



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:10 AM UTC

PDB ID : 2IRW / pdb_00002irw
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 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

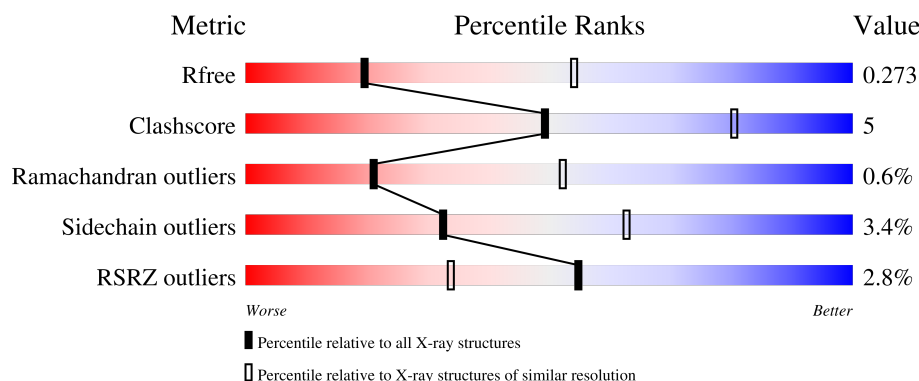
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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 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	264	 3% 90% 9% .
1	B	264	 2% 89% 10% .
1	C	264	 6% 83% 14% .
1	D	264	 3% 88% 12% .
1	E	264	 2% 83% 14% .

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Mol	Chain	Length	Quality of chain
1	F	264	% 82% 18%
1	G	264	3% 84% 14%
1	H	264	2% 78% 20%

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.

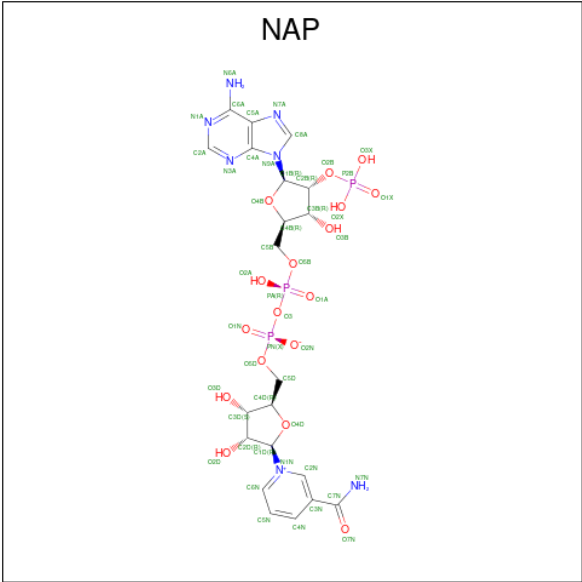
- Molecule 1 is a protein called Corticosteroid 11-beta-dehydrogenase isozyme 1.

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:

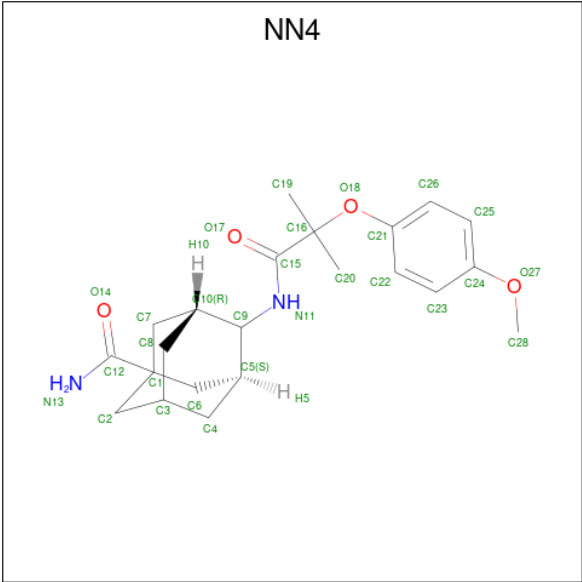
Chain	Residue	Modelled	Actual	Comment	Reference
A	272	SER	CYS	conflict	UNP P28845
B	272	SER	CYS	conflict	UNP P28845
C	272	SER	CYS	conflict	UNP P28845
D	272	SER	CYS	conflict	UNP P28845
E	272	SER	CYS	conflict	UNP P28845
F	272	SER	CYS	conflict	UNP P28845
G	272	SER	CYS	conflict	UNP P28845
H	272	SER	CYS	conflict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

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



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-METHYLPROPANOYL]AMINO}ADAMANTANE-1-CARBOXAMIDE (CCD ID: 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		

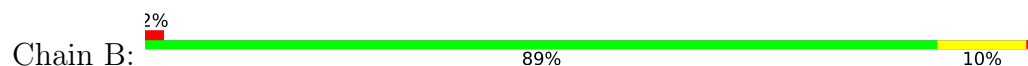
3 Residue-property plots

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.

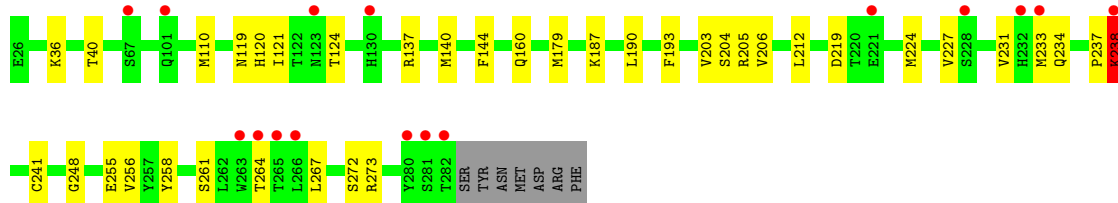
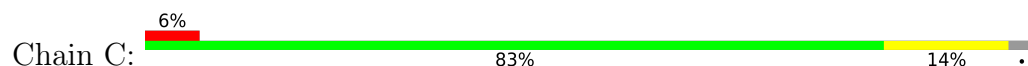
- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1



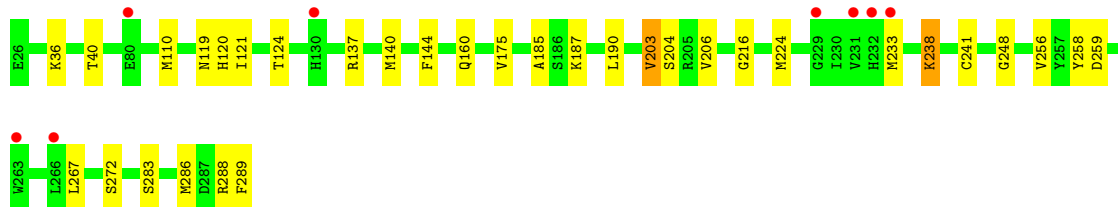
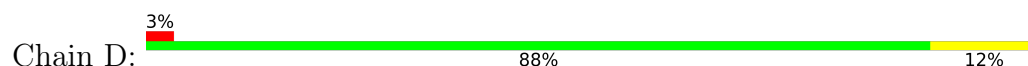
- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1



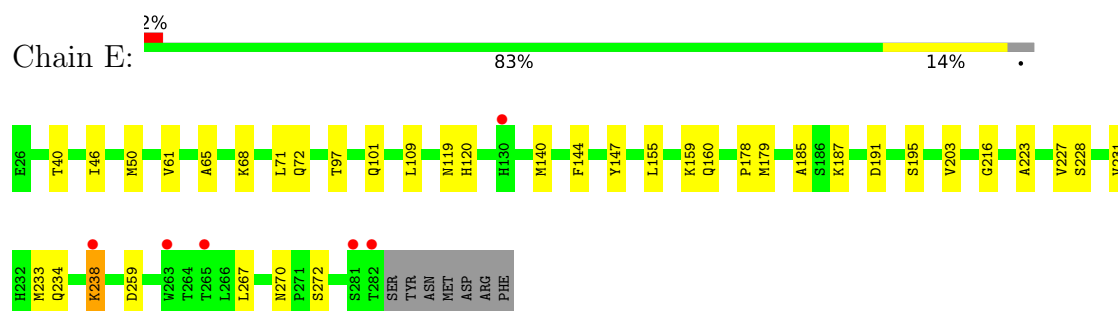
- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1



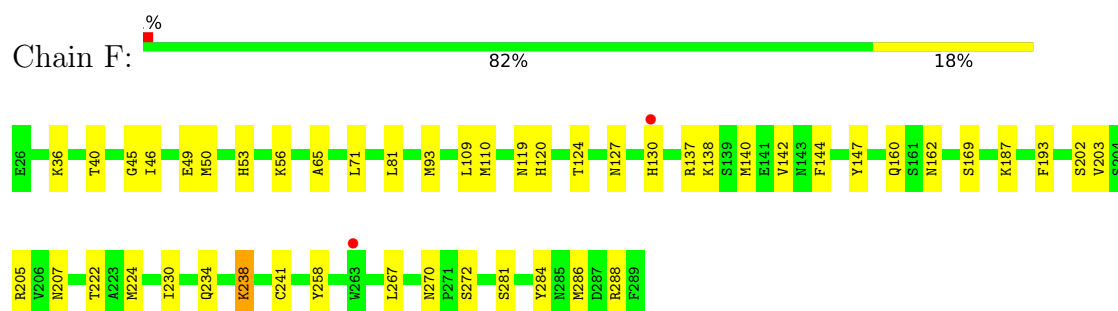
- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1



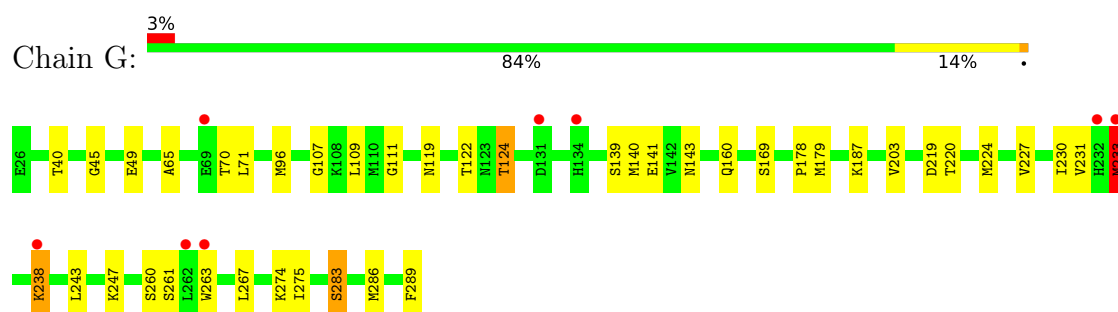
- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1



