



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 07:55 AM EDT

PDB ID : 6T6N  
Title : Crystal structure of *Klebsiella pneumoniae* FabG2(NADH-dependent) in complex with NADH at 2.5 Å resolution  
Authors : Vella, P.; Schnell, R.; Lindqvist, Y.; Schneider, G.  
Deposited on : 2019-10-18  
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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 : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
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

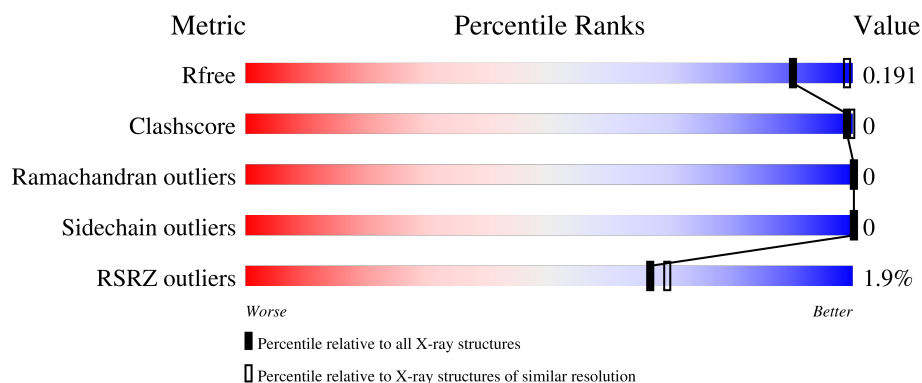
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



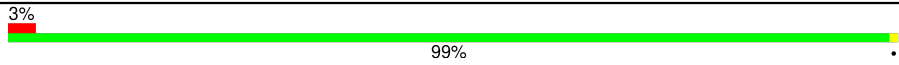
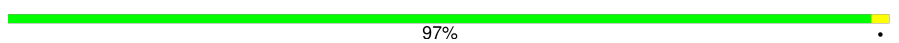
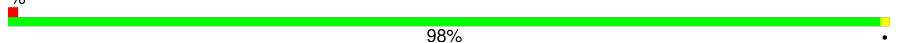
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	245	<div> <div>4%</div> <div>98%</div> <div>.</div> </div>
1	B	245	<div> <div>2%</div> <div>99%</div> <div>.</div> </div>
1	C	245	<div> <div>97%</div> <div>..</div> </div>
1	D	245	<div> <div>98%</div> <div>.</div> </div>
1	E	245	<div> <div>4%</div> <div>99%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	245	
1	G	245	
1	H	245	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	F	302	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15171 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 3-oxoacyl-[acyl-carrier protein] reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	4	0
			1812	1133	322	344	13			
1	B	244	Total	C	N	O	S	0	1	0
			1792	1117	321	341	13			
1	C	244	Total	C	N	O	S	0	4	0
			1814	1130	329	342	13			
1	D	244	Total	C	N	O	S	0	2	0
			1798	1120	323	342	13			
1	E	244	Total	C	N	O	S	0	1	0
			1797	1118	324	342	13			
1	F	244	Total	C	N	O	S	0	2	0
			1795	1118	321	343	13			
1	G	244	Total	C	N	O	S	0	3	0
			1807	1125	326	343	13			
1	H	244	Total	C	N	O	S	0	1	0
			1791	1116	320	341	14			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP W8VGR4
A	2	ALA	LYS	engineered mutation	UNP W8VGR4
B	0	SER	-	expression tag	UNP W8VGR4
B	2	ALA	LYS	engineered mutation	UNP W8VGR4
C	0	SER	-	expression tag	UNP W8VGR4
C	2	ALA	LYS	engineered mutation	UNP W8VGR4
D	0	SER	-	expression tag	UNP W8VGR4
D	2	ALA	LYS	engineered mutation	UNP W8VGR4
E	0	SER	-	expression tag	UNP W8VGR4
E	2	ALA	LYS	engineered mutation	UNP W8VGR4
F	0	SER	-	expression tag	UNP W8VGR4
F	2	ALA	LYS	engineered mutation	UNP W8VGR4
G	0	SER	-	expression tag	UNP W8VGR4

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Chain	Residue	Modelled	Actual	Comment	Reference
G	2	ALA	LYS	engineered mutation	UNP W8VGR4
H	0	SER	-	expression tag	UNP W8VGR4
H	2	ALA	LYS	engineered mutation	UNP W8VGR4

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



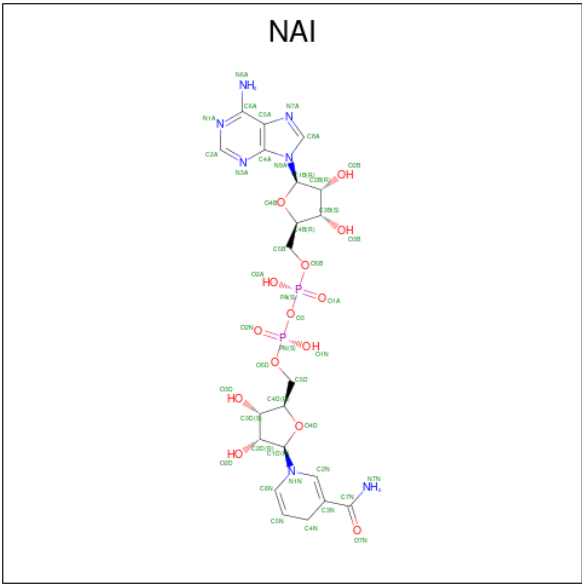
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	E	1	6	3	3	0	0
2	F	1	6	3	3	0	0
2	F	1	6	3	3	0	0
2	G	1	6	3	3	0	0
2	G	1	6	3	3	0	0
2	G	1	6	3	3	0	0
2	G	1	6	3	3	0	0
2	H	1	6	3	3	0	0
2	H	1	6	3	3	0	0

- Molecule 3 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C<sub>21</sub>H<sub>29</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



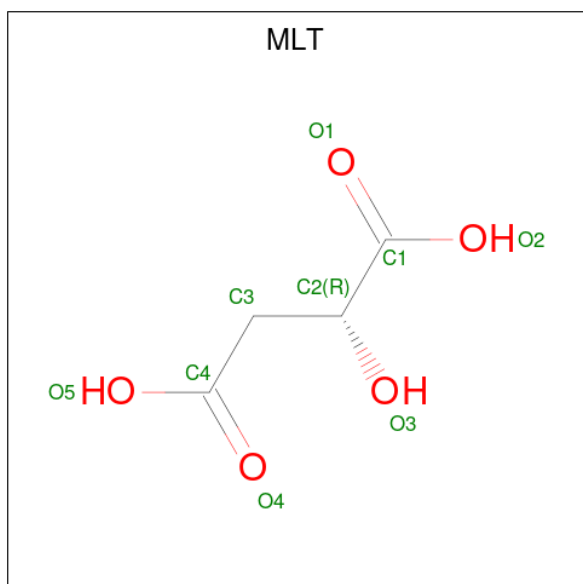
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	44	21	7	14	2	0
3	B	1	44	21	7	14	2	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is D-MALATE (three-letter code: MLT) (formula:  $C_4H_6O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			9	4	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	27	Total	O	0	0
			27	27		
5	B	22	Total	O	0	0
			22	22		

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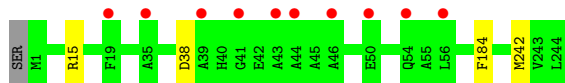
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	44	Total 44	O 44	0	0
5	D	50	Total 50	O 50	0	0
5	E	11	Total 11	O 11	0	0
5	F	16	Total 16	O 16	0	0
5	G	52	Total 52	O 52	0	0
5	H	68	Total 68	O 68	0	0



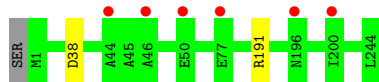
### 3 Residue-property plots [i](#)

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: 3-oxoacyl-[acyl-carrier protein] reductase



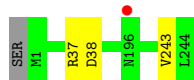
- Molecule 1: 3-oxoacyl-[acyl-carrier protein] reductase



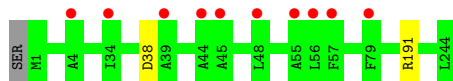
- Molecule 1: 3-oxoacyl-[acyl-carrier protein] reductase



- Molecule 1: 3-oxoacyl-[acyl-carrier protein] reductase



- Molecule 1: 3-oxoacyl-[acyl-carrier protein] reductase



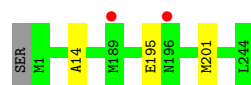
- Molecule 1: 3-oxoacyl-[acyl-carrier protein] reductase



- Molecule 1: 3-oxoacyl-[acyl-carrier protein] reductase



- Molecule 1: 3-oxoacyl-[acyl-carrier protein] reductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	161.11Å 255.32Å 262.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 48.96 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (30.00-2.50) 99.2 (48.96-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.192 , 0.211 0.198 , 0.191	Depositor DCC
$R_{free}$ test set	4604 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.0	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 40.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15171	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.93 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2318e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: GOL, NAI, MLT

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	0.48	0/1846	0.76	3/2491 (0.1%)
1	B	0.49	0/1816	0.72	2/2451 (0.1%)
1	C	0.54	0/1847	0.83	8/2492 (0.3%)
1	D	0.51	0/1825	0.74	3/2464 (0.1%)
1	E	0.52	2/1818 (0.1%)	0.75	4/2454 (0.2%)
1	F	0.46	0/1822	0.72	2/2461 (0.1%)
1	G	0.52	0/1837	0.75	2/2479 (0.1%)
1	H	0.53	0/1815	0.76	2/2450 (0.1%)
All	All	0.51	2/14626 (0.0%)	0.75	26/19742 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	191[A]	ARG	CZ-NH2	-5.04	1.26	1.33
1	E	191[B]	ARG	CZ-NH2	-5.04	1.26	1.33

