



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 10:27 PM BST

PDB ID : 6TBB  
Title : Crystal structure of *S. aureus* FabI in complex with NADPH and kalimantacin A (batumin)  
Authors : Fage, C.D.; Masschelein, J.  
Deposited on : 2019-11-01  
Resolution : 2.45 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 : 2.13.1  
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) : 2.13.1

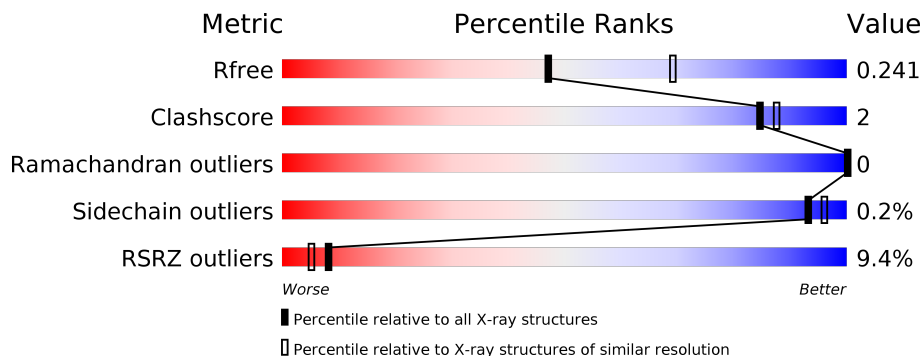
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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.



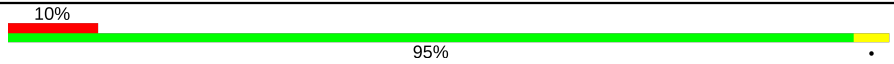
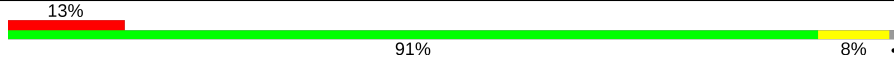
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	261	
1	B	261	
1	C	261	
1	D	261	
1	E	261	
1	F	261	

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Mol	Chain	Length	Quality of chain
1	G	261	 <p>10% 95% .</p>
1	H	261	 <p>13% 91% 8% .</p>

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 16633 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 Enoyl-[acyl-carrier-protein] reductase [NADPH].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	259	1992	1255	345	387	5	0	0	0
1	B	261	2002	1260	347	390	5	0	0	0
1	C	259	1992	1255	345	387	5	0	0	0
1	D	258	1982	1249	342	386	5	0	0	0
1	E	258	1982	1249	342	386	5	0	0	0
1	F	258	1982	1249	342	386	5	0	0	0
1	G	260	1998	1258	346	389	5	0	0	0
1	H	259	1992	1255	345	387	5	0	0	0

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP A0A0J9X1X7
A	-3	SER	-	expression tag	UNP A0A0J9X1X7
A	-2	HIS	-	expression tag	UNP A0A0J9X1X7
A	-1	MET	-	expression tag	UNP A0A0J9X1X7
A	0	ALA	-	expression tag	UNP A0A0J9X1X7
A	1	SER	-	expression tag	UNP A0A0J9X1X7
A	2	LEU	-	expression tag	UNP A0A0J9X1X7
B	-4	GLY	-	expression tag	UNP A0A0J9X1X7
B	-3	SER	-	expression tag	UNP A0A0J9X1X7
B	-2	HIS	-	expression tag	UNP A0A0J9X1X7
B	-1	MET	-	expression tag	UNP A0A0J9X1X7
B	0	ALA	-	expression tag	UNP A0A0J9X1X7
B	1	SER	-	expression tag	UNP A0A0J9X1X7

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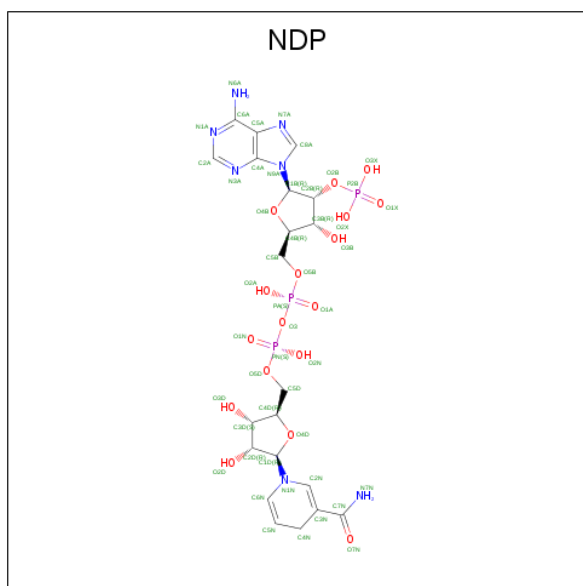
Chain	Residue	Modelled	Actual	Comment	Reference
B	2	LEU	-	expression tag	UNP A0A0J9X1X7
C	-4	GLY	-	expression tag	UNP A0A0J9X1X7
C	-3	SER	-	expression tag	UNP A0A0J9X1X7
C	-2	HIS	-	expression tag	UNP A0A0J9X1X7
C	-1	MET	-	expression tag	UNP A0A0J9X1X7
C	0	ALA	-	expression tag	UNP A0A0J9X1X7
C	1	SER	-	expression tag	UNP A0A0J9X1X7
C	2	LEU	-	expression tag	UNP A0A0J9X1X7
D	-4	GLY	-	expression tag	UNP A0A0J9X1X7
D	-3	SER	-	expression tag	UNP A0A0J9X1X7
D	-2	HIS	-	expression tag	UNP A0A0J9X1X7
D	-1	MET	-	expression tag	UNP A0A0J9X1X7
D	0	ALA	-	expression tag	UNP A0A0J9X1X7
D	1	SER	-	expression tag	UNP A0A0J9X1X7
D	2	LEU	-	expression tag	UNP A0A0J9X1X7
E	-4	GLY	-	expression tag	UNP A0A0J9X1X7
E	-3	SER	-	expression tag	UNP A0A0J9X1X7
E	-2	HIS	-	expression tag	UNP A0A0J9X1X7
E	-1	MET	-	expression tag	UNP A0A0J9X1X7
E	0	ALA	-	expression tag	UNP A0A0J9X1X7
E	1	SER	-	expression tag	UNP A0A0J9X1X7
E	2	LEU	-	expression tag	UNP A0A0J9X1X7
F	-4	GLY	-	expression tag	UNP A0A0J9X1X7
F	-3	SER	-	expression tag	UNP A0A0J9X1X7
F	-2	HIS	-	expression tag	UNP A0A0J9X1X7
F	-1	MET	-	expression tag	UNP A0A0J9X1X7
F	0	ALA	-	expression tag	UNP A0A0J9X1X7
F	1	SER	-	expression tag	UNP A0A0J9X1X7
F	2	LEU	-	expression tag	UNP A0A0J9X1X7
G	-4	GLY	-	expression tag	UNP A0A0J9X1X7
G	-3	SER	-	expression tag	UNP A0A0J9X1X7
G	-2	HIS	-	expression tag	UNP A0A0J9X1X7
G	-1	MET	-	expression tag	UNP A0A0J9X1X7
G	0	ALA	-	expression tag	UNP A0A0J9X1X7
G	1	SER	-	expression tag	UNP A0A0J9X1X7
G	2	LEU	-	expression tag	UNP A0A0J9X1X7
H	-4	GLY	-	expression tag	UNP A0A0J9X1X7
H	-3	SER	-	expression tag	UNP A0A0J9X1X7
H	-2	HIS	-	expression tag	UNP A0A0J9X1X7
H	-1	MET	-	expression tag	UNP A0A0J9X1X7
H	0	ALA	-	expression tag	UNP A0A0J9X1X7
H	1	SER	-	expression tag	UNP A0A0J9X1X7

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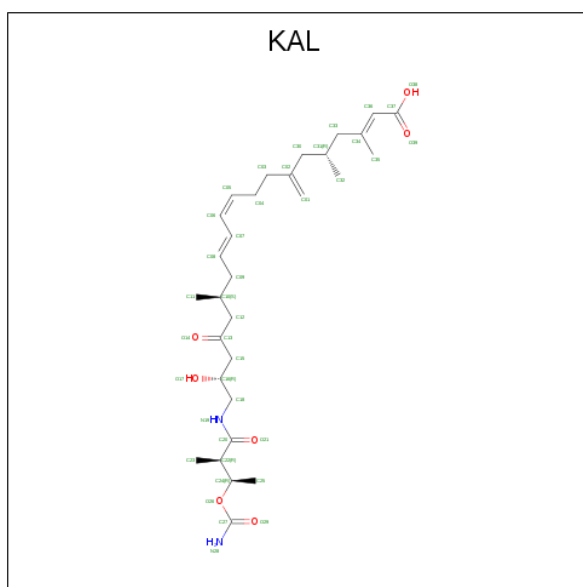
Chain	Residue	Modelled	Actual	Comment	Reference
H	2	LEU	-	expression tag	UNP A0A0J9X1X7

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
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 Kalimantacin (three-letter code: KAL) (formula:  $C_{30}H_{48}N_2O_7$ ) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	39	30	2	7	0	0
3	B	1	39	30	2	7	0	0
3	C	1	39	30	2	7	0	0
3	D	1	39	30	2	7	0	0
3	E	1	39	30	2	7	0	0
3	F	1	39	30	2	7	0	0
3	G	1	39	30	2	7	0	0
3	H	1	39	30	2	7	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total 4 4	0	0
4	C	1	Total 1 1	0	0
4	D	1	Total 1 1	0	0
4	E	3	Total 3 3	0	0

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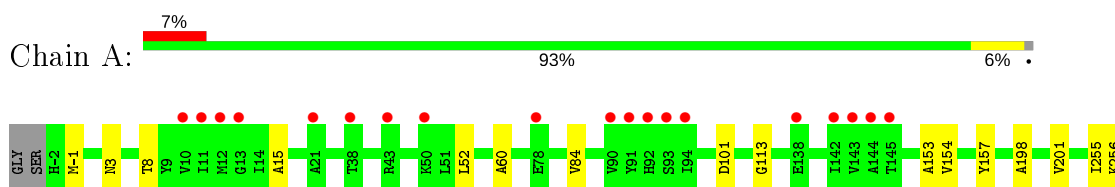
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
4	F	1	Total O 1 1	0	0
4	G	2	Total O 2 2	0	0
4	H	3	Total O 3 3	0	0



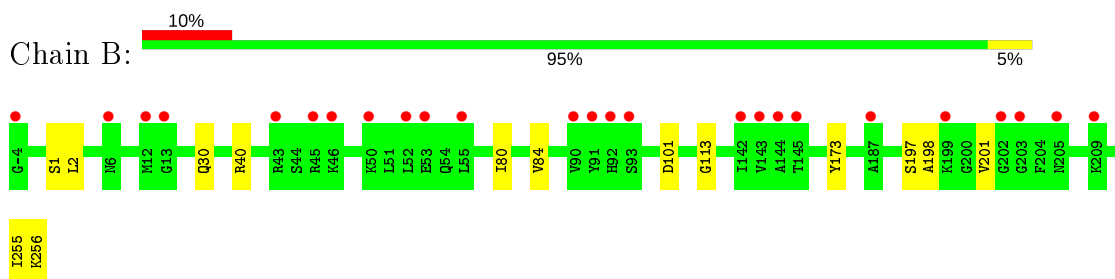
### 3 Residue-property plots [i](#)

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.

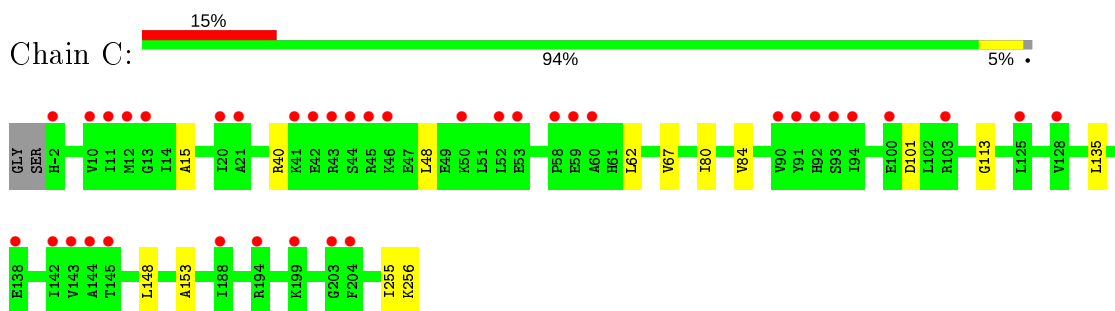
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADPH]



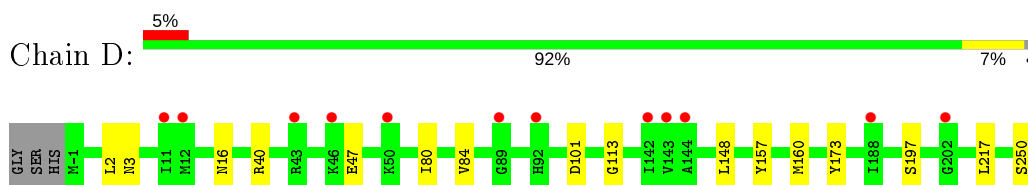
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADPH]



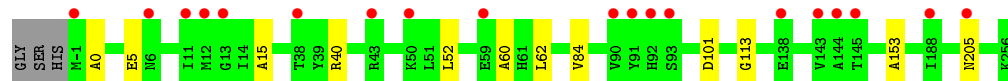
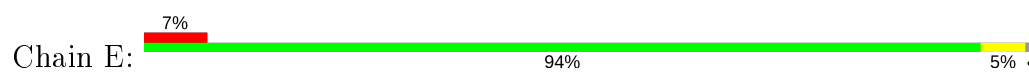
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADPH]



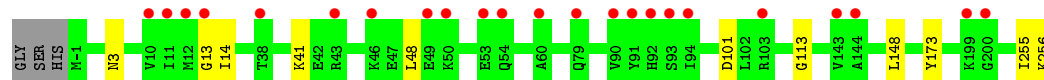
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADPH]



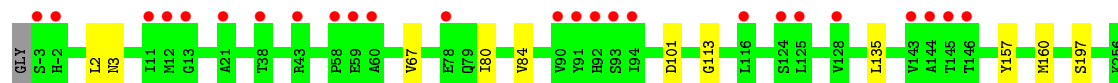
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADPH]



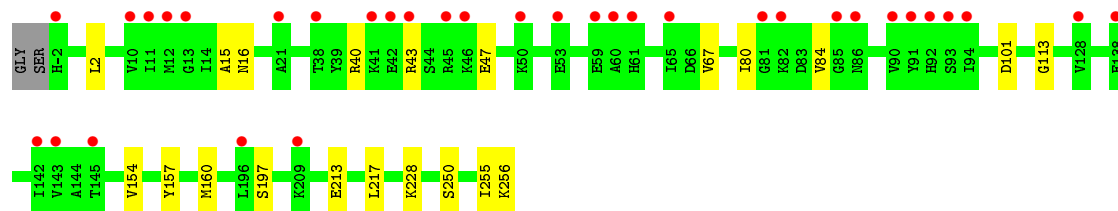
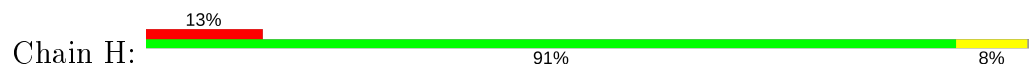
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADPH]



- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADPH]



- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADPH]



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.91Å 107.92Å 294.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 2.45 29.86 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.88-2.45) 99.9 (29.86-2.45)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.25 (at 2.45Å)	Xtrriage
Refinement program	REFMAC 5.8.0253	Depositor
R, $R_{free}$	0.196 , 0.247 0.195 , 0.241	Depositor DCC
$R_{free}$ test set	3746 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	81.8	Xtrriage
Anisotropy	0.200	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 55.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	16633	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	91.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.70% 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: NDP, KAL

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	0.70	0/2020	0.80	0/2722
1	B	0.70	0/2030	0.80	0/2735
1	C	0.72	0/2020	0.79	0/2722
1	D	0.72	0/2009	0.79	0/2707
1	E	0.70	0/2009	0.82	0/2707
1	F	0.73	0/2009	0.80	0/2707
1	G	0.71	0/2026	0.82	0/2730
1	H	0.70	0/2020	0.80	0/2722
All	All	0.71	0/16143	0.80	0/21752

There are no bond length outliers.

There are no bond angle outliers.

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	1992	0	2008	13	0
1	B	2002	0	2016	11	1
1	C	1992	0	2008	10	0
1	D	1982	0	2001	14	0
1	E	1982	0	2001	9	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1982	0	2001	8	1
1	G	1998	0	2013	10	0
1	H	1992	0	2008	15	1
2	A	48	0	26	1	0
2	B	48	0	26	2	0
2	C	48	0	26	4	0
2	D	48	0	26	2	0
2	E	48	0	26	2	0
2	F	48	0	26	1	0
2	G	48	0	26	3	0
2	H	48	0	26	4	0
3	A	39	0	0	0	0
3	B	39	0	0	0	0
3	C	39	0	0	2	0
3	D	39	0	0	1	0
3	E	39	0	0	0	0
3	F	39	0	0	0	0
3	G	39	0	0	0	0
3	H	39	0	0	0	0
4	A	4	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	3	0	0	0	0
4	F	1	0	0	0	0
4	G	2	0	0	0	0
4	H	3	0	0	0	0
All	All	16633	0	16264	77	2

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 2.

