



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:13 AM UTC

PDB ID : 4Q9N / pdb_00004q9n
Title : Crystal structure of Chlamydia trachomatis enoyl-ACP reductase (FabI) in complex with NADH and AFN-1252
Authors : Yao, J.; Abdelrahman, Y.; Robertson, R.M.; Cox, J.V.; Belland, R.J.; White, S.W.; Rock, C.O.
Deposited on : 2014-05-01
Resolution : 1.79 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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

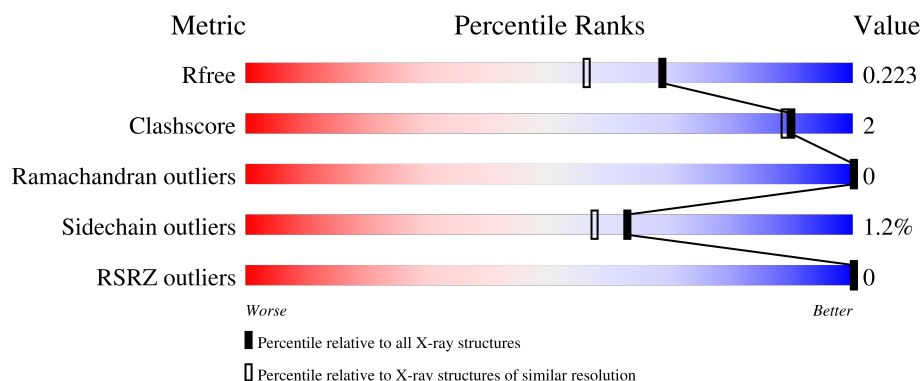
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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.



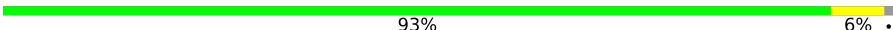
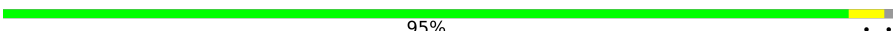
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 ≥ 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	298	96% 96% 96% 96% 96% 96%
1	B	298	94% 94% 94% 94% 94% 94%
1	C	298	93% 93% 93% 93% 93% 93%
1	D	298	92% 92% 92% 92% 92% 92%

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Mol	Chain	Length	Quality of chain
1	E	298	 93% 6% .
1	F	298	 95% . .
1	G	298	 91% 7% .
1	H	298	 94% 5% .

2 Entry composition

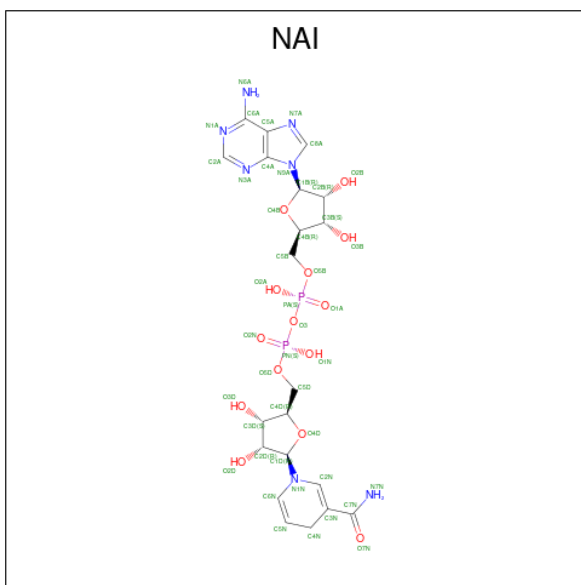
There are 4 unique types of molecules in this entry. The entry contains 19232 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 [NADH].

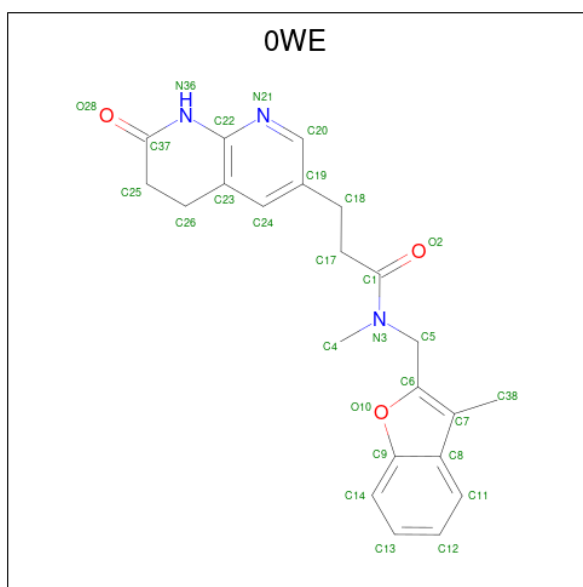
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	0	0
			2212	1421	364	418	9			
1	B	295	Total	C	N	O	S	0	0	0
			2206	1420	362	415	9			
1	C	295	Total	C	N	O	S	0	0	0
			2220	1427	366	418	9			
1	D	295	Total	C	N	O	S	0	0	0
			2216	1425	366	416	9			
1	E	295	Total	C	N	O	S	0	0	0
			2202	1418	362	413	9			
1	F	295	Total	C	N	O	S	0	0	0
			2220	1427	366	418	9			
1	G	295	Total	C	N	O	S	0	0	0
			2210	1422	363	416	9			
1	H	295	Total	C	N	O	S	0	0	0
			2214	1424	363	418	9			

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).



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

- Molecule 3 is N-methyl-N-[(3-methyl-1-benzofuran-2-yl)methyl]-3-(7-oxo-5,6,7,8-tetrahydro-1,8-naphthyridin-3-yl)propanamide (CCD ID: 0WE) (formula: $C_{22}H_{23}N_3O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			28	22	3	3		
3	B	1	Total	C	N	O	0	0
			28	22	3	3		
3	C	1	Total	C	N	O	0	0
			28	22	3	3		
3	D	1	Total	C	N	O	0	0
			28	22	3	3		
3	E	1	Total	C	N	O	0	0
			28	22	3	3		
3	F	1	Total	C	N	O	0	0
			28	22	3	3		
3	G	1	Total	C	N	O	0	0
			28	22	3	3		
3	H	1	Total	C	N	O	0	0
			28	22	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	120	Total	O	0	0
			120	120		
4	B	106	Total	O	0	0
			106	106		
4	C	110	Total	O	0	0
			110	110		
4	D	99	Total	O	0	0
			99	99		

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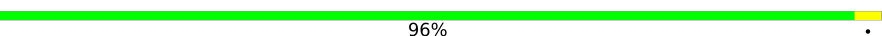
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	119	Total 119	O 119	0	0
4	F	129	Total 129	O 129	0	0
4	G	132	Total 132	O 132	0	0
4	H	141	Total 141	O 141	0	0

3 Residue-property plots

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

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

Chain A:  96% ..



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

Chain B:  94% 5% ..

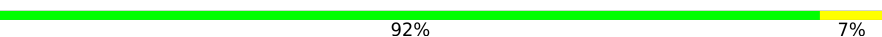


- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain C:  93% 6% ..

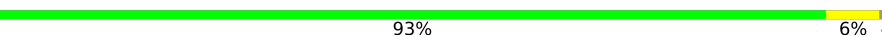


- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain D:  92% 7% ..

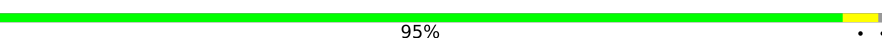


- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain E:  93% 6% ..



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

Chain F:  95% ..



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

Chain G: 91% 7% •



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

Chain H: 94% 5% •



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	96.15Å 96.15Å 263.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.61 – 1.79 38.61 – 1.79	Depositor EDS
% Data completeness (in resolution range)	98.6 (38.61-1.79) 98.7 (38.61-1.79)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.186 , 0.229 0.181 , 0.223	Depositor DCC
R_{free} test set	10949 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 22.8	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	19232	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 0WE, NAI

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	0.44	0/2263	0.73	0/3075
1	B	0.44	1/2257 (0.0%)	0.77	0/3066
1	C	0.44	0/2271	0.78	2/3083 (0.1%)
1	D	0.47	0/2267	0.75	0/3078
1	E	0.44	0/2253	0.76	2/3061 (0.1%)
1	F	0.43	0/2271	0.76	2/3083 (0.1%)
1	G	0.47	0/2261	0.74	0/3071
1	H	0.45	0/2265	0.75	0/3076
All	All	0.45	1/18108 (0.0%)	0.76	6/24593 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	43	VAL	CA-CB	5.02	1.56	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	291	GLY	CA-C-N	8.28	128.76	119.32
1	C	291	GLY	C-N-CA	8.28	128.76	119.32
1	F	291	GLY	CA-C-N	5.33	125.65	119.47
1	F	291	GLY	C-N-CA	5.33	125.65	119.47
1	E	291	GLY	CA-C-N	5.14	124.94	119.28
1	E	291	GLY	C-N-CA	5.14	124.94	119.28

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	2212	0	2193	6	0
1	B	2206	0	2194	12	0
1	C	2220	0	2215	13	0
1	D	2216	0	2211	11	0
1	E	2202	0	2190	8	0
1	F	2220	0	2215	9	0
1	G	2210	0	2200	14	0
1	H	2214	0	2204	7	0
2	A	44	0	27	0	0
2	B	44	0	27	0	0
2	C	44	0	27	0	0
2	D	44	0	27	0	0
2	E	44	0	27	0	0
2	F	44	0	27	0	0
2	G	44	0	27	0	0
2	H	44	0	27	0	0
3	A	28	0	23	0	0
3	B	28	0	23	0	0
3	C	28	0	23	0	0
3	D	28	0	23	0	0
3	E	28	0	23	0	0
3	F	28	0	23	0	0
3	G	28	0	23	0	0
3	H	28	0	23	0	0
4	A	120	0	0	0	0
4	B	106	0	0	1	0
4	C	110	0	0	1	0
4	D	99	0	0	0	0
4	E	119	0	0	0	0
4	F	129	0	0	2	0
4	G	132	0	0	0	0
4	H	141	0	0	0	0
All	All	19232	0	18022	66	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 2.

All (66) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:LYS:HE3	1:B:5:ASP:HA	1.77	0.66
1:B:3:LYS:NZ	1:C:2:LEU:H	1.94	0.66
1:E:240:MET:HE2	1:G:294:MET:HE2	1.79	0.63
1:G:149:LEU:HD13	1:H:149:LEU:HD13	1.79	0.63
1:H:74:LYS:HG2	1:H:76:TYR:CZ	2.34	0.62
1:D:245:GLN:HG3	1:D:251:PRO:O	2.01	0.61
1:F:250:LEU:HD11	1:G:217:ARG:HG2	1.83	0.60
1:B:217:ARG:HG2	1:C:250:LEU:HD11	1.84	0.60
1:H:290:ILE:HD12	1:H:294:MET:HB2	1.81	0.60
1:C:74:LYS:HG2	1:C:76:TYR:CZ	2.40	0.56
1:C:290:ILE:HD12	1:C:294:MET:HB2	1.90	0.54
1:G:86:GLU:OE1	1:G:86:GLU:N	2.37	0.53
1:G:133:ILE:HD13	1:G:234:ILE:HD11	1.91	0.52
1:B:3:LYS:HZ2	1:C:2:LEU:H	1.56	0.51
1:C:231:GLY:O	1:C:234:ILE:HG12	2.11	0.51
1:G:43:VAL:HG13	1:G:101:LEU:HD12	1.92	0.51
1:F:217:ARG:HG2	1:G:250:LEU:HD11	1.93	0.50
1:C:149:LEU:HD13	1:D:149:LEU:HD13	1.93	0.50
1:B:257:GLU:OE1	1:B:257:GLU:N	2.43	0.50
1:E:294:MET:HE2	1:G:240:MET:HE2	1.93	0.50
1:F:231:GLY:O	1:F:234:ILE:HG12	2.13	0.49
1:D:68:GLU:HG2	1:D:69:LEU:N	2.28	0.48
1:A:89:PRO:HG2	1:A:92:ILE:HG12	1.95	0.48
1:C:135:LYS:HD3	4:C:424:HOH:O	2.14	0.48
1:G:74:LYS:HG2	1:G:76:TYR:CZ	2.49	0.48
1:E:93:LEU:O	1:E:99:LYS:HD3	2.14	0.48
1:A:132:GLU:HB3	1:A:135:LYS:HD2	1.96	0.47
1:F:28:LYS:HG3	1:F:70:LEU:HD22	1.96	0.47
1:C:135:LYS:HD2	1:C:135:LYS:N	2.30	0.47
1:B:43:VAL:HG13	1:B:101:LEU:HD12	1.96	0.47
1:F:42:TRP:HA	1:F:78:MET:O	2.15	0.47
1:F:183:ARG:NH2	4:F:463:HOH:O	2.49	0.46
1:C:52:SER:HA	1:C:57:LYS:HD2	1.98	0.46
1:E:290:ILE:HD12	1:E:294:MET:HB2	1.97	0.46
1:G:108:GLU:O	1:G:111:GLU:HG2	2.17	0.45
1:B:3:LYS:HZ3	1:C:2:LEU:H	1.63	0.45
1:H:284:GLY:O	1:H:287:VAL:HG22	2.17	0.45
1:B:10:ILE:HD13	1:B:36:THR:HB	1.98	0.45
1:E:42:TRP:CG	1:E:44:PRO:HD2	2.52	0.44
1:H:247:TRP:CD1	1:H:292:PRO:HD3	2.53	0.44
1:G:91:GLU:CD	1:G:91:GLU:H	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:ILE:HD12	1:D:236:PHE:H	1.83	0.43
1:G:123:LEU:HB3	1:G:173:THR:HG22	2.01	0.43
1:A:231:GLY:O	1:A:234:ILE:HG12	2.20	0.42
1:H:108:GLU:O	1:H:112:GLN:HG3	2.19	0.42
1:A:250:LEU:HD11	1:D:217:ARG:HG2	2.01	0.42
1:B:3:LYS:HG3	1:B:5:ASP:HB2	2.01	0.42
1:D:231:GLY:O	1:D:234:ILE:HG13	2.20	0.42
1:C:42:TRP:CG	1:C:44:PRO:HD2	2.54	0.42
1:E:149:LEU:HD13	1:F:149:LEU:HD13	2.01	0.42
1:G:4:ILE:HG23	1:G:268:SER:HB3	2.01	0.42
1:F:86:GLU:OE1	4:F:481:HOH:O	2.22	0.42
1:B:48:ILE:HG12	4:B:425:HOH:O	2.21	0.41
1:D:52:SER:HB3	1:D:57:LYS:HG2	2.03	0.41
1:E:245:GLN:HG2	1:E:251:PRO:O	2.20	0.41
1:C:24:TRP:HE1	1:C:28:LYS:HD2	1.85	0.41
1:E:42:TRP:HA	1:E:78:MET:O	2.21	0.41
1:A:47:LYS:O	1:A:51:GLN:HB2	2.20	0.41
1:A:217:ARG:HG2	1:D:250:LEU:HD11	2.01	0.41
1:B:159:LEU:O	1:B:163:PHE:HB2	2.21	0.41
1:D:4:ILE:HG23	1:D:268:SER:HB3	2.02	0.41
1:B:230:ALA:O	1:B:234:ILE:HD12	2.20	0.41
1:F:290:ILE:HD11	1:H:240:MET:HE1	2.03	0.41
1:G:42:TRP:CD2	1:G:44:PRO:HD2	2.56	0.40
1:D:74:LYS:HG2	1:D:76:TYR:CZ	2.57	0.40
1:D:42:TRP:CD2	1:D:44:PRO:HD2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	293/298 (98%)	283 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	293/298 (98%)	285 (97%)	8 (3%)	0	100	100
1	C	293/298 (98%)	285 (97%)	8 (3%)	0	100	100
1	D	293/298 (98%)	285 (97%)	8 (3%)	0	100	100
1	E	293/298 (98%)	284 (97%)	9 (3%)	0	100	100
1	F	293/298 (98%)	282 (96%)	11 (4%)	0	100	100
1	G	293/298 (98%)	287 (98%)	6 (2%)	0	100	100
1	H	293/298 (98%)	286 (98%)	7 (2%)	0	100	100
All	All	2344/2384 (98%)	2277 (97%)	67 (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	226/233 (97%)	226 (100%)	0	100	100
1	B	225/233 (97%)	221 (98%)	4 (2%)	51	43
1	C	228/233 (98%)	226 (99%)	2 (1%)	70	67
1	D	227/233 (97%)	225 (99%)	2 (1%)	70	67
1	E	224/233 (96%)	218 (97%)	6 (3%)	39	27
1	F	228/233 (98%)	228 (100%)	0	100	100
1	G	226/233 (97%)	223 (99%)	3 (1%)	61	54
1	H	227/233 (97%)	223 (98%)	4 (2%)	51	43
All	All	1811/1864 (97%)	1790 (99%)	21 (1%)	63	57