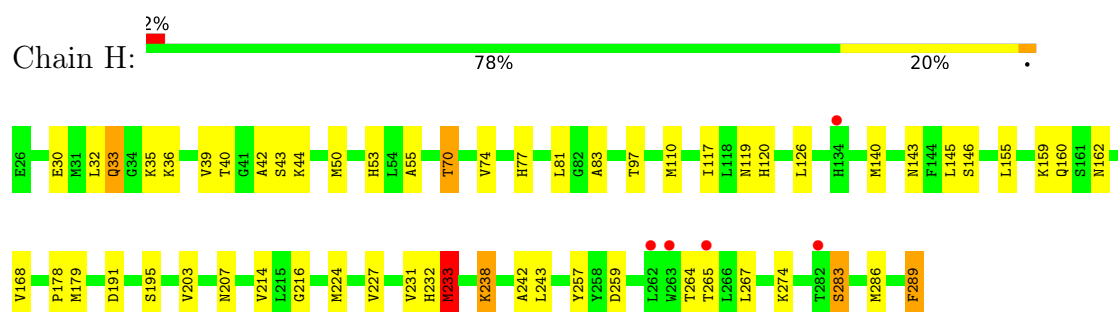
- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1



- 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 – 3.10 182.57 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (182.57-3.10) 99.9 (182.57-3.10)	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 , 0.273	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 , 18.2	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	0.67	1/2066 (0.0%)	0.85	1/2788 (0.0%)
1	B	0.67	2/2066 (0.1%)	0.85	1/2788 (0.0%)
1	C	0.66	1/2000 (0.1%)	0.86	0/2700
1	D	0.66	1/2066 (0.0%)	0.85	0/2788
1	E	0.72	1/2000 (0.1%)	0.89	0/2700
1	F	0.61	1/2066 (0.0%)	0.87	0/2788
1	G	0.75	2/2066 (0.1%)	0.88	1/2788 (0.0%)
1	H	0.60	1/2066 (0.0%)	0.89	1/2788 (0.0%)
All	All	0.67	10/16396 (0.1%)	0.87	4/22128 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	238	LYS	CE-NZ	21.01	2.12	1.49
1	E	238	LYS	CE-NZ	19.22	2.07	1.49
1	B	238	LYS	CE-NZ	16.28	1.98	1.49
1	A	238	LYS	CE-NZ	16.13	1.97	1.49
1	D	238	LYS	CE-NZ	15.69	1.96	1.49
1	C	238	LYS	CE-NZ	15.53	1.96	1.49
1	F	238	LYS	CE-NZ	11.96	1.85	1.49
1	H	238	LYS	CE-NZ	7.19	1.71	1.49
1	B	238	LYS	CD-CE	5.63	1.69	1.52
1	G	238	LYS	CD-CE	5.01	1.67	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	233	MET	N-CA-C	7.14	119.19	110.41
1	A	233	MET	N-CA-C	6.98	119.00	110.41
1	H	233	MET	N-CA-C	6.77	119.07	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	233	MET	N-CA-C	5.33	122.14	110.80

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	16	0
1	B	2031	0	2075	19	0
1	C	1967	0	2020	27	0
1	D	2031	0	2075	24	0
1	E	1967	0	2020	26	0
1	F	2031	0	2075	32	0
1	G	2031	0	2075	26	0
1	H	2031	0	2075	38	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	182	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 (182) 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:CE	1:H:238:LYS:NZ	1.70	1.50
1:F:238:LYS:CE	1:F:238:LYS:NZ	1.85	1.39
1:A:238:LYS:CE	1:A:238:LYS:NZ	1.97	1.27
1:C:238:LYS:NZ	1:C:238:LYS:CE	1.95	1.27
1:D:238:LYS:CE	1:D:238:LYS:NZ	1.96	1.27
1:B:238:LYS:CE	1:B:238:LYS:NZ	1.98	1.25
1:E:238:LYS:CE	1:E:238:LYS:NZ	2.07	1.17
1:G:238:LYS:NZ	1:G:238:LYS:CE	2.12	1.11
1:C:140:MET:HE2	1:D:140:MET:HE2	1.39	1.04
1:A:140:MET:HE2	1:B:140:MET:HE2	1.45	0.95
1:G:140:MET:HE2	1:H:140:MET:HE2	1.55	0.87
1:E:140:MET:HE2	1:F:140:MET:HE2	1.58	0.83
1:H:232:HIS:HB2	1:H:233:MET:SD	2.21	0.79
1:E:179:MET:SD	1:F:286:MET:HE1	2.23	0.78
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:SD	1:B:233:MET:N	2.61	0.74
1:A:233:MET:SD	1:A:233:MET:N	2.63	0.71
1:H:203:VAL:HG21	1:H:286:MET:HE3	1.72	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: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:F:93:MET:HG3	1:F:120:HIS:CE1	2.35	0.61
1:H:224:MET:HA	1:H:224:MET:HE2	1.83	0.61
1:G:179:MET:HE3	1:H:289:PHE:CE1	2.36	0.60
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:G:286:MET:HE1	1:H:178:PRO:HB2	1.86	0.57
1:D:241:CYS:HB2	1:D:258:TYR:CE1	2.39	0.57
1:H:126:LEU:HB3	1:H:179:MET:HE2	1.87	0.56
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:F:46:ILE:HG22	1:F:50:MET:HE2	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:MET:HE2	1:D:140:MET:CE	2.27	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:G:179:MET:HE1	1:G:230:ILE:HG21	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:A:224:MET:HA	1:A:224:MET:HE2	1.89	0.53
1:F:119:ASN:ND2	2:F:901:NAP:H4D	2.24	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:224:MET:HA	1:B:224:MET:HE2	1.91	0.52
1:B:227:VAL:HB	1:B:231:VAL:HB	1.91	0.52
1:C:179:MET:HG3	1:D:286:MET:HE1	1.91	0.51
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:224:MET:HA	1:G:224:MET:HE2	1.90	0.51
1:H:203:VAL:CG2	1:H:286:MET:HE3	2.40	0.51
1:E:270:ASN:HD22	1:E:270:ASN:C	2.19	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:E:140:MET:CE	1:F:140:MET:HE2	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:224:MET:HA	1:F:224:MET:HE2	1.96	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:224:MET:HA	1:C:224:MET:HE2	1.94	0.48
1:C:261:SER:HB3	1:C:264:THR:OG1	2.13	0.48
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:H:264:THR:O	1:H:265:THR:C	2.58	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: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
1:C:273:ARG:HG3	1:D:175:VAL:HG12	1.97	0.46
1:A:286:MET:HE1	1:B:179:MET:SD	2.56	0.45
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:55:ALA:HA	1:H:83:ALA:HB2	1.98	0.45
1:H:231:VAL:HG12	1:H:232:HIS:N	2.31	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:68:LYS:O	1:E:72:GLN:HG3	2.18	0.44
1:E:191:ASP:O	1:E:195:SER:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:203:VAL:C	1:F:205:ARG:H	2.25	0.44
1:C:219:ASP:OD1	1:C:237:PRO:HA	2.18	0.44
1:H:53:HIS:ND1	1:H:243:LEU:HD13	2.33	0.43
1:D:224:MET:HA	1:D:224:MET:HE2	1.99	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: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: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:E:46:ILE:HG22	1:E:50:MET:HE2	2.00	0.42
1:G:187:LYS:HE3	2:G:901:NAP:O2D	2.19	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:G:178:PRO:HB2	1:H:286:MET:HE1	2.01	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:F:56:LYS:HE3	1:F:81:LEU:HD22	2.02	0.42
1:A:40:THR:CB	1:A:120:HIS:HD2	2.33	0.42
1:A:231:VAL:HG12	1:A:232:HIS:N	2.35	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:C:179:MET:SD	1:D:286:MET:HE1	2.60	0.41
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:G:96:MET:HE1	1:G:141:GLU:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:203:VAL:HG21	1:G:286:MET:HE3	2.02	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
1:E:40:THR:HG1	1:E:119:ASN:H	1.69	0.41
3:G:911:NN4:H283	3:G:911:NN4:H23	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	262/264 (99%)	247 (94%)	12 (5%)	3 (1%)	11	39
1	B	262/264 (99%)	244 (93%)	16 (6%)	2 (1%)	16	47
1	C	255/264 (97%)	243 (95%)	11 (4%)	1 (0%)	30	61
1	D	262/264 (99%)	251 (96%)	10 (4%)	1 (0%)	30	61
1	E	255/264 (97%)	242 (95%)	13 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	262/264 (99%)	249 (95%)	13 (5%)	0	100	100
1	G	262/264 (99%)	245 (94%)	14 (5%)	3 (1%)	11	39
1	H	262/264 (99%)	233 (89%)	27 (10%)	2 (1%)	16	47
All	All	2082/2112 (99%)	1954 (94%)	116 (6%)	12 (1%)	21	52

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%)	214 (97%)	7 (3%)	34	64
1	B	221/221 (100%)	213 (96%)	8 (4%)	31	62
1	C	214/221 (97%)	209 (98%)	5 (2%)	44	70
1	D	221/221 (100%)	216 (98%)	5 (2%)	44	70
1	E	214/221 (97%)	209 (98%)	5 (2%)	44	70
1	F	221/221 (100%)	211 (96%)	10 (4%)	24	56
1	G	221/221 (100%)	212 (96%)	9 (4%)	27	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	221/221 (100%)	210 (95%)	11 (5%)	22	53
All	All	1754/1768 (99%)	1694 (97%)	60 (3%)	32	63

All (60) 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	233	MET
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	233	MET
1	B	238	LYS
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	203	VAL
1	C	238	LYS
1	D	124	THR
1	D	137	ARG
1	D	160	GLN
1	D	203	VAL
1	D	283	SER
1	E	61	VAL
1	E	109	LEU
1	E	160	GLN
1	E	203	VAL
1	E	234	GLN
1	F	109	LEU
1	F	124	THR
1	F	127	ASN
1	F	130	HIS
1	F	137	ARG
1	F	160	GLN

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Mol	Chain	Res	Type
1	F	202	SER
1	F	222	THR
1	F	234	GLN
1	F	288	ARG
1	G	70	THR
1	G	109	LEU
1	G	124	THR
1	G	160	GLN
1	G	260	SER
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	117	ILE
1	H	143	ASN
1	H	145	LEU
1	H	160	GLN
1	H	233	MET
1	H	274	LYS
1	H	283	SER
1	H	289	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	A	119	ASN
1	A	120	HIS
1	A	130	HIS
1	A	207	ASN
1	A	270	ASN
1	B	77	HIS
1	B	101	GLN
1	B	119	ASN
1	B	120	HIS
1	B	130	HIS
1	B	207	ASN
1	B	270	ASN
1	C	101	GLN