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:G:197:SER:HB2	2:G:301:NDP:O1A	1.75	0.87
1:H:197:SER:HB2	2:H:301:NDP:O1A	1.81	0.79
1:D:197:SER:HB2	2:D:301:NDP:O2A	1.82	0.79
1:B:197:SER:HB2	2:B:301:NDP:O2A	1.84	0.77
1:H:16:ASN:HA	1:H:47:GLU:HG2	1.70	0.73
1:C:40:ARG:HB3	2:C:301:NDP:O2X	1.89	0.73
1:F:256:LYS:HE2	1:H:255:ILE:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:135:LEU:HD12	1:G:135:LEU:N	2.04	0.71
1:D:16:ASN:HA	1:D:47:GLU:HG2	1.73	0.69
1:A:198:ALA:O	1:A:201:VAL:HG22	1.98	0.63
1:H:15:ALA:HB2	2:H:301:NDP:H3B	1.84	0.58
1:C:48:LEU:HD13	1:C:62:LEU:HD22	1.86	0.57
1:D:157:TYR:OH	3:D:302:KAL:O38	2.17	0.56
1:B:256:LYS:HE2	1:D:255:ILE:O	2.07	0.55
1:E:40:ARG:HB3	2:E:301:NDP:O2X	2.07	0.53
1:E:84:VAL:HG12	1:E:84:VAL:O	2.08	0.53
1:E:205:ASN:OD1	1:E:205:ASN:O	2.27	0.52
1:G:135:LEU:CD1	1:G:135:LEU:N	2.72	0.52
1:A:52:LEU:HD13	1:A:60:ALA:HB2	1.93	0.50
1:A:8:THR:HG21	1:A:84:VAL:HG11	1.93	0.50
1:E:153:ALA:HA	1:F:173:TYR:CZ	2.47	0.50
1:H:40:ARG:HB3	2:H:301:NDP:O1X	2.11	0.50
1:E:52:LEU:HD11	1:E:62:LEU:HD11	1.94	0.50
1:C:153:ALA:HA	1:D:173:TYR:CZ	2.48	0.48
1:D:40:ARG:HD3	2:D:301:NDP:C6A	2.44	0.48
1:A:15:ALA:HB2	2:A:301:NDP:H3B	1.95	0.47
1:C:101:ASP:OD2	1:C:113:GLY:HA3	2.15	0.47
1:B:198:ALA:O	1:B:201:VAL:HG22	2.15	0.46
1:B:101:ASP:OD2	1:B:113:GLY:HA3	2.15	0.46
1:H:101:ASP:OD2	1:H:113:GLY:HA3	2.16	0.46
1:A:101:ASP:OD2	1:A:113:GLY:HA3	2.15	0.46
1:D:101:ASP:OD2	1:D:113:GLY:HA3	2.15	0.46
1:F:101:ASP:OD2	1:F:113:GLY:HA3	2.16	0.46
1:H:80:ILE:O	1:H:84:VAL:HG22	2.15	0.46
1:D:80:ILE:O	1:D:84:VAL:HG22	2.16	0.45
1:B:30:GLN:HA	1:B:30:GLN:OE1	2.17	0.45
1:G:101:ASP:OD2	1:G:113:GLY:HA3	2.17	0.45
1:F:148:LEU:HD21	1:H:256:LYS:HG2	1.99	0.45
1:C:67:VAL:HG22	2:C:301:NDP:N1A	2.32	0.45
3:C:302:KAL:O39	3:C:302:KAL:C35	2.65	0.45
1:E:101:ASP:OD2	1:E:113:GLY:HA3	2.15	0.44
1:E:52:LEU:HD13	1:E:60:ALA:HB2	1.98	0.44
1:H:154:VAL:HG13	1:H:157:TYR:HB2	1.99	0.44
1:F:14:ILE:HB	1:F:48:LEU:HD21	2.00	0.44
1:G:67:VAL:HG22	2:G:301:NDP:N1A	2.33	0.44
1:B:40:ARG:HB3	2:B:301:NDP:O1X	2.18	0.43
1:F:255:ILE:O	1:H:256:LYS:HE2	2.18	0.43
1:E:15:ALA:HB2	2:E:301:NDP:H3B	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ASN:HD22	1:F:3:ASN:CG	2.21	0.43
1:A:256:LYS:HE2	1:C:255:ILE:O	2.17	0.43
1:G:2:LEU:HA	1:G:2:LEU:HD12	1.91	0.43
1:A:153:ALA:HA	1:B:173:TYR:CZ	2.54	0.43
2:C:301:NDP:H51A	3:C:302:KAL:C27	2.49	0.43
1:A:154:VAL:HG23	1:A:157:TYR:HB2	1.99	0.42
1:D:3:ASN:ND2	1:G:3:ASN:HB2	2.34	0.42
1:G:80:ILE:O	1:G:84:VAL:HG22	2.20	0.42
1:B:80:ILE:O	1:B:84:VAL:HG22	2.19	0.42
1:C:15:ALA:HB2	2:C:301:NDP:H3B	2.01	0.42
1:C:80:ILE:O	1:C:84:VAL:HG22	2.20	0.42
1:A:84:VAL:HG12	1:A:84:VAL:O	2.19	0.41
1:H:2:LEU:HA	1:H:2:LEU:HD12	1.91	0.41
1:A:255:ILE:O	1:C:256:LYS:HE2	2.20	0.41
1:H:67:VAL:HG22	2:H:301:NDP:N1A	2.36	0.41
1:B:255:ILE:O	1:D:256:LYS:HE2	2.20	0.41
1:B:256:LYS:HG2	1:D:148:LEU:HD21	2.02	0.41
1:D:217:LEU:HB2	1:D:250:SER:HB3	2.02	0.41
1:G:197:SER:CB	2:G:301:NDP:O1A	2.60	0.41
1:H:217:LEU:HB2	1:H:250:SER:HB3	2.02	0.41
1:D:157:TYR:CZ	1:D:160:MET:HG3	2.56	0.41
1:E:0:ALA:HB2	1:H:228:LYS:HG2	2.03	0.41
1:A:256:LYS:HG2	1:C:148:LEU:HD21	2.02	0.41
1:A:52:LEU:HD13	1:A:60:ALA:CB	2.51	0.40
1:D:2:LEU:HA	1:D:2:LEU:HD12	1.91	0.40
1:B:2:LEU:HA	1:B:2:LEU:HD12	1.91	0.40
1:F:13:GLY:O	2:F:301:NDP:O3B	2.37	0.40
1:G:157:TYR:CZ	1:G:160:MET:HG3	2.57	0.40
1:H:157:TYR:CZ	1:H:160:MET:HG3	2.56	0.40

All (2) 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:B:1:SER:OG	1:E:5:GLU:OE1[2_455]	1.98	0.22
1:F:41:LYS:NZ	1:H:213:GLU:OE2[4_554]	2.17	0.03

## 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	257/261 (98%)	246 (96%)	11 (4%)	0	100	100
1	B	259/261 (99%)	247 (95%)	12 (5%)	0	100	100
1	C	257/261 (98%)	247 (96%)	10 (4%)	0	100	100
1	D	256/261 (98%)	244 (95%)	12 (5%)	0	100	100
1	E	256/261 (98%)	244 (95%)	12 (5%)	0	100	100
1	F	256/261 (98%)	243 (95%)	13 (5%)	0	100	100
1	G	258/261 (99%)	247 (96%)	11 (4%)	0	100	100
1	H	257/261 (98%)	245 (95%)	12 (5%)	0	100	100
All	All	2056/2088 (98%)	1963 (96%)	93 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	212/213 (100%)	211 (100%)	1 (0%)	88	93
1	B	213/213 (100%)	213 (100%)	0	100	100
1	C	212/213 (100%)	211 (100%)	1 (0%)	88	93
1	D	211/213 (99%)	211 (100%)	0	100	100
1	E	211/213 (99%)	211 (100%)	0	100	100
1	F	211/213 (99%)	211 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	213/213 (100%)	213 (100%)	0	100	100
1	H	212/213 (100%)	211 (100%)	1 (0%)	88	93
All	All	1695/1704 (100%)	1692 (100%)	3 (0%)	93	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	MET
1	C	135	LEU
1	H	43	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	F	155	GLN
1	G	30	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	E	301	-	45,52,52	1.51	6 (13%)	53,80,80	1.55	11 (20%)
3	KAL	H	302	-	35,38,38	1.94	6 (17%)	38,48,48	1.68	6 (15%)
2	NDP	C	301	-	45,52,52	1.40	4 (8%)	53,80,80	1.61	10 (18%)
2	NDP	A	301	-	45,52,52	1.34	4 (8%)	53,80,80	1.70	16 (30%)
2	NDP	H	301	-	45,52,52	1.35	5 (11%)	53,80,80	1.70	15 (28%)
2	NDP	F	301	-	45,52,52	1.47	5 (11%)	53,80,80	1.51	8 (15%)
2	NDP	D	301	-	45,52,52	1.46	4 (8%)	53,80,80	1.55	12 (22%)
2	NDP	B	301	-	45,52,52	1.34	4 (8%)	53,80,80	1.68	12 (22%)
3	KAL	B	302	-	35,38,38	2.04	9 (25%)	38,48,48	1.68	7 (18%)
3	KAL	A	302	-	35,38,38	2.15	7 (20%)	38,48,48	1.94	11 (28%)
3	KAL	G	302	-	35,38,38	1.89	6 (17%)	38,48,48	1.44	4 (10%)
3	KAL	F	302	-	35,38,38	1.91	6 (17%)	38,48,48	1.69	8 (21%)
3	KAL	E	302	-	35,38,38	1.80	7 (20%)	38,48,48	1.65	7 (18%)
3	KAL	D	302	-	35,38,38	1.86	5 (14%)	38,48,48	1.56	8 (21%)
2	NDP	G	301	-	45,52,52	1.50	6 (13%)	53,80,80	1.83	14 (26%)
3	KAL	C	302	-	35,38,38	2.06	6 (17%)	38,48,48	1.64	7 (18%)

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	E	301	-	-	5/30/77/77	0/5/5/5
3	KAL	H	302	-	-	7/45/47/47	-
2	NDP	C	301	-	-	10/30/77/77	0/5/5/5
2	NDP	A	301	-	-	13/30/77/77	0/5/5/5
2	NDP	H	301	-	-	7/30/77/77	0/5/5/5
2	NDP	F	301	-	-	9/30/77/77	0/5/5/5
2	NDP	D	301	-	-	2/30/77/77	0/5/5/5
2	NDP	B	301	-	-	5/30/77/77	0/5/5/5
3	KAL	B	302	-	-	7/45/47/47	-
3	KAL	A	302	-	-	5/45/47/47	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	KAL	G	302	-	-	1/45/47/47	-
3	KAL	F	302	-	-	2/45/47/47	-
3	KAL	E	302	-	-	1/45/47/47	-
3	KAL	D	302	-	-	2/45/47/47	-
2	NDP	G	301	-	-	8/30/77/77	0/5/5/5
3	KAL	C	302	-	-	2/45/47/47	-

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	302	KAL	C27-N28	7.07	1.46	1.33
3	H	302	KAL	C27-N28	6.73	1.46	1.33
3	B	302	KAL	C27-N28	6.64	1.45	1.33
3	G	302	KAL	C27-N28	6.48	1.45	1.33
3	A	302	KAL	C27-N28	6.45	1.45	1.33
3	A	302	KAL	C20-N19	6.42	1.47	1.33
3	C	302	KAL	C20-N19	6.30	1.47	1.33
3	F	302	KAL	C27-N28	6.29	1.45	1.33
2	D	301	NDP	C4N-C3N	-6.09	1.37	1.49
3	C	302	KAL	C27-N28	6.02	1.44	1.33
3	G	302	KAL	C20-N19	5.92	1.46	1.33
3	F	302	KAL	C20-N19	5.85	1.46	1.33
2	F	301	NDP	C4N-C3N	-5.78	1.38	1.49
2	C	301	NDP	C4N-C3N	-5.73	1.38	1.49
3	H	302	KAL	C20-N19	5.55	1.45	1.33
2	G	301	NDP	C4N-C3N	-5.37	1.39	1.49
3	E	302	KAL	C27-N28	5.37	1.43	1.33
2	E	301	NDP	C4N-C3N	-5.22	1.39	1.49
3	D	302	KAL	C20-N19	5.21	1.45	1.33
2	H	301	NDP	C4N-C3N	-5.04	1.40	1.49
2	B	301	NDP	C4N-C3N	-5.02	1.40	1.49
3	B	302	KAL	C20-N19	4.79	1.44	1.33
3	E	302	KAL	C20-N19	4.74	1.44	1.33
3	A	302	KAL	C15-C13	4.47	1.57	1.51
2	D	301	NDP	C4N-C5N	-4.35	1.37	1.48
3	C	302	KAL	O26-C24	-4.33	1.39	1.46
2	A	301	NDP	C4N-C5N	-4.23	1.37	1.48
2	C	301	NDP	C4N-C5N	-4.21	1.37	1.48
3	E	302	KAL	C07-C06	4.04	1.55	1.44
3	B	302	KAL	C07-C06	4.03	1.55	1.44
2	E	301	NDP	C4N-C5N	-3.99	1.38	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	KAL	O26-C24	-3.95	1.40	1.46
2	B	301	NDP	C4N-C5N	-3.94	1.38	1.48
3	D	302	KAL	O26-C24	-3.94	1.40	1.46
2	G	301	NDP	C4N-C5N	-3.93	1.38	1.48
2	F	301	NDP	C4N-C5N	-3.92	1.38	1.48
3	F	302	KAL	O26-C24	-3.91	1.40	1.46
3	B	302	KAL	O26-C24	-3.89	1.40	1.46
2	A	301	NDP	C4N-C3N	-3.87	1.42	1.49
3	C	302	KAL	C07-C06	3.59	1.54	1.44
2	H	301	NDP	C4N-C5N	-3.46	1.39	1.48
2	E	301	NDP	O4B-C1B	3.44	1.45	1.41
3	F	302	KAL	C07-C06	3.43	1.54	1.44
3	D	302	KAL	C07-C06	3.43	1.54	1.44
2	G	301	NDP	C6N-C5N	3.40	1.39	1.33
3	B	302	KAL	C15-C13	3.39	1.56	1.51
3	H	302	KAL	O26-C24	-3.35	1.41	1.46
3	G	302	KAL	O26-C24	-3.30	1.41	1.46
3	C	302	KAL	C15-C13	3.23	1.55	1.51
3	H	302	KAL	C07-C06	3.18	1.53	1.44
2	A	301	NDP	C6N-C5N	3.16	1.39	1.33
3	A	302	KAL	O29-C27	-3.15	1.17	1.21
3	G	302	KAL	C07-C06	3.12	1.53	1.44
2	B	301	NDP	C6N-C5N	3.12	1.38	1.33
3	C	302	KAL	O29-C27	-3.07	1.17	1.21
2	H	301	NDP	C6N-C5N	3.06	1.38	1.33
2	F	301	NDP	P2B-O2B	3.03	1.65	1.59
3	E	302	KAL	O26-C24	-2.93	1.41	1.46
2	G	301	NDP	C5A-C4A	2.89	1.48	1.40
2	F	301	NDP	C6N-C5N	2.88	1.38	1.33
3	B	302	KAL	O29-C27	-2.85	1.18	1.21
2	E	301	NDP	C6N-C5N	2.85	1.38	1.33
2	H	301	NDP	C2A-N3A	2.77	1.36	1.32
3	H	302	KAL	O29-C27	-2.75	1.18	1.21
3	A	302	KAL	C07-C06	2.72	1.52	1.44
3	E	302	KAL	C15-C13	2.62	1.55	1.51
3	E	302	KAL	O26-C27	2.53	1.41	1.35
3	G	302	KAL	C15-C13	2.49	1.54	1.51
2	B	301	NDP	P2B-O2B	2.42	1.63	1.59
2	G	301	NDP	C2N-C3N	2.41	1.41	1.34
3	B	302	KAL	C12-C13	2.40	1.54	1.51
3	H	302	KAL	C12-C13	2.35	1.54	1.51
2	D	301	NDP	C6N-C5N	2.29	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	NDP	C5A-C4A	2.29	1.47	1.40
2	C	301	NDP	C2A-N3A	2.28	1.35	1.32
2	G	301	NDP	O4B-C1B	2.27	1.44	1.41
3	F	302	KAL	O21-C20	-2.27	1.18	1.23
3	F	302	KAL	C15-C13	2.26	1.54	1.51
3	G	302	KAL	C12-C13	2.21	1.54	1.51
2	F	301	NDP	C6N-N1N	-2.21	1.31	1.37
2	E	301	NDP	P2B-O2B	2.20	1.63	1.59
3	B	302	KAL	O21-C20	-2.17	1.19	1.23
3	E	302	KAL	O29-C27	-2.15	1.19	1.21
2	E	301	NDP	C2N-C3N	2.15	1.40	1.34
3	A	302	KAL	O26-C27	2.09	1.40	1.35
2	D	301	NDP	C3B-C2B	-2.05	1.48	1.52
2	A	301	NDP	C2N-C3N	2.04	1.40	1.34
2	H	301	NDP	C2N-C3N	2.04	1.40	1.34
3	D	302	KAL	O26-C27	2.03	1.40	1.35
3	B	302	KAL	O26-C27	2.02	1.40	1.35

