



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 10:25 am BST

PDB ID : 2IRW
Title : Human 11-beta-Hydroxysteroid Dehydrogenase (HSD1) with NADP and Adamantane Ether Inhibitor
Authors : Longenecker, K.L.; Patel, J.R.; Russell, J.; Qin, W.
Deposited on : 2006-10-16
Resolution : 3.10 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

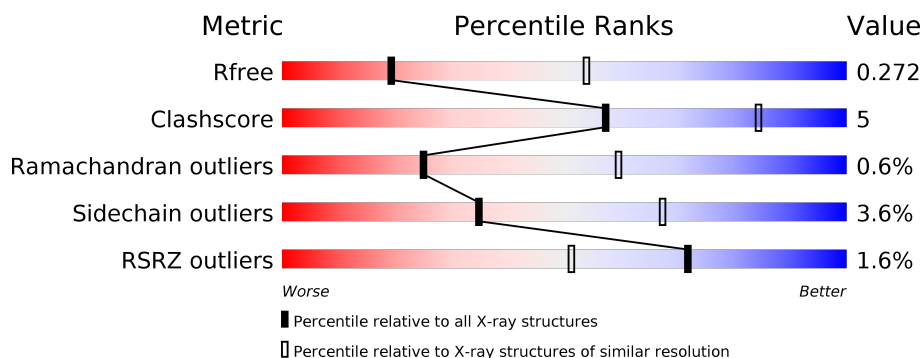
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	264	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>9%</div> <div>.</div> </div> </div>
1	B	264	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>11%</div> </div> </div>
1	C	264	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>.</div> </div> </div>
1	D	264	<div> <div>4%</div> <div> <div></div> <div>87%</div> <div>13%</div> </div> </div>
1	E	264	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>..</div> </div> </div>
1	F	264	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>15%</div> <div>.</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	264	<div><div></div><div>86%</div><div>13%</div><div></div></div>
1	H	264	<div>%<div><div></div><div>80%</div><div>18%</div><div></div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16728 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 Corticosteroid 11-beta-dehydrogenase isozyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2031	1296	344	375	16			
1	B	264	Total	C	N	O	S	0	0	0
			2031	1296	344	375	16			
1	C	257	Total	C	N	O	S	0	0	0
			1967	1256	333	363	15			
1	D	264	Total	C	N	O	S	0	0	0
			2031	1296	344	375	16			
1	E	257	Total	C	N	O	S	0	0	0
			1967	1256	333	363	15			
1	F	264	Total	C	N	O	S	0	0	0
			2031	1296	344	375	16			
1	G	264	Total	C	N	O	S	0	0	0
			2031	1296	344	375	16			
1	H	264	Total	C	N	O	S	0	0	0
			2031	1296	344	375	16			

There are 8 discrepancies between the modelled and reference sequences:

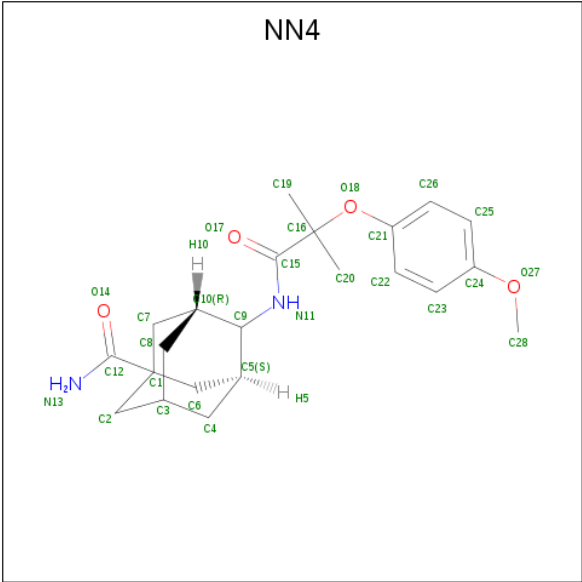
Chain	Residue	Modelled	Actual	Comment	Reference
A	272	SER	CYS	CONFLICT	UNP P28845
B	272	SER	CYS	CONFLICT	UNP P28845
C	272	SER	CYS	CONFLICT	UNP P28845
D	272	SER	CYS	CONFLICT	UNP P28845
E	272	SER	CYS	CONFLICT	UNP P28845
F	272	SER	CYS	CONFLICT	UNP P28845
G	272	SER	CYS	CONFLICT	UNP P28845
H	272	SER	CYS	CONFLICT	UNP P28845

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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

- Molecule 3 is (1S,3R,4S,5S,7S)-4-{[2-(4-METHOXYPHENOXY)-2-METHYLPROPAN OYL]AMINO} ADAMANTANE-1-CARBOXAMIDE (three-letter code: NN4) (formula: C₂₂H₃₀N₂O₄).

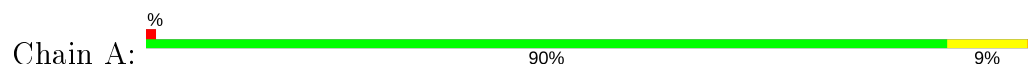


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			28	22	2	4		
3	B	1	Total	C	N	O	0	0
			28	22	2	4		
3	C	1	Total	C	N	O	0	0
			28	22	2	4		
3	D	1	Total	C	N	O	0	0
			28	22	2	4		
3	E	1	Total	C	N	O	0	0
			28	22	2	4		
3	F	1	Total	C	N	O	0	0
			28	22	2	4		
3	G	1	Total	C	N	O	0	0
			28	22	2	4		
3	H	1	Total	C	N	O	0	0
			28	22	2	4		

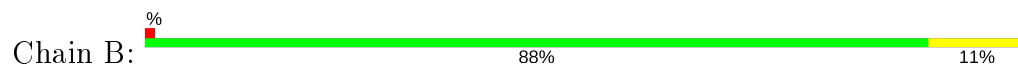
3 Residue-property plots [i](#)

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

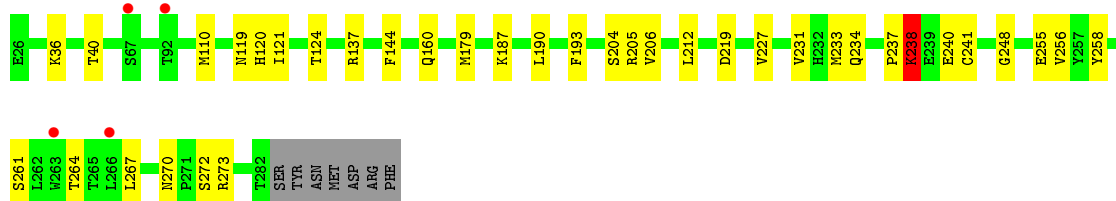
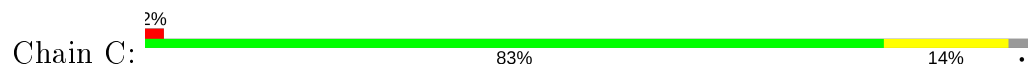
- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1



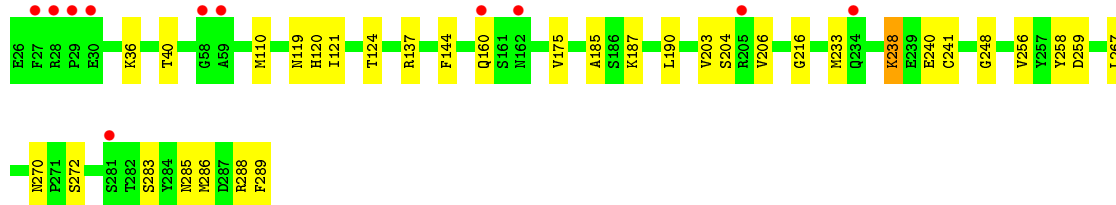
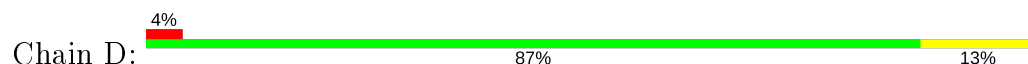
- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1



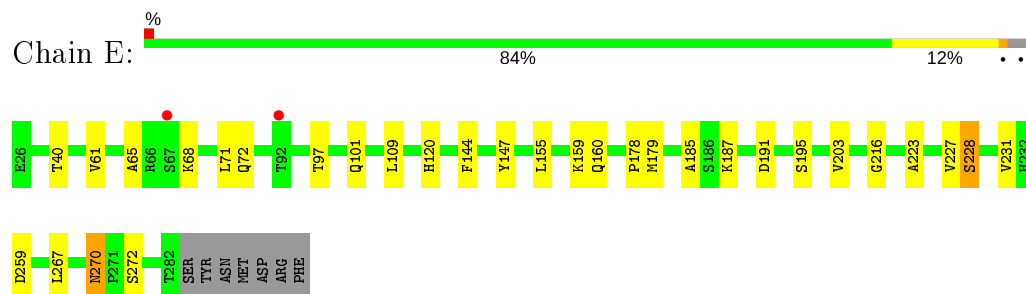
- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1



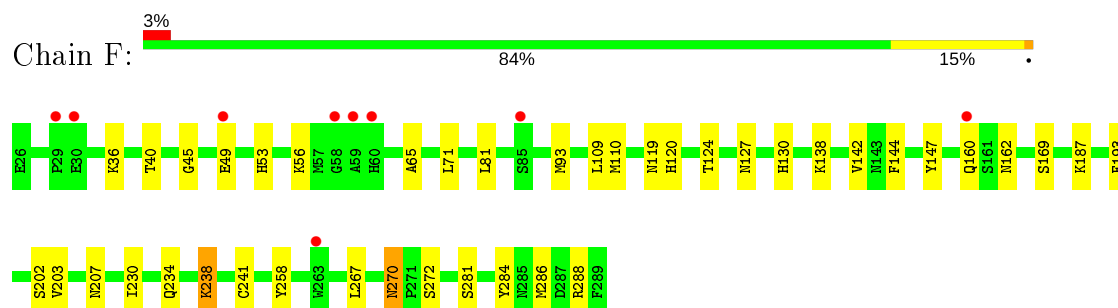
- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1



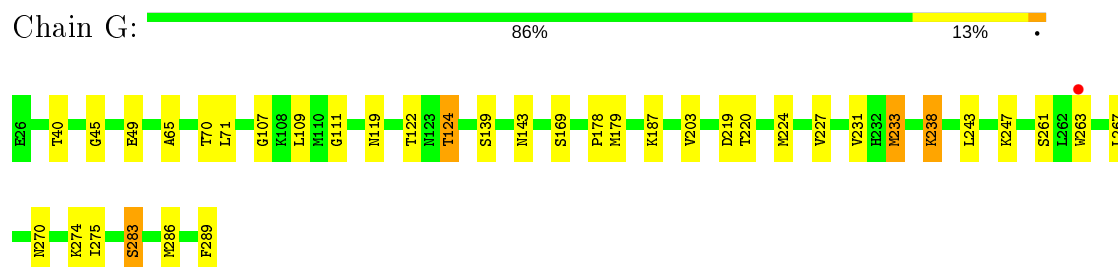
- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1



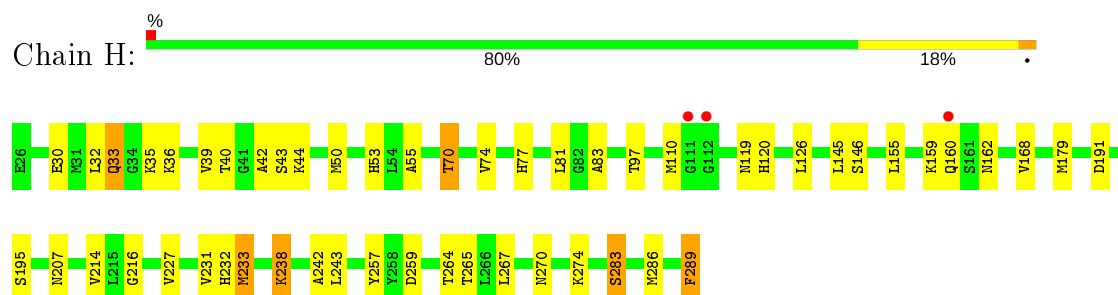
- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1



- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1



- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	184.54Å 184.54Å 558.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	182.57 – 3.10 48.35 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (182.57-3.10) 100.0 (48.35-3.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.99 (at 3.12Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.237 , 0.278 0.230 , 0.272	Depositor DCC
R_{free} test set	3377 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	51.5	Xtrriage
Anisotropy	0.537	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 20.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16728	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.27 % 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 8.8108e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: NAP, NN4

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	0.62	2/2066 (0.1%)	0.56	0/2788
1	B	0.65	2/2066 (0.1%)	0.57	0/2788
1	C	0.62	1/2000 (0.1%)	0.56	0/2700
1	D	0.64	2/2066 (0.1%)	0.55	0/2788
1	E	0.70	1/2000 (0.1%)	0.58	0/2700
1	F	0.56	1/2066 (0.0%)	0.57	0/2788
1	G	0.74	2/2066 (0.1%)	0.60	1/2788 (0.0%)
1	H	0.52	1/2066 (0.0%)	0.60	0/2788
All	All	0.63	12/16396 (0.1%)	0.58	1/22128 (0.0%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	238	LYS	CE-NZ	25.34	2.12	1.49
1	E	238	LYS	CE-NZ	23.19	2.07	1.49
1	B	238	LYS	CE-NZ	19.66	1.98	1.49
1	A	238	LYS	CE-NZ	19.47	1.97	1.49
1	D	238	LYS	CE-NZ	18.95	1.96	1.49
1	C	238	LYS	CE-NZ	18.76	1.96	1.49
1	F	238	LYS	CE-NZ	14.47	1.85	1.49
1	H	238	LYS	CE-NZ	8.74	1.71	1.49
1	B	238	LYS	CD-CE	7.24	1.69	1.51
1	G	238	LYS	CD-CE	6.49	1.67	1.51
1	A	238	LYS	CD-CE	5.79	1.65	1.51
1	D	238	LYS	CD-CE	5.76	1.65	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	238	LYS	CD-CE-NZ	-5.17	99.82	111.70