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Mol	Chain	Res	Type
1	C	105	GLN
1	C	119	ASN
1	C	120	HIS
1	C	234	GLN
1	C	270	ASN
1	D	77	HIS
1	D	101	GLN
1	D	105	GLN
1	D	119	ASN
1	D	120	HIS
1	D	127	ASN
1	D	270	ASN
1	D	285	ASN
1	E	119	ASN
1	E	120	HIS
1	E	270	ASN
1	F	53	HIS
1	F	101	GLN
1	F	119	ASN
1	F	120	HIS
1	F	127	ASN
1	F	134	HIS
1	F	270	ASN
1	F	285	ASN
1	G	119	ASN
1	G	120	HIS
1	G	207	ASN
1	G	270	ASN
1	H	33	GLN
1	H	119	ASN
1	H	120	HIS
1	H	130	HIS
1	H	207	ASN
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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NN4	B	911	-	31,31,31	1.28	3 (9%)	44,48,48	1.36	5 (11%)
3	NN4	D	911	-	31,31,31	1.14	4 (12%)	44,48,48	1.20	4 (9%)
3	NN4	F	911	-	31,31,31	1.06	4 (12%)	44,48,48	1.23	5 (11%)
2	NAP	E	901	-	50,52,52	1.65	5 (10%)	71,80,80	1.46	9 (12%)
2	NAP	A	901	-	50,52,52	1.63	4 (8%)	71,80,80	1.45	8 (11%)
2	NAP	F	901	-	50,52,52	1.77	6 (12%)	71,80,80	1.47	10 (14%)
2	NAP	H	901	-	50,52,52	1.64	6 (12%)	71,80,80	1.44	10 (14%)
3	NN4	A	911	-	31,31,31	1.17	3 (9%)	44,48,48	1.22	3 (6%)
2	NAP	C	901	-	50,52,52	1.61	5 (10%)	71,80,80	1.44	8 (11%)
3	NN4	C	911	-	31,31,31	1.17	4 (12%)	44,48,48	1.22	5 (11%)
2	NAP	G	901	-	50,52,52	1.65	6 (12%)	71,80,80	1.49	9 (12%)
3	NN4	E	911	-	31,31,31	1.27	3 (9%)	44,48,48	1.32	5 (11%)
3	NN4	H	911	-	31,31,31	1.23	2 (6%)	44,48,48	1.32	6 (13%)
3	NN4	G	911	-	31,31,31	1.03	3 (9%)	44,48,48	1.28	5 (11%)
2	NAP	B	901	-	50,52,52	1.64	5 (10%)	71,80,80	1.39	8 (11%)
2	NAP	D	901	-	50,52,52	1.77	6 (12%)	71,80,80	1.44	9 (12%)

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	B	911	-	-	5/23/54/54	0/5/4/4
3	NN4	D	911	-	-	3/23/54/54	0/5/4/4
3	NN4	F	911	-	-	3/23/54/54	0/5/4/4
2	NAP	E	901	-	-	4/35/67/67	0/5/5/5
2	NAP	A	901	-	-	1/35/67/67	0/5/5/5
2	NAP	F	901	-	-	6/35/67/67	0/5/5/5
2	NAP	H	901	-	-	3/35/67/67	0/5/5/5
3	NN4	A	911	-	-	3/23/54/54	0/5/4/4
2	NAP	C	901	-	-	5/35/67/67	0/5/5/5
3	NN4	C	911	-	-	4/23/54/54	0/5/4/4
2	NAP	G	901	-	-	5/35/67/67	0/5/5/5
3	NN4	E	911	-	-	7/23/54/54	0/5/4/4
3	NN4	H	911	-	-	5/23/54/54	0/5/4/4
3	NN4	G	911	-	-	3/23/54/54	0/5/4/4
2	NAP	B	901	-	-	1/35/67/67	0/5/5/5
2	NAP	D	901	-	-	5/35/67/67	0/5/5/5

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	901	NAP	O7N-C7N	9.82	1.42	1.24
2	F	901	NAP	O7N-C7N	9.12	1.41	1.24
2	A	901	NAP	O7N-C7N	9.07	1.41	1.24
2	B	901	NAP	O7N-C7N	9.07	1.41	1.24
2	E	901	NAP	O7N-C7N	9.04	1.41	1.24
2	G	901	NAP	O7N-C7N	9.00	1.40	1.24
2	H	901	NAP	O7N-C7N	8.85	1.40	1.24
2	C	901	NAP	O7N-C7N	8.80	1.40	1.24
3	B	911	NN4	C1-C12	-4.78	1.49	1.53
3	H	911	NN4	C1-C12	-4.61	1.50	1.53
3	A	911	NN4	C1-C12	-4.25	1.50	1.53
3	E	911	NN4	C16-C15	-4.24	1.49	1.53
2	F	901	NAP	PA-O3	3.91	1.63	1.59
3	E	911	NN4	C1-C12	-3.78	1.50	1.53
3	D	911	NN4	C16-C15	-3.77	1.50	1.53
3	C	911	NN4	C1-C12	-3.74	1.50	1.53
3	D	911	NN4	C12-N13	3.12	1.38	1.32
3	G	911	NN4	C1-C12	-3.03	1.51	1.53
2	H	901	NAP	C2A-N1A	3.01	1.39	1.33
3	F	911	NN4	C12-N13	3.01	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	NAP	C2A-N1A	2.99	1.39	1.33
3	B	911	NN4	C16-C15	-2.98	1.50	1.53
2	F	901	NAP	C2A-N1A	2.94	1.39	1.33
3	C	911	NN4	C16-C15	-2.92	1.50	1.53
3	G	911	NN4	C12-N13	2.91	1.38	1.32
2	F	901	NAP	C2A-N3A	2.84	1.39	1.33
3	F	911	NN4	C1-C12	-2.84	1.51	1.53
2	D	901	NAP	C2A-N1A	2.83	1.39	1.33
3	B	911	NN4	C12-N13	2.81	1.38	1.32
2	D	901	NAP	C2A-N3A	2.81	1.38	1.33
3	G	911	NN4	C16-C15	-2.76	1.51	1.53
3	F	911	NN4	C16-C15	-2.74	1.51	1.53
2	C	901	NAP	C2A-N3A	2.72	1.38	1.33
3	A	911	NN4	C12-N13	2.69	1.37	1.32
3	C	911	NN4	C12-N13	2.69	1.37	1.32
2	E	901	NAP	C2A-N3A	2.62	1.38	1.33
3	H	911	NN4	C12-N13	2.61	1.37	1.32
2	D	901	NAP	C8A-N7A	2.61	1.36	1.31
2	C	901	NAP	C2A-N1A	2.61	1.38	1.33
2	G	901	NAP	C2A-N1A	2.59	1.38	1.33
2	E	901	NAP	C2A-N1A	2.56	1.38	1.33
2	B	901	NAP	C2A-N3A	2.54	1.38	1.33
2	H	901	NAP	C2A-N3A	2.53	1.38	1.33
2	D	901	NAP	C2N-N1N	2.51	1.37	1.35
3	C	911	NN4	C15-N11	2.48	1.38	1.34
2	F	901	NAP	C8A-N7A	2.47	1.36	1.31
2	A	901	NAP	C2A-N1A	2.43	1.38	1.33
3	F	911	NN4	C15-N11	2.41	1.38	1.34
2	H	901	NAP	C2N-N1N	2.39	1.37	1.35
2	B	901	NAP	C2N-N1N	2.37	1.37	1.35
3	D	911	NN4	C15-N11	2.37	1.38	1.34
2	G	901	NAP	C2A-N3A	2.36	1.38	1.33
3	A	911	NN4	C16-C15	-2.35	1.51	1.53
3	D	911	NN4	C1-C12	-2.34	1.51	1.53
2	F	901	NAP	PN-O3	2.29	1.62	1.59
3	E	911	NN4	C12-N13	2.25	1.37	1.32
2	H	901	NAP	C8A-N7A	2.25	1.36	1.31
2	D	901	NAP	PA-O3	2.24	1.61	1.59
2	A	901	NAP	C8A-N7A	2.23	1.36	1.31
2	A	901	NAP	C2A-N3A	2.23	1.37	1.33
2	G	901	NAP	C2N-N1N	2.21	1.37	1.35
2	E	901	NAP	C8A-N7A	2.19	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	901	NAP	C5A-N7A	-2.16	1.35	1.39
2	B	901	NAP	C8A-N7A	2.13	1.35	1.31
2	C	901	NAP	C8A-N7A	2.10	1.35	1.31
2	H	901	NAP	C5A-N7A	-2.07	1.35	1.39
2	G	901	NAP	C8A-N7A	2.06	1.35	1.31
2	C	901	NAP	C2N-N1N	2.06	1.37	1.35
2	E	901	NAP	C2N-N1N	2.04	1.37	1.35