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	127	LEU
1	B	179	LEU

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Mol	Chain	Res	Type
1	B	234	ILE
1	B	287	VAL
1	C	45	ILE
1	C	179	LEU
1	D	127	LEU
1	D	179	LEU
1	E	45	ILE
1	E	50	SER
1	E	96	LYS
1	E	127	LEU
1	E	234	ILE
1	E	287	VAL
1	G	179	LEU
1	G	232	LYS
1	G	234	ILE
1	H	45	ILE
1	H	91	GLU
1	H	135	LYS
1	H	179	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	ASN
1	C	95	ASN
1	C	116	HIS
1	D	193	ASN
1	D	286	ASN
1	E	119	HIS
1	F	129	ASN
1	G	20	ASN
1	G	119	HIS
1	G	129	ASN
1	G	168	ASN
1	G	245	GLN
1	H	51	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAI	H	301	-	47,48,48	3.44	20 (42%)	64,73,73	2.67	18 (28%)
2	NAI	C	301	-	47,48,48	3.44	20 (42%)	64,73,73	2.70	19 (29%)
3	0WE	E	302	-	29,31,31	2.92	8 (27%)	40,44,44	2.21	15 (37%)
2	NAI	G	301	-	47,48,48	3.49	19 (40%)	64,73,73	2.77	22 (34%)
3	0WE	B	302	-	29,31,31	2.99	8 (27%)	40,44,44	2.28	18 (45%)
3	0WE	F	302	-	29,31,31	2.99	9 (31%)	40,44,44	2.13	16 (40%)
3	0WE	D	302	-	29,31,31	3.05	8 (27%)	40,44,44	2.24	16 (40%)
2	NAI	E	301	-	47,48,48	3.48	20 (42%)	64,73,73	2.72	22 (34%)
2	NAI	A	301	-	47,48,48	3.43	20 (42%)	64,73,73	2.71	21 (32%)
2	NAI	F	301	-	47,48,48	3.46	18 (38%)	64,73,73	2.74	22 (34%)
3	0WE	C	302	-	29,31,31	2.90	9 (31%)	40,44,44	2.25	19 (47%)
2	NAI	D	301	-	47,48,48	3.48	18 (38%)	64,73,73	2.73	22 (34%)
3	0WE	H	302	-	29,31,31	2.84	8 (27%)	40,44,44	2.19	19 (47%)
3	0WE	G	302	-	29,31,31	3.08	9 (31%)	40,44,44	2.15	17 (42%)
3	0WE	A	302	-	29,31,31	3.04	10 (34%)	40,44,44	2.14	16 (40%)
2	NAI	B	301	-	47,48,48	3.48	20 (42%)	64,73,73	2.73	22 (34%)

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	NAI	H	301	-	-	7/29/72/72	0/5/5/5
2	NAI	C	301	-	-	8/29/72/72	0/5/5/5
3	0WE	E	302	-	-	2/13/22/22	0/4/4/4
2	NAI	G	301	-	-	6/29/72/72	0/5/5/5
3	0WE	B	302	-	-	2/13/22/22	0/4/4/4
3	0WE	F	302	-	-	1/13/22/22	0/4/4/4
3	0WE	D	302	-	-	2/13/22/22	0/4/4/4
2	NAI	E	301	-	-	7/29/72/72	0/5/5/5
2	NAI	A	301	-	-	6/29/72/72	0/5/5/5
2	NAI	F	301	-	-	6/29/72/72	0/5/5/5
3	0WE	C	302	-	-	2/13/22/22	0/4/4/4
2	NAI	D	301	-	-	6/29/72/72	0/5/5/5
3	0WE	H	302	-	-	2/13/22/22	0/4/4/4
3	0WE	G	302	-	-	1/13/22/22	0/4/4/4
3	0WE	A	302	-	-	2/13/22/22	0/4/4/4
2	NAI	B	301	-	-	6/29/72/72	0/5/5/5

All (224) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	0WE	C1-N3	11.33	1.48	1.34
3	B	302	0WE	C1-N3	10.88	1.47	1.34
3	D	302	0WE	C1-N3	10.82	1.47	1.34
3	F	302	0WE	C1-N3	10.67	1.47	1.34
3	G	302	0WE	C1-N3	10.62	1.47	1.34
3	E	302	0WE	C1-N3	10.41	1.47	1.34
3	C	302	0WE	C1-N3	10.05	1.46	1.34
3	H	302	0WE	C1-N3	9.29	1.45	1.34
2	B	301	NAI	C2N-C3N	9.27	1.60	1.35
2	G	301	NAI	C2N-C3N	9.26	1.60	1.35
2	E	301	NAI	C2N-C3N	9.19	1.60	1.35
2	F	301	NAI	C2N-C3N	9.15	1.60	1.35
2	D	301	NAI	C2N-C3N	9.14	1.60	1.35
2	C	301	NAI	C2N-C3N	9.01	1.60	1.35
2	A	301	NAI	C2N-C3N	8.96	1.59	1.35
2	H	301	NAI	C2N-C3N	8.95	1.59	1.35
2	E	301	NAI	C2A-N1A	8.18	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	301	NAI	C2A-N1A	8.17	1.48	1.33
2	D	301	NAI	C2A-N1A	8.16	1.48	1.33
3	F	302	0WE	C23-C22	8.03	1.48	1.41
2	B	301	NAI	C2A-N1A	8.01	1.48	1.33
2	E	301	NAI	C8A-N7A	8.00	1.47	1.31
2	H	301	NAI	C2A-N1A	7.96	1.48	1.33
3	G	302	0WE	C23-C22	7.94	1.48	1.41
2	C	301	NAI	C8A-N7A	7.93	1.46	1.31
2	B	301	NAI	C8A-N7A	7.93	1.46	1.31
2	H	301	NAI	C8A-N7A	7.92	1.46	1.31
2	A	301	NAI	C2A-N1A	7.89	1.47	1.33
2	C	301	NAI	C2A-N1A	7.87	1.47	1.33
2	F	301	NAI	C8A-N7A	7.87	1.46	1.31
2	C	301	NAI	C2A-N3A	7.84	1.47	1.33
2	F	301	NAI	C2A-N1A	7.83	1.47	1.33
2	D	301	NAI	C2A-N3A	7.81	1.47	1.33
2	A	301	NAI	C8A-N7A	7.79	1.46	1.31
2	F	301	NAI	C2A-N3A	7.78	1.47	1.33
2	G	301	NAI	C8A-N7A	7.76	1.46	1.31
2	H	301	NAI	C2A-N3A	7.75	1.47	1.33
2	A	301	NAI	C2A-N3A	7.74	1.47	1.33
3	E	302	0WE	C23-C22	7.66	1.48	1.41
2	D	301	NAI	C8A-N7A	7.65	1.46	1.31
3	D	302	0WE	C23-C22	7.62	1.48	1.41
3	B	302	0WE	C23-C22	7.58	1.48	1.41
3	C	302	0WE	C23-C22	7.57	1.48	1.41
2	G	301	NAI	C2A-N3A	7.54	1.47	1.33
3	H	302	0WE	C23-C22	7.50	1.48	1.41
2	E	301	NAI	C2A-N3A	7.46	1.47	1.33
2	B	301	NAI	C2A-N3A	7.45	1.47	1.33
2	G	301	NAI	C4N-C5N	-7.44	1.29	1.49
3	A	302	0WE	C23-C22	7.41	1.48	1.41
2	H	301	NAI	C4N-C5N	-7.37	1.29	1.49
2	D	301	NAI	C4N-C5N	-7.33	1.30	1.49
2	E	301	NAI	C4N-C5N	-7.32	1.30	1.49
2	C	301	NAI	C4N-C5N	-7.31	1.30	1.49
2	B	301	NAI	C4N-C5N	-7.30	1.30	1.49
2	F	301	NAI	C4N-C5N	-7.14	1.30	1.49
2	A	301	NAI	C4N-C5N	-6.87	1.31	1.49
2	B	301	NAI	C4A-N9A	-6.45	1.24	1.37
2	H	301	NAI	C4A-N9A	-6.30	1.24	1.37
2	G	301	NAI	C4A-N9A	-6.26	1.24	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	NAI	C4A-N9A	-6.26	1.24	1.37
2	E	301	NAI	C4A-N9A	-6.26	1.24	1.37
2	D	301	NAI	C4A-N9A	-6.23	1.24	1.37
2	F	301	NAI	C4A-N9A	-5.97	1.25	1.37
2	C	301	NAI	C4A-N9A	-5.91	1.25	1.37
2	F	301	NAI	C4A-N3A	5.50	1.44	1.34
2	C	301	NAI	C4A-N3A	5.43	1.44	1.34
2	D	301	NAI	C4A-N3A	5.42	1.44	1.34
2	A	301	NAI	C4A-N3A	5.37	1.44	1.34
2	E	301	NAI	C4A-N3A	5.19	1.44	1.34
2	B	301	NAI	C4A-N3A	5.05	1.43	1.34
2	G	301	NAI	C4A-N3A	5.05	1.43	1.34
2	H	301	NAI	C4A-N3A	4.92	1.43	1.34
2	A	301	NAI	C5A-C4A	-4.86	1.30	1.39
2	F	301	NAI	C5A-C4A	-4.84	1.30	1.39
2	G	301	NAI	C5A-C4A	-4.52	1.31	1.39
2	G	301	NAI	C6A-N6A	4.48	1.45	1.34
2	D	301	NAI	C5A-C4A	-4.47	1.31	1.39
2	B	301	NAI	C5A-C4A	-4.44	1.31	1.39
2	H	301	NAI	C6A-N6A	4.41	1.45	1.34
2	C	301	NAI	C6A-N6A	4.39	1.45	1.34
2	E	301	NAI	C5A-C4A	-4.35	1.31	1.39
2	D	301	NAI	C6A-N6A	4.31	1.45	1.34
2	B	301	NAI	C6A-N6A	4.23	1.45	1.34
2	E	301	NAI	C6A-N6A	4.21	1.45	1.34
2	G	301	NAI	PA-O3	-4.20	1.55	1.59
2	G	301	NAI	C6N-N1N	-4.17	1.27	1.37
2	D	301	NAI	PA-O3	-4.12	1.55	1.59
2	H	301	NAI	C5A-C4A	-4.11	1.31	1.39
2	D	301	NAI	C6N-N1N	-4.04	1.27	1.37
3	D	302	0WE	C37-N36	4.03	1.39	1.35
2	C	301	NAI	C5A-C4A	-4.03	1.31	1.39
2	A	301	NAI	C6A-N6A	4.03	1.44	1.34
2	C	301	NAI	C5A-N7A	4.01	1.46	1.39
3	G	302	0WE	C37-N36	3.98	1.39	1.35
2	E	301	NAI	C5A-N7A	3.98	1.46	1.39
2	D	301	NAI	C5A-N7A	3.96	1.46	1.39
2	F	301	NAI	PA-O3	-3.94	1.55	1.59
3	H	302	0WE	C37-N36	3.92	1.39	1.35
2	B	301	NAI	C5A-N7A	3.92	1.46	1.39
2	F	301	NAI	C5A-N7A	3.90	1.46	1.39
2	C	301	NAI	C6N-N1N	-3.90	1.27	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	301	NAI	C6N-N1N	-3.89	1.27	1.37
2	H	301	NAI	C5A-N7A	3.87	1.46	1.39
3	E	302	0WE	C37-N36	3.87	1.39	1.35
2	A	301	NAI	C8A-N9A	-3.86	1.31	1.37
2	F	301	NAI	C6N-N1N	-3.85	1.27	1.37
2	A	301	NAI	C5A-N7A	3.84	1.46	1.39
3	D	302	0WE	C22-N36	3.82	1.42	1.38
3	G	302	0WE	O10-C6	-3.82	1.33	1.38
2	F	301	NAI	C6A-N6A	3.82	1.44	1.34
2	B	301	NAI	PA-O3	-3.81	1.55	1.59
2	B	301	NAI	C8A-N9A	-3.79	1.31	1.37
2	F	301	NAI	C8A-N9A	-3.79	1.31	1.37
2	G	301	NAI	C8A-N9A	-3.79	1.31	1.37
2	E	301	NAI	PA-O3	-3.78	1.55	1.59
3	C	302	0WE	C37-N36	3.74	1.39	1.35
2	G	301	NAI	C5A-N7A	3.74	1.45	1.39
2	E	301	NAI	C6N-N1N	-3.74	1.28	1.37
2	D	301	NAI	C8A-N9A	-3.73	1.31	1.37
2	H	301	NAI	PA-O3	-3.72	1.55	1.59
2	E	301	NAI	O7N-C7N	3.70	1.33	1.24
2	H	301	NAI	O7N-C7N	3.70	1.33	1.24
2	B	301	NAI	C6N-N1N	-3.69	1.28	1.37
2	E	301	NAI	C8A-N9A	-3.66	1.31	1.37
2	B	301	NAI	O7N-C7N	3.62	1.32	1.24
2	A	301	NAI	PA-O3	-3.61	1.55	1.59
2	A	301	NAI	C6N-N1N	-3.60	1.28	1.37
3	B	302	0WE	C37-N36	3.59	1.39	1.35
3	D	302	0WE	O10-C6	-3.58	1.33	1.38
2	C	301	NAI	O7N-C7N	3.58	1.32	1.24
3	A	302	0WE	O10-C6	-3.57	1.33	1.38
2	D	301	NAI	O7N-C7N	3.55	1.32	1.24
2	H	301	NAI	C8A-N9A	-3.54	1.31	1.37
3	G	302	0WE	C22-N36	3.51	1.42	1.38
3	G	302	0WE	C20-C19	3.50	1.46	1.38
3	H	302	0WE	O10-C6	-3.47	1.33	1.38
2	C	301	NAI	PA-O3	-3.46	1.55	1.59
3	C	302	0WE	C22-N36	3.43	1.42	1.38
3	B	302	0WE	O10-C6	-3.43	1.33	1.38
3	D	302	0WE	C20-C19	3.42	1.46	1.38
3	H	302	0WE	C22-N36	3.39	1.42	1.38
2	A	301	NAI	O7N-C7N	3.39	1.32	1.24
2	F	301	NAI	O7N-C7N	3.37	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	0WE	C20-C19	3.36	1.46	1.38
3	F	302	0WE	O10-C6	-3.33	1.33	1.38
3	C	302	0WE	C20-C19	3.30	1.46	1.38
3	A	302	0WE	C20-C19	3.30	1.46	1.38
2	G	301	NAI	O7N-C7N	3.29	1.32	1.24
2	A	301	NAI	C5A-C6A	3.28	1.50	1.41
3	E	302	0WE	C22-N36	3.28	1.42	1.38
2	F	301	NAI	C5A-C6A	3.27	1.50	1.41
3	H	302	0WE	C20-C19	3.26	1.46	1.38
2	C	301	NAI	C8A-N9A	-3.25	1.32	1.37
2	C	301	NAI	C5A-C6A	3.24	1.50	1.41
3	F	302	0WE	C20-C19	3.23	1.46	1.38
2	H	301	NAI	C5A-C6A	3.23	1.50	1.41
3	B	302	0WE	C22-N36	3.19	1.42	1.38
3	H	302	0WE	C24-C19	3.19	1.44	1.39
3	C	302	0WE	O10-C6	-3.16	1.33	1.38
2	C	301	NAI	C6N-C5N	-3.16	1.23	1.33
3	A	302	0WE	C22-N36	3.15	1.41	1.38
3	E	302	0WE	C18-C17	-3.14	1.37	1.52
3	F	302	0WE	C37-N36	3.14	1.38	1.35
3	C	302	0WE	C24-C19	3.13	1.44	1.39
3	H	302	0WE	C18-C17	-3.12	1.37	1.52
3	A	302	0WE	C18-C17	-3.11	1.37	1.52
3	F	302	0WE	C18-C17	-3.08	1.38	1.52
3	F	302	0WE	C24-C19	3.07	1.44	1.39
2	B	301	NAI	C5A-C6A	3.06	1.49	1.41
2	D	301	NAI	C5A-C6A	3.05	1.49	1.41
2	B	301	NAI	C2B-C3B	-3.04	1.45	1.53
3	E	302	0WE	C20-C19	3.04	1.45	1.38
2	G	301	NAI	C2B-C3B	-3.03	1.45	1.53
3	C	302	0WE	C18-C17	-3.02	1.38	1.52
2	F	301	NAI	C2B-C3B	-3.02	1.45	1.53
2	E	301	NAI	C5A-C6A	3.01	1.49	1.41
2	G	301	NAI	C6N-C5N	-3.00	1.23	1.33
2	H	301	NAI	C6N-C5N	-3.00	1.23	1.33
3	A	302	0WE	C24-C19	3.00	1.44	1.39
2	G	301	NAI	C5A-C6A	2.99	1.49	1.41
2	D	301	NAI	C2B-C3B	-2.98	1.45	1.53
2	C	301	NAI	C2B-C3B	-2.98	1.45	1.53
2	E	301	NAI	C6N-C5N	-2.97	1.23	1.33
2	A	301	NAI	C6N-C5N	-2.97	1.23	1.33
3	A	302	0WE	C37-N36	2.96	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	302	0WE	C18-C17	-2.95	1.38	1.52
2	H	301	NAI	C2B-C3B	-2.94	1.45	1.53
2	F	301	NAI	C6N-C5N	-2.94	1.23	1.33
3	B	302	0WE	C18-C17	-2.93	1.38	1.52
3	E	302	0WE	O10-C6	-2.92	1.34	1.38
2	E	301	NAI	C2B-C3B	-2.91	1.45	1.53
2	D	301	NAI	C6N-C5N	-2.90	1.24	1.33
3	D	302	0WE	C18-C17	-2.89	1.38	1.52
2	A	301	NAI	C2B-C3B	-2.83	1.45	1.53
3	G	302	0WE	C24-C19	2.79	1.44	1.39
3	D	302	0WE	C24-C19	2.78	1.44	1.39
2	B	301	NAI	C6N-C5N	-2.78	1.24	1.33
3	B	302	0WE	C24-C19	2.77	1.44	1.39
3	F	302	0WE	C22-N36	2.77	1.41	1.38
3	E	302	0WE	C24-C19	2.62	1.43	1.39
2	E	301	NAI	C7N-C3N	-2.46	1.43	1.48
2	G	301	NAI	O3B-C3B	-2.32	1.37	1.43
2	E	301	NAI	O3B-C3B	-2.29	1.37	1.43
2	H	301	NAI	C7N-C3N	-2.29	1.43	1.48
2	D	301	NAI	O3B-C3B	-2.23	1.37	1.43
2	B	301	NAI	O3B-C3B	-2.22	1.37	1.43
2	B	301	NAI	C7N-C3N	-2.21	1.44	1.48
2	A	301	NAI	C2D-C3D	-2.20	1.47	1.53
2	B	301	NAI	O4D-C4D	-2.16	1.40	1.45
2	C	301	NAI	C2D-C1D	-2.15	1.46	1.53
2	H	301	NAI	O3B-C3B	-2.14	1.37	1.43
2	G	301	NAI	C7N-C3N	-2.14	1.44	1.48
2	F	301	NAI	C2D-C1D	-2.12	1.46	1.53
3	G	302	0WE	C11-C8	2.11	1.43	1.39
2	C	301	NAI	O3B-C3B	-2.10	1.37	1.43
2	C	301	NAI	C7N-C3N	-2.10	1.44	1.48
2	A	301	NAI	O3B-C3B	-2.09	1.37	1.43
3	A	302	0WE	C14-C9	2.07	1.43	1.39
3	C	302	0WE	C11-C8	2.05	1.43	1.39
2	A	301	NAI	C2D-C1D	-2.03	1.47	1.53
3	A	302	0WE	C11-C8	2.02	1.43	1.39
2	E	301	NAI	O4D-C4D	-2.02	1.40	1.45
3	F	302	0WE	C11-C8	2.00	1.43	1.39
2	H	301	NAI	C2D-C1D	-2.00	1.47	1.53