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	38	ASP	CB-CG-OD2	-8.91	110.28	118.30
1	C	15[A]	ARG	NE-CZ-NH2	7.42	124.01	120.30
1	C	15[B]	ARG	NE-CZ-NH2	7.42	124.01	120.30
1	F	15	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	D	38	ASP	CB-CG-OD2	6.63	124.26	118.30
1	B	38	ASP	CB-CG-OD2	6.61	124.25	118.30
1	C	201	MET	CG-SD-CE	6.39	110.42	100.20
1	G	15	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	E	38	ASP	CB-CG-OD1	6.26	123.93	118.30
1	G	38	ASP	CB-CG-OD1	6.24	123.92	118.30
1	A	38	ASP	CB-CG-OD2	-6.08	112.83	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	38	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	A	38	ASP	CB-CG-OD1	5.98	123.68	118.30
1	E	191[A]	ARG	NE-CZ-NH2	5.80	123.20	120.30
1	E	191[B]	ARG	NE-CZ-NH2	5.80	123.20	120.30
1	D	38	ASP	CB-CG-OD1	-5.61	113.25	118.30
1	H	195	GLU	CG-CD-OE1	5.47	129.24	118.30
1	B	191	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	C	15[A]	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	C	15[B]	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	H	201	MET	CG-SD-CE	5.23	108.57	100.20
1	A	15	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	D	37	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	F	38	ASP	CB-CG-OD2	5.07	122.86	118.30
1	C	126[A]	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	C	126[B]	ARG	NE-CZ-NH1	5.02	122.81	120.30

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	1812	0	1840	2	0
1	B	1792	0	1817	0	0
1	C	1814	0	1850	3	0
1	D	1798	0	1824	1	0
1	E	1797	0	1816	0	0
1	F	1795	0	1817	0	0
1	G	1807	0	1834	3	0
1	H	1791	0	1813	1	0
2	A	6	0	8	0	0
2	B	12	0	16	0	0
2	C	18	0	24	0	0
2	D	18	0	24	1	0
2	E	12	0	16	0	0
2	F	12	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	24	0	32	1	0
2	H	12	0	16	1	0
3	A	44	0	27	0	0
3	B	44	0	27	0	0
3	C	44	0	27	0	0
3	D	44	0	27	0	0
3	E	44	0	27	0	0
3	F	44	0	27	0	0
3	G	44	0	27	1	0
3	H	44	0	27	0	0
4	H	9	0	4	0	0
5	A	27	0	0	0	0
5	B	22	0	0	0	0
5	C	44	0	0	0	0
5	D	50	0	0	0	0
5	E	11	0	0	0	0
5	F	16	0	0	0	0
5	G	52	0	0	0	0
5	H	68	0	0	0	0
All	All	15171	0	14983	10	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 0.

All (10) 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:VAL:O	1:G:200:ILE:HG13	1.59	1.02
1:H:14:ALA:O	2:H:301:GOL:O1	2.32	0.46
1:A:184[A]:PHE:CD2	1:A:242:MET:CE	2.99	0.46
1:C:76:GLU:OE1	1:C:126[B]:ARG:NH1	2.46	0.46
1:C:15[A]:ARG:NH1	1:C:38:ASP:OD2	2.37	0.44
1:G:141:ALA:HB1	2:G:301:GOL:H31	2.00	0.44
1:A:184[A]:PHE:CD2	1:A:242:MET:HE2	2.54	0.42
1:D:243:VAL:HA	2:D:302:GOL:H11	2.01	0.41
1:G:17:ILE:HB	3:G:305:NAI:H51N	2.01	0.40
1:C:204:LYS:HB3	1:C:204:LYS:HE3	1.99	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	246/245 (100%)	237 (96%)	9 (4%)	0	100	100
1	B	243/245 (99%)	235 (97%)	8 (3%)	0	100	100
1	C	246/245 (100%)	238 (97%)	8 (3%)	0	100	100
1	D	244/245 (100%)	236 (97%)	8 (3%)	0	100	100
1	E	243/245 (99%)	236 (97%)	7 (3%)	0	100	100
1	F	244/245 (100%)	236 (97%)	8 (3%)	0	100	100
1	G	245/245 (100%)	238 (97%)	7 (3%)	0	100	100
1	H	243/245 (99%)	235 (97%)	8 (3%)	0	100	100
All	All	1954/1960 (100%)	1891 (97%)	63 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	182/179 (102%)	182 (100%)	0	100	100
1	B	179/179 (100%)	179 (100%)	0	100	100
1	C	182/179 (102%)	182 (100%)	0	100	100
1	D	180/179 (101%)	180 (100%)	0	100	100
1	E	179/179 (100%)	179 (100%)	0	100	100
1	F	180/179 (101%)	180 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	181/179 (101%)	181 (100%)	0	100	100
1	H	179/179 (100%)	179 (100%)	0	100	100
All	All	1442/1432 (101%)	1442 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	C	67	GLN
1	D	92	ASN
1	E	67	GLN
1	G	67	GLN
1	G	92	ASN
1	H	92	ASN

### 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](#)

28 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	GOL	D	301	-	5,5,5	0.30	0	5,5,5	0.50	0
2	GOL	B	302	-	5,5,5	0.46	0	5,5,5	0.36	0
2	GOL	D	302	-	5,5,5	0.61	0	5,5,5	1.15	1 (20%)
2	GOL	C	301	-	5,5,5	0.15	0	5,5,5	0.37	0
3	NAI	G	305	-	43,48,48	0.89	1 (2%)	50,73,73	1.70	7 (14%)
2	GOL	D	303	-	5,5,5	0.32	0	5,5,5	0.49	0
3	NAI	D	304	-	43,48,48	0.95	2 (4%)	50,73,73	1.64	7 (14%)
2	GOL	E	301	-	5,5,5	0.38	0	5,5,5	0.67	0
2	GOL	G	303	-	5,5,5	0.67	0	5,5,5	0.52	0
3	NAI	E	303	-	43,48,48	1.06	2 (4%)	50,73,73	1.53	8 (16%)
2	GOL	H	301	-	5,5,5	0.50	0	5,5,5	0.36	0
2	GOL	A	301	-	5,5,5	0.58	0	5,5,5	0.87	0
2	GOL	F	302	-	5,5,5	0.57	0	5,5,5	0.41	0
3	NAI	C	304	-	43,48,48	0.92	1 (2%)	50,73,73	1.42	4 (8%)
3	NAI	B	303	-	43,48,48	0.98	0	50,73,73	1.70	5 (10%)
2	GOL	G	304	-	5,5,5	0.34	0	5,5,5	0.37	0
2	GOL	C	302	-	5,5,5	0.30	0	5,5,5	0.63	0
3	NAI	A	302	-	43,48,48	1.07	3 (6%)	50,73,73	1.53	8 (16%)
2	GOL	C	303	-	5,5,5	0.28	0	5,5,5	0.31	0
2	GOL	H	302	-	5,5,5	0.31	0	5,5,5	0.95	0
2	GOL	G	301	-	5,5,5	0.27	0	5,5,5	0.78	0
4	MLT	H	303	-	8,8,8	1.30	0	10,10,10	1.26	1 (10%)
2	GOL	E	302	-	5,5,5	0.29	0	5,5,5	0.49	0
2	GOL	F	301	-	5,5,5	0.39	0	5,5,5	0.66	0
3	NAI	H	304	-	43,48,48	0.85	0	50,73,73	1.70	10 (20%)
2	GOL	B	301	-	5,5,5	0.51	0	5,5,5	0.49	0
3	NAI	F	303	-	43,48,48	0.93	3 (6%)	50,73,73	1.78	8 (16%)
2	GOL	G	302	-	5,5,5	0.38	0	5,5,5	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	D	301	-	-	0/4/4/4	-
2	GOL	B	302	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	D	302	-	-	3/4/4/4	-
2	GOL	C	301	-	-	0/4/4/4	-
3	NAI	G	305	-	-	2/25/72/72	0/5/5/5
2	GOL	D	303	-	-	2/4/4/4	-
3	NAI	D	304	-	-	3/25/72/72	0/5/5/5
2	GOL	E	301	-	-	2/4/4/4	-
2	GOL	G	303	-	-	0/4/4/4	-
3	NAI	E	303	-	-	4/25/72/72	0/5/5/5
2	GOL	H	301	-	-	2/4/4/4	-
2	GOL	A	301	-	-	2/4/4/4	-
2	GOL	F	302	-	-	0/4/4/4	-
3	NAI	C	304	-	-	4/25/72/72	0/5/5/5
3	NAI	B	303	-	-	6/25/72/72	0/5/5/5
2	GOL	G	304	-	-	2/4/4/4	-
2	GOL	C	302	-	-	2/4/4/4	-
3	NAI	A	302	-	-	3/25/72/72	0/5/5/5
2	GOL	C	303	-	-	4/4/4/4	-
2	GOL	H	302	-	-	2/4/4/4	-
2	GOL	G	301	-	-	2/4/4/4	-
4	MLT	H	303	-	-	1/8/8/8	-
2	GOL	E	302	-	-	0/4/4/4	-
2	GOL	F	301	-	-	2/4/4/4	-
3	NAI	H	304	-	-	3/25/72/72	0/5/5/5
2	GOL	B	301	-	-	2/4/4/4	-
3	NAI	F	303	-	-	3/25/72/72	0/5/5/5
2	GOL	G	302	-	-	0/4/4/4	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	NAI	PA-O3	3.71	1.63	1.59
3	E	303	NAI	PA-O3	2.98	1.62	1.59
3	C	304	NAI	C6N-C5N	2.45	1.40	1.33
3	A	302	NAI	PN-O3	2.45	1.62	1.59
3	F	303	NAI	C2A-N3A	2.45	1.35	1.32
3	E	303	NAI	PN-O3	2.37	1.62	1.59
3	G	305	NAI	C2A-N3A	2.37	1.35	1.32
3	D	304	NAI	C2N-C3N	2.26	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	304	NAI	O4B-C1B	2.20	1.43	1.40
3	F	303	NAI	C2N-C3N	2.15	1.41	1.35
3	A	302	NAI	C6N-C5N	2.10	1.39	1.33
3	F	303	NAI	C6N-C5N	2.01	1.39	1.33