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	901	NAP	N3A-C2A-N1A	-5.81	119.78	128.58
2	E	901	NAP	N3A-C2A-N1A	-5.80	119.81	128.58
2	H	901	NAP	N3A-C2A-N1A	-5.67	120.00	128.58
2	G	901	NAP	N3A-C2A-N1A	-5.65	120.03	128.58
2	B	901	NAP	N3A-C2A-N1A	-5.53	120.20	128.58
2	D	901	NAP	N3A-C2A-N1A	-5.46	120.31	128.58
2	A	901	NAP	N3A-C2A-N1A	-5.39	120.43	128.58
2	F	901	NAP	N3A-C2A-N1A	-5.30	120.56	128.58
3	G	911	NN4	C28-O27-C24	-5.11	106.55	117.50
3	H	911	NN4	C1-C12-N13	-4.86	112.28	117.54
3	D	911	NN4	C16-O18-C21	-4.65	114.16	120.98
3	F	911	NN4	C28-O27-C24	-4.61	107.61	117.50
2	G	901	NAP	C5A-C4A-N3A	-4.27	120.84	126.72
2	F	901	NAP	N9A-C8A-N7A	-4.27	107.88	113.94
2	G	901	NAP	N9A-C8A-N7A	-4.24	107.91	113.94
3	E	911	NN4	C16-O18-C21	-4.24	114.76	120.98
2	E	901	NAP	N9A-C8A-N7A	-4.23	107.93	113.94
3	D	911	NN4	C28-O27-C24	-4.22	108.44	117.50
2	D	901	NAP	C5A-C4A-N3A	-4.20	120.93	126.72
2	A	901	NAP	N9A-C8A-N7A	-4.19	108.00	113.94
3	B	911	NN4	C1-C12-N13	-4.16	113.04	117.54
2	A	901	NAP	C5A-C4A-N3A	-4.09	121.08	126.72
3	E	911	NN4	C28-O27-C24	-4.08	108.75	117.50
2	H	901	NAP	C5A-C4A-N3A	-4.08	121.10	126.72
3	A	911	NN4	C28-O27-C24	-4.08	108.76	117.50
2	C	901	NAP	C5A-C4A-N3A	-4.06	121.12	126.72
2	D	901	NAP	N9A-C8A-N7A	-4.04	108.21	113.94
2	E	901	NAP	C5A-C4A-N3A	-4.01	121.20	126.72
3	B	911	NN4	C16-O18-C21	-3.97	115.16	120.98
2	F	901	NAP	C5A-C4A-N3A	-3.95	121.28	126.72
3	A	911	NN4	C16-O18-C21	-3.89	115.27	120.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	911	NN4	C28-O27-C24	-3.88	109.17	117.50
2	B	901	NAP	C5A-C4A-N3A	-3.82	121.45	126.72
3	C	911	NN4	C28-O27-C24	-3.82	109.31	117.50
3	C	911	NN4	C16-O18-C21	-3.79	115.42	120.98
2	H	901	NAP	N9A-C8A-N7A	-3.78	108.58	113.94
2	C	901	NAP	N9A-C8A-N7A	-3.75	108.61	113.94
2	B	901	NAP	N9A-C8A-N7A	-3.69	108.70	113.94
2	G	901	NAP	C5A-N7A-C8A	3.67	109.22	103.45
2	F	901	NAP	C5A-N7A-C8A	3.65	109.19	103.45
3	G	911	NN4	C16-O18-C21	-3.64	115.64	120.98
2	A	901	NAP	C5A-N7A-C8A	3.53	109.00	103.45
2	H	901	NAP	C5A-N7A-C8A	3.53	108.99	103.45
3	C	911	NN4	C1-C12-N13	-3.51	113.74	117.54
2	D	901	NAP	C5A-N7A-C8A	3.47	108.90	103.45
3	F	911	NN4	C16-O18-C21	-3.46	115.90	120.98
3	H	911	NN4	C28-O27-C24	-3.35	110.31	117.50
2	C	901	NAP	C2A-N3A-C4A	3.34	119.99	111.83
2	E	901	NAP	C2A-N3A-C4A	3.34	119.98	111.83
2	G	901	NAP	C2A-N3A-C4A	3.30	119.88	111.83
2	E	901	NAP	C5A-N7A-C8A	3.29	108.62	103.45
3	E	911	NN4	C1-C12-N13	-3.27	114.00	117.54
2	D	901	NAP	C2A-N3A-C4A	3.26	119.79	111.83
2	B	901	NAP	C5A-N7A-C8A	3.24	108.55	103.45
2	F	901	NAP	C2A-N3A-C4A	3.18	119.61	111.83
2	A	901	NAP	C2A-N3A-C4A	3.16	119.56	111.83
2	H	901	NAP	C2A-N3A-C4A	3.13	119.47	111.83
2	B	901	NAP	C2A-N3A-C4A	3.12	119.46	111.83
2	C	901	NAP	C5A-N7A-C8A	3.10	108.33	103.45
3	H	911	NN4	C16-O18-C21	-3.01	116.56	120.98
3	A	911	NN4	C1-C12-N13	-2.90	114.41	117.54
2	F	901	NAP	C4A-C5A-N7A	-2.89	107.28	110.58
2	G	901	NAP	N3A-C4A-N9A	2.74	131.83	127.17
2	G	901	NAP	C4A-C5A-N7A	-2.69	107.51	110.58
2	C	901	NAP	N3A-C4A-N9A	2.67	131.70	127.17
2	D	901	NAP	N3A-C4A-N9A	2.66	131.69	127.17
3	E	911	NN4	O14-C12-C1	2.64	122.98	120.62
2	A	901	NAP	C4A-C5A-N7A	-2.64	107.57	110.58
2	E	901	NAP	N3A-C4A-N9A	2.63	131.63	127.17
2	D	901	NAP	C4A-C5A-N7A	-2.62	107.59	110.58
2	H	901	NAP	C4A-C5A-N7A	-2.61	107.60	110.58
2	A	901	NAP	N3A-C4A-N9A	2.61	131.60	127.17
3	H	911	NN4	O14-C12-C1	2.58	122.93	120.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	901	NAP	N3A-C4A-N9A	2.57	131.53	127.17
3	B	911	NN4	O17-C15-C16	2.55	124.12	120.88
3	G	911	NN4	C1-C12-N13	-2.53	114.81	117.54
3	H	911	NN4	O17-C15-C16	2.51	124.05	120.88
3	F	911	NN4	C1-C12-N13	-2.50	114.83	117.54
2	F	901	NAP	N3A-C4A-N9A	2.47	131.37	127.17
2	E	901	NAP	C4A-N9A-C8A	2.47	108.33	105.74
2	F	901	NAP	C4A-N9A-C8A	2.44	108.30	105.74
2	B	901	NAP	C4A-C5A-N7A	-2.44	107.80	110.58
2	B	901	NAP	N3A-C4A-N9A	2.41	131.26	127.17
2	F	901	NAP	P2B-O2B-C2B	-2.38	117.06	123.43
3	C	911	NN4	O14-C12-C1	2.35	122.72	120.62
3	G	911	NN4	O17-C15-C16	2.34	123.84	120.88
2	E	901	NAP	C4A-C5A-N7A	-2.31	107.94	110.58
2	A	901	NAP	C4A-N9A-C8A	2.27	108.12	105.74
3	F	911	NN4	O17-C15-N11	2.23	127.20	122.71
3	D	911	NN4	C1-C12-N13	-2.22	115.14	117.54
2	H	901	NAP	O2N-PN-O1N	2.20	122.67	112.44
2	G	901	NAP	C4A-N9A-C8A	2.18	108.02	105.74
2	B	901	NAP	O2N-PN-O1N	2.17	122.53	112.44
2	C	901	NAP	C4A-C5A-N7A	-2.16	108.12	110.58
2	E	901	NAP	O2N-PN-O1N	2.13	122.35	112.44
2	D	901	NAP	P2B-O2B-C2B	-2.13	117.75	123.43
3	F	911	NN4	O18-C16-C19	2.13	116.76	107.74
2	H	901	NAP	O3-PN-O1N	-2.12	104.32	110.70
2	C	901	NAP	O2N-PN-O1N	2.11	122.27	112.44
3	C	911	NN4	O18-C16-C19	2.09	116.61	107.74
2	D	901	NAP	C4A-N9A-C8A	2.09	107.93	105.74
2	F	901	NAP	O5D-C5D-C4D	2.07	116.03	108.99
3	E	911	NN4	O18-C16-C19	2.06	116.48	107.74
3	H	911	NN4	O18-C16-C19	2.06	116.48	107.74
3	G	911	NN4	O18-C16-C19	2.05	116.44	107.74
2	H	901	NAP	O4B-C1B-N9A	2.05	112.02	108.09
2	G	901	NAP	O4B-C1B-N9A	2.01	111.95	108.09
3	D	911	NN4	O18-C16-C19	2.01	116.26	107.74
3	B	911	NN4	O18-C16-C19	2.01	116.26	107.74

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	901	NAP	C5D-O5D-PN-O2N

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Mol	Chain	Res	Type	Atoms
2	F	901	NAP	O4D-C4D-C5D-O5D
3	A	911	NN4	C15-C16-O18-C21
3	A	911	NN4	C20-C16-O18-C21
3	B	911	NN4	C15-C16-O18-C21
3	B	911	NN4	C20-C16-O18-C21
3	C	911	NN4	C15-C16-O18-C21
3	C	911	NN4	C20-C16-O18-C21
3	D	911	NN4	C15-C16-O18-C21
3	D	911	NN4	C20-C16-O18-C21
3	E	911	NN4	C15-C16-O18-C21
3	E	911	NN4	C20-C16-O18-C21
3	F	911	NN4	C20-C16-O18-C21
3	G	911	NN4	C15-C16-O18-C21
3	G	911	NN4	C20-C16-O18-C21
3	H	911	NN4	C15-C16-O18-C21
3	H	911	NN4	C20-C16-O18-C21
2	D	901	NAP	O4D-C4D-C5D-O5D
3	H	911	NN4	C25-C24-O27-C28
3	H	911	NN4	C23-C24-O27-C28
2	C	901	NAP	O4D-C4D-C5D-O5D
2	F	901	NAP	C3D-C4D-C5D-O5D
2	F	901	NAP	O4B-C4B-C5B-O5B
3	F	911	NN4	C19-C16-O18-C21
3	F	911	NN4	C15-C16-O18-C21
2	D	901	NAP	C3D-C4D-C5D-O5D
3	A	911	NN4	C19-C16-O18-C21
3	B	911	NN4	C19-C16-O18-C21
3	C	911	NN4	C19-C16-O18-C21
3	D	911	NN4	C19-C16-O18-C21
3	E	911	NN4	C19-C16-O18-C21
3	G	911	NN4	C19-C16-O18-C21
3	H	911	NN4	C19-C16-O18-C21
2	G	901	NAP	PN-O3-PA-O1A
2	E	901	NAP	C2B-O2B-P2B-O3X
2	C	901	NAP	C3D-C4D-C5D-O5D
3	E	911	NN4	C25-C24-O27-C28
3	E	911	NN4	C23-C24-O27-C28
2	C	901	NAP	PN-O3-PA-O2A
2	D	901	NAP	PN-O3-PA-O2A
2	H	901	NAP	PN-O3-PA-O1A
2	G	901	NAP	O4D-C4D-C5D-O5D
2	F	901	NAP	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	E	901	NAP	PN-O3-PA-O2A
2	H	901	NAP	C2B-O2B-P2B-O3X
2	H	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	C	901	NAP	O4B-C4B-C5B-O5B
2	D	901	NAP	O4B-C4B-C5B-O5B
2	E	901	NAP	O4B-C4B-C5B-O5B
2	C	901	NAP	PN-O3-PA-O1A
2	D	901	NAP	PN-O3-PA-O1A
2	G	901	NAP	PN-O3-PA-O2A
3	C	911	NN4	C5-C9-N11-C15
3	E	911	NN4	C5-C9-N11-C15
2	G	901	NAP	O4B-C4B-C5B-O5B
2	A	901	NAP	C2B-O2B-P2B-O2X
2	F	901	NAP	C2B-O2B-P2B-O2X
2	G	901	NAP	C3D-C4D-C5D-O5D
3	E	911	NN4	C7-C1-C12-N13
2	E	901	NAP	PN-O3-PA-O1A