All (304) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	NAI	C4A-N9A-C8A	8.31	114.47	105.74
2	B	301	NAI	C4A-N9A-C8A	8.28	114.43	105.74
2	A	301	NAI	C4A-N9A-C8A	8.23	114.38	105.74
2	F	301	NAI	C4A-N9A-C8A	8.17	114.31	105.74
2	E	301	NAI	C4A-N9A-C8A	8.08	114.22	105.74
2	G	301	NAI	C4A-N9A-C8A	8.06	114.20	105.74
2	G	301	NAI	N3A-C2A-N1A	-7.61	117.07	128.58
2	H	301	NAI	C4A-N9A-C8A	7.37	113.47	105.74
2	C	301	NAI	C4A-N9A-C8A	7.34	113.45	105.74
2	B	301	NAI	N3A-C2A-N1A	-7.25	117.61	128.58
2	F	301	NAI	N3A-C2A-N1A	-7.25	117.61	128.58
2	E	301	NAI	N3A-C2A-N1A	-7.17	117.72	128.58
2	C	301	NAI	N3A-C2A-N1A	-7.14	117.77	128.58
2	H	301	NAI	N3A-C2A-N1A	-7.14	117.78	128.58
2	A	301	NAI	N3A-C2A-N1A	-7.09	117.86	128.58
2	F	301	NAI	C5A-C4A-N3A	-6.99	117.09	126.72
2	C	301	NAI	C5A-C4A-N3A	-6.96	117.14	126.72
2	D	301	NAI	N3A-C2A-N1A	-6.95	118.06	128.58
2	A	301	NAI	C5A-C4A-N3A	-6.80	117.36	126.72
2	D	301	NAI	C5A-C4A-N3A	-6.79	117.37	126.72
2	H	301	NAI	C5A-C4A-N3A	-6.77	117.39	126.72
2	E	301	NAI	C5A-C4A-N3A	-6.69	117.51	126.72
2	G	301	NAI	C5A-C4A-N3A	-6.68	117.51	126.72
2	B	301	NAI	C5A-C4A-N3A	-6.62	117.61	126.72
3	E	302	0WE	O10-C6-C5	6.32	126.03	116.06
3	B	302	0WE	O10-C6-C5	6.25	125.94	116.06
2	F	301	NAI	N9A-C8A-N7A	-6.14	105.23	113.94
2	B	301	NAI	N9A-C8A-N7A	-6.07	105.32	113.94
2	A	301	NAI	N9A-C8A-N7A	-6.05	105.35	113.94
2	C	301	NAI	O7N-C7N-C3N	-5.96	109.67	120.90
3	C	302	0WE	O10-C6-C5	5.88	125.34	116.06
2	D	301	NAI	N9A-C8A-N7A	-5.87	105.61	113.94
2	F	301	NAI	O7N-C7N-C3N	-5.86	109.85	120.90
2	G	301	NAI	N9A-C8A-N7A	-5.86	105.62	113.94
2	C	301	NAI	O7N-C7N-N7N	5.86	136.03	122.89
2	H	301	NAI	O7N-C7N-N7N	5.83	135.97	122.89
2	C	301	NAI	C6A-C5A-C4A	5.81	125.12	117.18
2	E	301	NAI	N9A-C8A-N7A	-5.80	105.71	113.94
2	D	301	NAI	C6A-C5A-C4A	5.77	125.06	117.18
2	E	301	NAI	O7N-C7N-N7N	5.74	135.77	122.89
2	H	301	NAI	C5A-C4A-N9A	5.73	112.05	105.81
2	G	301	NAI	O7N-C7N-C3N	-5.70	110.16	120.90
2	H	301	NAI	C6A-C5A-C4A	5.70	124.96	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	NAI	O7N-C7N-C3N	-5.70	110.16	120.90
2	G	301	NAI	C6A-C5A-C4A	5.67	124.92	117.18
2	G	301	NAI	O7N-C7N-N7N	5.66	135.59	122.89
2	D	301	NAI	O7N-C7N-C3N	-5.62	110.32	120.90
2	E	301	NAI	C6A-C5A-C4A	5.62	124.84	117.18
2	B	301	NAI	O7N-C7N-N7N	5.58	135.40	122.89
3	F	302	0WE	O10-C6-C5	5.57	124.86	116.06
2	D	301	NAI	C6N-N1N-C2N	-5.53	113.40	119.32
3	D	302	0WE	O10-C6-C5	5.49	124.73	116.06
2	A	301	NAI	C6A-C5A-C4A	5.49	124.67	117.18
2	B	301	NAI	C5A-C4A-N9A	5.46	111.76	105.81
2	B	301	NAI	C6A-C5A-C4A	5.46	124.63	117.18
2	C	301	NAI	N9A-C8A-N7A	-5.45	106.20	113.94
2	H	301	NAI	N9A-C8A-N7A	-5.45	106.21	113.94
2	C	301	NAI	C5A-C4A-N9A	5.44	111.74	105.81
2	F	301	NAI	O7N-C7N-N7N	5.42	135.05	122.89
2	H	301	NAI	O7N-C7N-C3N	-5.39	110.75	120.90
2	F	301	NAI	C6A-C5A-C4A	5.34	124.47	117.18
3	A	302	0WE	O10-C6-C5	5.30	124.42	116.06
2	F	301	NAI	C5A-C4A-N9A	5.29	111.58	105.81
2	A	301	NAI	O7N-C7N-N7N	5.26	134.70	122.89
2	A	301	NAI	C5A-C4A-N9A	5.25	111.53	105.81
2	E	301	NAI	C5A-C4A-N9A	5.23	111.51	105.81
2	G	301	NAI	C5A-C4A-N9A	5.17	111.44	105.81
2	H	301	NAI	C6N-N1N-C2N	-5.11	113.85	119.32
2	B	301	NAI	O7N-C7N-C3N	-5.11	111.27	120.90
3	H	302	0WE	O10-C6-C5	5.06	124.04	116.06
2	E	301	NAI	O7N-C7N-C3N	-5.05	111.38	120.90
2	G	301	NAI	C6N-N1N-C2N	-5.05	113.92	119.32
2	D	301	NAI	O7N-C7N-N7N	5.03	134.17	122.89
3	A	302	0WE	C9-O10-C6	5.00	110.97	106.04
3	H	302	0WE	C24-C19-C20	4.99	121.52	116.90
2	E	301	NAI	C6N-N1N-C2N	-4.98	113.98	119.32
3	G	302	0WE	O10-C6-C5	4.94	123.86	116.06
2	B	301	NAI	C6N-N1N-C2N	-4.91	114.06	119.32
2	D	301	NAI	C5A-C4A-N9A	4.89	111.14	105.81
3	B	302	0WE	C9-O10-C6	4.85	110.83	106.04
3	D	302	0WE	C9-O10-C6	4.69	110.67	106.04
3	F	302	0WE	C9-O10-C6	4.69	110.67	106.04
3	C	302	0WE	C24-C19-C20	4.68	121.23	116.90
3	D	302	0WE	C24-C19-C20	4.55	121.11	116.90
2	A	301	NAI	C6N-N1N-C2N	-4.52	114.48	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	302	0WE	C24-C19-C20	4.52	121.08	116.90
3	G	302	0WE	C9-O10-C6	4.50	110.48	106.04
3	D	302	0WE	C6-C5-N3	-4.36	106.24	113.11
2	F	301	NAI	C6N-N1N-C2N	-4.31	114.71	119.32
3	F	302	0WE	C24-C19-C20	4.30	120.88	116.90
3	G	302	0WE	C24-C19-C20	4.11	120.71	116.90
3	A	302	0WE	C24-C19-C20	4.10	120.70	116.90
2	C	301	NAI	C6N-N1N-C2N	-4.07	114.96	119.32
2	C	301	NAI	C3N-C2N-N1N	-4.07	117.23	123.20
3	H	302	0WE	C9-O10-C6	4.04	110.03	106.04
2	D	301	NAI	C1D-N1N-C6N	3.94	129.11	120.77
2	A	301	NAI	C1D-N1N-C6N	3.87	128.96	120.77
2	F	301	NAI	C2A-N3A-C4A	3.85	121.23	111.83
3	E	302	0WE	O28-C37-N36	-3.79	117.37	121.39
2	G	301	NAI	C2A-N3A-C4A	3.76	121.01	111.83
2	G	301	NAI	C1D-N1N-C6N	3.76	128.72	120.77
3	A	302	0WE	O28-C37-N36	-3.71	117.46	121.39
3	B	302	0WE	C24-C19-C20	3.71	120.33	116.90
3	C	302	0WE	C6-C5-N3	-3.70	107.28	113.11
2	A	301	NAI	C2A-N3A-C4A	3.67	120.80	111.83
3	G	302	0WE	C25-C37-N36	3.66	120.42	116.31
2	H	301	NAI	C2A-N3A-C4A	3.65	120.75	111.83
2	B	301	NAI	C1D-N1N-C6N	3.65	128.49	120.77
2	B	301	NAI	C2A-N3A-C4A	3.64	120.72	111.83
2	C	301	NAI	C2A-N3A-C4A	3.63	120.69	111.83
2	E	301	NAI	C2A-N3A-C4A	3.61	120.65	111.83
2	D	301	NAI	C2A-N3A-C4A	3.58	120.57	111.83
2	E	301	NAI	O4B-C1B-C2B	-3.58	98.96	106.62
3	E	302	0WE	C9-O10-C6	3.57	109.57	106.04
3	G	302	0WE	C6-C5-N3	-3.57	107.49	113.11
3	B	302	0WE	O28-C37-N36	-3.54	117.64	121.39
3	H	302	0WE	C6-C5-N3	-3.50	107.59	113.11
3	C	302	0WE	C14-C9-C8	-3.50	119.56	123.58
3	C	302	0WE	C9-O10-C6	3.43	109.43	106.04
3	H	302	0WE	C23-C24-C19	-3.39	116.45	121.76
2	H	301	NAI	C1D-N1N-C6N	3.38	127.93	120.77
2	B	301	NAI	C3N-C2N-N1N	-3.38	118.25	123.20
2	G	301	NAI	C3N-C2N-N1N	-3.35	118.29	123.20
3	B	302	0WE	C25-C37-N36	3.34	120.06	116.31
2	F	301	NAI	C3B-C2B-C1B	3.33	107.77	101.46
2	E	301	NAI	C1D-N1N-C6N	3.31	127.78	120.77
2	F	301	NAI	C1D-N1N-C6N	3.30	127.75	120.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	301	NAI	C3N-C2N-N1N	-3.25	118.43	123.20
2	C	301	NAI	C3B-C2B-C1B	3.25	107.61	101.46
3	G	302	0WE	C17-C18-C19	3.24	124.10	112.70
2	B	301	NAI	O4B-C1B-C2B	-3.22	99.72	106.62
2	E	301	NAI	C3N-C2N-N1N	-3.22	118.48	123.20
3	F	302	0WE	O28-C37-N36	-3.19	118.01	121.39
3	E	302	0WE	C6-C5-N3	-3.18	108.09	113.11
3	A	302	0WE	C19-C20-N21	-3.18	119.27	123.99
2	G	301	NAI	O4B-C1B-C2B	-3.17	99.83	106.62
2	A	301	NAI	C3B-C2B-C1B	3.16	107.45	101.46
2	B	301	NAI	C4A-C5A-N7A	-3.16	106.97	110.58
3	C	302	0WE	O28-C37-N36	-3.15	118.06	121.39
3	E	302	0WE	C14-C9-C8	-3.13	119.98	123.58
3	F	302	0WE	C17-C1-N3	3.11	123.39	118.08
3	D	302	0WE	C23-C24-C19	-3.08	116.94	121.76
2	C	301	NAI	C1D-N1N-C6N	3.07	127.26	120.77
3	B	302	0WE	C17-C18-C19	3.06	123.46	112.70
3	E	302	0WE	C25-C37-N36	3.05	119.73	116.31
3	H	302	0WE	O2-C1-N3	-3.03	117.79	122.19
2	H	301	NAI	C4A-C5A-N7A	-3.03	107.12	110.58
3	F	302	0WE	C23-C24-C19	-3.03	117.02	121.76
3	A	302	0WE	C17-C1-N3	3.03	123.25	118.08
2	F	301	NAI	C3N-C2N-N1N	-3.03	118.76	123.20
3	C	302	0WE	C23-C24-C19	-3.02	117.04	121.76
3	D	302	0WE	C17-C18-C19	2.98	123.19	112.70
3	C	302	0WE	O2-C1-N3	-2.98	117.86	122.19
3	C	302	0WE	C19-C20-N21	-2.98	119.56	123.99
3	H	302	0WE	C14-C9-C8	-2.97	120.17	123.58
3	F	302	0WE	C17-C18-C19	2.96	123.12	112.70
2	H	301	NAI	C3B-C2B-C1B	2.95	107.05	101.46
3	G	302	0WE	C17-C1-N3	2.94	123.09	118.08
2	F	301	NAI	C4A-C5A-N7A	-2.93	107.23	110.58
3	G	302	0WE	C22-N36-C37	-2.92	119.88	124.50
3	H	302	0WE	C25-C37-N36	2.92	119.59	116.31
3	H	302	0WE	C19-C20-N21	-2.90	119.68	123.99
3	B	302	0WE	C6-C5-N3	-2.89	108.55	113.11
3	E	302	0WE	C18-C19-C20	-2.89	116.59	121.73
2	C	301	NAI	O4B-C1B-C2B	-2.88	100.45	106.62
3	A	302	0WE	C20-N21-C22	2.86	121.80	116.19
2	D	301	NAI	O4B-C1B-C2B	-2.86	100.49	106.62
2	A	301	NAI	C4A-C5A-N7A	-2.82	107.35	110.58
3	F	302	0WE	C18-C19-C20	-2.82	116.71	121.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	302	0WE	C17-C1-N3	2.81	122.88	118.08
2	C	301	NAI	C4A-C5A-N7A	-2.81	107.37	110.58
3	A	302	0WE	C17-C18-C19	2.81	122.58	112.70
3	G	302	0WE	C23-C24-C19	-2.81	117.37	121.76
3	E	302	0WE	C19-C20-N21	-2.80	119.83	123.99
2	G	301	NAI	C4A-C5A-N7A	-2.79	107.39	110.58
2	A	301	NAI	C1D-N1N-C2N	-2.78	116.55	121.14
3	G	302	0WE	C14-C9-C8	-2.77	120.39	123.58
2	E	301	NAI	O3-PA-O1A	-2.77	102.37	110.70
2	E	301	NAI	C4A-C5A-N7A	-2.76	107.43	110.58
3	F	302	0WE	C25-C37-N36	2.75	119.40	116.31
3	C	302	0WE	C18-C19-C20	-2.74	116.85	121.73
3	D	302	0WE	C25-C37-N36	2.74	119.38	116.31
3	B	302	0WE	C19-C20-N21	-2.73	119.93	123.99
2	B	301	NAI	O3-PA-O1A	-2.72	102.52	110.70
3	C	302	0WE	C4-N3-C5	2.72	120.90	116.89
2	E	301	NAI	C3N-C7N-N7N	-2.71	112.85	117.67
3	B	302	0WE	C18-C19-C20	-2.71	116.91	121.73
3	D	302	0WE	C14-C9-C8	-2.70	120.47	123.58
2	D	301	NAI	C4A-C5A-N7A	-2.69	107.50	110.58
3	H	302	0WE	C4-N3-C5	2.62	120.76	116.89
3	A	302	0WE	O10-C9-C8	-2.62	108.27	110.84
3	B	302	0WE	C14-C9-C8	-2.62	120.57	123.58
2	B	301	NAI	C4A-N9A-C1B	-2.62	120.52	126.63
3	H	302	0WE	C18-C19-C20	-2.61	117.09	121.73
3	E	302	0WE	C23-C24-C19	-2.61	117.67	121.76
3	E	302	0WE	C17-C18-C19	2.61	121.86	112.70
3	F	302	0WE	O10-C9-C8	-2.61	108.28	110.84
3	C	302	0WE	C20-N21-C22	2.60	121.29	116.19
3	A	302	0WE	C14-C9-C8	-2.59	120.60	123.58
3	A	302	0WE	C23-C24-C19	-2.58	117.72	121.76
2	F	301	NAI	O4B-C1B-C2B	-2.58	101.10	106.62
3	C	302	0WE	C25-C37-N36	2.58	119.21	116.31
3	D	302	0WE	C18-C19-C20	-2.56	117.18	121.73
3	C	302	0WE	C17-C1-N3	2.54	122.43	118.08
3	C	302	0WE	C17-C18-C19	2.54	121.65	112.70
2	D	301	NAI	N3A-C4A-N9A	2.54	131.48	127.17
3	B	302	0WE	O2-C1-N3	-2.52	118.53	122.19
2	A	301	NAI	C4A-N9A-C1B	-2.52	120.74	126.63
3	D	302	0WE	C19-C20-N21	-2.51	120.25	123.99
3	A	302	0WE	C6-C5-N3	-2.50	109.16	113.11
3	A	302	0WE	C18-C19-C20	-2.50	117.28	121.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	302	0WE	O10-C9-C8	-2.50	108.39	110.84
2	A	301	NAI	O4D-C1D-C2D	-2.50	101.27	106.62
3	B	302	0WE	C20-N21-C22	2.48	121.05	116.19
2	D	301	NAI	O4D-C1D-C2D	-2.47	101.32	106.62
3	B	302	0WE	C17-C1-N3	2.47	122.30	118.08
2	H	301	NAI	C3N-C7N-N7N	-2.47	113.28	117.67
2	F	301	NAI	O3-PA-O1A	-2.46	103.29	110.70
2	D	301	NAI	C3N-C2N-N1N	-2.46	119.59	123.20
2	H	301	NAI	O4B-C1B-C2B	-2.46	101.35	106.62
3	B	302	0WE	O10-C9-C8	-2.46	108.43	110.84
2	B	301	NAI	C3N-C7N-N7N	-2.45	113.32	117.67
2	G	301	NAI	O4D-C1D-C2D	-2.45	101.38	106.62
2	F	301	NAI	N3A-C4A-N9A	2.44	131.32	127.17
3	F	302	0WE	C14-C9-C8	-2.43	120.79	123.58
3	F	302	0WE	C19-C20-N21	-2.42	120.39	123.99
3	D	302	0WE	O28-C37-N36	-2.42	118.82	121.39
2	D	301	NAI	C6A-C5A-N7A	-2.41	127.44	132.09
3	H	302	0WE	C20-N21-C22	2.41	120.92	116.19
2	B	301	NAI	C3B-C2B-C1B	2.39	105.99	101.46
2	H	301	NAI	C4A-N9A-C1B	-2.38	121.06	126.63
2	C	301	NAI	C6A-C5A-N7A	-2.37	127.51	132.09
3	F	302	0WE	O2-C1-N3	-2.37	118.75	122.19
3	E	302	0WE	C20-N21-C22	2.37	120.84	116.19
2	E	301	NAI	C3B-C2B-C1B	2.37	105.95	101.46
2	D	301	NAI	O4D-C1D-N1N	-2.37	103.57	108.08
3	D	302	0WE	C22-N36-C37	-2.36	120.77	124.50
2	F	301	NAI	C4A-N9A-C1B	-2.36	121.11	126.63
3	G	302	0WE	O10-C9-C8	-2.36	108.53	110.84
3	G	302	0WE	C19-C20-N21	-2.35	120.49	123.99
3	H	302	0WE	O28-C37-N36	-2.35	118.90	121.39
2	A	301	NAI	O4B-C1B-C2B	-2.35	101.59	106.62
2	A	301	NAI	C4B-O4B-C1B	-2.34	104.31	109.47
3	H	302	0WE	C17-C1-N3	2.33	122.07	118.08
2	A	301	NAI	C3N-C2N-N1N	-2.33	119.78	123.20
2	G	301	NAI	O2A-PA-O3	2.33	113.58	107.27
2	D	301	NAI	O1N-PN-O3	-2.33	100.98	107.27
2	C	301	NAI	N3A-C4A-N9A	2.32	131.11	127.17
2	A	301	NAI	N3A-C4A-N9A	2.32	131.11	127.17
2	C	301	NAI	O3-PA-O1A	-2.31	103.74	110.70
2	F	301	NAI	C4B-O4B-C1B	-2.31	104.36	109.47
2	B	301	NAI	O4D-C1D-C2D	-2.31	101.68	106.62
2	G	301	NAI	O4D-C1D-N1N	-2.29	103.71	108.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	301	NAI	C1D-N1N-C2N	-2.29	117.37	121.14
3	B	302	0WE	C22-N36-C37	-2.29	120.88	124.50
2	E	301	NAI	C4A-N9A-C1B	-2.28	121.29	126.63
2	G	301	NAI	C6A-C5A-N7A	-2.28	127.69	132.09
3	E	302	0WE	C4-N3-C5	2.28	120.25	116.89
2	G	301	NAI	N3A-C4A-N9A	2.27	131.03	127.17
3	B	302	0WE	C23-C24-C19	-2.27	118.21	121.76
2	E	301	NAI	C6A-C5A-N7A	-2.26	127.73	132.09
3	D	302	0WE	O2-C1-N3	-2.26	118.91	122.19
3	C	302	0WE	O10-C9-C14	2.25	131.23	126.49
3	A	302	0WE	O2-C1-N3	-2.25	118.92	122.19
2	E	301	NAI	N3A-C4A-N9A	2.24	130.98	127.17
2	D	301	NAI	C4A-N9A-C1B	-2.24	121.39	126.63
2	B	301	NAI	C1D-N1N-C2N	-2.24	117.45	121.14
2	B	301	NAI	C4B-O4B-C1B	-2.24	104.53	109.47
2	D	301	NAI	C1D-N1N-C2N	-2.22	117.48	121.14
2	G	301	NAI	C4A-N9A-C1B	-2.22	121.45	126.63
3	D	302	0WE	O10-C9-C14	2.21	131.14	126.49
3	A	302	0WE	O10-C9-C14	2.21	131.13	126.49
3	H	302	0WE	C22-N36-C37	-2.21	121.01	124.50
2	F	301	NAI	O4D-C1D-C2D	-2.20	101.91	106.62
3	G	302	0WE	C18-C19-C20	-2.18	117.85	121.73
2	F	301	NAI	C1D-N1N-C2N	-2.18	117.54	121.14
3	G	302	0WE	O10-C9-C14	2.18	131.08	126.49
3	F	302	0WE	C20-N21-C22	2.18	120.46	116.19
3	B	302	0WE	C4-N3-C5	2.17	120.10	116.89
3	H	302	0WE	C26-C23-C24	2.17	124.20	119.91
2	H	301	NAI	C6A-C5A-N7A	-2.16	127.92	132.09
3	C	302	0WE	C26-C23-C24	2.16	124.17	119.91
2	F	301	NAI	O1N-PN-O3	-2.15	101.46	107.27
3	G	302	0WE	O2-C1-N3	-2.15	119.08	122.19
3	B	302	0WE	O10-C9-C14	2.15	131.00	126.49
3	H	302	0WE	O10-C9-C14	2.14	130.99	126.49
3	H	302	0WE	C17-C18-C19	2.14	120.22	112.70
3	G	302	0WE	O28-C37-N36	-2.14	119.12	121.39
2	A	301	NAI	C6A-C5A-N7A	-2.14	127.97	132.09
3	E	302	0WE	C17-C1-N3	2.12	121.71	118.08
3	E	302	0WE	O10-C9-C14	2.12	130.95	126.49
2	G	301	NAI	C3B-C2B-C1B	2.11	105.46	101.46
3	F	302	0WE	O10-C9-C14	2.11	130.92	126.49
2	E	301	NAI	O4D-C1D-C2D	-2.10	102.13	106.62
3	A	302	0WE	C25-C37-N36	2.09	118.66	116.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	NAI	O2A-PA-O3	2.09	112.93	107.27
3	C	302	0WE	C22-N36-C37	-2.08	121.21	124.50
2	C	301	NAI	C1D-N1N-C2N	-2.05	117.77	121.14
3	F	302	0WE	C6-C5-N3	-2.05	109.88	113.11
3	H	302	0WE	O10-C9-C8	-2.04	108.84	110.84
2	B	301	NAI	N3A-C4A-N9A	2.04	130.63	127.17
3	G	302	0WE	N36-C22-N21	2.03	119.41	116.38
3	C	302	0WE	C11-C8-C9	2.03	121.17	118.88
2	E	301	NAI	C4B-O4B-C1B	-2.02	105.01	109.47