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	2031	0	2075	14	0
1	B	2031	0	2075	17	0
1	C	1967	0	2020	24	0
1	D	2031	0	2075	21	0
1	E	1967	0	2020	23	0
1	F	2031	0	2075	28	0
1	G	2031	0	2075	23	0
1	H	2031	0	2075	36	0
2	A	48	0	25	0	0
2	B	48	0	25	0	0
2	C	48	0	25	2	0
2	D	48	0	25	3	0
2	E	48	0	25	1	0
2	F	48	0	25	3	0
2	G	48	0	25	1	0
2	H	48	0	25	0	0
3	A	28	0	30	0	0
3	B	28	0	30	0	0
3	C	28	0	30	0	0
3	D	28	0	30	0	0
3	E	28	0	30	0	0
3	F	28	0	30	0	0
3	G	28	0	30	1	0
3	H	28	0	30	0	0
All	All	16728	0	16930	164	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (164) 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:H:238:LYS:NZ	1:H:238:LYS:CE	1.70	1.50
1:F:238:LYS:NZ	1:F:238:LYS:CE	1.85	1.39
1:A:238:LYS:NZ	1:A:238:LYS:CE	1.97	1.27
1:C:238:LYS:NZ	1:C:238:LYS:CE	1.95	1.27
1:D:238:LYS:NZ	1:D:238:LYS:CE	1.96	1.27
1:B:238:LYS:CE	1:B:238:LYS:NZ	1.98	1.25
1:E:238:LYS:NZ	1:E:238:LYS:CE	2.07	1.17
1:G:238:LYS:NZ	1:G:238:LYS:CE	2.12	1.11
1:H:232:HIS:HB2	1:H:233:MET:SD	2.21	0.79
1:H:162:ASN:OD1	1:H:207:ASN:HB3	1.83	0.78
1:H:233:MET:SD	1:H:233:MET:N	2.59	0.75
1:B:233:MET:N	1:B:233:MET:SD	2.61	0.74
1:A:233:MET:SD	1:A:233:MET:N	2.63	0.71
1:E:228:SER:HB2	1:G:219:ASP:OD1	1.92	0.69
1:G:233:MET:SD	1:G:233:MET:N	2.66	0.67
1:F:241:CYS:HB2	1:F:258:TYR:CE1	2.30	0.66
1:G:179:MET:HE1	1:H:289:PHE:HE1	1.65	0.62
1:E:227:VAL:HB	1:E:231:VAL:HB	1.81	0.62
1:D:203:VAL:HG11	1:D:286:MET:HG3	1.80	0.62
1:G:178:PRO:HB2	1:H:286:MET:HE1	1.82	0.61
1:F:93:MET:HG3	1:F:120:HIS:CE1	2.35	0.61
1:E:179:MET:SD	1:F:286:MET:CE	2.89	0.60
1:B:232:HIS:HB2	1:B:233:MET:SD	2.41	0.60
1:G:227:VAL:HB	1:G:231:VAL:HB	1.83	0.59
1:A:232:HIS:HB2	1:A:233:MET:SD	2.42	0.58
1:H:126:LEU:HB3	1:H:179:MET:HE2	1.86	0.57
1:E:179:MET:SD	1:F:286:MET:HE2	2.44	0.57
1:D:241:CYS:HB2	1:D:258:TYR:CE1	2.39	0.57
1:B:162:ASN:OD1	1:B:207:ASN:HB3	2.06	0.56
1:G:139:SER:O	1:G:143:ASN:HB2	2.04	0.56
1:E:97:THR:O	1:E:101:GLN:HB2	2.05	0.56
1:H:50:MET:HG3	1:H:242:ALA:HB1	1.87	0.56
1:A:227:VAL:HB	1:A:231:VAL:HB	1.89	0.55
1:H:36:LYS:HG2	1:H:110:MET:HB3	1.88	0.55
1:B:119:ASN:HD22	1:B:168:VAL:HG21	1.70	0.55
1:H:119:ASN:HD22	1:H:168:VAL:HG21	1.72	0.55
1:C:204:SER:HB2	1:C:206:VAL:HG23	1.87	0.55
1:G:169:SER:HA	1:G:187:LYS:HD2	1.90	0.54
1:E:185:ALA:HB2	1:F:193:PHE:HB2	1.88	0.54
1:E:178:PRO:O	1:E:179:MET:HB2	2.08	0.54
1:H:232:HIS:CB	1:H:233:MET:SD	2.96	0.54
1:F:119:ASN:ND2	2:F:901:NAP:H4D	2.24	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:MET:SD	1:D:286:MET:HE2	2.48	0.53
1:E:155:LEU:HG	1:E:159:LYS:HE2	1.91	0.53
1:E:267:LEU:O	1:F:272:SER:HB3	2.07	0.53
1:D:288:ARG:HG3	1:D:289:PHE:CE1	2.44	0.53
1:E:40:THR:OG1	1:E:120:HIS:HD2	1.92	0.52
1:F:203:VAL:HG21	1:F:286:MET:HG3	1.89	0.52
1:D:248:GLY:HA3	1:D:256:VAL:HG21	1.92	0.52
1:B:227:VAL:HB	1:B:231:VAL:HB	1.91	0.52
1:F:45:GLY:HA3	2:F:901:NAP:O2N	2.10	0.51
1:H:216:GLY:HA3	1:H:259:ASP:OD2	2.10	0.51
1:G:178:PRO:O	1:G:179:MET:HB2	2.11	0.50
1:E:223:ALA:O	1:E:227:VAL:HG22	2.11	0.50
1:H:227:VAL:HB	1:H:231:VAL:HB	1.92	0.50
1:H:231:VAL:HG12	1:H:232:HIS:H	1.75	0.50
1:H:43:SER:O	1:H:44:LYS:HB3	2.11	0.50
1:A:40:THR:O	1:A:119:ASN:HB3	2.12	0.50
1:F:138:LYS:O	1:F:142:VAL:HG23	2.12	0.50
1:G:261:SER:OG	1:G:263:TRP:HB2	2.12	0.49
1:H:36:LYS:HD3	1:H:110:MET:O	2.12	0.49
1:F:49:GLU:O	1:F:53:HIS:HD2	1.96	0.49
1:C:248:GLY:HA3	1:C:256:VAL:HG21	1.95	0.49
1:D:204:SER:HB2	1:D:206:VAL:HG23	1.94	0.48
1:H:238:LYS:NZ	1:H:238:LYS:CD	2.70	0.48
1:F:162:ASN:OD1	1:F:207:ASN:HB3	2.12	0.48
1:E:272:SER:HB3	1:F:267:LEU:O	2.14	0.48
1:F:241:CYS:HB2	1:F:258:TYR:HE1	1.76	0.48
1:C:261:SER:HB3	1:C:264:THR:OG1	2.13	0.48
1:G:179:MET:HE1	1:H:289:PHE:CE1	2.47	0.47
1:A:119:ASN:HD22	1:A:168:VAL:HG21	1.79	0.47
1:E:216:GLY:HA3	1:E:259:ASP:OD2	2.14	0.47
1:C:205:ARG:HB3	1:F:230:ILE:HG23	1.97	0.47
1:G:49:GLU:HG3	1:G:238:LYS:HG3	1.97	0.47
1:C:267:LEU:O	1:D:272:SER:HB3	2.14	0.47
1:C:179:MET:SD	1:D:286:MET:CE	3.03	0.46
1:G:220:THR:O	1:G:224:MET:HG2	2.16	0.46
1:C:227:VAL:HB	1:C:231:VAL:HB	1.96	0.46
1:E:270:ASN:C	1:E:270:ASN:HD22	2.19	0.46
1:D:119:ASN:ND2	2:D:901:NAP:H4D	2.31	0.46
1:F:270:ASN:HD21	1:F:272:SER:HB2	1.79	0.46
1:C:241:CYS:HB2	1:C:258:TYR:CE1	2.51	0.46
1:D:40:THR:OG1	1:D:120:HIS:HD2	1.99	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:ARG:HG3	1:D:175:VAL:HG12	1.97	0.46
1:C:193:PHE:HB2	1:D:185:ALA:HB2	1.98	0.45
1:F:49:GLU:O	1:F:53:HIS:CD2	2.69	0.45
1:B:36:LYS:HG2	1:B:110:MET:HB3	1.99	0.45
1:H:231:VAL:HG12	1:H:232:HIS:N	2.31	0.45
1:H:55:ALA:HA	1:H:83:ALA:HB2	1.98	0.45
1:E:187:LYS:HE3	2:E:901:NAP:O2D	2.16	0.45
1:H:214:VAL:HB	1:H:257:TYR:HD2	1.82	0.45
1:A:232:HIS:HB3	1:C:234:GLN:NE2	2.31	0.45
1:F:36:LYS:HG2	1:F:110:MET:HB3	1.99	0.45
1:F:187:LYS:HE3	2:F:901:NAP:O2D	2.17	0.45
1:B:216:GLY:HA3	1:B:259:ASP:OD2	2.17	0.45
1:E:65:ALA:H	1:E:71:LEU:HD11	1.81	0.45
1:E:144:PHE:O	1:E:147:TYR:HB2	2.17	0.45
1:H:191:ASP:O	1:H:195:SER:HB2	2.17	0.45
1:C:205:ARG:HD3	1:F:230:ILE:O	2.17	0.45
1:F:40:THR:OG1	1:F:120:HIS:HD2	2.00	0.44
1:A:162:ASN:OD1	1:A:207:ASN:HB3	2.17	0.44
1:B:231:VAL:HG12	1:B:232:HIS:N	2.33	0.44
1:H:39:VAL:HG12	1:H:42:ALA:HB2	1.99	0.44
1:E:191:ASP:O	1:E:195:SER:HB2	2.18	0.44
1:E:68:LYS:O	1:E:72:GLN:HG3	2.18	0.44
1:C:219:ASP:OD1	1:C:237:PRO:HA	2.18	0.44
1:A:280:TYR:HH	1:B:264:THR:HG1	1.62	0.43
1:H:53:HIS:ND1	1:H:243:LEU:HD13	2.33	0.43
1:F:281:SER:HA	1:F:284:TYR:CZ	2.52	0.43
1:D:40:THR:O	1:D:119:ASN:HB3	2.19	0.43
1:H:155:LEU:HG	1:H:159:LYS:HE3	1.99	0.43
1:C:40:THR:O	1:C:119:ASN:HB3	2.19	0.43
1:G:107:GLY:O	1:G:111:GLY:N	2.51	0.43
1:C:212:LEU:O	1:C:255:GLU:HA	2.19	0.43
1:G:178:PRO:CB	1:H:286:MET:HE1	2.48	0.43
1:E:65:ALA:N	1:E:71:LEU:HD11	2.33	0.43
1:G:40:THR:O	1:G:119:ASN:HB3	2.19	0.43
1:G:45:GLY:HA2	1:G:238:LYS:NZ	2.34	0.43
1:G:203:VAL:HG21	1:G:286:MET:HG3	2.01	0.43
1:E:179:MET:SD	1:F:286:MET:HE1	2.59	0.43
1:H:126:LEU:CB	1:H:179:MET:HE2	2.48	0.43
1:H:53:HIS:CE1	1:H:243:LEU:HB2	2.54	0.43
1:C:144:PHE:HD1	1:C:190:LEU:HD23	1.84	0.42
1:G:187:LYS:HE3	2:G:901:NAP:O2D	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:MET:HG3	1:D:286:MET:HE1	1.99	0.42
1:B:169:SER:HA	1:B:187:LYS:HD2	2.00	0.42
1:D:187:LYS:HE3	2:D:901:NAP:O2D	2.20	0.42
1:A:178:PRO:O	1:A:179:MET:HB2	2.19	0.42
1:C:121:ILE:HG12	2:C:901:NAP:H3D	2.02	0.42
1:A:169:SER:HA	1:A:187:LYS:HD2	2.02	0.42
1:D:216:GLY:HA3	1:D:259:ASP:OD2	2.19	0.42
1:F:65:ALA:N	1:F:71:LEU:HD11	2.34	0.42
1:H:40:THR:CB	1:H:120:HIS:HD2	2.33	0.42
1:H:264:THR:O	1:H:265:THR:C	2.58	0.42
1:F:56:LYS:HE3	1:F:81:LEU:HD22	2.02	0.42
1:A:231:VAL:HG12	1:A:232:HIS:N	2.35	0.42
1:A:40:THR:CB	1:A:120:HIS:HD2	2.33	0.42
1:D:36:LYS:HG2	1:D:110:MET:HB3	2.01	0.42
1:C:187:LYS:HE3	2:C:901:NAP:O2D	2.20	0.42
1:F:169:SER:HA	1:F:187:LYS:HD2	2.02	0.42
1:H:70:THR:O	1:H:74:VAL:HG23	2.20	0.41
1:H:77:HIS:CD2	1:H:81:LEU:HD11	2.55	0.41
1:H:120:HIS:HE1	1:H:146:SER:OG	2.03	0.41
1:B:40:THR:O	1:B:119:ASN:HB3	2.20	0.41
1:H:32:LEU:HA	1:H:35:LYS:HG3	2.02	0.41
1:B:36:LYS:HA	1:B:60:HIS:HB2	2.02	0.41
1:G:203:VAL:HG21	1:G:286:MET:HE3	2.03	0.41
1:D:144:PHE:HD1	1:D:190:LEU:HD23	1.85	0.41
1:G:65:ALA:H	1:G:71:LEU:HD11	1.86	0.41
1:B:31:MET:O	1:B:35:LYS:HE2	2.21	0.41
1:H:36:LYS:HB3	1:H:110:MET:SD	2.61	0.41
1:A:286:MET:CE	1:B:179:MET:SD	3.09	0.41
1:E:231:VAL:HG12	1:E:233:MET:HG2	2.03	0.41
1:C:40:THR:OG1	1:C:120:HIS:HD2	2.04	0.41
3:G:911:NN4:H23	3:G:911:NN4:H283	1.72	0.40
1:C:36:LYS:HG2	1:C:110:MET:HB3	2.04	0.40
1:F:144:PHE:O	1:F:147:TYR:HB2	2.22	0.40
1:G:122:THR:O	1:G:124:THR:HG22	2.22	0.40
1:H:30:GLU:O	1:H:33:GLN:HB2	2.22	0.40
1:B:40:THR:OG1	1:B:120:HIS:HD2	2.04	0.40
1:C:272:SER:HB3	1:D:267:LEU:O	2.22	0.40
1:B:40:THR:CB	1:B:120:HIS:HD2	2.35	0.40
1:D:121:ILE:HG12	2:D:901:NAP:H3D	2.03	0.40
1:G:243:LEU:HG	1:G:247:LYS:HE3	2.04	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	262/264 (99%)	247 (94%)	12 (5%)	3 (1%)	14	46
1	B	262/264 (99%)	244 (93%)	16 (6%)	2 (1%)	19	54
1	C	255/264 (97%)	243 (95%)	11 (4%)	1 (0%)	34	69
1	D	262/264 (99%)	251 (96%)	10 (4%)	1 (0%)	34	69
1	E	255/264 (97%)	242 (95%)	13 (5%)	0	100	100
1	F	262/264 (99%)	249 (95%)	13 (5%)	0	100	100
1	G	262/264 (99%)	245 (94%)	14 (5%)	3 (1%)	14	46
1	H	262/264 (99%)	233 (89%)	27 (10%)	2 (1%)	19	54
All	All	2082/2112 (99%)	1954 (94%)	116 (6%)	12 (1%)	25	59

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	LEU
1	B	267	LEU
1	G	283	SER
1	H	283	SER
1	A	283	SER
1	B	283	SER
1	D	233	MET
1	G	267	LEU
1	H	267	LEU
1	C	233	MET
1	G	233	MET
1	A	287	ASP

5.3.2 Protein sidechains

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	221/221 (100%)	213 (96%)	8 (4%)	35	67
1	B	221/221 (100%)	212 (96%)	9 (4%)	30	64
1	C	214/221 (97%)	208 (97%)	6 (3%)	43	73
1	D	221/221 (100%)	214 (97%)	7 (3%)	39	69
1	E	214/221 (97%)	207 (97%)	7 (3%)	38	69
1	F	221/221 (100%)	212 (96%)	9 (4%)	30	64
1	G	221/221 (100%)	213 (96%)	8 (4%)	35	67
1	H	221/221 (100%)	211 (96%)	10 (4%)	27	60
All	All	1754/1768 (99%)	1690 (96%)	64 (4%)	35	67

