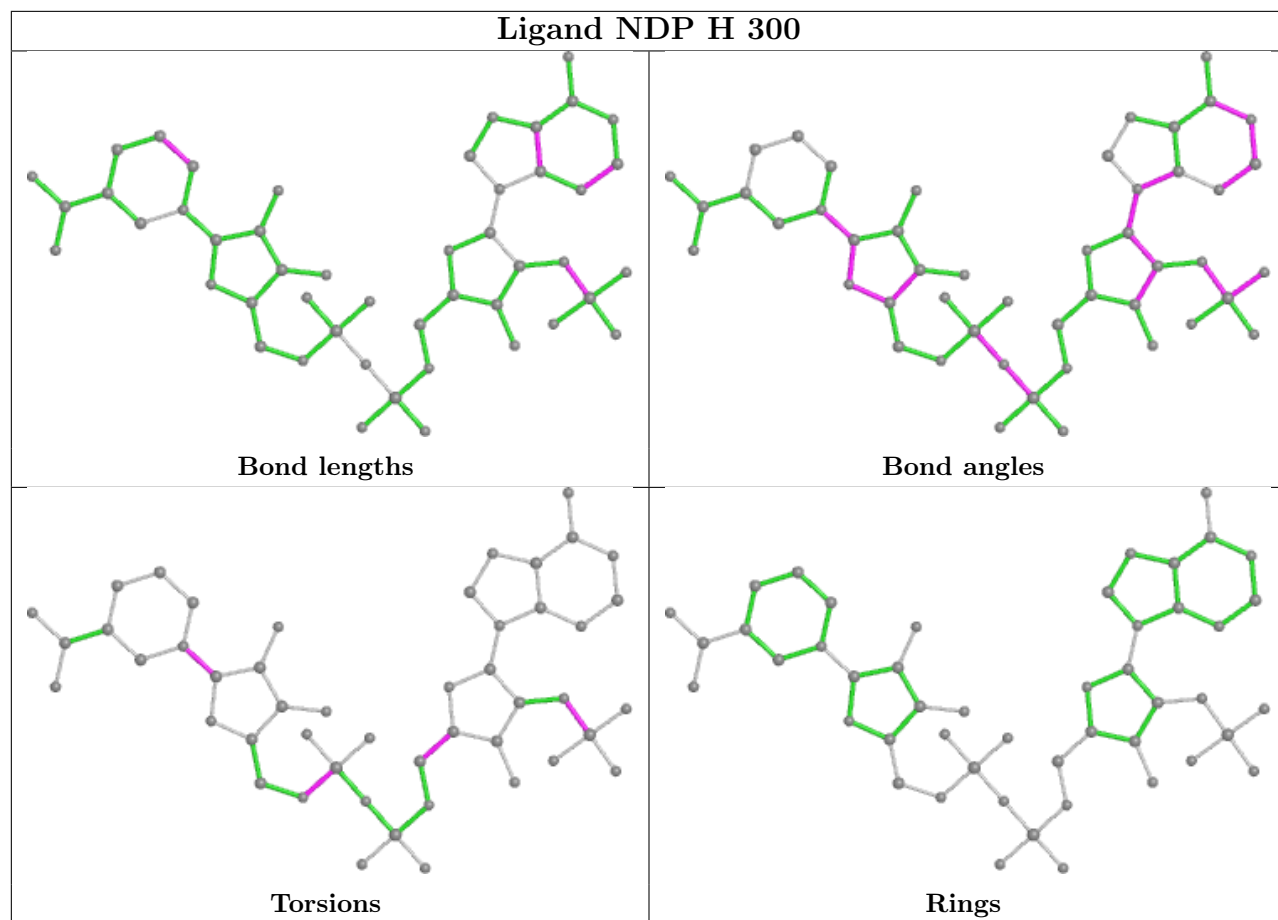


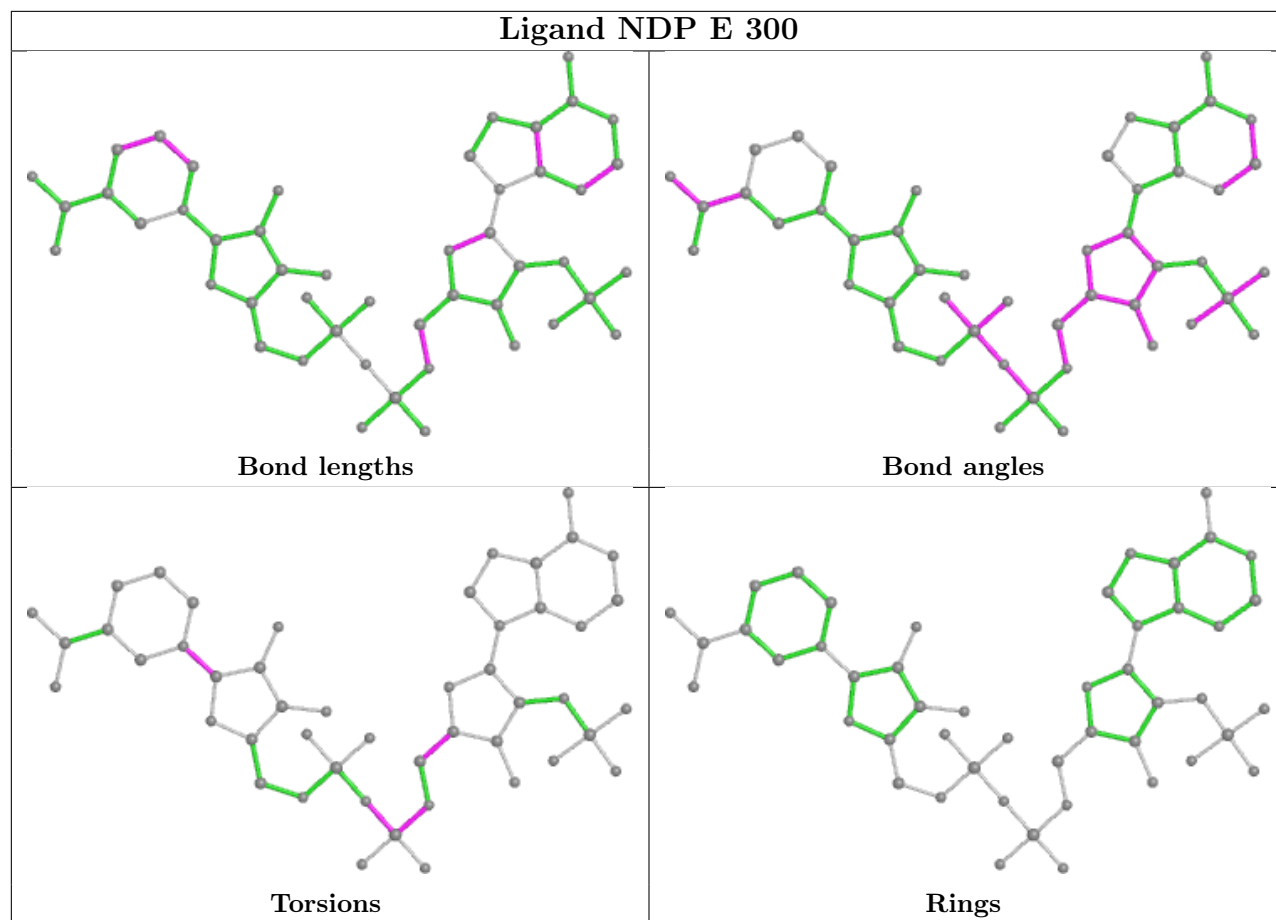












## 5.7 Other polymers [i](#)

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 [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	289/295 (97%)	-0.65	0 100 100	24, 36, 55, 85	0
1	B	289/295 (97%)	-0.58	0 100 100	25, 38, 57, 78	0
1	C	288/295 (97%)	-0.64	0 100 100	25, 37, 53, 72	0
1	D	288/295 (97%)	-0.64	0 100 100	25, 37, 55, 74	0
1	E	288/295 (97%)	-0.63	0 100 100	24, 37, 54, 71	0
1	F	289/295 (97%)	-0.59	0 100 100	24, 37, 55, 82	0
1	G	289/295 (97%)	-0.60	0 100 100	25, 38, 57, 75	0
1	H	289/295 (97%)	-0.60	0 100 100	26, 37, 56, 81	0
All	All	2309/2360 (97%)	-0.62	0 100 100	24, 37, 56, 85	0