All (156) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	302	KAL	O26-C27-N28	5.47	119.09	110.58
3	A	302	KAL	O26-C27-N28	5.38	118.94	110.58
3	E	302	KAL	O26-C27-N28	5.24	118.73	110.58
3	B	302	KAL	O26-C27-N28	4.94	118.26	110.58
3	C	302	KAL	O26-C27-N28	4.81	118.06	110.58
2	H	301	NDP	O2B-P2B-O1X	-4.67	91.38	109.39
2	F	301	NDP	N3A-C2A-N1A	-4.62	121.45	128.68
2	G	301	NDP	O5B-PA-O1A	-4.59	91.12	109.07
2	C	301	NDP	O4B-C1B-C2B	-4.54	98.71	106.59
3	G	302	KAL	C09-C08-C07	-4.52	119.58	125.41
3	E	302	KAL	O29-C27-N28	-4.49	118.11	125.51
3	F	302	KAL	C09-C08-C07	-4.45	119.67	125.41
3	D	302	KAL	C15-C13-C12	-4.38	112.20	116.48
2	A	301	NDP	O5B-C5B-C4B	-4.16	94.67	108.99
2	G	301	NDP	N3A-C2A-N1A	-4.05	122.35	128.68
2	A	301	NDP	O2B-P2B-O1X	-4.04	93.81	109.39
2	B	301	NDP	N3A-C2A-N1A	-4.01	122.41	128.68
3	H	302	KAL	O26-C27-O29	-4.01	119.64	123.69
2	E	301	NDP	C3N-C2N-N1N	-3.98	117.42	123.10
2	C	301	NDP	O2B-P2B-O1X	-3.93	94.22	109.39
3	A	302	KAL	O29-C27-N28	-3.91	119.06	125.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	NDP	N3A-C2A-N1A	-3.85	122.66	128.68
2	G	301	NDP	O5B-C5B-C4B	-3.82	95.83	108.99
3	C	302	KAL	C31-C30-C02	-3.81	106.62	116.69
2	B	301	NDP	C1B-N9A-C4A	-3.81	119.95	126.64
3	E	302	KAL	C09-C10-C12	-3.78	105.81	110.80
3	A	302	KAL	C23-C22-C20	3.76	116.33	108.78
3	A	302	KAL	O14-C13-C15	3.70	126.82	121.55
2	B	301	NDP	C2D-C1D-N1N	3.69	122.55	113.30
3	A	302	KAL	C09-C08-C07	-3.65	120.70	125.41
2	C	301	NDP	C2D-C1D-N1N	3.65	122.44	113.30
3	A	302	KAL	O26-C24-C25	3.62	115.42	108.21
3	F	302	KAL	C09-C10-C12	-3.61	106.03	110.80
2	D	301	NDP	C3N-C2N-N1N	-3.61	117.94	123.10
2	F	301	NDP	O4B-C1B-C2B	-3.58	100.38	106.59
3	C	302	KAL	C09-C08-C07	-3.51	120.88	125.41
3	G	302	KAL	O26-C27-N28	3.50	116.03	110.58
3	H	302	KAL	C09-C08-C07	-3.45	120.96	125.41
2	D	301	NDP	O2N-PN-O1N	3.44	129.25	112.24
2	E	301	NDP	N3A-C2A-N1A	-3.43	123.32	128.68
3	B	302	KAL	O29-C27-N28	-3.40	119.89	125.51
3	B	302	KAL	C18-N19-C20	-3.40	116.17	122.67
3	B	302	KAL	C22-C20-N19	3.36	121.47	116.44
3	D	302	KAL	O26-C27-N28	3.29	115.70	110.58
3	F	302	KAL	O26-C27-N28	3.27	115.66	110.58
2	F	301	NDP	O2N-PN-O1N	3.25	128.33	112.24
2	A	301	NDP	C3N-C2N-N1N	-3.25	118.46	123.10
2	D	301	NDP	O2B-P2B-O1X	-3.17	97.17	109.39
2	C	301	NDP	C3N-C2N-N1N	-3.17	118.58	123.10
2	H	301	NDP	C2D-C1D-N1N	3.16	121.23	113.30
2	G	301	NDP	O2B-P2B-O1X	-3.10	97.44	109.39
2	C	301	NDP	O4D-C1D-N1N	-3.08	102.03	108.06
2	H	301	NDP	N3A-C2A-N1A	-3.03	123.94	128.68
2	H	301	NDP	C1B-N9A-C4A	-3.03	121.33	126.64
3	C	302	KAL	O29-C27-N28	-3.02	120.52	125.51
2	H	301	NDP	C4A-C5A-N7A	-3.02	106.26	109.40
3	F	302	KAL	C22-C20-N19	3.01	120.95	116.44
2	F	301	NDP	O3X-P2B-O2X	3.00	119.09	107.64
3	D	302	KAL	O26-C27-O29	-2.99	120.67	123.69
2	B	301	NDP	O2A-PA-O5B	-2.99	93.86	107.75
2	B	301	NDP	O3B-C3B-C4B	-2.97	102.45	111.05
2	E	301	NDP	O2B-P2B-O1X	-2.96	97.96	109.39
2	G	301	NDP	C2A-N1A-C6A	2.96	123.81	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	302	KAL	C09-C10-C12	-2.95	106.90	110.80
3	F	302	KAL	O21-C20-C22	-2.91	115.76	121.02
2	A	301	NDP	C3N-C7N-N7N	2.91	122.83	117.67
2	G	301	NDP	O4B-C4B-C5B	2.89	118.89	109.37
2	H	301	NDP	O4B-C4B-C3B	2.88	110.81	105.11
3	B	302	KAL	C03-C02-C30	2.88	125.02	115.88
2	E	301	NDP	O2N-PN-O1N	2.84	126.27	112.24
3	G	302	KAL	C22-C20-N19	-2.84	112.19	116.44
2	G	301	NDP	C5B-C4B-C3B	-2.82	104.60	115.18
2	G	301	NDP	C1D-N1N-C6N	-2.77	114.87	120.83
2	D	301	NDP	O4B-C1B-C2B	-2.73	101.86	106.59
3	C	302	KAL	C09-C10-C12	-2.70	107.23	110.80
2	A	301	NDP	C4A-C5A-N7A	-2.70	106.58	109.40
3	F	302	KAL	O26-C27-O29	-2.69	120.97	123.69
2	H	301	NDP	C3N-C2N-N1N	-2.69	119.26	123.10
2	A	301	NDP	C3D-C2D-C1D	-2.67	96.36	101.43
2	E	301	NDP	N6A-C6A-N1A	2.67	124.11	118.57
2	D	301	NDP	PA-O5B-C5B	-2.66	106.08	121.68
2	A	301	NDP	N3A-C2A-N1A	-2.65	124.54	128.68
2	A	301	NDP	C1B-N9A-C4A	-2.62	122.04	126.64
2	H	301	NDP	C1D-N1N-C6N	-2.62	115.19	120.83
2	E	301	NDP	C2A-N1A-C6A	2.59	123.19	118.75
3	E	302	KAL	C31-C30-C02	-2.59	109.85	116.69
2	E	301	NDP	C1B-N9A-C4A	-2.59	122.09	126.64
2	D	301	NDP	C1D-N1N-C6N	-2.58	115.27	120.83
3	H	302	KAL	C31-C30-C02	-2.58	109.89	116.69
2	G	301	NDP	O2X-P2B-O1X	2.57	120.75	110.68
3	H	302	KAL	O29-C27-N28	-2.57	121.27	125.51
2	H	301	NDP	O4B-C1B-C2B	-2.53	102.20	106.59
2	C	301	NDP	C1D-N1N-C6N	-2.52	115.39	120.83
3	F	302	KAL	C31-C30-C02	-2.52	110.04	116.69
3	A	302	KAL	C03-C02-C30	2.50	123.83	115.88
3	E	302	KAL	O14-C13-C15	2.50	125.11	121.55
2	E	301	NDP	C1D-N1N-C6N	-2.50	115.45	120.83
2	A	301	NDP	O5B-PA-O1A	-2.49	99.32	109.07
2	B	301	NDP	O3X-P2B-O2X	2.49	117.17	107.64
3	A	302	KAL	C09-C10-C12	-2.48	107.52	110.80
2	C	301	NDP	N3A-C2A-N1A	-2.48	124.80	128.68
3	D	302	KAL	C09-C08-C07	-2.46	122.23	125.41
2	G	301	NDP	C1B-N9A-C4A	-2.46	122.32	126.64
2	H	301	NDP	O2N-PN-O1N	2.45	124.36	112.24
2	F	301	NDP	C1B-N9A-C4A	-2.45	122.34	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	301	NDP	PA-O5B-C5B	-2.45	107.33	121.68
2	E	301	NDP	O2A-PA-O1A	2.45	124.34	112.24
2	B	301	NDP	C2A-N1A-C6A	2.45	122.94	118.75
2	A	301	NDP	C1D-N1N-C6N	-2.44	115.57	120.83
2	A	301	NDP	O2A-PA-O1A	2.44	124.31	112.24
2	H	301	NDP	O2X-P2B-O1X	2.43	120.17	110.68
2	C	301	NDP	O2A-PA-O1A	2.41	124.17	112.24
2	B	301	NDP	C1D-N1N-C6N	-2.37	115.72	120.83
3	G	302	KAL	O29-C27-N28	-2.34	121.65	125.51
2	C	301	NDP	O2N-PN-O1N	2.34	123.80	112.24
2	B	301	NDP	PA-O5B-C5B	-2.34	107.98	121.68
3	H	302	KAL	O26-C24-C25	2.34	112.86	108.21
2	G	301	NDP	O2A-PA-O5B	2.33	118.55	107.75
3	B	302	KAL	O26-C24-C22	2.32	110.89	106.40
3	B	302	KAL	O21-C20-N19	-2.29	118.08	122.99
3	C	302	KAL	O14-C13-C15	2.24	124.75	121.55
3	C	302	KAL	O26-C27-O29	-2.24	121.42	123.69
2	C	301	NDP	C4A-C5A-N7A	-2.23	107.07	109.40
2	E	301	NDP	PN-O3-PA	-2.23	125.16	132.83
2	G	301	NDP	C3N-C2N-N1N	-2.23	119.91	123.10
3	A	302	KAL	C25-C24-C22	-2.22	108.15	113.10
2	A	301	NDP	O7N-C7N-C3N	-2.22	116.72	120.90
2	D	301	NDP	N6A-C6A-N1A	2.21	123.15	118.57
3	E	302	KAL	C15-C13-C12	-2.20	114.33	116.48
2	H	301	NDP	O3X-P2B-O1X	2.18	119.21	110.68
3	D	302	KAL	C23-C22-C24	-2.15	109.51	111.79
2	A	301	NDP	O2N-PN-O1N	2.15	122.86	112.24
2	E	301	NDP	O3X-P2B-O1X	2.14	119.07	110.68
2	D	301	NDP	O7N-C7N-C3N	-2.14	116.87	120.90
3	A	302	KAL	O14-C13-C12	-2.13	118.52	121.55
2	B	301	NDP	O5B-PA-O1A	2.13	117.38	109.07
2	G	301	NDP	C3D-C2D-C1D	-2.12	97.39	101.43
2	F	301	NDP	C2A-N1A-C6A	2.12	122.39	118.75
2	A	301	NDP	C3B-C2B-C1B	-2.12	98.90	102.89
3	A	302	KAL	C04-C03-C02	2.10	118.39	112.16
3	D	302	KAL	O14-C13-C15	2.09	124.53	121.55
2	F	301	NDP	PN-O3-PA	-2.08	125.69	132.83
3	E	302	KAL	C09-C08-C07	-2.08	122.73	125.41
2	B	301	NDP	C3N-C2N-N1N	-2.07	120.14	123.10
2	F	301	NDP	O3D-C3D-C4D	-2.07	105.06	111.05
2	H	301	NDP	N6A-C6A-N1A	2.06	122.86	118.57
2	A	301	NDP	O2X-P2B-O1X	2.06	118.75	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	NDP	O5B-PA-O1A	2.06	117.12	109.07
2	B	301	NDP	C5B-C4B-C3B	-2.05	107.50	115.18
2	G	301	NDP	O7N-C7N-N7N	-2.03	118.14	122.88
3	D	302	KAL	C31-C30-C02	-2.03	111.34	116.69
2	H	301	NDP	PN-O3-PA	-2.02	125.88	132.83
2	A	301	NDP	O2D-C2D-C1D	2.02	116.78	110.02
2	D	301	NDP	O4B-C4B-C5B	2.01	115.98	109.37
3	F	302	KAL	O17-C16-C15	-2.00	104.34	109.65
2	D	301	NDP	O3X-P2B-O1X	2.00	118.51	110.68

There are no chirality outliers.

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	301	NDP	C4B-C5B-O5B-PA
2	E	301	NDP	C2B-O2B-P2B-O1X
3	H	302	KAL	C22-C24-O26-C27
3	H	302	KAL	N28-C27-O26-C24
2	C	301	NDP	C4B-C5B-O5B-PA
2	C	301	NDP	C2B-O2B-P2B-O1X
2	C	301	NDP	C5D-O5D-PN-O2N
2	A	301	NDP	C5B-O5B-PA-O1A
2	A	301	NDP	C5B-O5B-PA-O2A
2	A	301	NDP	C5D-O5D-PN-O2N
2	H	301	NDP	C5D-O5D-PN-O2N
2	F	301	NDP	C5D-O5D-PN-O1N
3	B	302	KAL	C01-C02-C30-C31
3	B	302	KAL	C03-C02-C30-C31
3	B	302	KAL	C08-C09-C10-C11
3	B	302	KAL	C08-C09-C10-C12
3	A	302	KAL	C22-C24-O26-C27
3	A	302	KAL	N28-C27-O26-C24
3	A	302	KAL	C02-C30-C31-C32
2	G	301	NDP	C2B-O2B-P2B-O1X
2	A	301	NDP	O4B-C4B-C5B-O5B
2	A	301	NDP	C3B-C4B-C5B-O5B
2	F	301	NDP	O4B-C4B-C5B-O5B
2	G	301	NDP	O4D-C4D-C5D-O5D
3	H	302	KAL	O29-C27-O26-C24
2	G	301	NDP	C3D-C4D-C5D-O5D
3	D	302	KAL	C05-C06-C07-C08
3	F	302	KAL	C05-C06-C07-C08

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Mol	Chain	Res	Type	Atoms
3	H	302	KAL	C25-C24-O26-C27
3	G	302	KAL	C15-C16-C18-N19
3	F	302	KAL	C15-C16-C18-N19
2	F	301	NDP	C4B-C5B-O5B-PA
3	A	302	KAL	O29-C27-O26-C24
2	A	301	NDP	PA-O3-PN-O1N
2	H	301	NDP	PN-O3-PA-O1A
3	B	302	KAL	C11-C10-C12-C13
3	D	302	KAL	C11-C10-C12-C13
3	C	302	KAL	C01-C02-C03-C04
2	F	301	NDP	C2D-C1D-N1N-C6N
2	E	301	NDP	C2B-O2B-P2B-O2X
2	C	301	NDP	C5D-O5D-PN-O3
2	A	301	NDP	C5B-O5B-PA-O3
2	A	301	NDP	C2B-O2B-P2B-O2X
2	A	301	NDP	C5D-O5D-PN-O3
2	H	301	NDP	C5D-O5D-PN-O3
2	G	301	NDP	C2B-O2B-P2B-O2X
2	G	301	NDP	C5D-O5D-PN-O3
2	B	301	NDP	PN-O3-PA-O1A
2	F	301	NDP	C5D-O5D-PN-O2N
2	F	301	NDP	O4D-C1D-N1N-C6N
2	B	301	NDP	O4D-C1D-N1N-C6N
2	C	301	NDP	C2D-C1D-N1N-C6N
2	C	301	NDP	O4D-C1D-N1N-C6N
2	A	301	NDP	O4D-C1D-N1N-C6N
2	H	301	NDP	O4D-C1D-N1N-C6N
2	D	301	NDP	O4D-C1D-N1N-C6N
2	A	301	NDP	PA-O3-PN-O2N
3	B	302	KAL	C05-C06-C07-C08
2	E	301	NDP	O4D-C1D-N1N-C6N
3	H	302	KAL	C15-C16-C18-N19
2	G	301	NDP	O4D-C1D-N1N-C6N
2	B	301	NDP	O4B-C4B-C5B-O5B
3	H	302	KAL	C05-C06-C07-C08
3	E	302	KAL	C05-C06-C07-C08
3	C	302	KAL	C05-C06-C07-C08
2	D	301	NDP	O4B-C4B-C5B-O5B
2	B	301	NDP	C2D-C1D-N1N-C6N
2	H	301	NDP	PN-O3-PA-O2A
3	A	302	KAL	C25-C24-O26-C27
2	H	301	NDP	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	A	301	NDP	C2D-C1D-N1N-C6N
3	H	302	KAL	C01-C02-C03-C04
2	C	301	NDP	C2B-O2B-P2B-O3X
2	F	301	NDP	C5D-O5D-PN-O3
2	C	301	NDP	O4B-C4B-C5B-O5B
2	A	301	NDP	PN-O3-PA-O1A
2	C	301	NDP	C5B-O5B-PA-O1A
2	C	301	NDP	C5D-O5D-PN-O1N
2	H	301	NDP	C5D-O5D-PN-O1N
2	F	301	NDP	C5B-O5B-PA-O1A
3	B	302	KAL	C09-C10-C12-C13
2	G	301	NDP	C5D-O5D-PN-O1N
2	E	301	NDP	O4B-C4B-C5B-O5B
2	B	301	NDP	O4D-C4D-C5D-O5D
2	G	301	NDP	O4B-C4B-C5B-O5B
2	F	301	NDP	C2D-C1D-N1N-C2N