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	THR
1	A	109	LEU
1	A	124	THR
1	A	160	GLN
1	A	270	ASN
1	A	274	LYS
1	A	283	SER
1	A	288	ARG
1	B	70	THR
1	B	109	LEU
1	B	124	THR
1	B	160	GLN
1	B	238	LYS
1	B	270	ASN
1	B	274	LYS
1	B	283	SER
1	B	288	ARG
1	C	124	THR
1	C	137	ARG
1	C	160	GLN
1	C	238	LYS
1	C	240	GLU
1	C	270	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	124	THR
1	D	137	ARG
1	D	160	GLN
1	D	240	GLU
1	D	270	ASN
1	D	283	SER
1	D	285	ASN
1	E	61	VAL
1	E	109	LEU
1	E	160	GLN
1	E	203	VAL
1	E	228	SER
1	E	234	GLN
1	E	270	ASN
1	F	109	LEU
1	F	124	THR
1	F	127	ASN
1	F	130	HIS
1	F	160	GLN
1	F	202	SER
1	F	234	GLN
1	F	270	ASN
1	F	288	ARG
1	G	70	THR
1	G	109	LEU
1	G	124	THR
1	G	270	ASN
1	G	274	LYS
1	G	275	ILE
1	G	283	SER
1	G	289	PHE
1	H	33	GLN
1	H	70	THR
1	H	97	THR
1	H	145	LEU
1	H	160	GLN
1	H	233	MET
1	H	270	ASN
1	H	274	LYS
1	H	283	SER
1	H	289	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	120	HIS
1	A	270	ASN
1	B	119	ASN
1	B	120	HIS
1	B	270	ASN
1	C	119	ASN
1	C	120	HIS
1	C	127	ASN
1	C	234	GLN
1	C	270	ASN
1	D	77	HIS
1	D	119	ASN
1	D	120	HIS
1	D	127	ASN
1	D	270	ASN
1	E	119	ASN
1	E	120	HIS
1	E	270	ASN
1	F	53	HIS
1	F	119	ASN
1	F	120	HIS
1	F	270	ASN
1	G	119	ASN
1	G	120	HIS
1	G	127	ASN
1	G	270	ASN
1	H	77	HIS
1	H	119	ASN
1	H	120	HIS
1	H	130	HIS
1	H	270	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates 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$
3	NN4	C	911	-	29,31,31	0.81	2 (6%)	39,48,48	1.07	3 (7%)
3	NN4	H	911	-	29,31,31	0.86	1 (3%)	39,48,48	1.01	3 (7%)
3	NN4	E	911	-	29,31,31	0.76	1 (3%)	39,48,48	1.16	3 (7%)
2	NAP	H	901	-	45,52,52	1.66	4 (8%)	56,80,80	1.10	2 (3%)
2	NAP	D	901	-	45,52,52	1.79	4 (8%)	56,80,80	1.03	1 (1%)
2	NAP	G	901	-	45,52,52	1.67	4 (8%)	56,80,80	1.05	1 (1%)
3	NN4	B	911	-	29,31,31	0.79	1 (3%)	39,48,48	1.14	2 (5%)
2	NAP	E	901	-	45,52,52	1.69	3 (6%)	56,80,80	1.09	2 (3%)
3	NN4	D	911	-	29,31,31	0.83	2 (6%)	39,48,48	1.15	2 (5%)
2	NAP	C	901	-	45,52,52	1.67	3 (6%)	56,80,80	1.08	2 (3%)
2	NAP	F	901	-	45,52,52	1.70	3 (6%)	56,80,80	1.08	4 (7%)
2	NAP	A	901	-	45,52,52	1.65	3 (6%)	56,80,80	1.07	1 (1%)
2	NAP	B	901	-	45,52,52	1.68	4 (8%)	56,80,80	1.09	2 (3%)
3	NN4	G	911	-	29,31,31	0.72	1 (3%)	39,48,48	1.18	2 (5%)
3	NN4	F	911	-	29,31,31	0.80	2 (6%)	39,48,48	1.16	4 (10%)
3	NN4	A	911	-	29,31,31	0.78	1 (3%)	39,48,48	1.11	2 (5%)

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
3	NN4	C	911	-	-	4/23/54/54	0/5/4/4
3	NN4	H	911	-	-	5/23/54/54	0/5/4/4
3	NN4	E	911	-	-	6/23/54/54	0/5/4/4
2	NAP	H	901	-	-	4/31/67/67	0/5/5/5
2	NAP	D	901	-	-	6/31/67/67	0/5/5/5
2	NAP	G	901	-	-	6/31/67/67	0/5/5/5
3	NN4	B	911	-	-	5/23/54/54	0/5/4/4
2	NAP	E	901	-	-	4/31/67/67	0/5/5/5
3	NN4	D	911	-	-	3/23/54/54	0/5/4/4
2	NAP	C	901	-	-	6/31/67/67	0/5/5/5
2	NAP	F	901	-	-	6/31/67/67	0/5/5/5
2	NAP	A	901	-	-	3/31/67/67	0/5/5/5
2	NAP	B	901	-	-	5/31/67/67	0/5/5/5
3	NN4	G	911	-	-	3/23/54/54	0/5/4/4
3	NN4	F	911	-	-	3/23/54/54	0/5/4/4
3	NN4	A	911	-	-	3/23/54/54	0/5/4/4

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	901	NAP	O7N-C7N	9.54	1.42	1.24
2	F	901	NAP	O7N-C7N	8.86	1.41	1.24
2	A	901	NAP	O7N-C7N	8.81	1.41	1.24
2	B	901	NAP	O7N-C7N	8.81	1.41	1.24
2	E	901	NAP	O7N-C7N	8.78	1.41	1.24
2	G	901	NAP	O7N-C7N	8.74	1.40	1.24
2	H	901	NAP	O7N-C7N	8.59	1.40	1.24
2	C	901	NAP	O7N-C7N	8.55	1.40	1.24
2	F	901	NAP	C2A-N3A	4.27	1.39	1.32
2	D	901	NAP	C2A-N3A	4.23	1.38	1.32
2	C	901	NAP	C2A-N3A	4.13	1.38	1.32
2	E	901	NAP	C2A-N3A	4.03	1.38	1.32
2	B	901	NAP	C2A-N3A	3.93	1.38	1.32
2	H	901	NAP	C2A-N3A	3.93	1.38	1.32
2	G	901	NAP	C2A-N3A	3.74	1.38	1.32
2	A	901	NAP	C2A-N3A	3.60	1.37	1.32
3	D	911	NN4	C12-N13	3.10	1.38	1.32
3	F	911	NN4	C12-N13	2.99	1.38	1.32
3	G	911	NN4	C12-N13	2.89	1.38	1.32
2	H	901	NAP	C2A-N1A	2.89	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	NAP	C2A-N1A	2.87	1.39	1.33
2	F	901	NAP	C2A-N1A	2.83	1.39	1.33
3	B	911	NN4	C12-N13	2.79	1.38	1.32
2	D	901	NAP	C2A-N1A	2.71	1.39	1.33
3	A	911	NN4	C12-N13	2.68	1.37	1.32
3	C	911	NN4	C12-N13	2.67	1.37	1.32
3	H	911	NN4	C12-N13	2.60	1.37	1.32
2	C	901	NAP	C2A-N1A	2.50	1.38	1.33
2	G	901	NAP	C2A-N1A	2.49	1.38	1.33
2	E	901	NAP	C2A-N1A	2.46	1.38	1.33
3	C	911	NN4	C15-N11	2.42	1.38	1.34
3	F	911	NN4	C15-N11	2.35	1.38	1.34
2	A	901	NAP	C2A-N1A	2.33	1.38	1.33
3	D	911	NN4	C15-N11	2.31	1.38	1.34
2	D	901	NAP	C2N-N1N	2.29	1.37	1.35
3	E	911	NN4	C12-N13	2.24	1.37	1.32
2	H	901	NAP	C2N-N1N	2.18	1.37	1.35
2	B	901	NAP	C2N-N1N	2.16	1.37	1.35
2	G	901	NAP	C2N-N1N	2.02	1.37	1.35

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	901	NAP	N3A-C2A-N1A	-5.69	119.78	128.68
2	E	901	NAP	N3A-C2A-N1A	-5.68	119.81	128.68
2	H	901	NAP	N3A-C2A-N1A	-5.55	120.00	128.68
2	G	901	NAP	N3A-C2A-N1A	-5.53	120.03	128.68
2	B	901	NAP	N3A-C2A-N1A	-5.42	120.20	128.68
2	D	901	NAP	N3A-C2A-N1A	-5.35	120.31	128.68
2	A	901	NAP	N3A-C2A-N1A	-5.28	120.43	128.68
2	F	901	NAP	N3A-C2A-N1A	-5.19	120.56	128.68
3	G	911	NN4	C28-O27-C24	-5.05	106.55	117.51
3	F	911	NN4	C28-O27-C24	-4.56	107.61	117.51
3	D	911	NN4	C16-O18-C21	-4.23	114.16	120.95
3	D	911	NN4	C28-O27-C24	-4.18	108.44	117.51
3	E	911	NN4	C28-O27-C24	-4.04	108.75	117.51
3	A	911	NN4	C28-O27-C24	-4.03	108.76	117.51
3	E	911	NN4	C16-O18-C21	-3.86	114.76	120.95
3	B	911	NN4	C28-O27-C24	-3.84	109.17	117.51
3	C	911	NN4	C28-O27-C24	-3.78	109.31	117.51
3	B	911	NN4	C16-O18-C21	-3.61	115.16	120.95
3	A	911	NN4	C16-O18-C21	-3.54	115.27	120.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	911	NN4	C16-O18-C21	-3.45	115.42	120.95
3	H	911	NN4	C28-O27-C24	-3.32	110.31	117.51
3	G	911	NN4	C16-O18-C21	-3.31	115.64	120.95
3	F	911	NN4	C16-O18-C21	-3.15	115.90	120.95
3	H	911	NN4	C16-O18-C21	-2.74	116.56	120.95
2	F	901	NAP	C1B-N9A-C4A	-2.21	122.76	126.64
3	F	911	NN4	O17-C15-N11	2.19	127.20	122.74
2	H	901	NAP	O2N-PN-O1N	2.11	122.67	112.24
2	B	901	NAP	O2N-PN-O1N	2.08	122.53	112.24
3	F	911	NN4	O18-C16-C19	2.07	116.76	107.80
2	E	901	NAP	O2N-PN-O1N	2.04	122.35	112.24
2	F	901	NAP	O5D-C5D-C4D	2.04	116.03	108.99
2	F	901	NAP	C4A-C5A-N7A	-2.04	107.28	109.40
3	C	911	NN4	O18-C16-C19	2.03	116.61	107.80
2	C	901	NAP	O2N-PN-O1N	2.03	122.27	112.24
3	E	911	NN4	O18-C16-C19	2.00	116.48	107.80
3	H	911	NN4	O18-C16-C19	2.00	116.48	107.80

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	911	NN4	C15-C16-O18-C21
3	H	911	NN4	C20-C16-O18-C21
3	E	911	NN4	C15-C16-O18-C21
3	E	911	NN4	C20-C16-O18-C21
3	G	911	NN4	C15-C16-O18-C21
3	G	911	NN4	C20-C16-O18-C21
3	B	911	NN4	C15-C16-O18-C21
3	B	911	NN4	C20-C16-O18-C21
2	E	901	NAP	C2B-O2B-P2B-O3X
3	D	911	NN4	C15-C16-O18-C21
3	D	911	NN4	C20-C16-O18-C21
2	F	901	NAP	O4B-C4B-C5B-O5B
2	F	901	NAP	O4D-C4D-C5D-O5D
2	B	901	NAP	C5D-O5D-PN-O2N
3	F	911	NN4	C20-C16-O18-C21
3	C	911	NN4	C15-C16-O18-C21
3	C	911	NN4	C20-C16-O18-C21
3	A	911	NN4	C15-C16-O18-C21
3	A	911	NN4	C20-C16-O18-C21
2	D	901	NAP	O4D-C4D-C5D-O5D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	F	901	NAP	C3D-C4D-C5D-O5D
3	H	911	NN4	C25-C24-O27-C28
3	H	911	NN4	C23-C24-O27-C28
2	D	901	NAP	C3D-C4D-C5D-O5D
2	C	901	NAP	O4D-C4D-C5D-O5D
2	C	901	NAP	C3D-C4D-C5D-O5D
3	H	911	NN4	C19-C16-O18-C21
3	E	911	NN4	C19-C16-O18-C21
3	G	911	NN4	C19-C16-O18-C21
3	B	911	NN4	C19-C16-O18-C21
3	D	911	NN4	C19-C16-O18-C21
3	F	911	NN4	C19-C16-O18-C21
3	C	911	NN4	C19-C16-O18-C21
3	A	911	NN4	C19-C16-O18-C21
3	F	911	NN4	C15-C16-O18-C21
2	G	901	NAP	PN-O3-PA-O1A
3	E	911	NN4	C23-C24-O27-C28
3	E	911	NN4	C25-C24-O27-C28
2	H	901	NAP	C2B-O2B-P2B-O3X
2	H	901	NAP	O4B-C4B-C5B-O5B
2	H	901	NAP	PN-O3-PA-O1A
2	D	901	NAP	PN-O3-PA-O2A
2	C	901	NAP	PN-O3-PA-O2A
2	G	901	NAP	O4D-C4D-C5D-O5D
2	E	901	NAP	PN-O3-PA-O2A
2	D	901	NAP	O4B-C4B-C5B-O5B
2	E	901	NAP	O4B-C4B-C5B-O5B
2	C	901	NAP	O4B-C4B-C5B-O5B
2	G	901	NAP	O4B-C4B-C5B-O5B
2	F	901	NAP	PN-O3-PA-O1A
3	B	911	NN4	C23-C24-O27-C28
3	B	911	NN4	C25-C24-O27-C28
2	G	901	NAP	C3D-C4D-C5D-O5D
3	E	911	NN4	C5-C9-N11-C15
3	C	911	NN4	C5-C9-N11-C15
2	H	901	NAP	C2B-O2B-P2B-O2X
2	D	901	NAP	C2B-O2B-P2B-O2X
2	G	901	NAP	C2B-O2B-P2B-O2X
2	E	901	NAP	C2B-O2B-P2B-O2X
2	C	901	NAP	C2B-O2B-P2B-O2X
2	F	901	NAP	C2B-O2B-P2B-O2X
2	A	901	NAP	C2B-O2B-P2B-O2X

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	901	NAP	C5D-O5D-PN-O3
2	B	901	NAP	C2B-O2B-P2B-O2X
2	B	901	NAP	C5D-O5D-PN-O3
2	D	901	NAP	PN-O3-PA-O1A
2	G	901	NAP	PN-O3-PA-O2A
2	C	901	NAP	PN-O3-PA-O1A
2	F	901	NAP	C5B-O5B-PA-O1A
2	B	901	NAP	C5D-O5D-PN-O1N
2	A	901	NAP	O4B-C4B-C5B-O5B
2	B	901	NAP	O4B-C4B-C5B-O5B

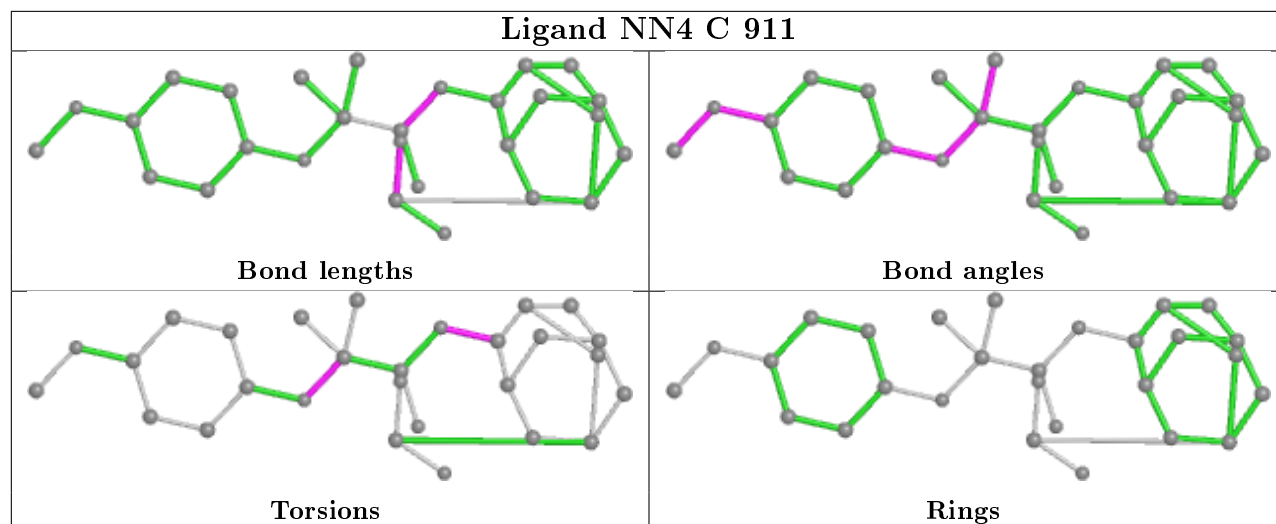
There are no ring outliers.