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	303	NAI	O4B-C1B-N9A	7.67	118.91	108.75
3	D	304	NAI	O4B-C1B-N9A	6.72	117.65	108.75
3	F	303	NAI	O4B-C1B-N9A	6.42	117.26	108.75
3	G	305	NAI	O4B-C1B-N9A	6.31	117.11	108.75
3	E	303	NAI	N3A-C2A-N1A	-5.21	121.60	128.67
3	C	304	NAI	O4B-C1B-N9A	5.13	115.55	108.75
3	H	304	NAI	O4B-C1B-N9A	5.07	115.47	108.75
3	C	304	NAI	N3A-C2A-N1A	-4.84	122.11	128.67
3	G	305	NAI	N3A-C2A-N1A	-4.83	122.11	128.67
3	H	304	NAI	N3A-C2A-N1A	-4.67	122.34	128.67
3	D	304	NAI	N3A-C2A-N1A	-4.58	122.45	128.67
3	A	302	NAI	N3A-C2A-N1A	-4.58	122.46	128.67
3	F	303	NAI	N3A-C2A-N1A	-4.43	122.66	128.67
3	A	302	NAI	O4B-C1B-N9A	4.28	114.42	108.75
3	B	303	NAI	N3A-C2A-N1A	-4.22	122.94	128.67
3	F	303	NAI	O3-PA-O1A	-4.11	98.33	110.70
3	E	303	NAI	C1B-N9A-C4A	-4.04	119.55	126.64
3	G	305	NAI	C1B-N9A-C4A	-3.83	119.90	126.64
3	A	302	NAI	C3N-C7N-N7N	3.23	123.40	117.67
3	A	302	NAI	O7N-C7N-C3N	-3.22	114.84	120.90
3	H	304	NAI	C6N-N1N-C2N	3.16	122.70	119.32
3	B	303	NAI	O3-PA-O1A	-3.14	101.26	110.70
3	F	303	NAI	O2A-PA-O1A	3.08	126.77	112.44
3	F	303	NAI	O1N-PN-O2N	3.07	126.70	112.44
3	E	303	NAI	O2A-PA-O1A	2.91	125.99	112.44
3	F	303	NAI	C1B-N9A-C4A	-2.89	121.56	126.64
3	E	303	NAI	C6N-N1N-C2N	2.85	122.37	119.32
3	H	304	NAI	C1B-N9A-C4A	-2.83	121.67	126.64
3	H	304	NAI	C3N-C7N-N7N	2.81	122.66	117.67
4	H	303	MLT	O2-C1-C2	2.79	118.64	112.74
3	H	304	NAI	N6A-C6A-N1A	2.77	124.26	118.33
3	H	304	NAI	C4B-O4B-C1B	-2.77	107.39	109.92
3	G	305	NAI	O1N-PN-O2N	2.76	125.28	112.44
3	G	305	NAI	C6N-N1N-C2N	2.69	122.20	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	305	NAI	O2A-PA-O1A	2.67	124.86	112.44
3	F	303	NAI	C3N-C7N-N7N	2.66	122.39	117.67
3	B	303	NAI	O1N-PN-O2N	2.63	124.67	112.44
3	F	303	NAI	C4A-C5A-N7A	-2.62	106.57	109.34
3	E	303	NAI	O1N-PN-O2N	2.51	124.14	112.44
3	A	302	NAI	O3-PA-O1A	-2.51	103.14	110.70
3	D	304	NAI	O1N-PN-O2N	2.51	124.12	112.44
2	D	302	GOL	O3-C3-C2	2.43	121.30	110.38
3	D	304	NAI	N6A-C6A-N1A	2.35	123.36	118.33
3	H	304	NAI	O2A-PA-O1A	2.35	123.37	112.44
3	E	303	NAI	O4B-C4B-C3B	2.29	109.69	105.15
3	H	304	NAI	O4D-C1D-N1N	-2.28	103.73	108.08
3	D	304	NAI	O3D-C3D-C4D	-2.25	104.61	111.08
3	E	303	NAI	C4B-O4B-C1B	-2.24	107.87	109.92
3	C	304	NAI	C3N-C7N-N7N	2.24	121.64	117.67
3	C	304	NAI	O2A-PA-O1A	2.22	122.77	112.44
3	B	303	NAI	O2A-PA-O1A	2.20	122.69	112.44
3	D	304	NAI	O1N-PN-O3	2.19	113.20	107.27
3	A	302	NAI	C1B-N9A-C4A	-2.16	122.84	126.64
3	H	304	NAI	C2D-C1D-N1N	2.12	118.53	113.31
3	G	305	NAI	C2D-C1D-N1N	2.09	118.46	113.31
3	A	302	NAI	C4B-O4B-C1B	-2.08	108.02	109.92
3	D	304	NAI	O2A-PA-O1A	2.08	122.10	112.44
3	E	303	NAI	O3-PA-O1A	-2.04	104.58	110.70
3	A	302	NAI	O2A-PA-O1A	2.01	121.81	112.44

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	GOL	C1-C2-C3-O3
2	C	302	GOL	C1-C2-C3-O3
2	C	302	GOL	O2-C2-C3-O3
2	D	302	GOL	C1-C2-C3-O3
2	D	303	GOL	O1-C1-C2-C3
2	F	301	GOL	O1-C1-C2-C3
2	G	301	GOL	O1-C1-C2-O2
2	G	301	GOL	O1-C1-C2-C3
2	G	304	GOL	C1-C2-C3-O3
2	H	301	GOL	C1-C2-C3-O3
2	H	302	GOL	C1-C2-C3-O3
3	B	303	NAI	C5D-O5D-PN-O3

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Mol	Chain	Res	Type	Atoms
3	B	303	NAI	C5D-O5D-PN-O2N
3	C	304	NAI	C5D-O5D-PN-O3
3	C	304	NAI	C5D-O5D-PN-O2N
3	E	303	NAI	C5B-O5B-PA-O1A
2	B	302	GOL	O2-C2-C3-O3
2	D	303	GOL	O1-C1-C2-O2
2	B	301	GOL	O1-C1-C2-C3
2	B	302	GOL	O1-C1-C2-C3
2	B	302	GOL	C1-C2-C3-O3
2	C	303	GOL	O1-C1-C2-C3
2	C	303	GOL	C1-C2-C3-O3
2	D	302	GOL	O1-C1-C2-C3
2	E	301	GOL	C1-C2-C3-O3
2	A	301	GOL	O2-C2-C3-O3
2	D	302	GOL	O2-C2-C3-O3
2	F	301	GOL	O1-C1-C2-O2
2	G	304	GOL	O2-C2-C3-O3
2	H	302	GOL	O2-C2-C3-O3
2	C	303	GOL	O1-C1-C2-O2
2	H	301	GOL	O2-C2-C3-O3
3	F	303	NAI	O4D-C1D-N1N-C6N
2	B	302	GOL	O1-C1-C2-O2
2	E	301	GOL	O2-C2-C3-O3
2	C	303	GOL	O2-C2-C3-O3
3	A	302	NAI	PN-O3-PA-O1A
3	H	304	NAI	PN-O3-PA-O2A
3	A	302	NAI	O4D-C1D-N1N-C6N
3	B	303	NAI	O4D-C1D-N1N-C6N
3	D	304	NAI	O4D-C1D-N1N-C6N
3	E	303	NAI	O4D-C1D-N1N-C6N
3	G	305	NAI	O4D-C1D-N1N-C6N
3	H	304	NAI	O4D-C1D-N1N-C6N
3	B	303	NAI	C5D-O5D-PN-O1N
3	C	304	NAI	C5D-O5D-PN-O1N
3	C	304	NAI	O4D-C1D-N1N-C6N
3	B	303	NAI	C2N-C3N-C7N-N7N
3	D	304	NAI	C2N-C3N-C7N-N7N
3	F	303	NAI	PN-O3-PA-O1A
3	G	305	NAI	PN-O3-PA-O2A
3	H	304	NAI	PN-O3-PA-O1A
3	E	303	NAI	O4D-C4D-C5D-O5D
3	E	303	NAI	O4B-C4B-C5B-O5B