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	NAI	PN-O3-PA-O5B
2	A	301	NAI	C5D-O5D-PN-O3
2	A	301	NAI	C5D-O5D-PN-O1N
2	A	301	NAI	C5D-O5D-PN-O2N
2	B	301	NAI	C5D-O5D-PN-O3
2	B	301	NAI	C5D-O5D-PN-O2N
2	C	301	NAI	PN-O3-PA-O5B
2	C	301	NAI	C5D-O5D-PN-O3
2	C	301	NAI	C5D-O5D-PN-O1N
2	C	301	NAI	C5D-O5D-PN-O2N
2	D	301	NAI	C5D-O5D-PN-O3
2	D	301	NAI	C5D-O5D-PN-O2N
2	E	301	NAI	C5D-O5D-PN-O3
2	E	301	NAI	C5D-O5D-PN-O2N
2	F	301	NAI	PN-O3-PA-O5B
2	F	301	NAI	C5D-O5D-PN-O3
2	F	301	NAI	C5D-O5D-PN-O1N
2	F	301	NAI	C5D-O5D-PN-O2N
2	G	301	NAI	C5D-O5D-PN-O3
2	G	301	NAI	C5D-O5D-PN-O1N
2	G	301	NAI	C5D-O5D-PN-O2N
2	H	301	NAI	PN-O3-PA-O5B
2	H	301	NAI	C5D-O5D-PN-O3
2	H	301	NAI	C5D-O5D-PN-O1N
2	H	301	NAI	C5D-O5D-PN-O2N
2	B	301	NAI	PN-O3-PA-O5B
2	D	301	NAI	PN-O3-PA-O5B
2	E	301	NAI	PN-O3-PA-O5B

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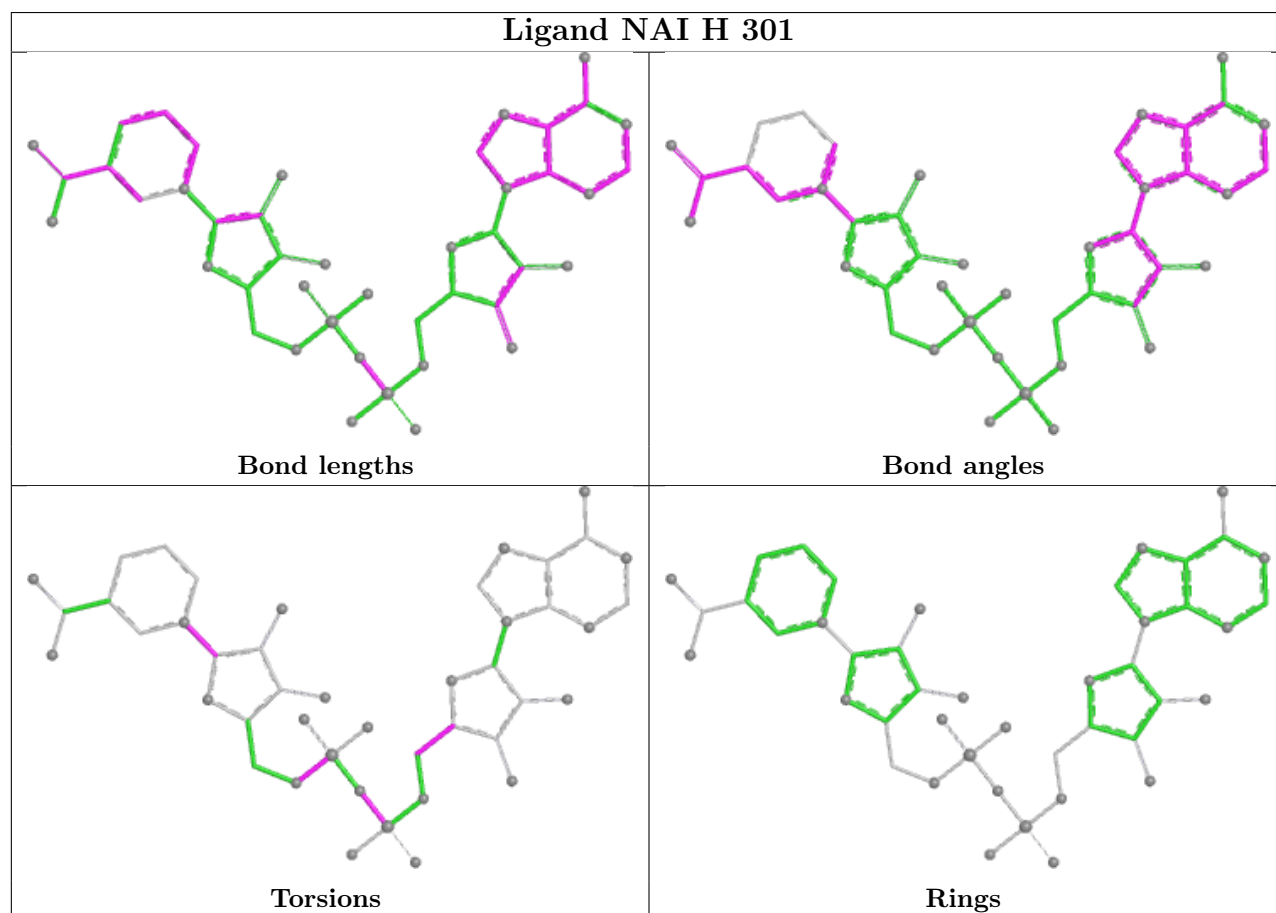
Mol	Chain	Res	Type	Atoms
2	G	301	NAI	PN-O3-PA-O5B
3	E	302	0WE	C17-C18-C19-C20
2	B	301	NAI	C5D-O5D-PN-O1N
2	C	301	NAI	C5B-O5B-PA-O2A
2	D	301	NAI	C5D-O5D-PN-O1N
2	E	301	NAI	C5D-O5D-PN-O1N
2	A	301	NAI	O4D-C1D-N1N-C6N
2	C	301	NAI	O4D-C1D-N1N-C6N
2	F	301	NAI	O4D-C1D-N1N-C6N
3	B	302	0WE	C17-C18-C19-C24
2	B	301	NAI	O4D-C1D-N1N-C6N
2	D	301	NAI	O4D-C1D-N1N-C6N
2	E	301	NAI	O4D-C1D-N1N-C6N
2	G	301	NAI	O4D-C1D-N1N-C6N
2	H	301	NAI	O4D-C1D-N1N-C6N
3	A	302	0WE	C17-C18-C19-C20
3	B	302	0WE	C17-C18-C19-C20
3	E	302	0WE	C17-C18-C19-C24
3	C	302	0WE	C17-C18-C19-C20
3	H	302	0WE	C17-C18-C19-C20
3	D	302	0WE	C17-C18-C19-C20
3	F	302	0WE	C17-C18-C19-C20
3	G	302	0WE	C17-C18-C19-C20
2	D	301	NAI	C2D-C1D-N1N-C6N
2	G	301	NAI	C2D-C1D-N1N-C6N
2	C	301	NAI	O4B-C4B-C5B-O5B
2	E	301	NAI	C2D-C1D-N1N-C6N
2	A	301	NAI	C2D-C1D-N1N-C6N
2	B	301	NAI	C2D-C1D-N1N-C6N
2	C	301	NAI	C2D-C1D-N1N-C6N
2	F	301	NAI	C2D-C1D-N1N-C6N
2	H	301	NAI	C2D-C1D-N1N-C6N
3	D	302	0WE	C17-C18-C19-C24
2	H	301	NAI	O4B-C4B-C5B-O5B
3	A	302	0WE	C17-C18-C19-C24
3	H	302	0WE	C17-C18-C19-C24
3	C	302	0WE	C17-C18-C19-C24
2	E	301	NAI	C2N-C3N-C7N-O7N

There are no ring outliers.