6 monomers are involved in 11 short contacts:

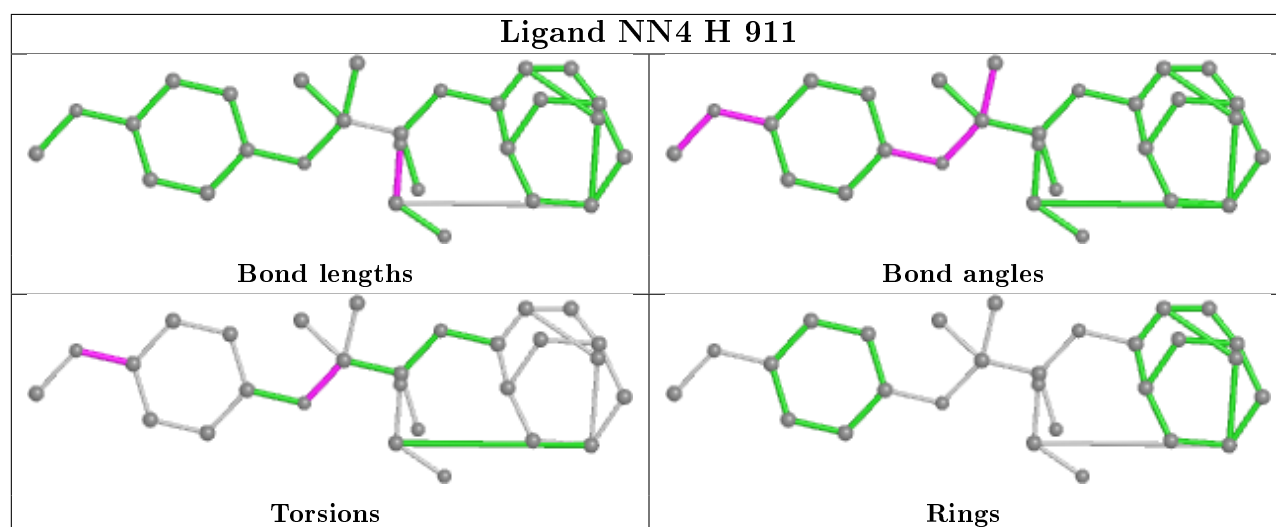
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	901	NAP	3	0
2	G	901	NAP	1	0
2	E	901	NAP	1	0
2	C	901	NAP	2	0
2	F	901	NAP	3	0
3	G	911	NN4	1	0

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.