There are no RSRZ outliers to report.

### 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](#)

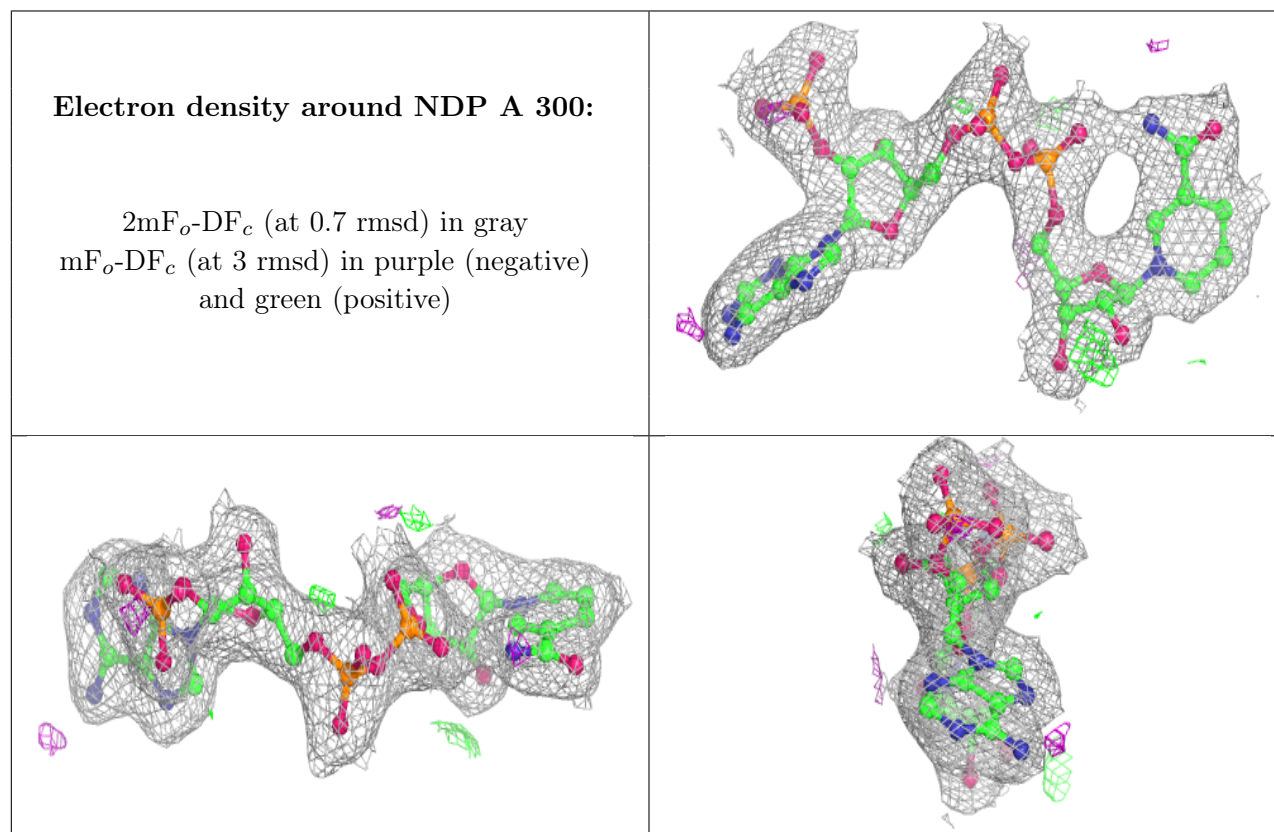
There are no monosaccharides in this entry.