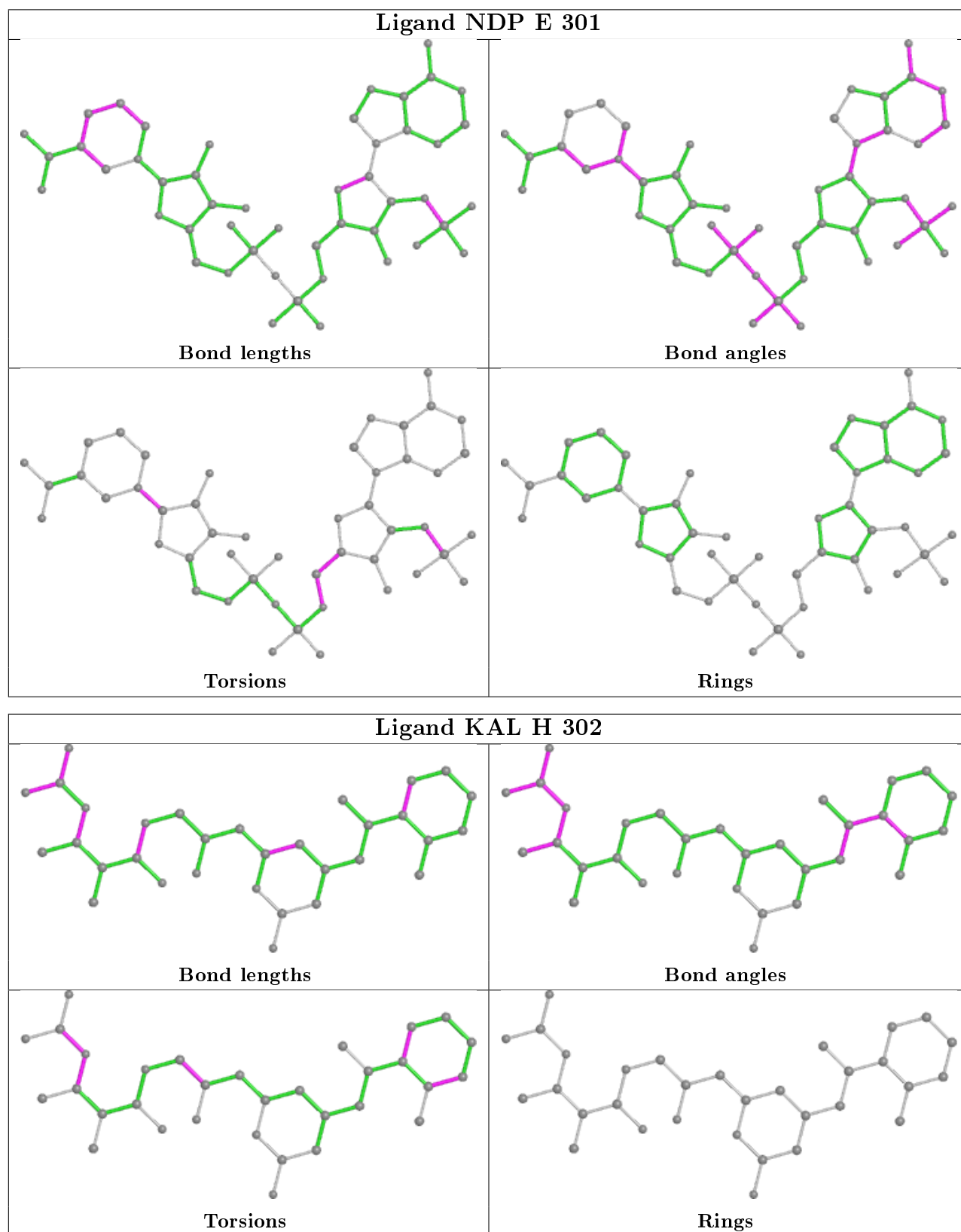
There are no ring outliers.

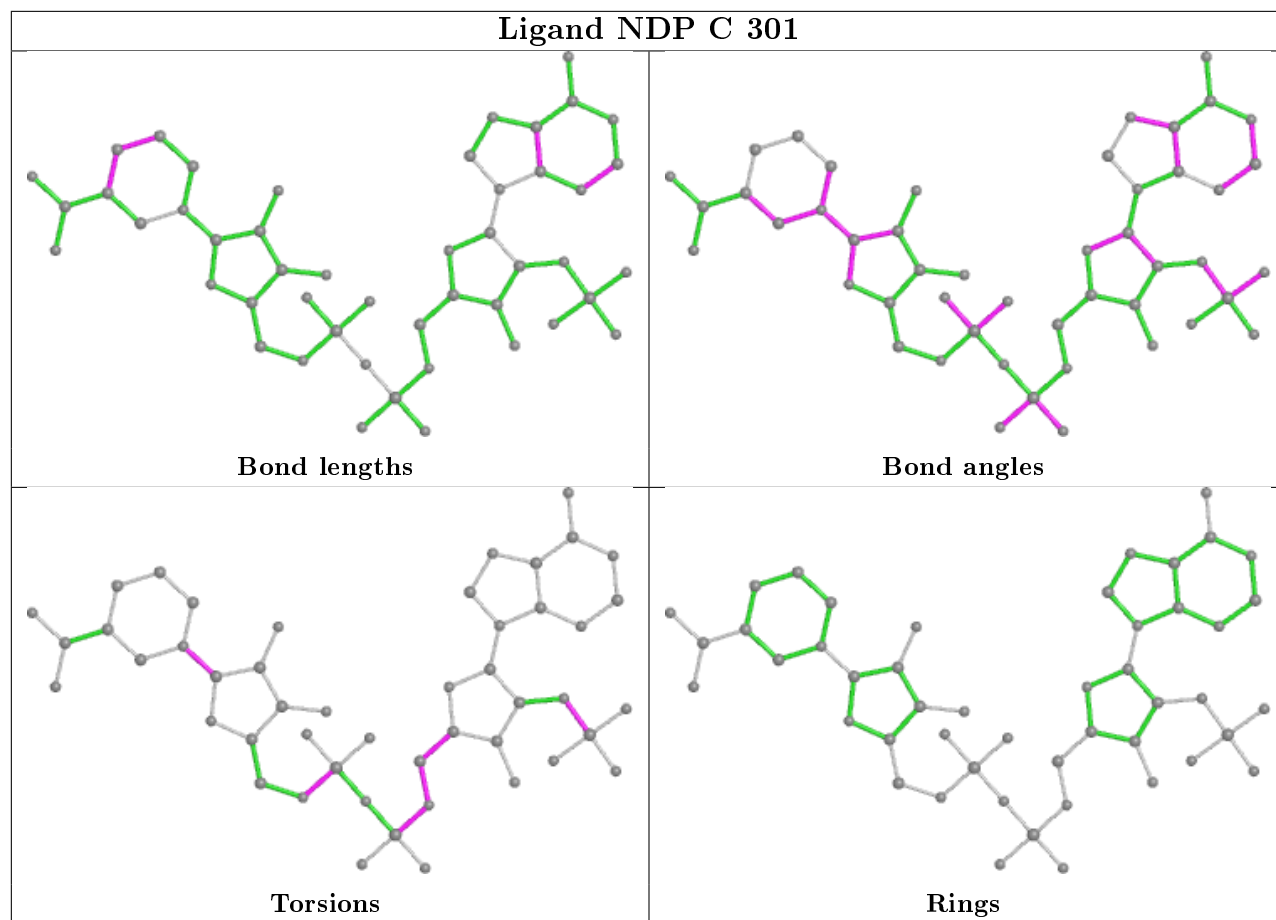
10 monomers are involved in 21 short contacts:

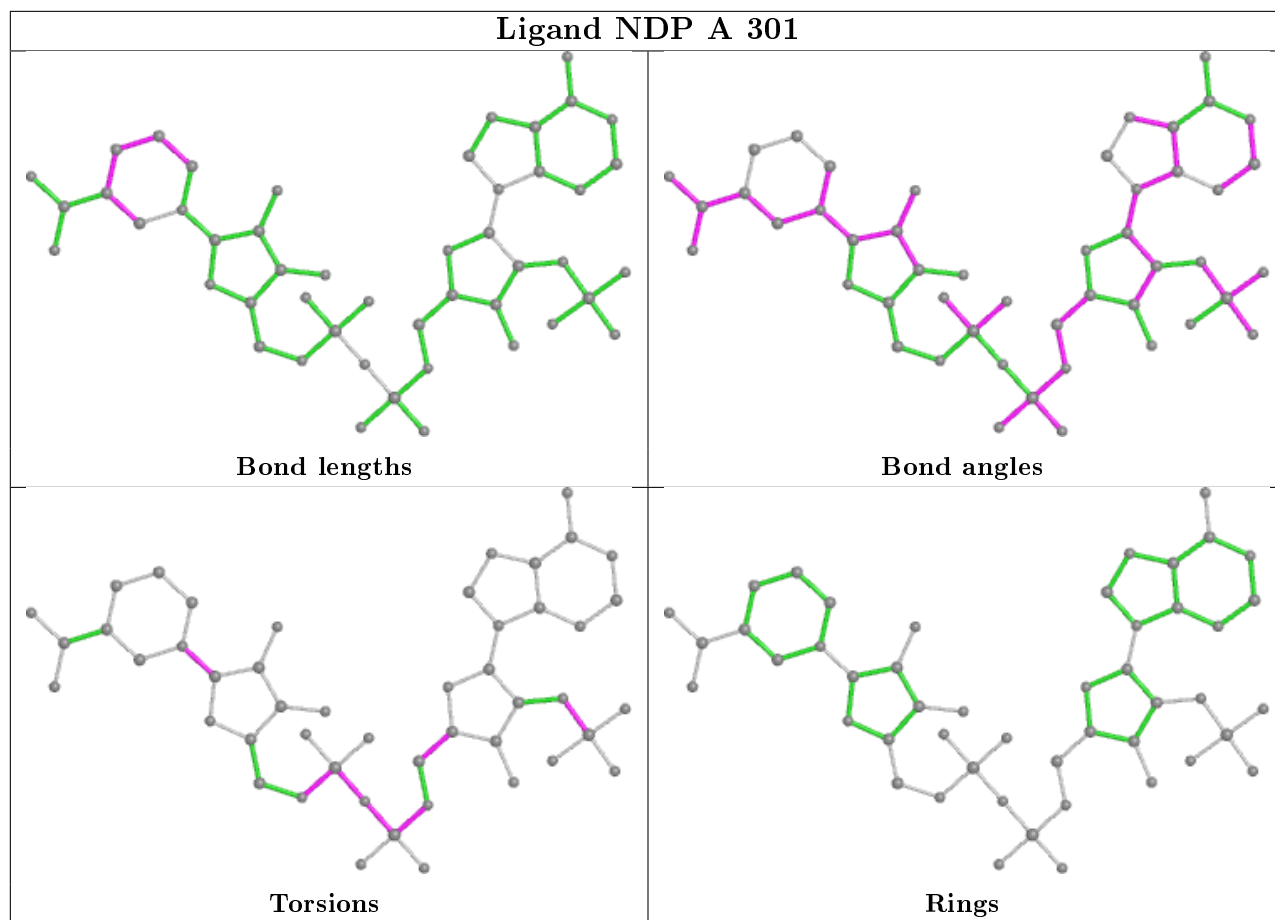
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301	NDP	2	0
2	C	301	NDP	4	0
2	A	301	NDP	1	0
2	H	301	NDP	4	0
2	F	301	NDP	1	0
2	D	301	NDP	2	0
2	B	301	NDP	2	0
3	D	302	KAL	1	0
2	G	301	NDP	3	0
3	C	302	KAL	2	0

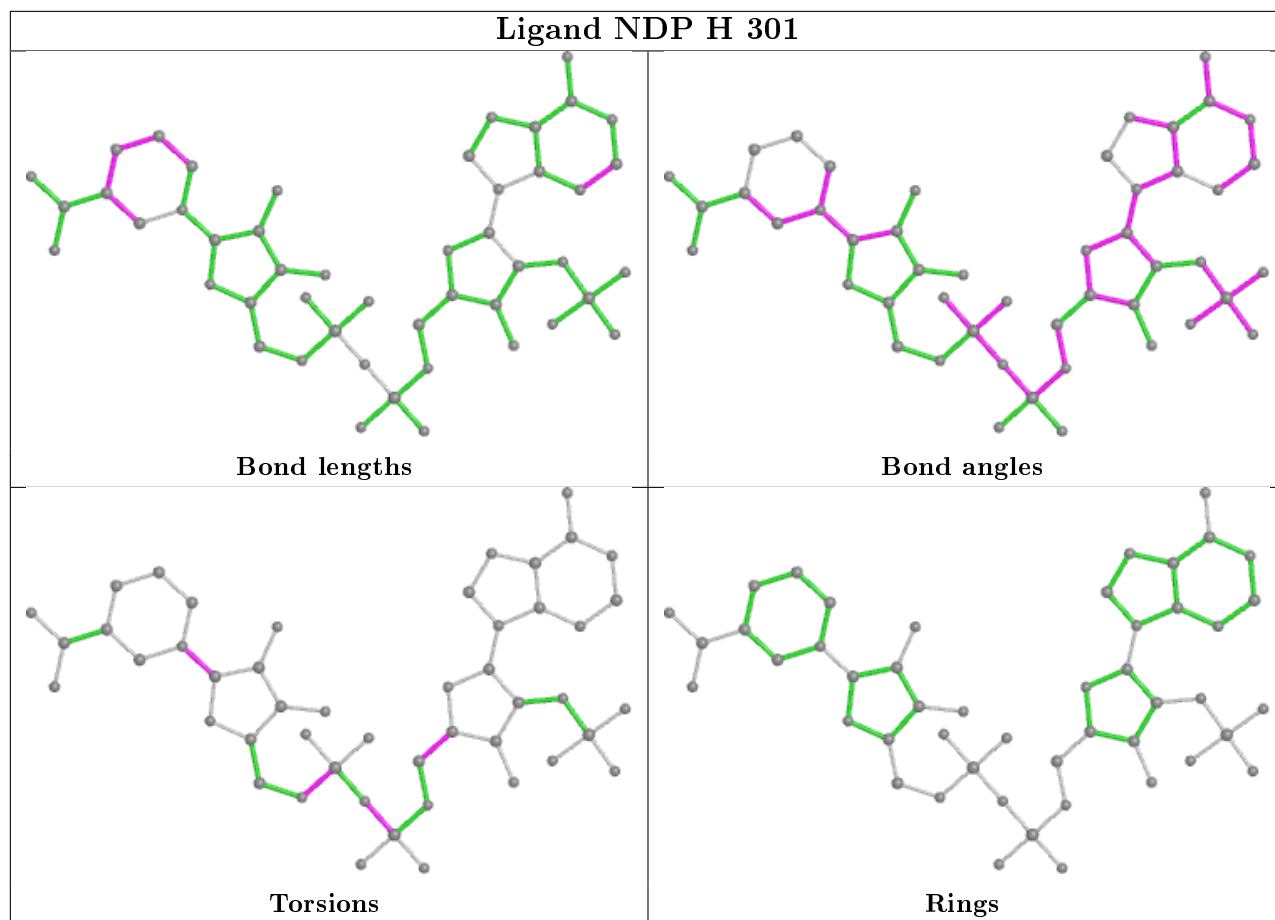
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