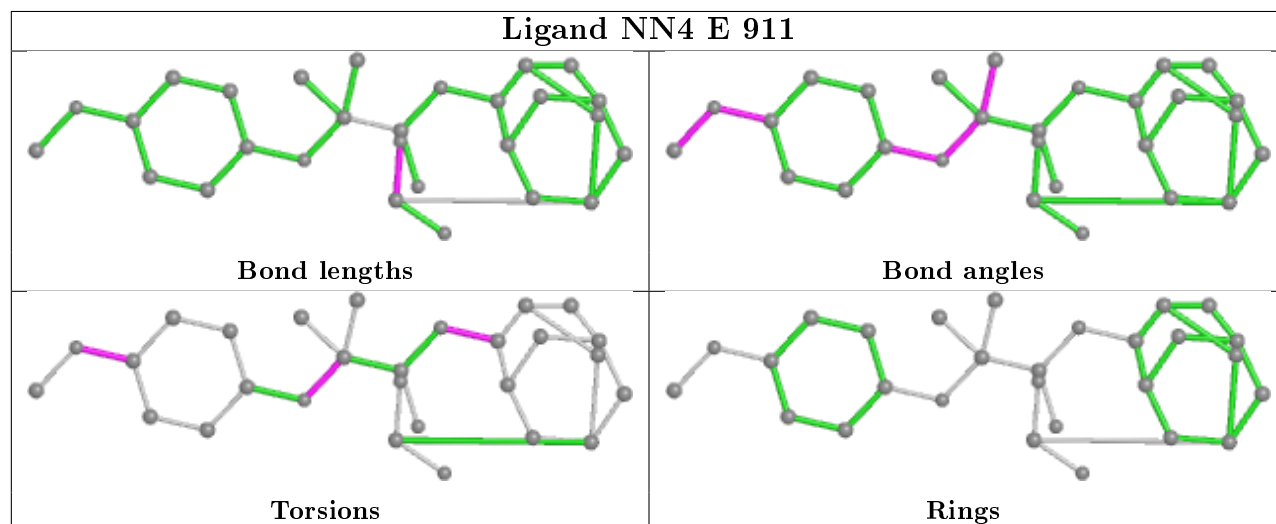
Ligand NN4 C 911

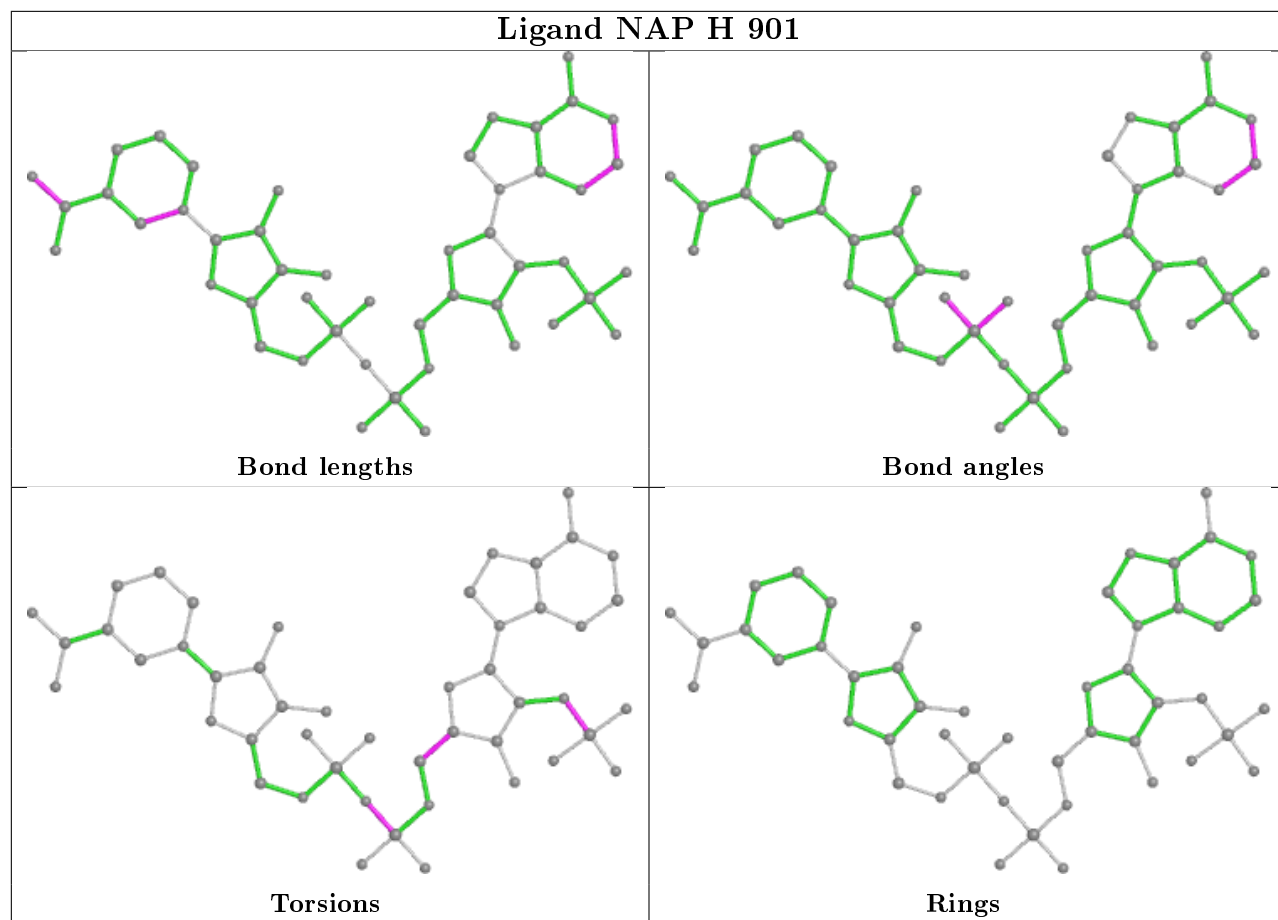


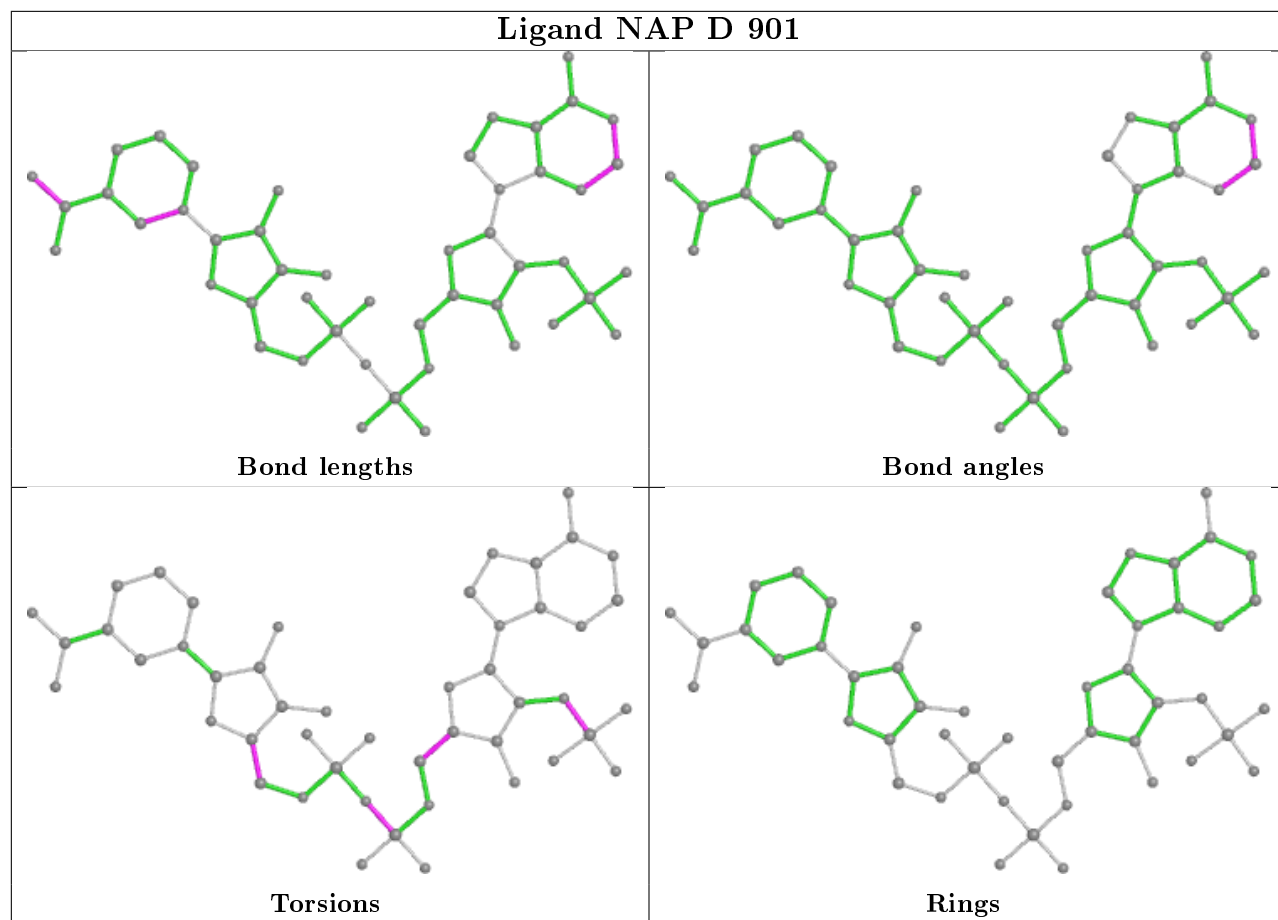
Ligand NN4 H 911

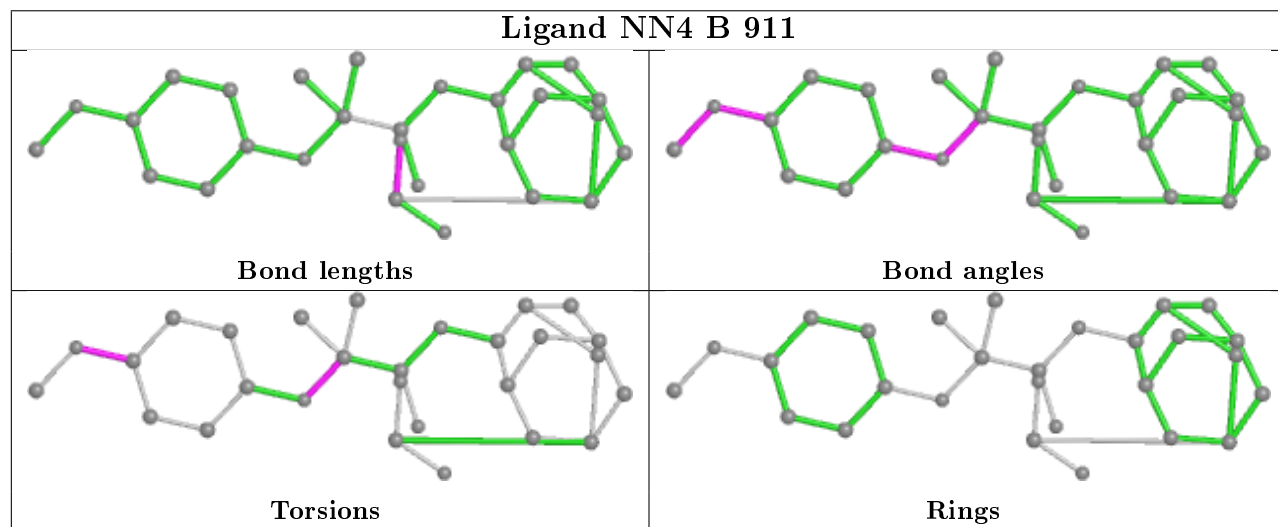
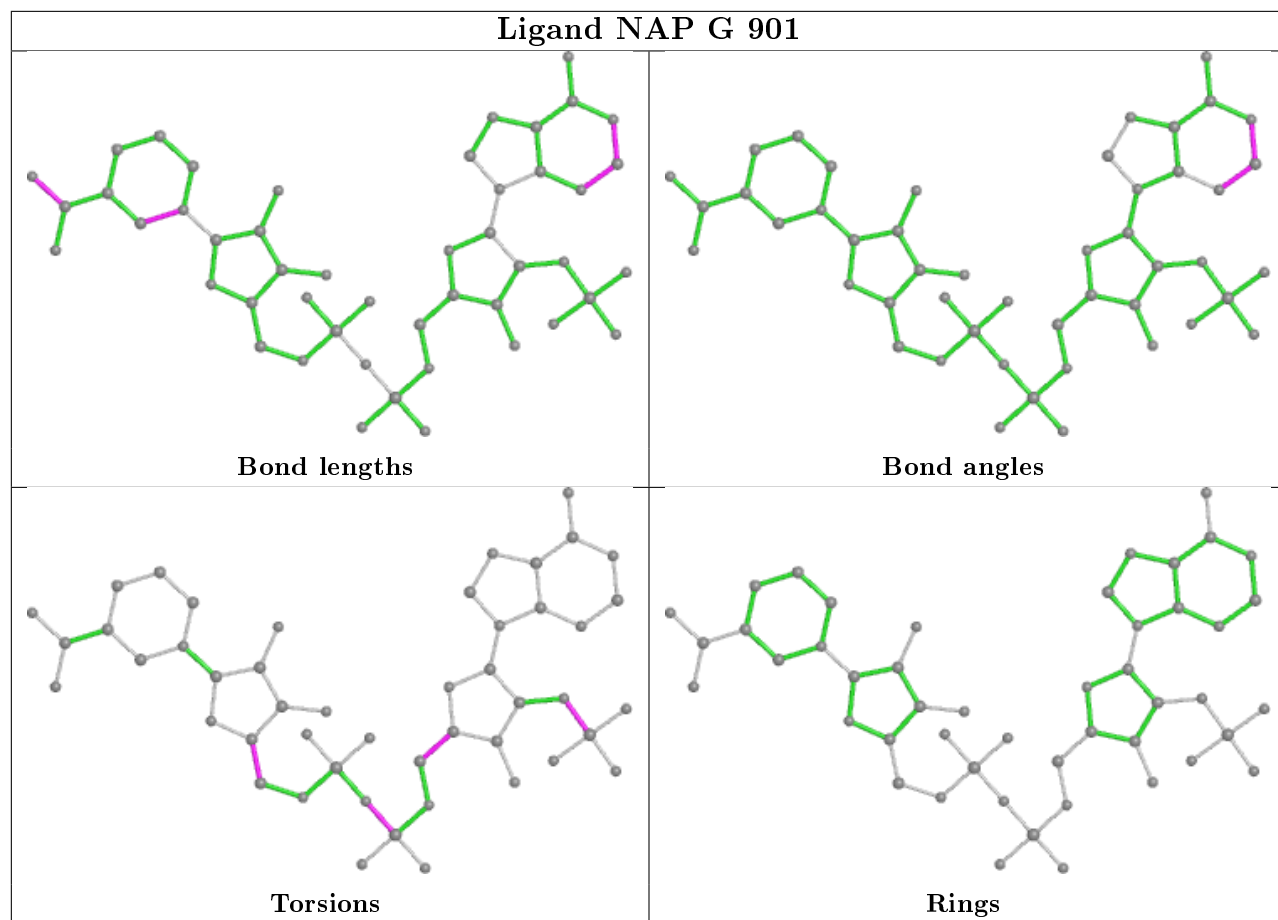