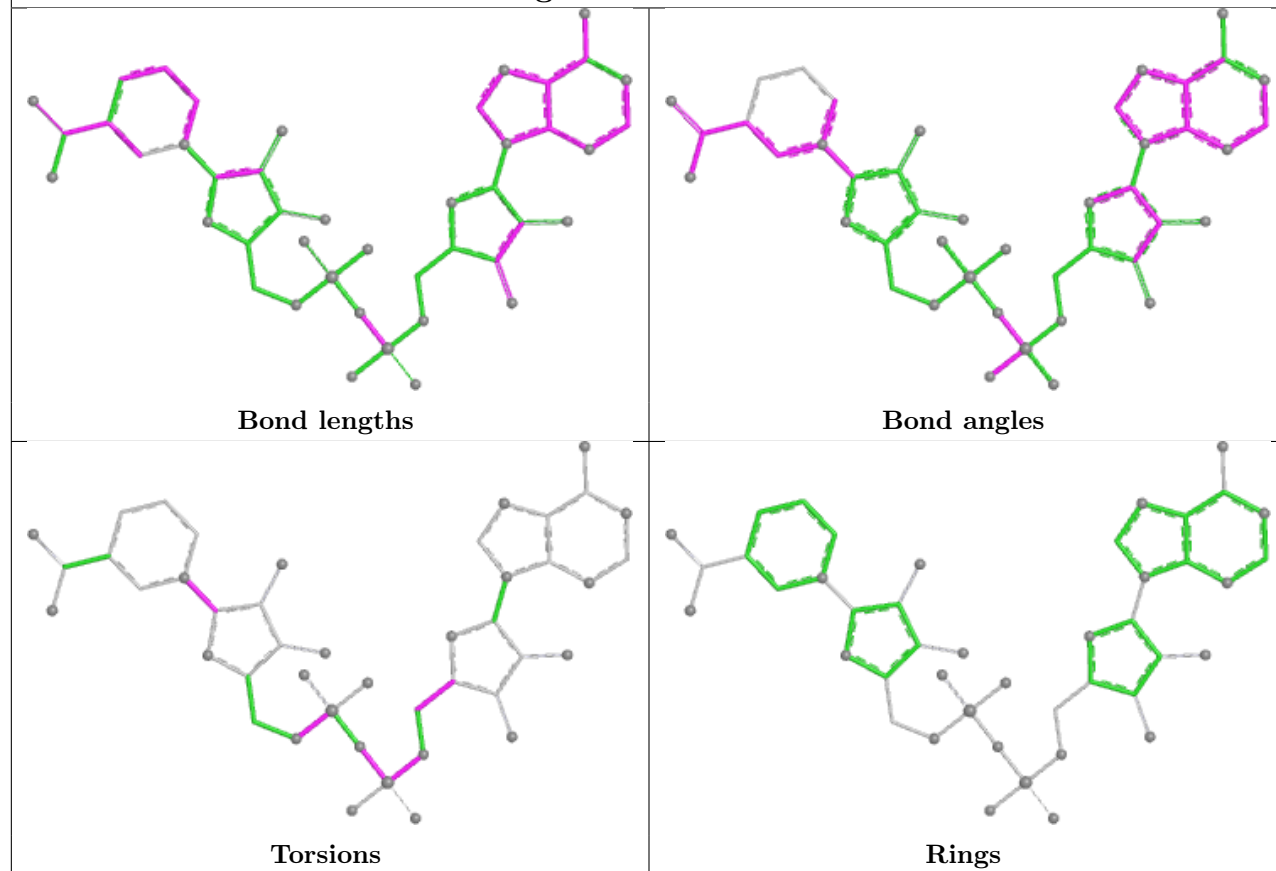
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

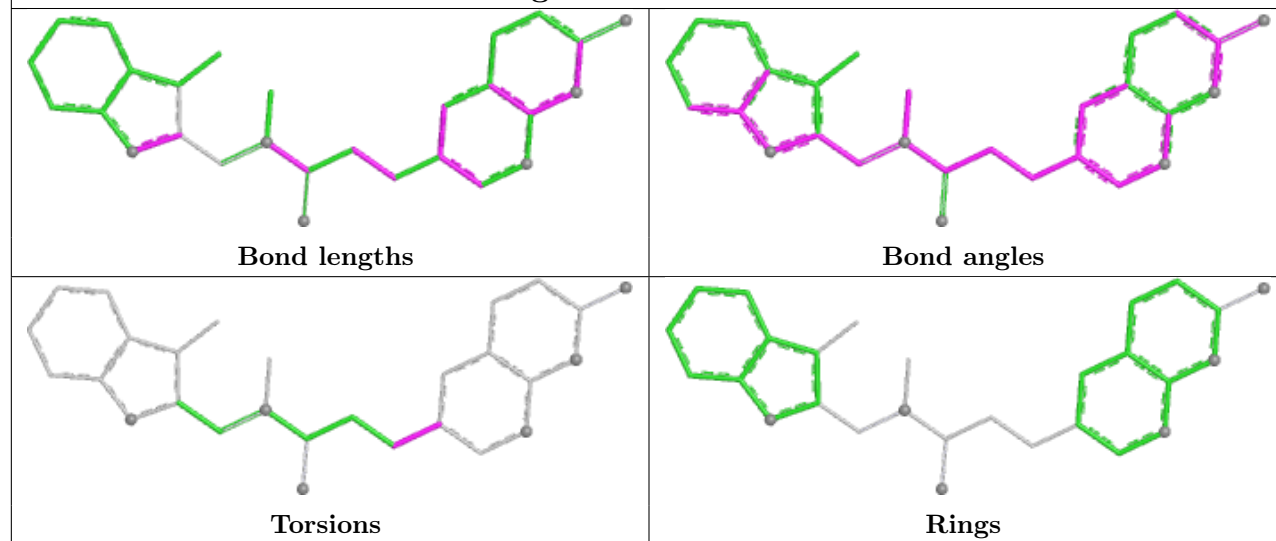
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.