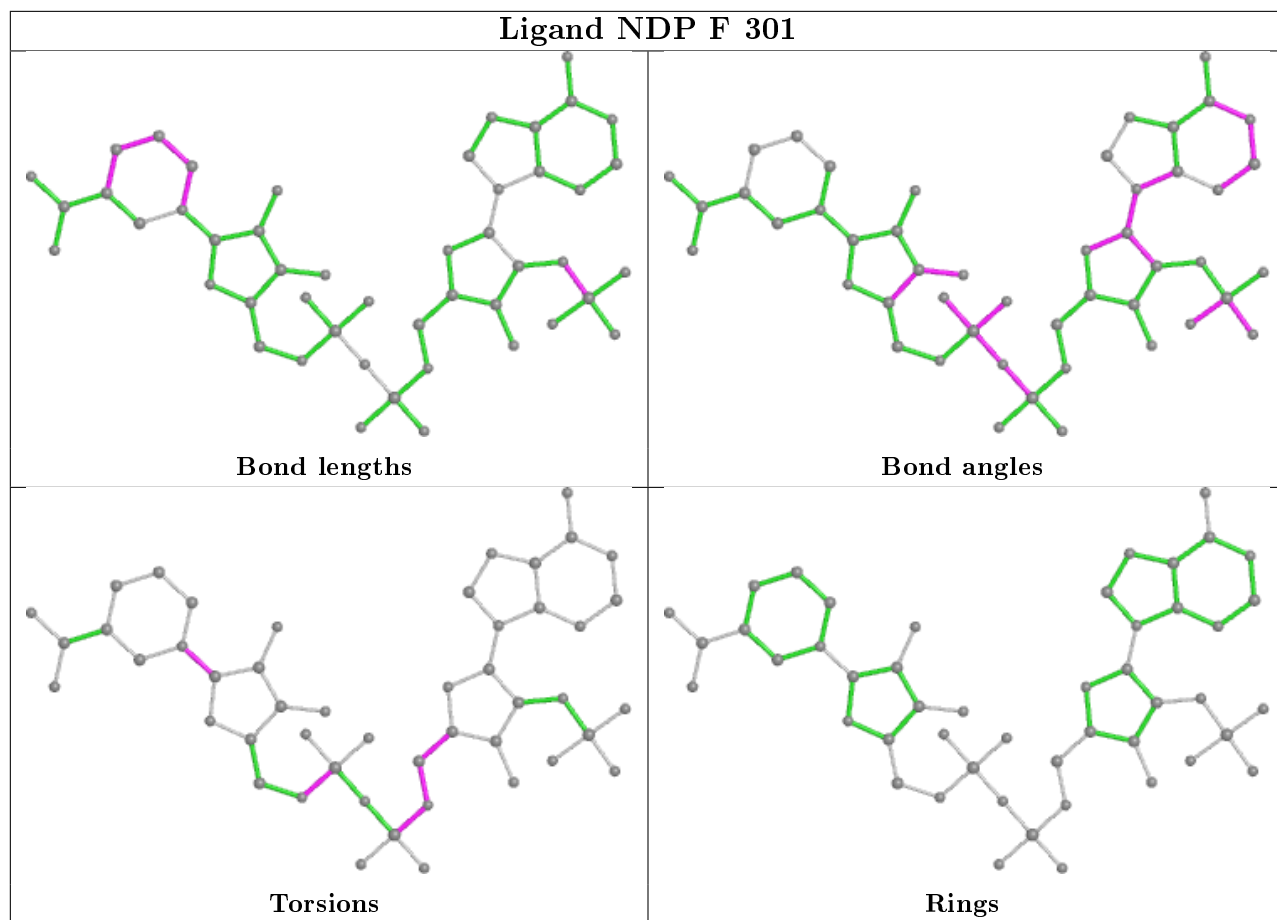
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



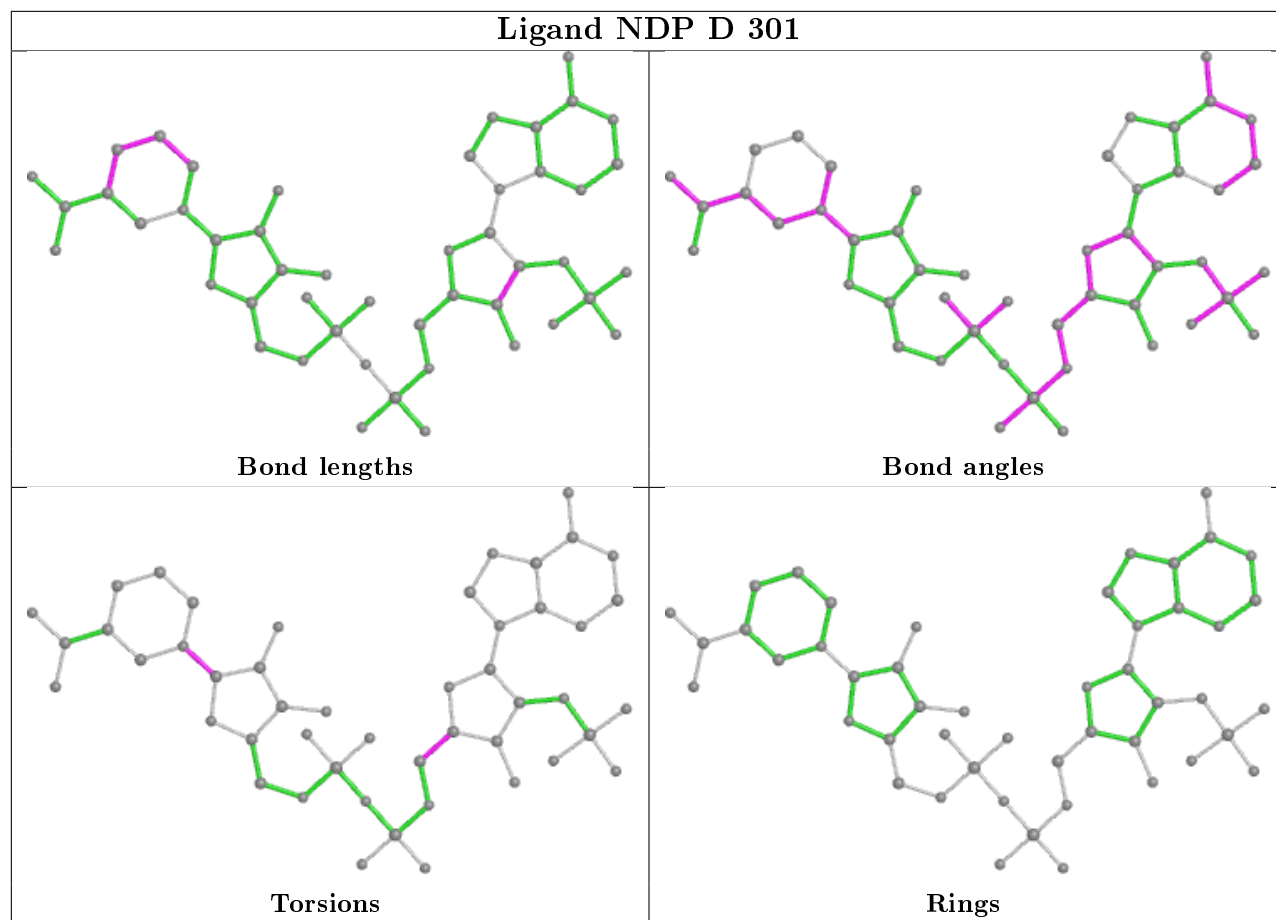


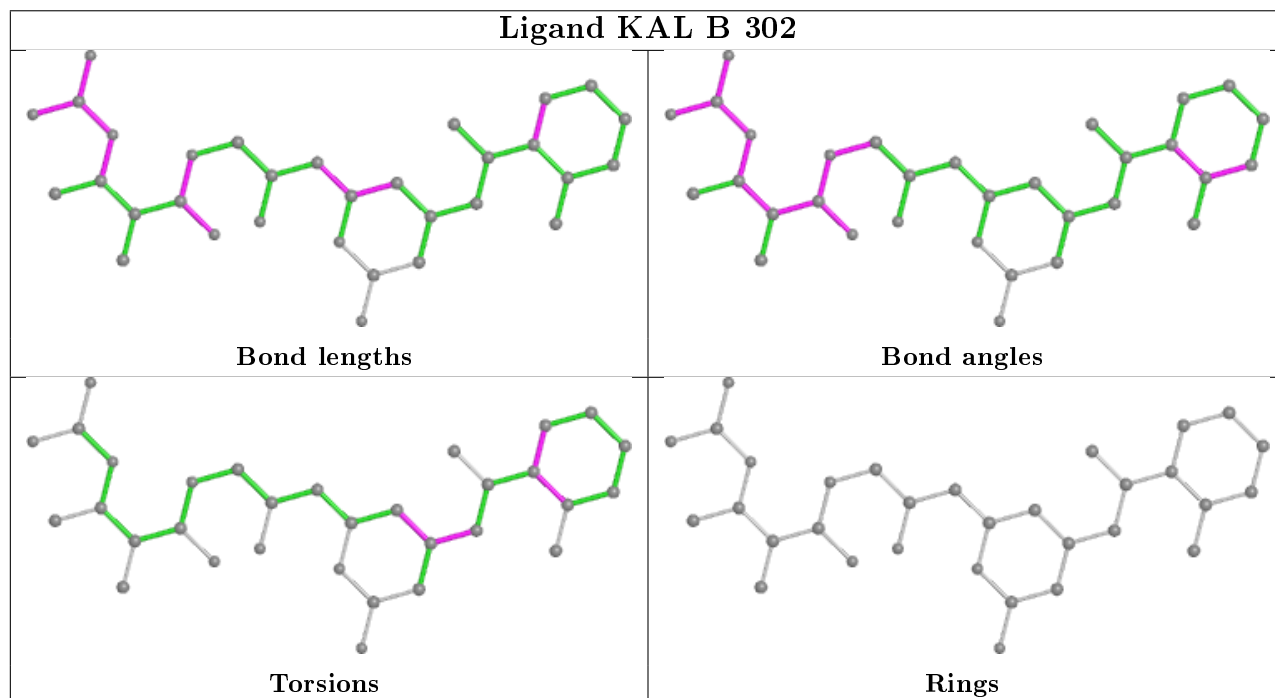
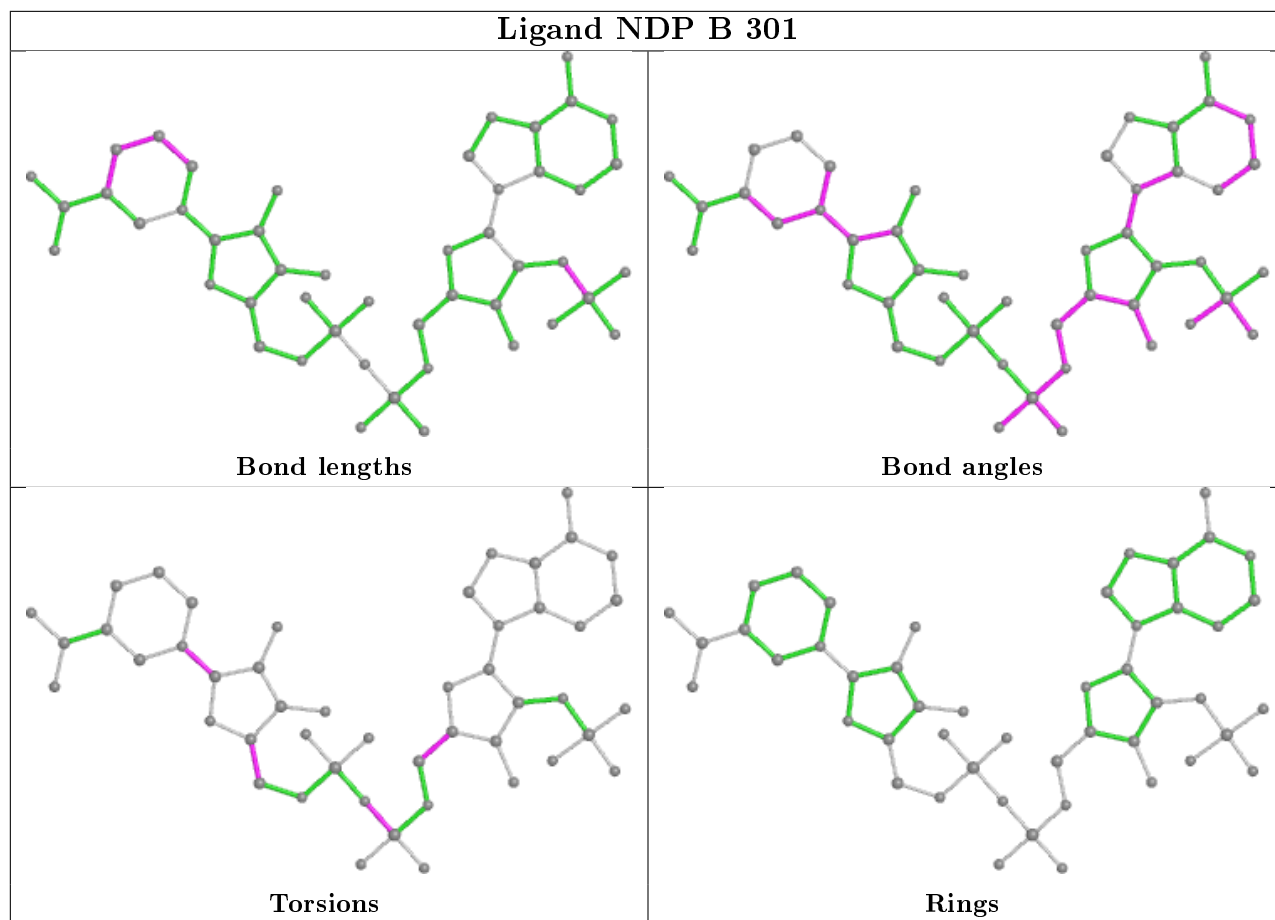