Ligand NN4 E 911

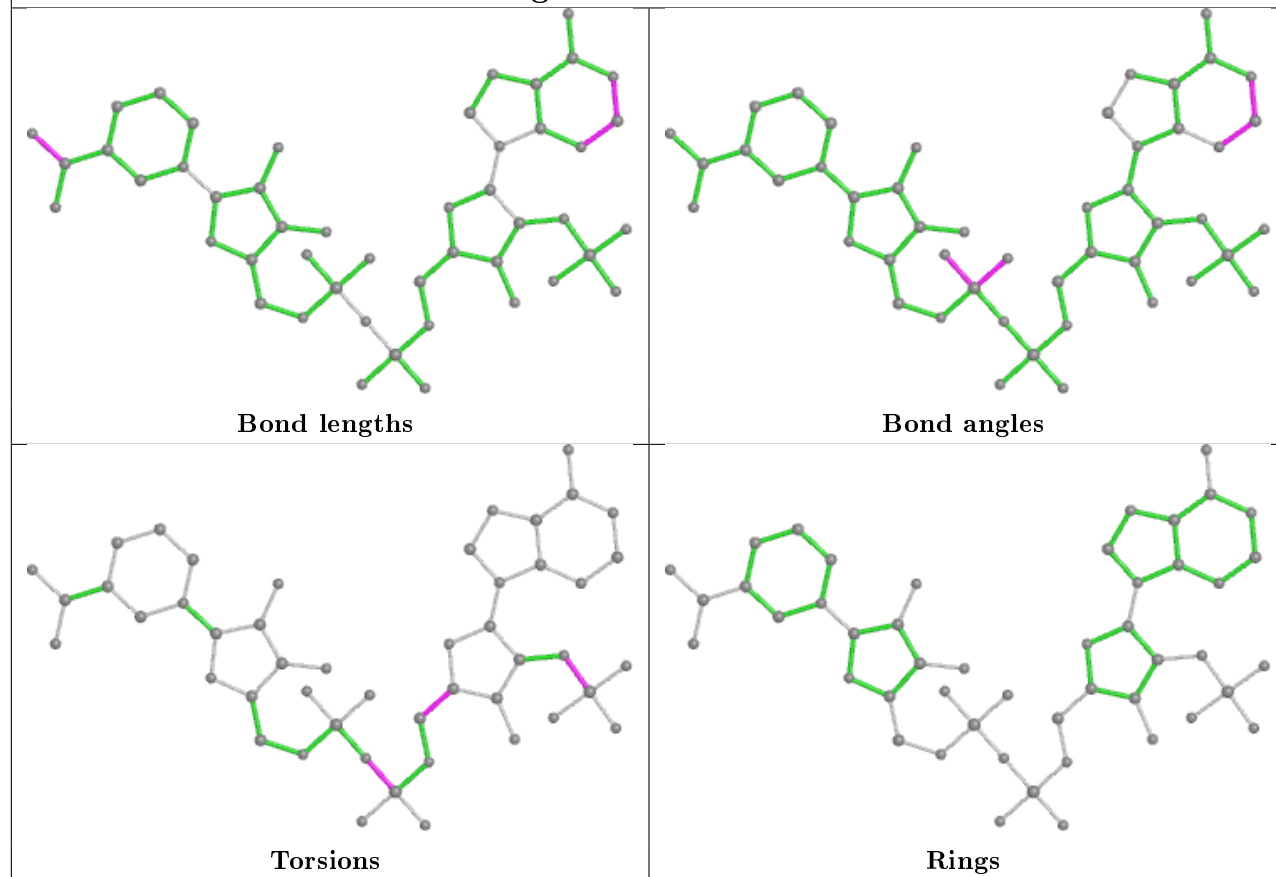




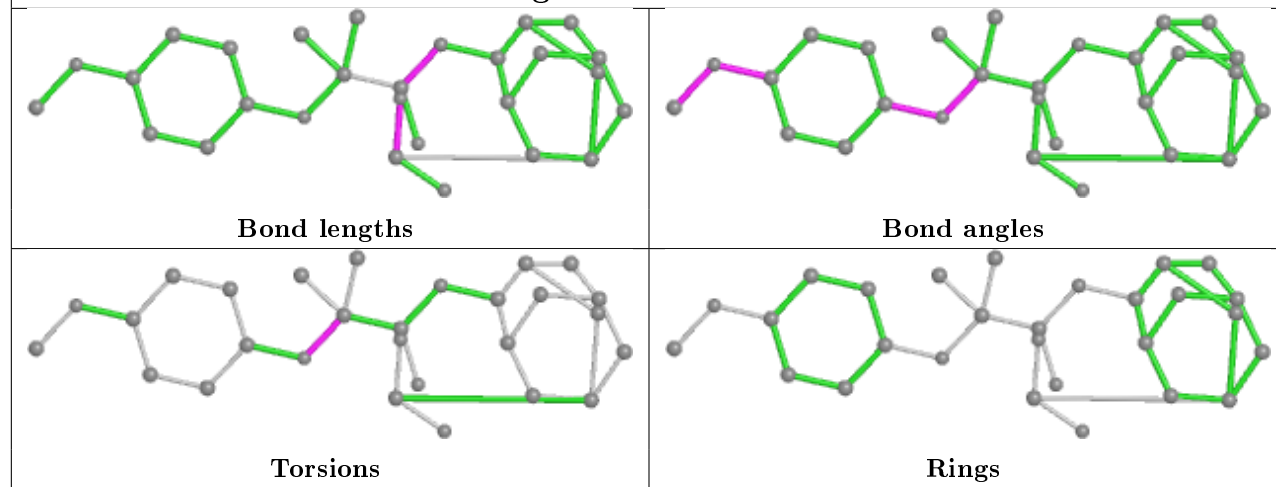


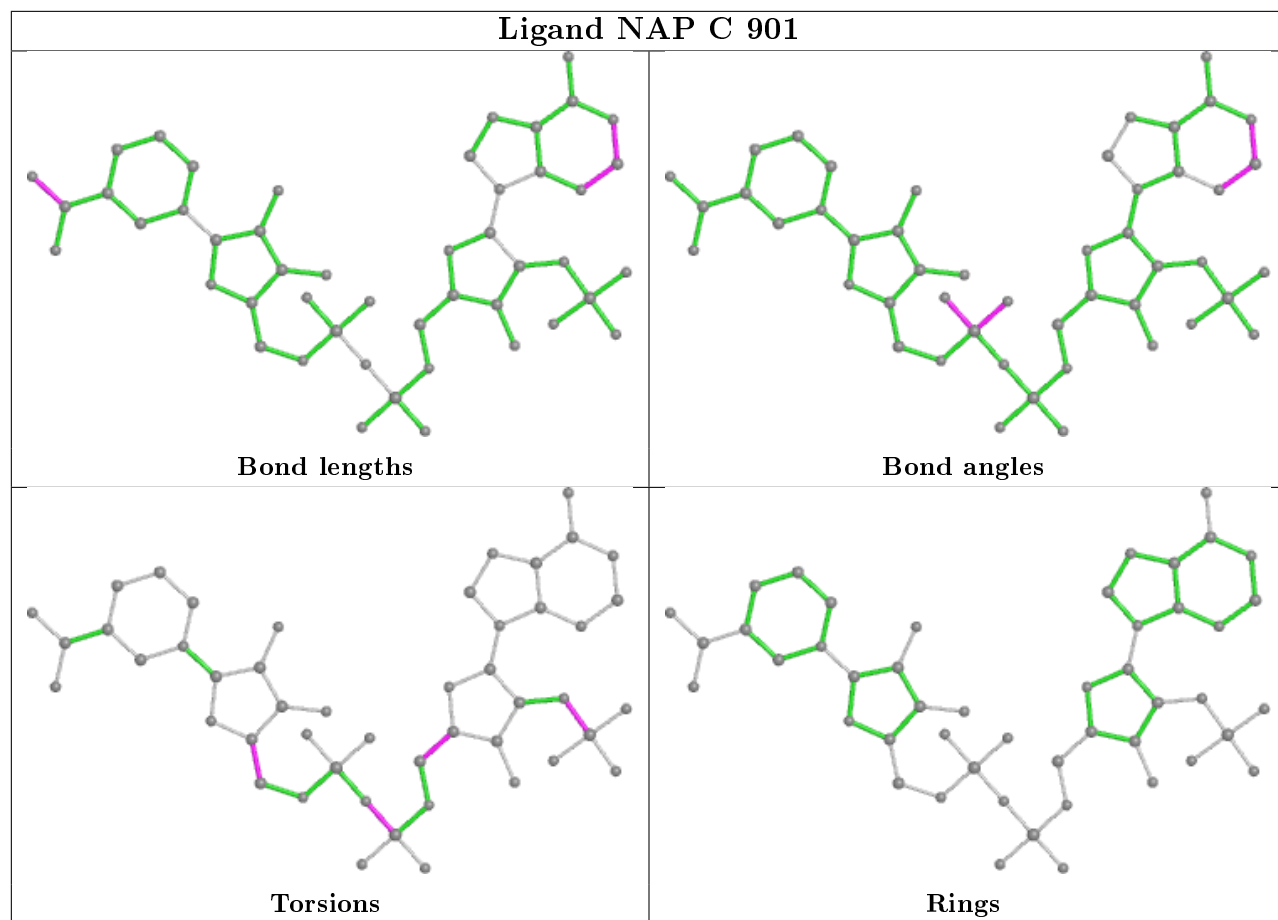


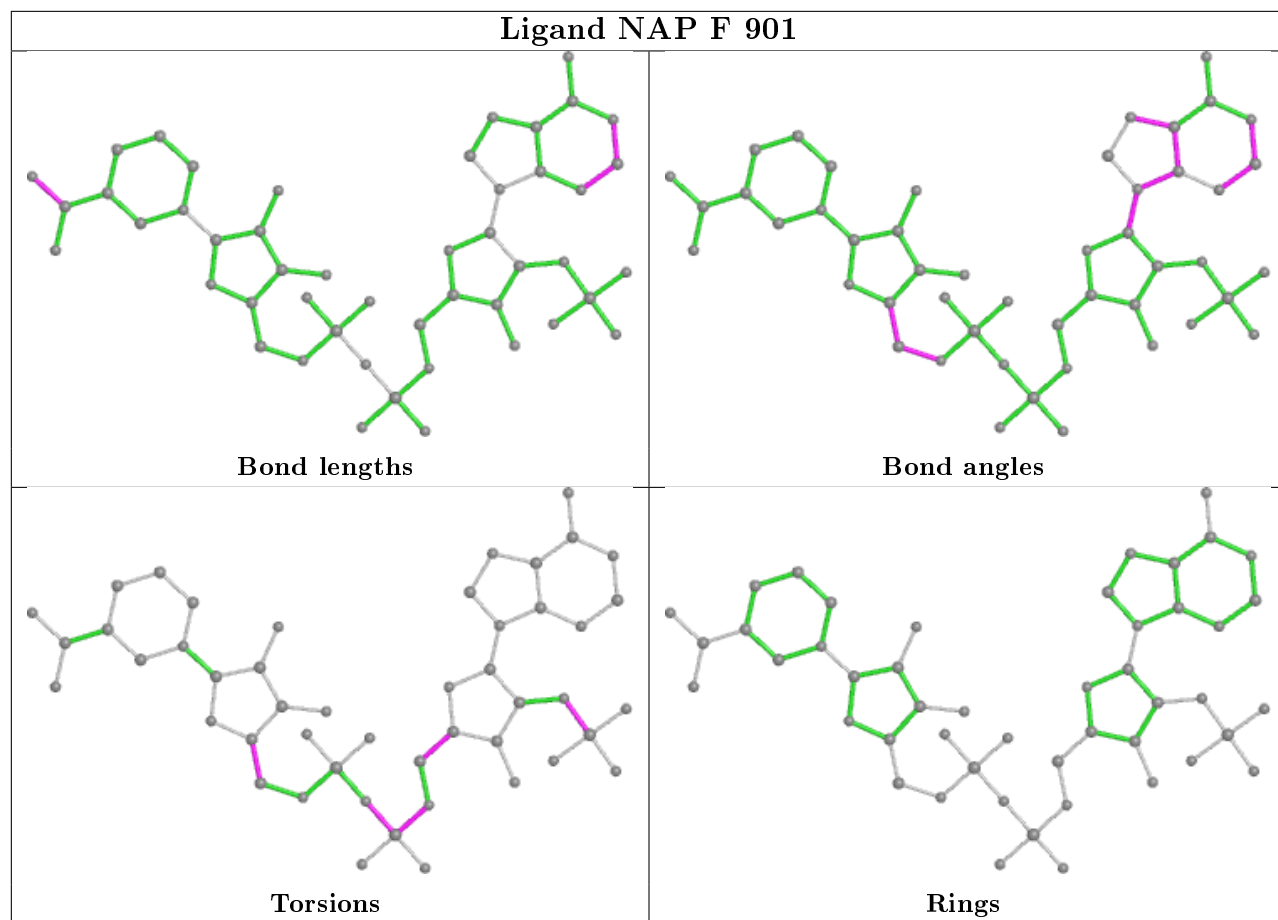
Ligand NAP E 901

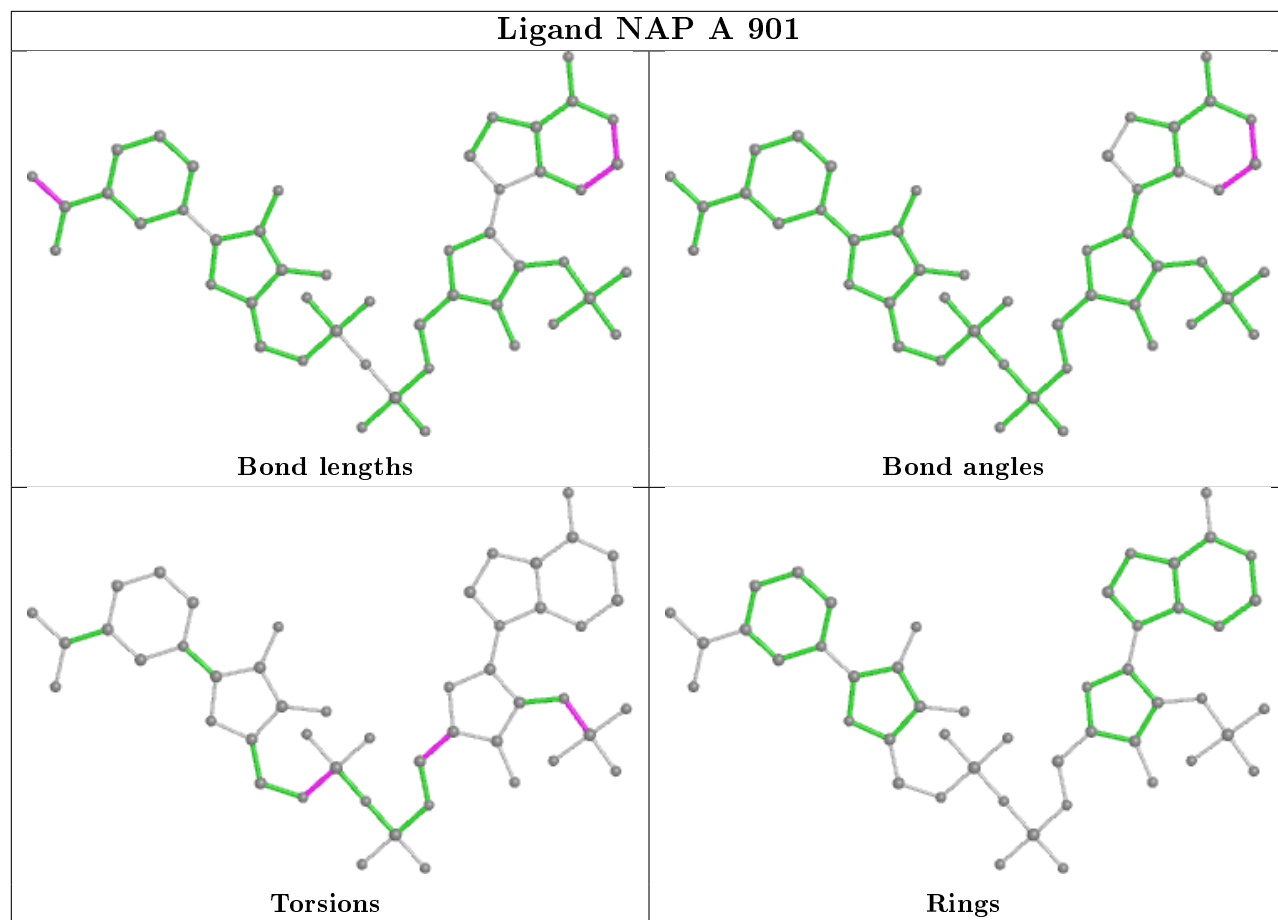


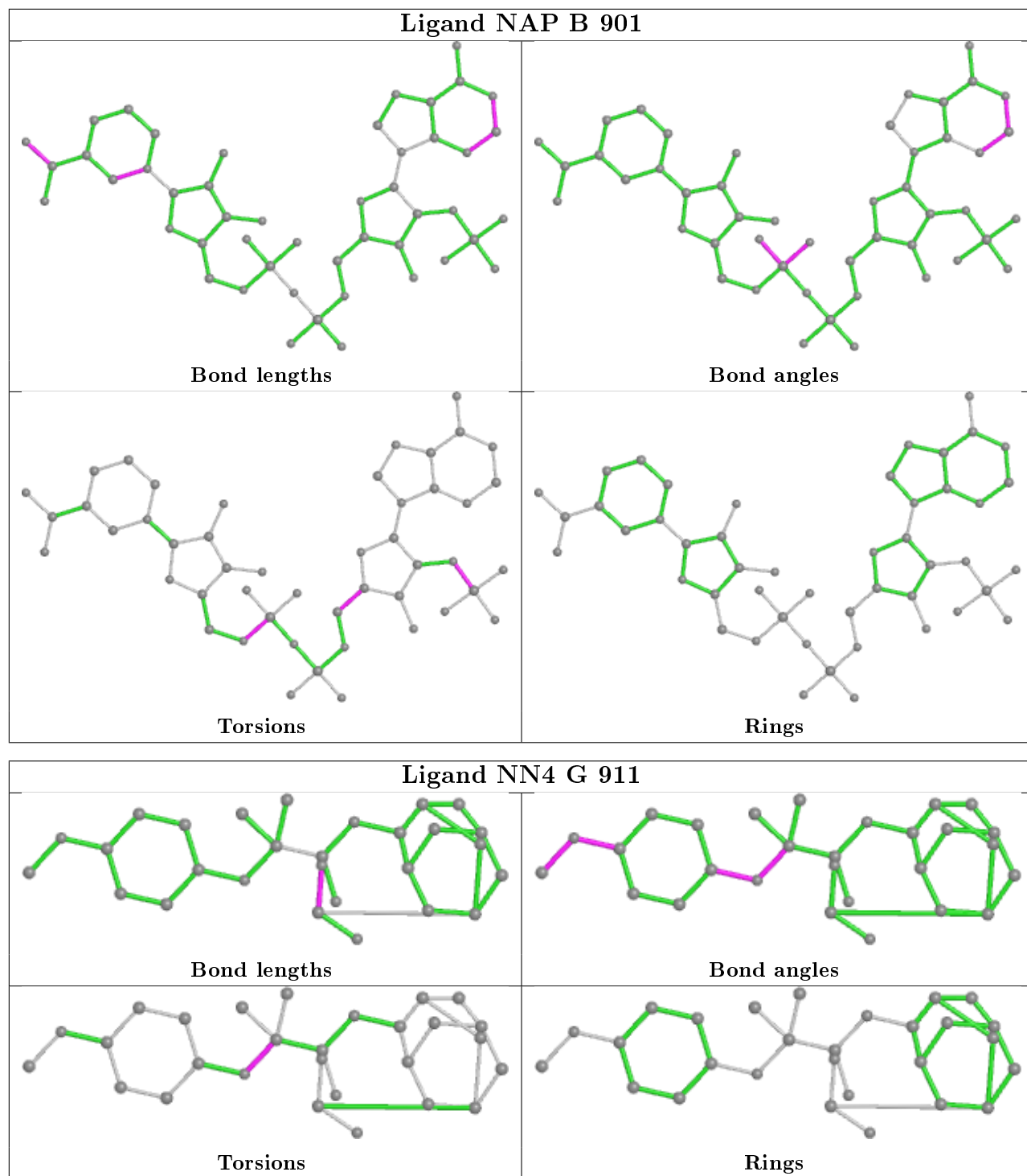
Ligand NN4 D 911

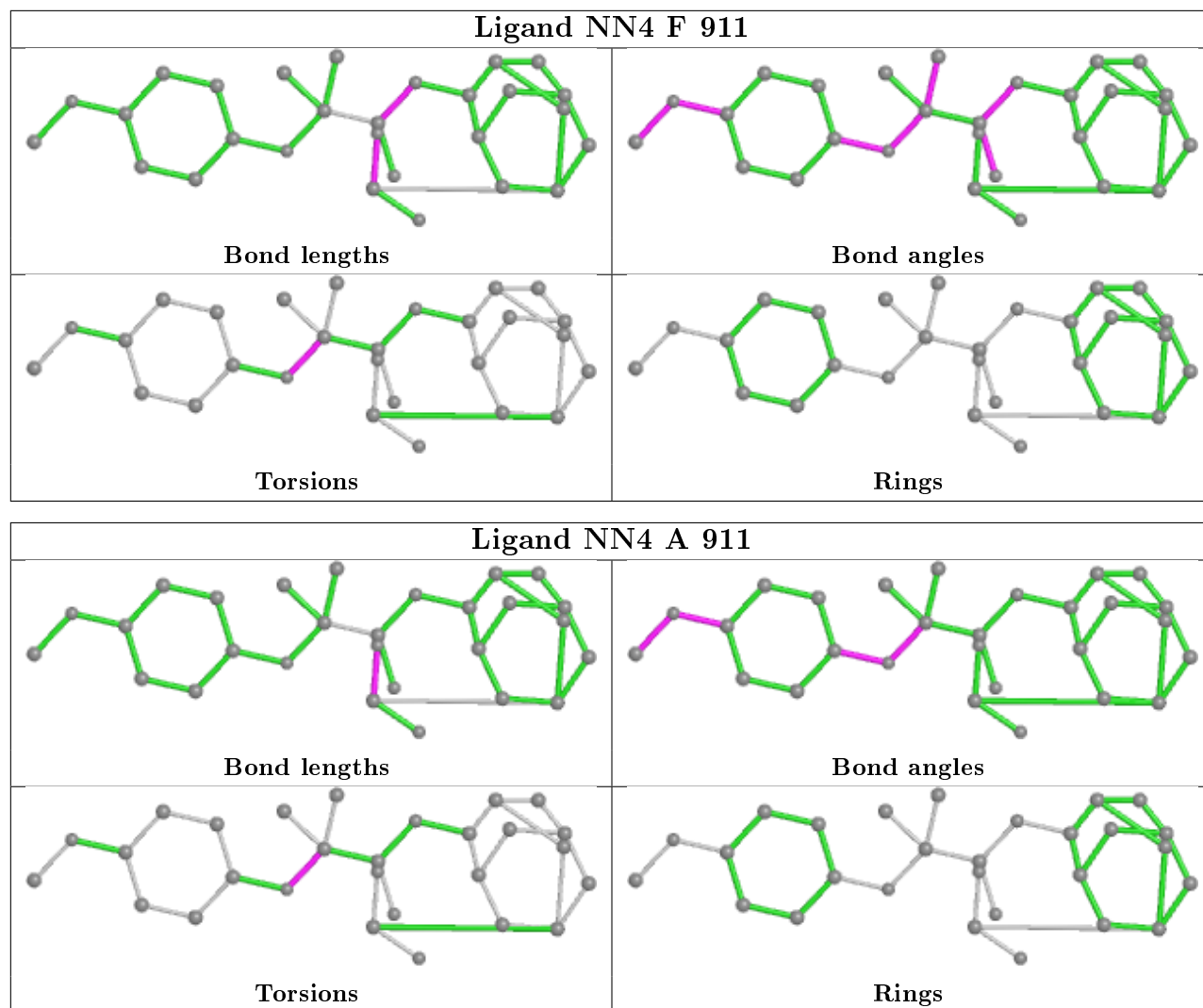












5.7 Other polymers [i](#)

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, 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	264/264 (100%)	-0.14	2 (0%)	86 72	34, 41, 49, 55	0
1	B	264/264 (100%)	-0.01	2 (0%)	86 72	34, 41, 49, 55	0
1	C	257/264 (97%)	-0.08	4 (1%)	72 51	35, 42, 49, 54	0
1	D	264/264 (100%)	0.16	11 (4%)	36 18	35, 42, 51, 67	0
1	E	257/264 (97%)	-0.19	2 (0%)	86 72	29, 40, 54, 62	0
1	F	264/264 (100%)	0.07	9 (3%)	45 24	30, 41, 57, 65	0
1	G	264/264 (100%)	-0.19	1 (0%)	92 84	29, 38, 54, 64	0
1	H	264/264 (100%)	-0.12	3 (1%)	80 64	30, 40, 54, 63	0
All	All	2098/2112 (99%)	-0.06	34 (1%)	72 51	29, 41, 52, 67	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	263	TRP	3.2
1	C	67	SER	3.1
1	D	30	GLU	3.1
1	D	28	ARG	2.9
1	E	92	THR	2.7
1	F	30	GLU	2.7
1	D	59	ALA	2.7
1	D	29	PRO	2.6
1	E	67	SER	2.5
1	F	263	TRP	2.5
1	F	59	ALA	2.4
1	F	58	GLY	2.4
1	F	60	HIS	2.4
1	F	49	GLU	2.4
1	D	162	ASN	2.4
1	D	27	PHE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	234	GLN	2.3
1	D	160	GLN	2.3
1	F	29	PRO	2.3
1	H	160	GLN	2.3
1	C	92	THR	2.3
1	F	85	SER	2.2
1	H	111	GLY	2.2
1	A	263	TRP	2.2
1	B	263	TRP	2.1
1	C	266	LEU	2.1
1	H	112	GLY	2.1
1	D	205	ARG	2.1
1	D	281	SER	2.1
1	C	263	TRP	2.1
1	F	160	GLN	2.1
1	B	80	GLU	2.1
1	D	58	GLY	2.1
1	A	160	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.