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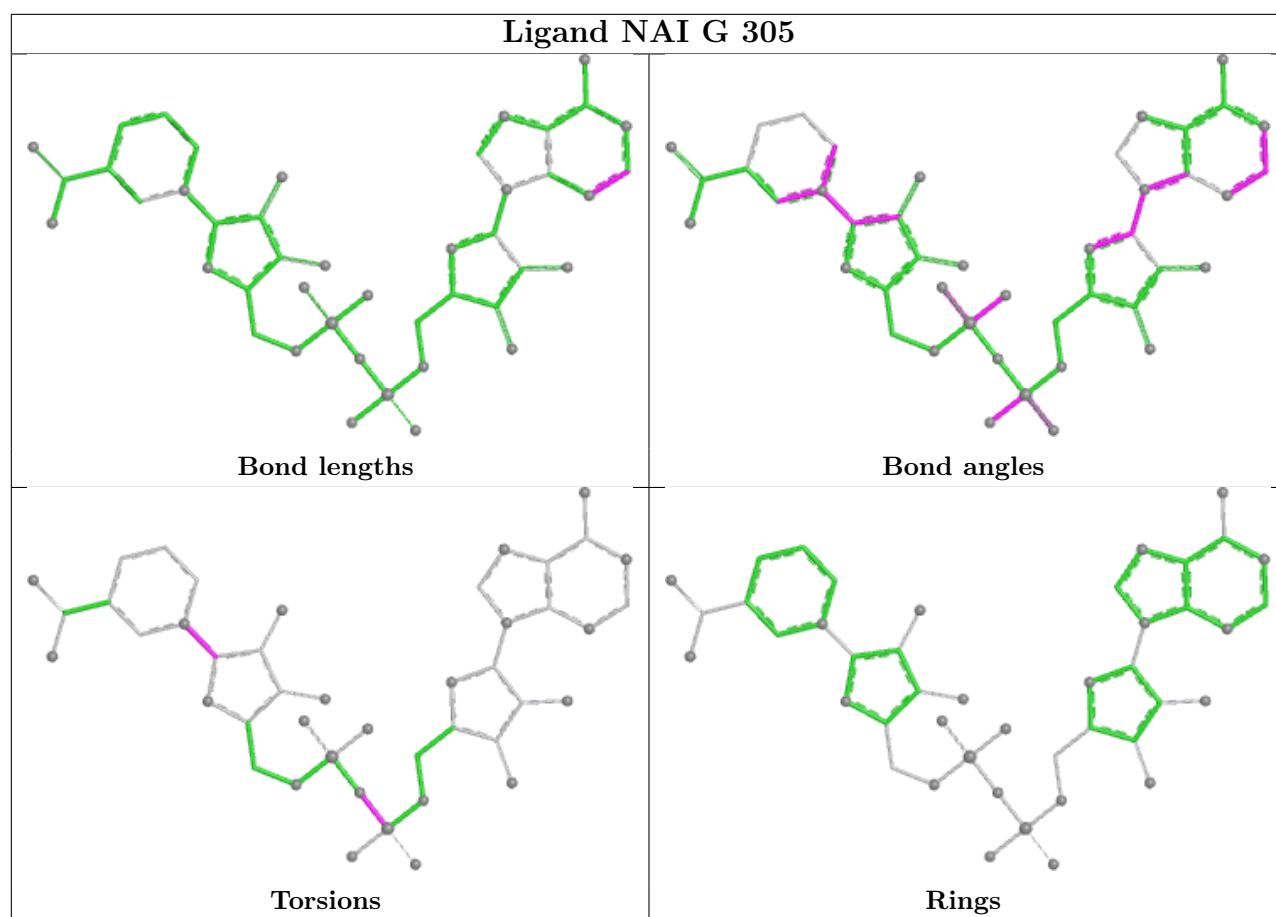
Mol	Chain	Res	Type	Atoms
3	A	302	NAI	PN-O3-PA-O2A
3	D	304	NAI	PN-O3-PA-O2A
3	F	303	NAI	PN-O3-PA-O2A
4	H	303	MLT	C2-C3-C4-O5
2	B	301	GOL	O1-C1-C2-O2
3	B	303	NAI	O4B-C4B-C5B-O5B

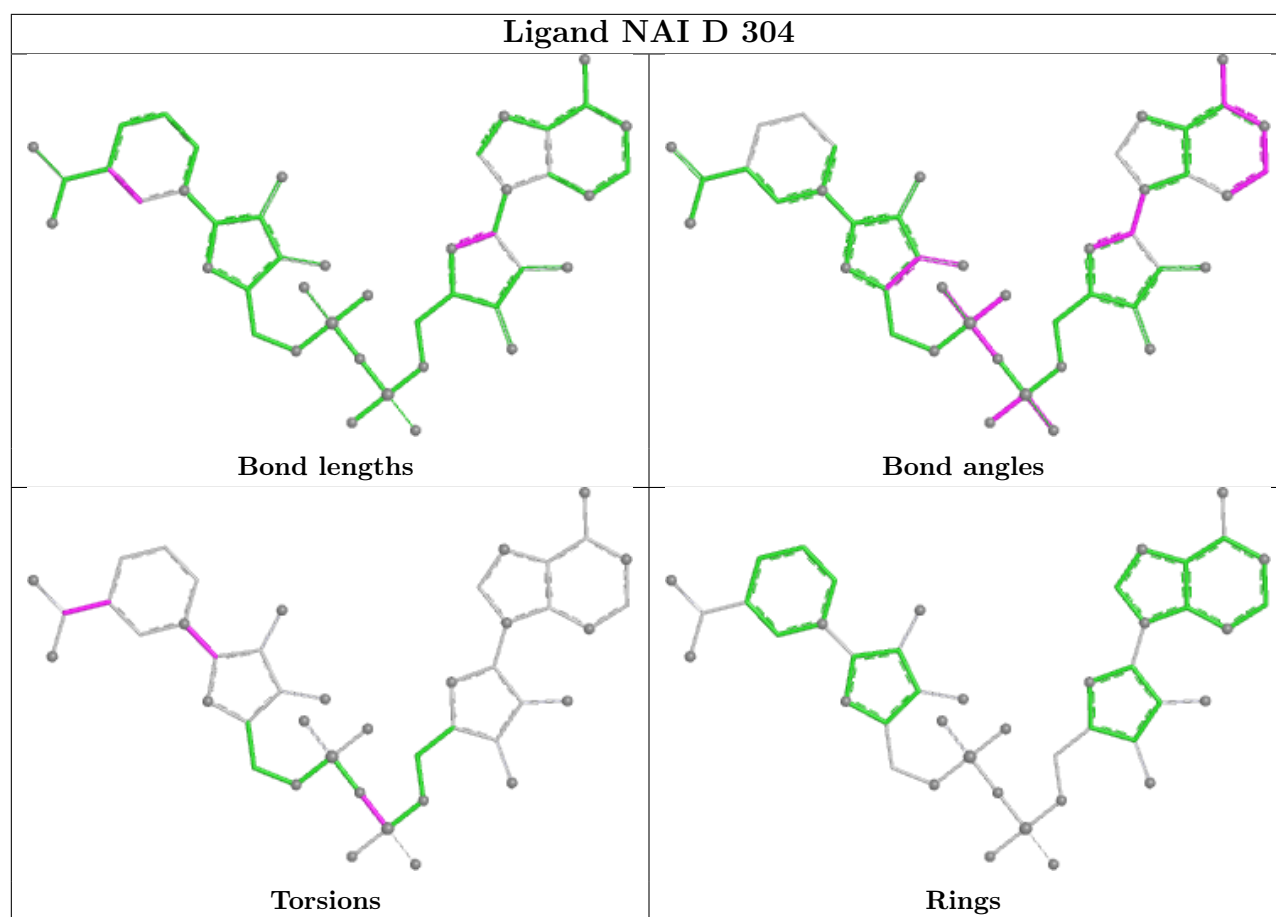
There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	302	GOL	1	0
3	G	305	NAI	1	0
2	H	301	GOL	1	0
2	G	301	GOL	1	0

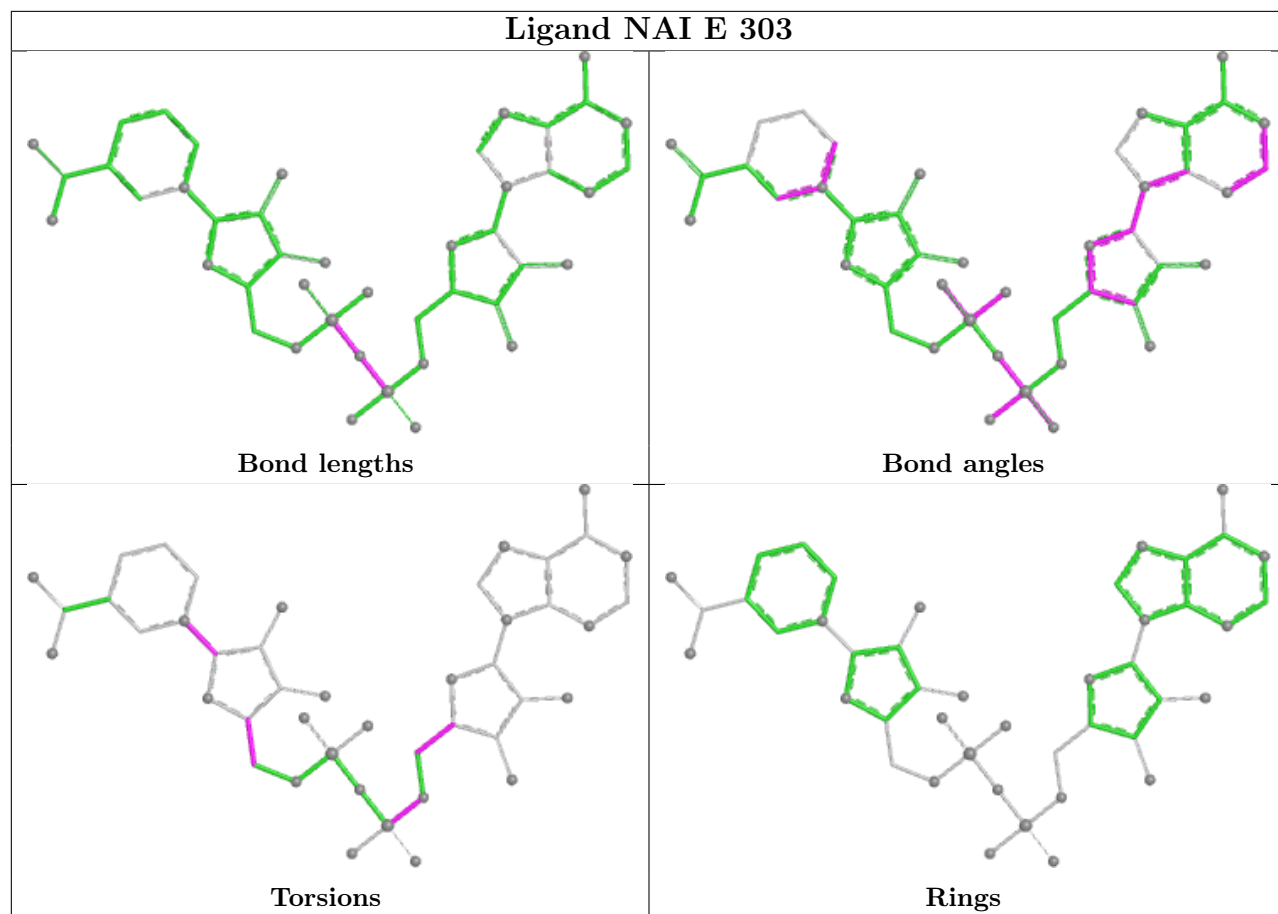
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