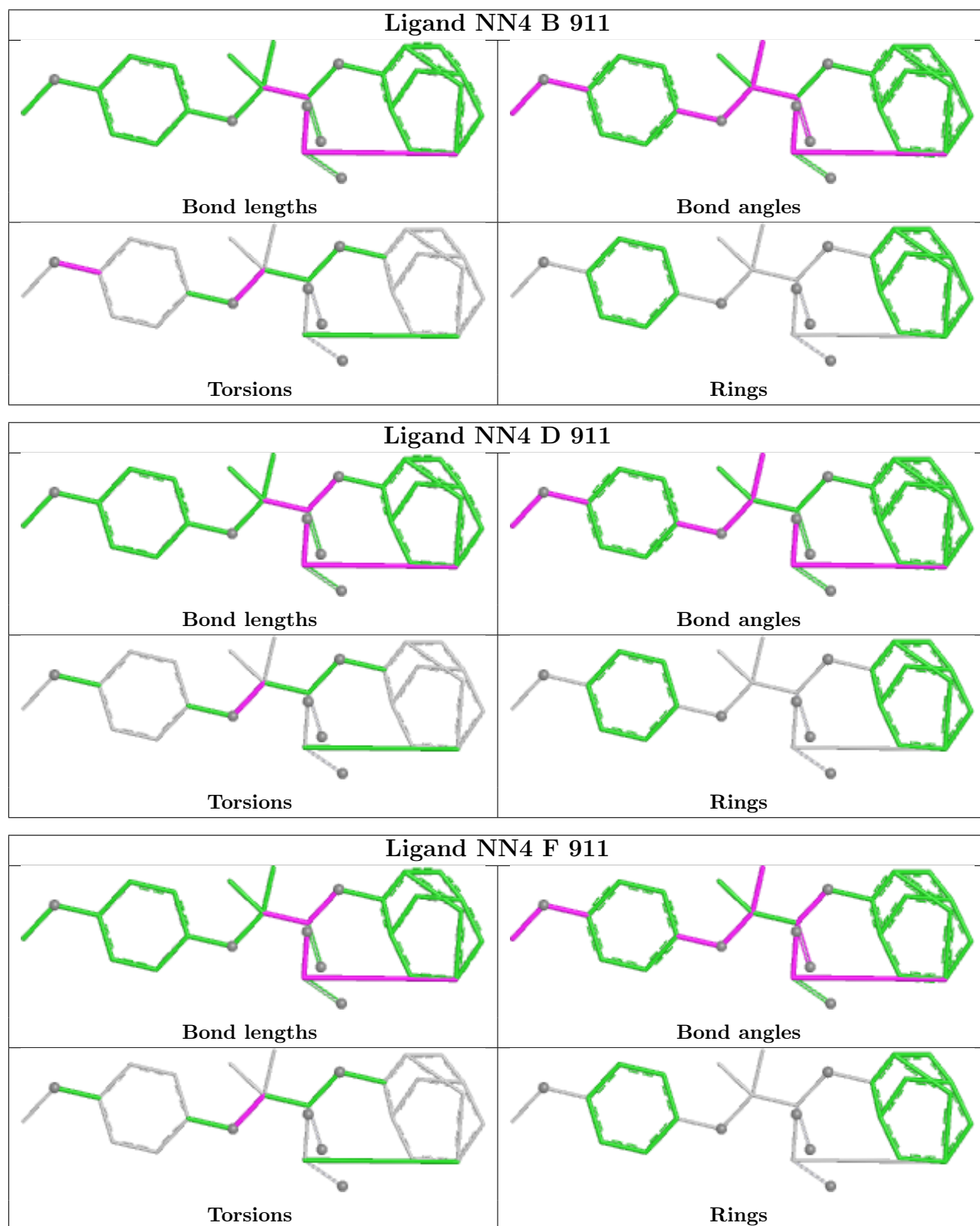
There are no ring outliers.

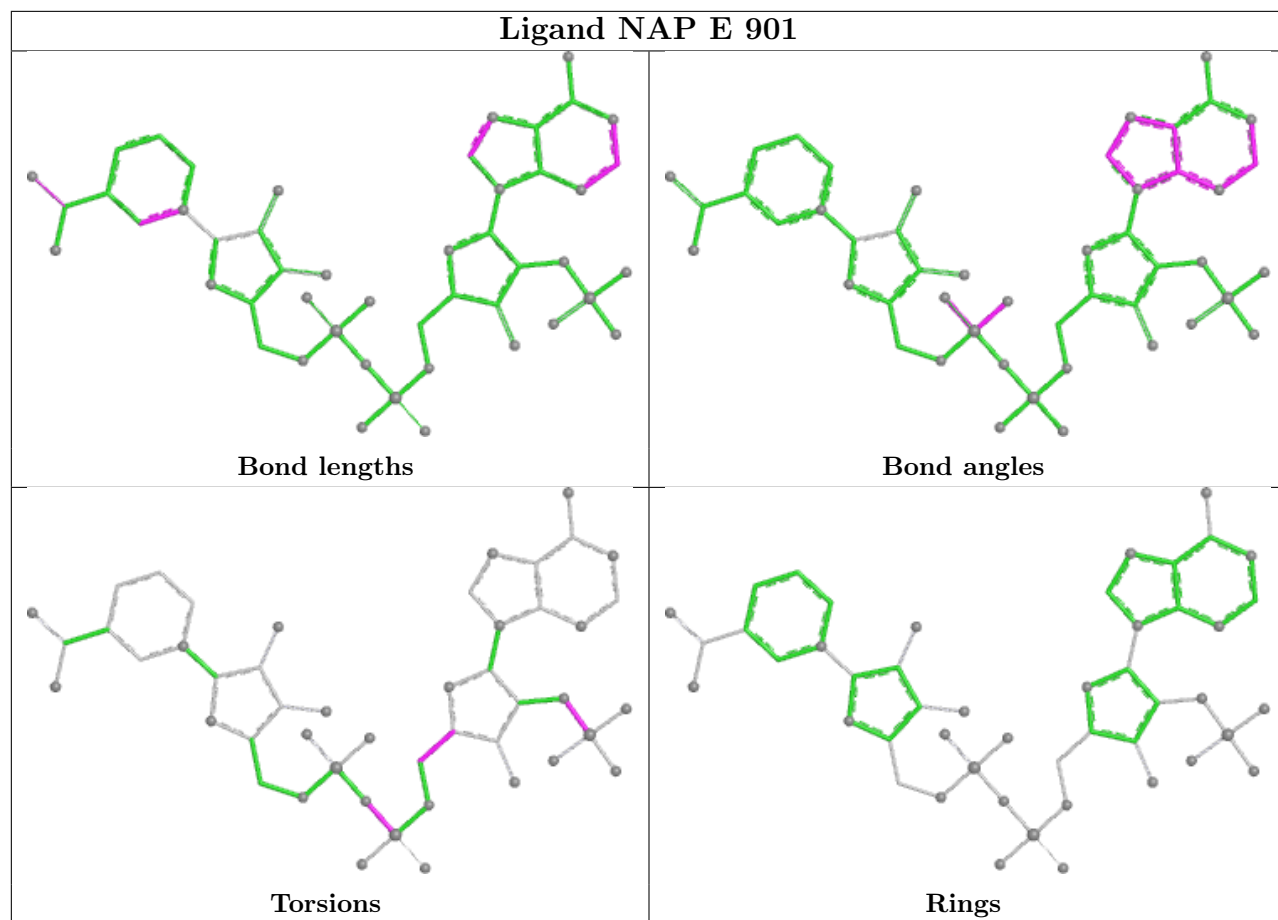
6 monomers are involved in 11 short contacts:

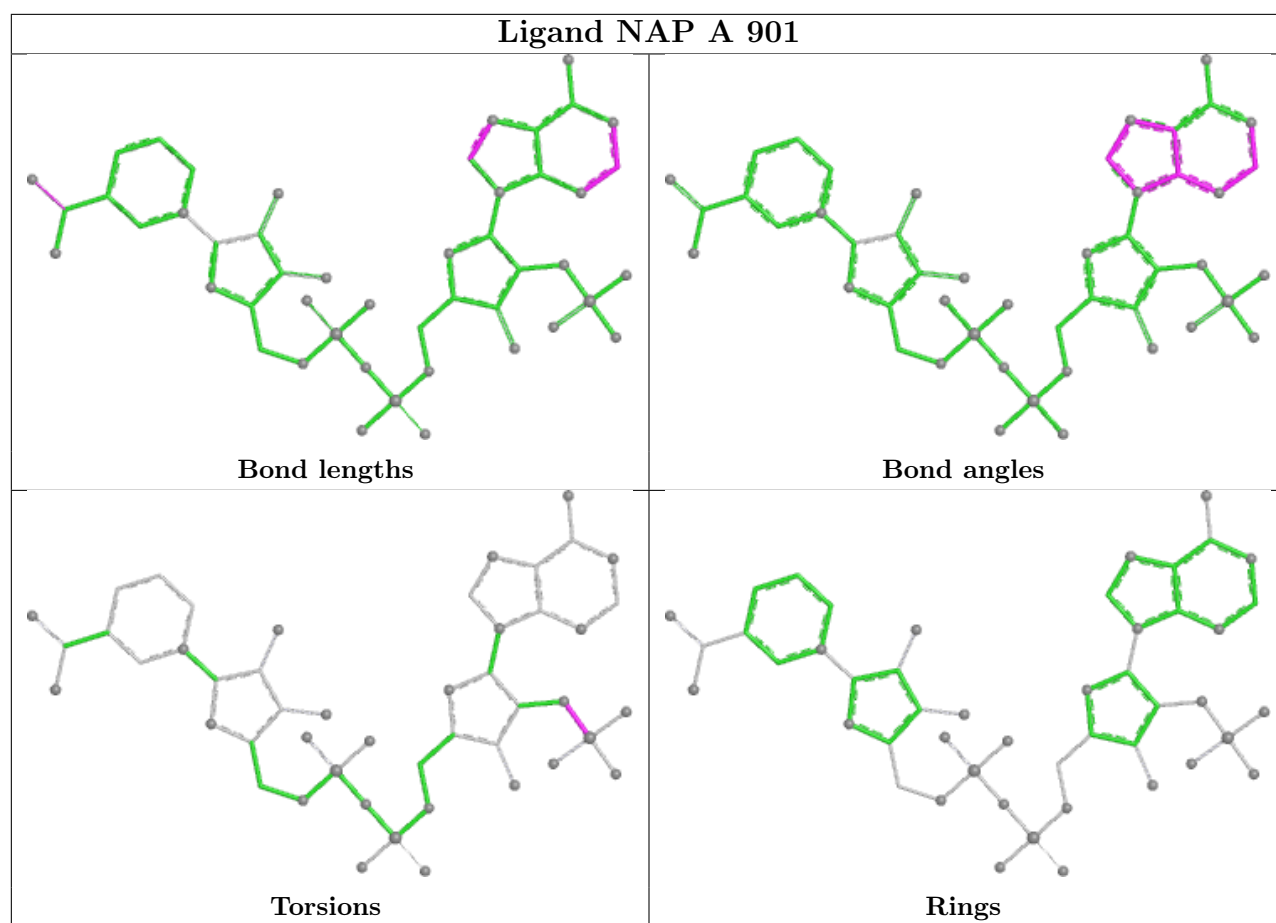
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	901	NAP	1	0
2	F	901	NAP	3	0
2	C	901	NAP	2	0
2	G	901	NAP	1	0
3	G	911	NN4	1	0
2	D	901	NAP	3	0