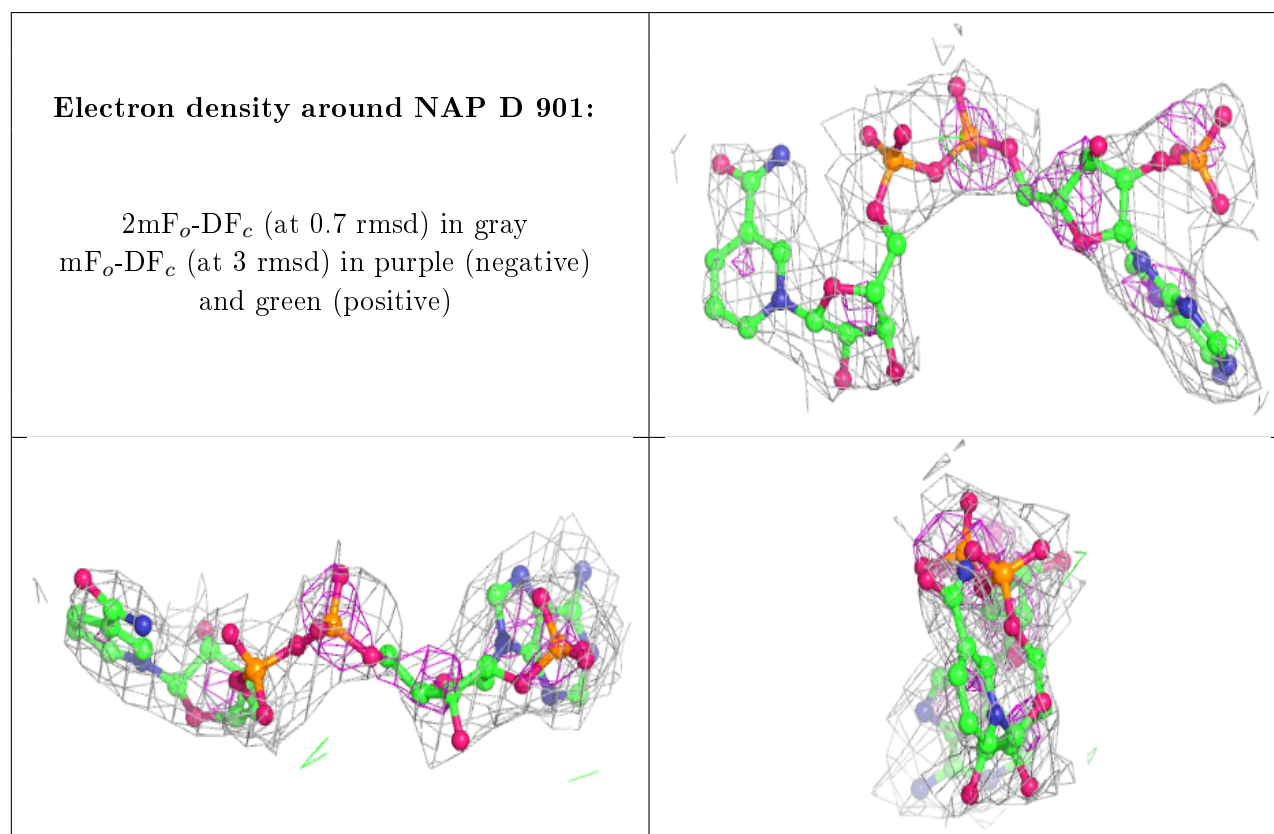
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAP	D	901	48/48	0.92	0.23	43,45,47,47	0
2	NAP	F	901	48/48	0.92	0.28	42,47,49,49	0
2	NAP	C	901	48/48	0.94	0.23	43,45,46,47	0
2	NAP	E	901	48/48	0.94	0.22	41,43,47,47	0
2	NAP	H	901	48/48	0.95	0.15	37,40,43,45	0

Continued on next page...

Continued from previous page...

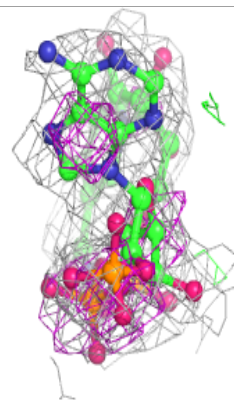
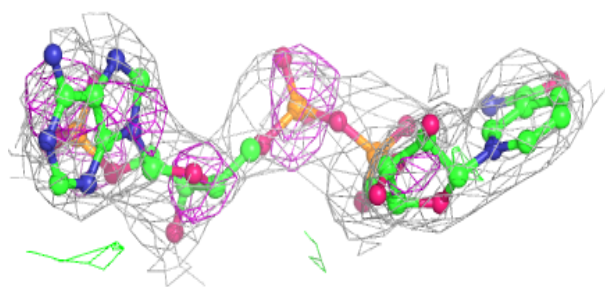
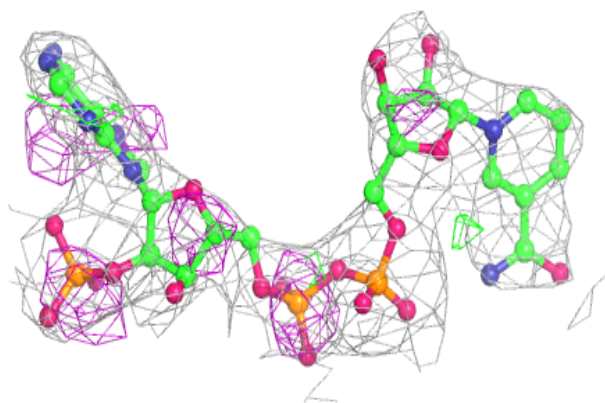
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NN4	D	911	28/28	0.95	0.17	27,28,30,31	0
3	NN4	F	911	28/28	0.95	0.21	30,32,36,36	0
3	NN4	B	911	28/28	0.96	0.20	25,27,30,32	0
2	NAP	B	901	48/48	0.96	0.19	38,40,43,44	0
3	NN4	H	911	28/28	0.96	0.19	27,28,30,31	0
3	NN4	C	911	28/28	0.96	0.21	27,28,30,31	0
2	NAP	A	901	48/48	0.97	0.17	38,40,43,44	0
2	NAP	G	901	48/48	0.97	0.19	37,40,42,43	0
3	NN4	G	911	28/28	0.97	0.15	27,28,30,31	0
3	NN4	E	911	28/28	0.97	0.18	28,32,34,35	0
3	NN4	A	911	28/28	0.97	0.17	25,27,30,32	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.

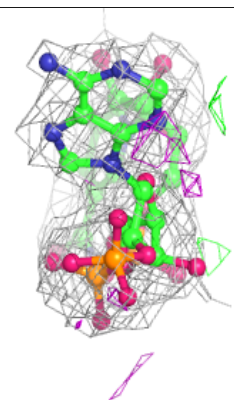
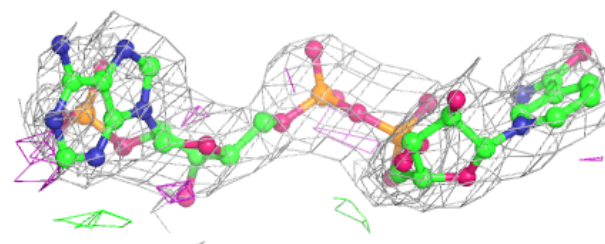
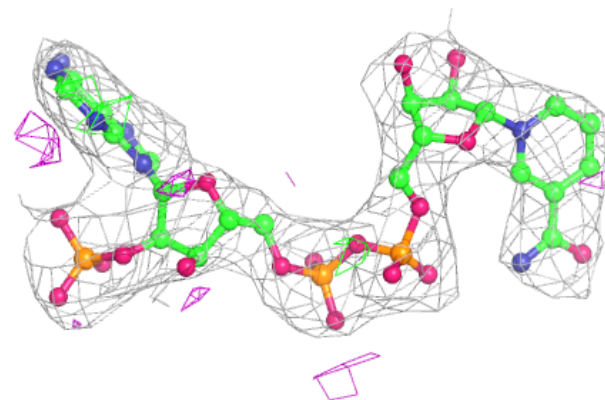


Electron density around NAP F 901:

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

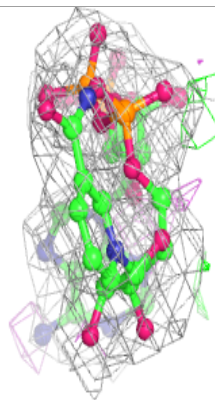
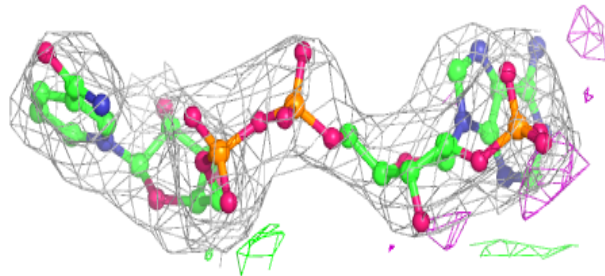
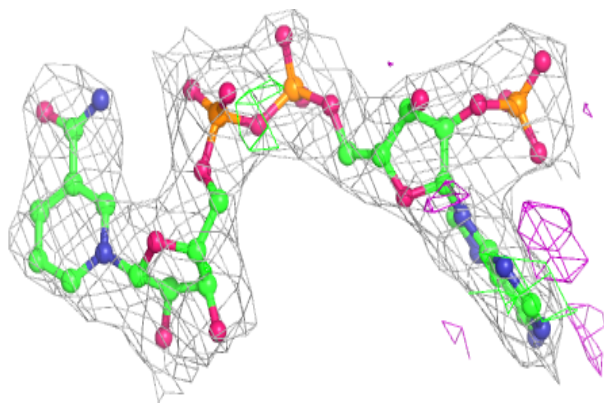
**Electron density around NAP C 901:**

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

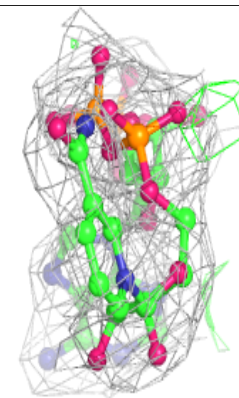
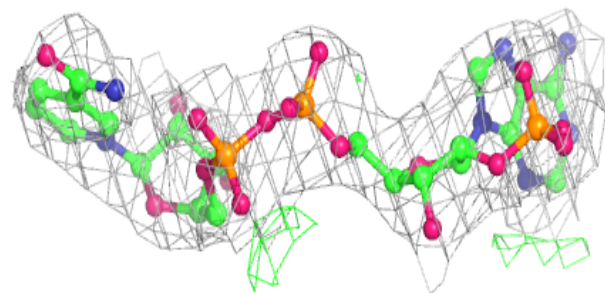
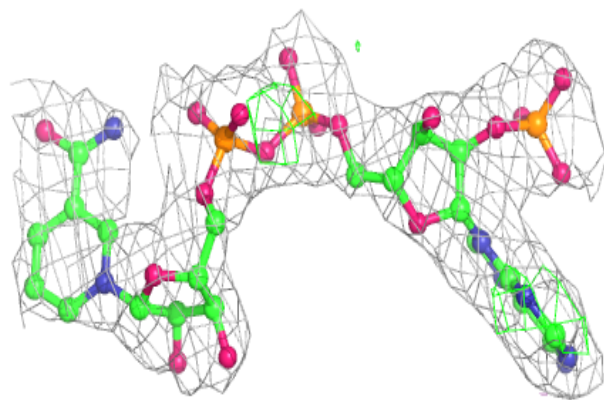


Electron density around NAP E 901:

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

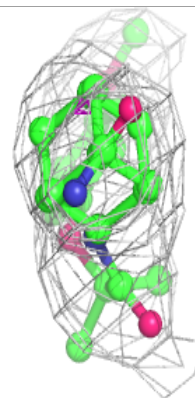
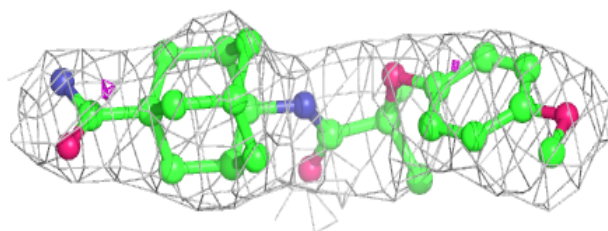
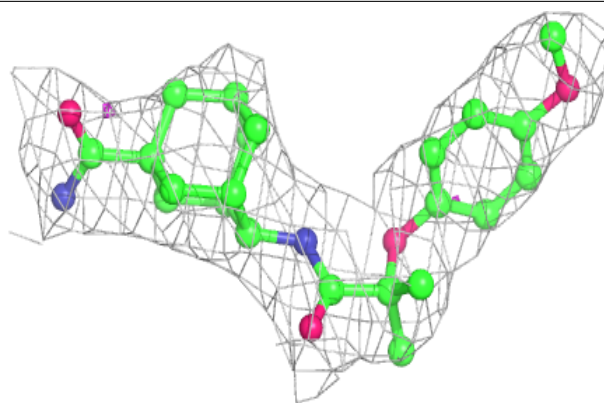
**Electron density around NAP H 901:**

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

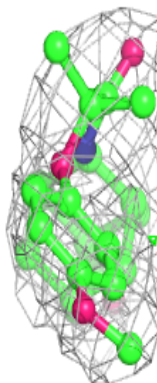
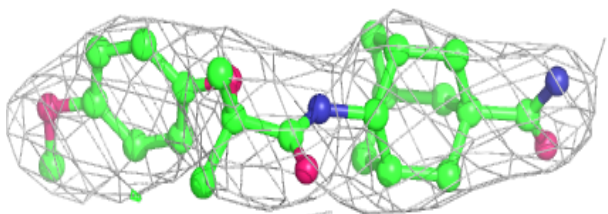
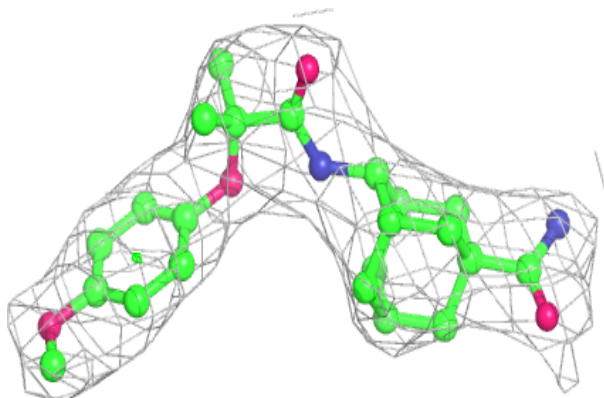


Electron density around NN4 D 911:

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

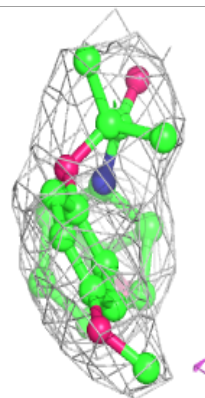
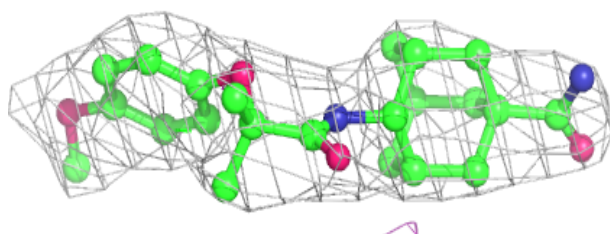
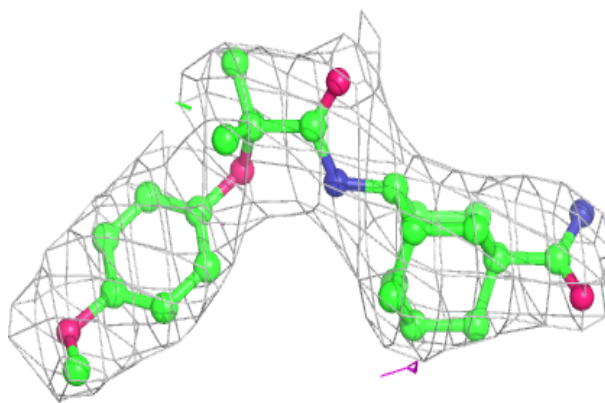
**Electron density around NN4 F 911:**