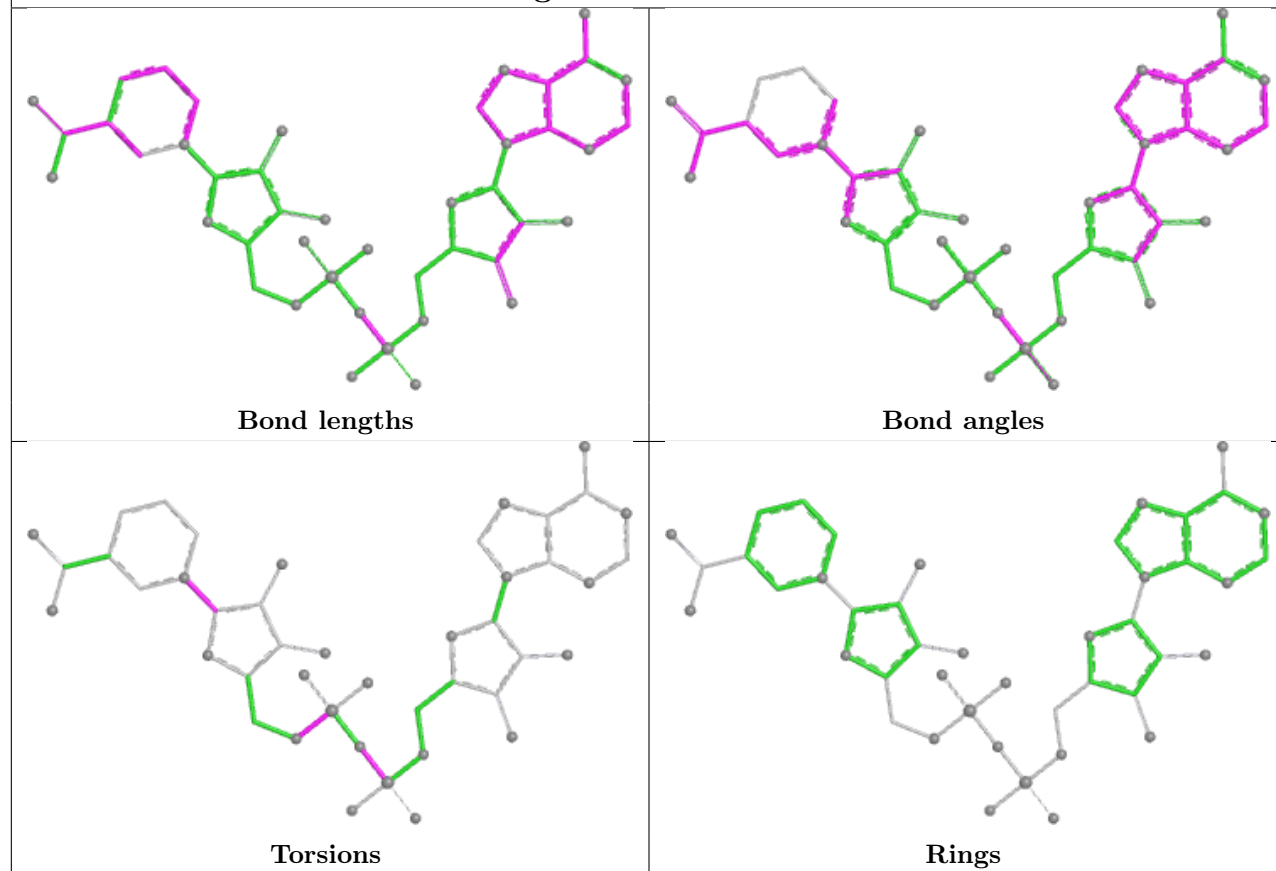
Ligand NAI C 301



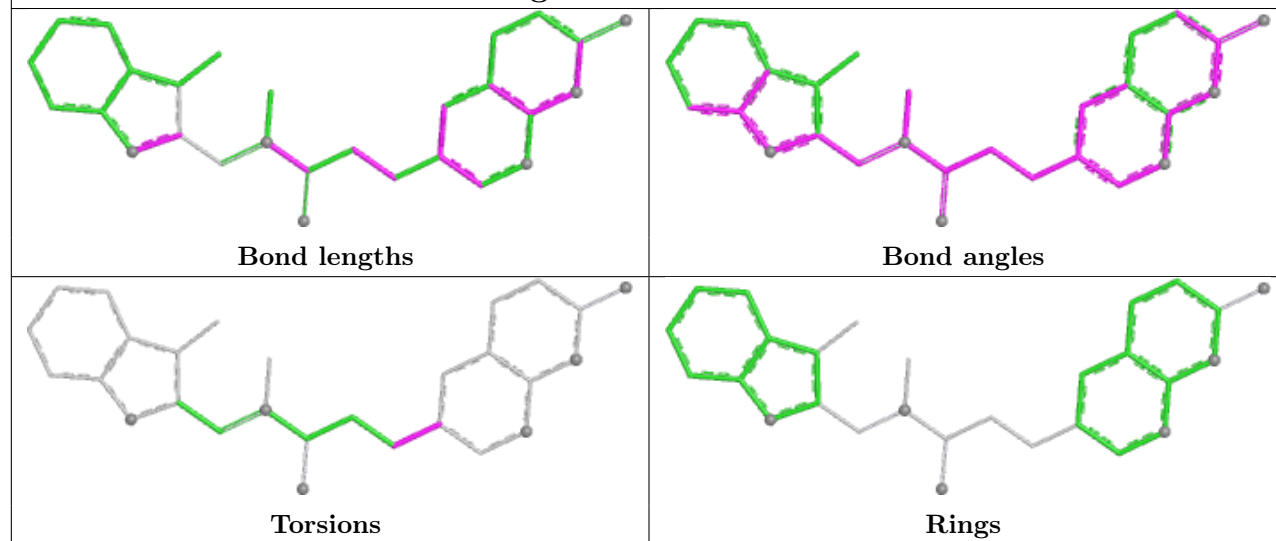
Ligand 0WE E 302



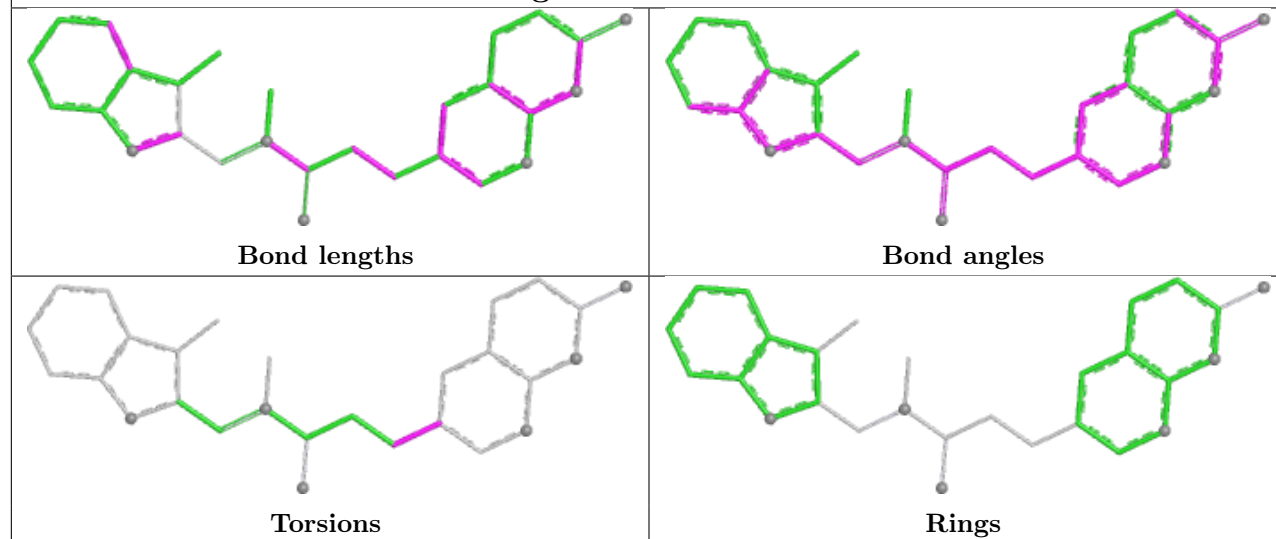
Ligand NAI G 301



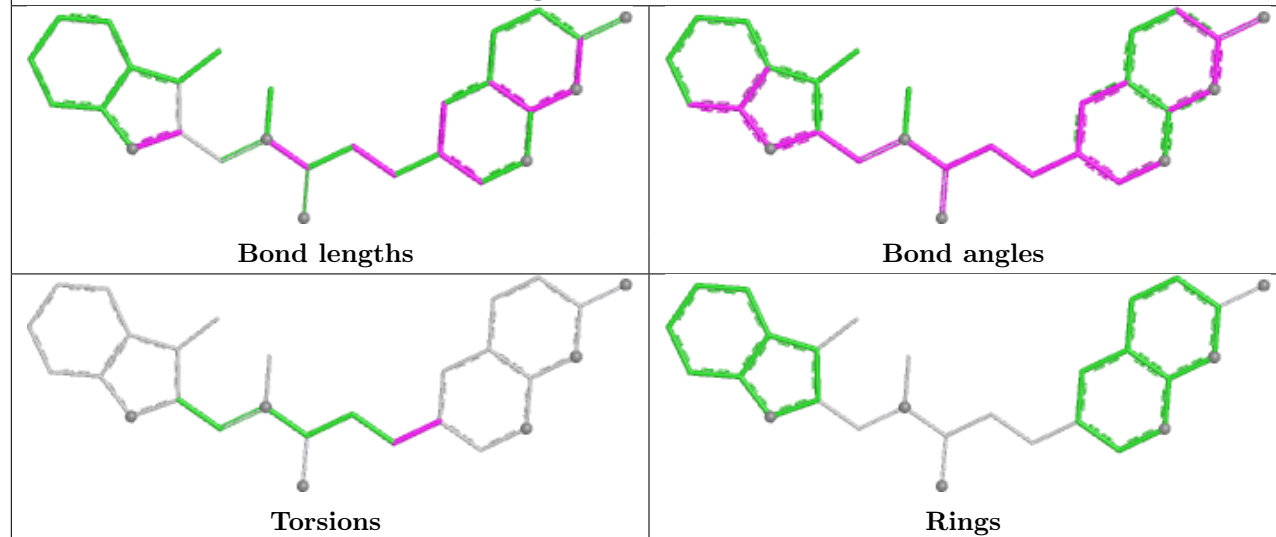
Ligand 0WE B 302

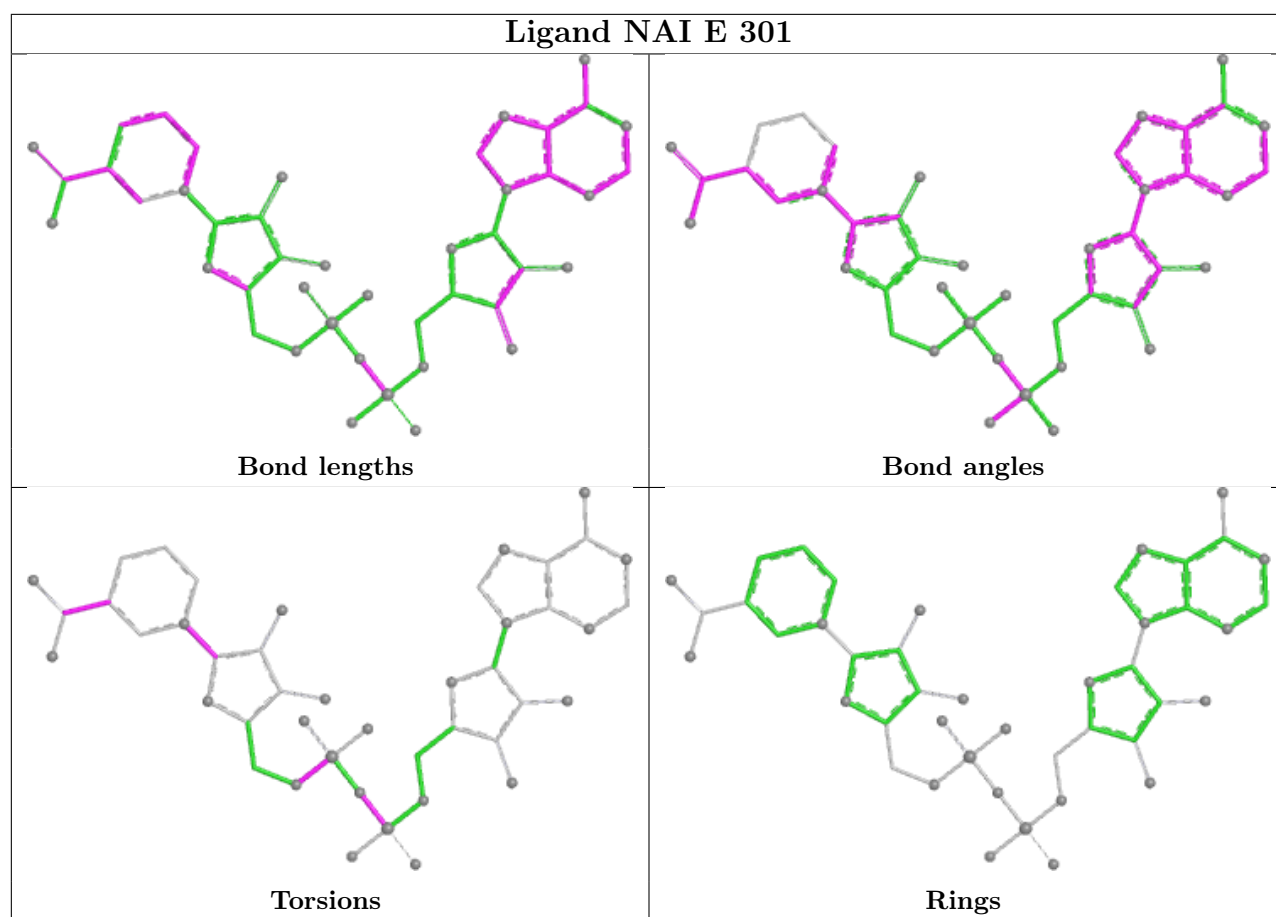


Ligand 0WE F 302

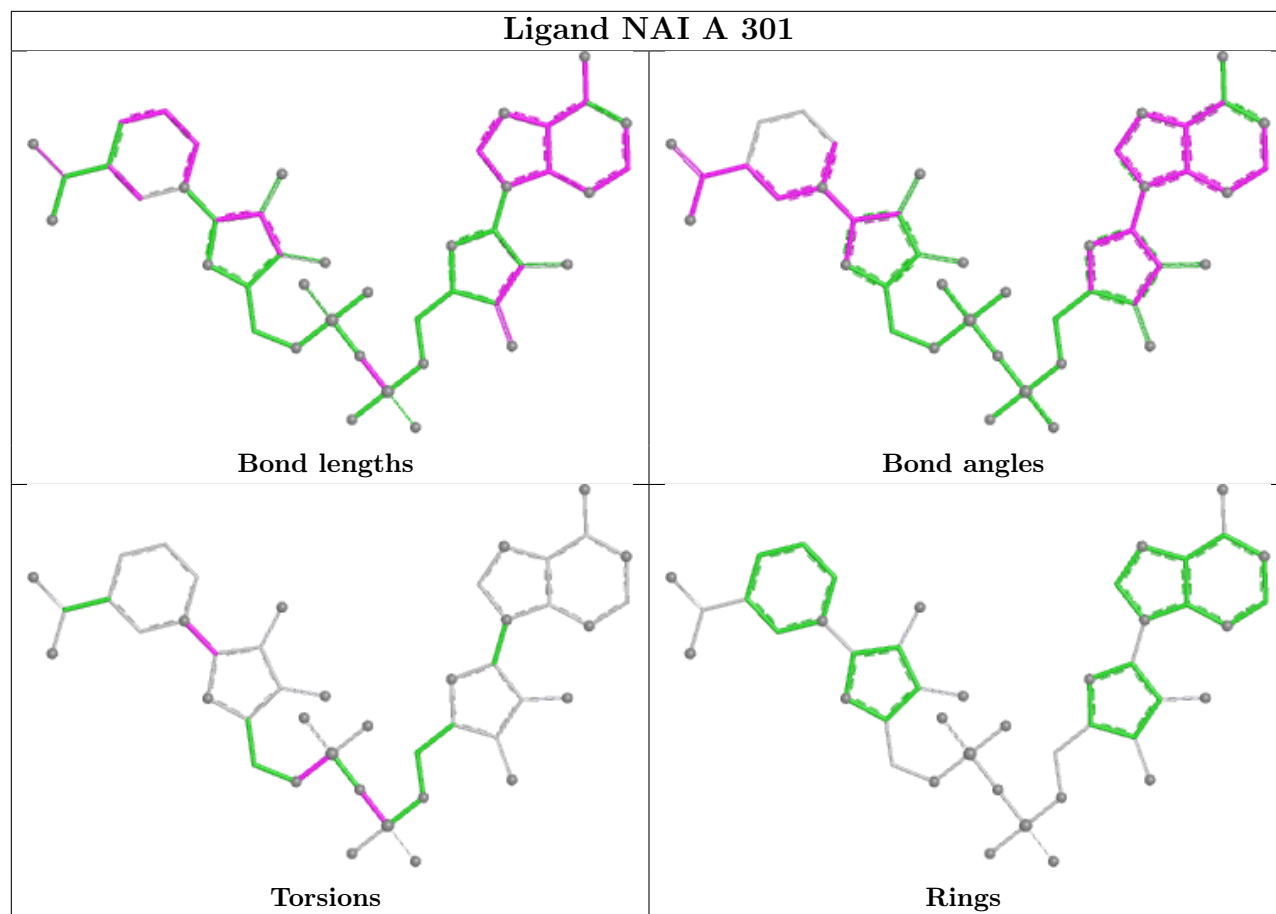


Ligand 0WE D 302

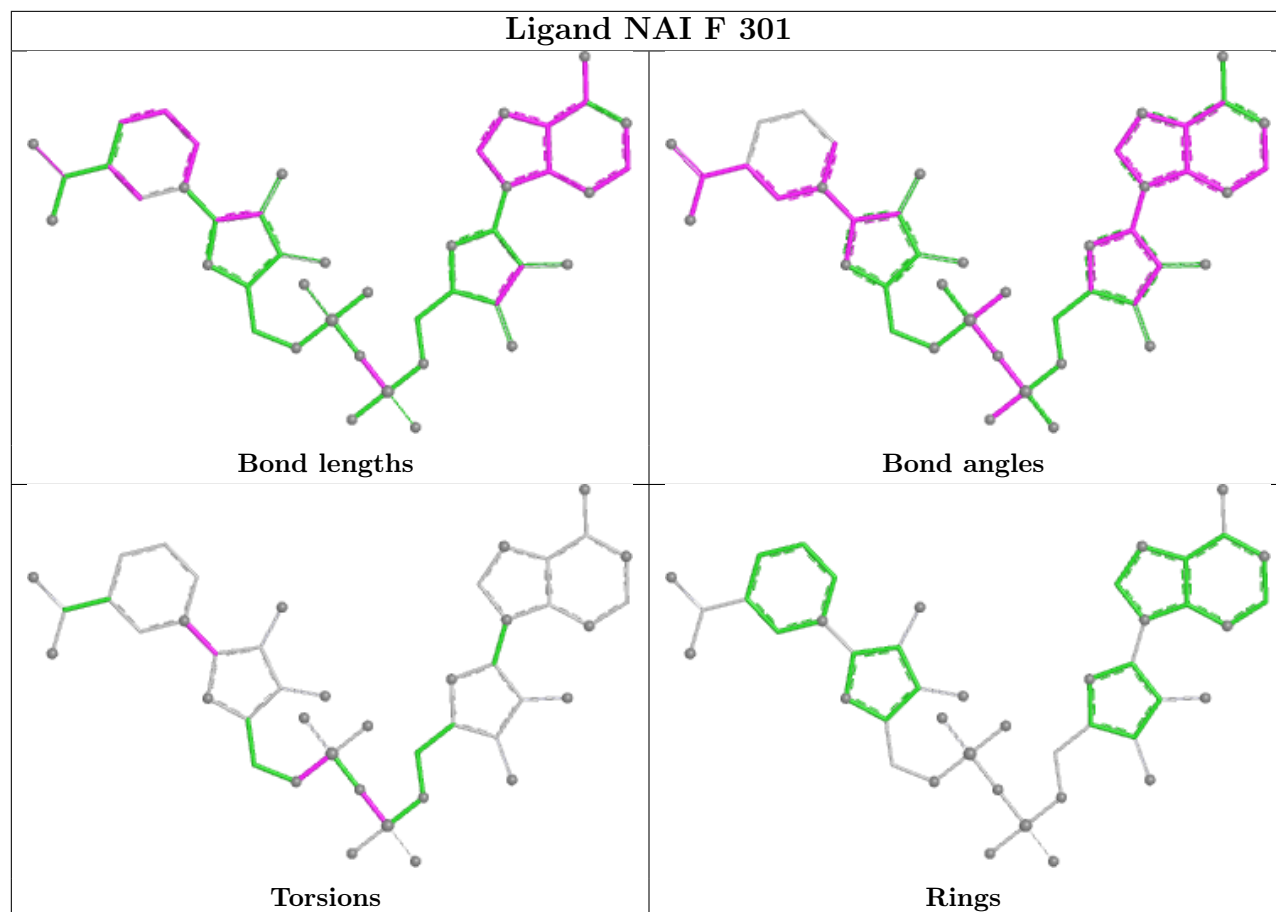




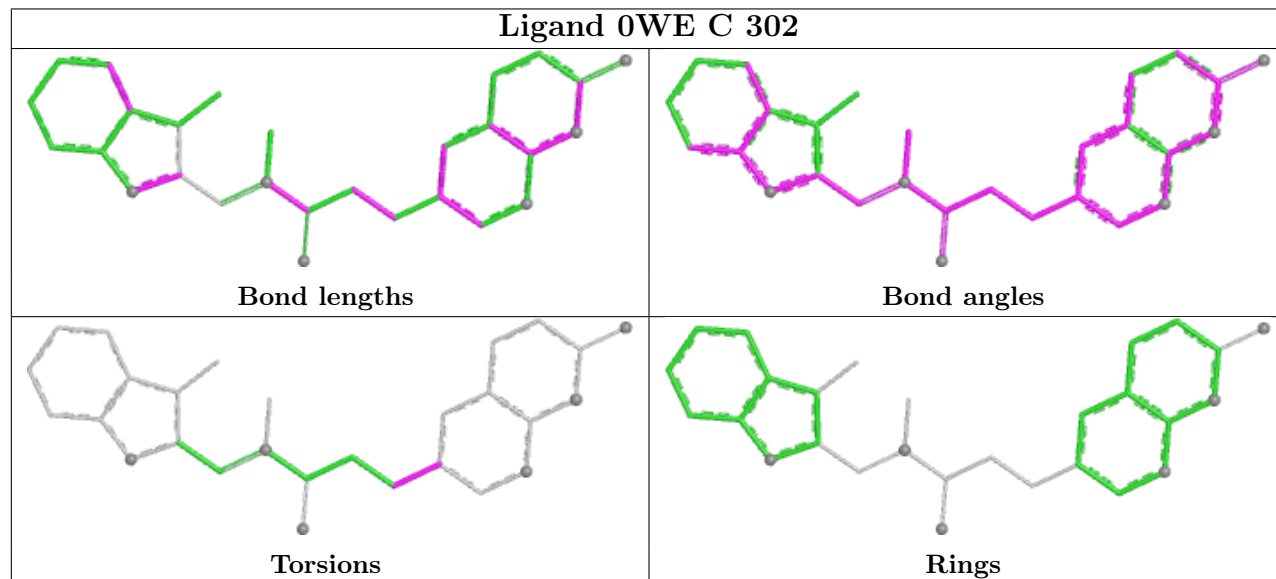
Ligand NAI A 301



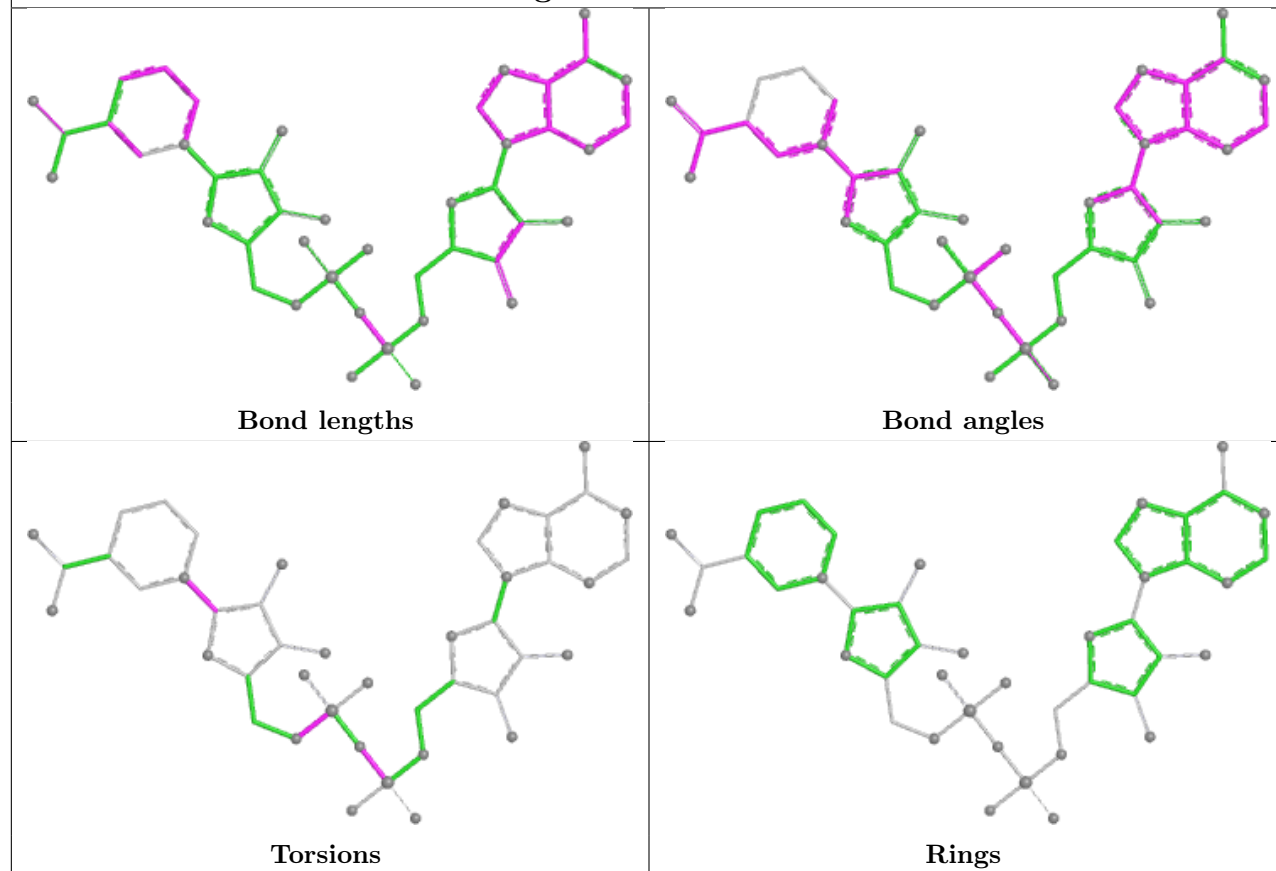
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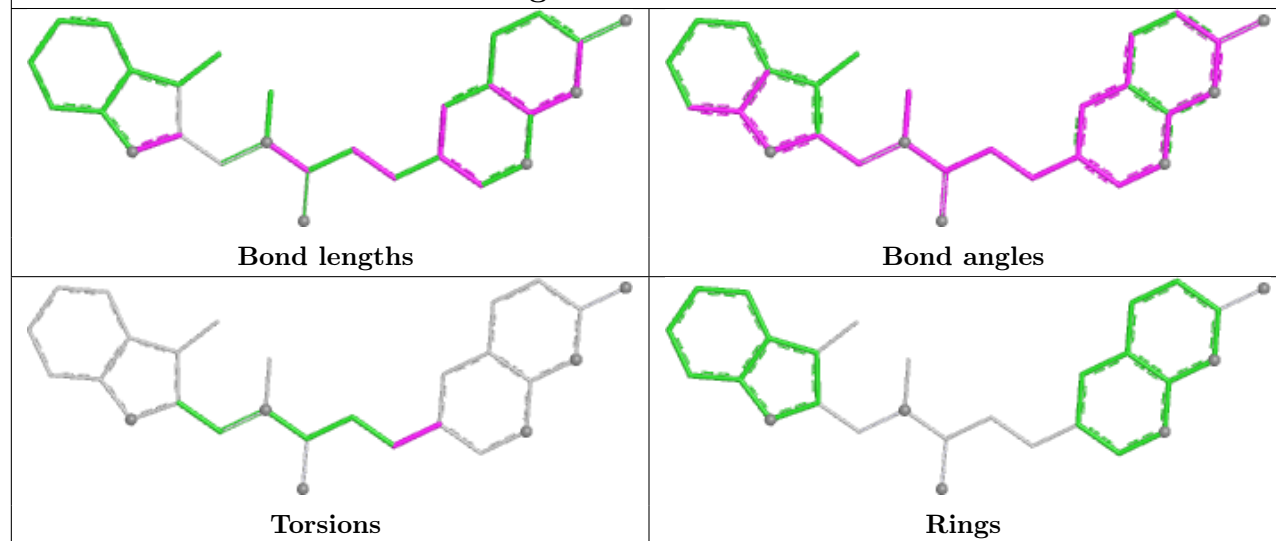
Ligand 0WE C 302