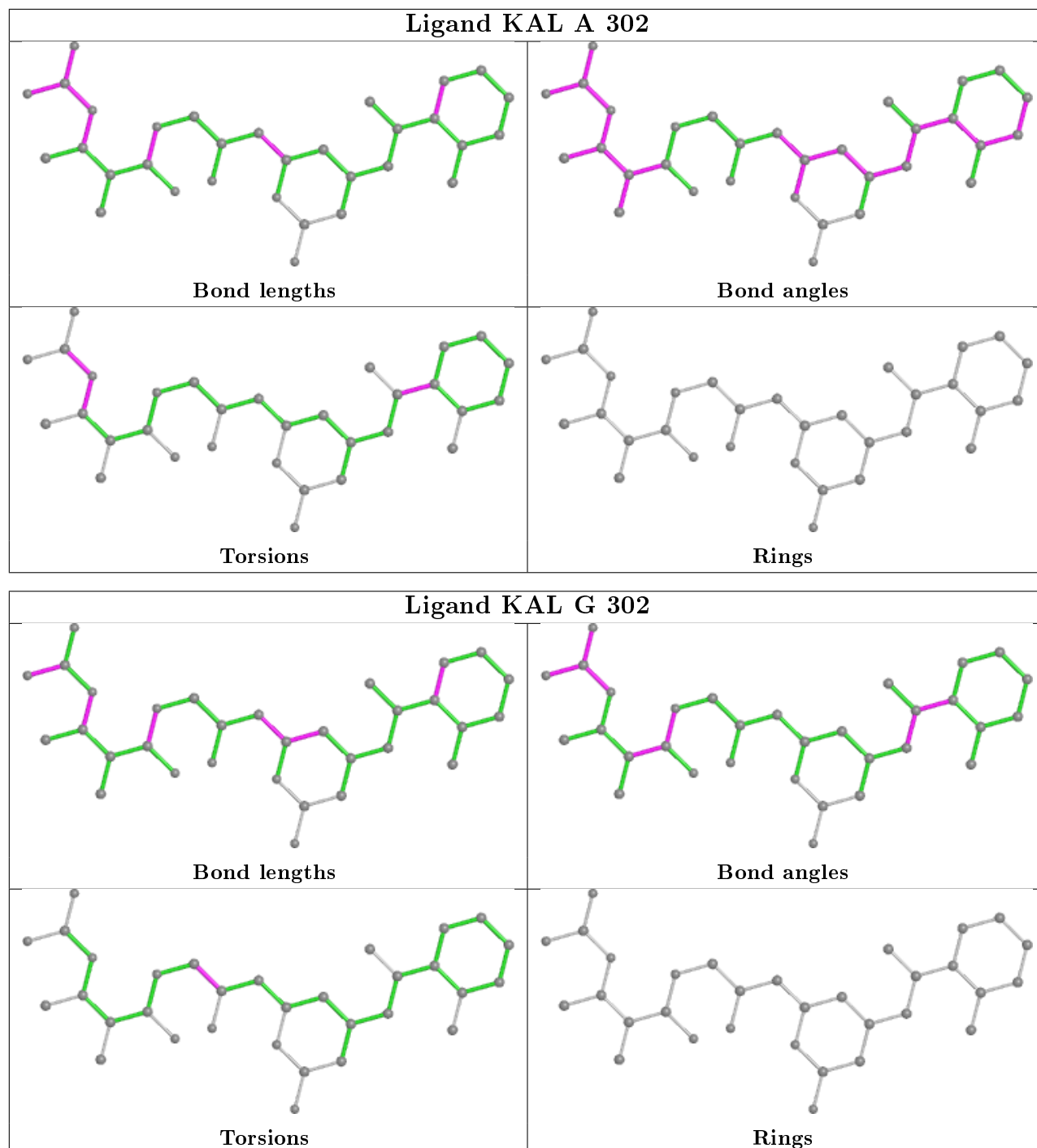


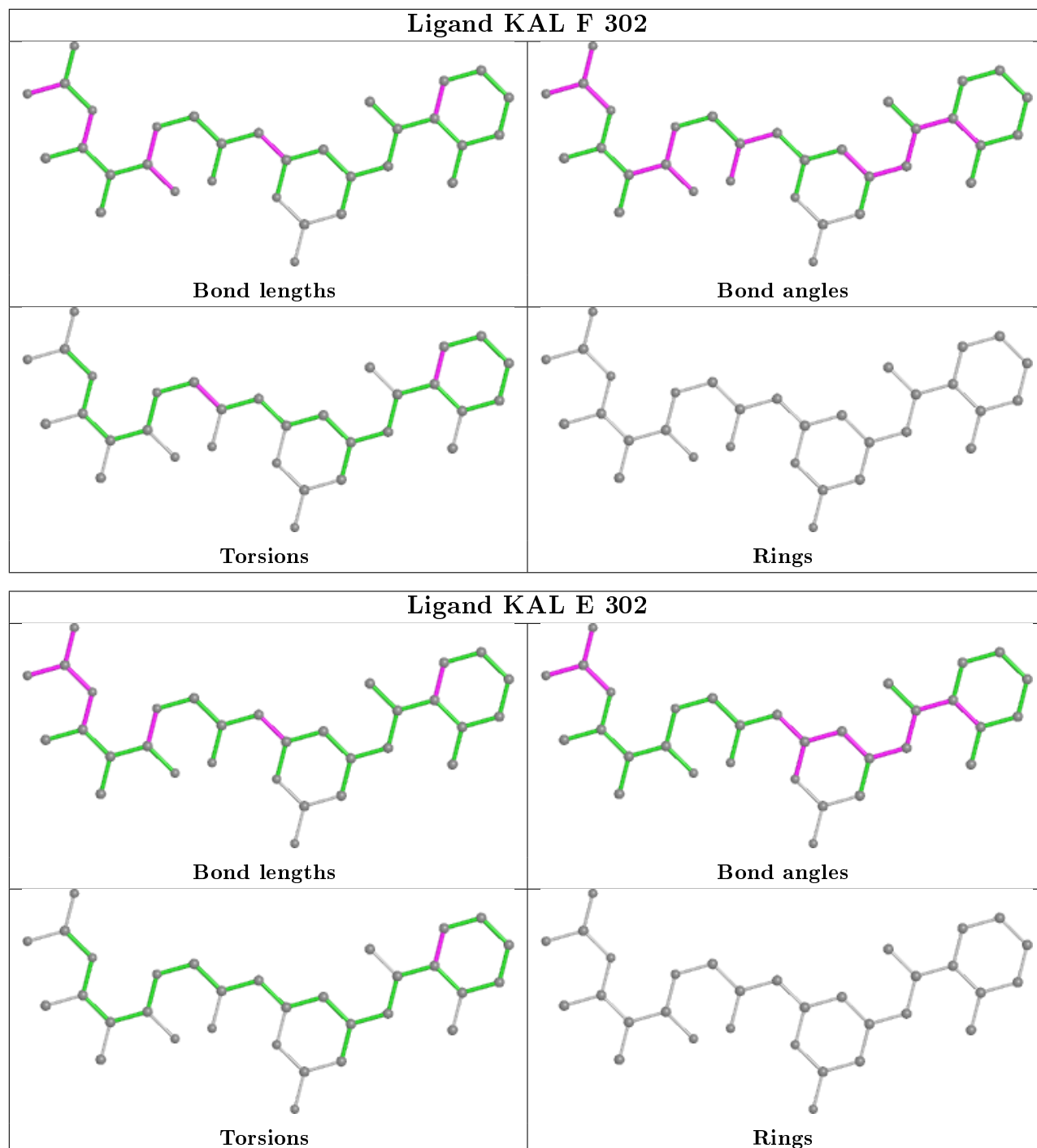


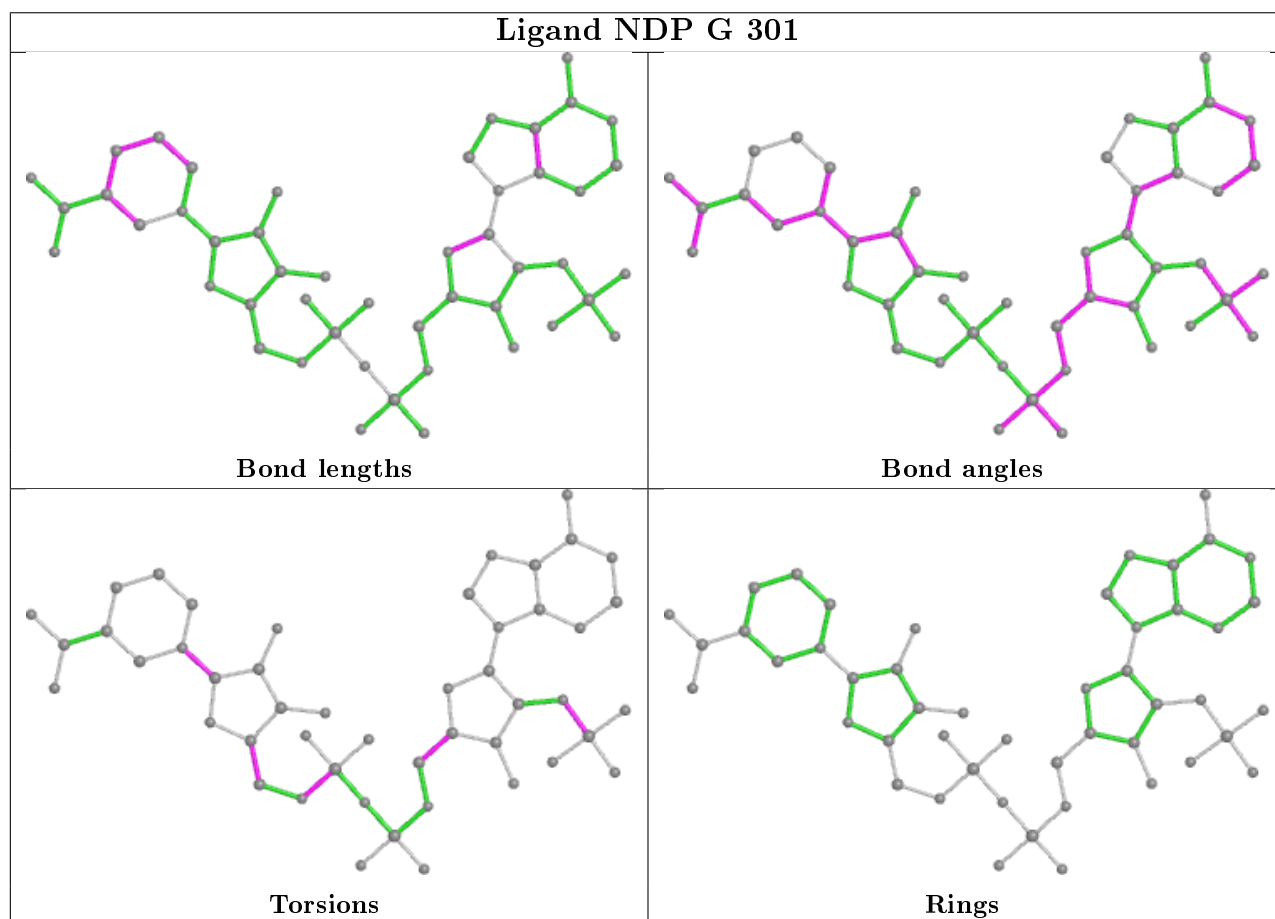
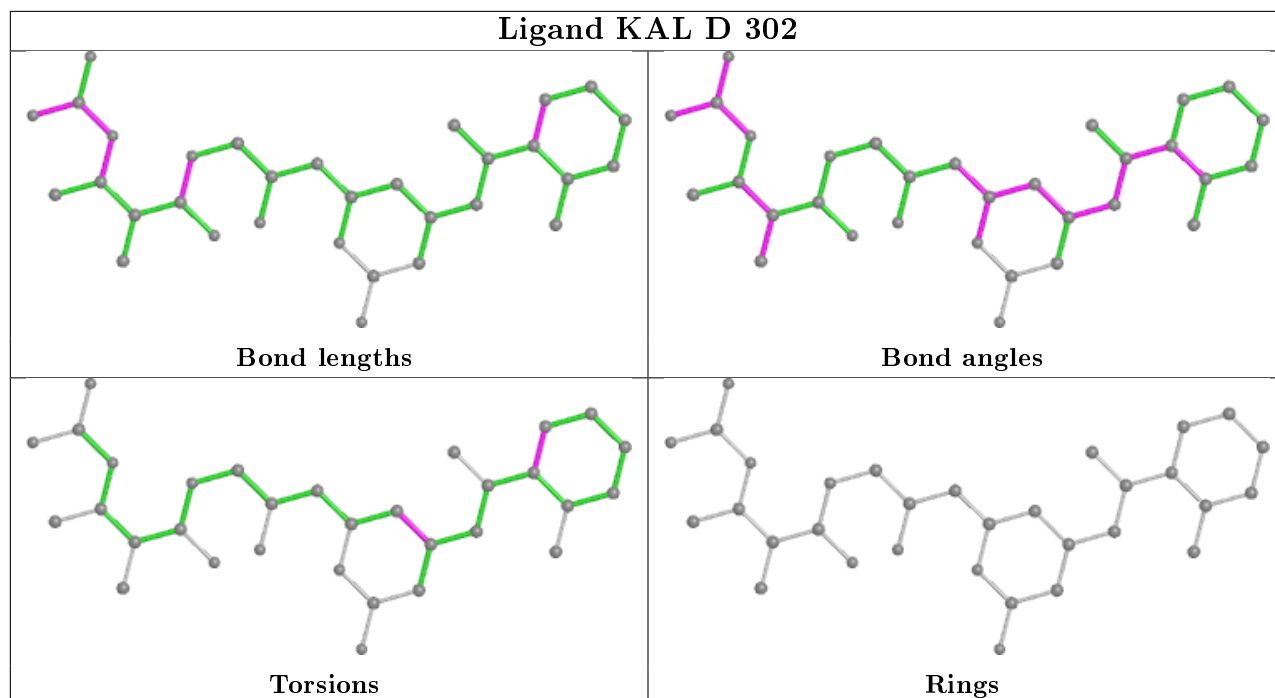


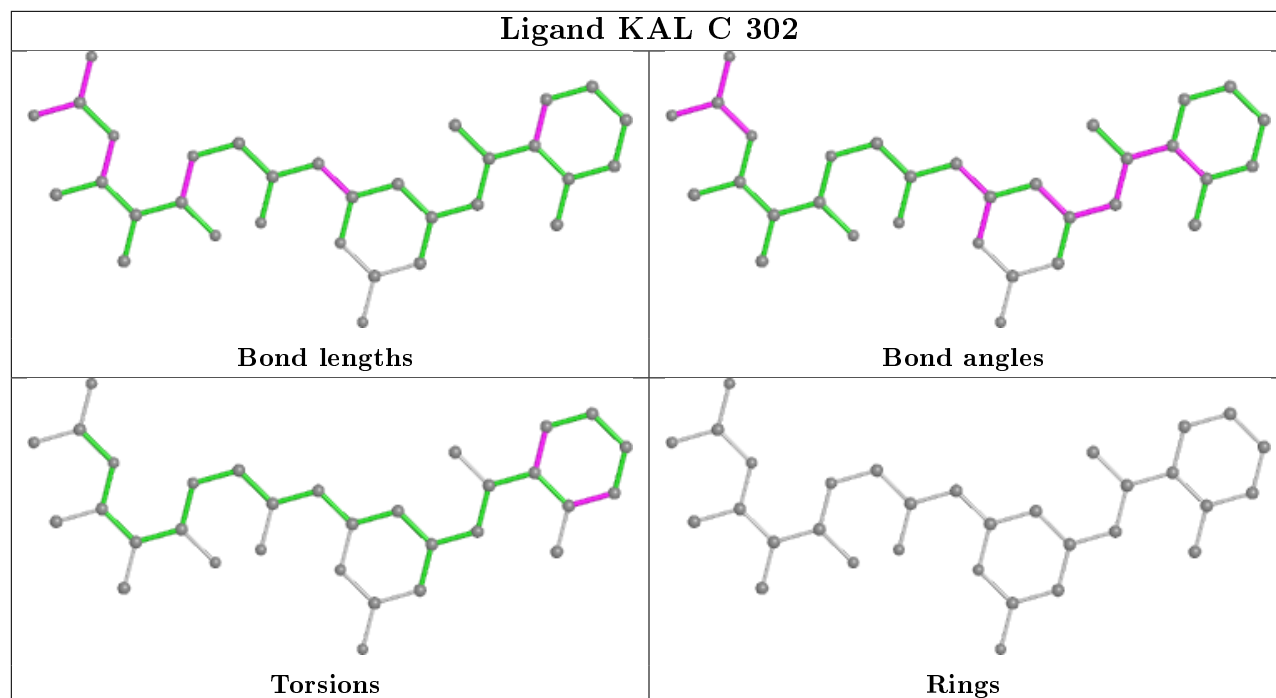












## 5.7 Other polymers [\(i\)](#)

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	259/261 (99%)	0.24	19 (7%) 15 11	61, 85, 134, 160	0
1	B	261/261 (100%)	0.25	25 (9%) 8 5	63, 88, 134, 191	1 (0%)
1	C	259/261 (99%)	0.35	38 (14%) 2 1	65, 86, 141, 172	0
1	D	258/261 (98%)	0.06	12 (4%) 31 29	59, 83, 131, 151	0
1	E	258/261 (98%)	0.20	19 (7%) 14 11	54, 80, 130, 146	0
1	F	258/261 (98%)	0.20	23 (8%) 9 6	55, 82, 127, 152	1 (0%)
1	G	260/261 (99%)	0.36	25 (9%) 8 5	57, 83, 128, 176	0
1	H	259/261 (99%)	0.54	34 (13%) 3 2	61, 92, 147, 176	0
All	All	2072/2088 (99%)	0.27	195 (9%) 8 5	54, 85, 135, 191	2 (0%)

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	93	SER	6.1
1	G	12	MET	6.1
1	H	12	MET	5.5
1	G	92	HIS	5.4
1	G	94	ILE	5.3
1	F	60	ALA	5.3
1	H	91	TYR	5.2
1	C	90	VAL	5.2
1	G	91	TYR	5.1
1	H	38	THR	5.1
1	A	12	MET	5.1
1	C	12	MET	5.1
1	B	203	GLY	4.9
1	G	13	GLY	4.9
1	B	-4	GLY	4.8
1	C	93	SER	4.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	11	ILE	4.6
1	F	12	MET	4.6
1	B	93	SER	4.4
1	G	145	THR	4.4
1	G	11	ILE	4.4
1	H	-2	HIS	4.4
1	H	92	HIS	4.4
1	F	199	LYS	4.3
1	H	43	ARG	4.3
1	F	46	LYS	4.3
1	G	90	VAL	4.3
1	H	60	ALA	4.2
1	H	10	VAL	4.2
1	B	12	MET	4.1
1	C	92	HIS	4.1
1	H	42	GLU	4.1
1	H	13	GLY	4.0
1	C	144	ALA	4.0
1	G	-2	HIS	4.0
1	B	46	LYS	4.0
1	H	93	SER	3.9
1	C	91	TYR	3.9
1	A	93	SER	3.9
1	C	45	ARG	3.8
1	G	-3	SER	3.8
1	G	125	LEU	3.8
1	H	46	LYS	3.8
1	C	41	LYS	3.7
1	E	93	SER	3.7
1	C	94	ILE	3.7
1	H	143	VAL	3.7
1	E	11	ILE	3.7
1	F	93	SER	3.6
1	A	144	ALA	3.5
1	C	143	VAL	3.5
1	F	143	VAL	3.5
1	B	92	HIS	3.5
1	A	92	HIS	3.5
1	F	53	GLU	3.5
1	F	90	VAL	3.5
1	C	13	GLY	3.4
1	C	199	LYS	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	91	TYR	3.3
1	E	12	MET	3.3
1	G	128	VAL	3.3
1	E	6	ASN	3.3
1	E	13	GLY	3.3
1	A	50	LYS	3.3
1	B	50	LYS	3.3
1	E	50	LYS	3.3
1	E	92	HIS	3.3
1	B	90	VAL	3.3
1	G	59	GLU	3.2
1	F	91	TYR	3.2
1	C	21	ALA	3.2
1	H	11	ILE	3.2
1	F	43	ARG	3.2
1	C	11	ILE	3.2
1	C	50	LYS	3.2
1	G	116	LEU	3.2
1	E	188	ILE	3.2
1	F	92	HIS	3.1
1	H	209	LYS	3.1
1	A	38	THR	3.1
1	G	143	VAL	3.1
1	C	203	GLY	3.1
1	F	11	ILE	3.1
1	A	91	TYR	3.1
1	C	43	ARG	3.1
1	B	202	GLY	3.1
1	A	143	VAL	3.0
1	H	90	VAL	3.0
1	E	43	ARG	3.0
1	A	10	VAL	3.0
1	E	143	VAL	2.9
1	H	61	HIS	2.9
1	B	199	LYS	2.9
1	F	94	ILE	2.9
1	B	143	VAL	2.9
1	H	45	ARG	2.9
1	E	91	TYR	2.9
1	D	89	GLY	2.9
1	C	145	THR	2.9
1	D	144	ALA	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	G	43	ARG	2.9
1	C	194	ARG	2.8
1	A	142	ILE	2.8
1	F	50	LYS	2.8
1	F	10	VAL	2.8
1	H	65	ILE	2.8
1	B	144	ALA	2.8
1	H	138	GLU	2.8
1	H	94	ILE	2.8
1	D	11	ILE	2.8
1	A	13	GLY	2.8
1	D	202	GLY	2.8
1	C	100	GLU	2.8
1	H	145	THR	2.7
1	H	53	GLU	2.7
1	C	10	VAL	2.7
1	E	90	VAL	2.7
1	B	187	ALA	2.7
1	H	50	LYS	2.7
1	E	144	ALA	2.6
1	G	38	THR	2.6
1	G	58	PRO	2.6
1	B	13	GLY	2.6
1	B	53	GLU	2.6
1	A	90	VAL	2.6
1	C	142	ILE	2.6
1	D	12	MET	2.6
1	C	59	GLU	2.6
1	B	145	THR	2.6
1	G	144	ALA	2.5
1	B	52	LEU	2.5
1	C	204	PHE	2.5
1	A	94	ILE	2.5
1	D	143	VAL	2.5
1	C	20	ILE	2.5
1	H	128	VAL	2.5
1	H	142	ILE	2.5
1	C	46	LYS	2.5
1	C	58	PRO	2.5
1	C	-2	HIS	2.4
1	D	43	ARG	2.4
1	B	6	ASN	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	144	ALA	2.4
1	H	21	ALA	2.4
1	E	-1	MET	2.4
1	F	13	GLY	2.3
1	G	60	ALA	2.3
1	E	138	GLU	2.3
1	A	43	ARG	2.3
1	C	53	GLU	2.3
1	F	103	ARG	2.3
1	H	196	LEU	2.3
1	H	85	GLY	2.3
1	F	54	GLN	2.3
1	C	44	SER	2.3
1	A	21	ALA	2.3
1	F	49	GLU	2.3
1	G	78	GLU	2.3
1	E	38	THR	2.2
1	F	38	THR	2.2
1	B	43	ARG	2.2
1	C	138	GLU	2.2
1	G	124	SER	2.2
1	G	21	ALA	2.2
1	B	45	ARG	2.2
1	H	86	ASN	2.2
1	C	103	ARG	2.2
1	D	92	HIS	2.2
1	D	46	LYS	2.2
1	C	60	ALA	2.2
1	F	200	GLY	2.2
1	H	81	GLY	2.2
1	C	52	LEU	2.2
1	B	209	LYS	2.1
1	B	142	ILE	2.1
1	D	142	ILE	2.1
1	B	205	ASN	2.1
1	D	50	LYS	2.1
1	B	55	LEU	2.1
1	A	145	THR	2.1
1	F	79	GLN	2.1
1	A	78	GLU	2.1
1	H	41	LYS	2.1
1	E	205	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	82	LYS	2.1
1	C	188	ILE	2.1
1	C	42	GLU	2.1
1	E	145	THR	2.0
1	D	188	ILE	2.0
1	C	125	LEU	2.0
1	H	59	GLU	2.0
1	G	146	THR	2.0
1	E	59	GLU	2.0
1	C	128	VAL	2.0
1	A	138	GLU	2.0