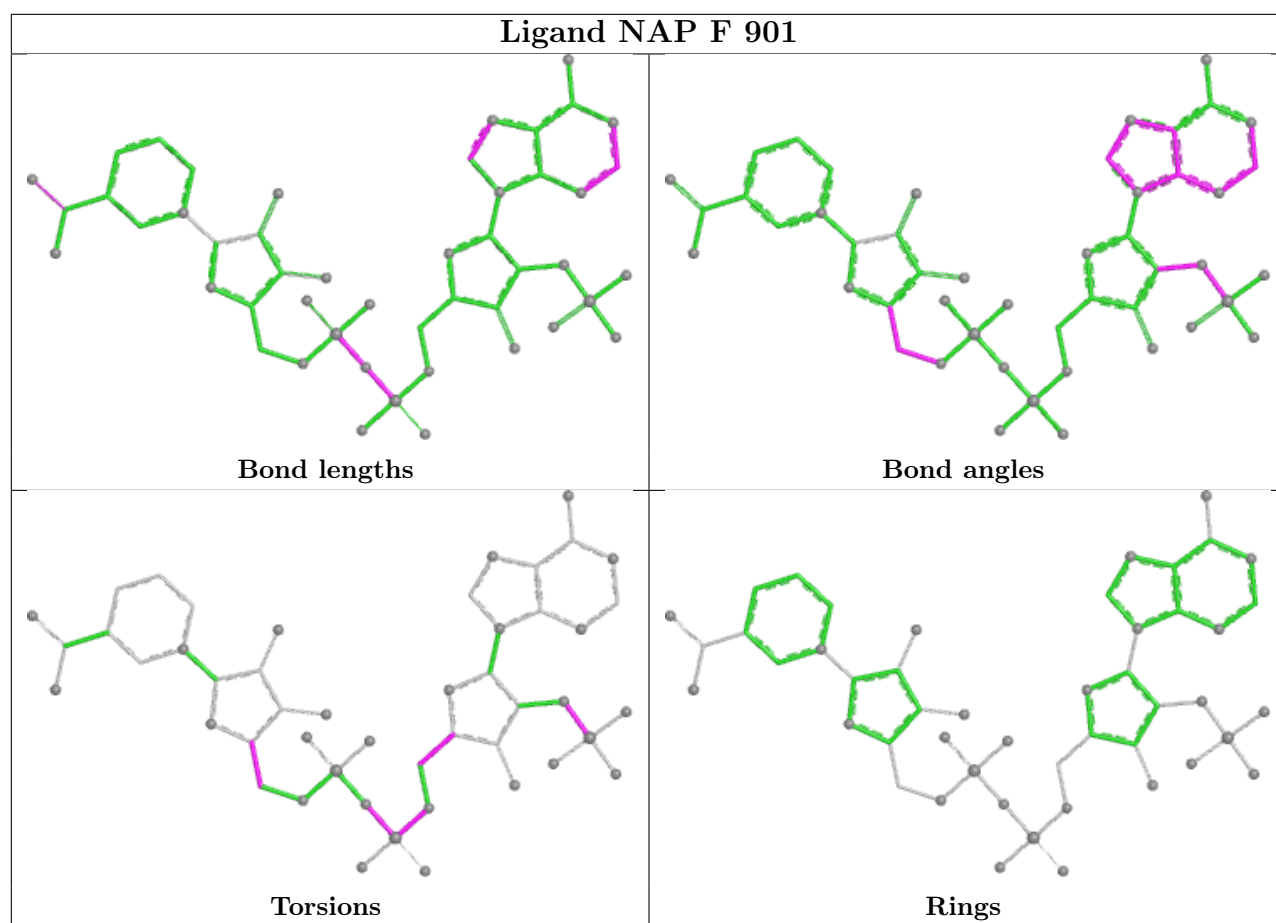
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

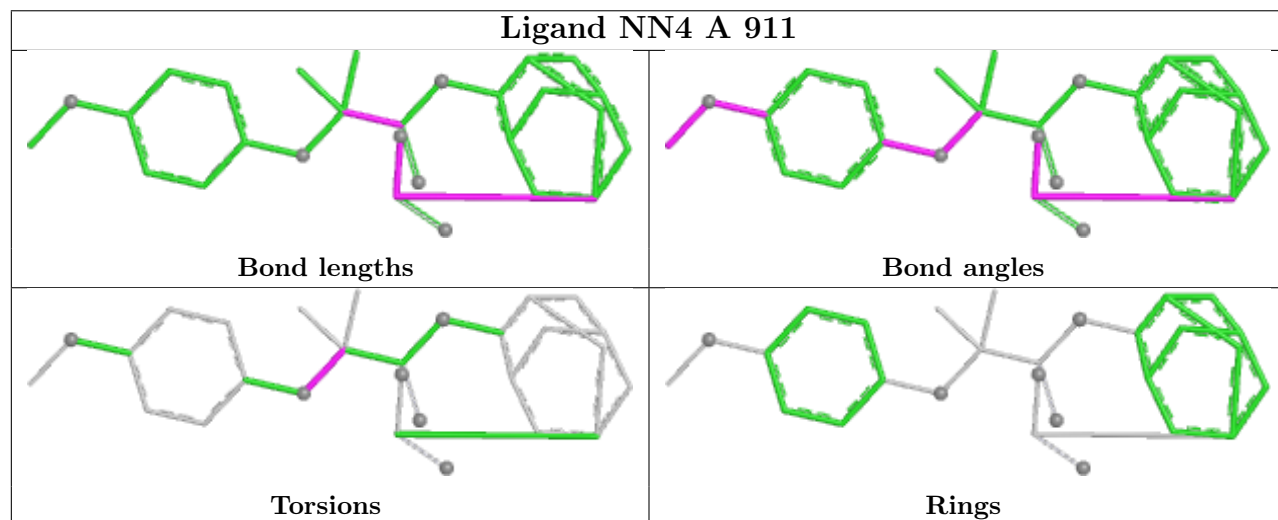
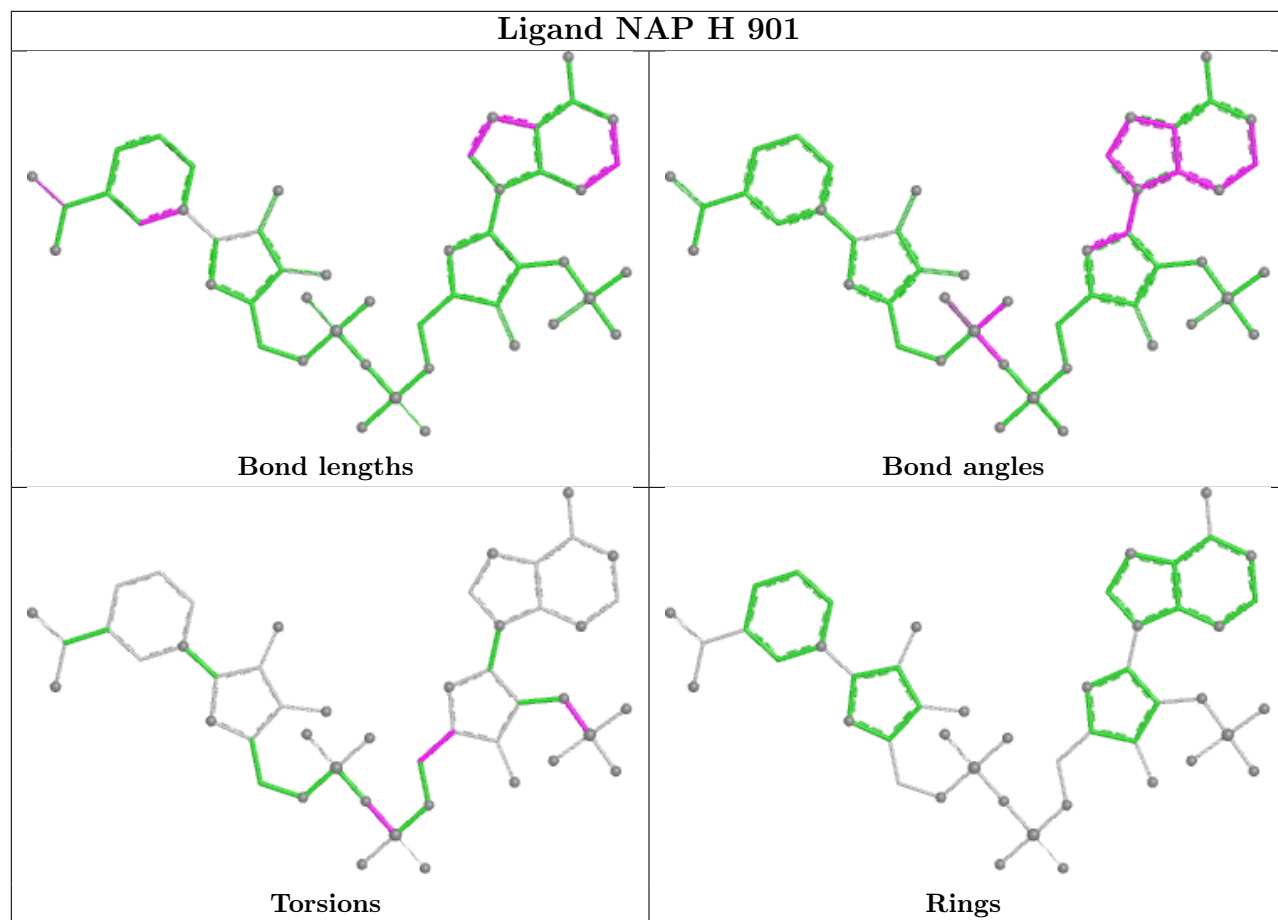
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