### 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
3	RAU	D	400	13/13	0.93	0.35	64,69,79,80	0
3	RAU	E	400	13/13	0.93	0.28	58,66,80,83	0
3	RAU	F	400	13/13	0.93	0.33	60,67,76,80	0
3	RAU	C	400	13/13	0.94	0.29	60,63,81,82	0
3	RAU	G	400	13/13	0.94	0.26	56,59,64,67	0
3	RAU	B	400	13/13	0.95	0.23	56,61,66,66	0
3	RAU	A	400	13/13	0.95	0.22	54,61,71,73	0
3	RAU	H	400	13/13	0.96	0.27	62,66,71,71	0
2	NDP	A	300	48/48	0.99	0.08	23,28,36,39	0
2	NDP	B	300	48/48	0.99	0.08	31,36,39,41	0
2	NDP	C	300	48/48	0.99	0.08	24,27,34,40	0
2	NDP	D	300	48/48	0.99	0.09	22,28,36,44	0
2	NDP	E	300	48/48	0.99	0.08	22,27,37,43	0
2	NDP	F	300	48/48	0.99	0.09	27,33,38,40	0
2	NDP	G	300	48/48	0.99	0.08	31,35,39,41	0
2	NDP	H	300	48/48	0.99	0.09	29,31,35,38	0

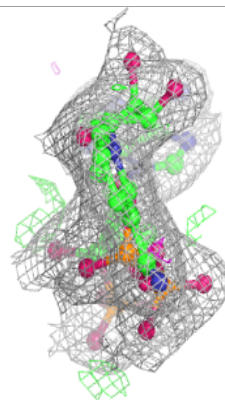
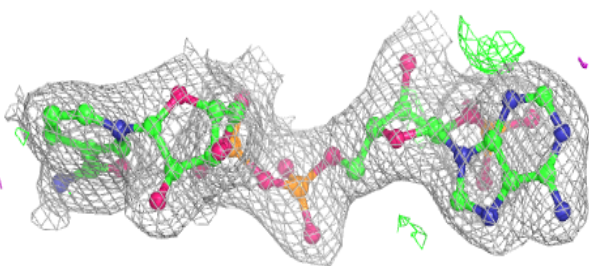
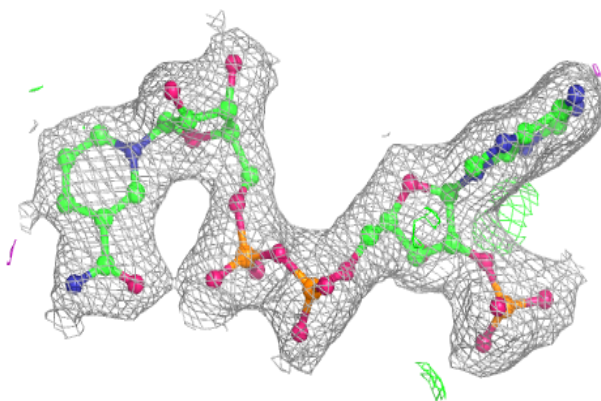
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