## 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.

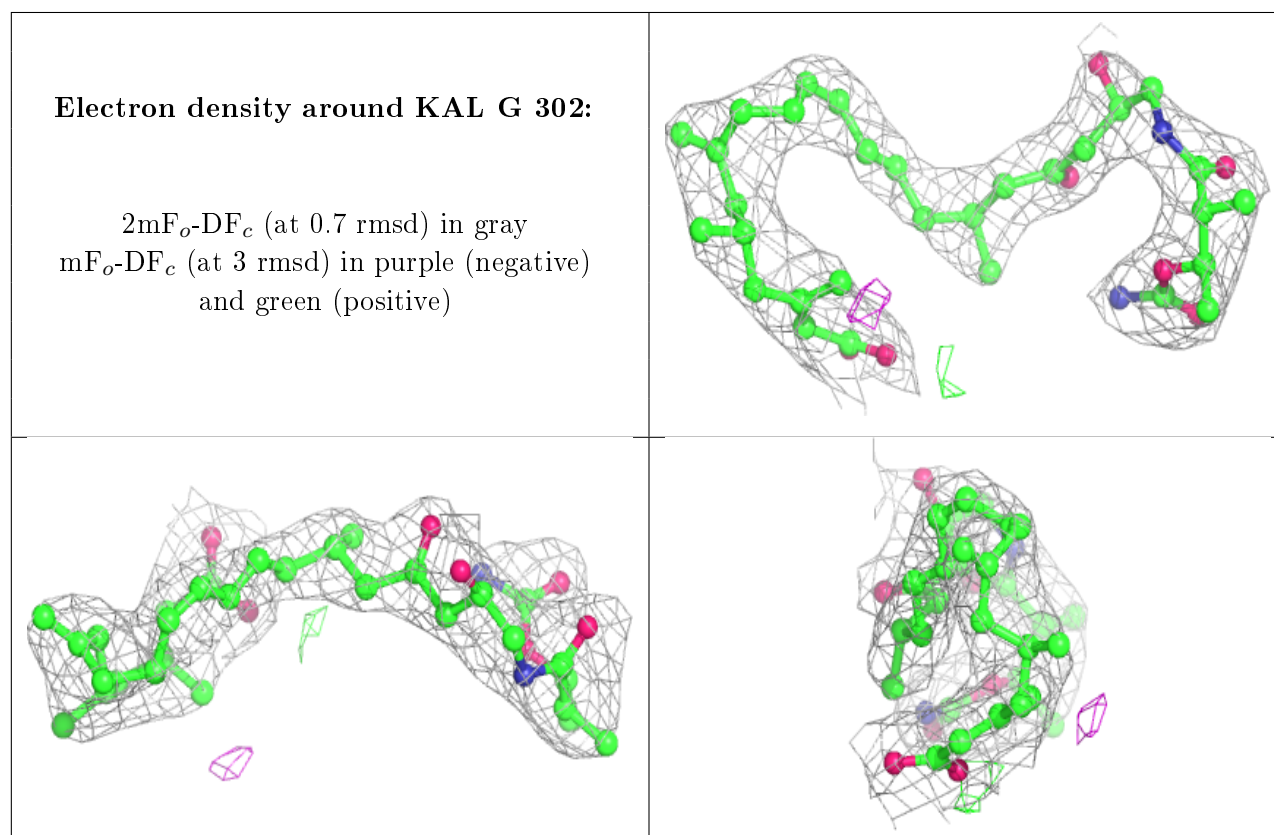
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	KAL	G	302	39/39	0.87	0.19	57,72,93,98	0
3	KAL	A	302	39/39	0.92	0.19	74,88,94,95	0
3	KAL	B	302	39/39	0.93	0.18	73,86,101,104	0
3	KAL	H	302	39/39	0.93	0.17	68,92,107,108	0
2	NDP	H	301	48/48	0.93	0.14	61,92,123,143	0
3	KAL	F	302	39/39	0.93	0.16	69,82,99,103	0
3	KAL	C	302	39/39	0.93	0.15	71,81,102,111	0
3	KAL	D	302	39/39	0.94	0.15	59,74,92,100	0
3	KAL	E	302	39/39	0.94	0.15	53,73,87,94	0
2	NDP	B	301	48/48	0.95	0.16	63,82,98,104	0
2	NDP	C	301	48/48	0.96	0.14	64,79,101,104	0
2	NDP	A	301	48/48	0.96	0.15	65,78,97,107	0

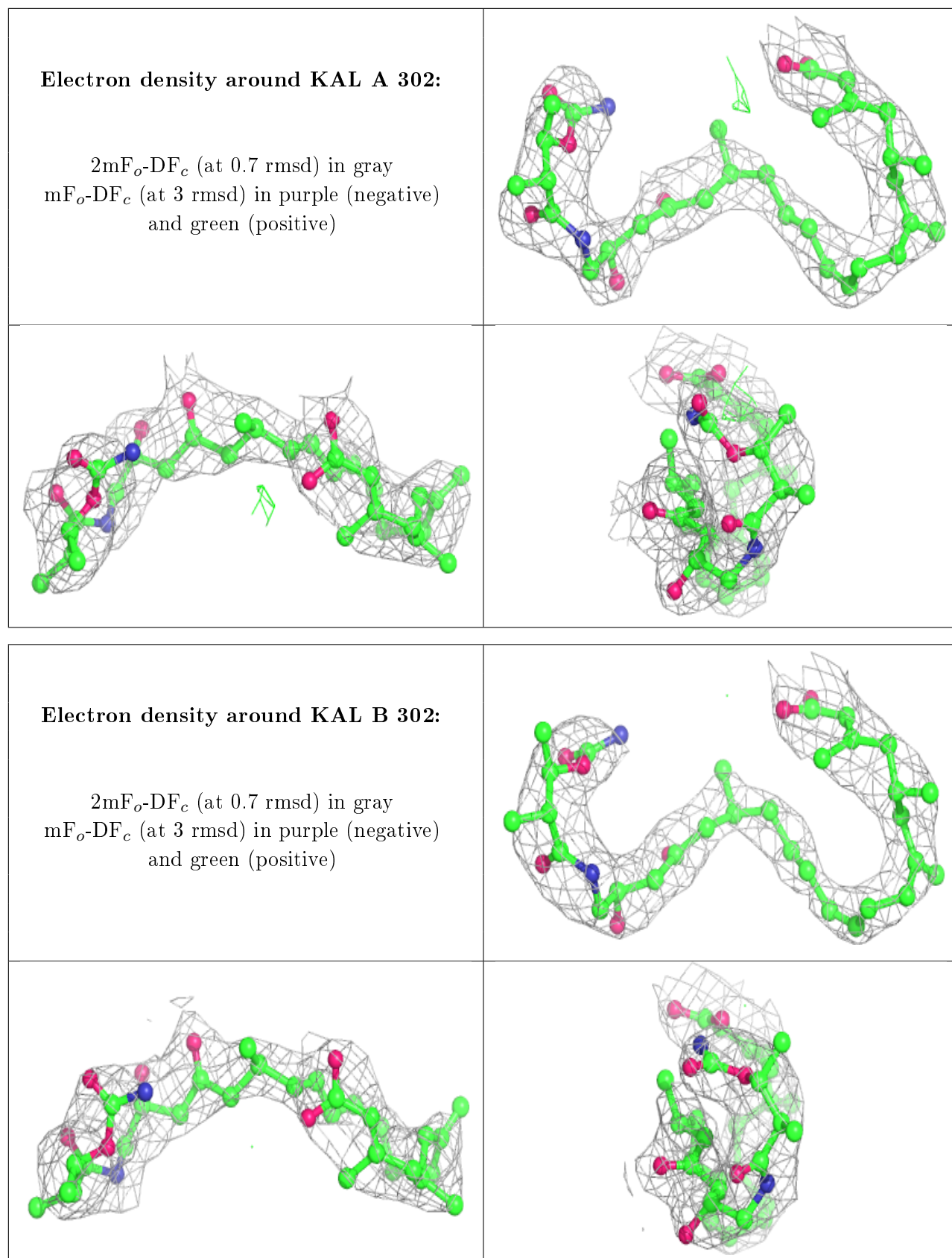
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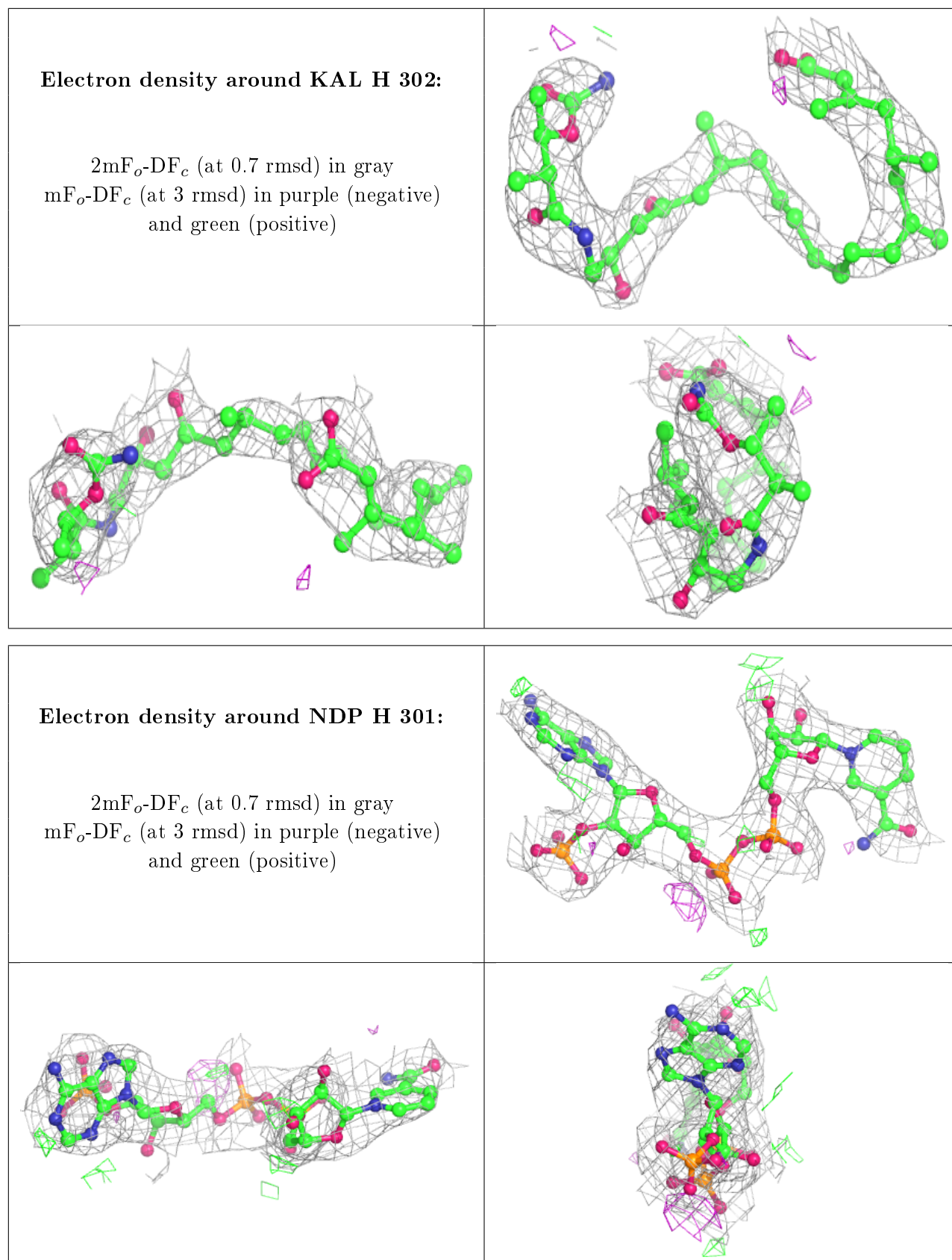
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NDP	E	301	48/48	0.96	0.15	59,72,87,93	0
2	NDP	G	301	48/48	0.96	0.16	63,73,85,97	0
2	NDP	F	301	48/48	0.96	0.14	55,82,98,104	0
2	NDP	D	301	48/48	0.98	0.14	68,78,94,110	0

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.

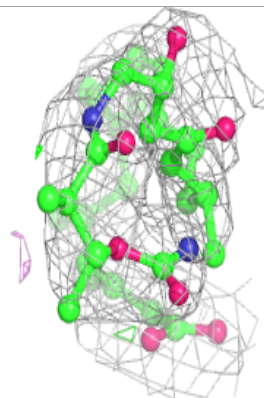
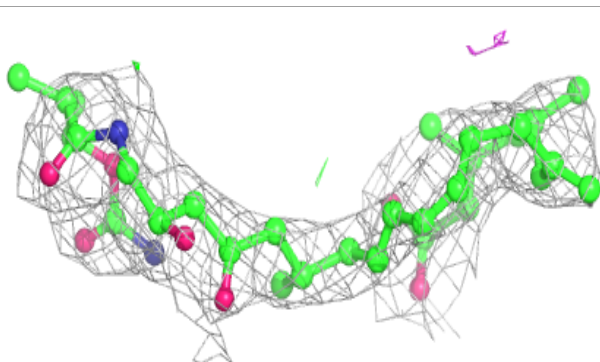
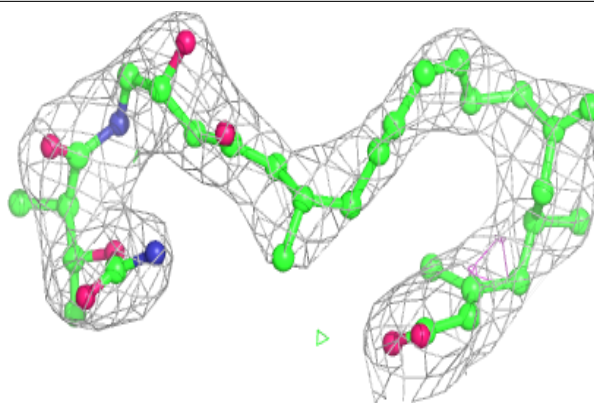




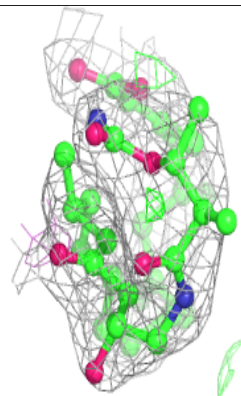
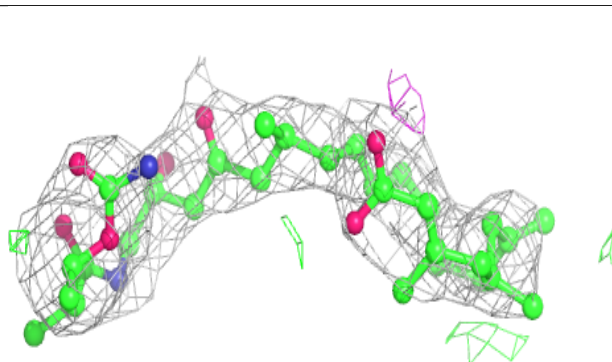
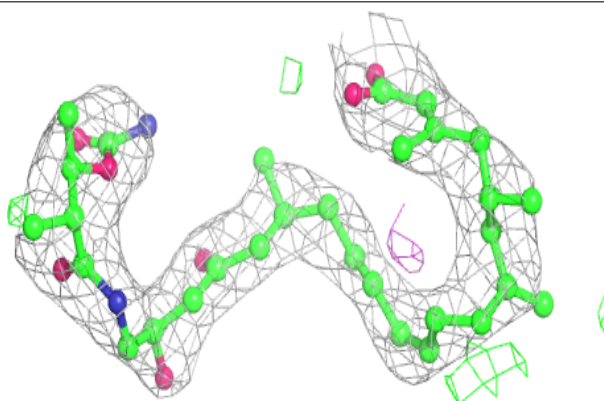