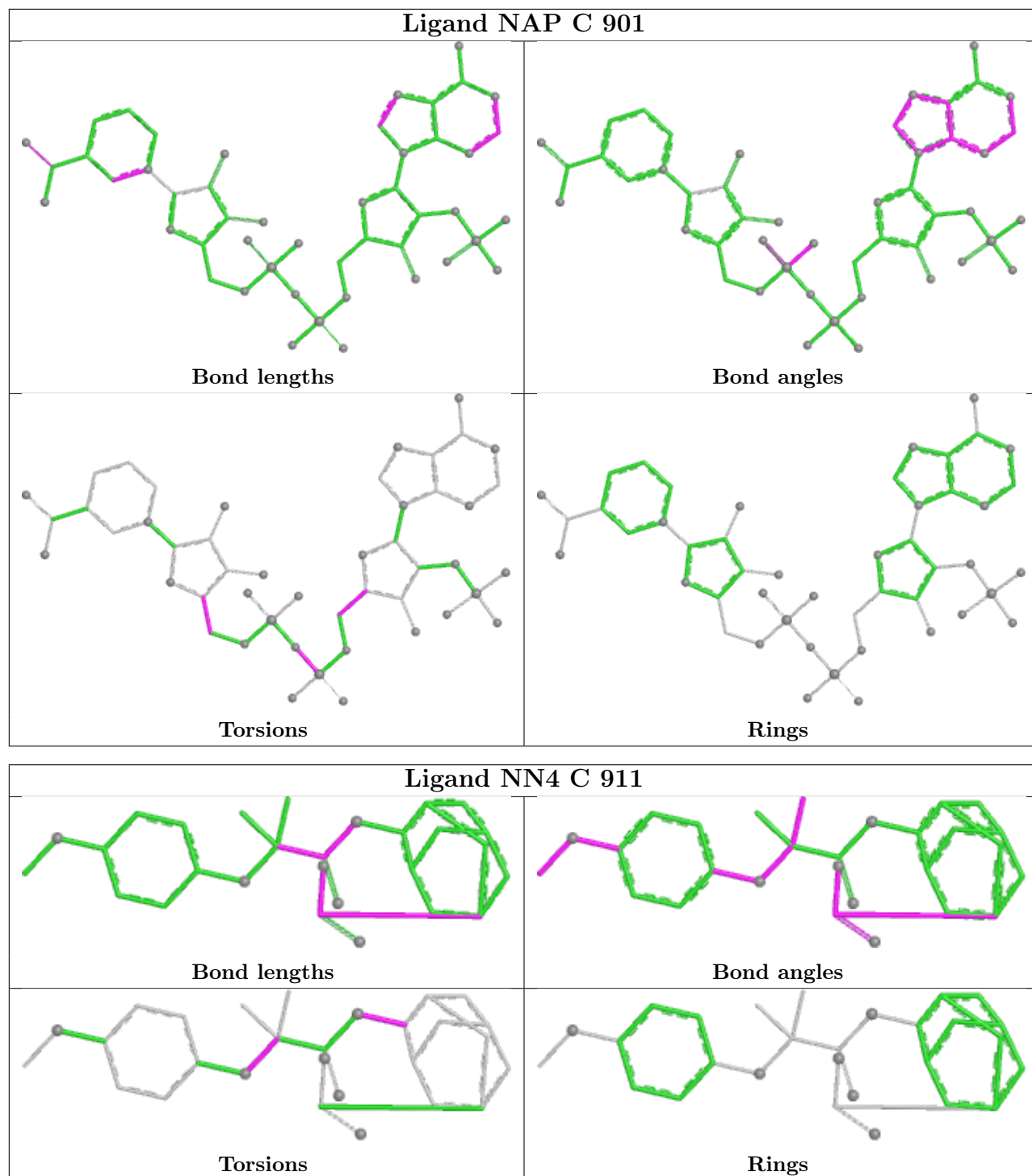


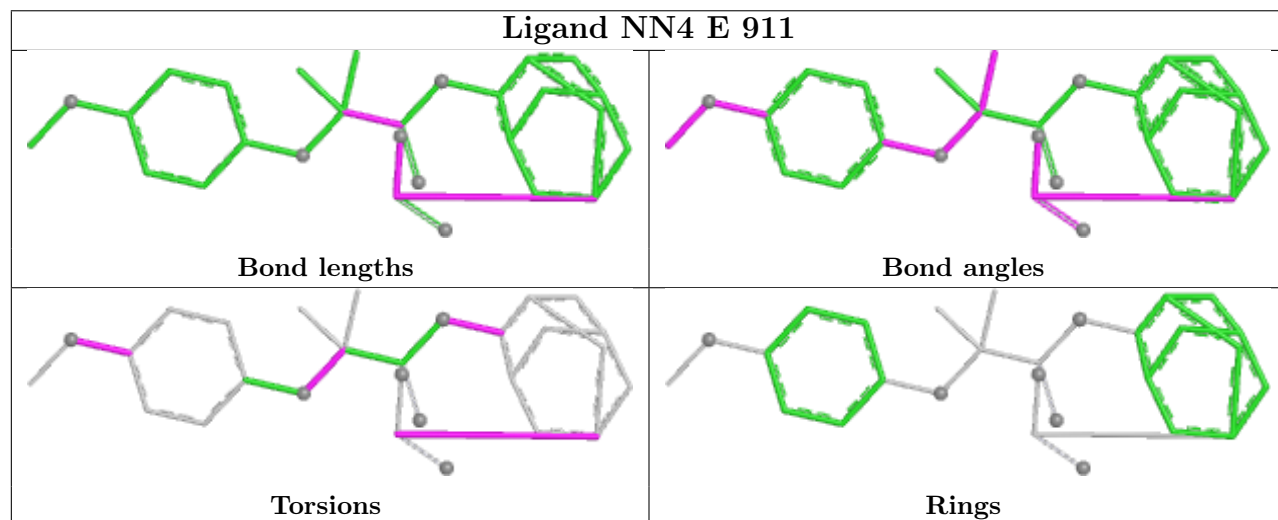
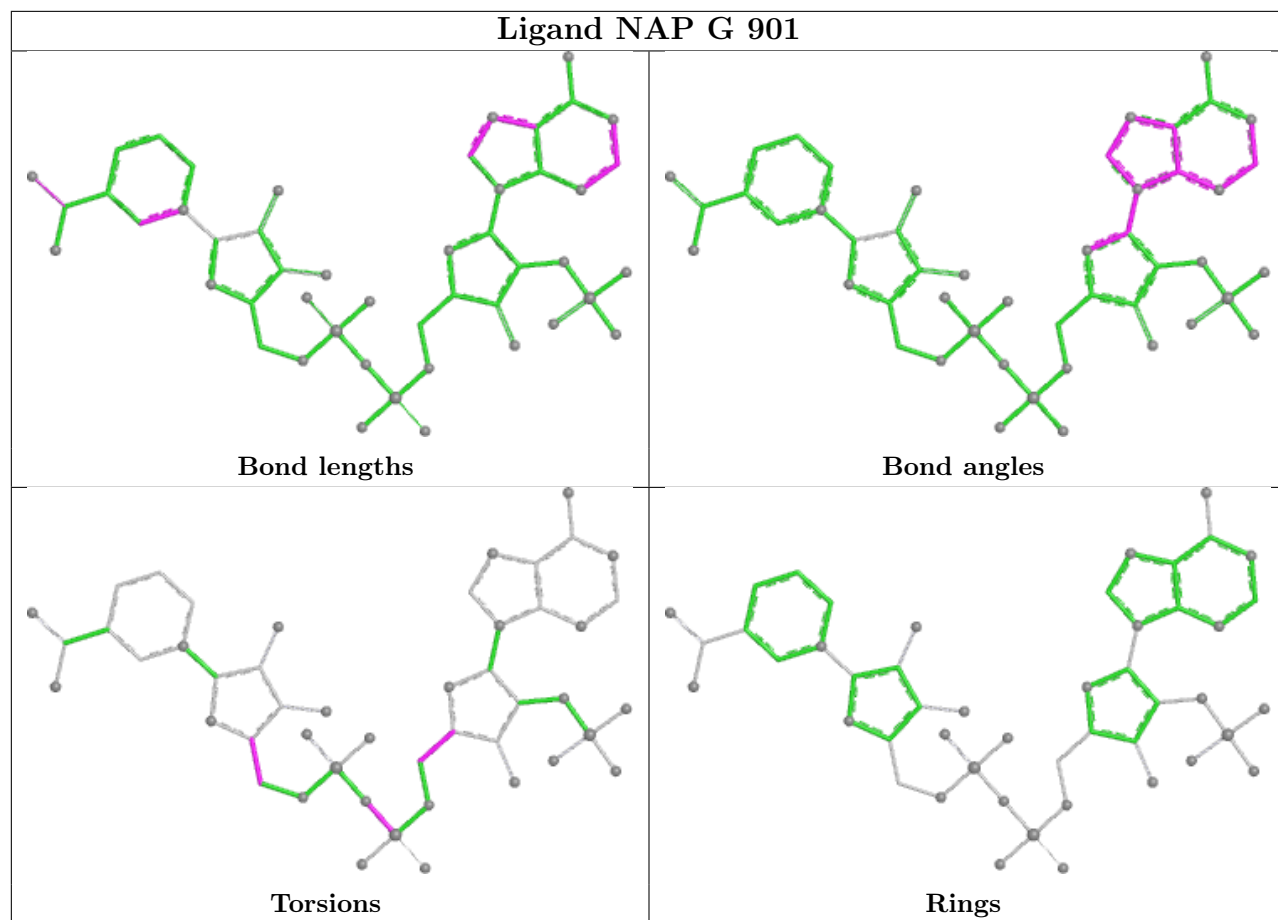


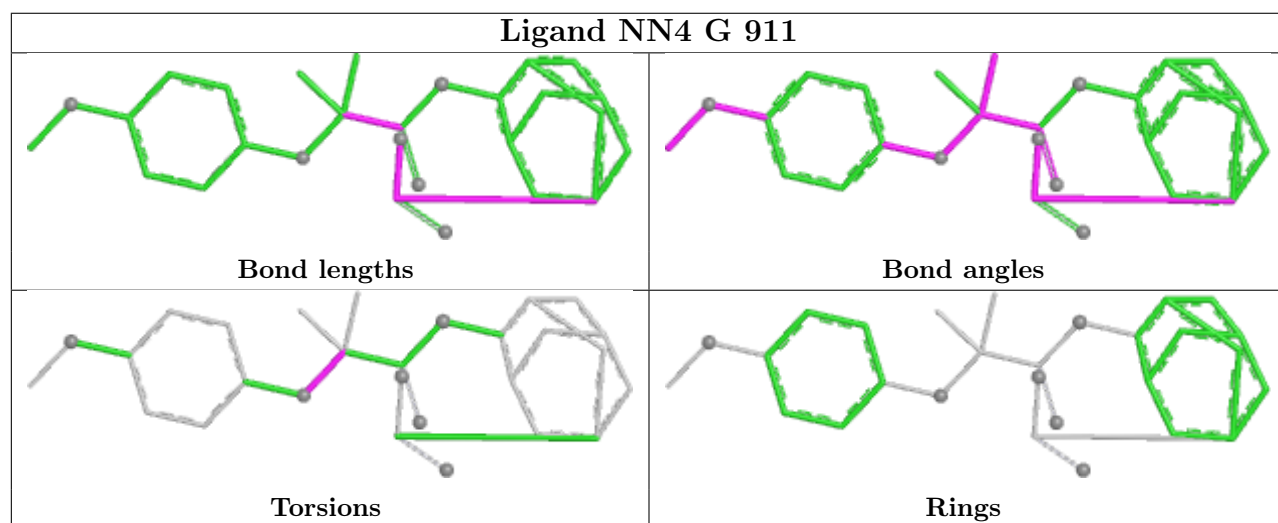
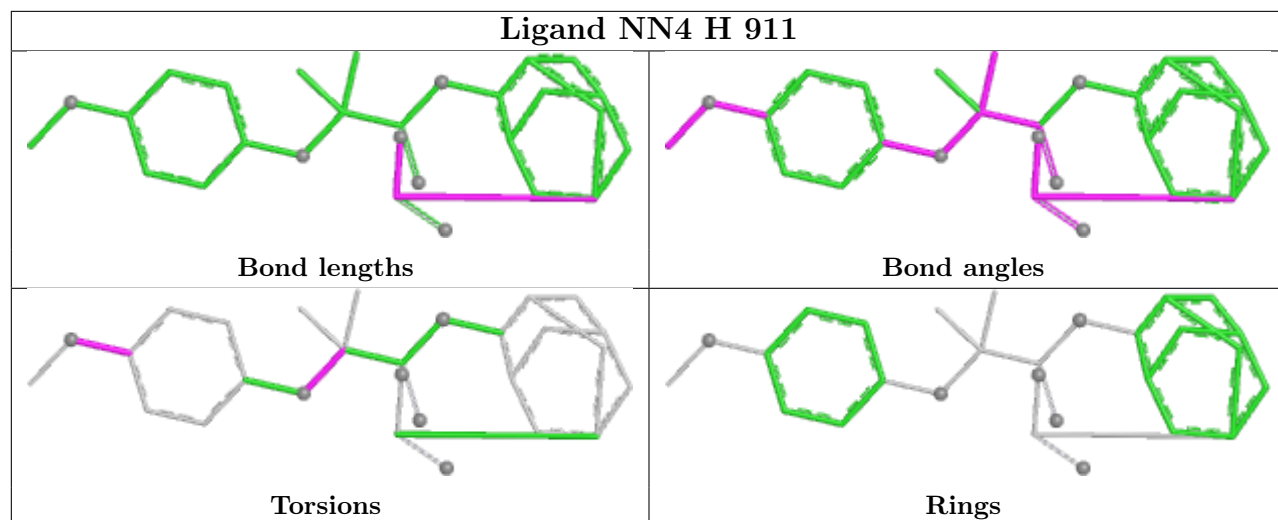