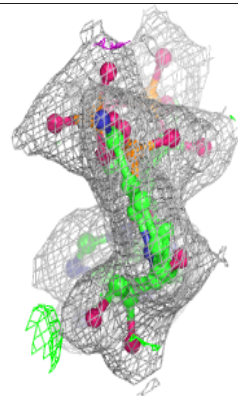
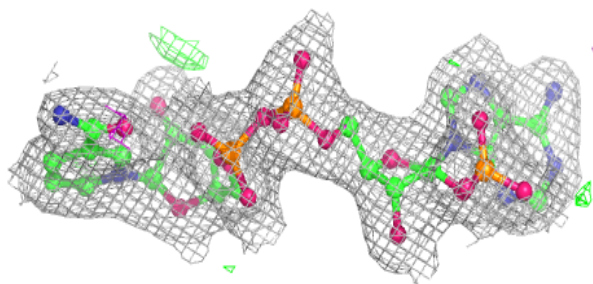
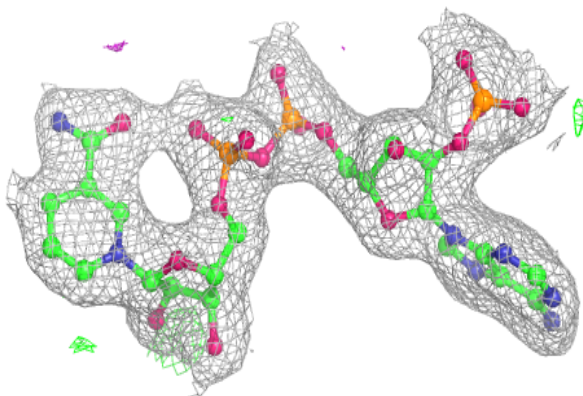


**Electron density around NDP B 300:**

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

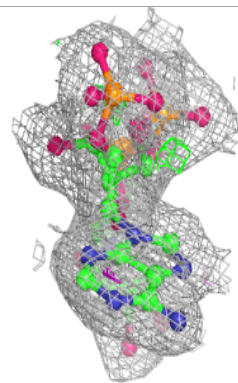
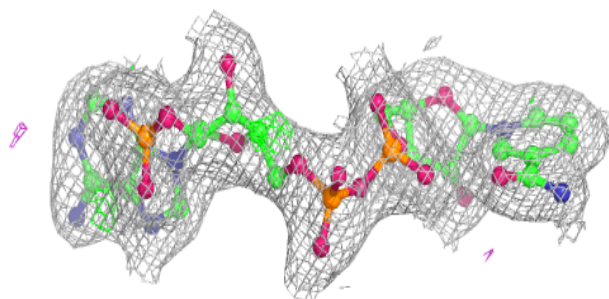
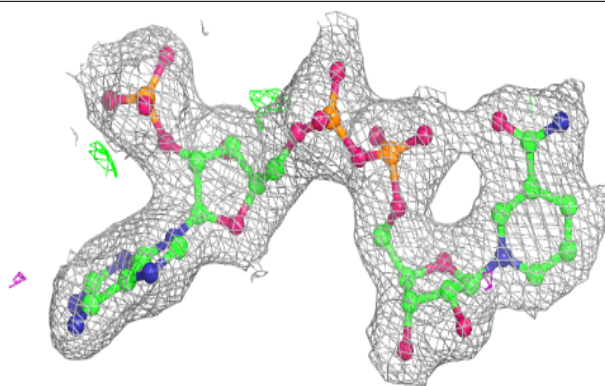
**Electron density around NDP C 300:**

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

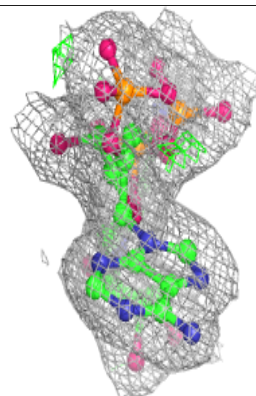
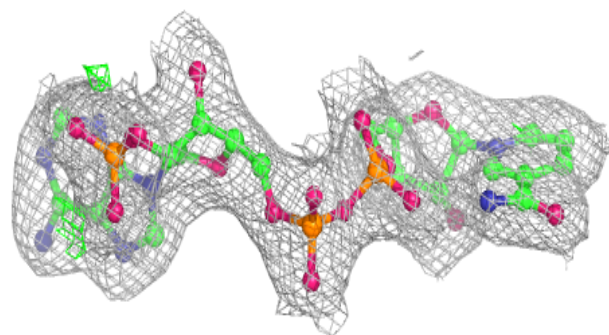
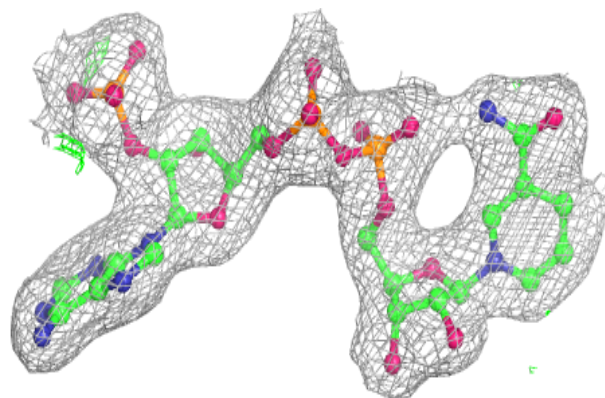