**Electron density around KAL F 302:**

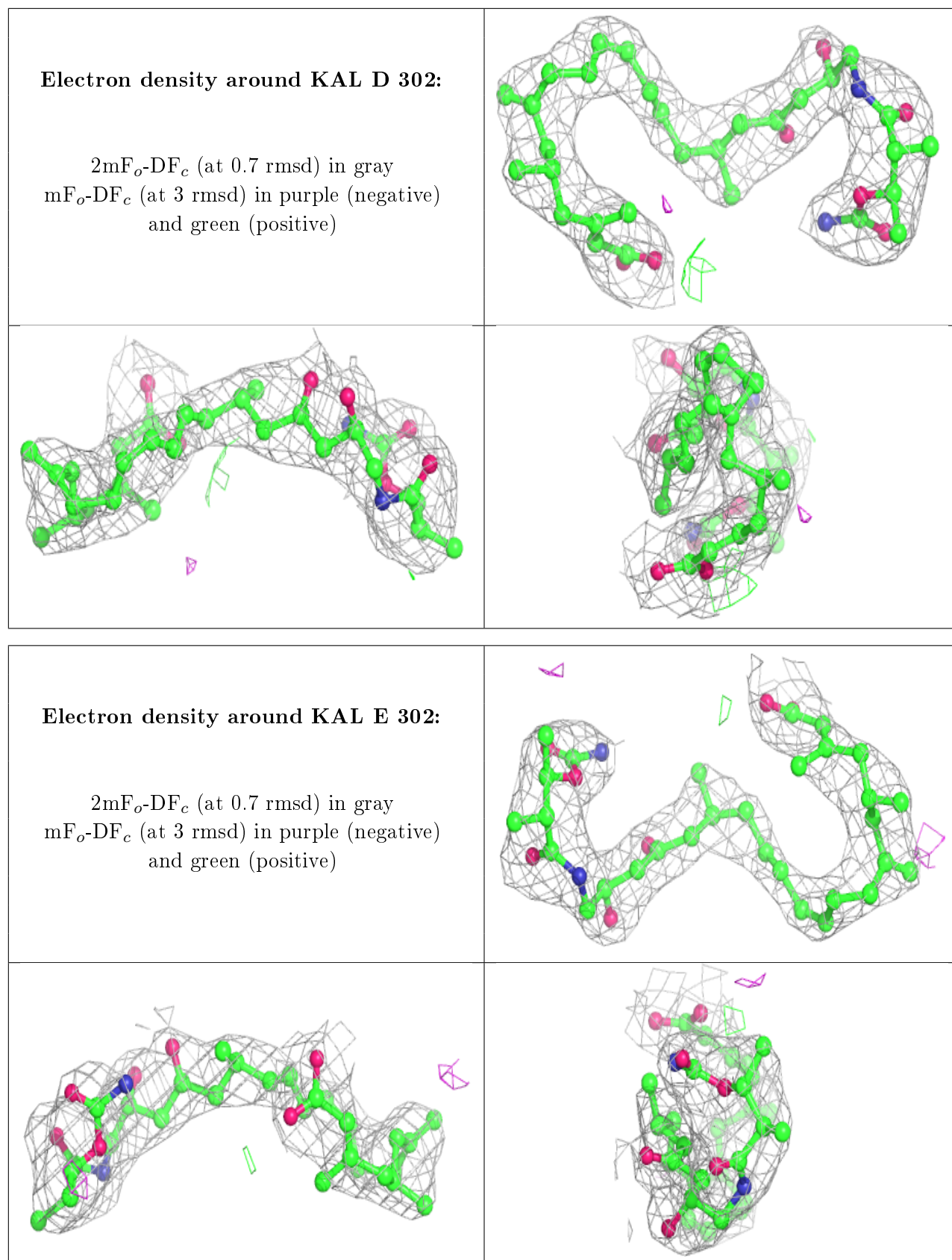
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around KAL C 302:**

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

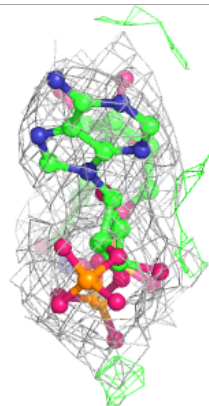
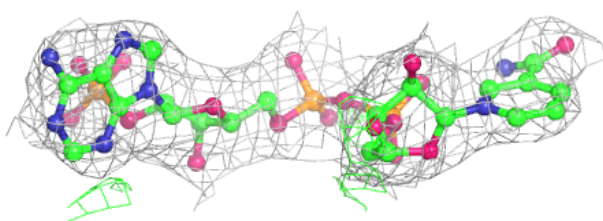
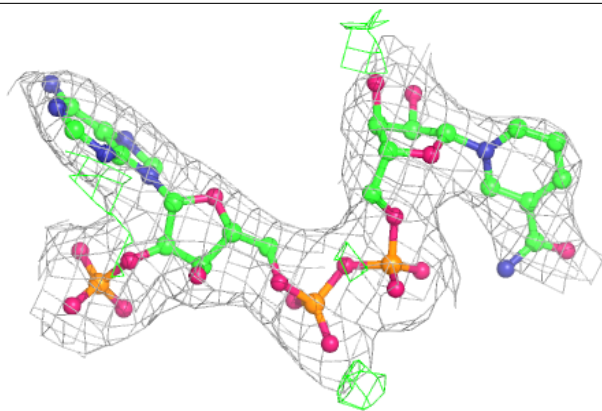




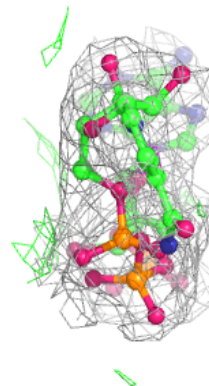
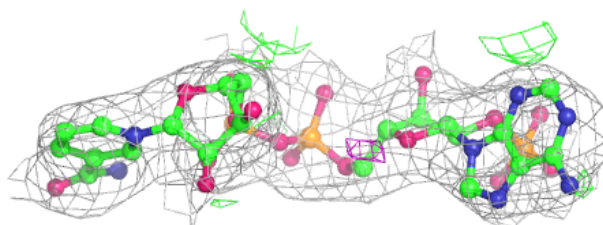
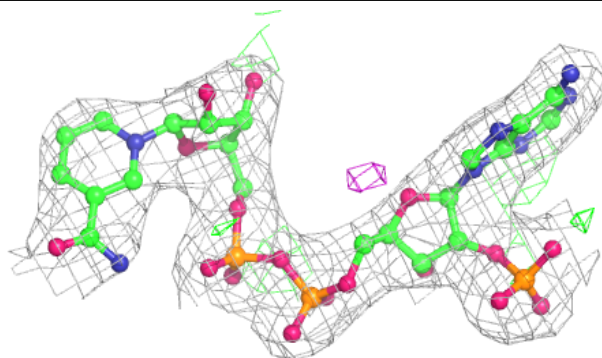


**Electron density around NDP B 301:**

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

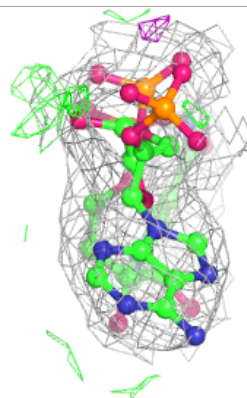
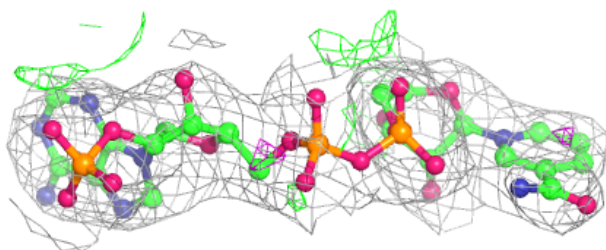
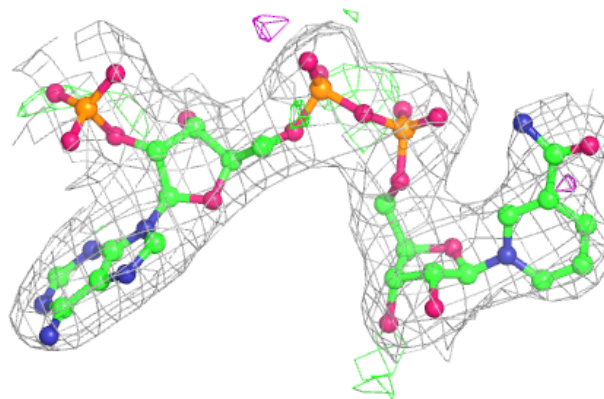
**Electron density around NDP C 301:**

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

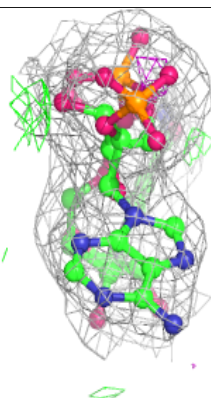
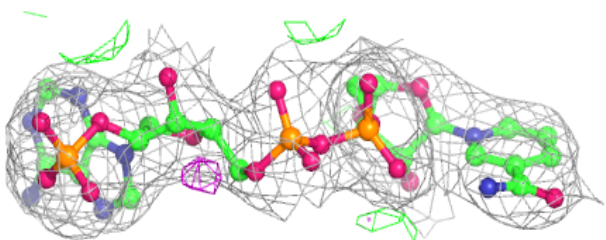
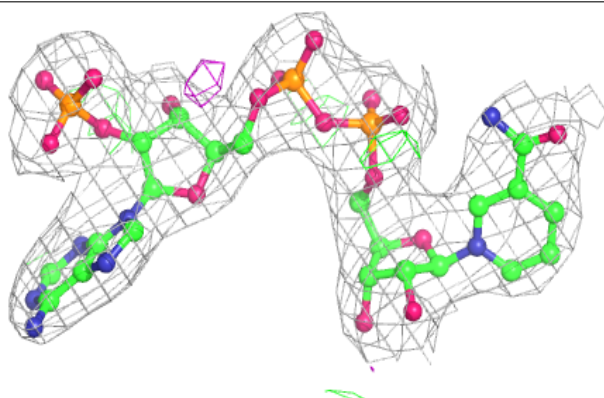


**Electron density around NDP A 301:**

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

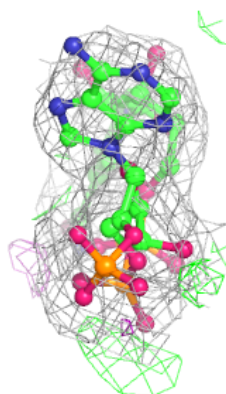
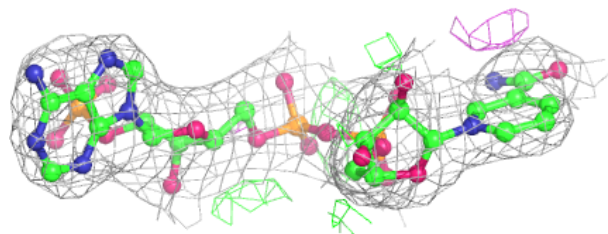
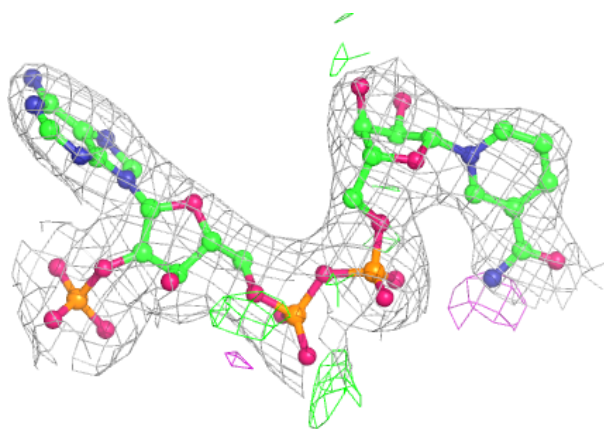
**Electron density around NDP E 301:**

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

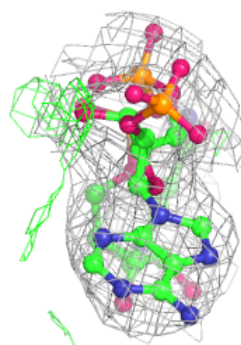
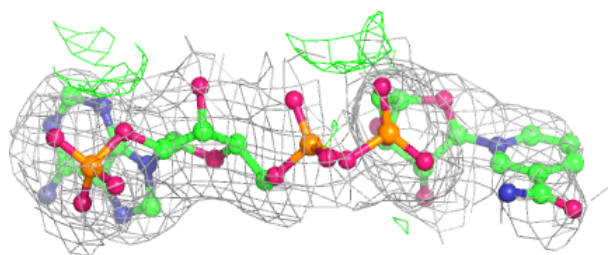
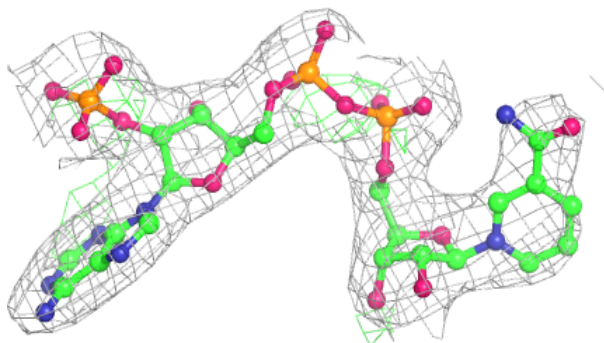


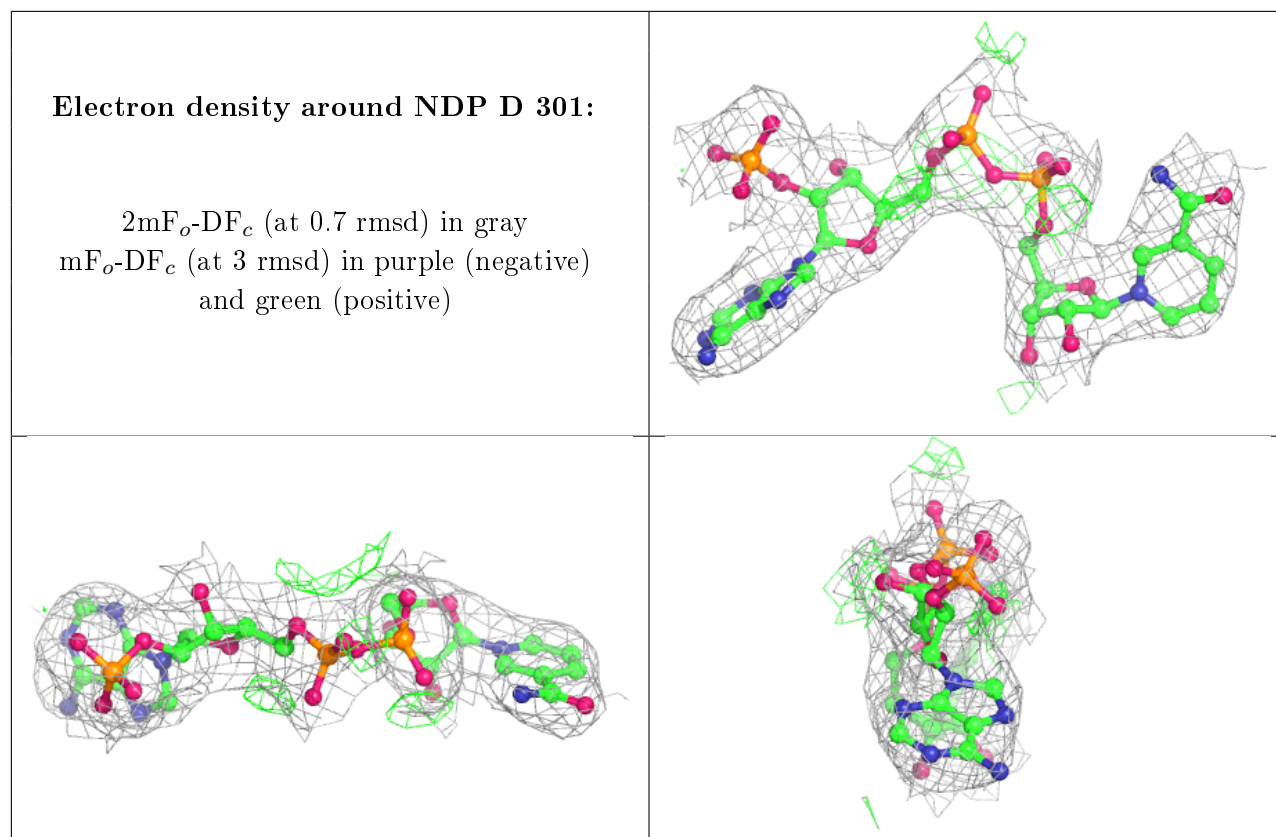
**Electron density around NDP G 301:**

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

**Electron density around NDP F 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.