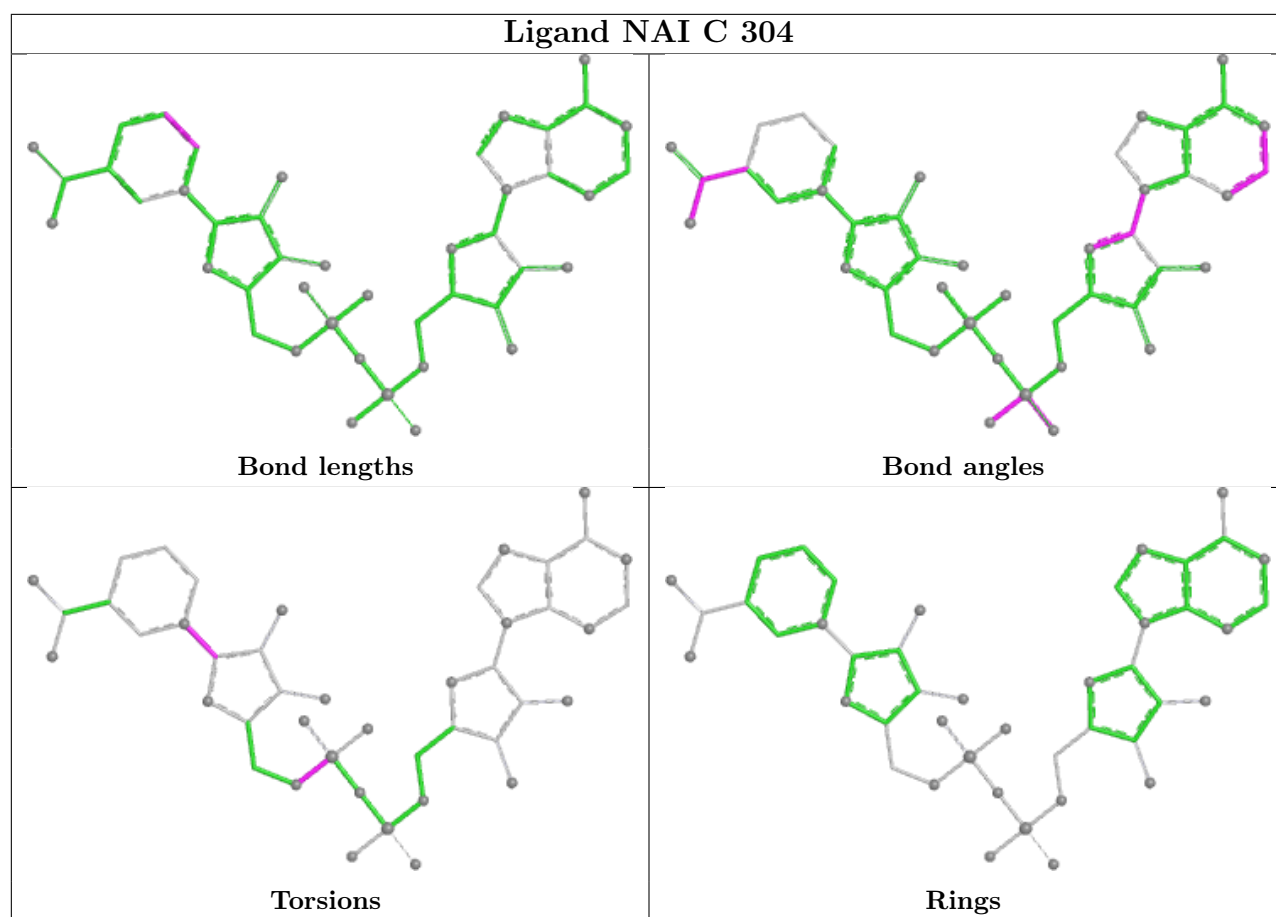


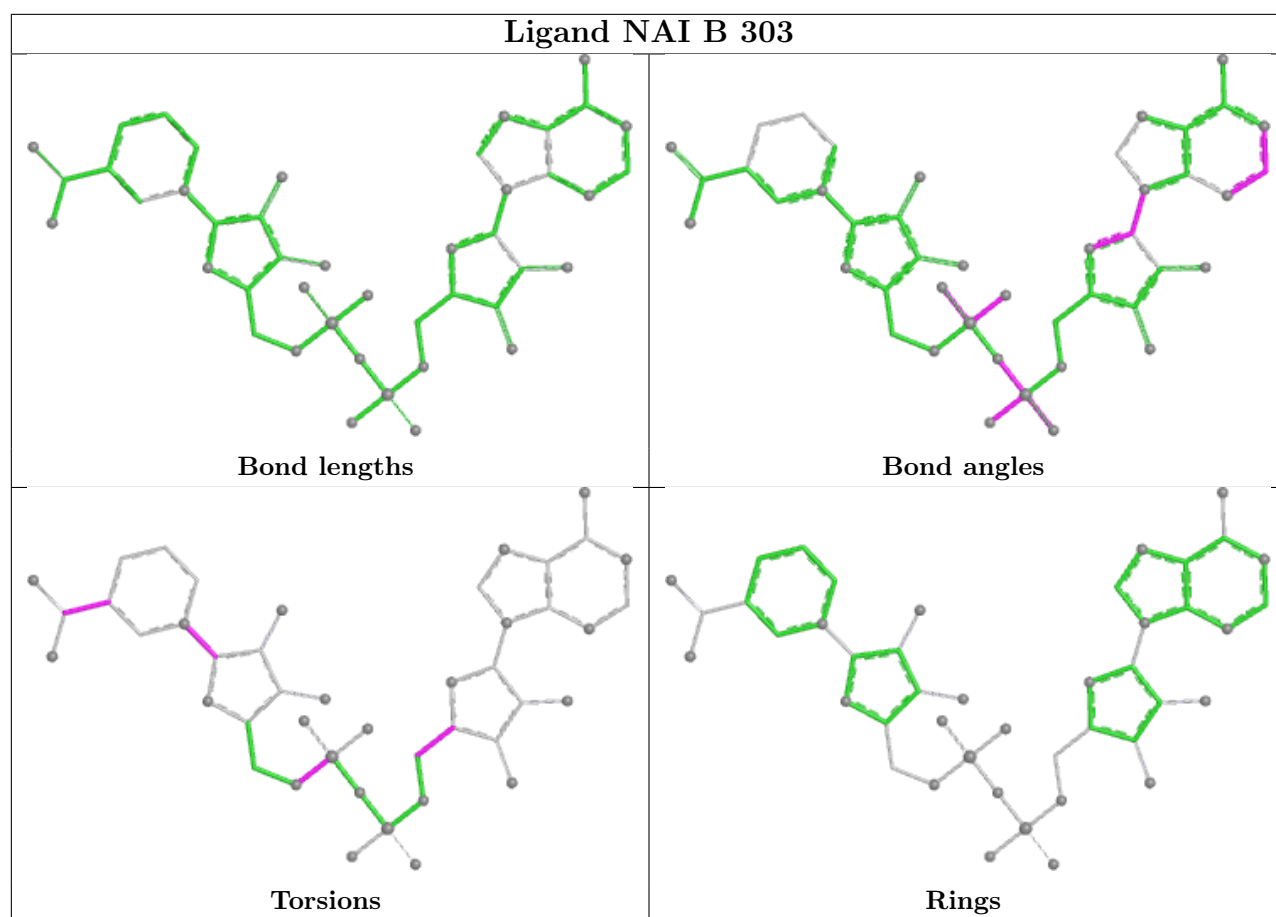


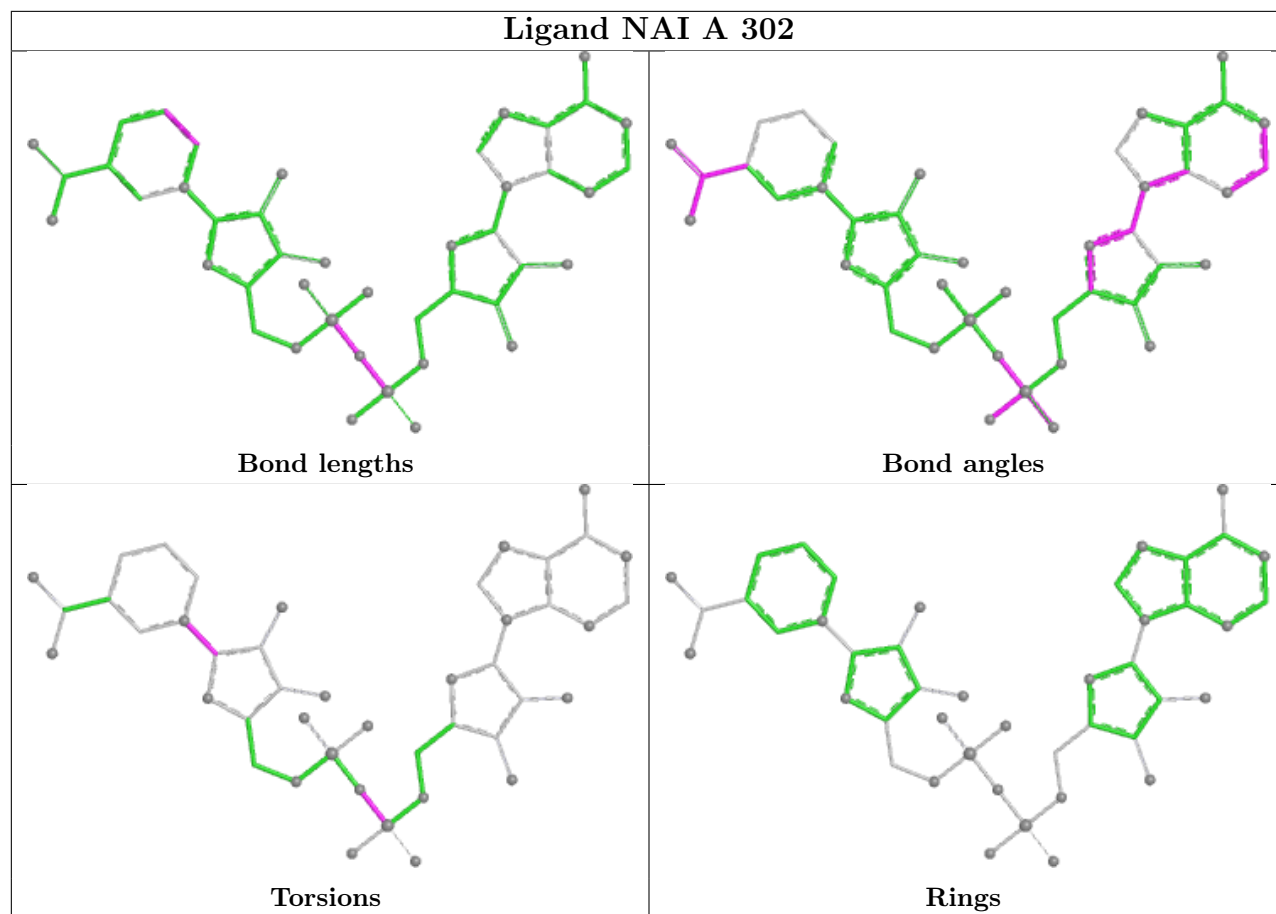


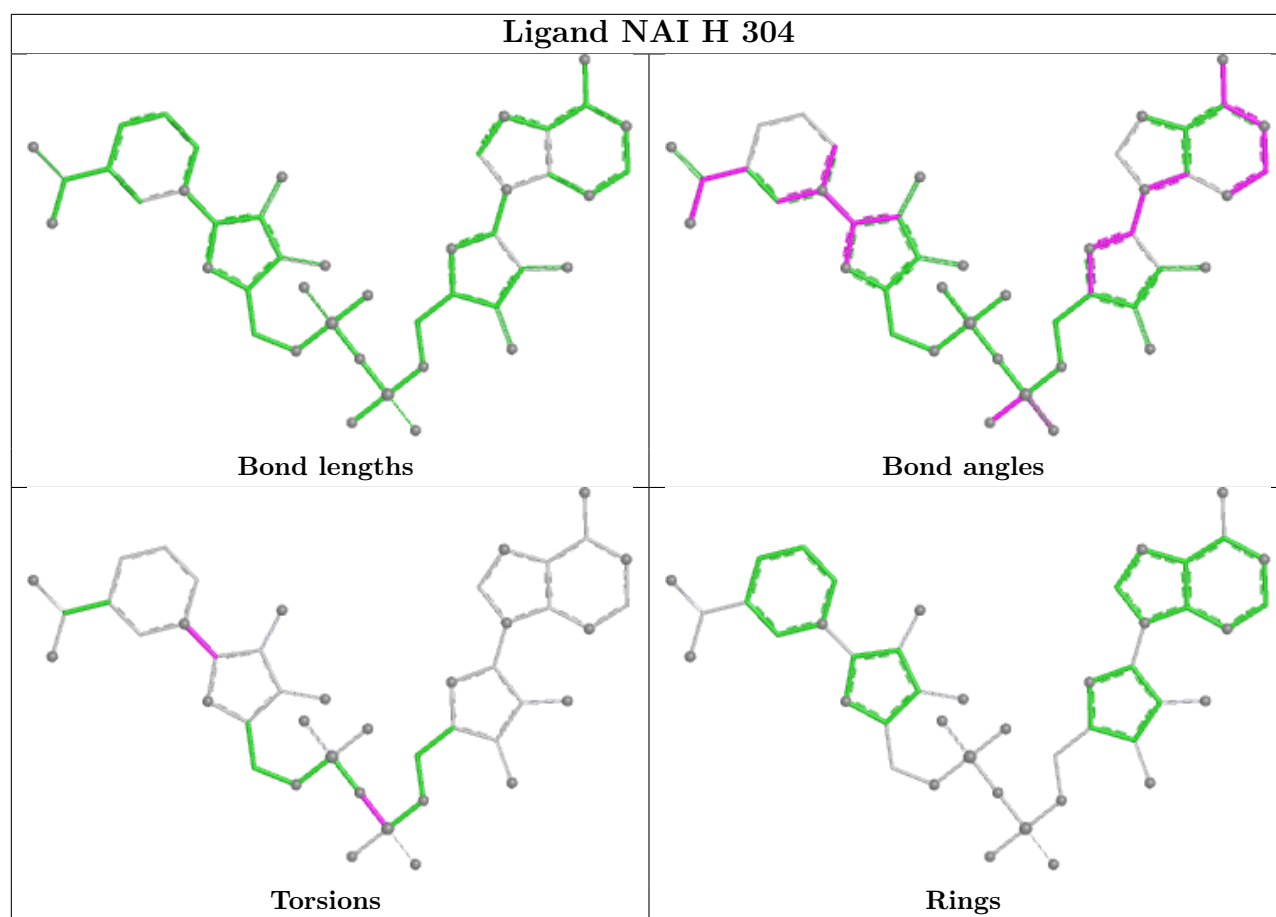
## Ligand NAI E 303

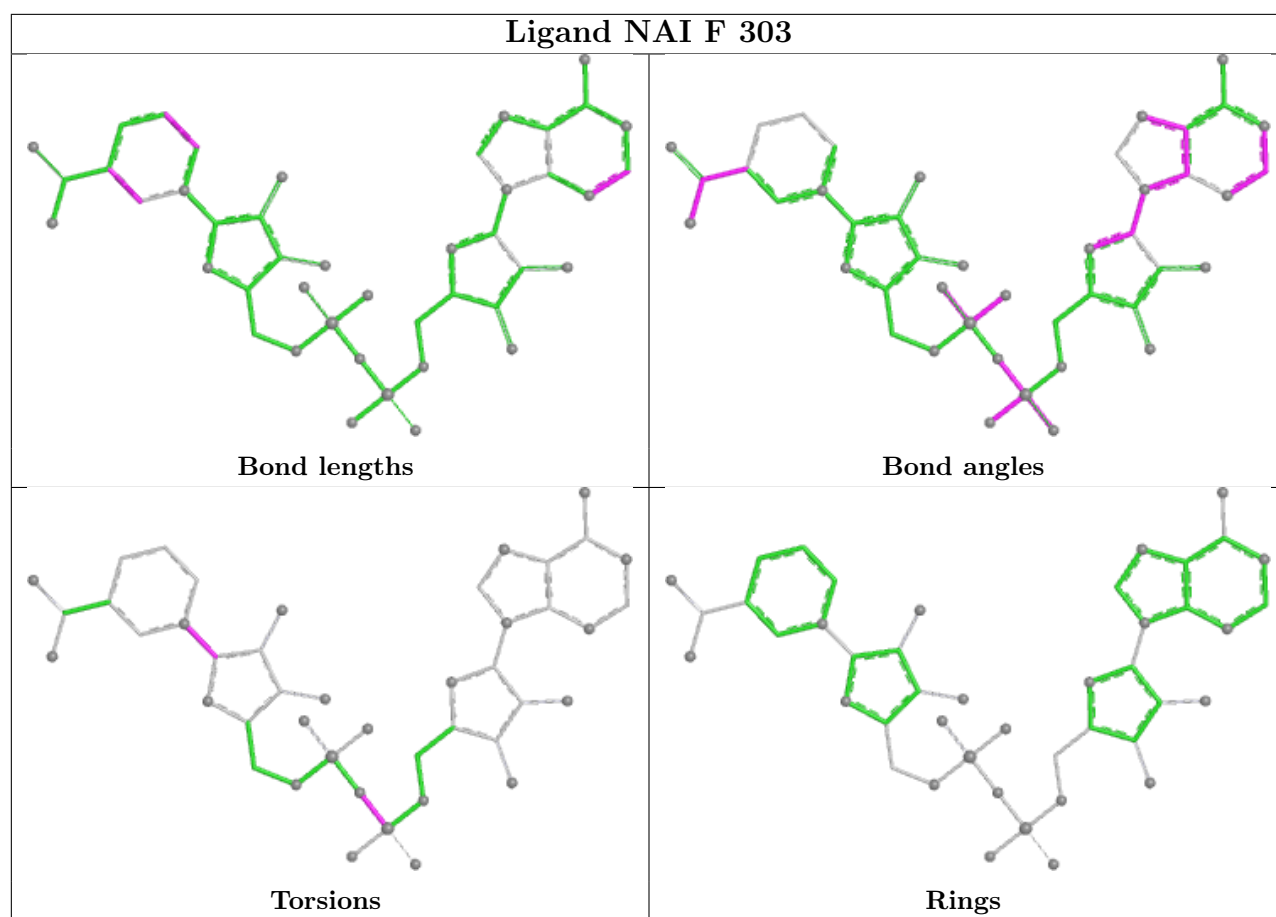












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	244/245 (99%)	0.10	10 (4%) 37 40	37, 57, 87, 117	0
1	B	244/245 (99%)	0.04	6 (2%) 57 61	37, 60, 87, 115	0
1	C	244/245 (99%)	-0.25	0 100 100	33, 43, 72, 102	0
1	D	244/245 (99%)	-0.20	1 (0%) 92 93	33, 46, 72, 102	0
1	E	244/245 (99%)	0.21	10 (4%) 37 40	42, 63, 94, 107	0
1	F	244/245 (99%)	0.02	7 (2%) 51 55	44, 62, 95, 121	0
1	G	244/245 (99%)	-0.23	1 (0%) 92 93	31, 45, 79, 100	0
1	H	244/245 (99%)	-0.25	2 (0%) 86 87	29, 40, 74, 118	0
All	All	1952/1960 (99%)	-0.07	37 (1%) 66 69	29, 52, 87, 121	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	196	ASN	4.8
1	E	56	LEU	3.6
1	A	44	ALA	3.6
1	D	196	ASN	3.1
1	A	41	GLY	3.1
1	A	50	GLU	3.0
1	E	55	ALA	2.9
1	F	77	GLU	2.9
1	B	196	ASN	2.9
1	E	79	PHE	2.8
1	E	4	ALA	2.8
1	F	78	ALA	2.7