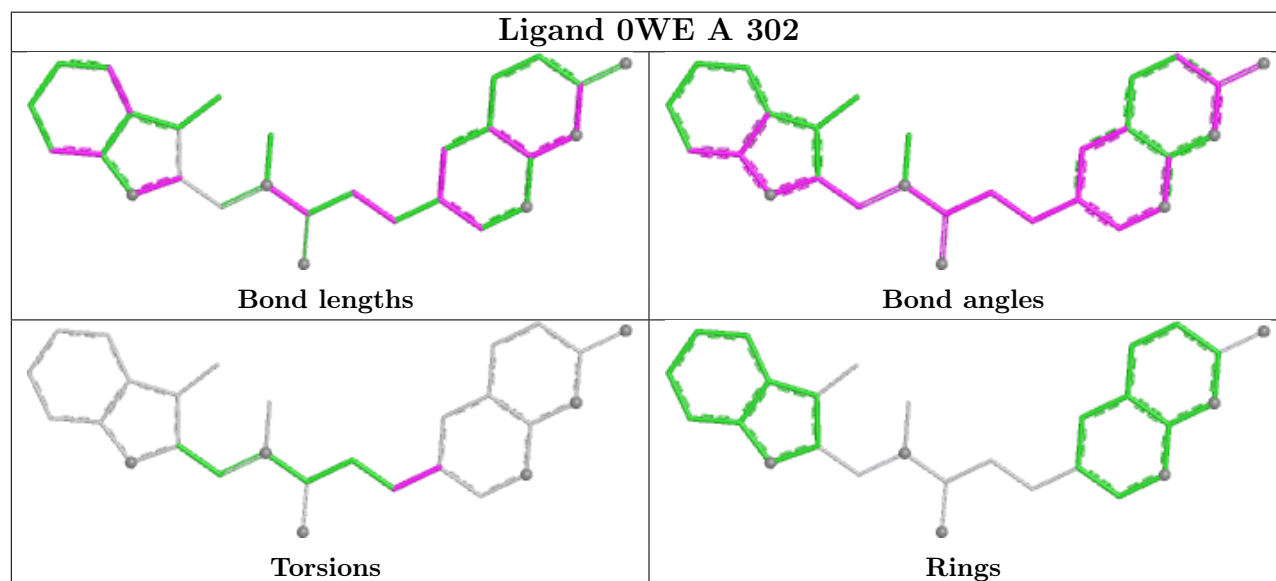
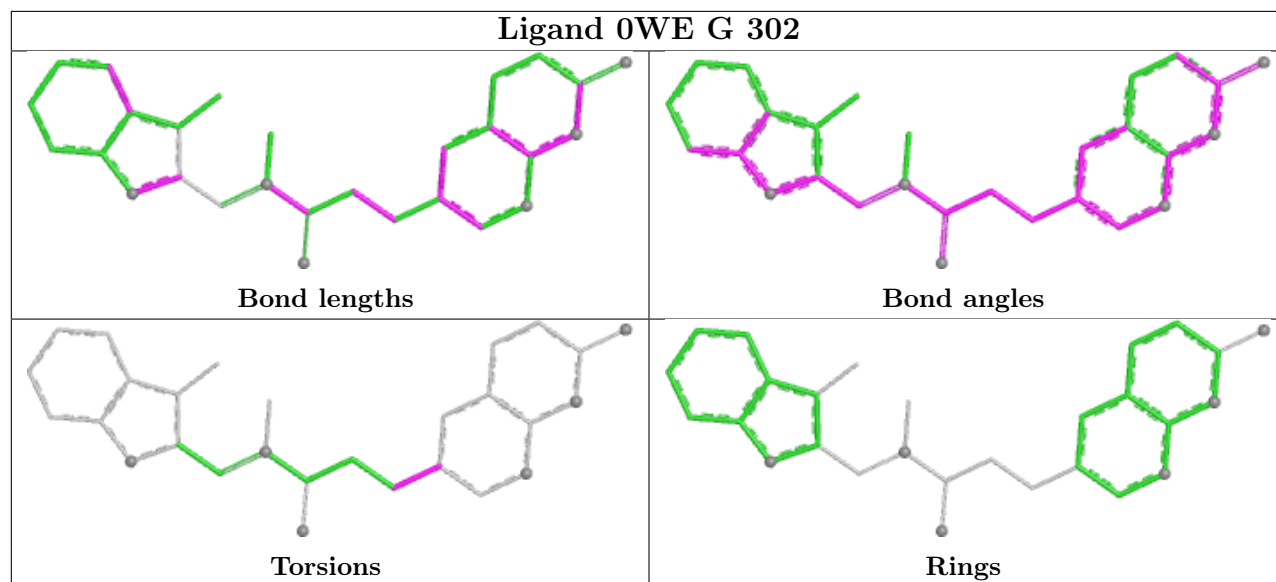


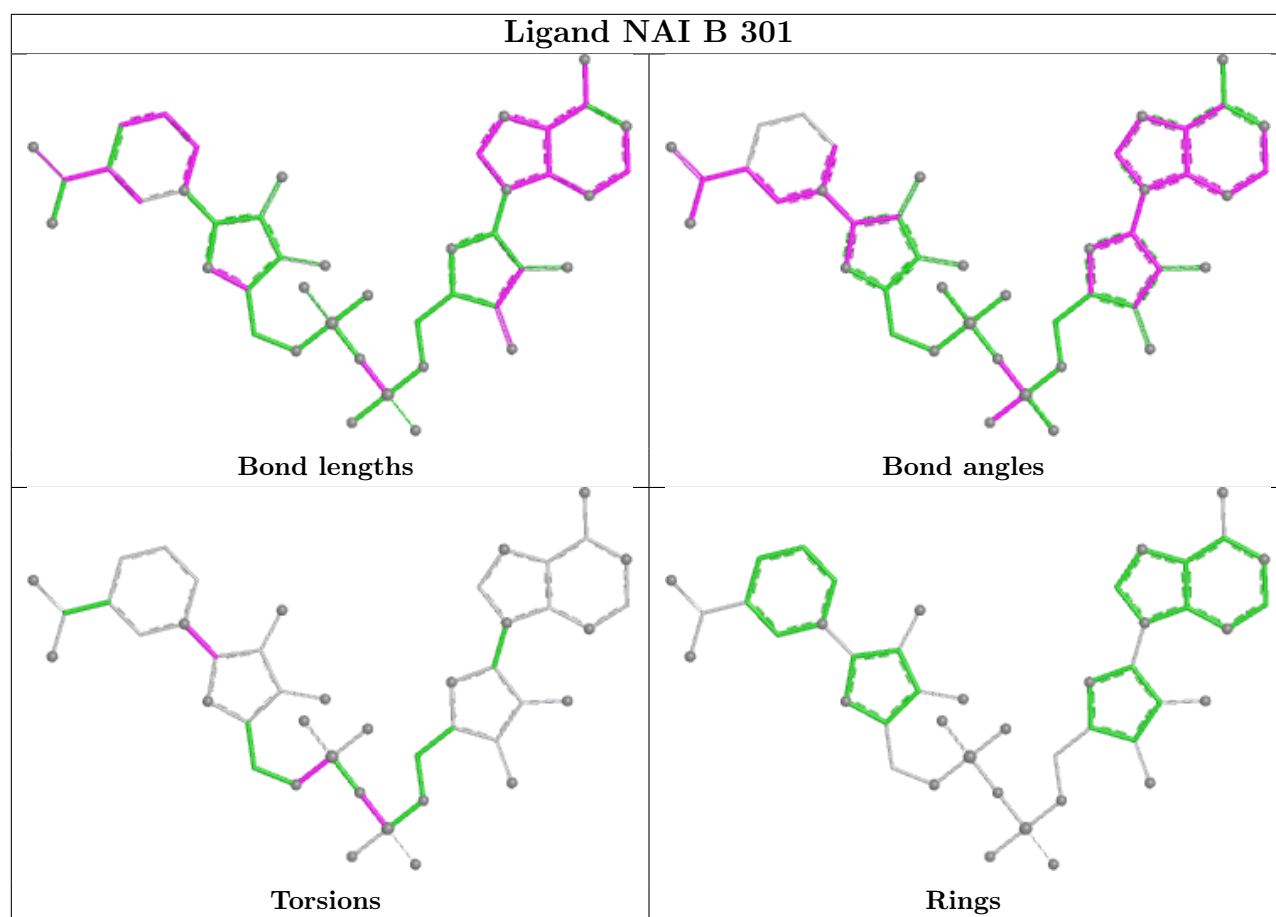
Ligand NAI D 301



Ligand OWE H 302







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, 95th 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 ²)	Q<0.9
1	A	295/298 (98%)	-1.23	0 100 100	13, 22, 41, 53	0
1	B	295/298 (98%)	-1.14	0 100 100	12, 24, 47, 64	0
1	C	295/298 (98%)	-1.21	0 100 100	12, 22, 42, 56	0
1	D	295/298 (98%)	-1.23	0 100 100	12, 22, 43, 58	0
1	E	295/298 (98%)	-1.14	0 100 100	11, 23, 46, 60	0
1	F	295/298 (98%)	-1.25	0 100 100	12, 22, 43, 57	0
1	G	295/298 (98%)	-1.23	0 100 100	13, 21, 43, 71	0
1	H	295/298 (98%)	-1.22	0 100 100	12, 22, 42, 55	0
All	All	2360/2384 (98%)	-1.21	0 100 100	11, 22, 44, 71	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

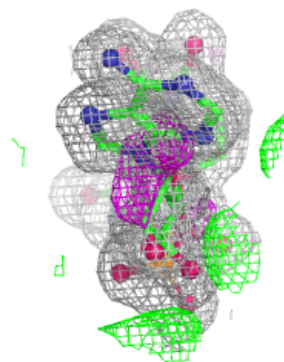
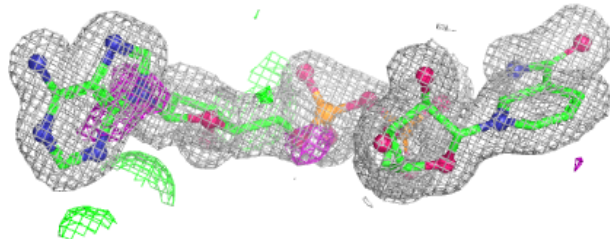
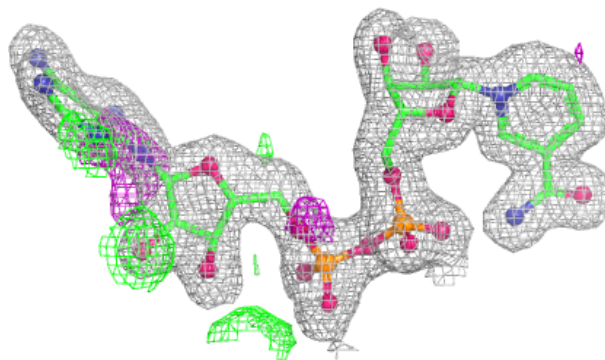
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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	NAI	A	301	44/44	0.99	0.03	13,19,27,35	0
2	NAI	B	301	44/44	0.99	0.03	14,24,31,37	0
2	NAI	C	301	44/44	0.99	0.03	13,20,30,31	0
2	NAI	D	301	44/44	0.99	0.03	14,22,28,32	0
2	NAI	E	301	44/44	0.99	0.03	14,23,28,35	0
2	NAI	F	301	44/44	0.99	0.03	11,20,29,32	0
3	0WE	A	302	28/28	0.99	0.03	17,23,30,34	0
3	0WE	B	302	28/28	0.99	0.02	14,23,29,33	0
3	0WE	C	302	28/28	0.99	0.03	16,22,31,34	0
3	0WE	D	302	28/28	0.99	0.03	16,22,28,40	0
3	0WE	E	302	28/28	0.99	0.03	16,23,28,34	0
3	0WE	F	302	28/28	0.99	0.03	14,21,34,38	0
3	0WE	G	302	28/28	0.99	0.03	17,21,26,39	0
3	0WE	H	302	28/28	0.99	0.03	14,23,30,36	0
2	NAI	G	301	44/44	1.00	0.02	11,21,29,31	0
2	NAI	H	301	44/44	1.00	0.02	10,20,27,29	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.

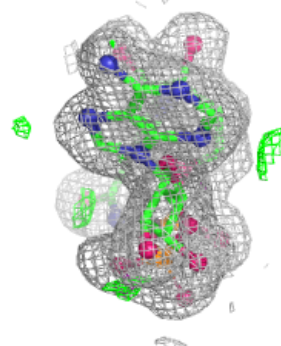
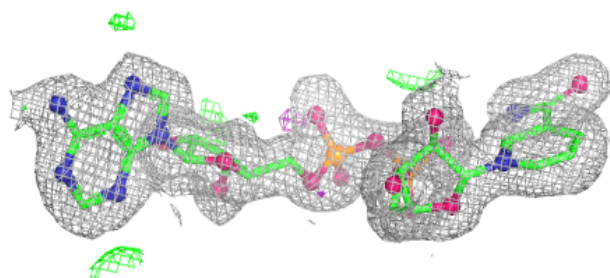
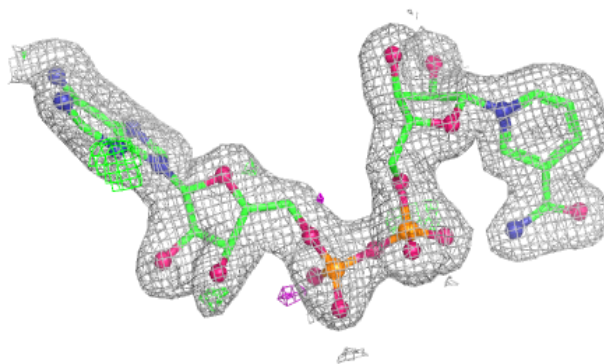
Electron density around NAI A 301:

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

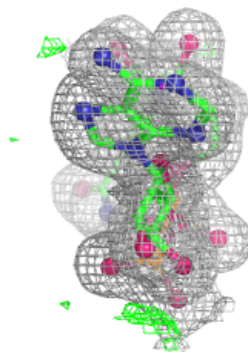
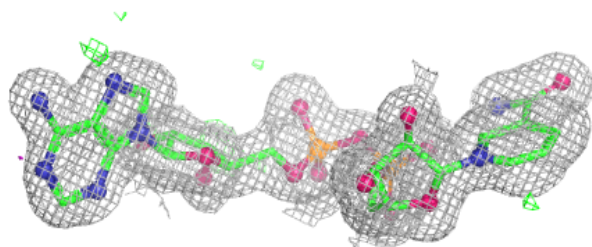
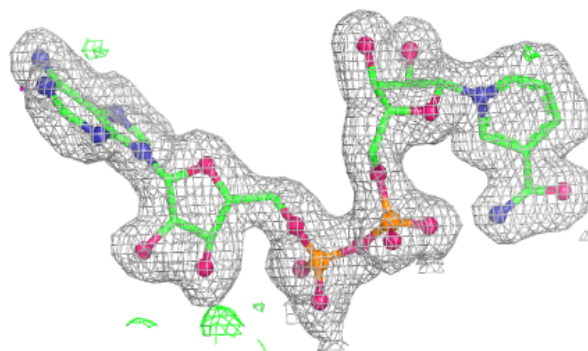


Electron density around NAI B 301:

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

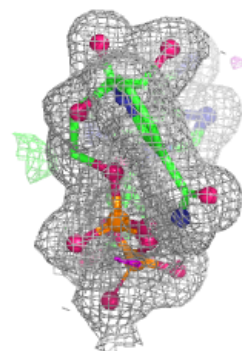
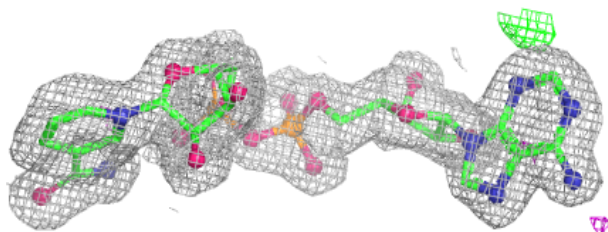
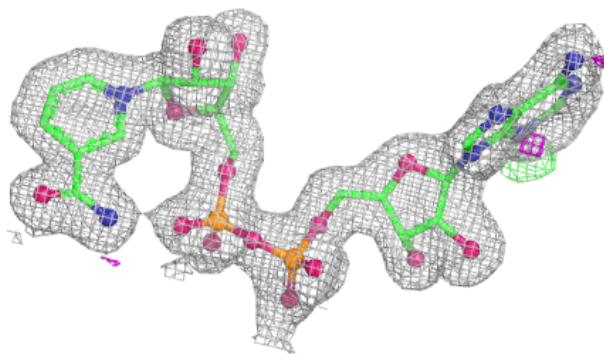
**Electron density around NAI C 301:**

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

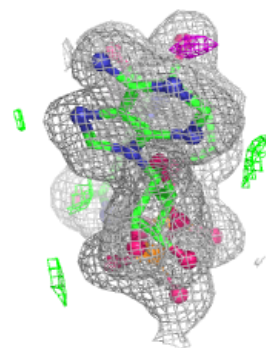
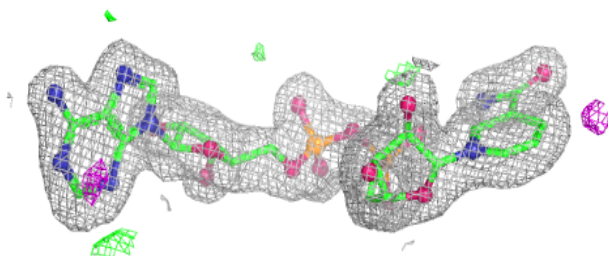
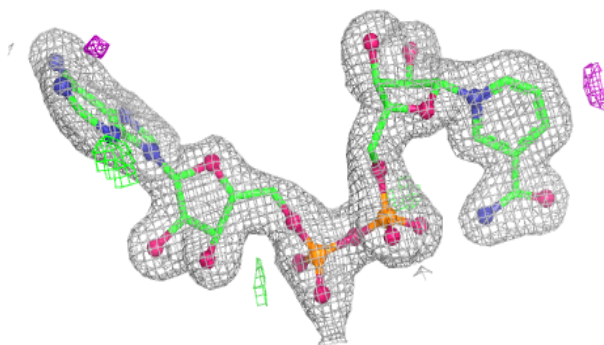