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

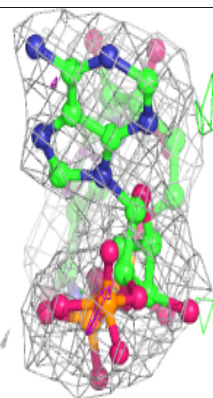
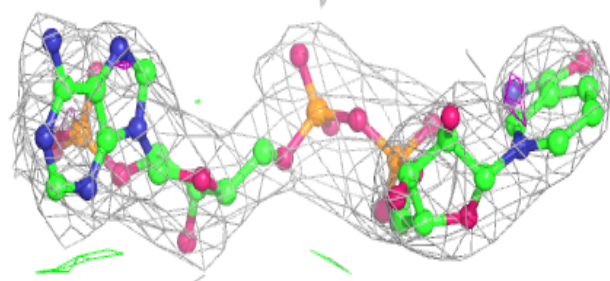
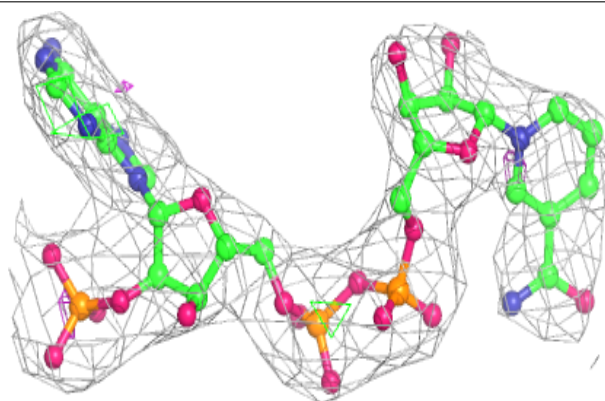


Electron density around NN4 B 911:

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

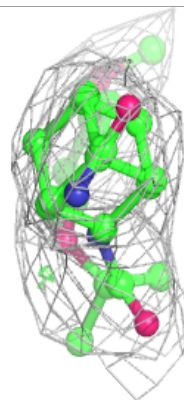
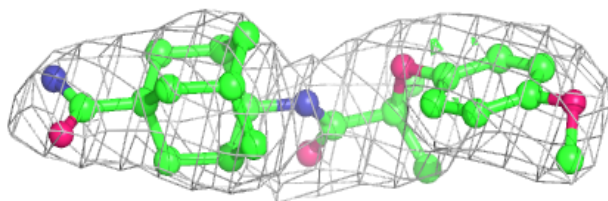
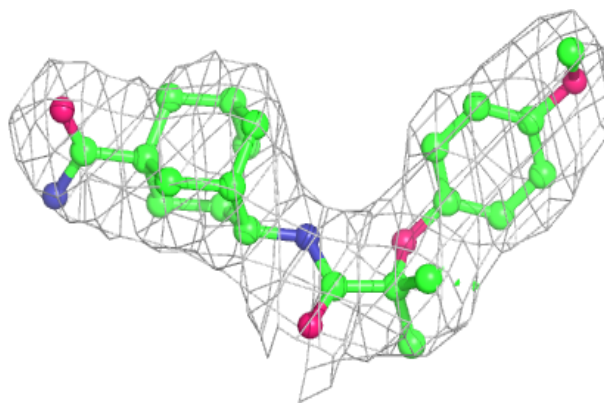
**Electron density around NAP B 901:**

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

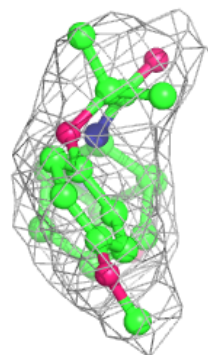
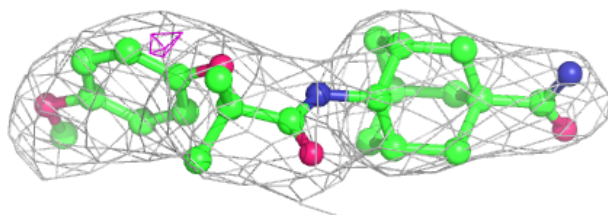
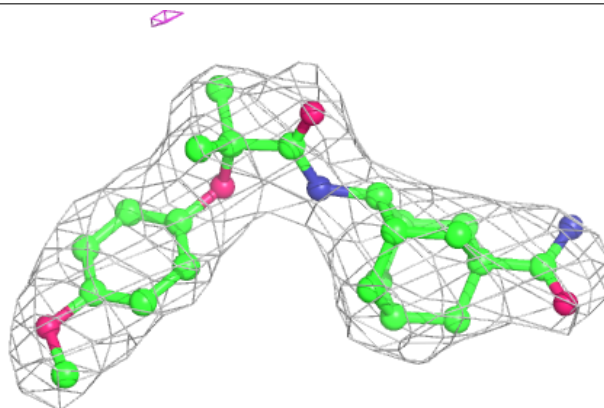


Electron density around NN4 H 911:

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

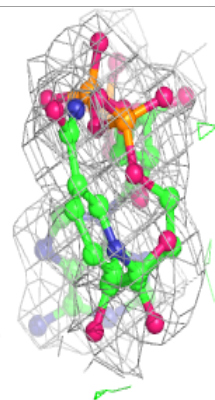
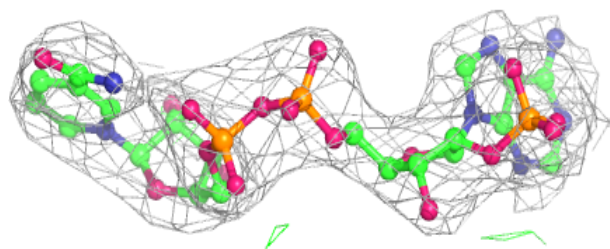
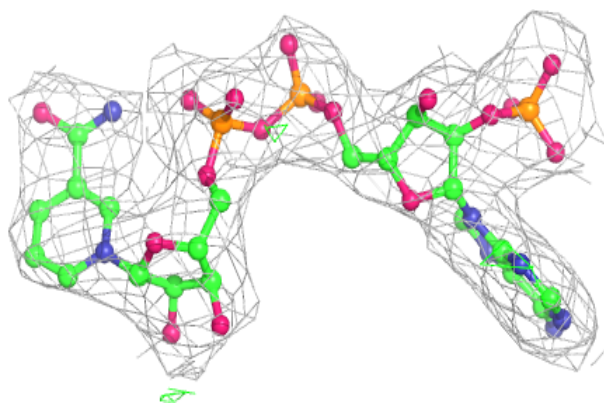
**Electron density around NN4 C 911:**

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

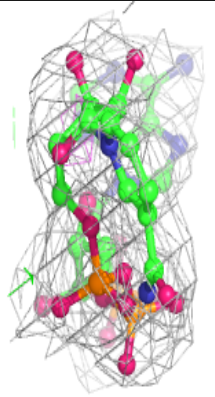
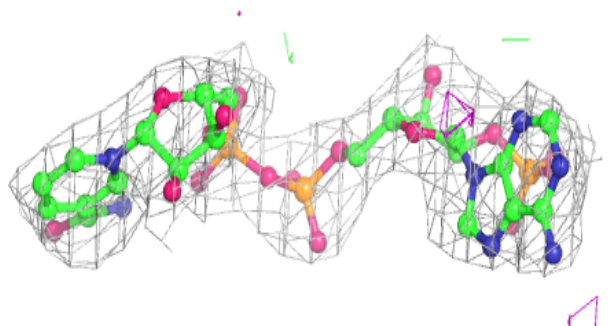
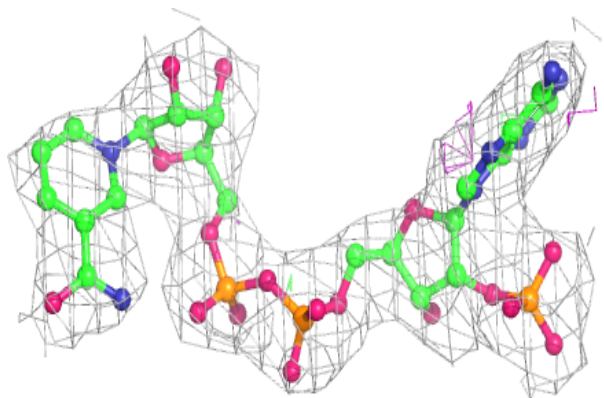


Electron density around NAP A 901:

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

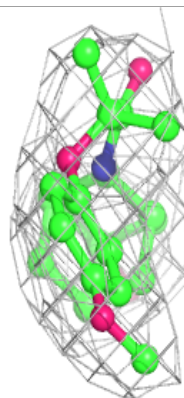
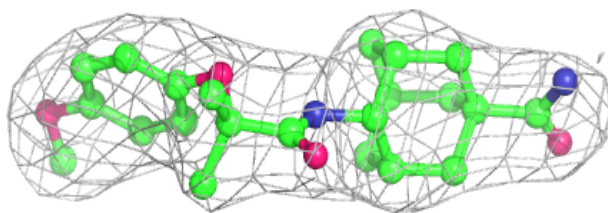
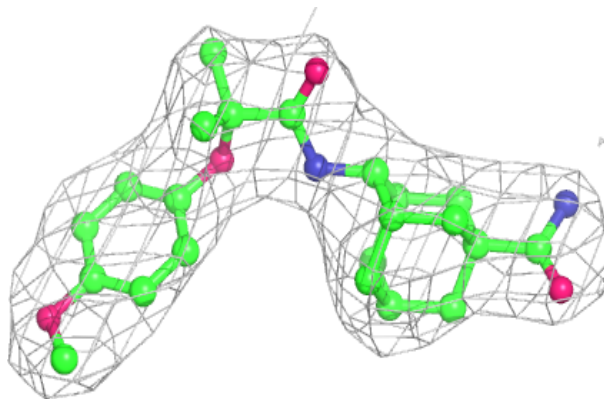
**Electron density around NAP G 901:**

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

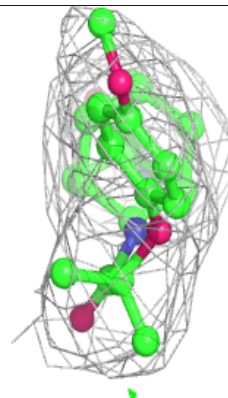
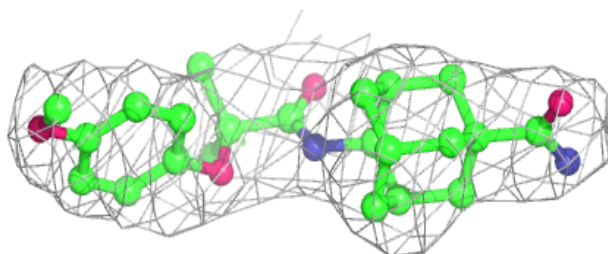
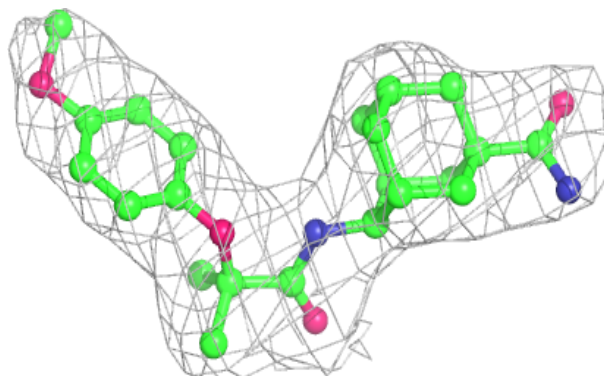


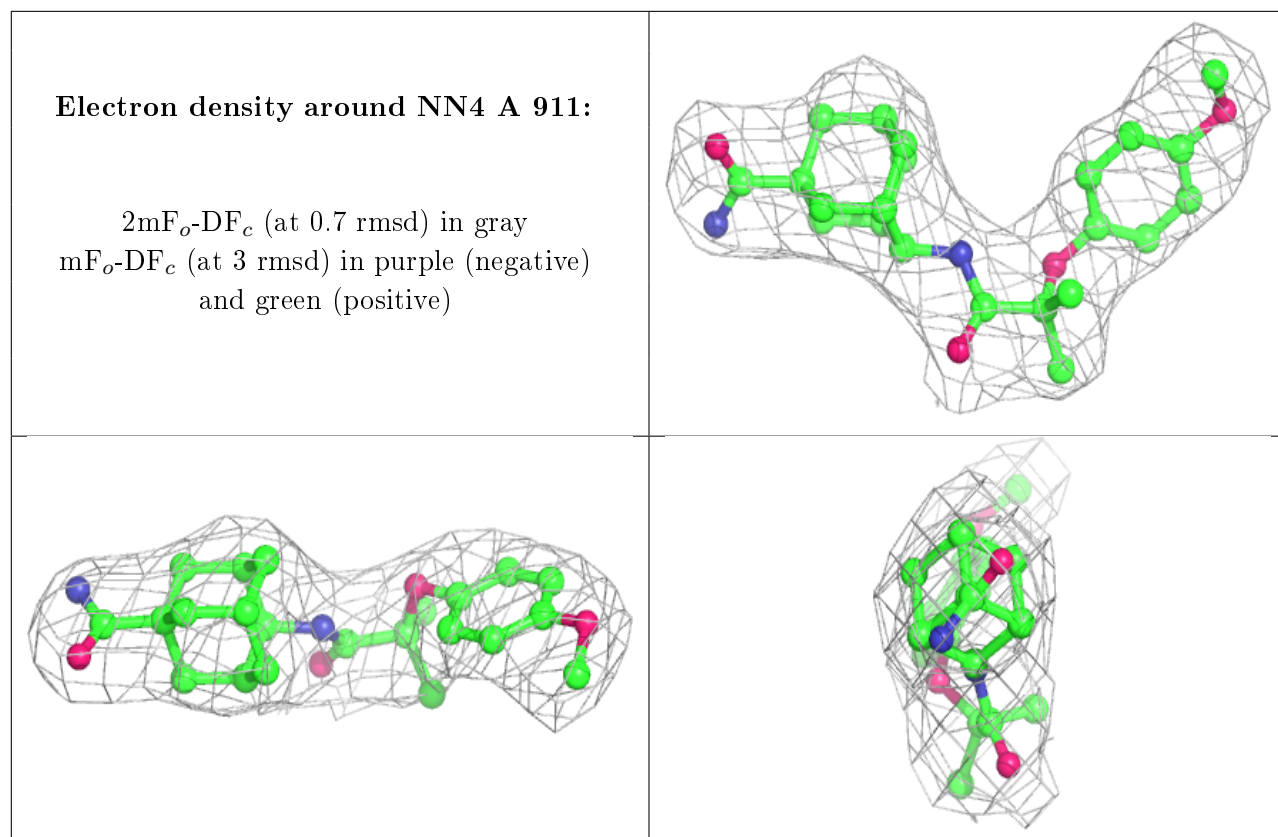
Electron density around NN4 G 911:

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

**Electron density around NN4 E 911:**

$2mF_o-DF_c$ (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.