1	A	39	ALA	2.7
1	G	197	VAL	2.6
1	B	44	ALA	2.6
1	E	45	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	46	ALA	2.6
1	B	46	ALA	2.6
1	E	39	ALA	2.5
1	F	196[A]	ASN	2.4
1	B	77	GLU	2.4
1	B	200	ILE	2.4
1	F	75	ALA	2.4
1	A	54	GLN	2.4
1	A	35	ALA	2.3
1	H	189[A]	MET	2.3
1	E	57	PHE	2.3
1	F	50	GLU	2.3
1	A	19	PHE	2.3
1	F	5	SER	2.3
1	A	56	LEU	2.2
1	F	197	VAL	2.2
1	E	48	LEU	2.2
1	A	43	ALA	2.1
1	E	34	ILE	2.1
1	B	50	GLU	2.1
1	E	44	ALA	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	F	302	6/6	0.75	0.73	76,81,83,83	0
2	GOL	G	303	6/6	0.81	0.22	73,79,82,84	0

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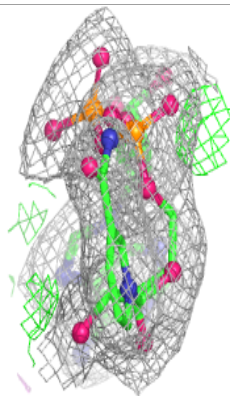
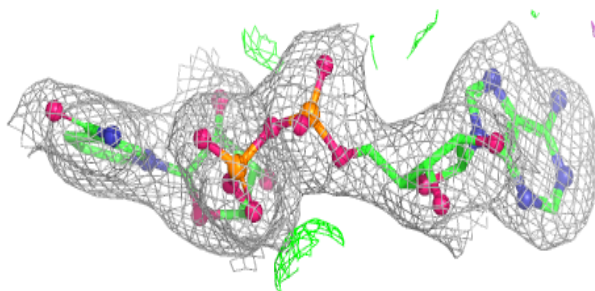
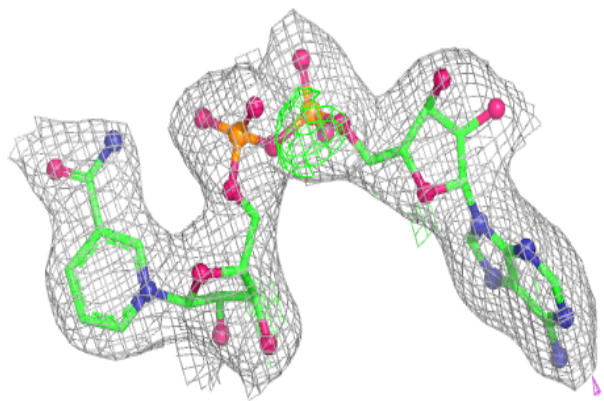
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MLT	H	303	9/9	0.81	0.44	75,82,85,92	0
2	GOL	B	302	6/6	0.82	0.22	86,88,90,91	0
2	GOL	C	303	6/6	0.86	0.31	76,79,84,84	0
2	GOL	D	303	6/6	0.89	0.23	63,68,84,84	0
2	GOL	D	301	6/6	0.89	0.20	57,59,64,67	0
2	GOL	G	304	6/6	0.91	0.21	64,67,69,72	0