Electron density around NAI D 301:

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

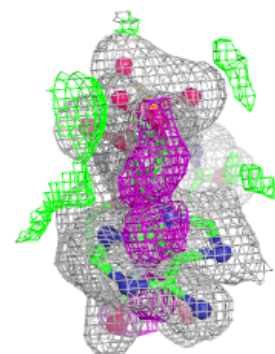
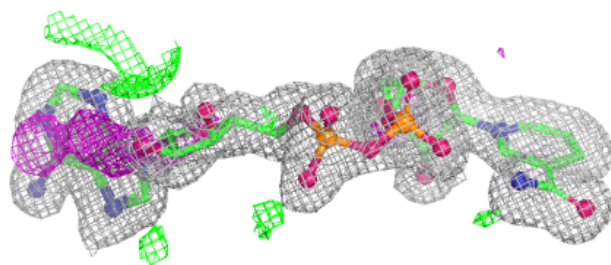
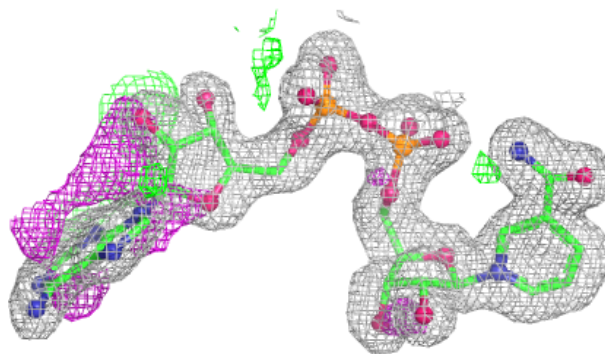
**Electron density around NAI E 301:**

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

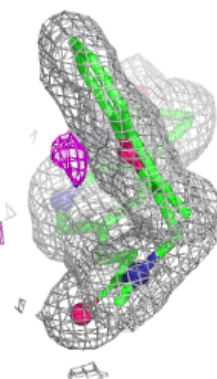
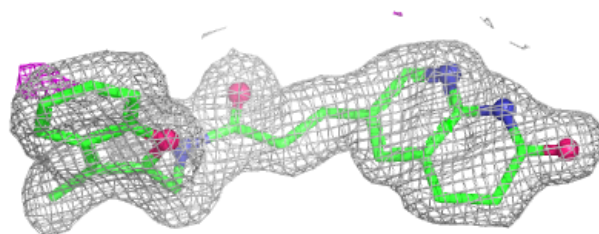
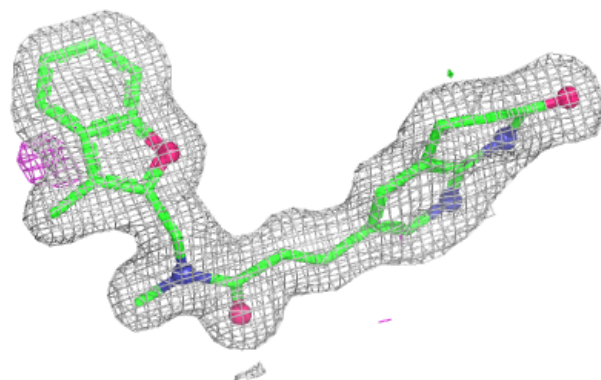


Electron density around NAI F 301:

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

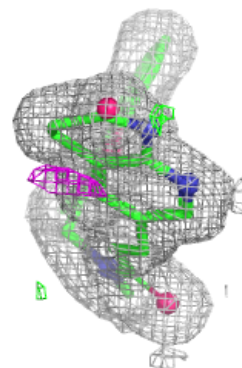
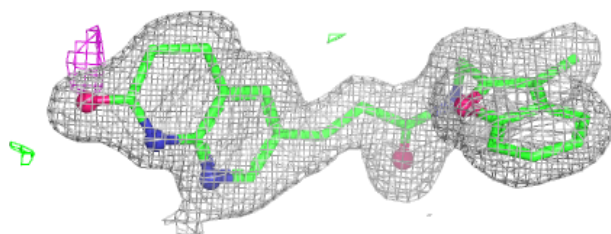
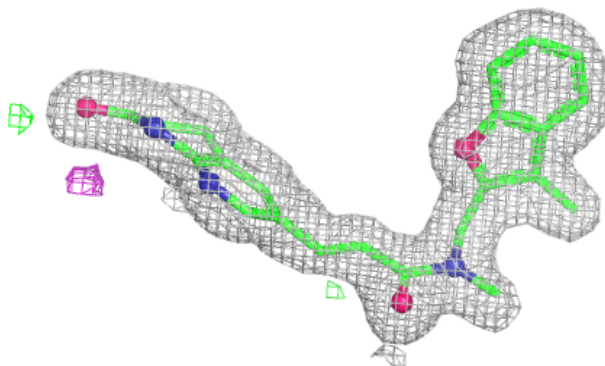
**Electron density around 0WE A 302:**

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

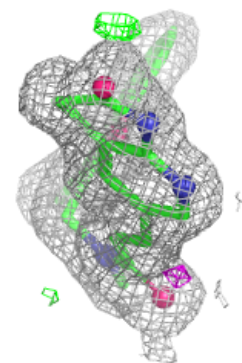
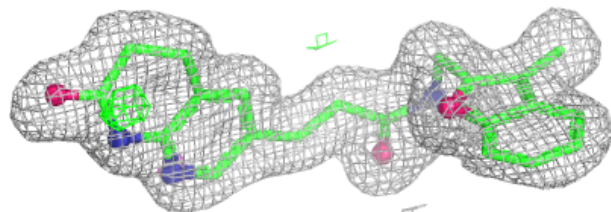
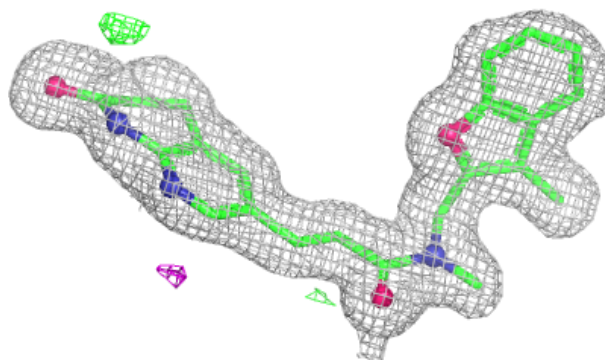


Electron density around 0WE B 302:

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

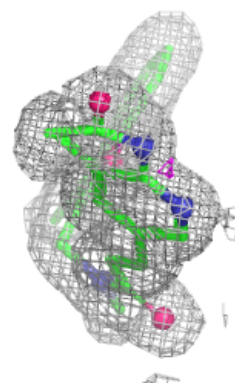
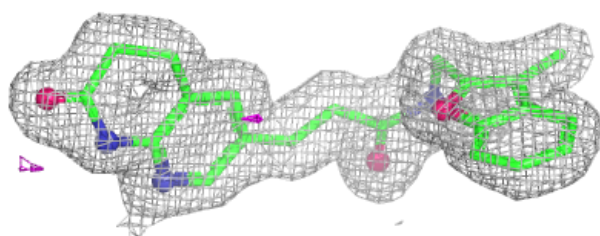
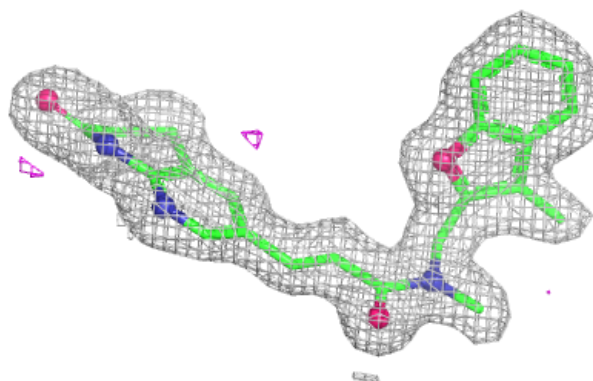
**Electron density around 0WE C 302:**

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

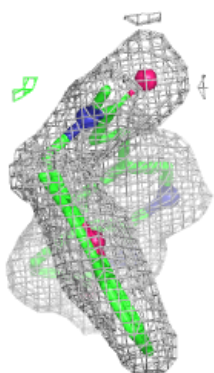
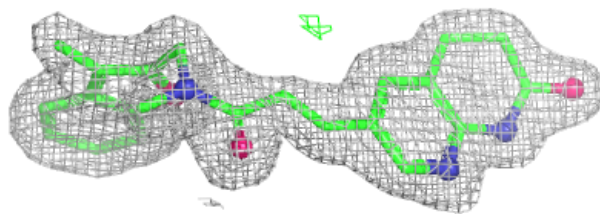
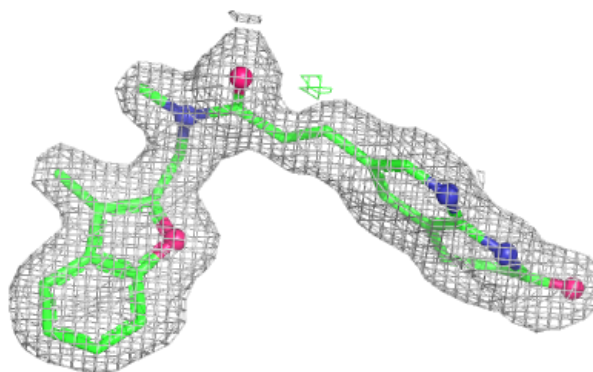


Electron density around 0WE D 302:

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

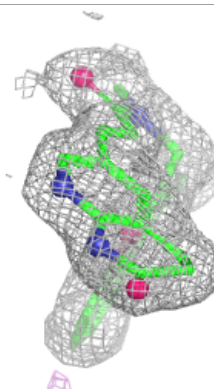
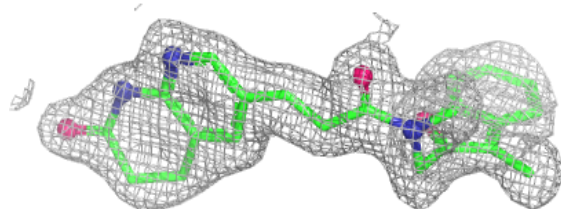
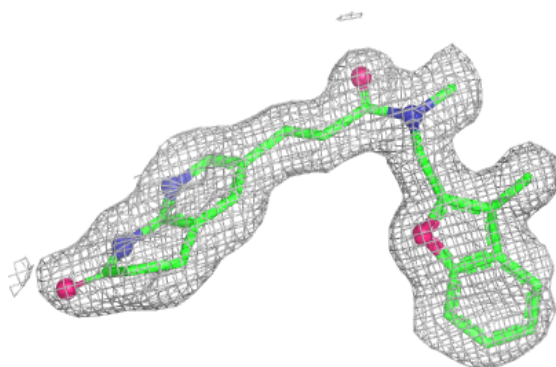
**Electron density around 0WE E 302:**

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

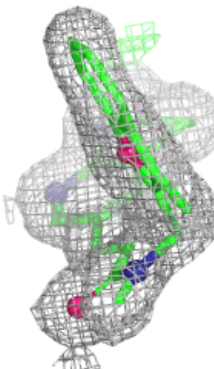
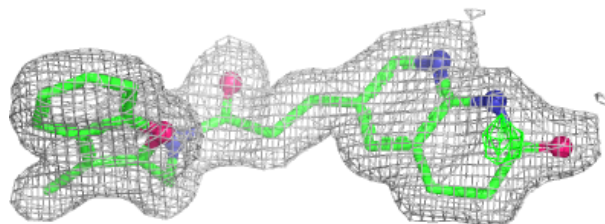
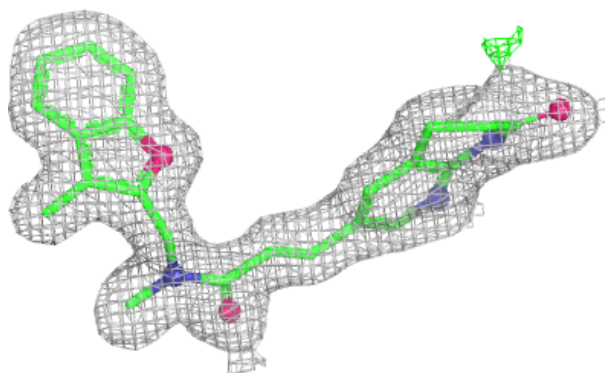


Electron density around 0WE F 302:

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

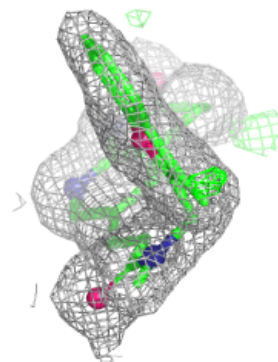
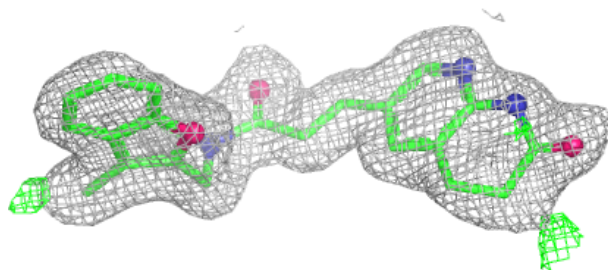
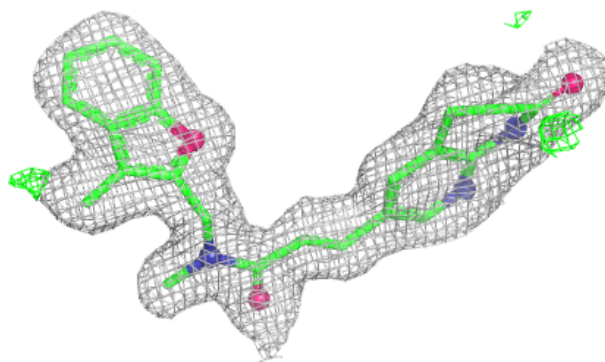
**Electron density around 0WE G 302:**

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

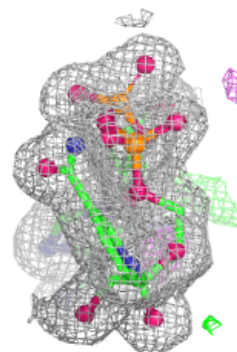
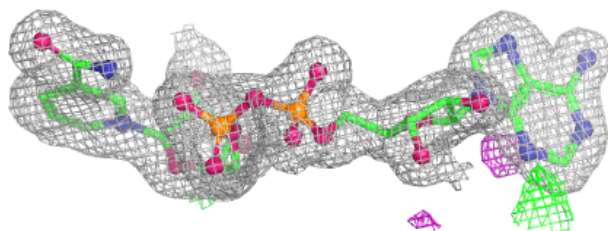
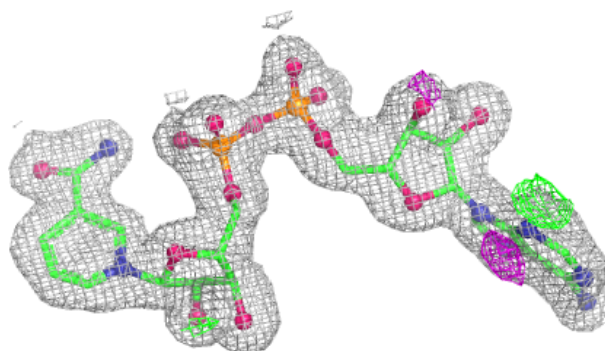


Electron density around OWE H 302:

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

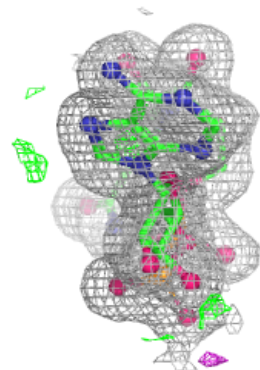
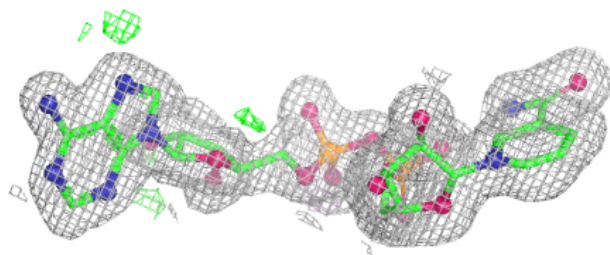
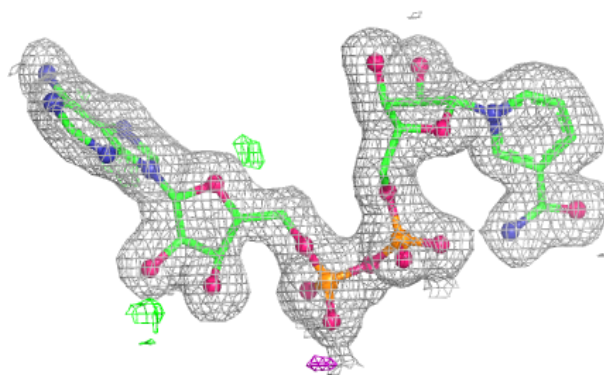
**Electron density around NAI G 301:**

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



Electron density around NAI H 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.