**Electron density around NDP D 300:**

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

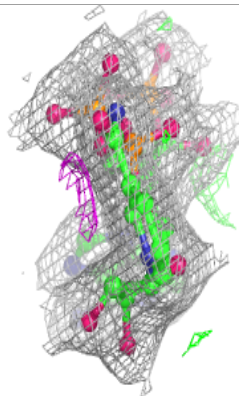
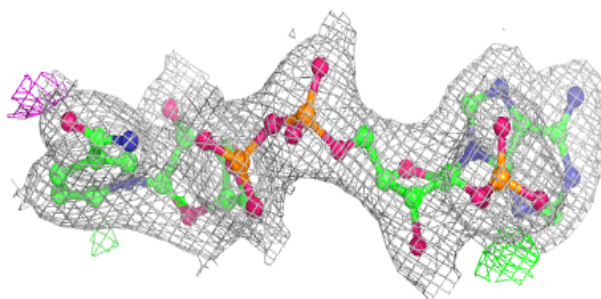
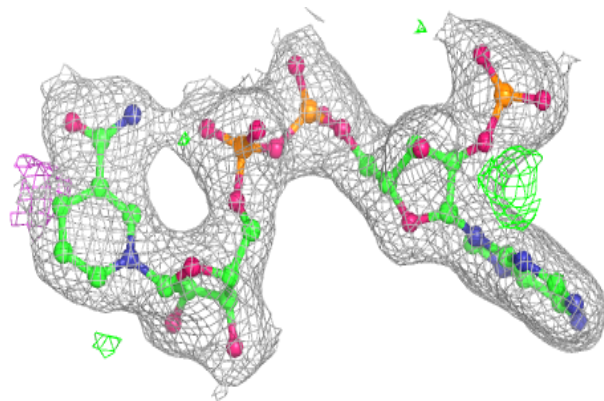
**Electron density around NDP E 300:**

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

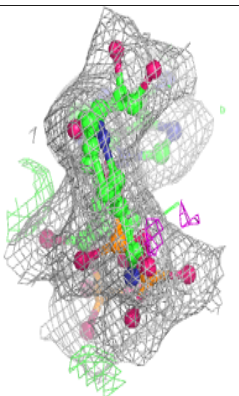
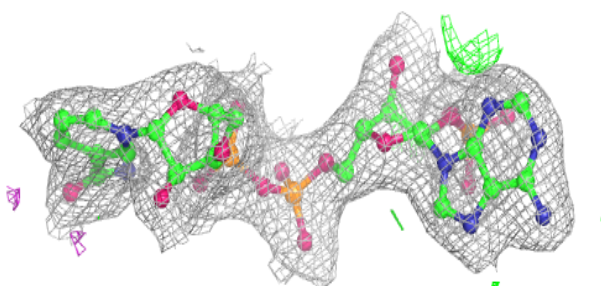
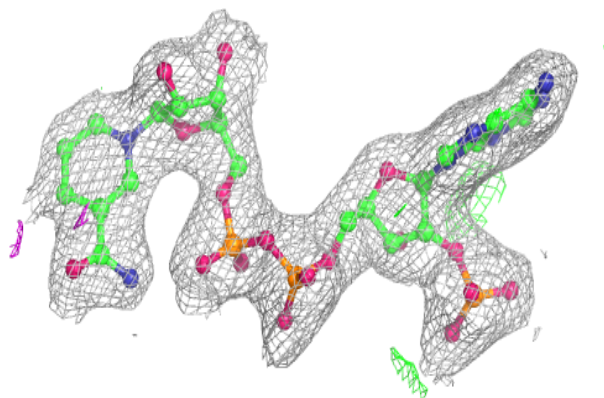