2	GOL	A	301	6/6	0.92	0.35	54,58,64,64	0
2	GOL	H	301	6/6	0.92	0.19	52,59,63,65	0
2	GOL	E	301	6/6	0.92	0.30	64,65,69,74	0
2	GOL	E	302	6/6	0.93	0.42	80,85,86,87	0
2	GOL	H	302	6/6	0.93	0.22	50,52,55,62	0
2	GOL	D	302	6/6	0.93	0.25	58,64,67,71	0
2	GOL	B	301	6/6	0.94	0.15	75,79,83,83	0
2	GOL	G	301	6/6	0.94	0.37	52,54,55,60	0
2	GOL	G	302	6/6	0.94	0.23	64,66,69,72	0
2	GOL	F	301	6/6	0.94	0.26	64,67,71,73	0
2	GOL	C	302	6/6	0.95	0.25	53,61,67,68	0
2	GOL	C	301	6/6	0.95	0.19	68,71,73,74	0
3	NAI	E	303	44/44	0.96	0.11	49,58,66,69	0
3	NAI	A	302	44/44	0.96	0.12	47,58,66,72	0
3	NAI	F	303	44/44	0.97	0.13	43,56,65,68	0
3	NAI	G	305	44/44	0.97	0.10	33,45,49,54	0
3	NAI	B	303	44/44	0.97	0.12	41,49,58,61	0
3	NAI	C	304	44/44	0.98	0.10	34,43,50,54	0
3	NAI	D	304	44/44	0.98	0.11	31,36,42,47	0
3	NAI	H	304	44/44	0.99	0.12	30,36,42,44	0

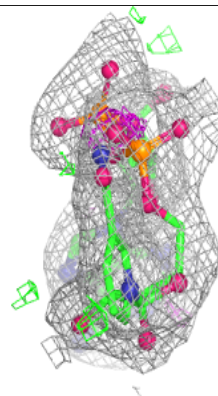
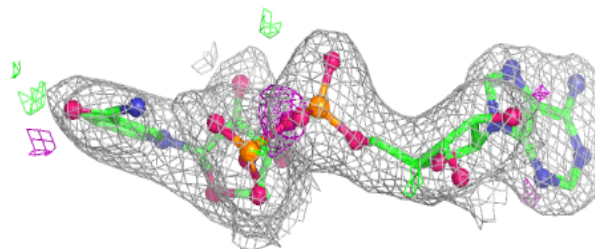
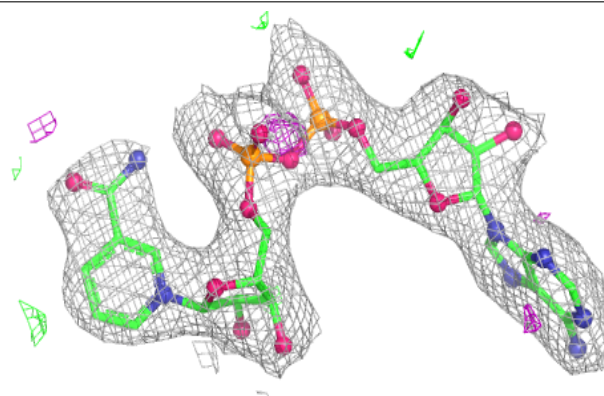
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAI E 303:**

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

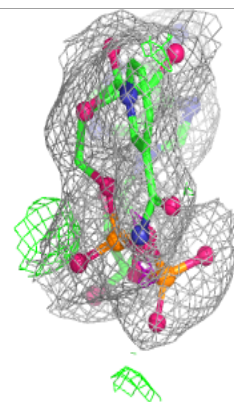
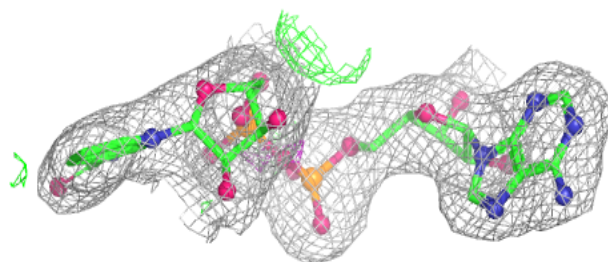
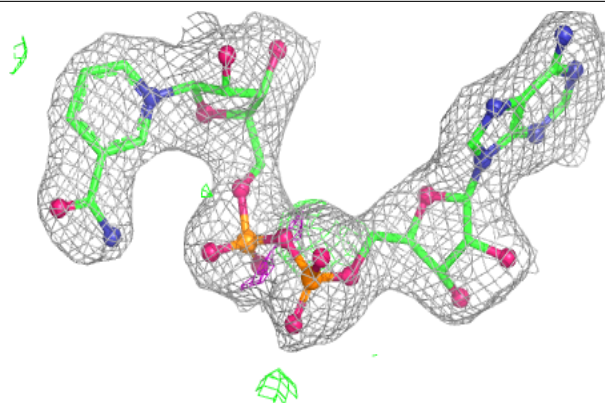
**Electron density around NAI A 302:**

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

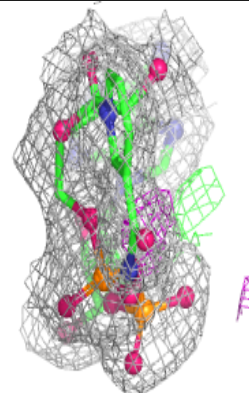
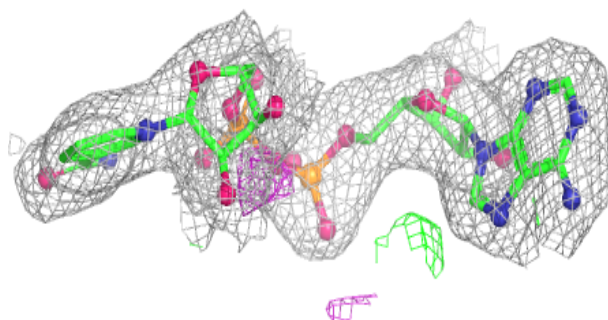
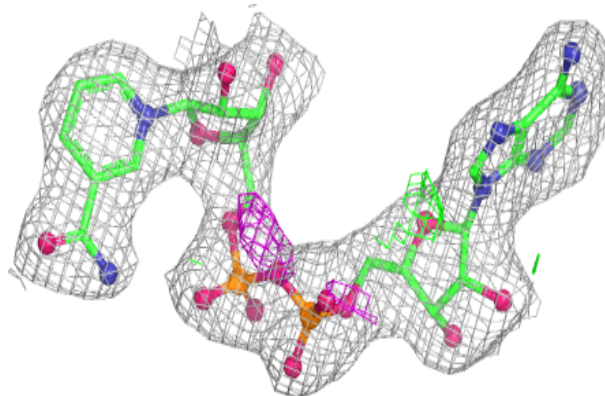


**Electron density around NAI F 303:**

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

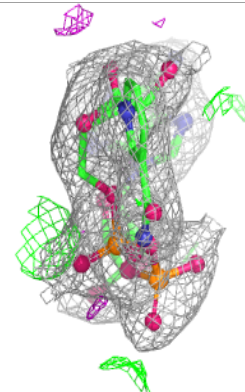
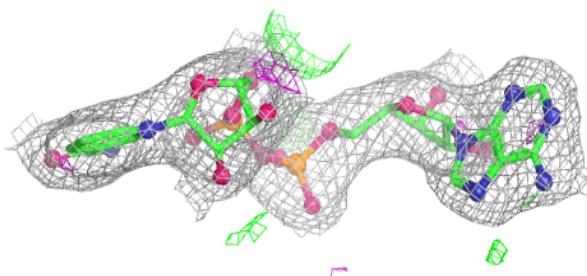
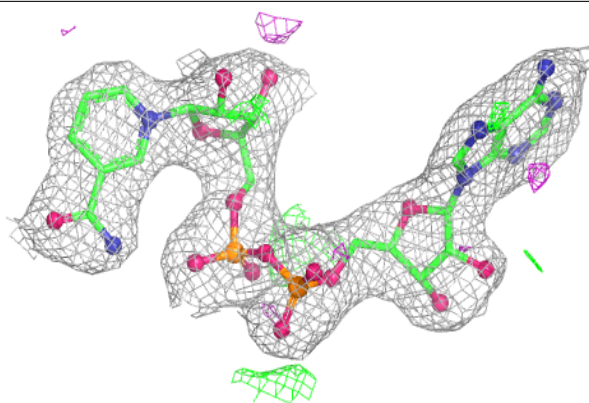
**Electron density around NAI G 305:**

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

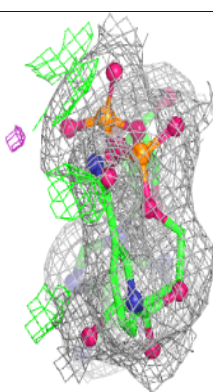
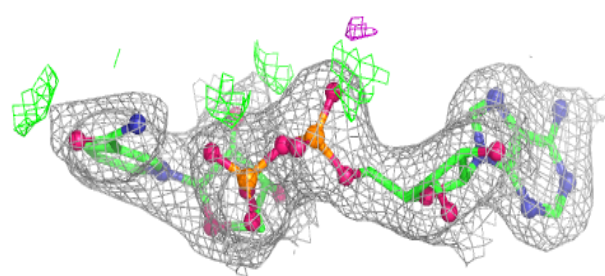
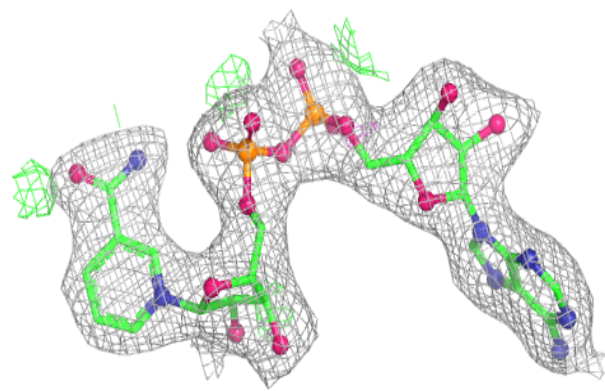


**Electron density around NAI B 303:**

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

**Electron density around NAI C 304:**

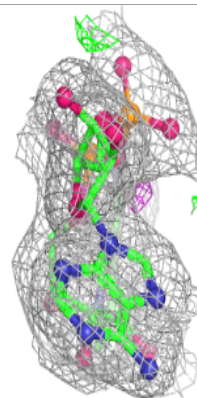
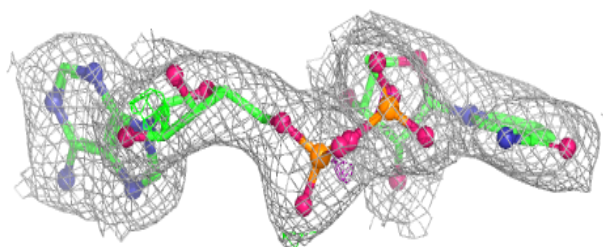
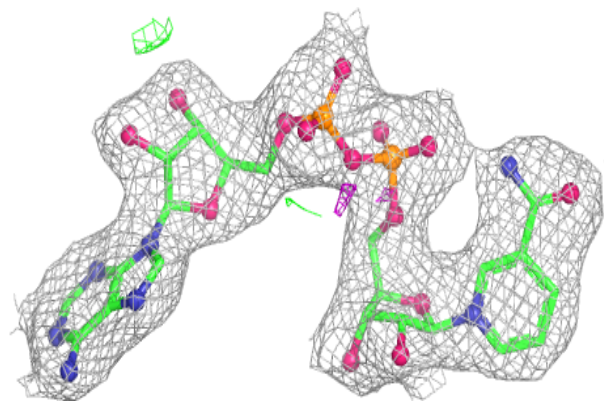
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



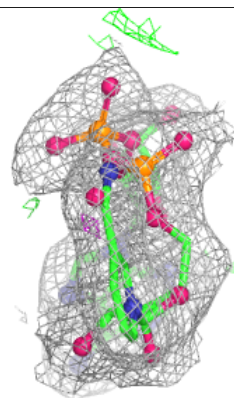
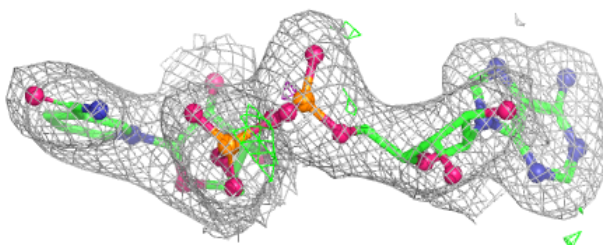
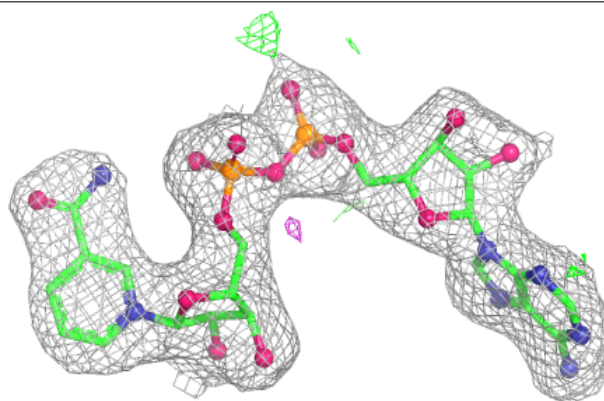


**Electron density around NAI D 304:**

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

**Electron density around NAI H 304:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.