**Electron density around NDP F 300:**

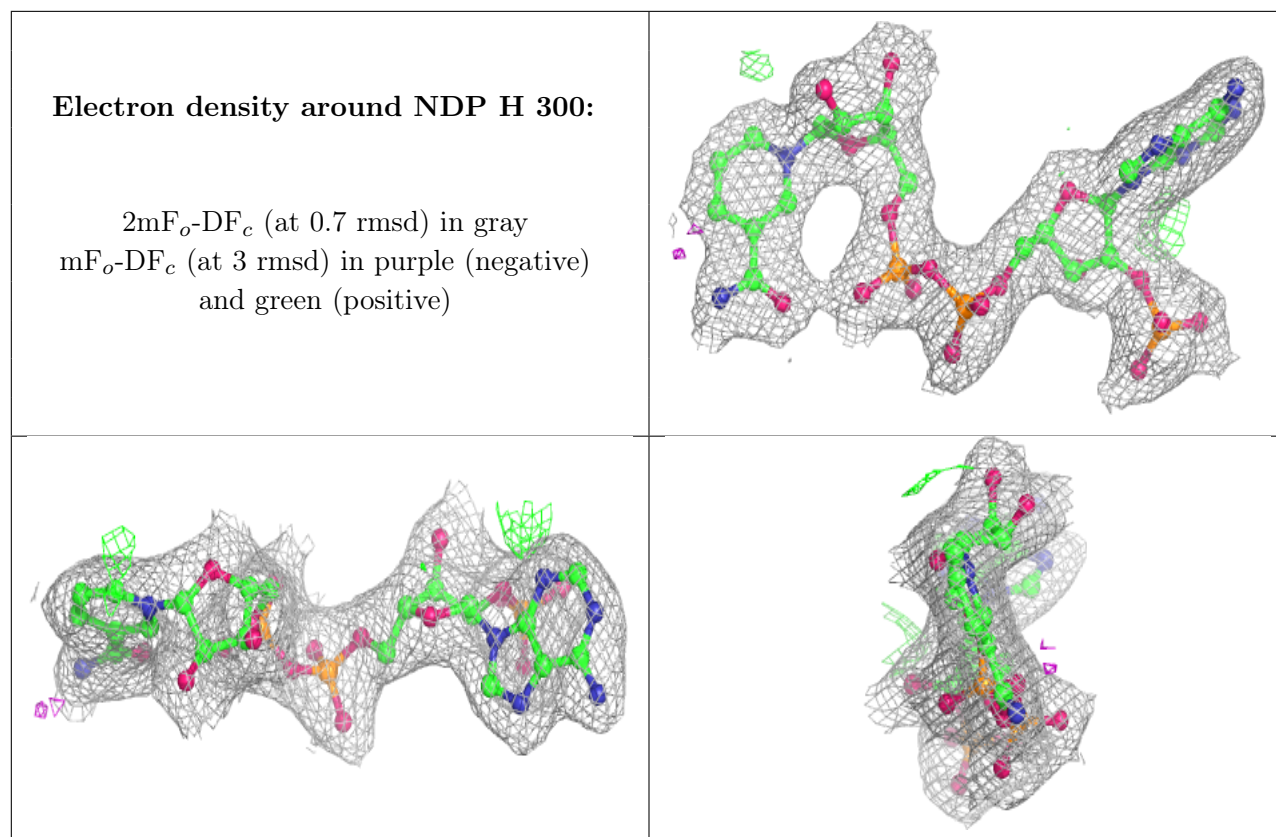
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around NDP G 300:**

$2mF_o-DF_c$  (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.