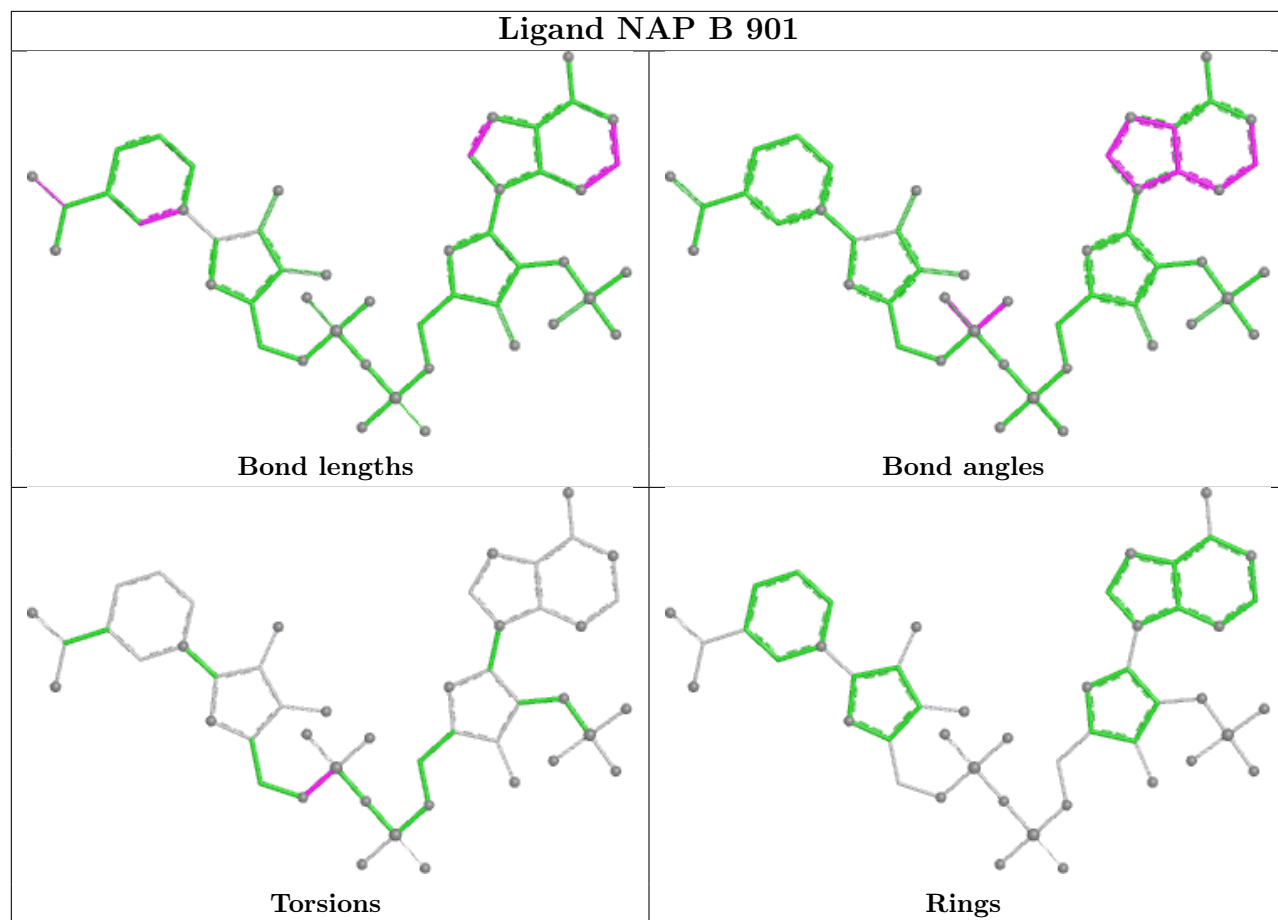


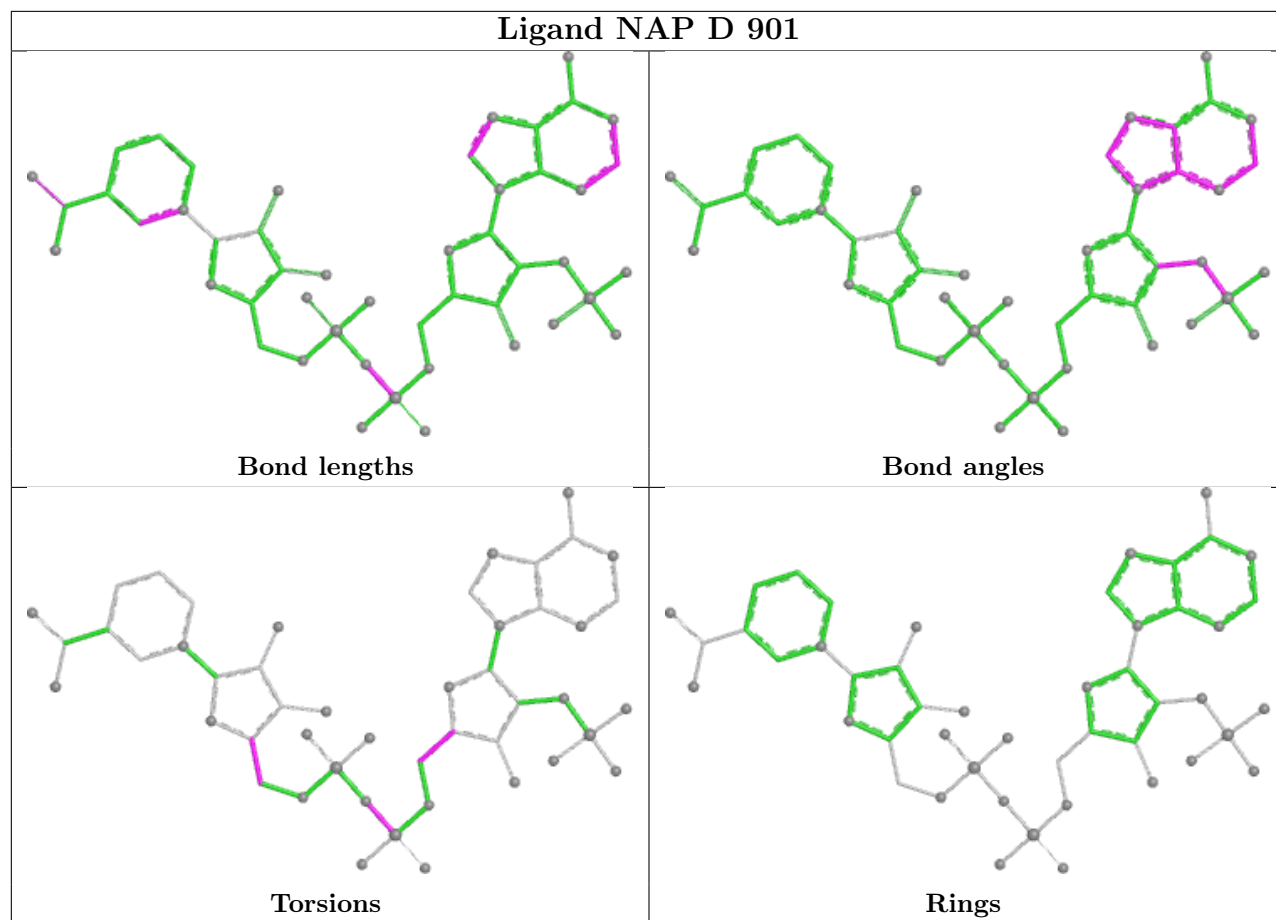












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	0.15	9 (3%)	48	28	34, 41, 49, 55	0
1	B	264/264 (100%)	0.10	5 (1%)	66	45	34, 41, 49, 55	0
1	C	257/264 (97%)	0.18	16 (6%)	26	14	35, 42, 49, 54	0
1	D	264/264 (100%)	0.20	8 (3%)	52	31	35, 42, 51, 67	0
1	E	257/264 (97%)	-0.07	6 (2%)	61	39	29, 40, 54, 62	0
1	F	264/264 (100%)	-0.10	2 (0%)	82	65	30, 41, 57, 65	0
1	G	264/264 (100%)	-0.03	8 (3%)	52	31	29, 38, 54, 64	0
1	H	264/264 (100%)	0.04	5 (1%)	66	45	30, 40, 54, 63	0
All	All	2098/2112 (99%)	0.06	59 (2%)	55	34	29, 41, 52, 67	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	263	TRP	4.6
1	C	282	THR	4.3
1	G	262	LEU	4.1
1	C	281	SER	4.0
1	H	263	TRP	3.9
1	G	233	MET	3.8
1	A	233	MET	3.6
1	A	263	TRP	3.5
1	E	282	THR	3.5
1	D	130	HIS	3.4
1	C	263	TRP	3.3
1	H	134	HIS	3.2
1	A	123	ASN	3.1
1	D	233	MET	3.1
1	C	266	LEU	3.0
1	E	281	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	130	HIS	3.0
1	E	238	LYS	3.0
1	F	130	HIS	3.0
1	G	238	LYS	2.8
1	G	134	HIS	2.8
1	A	238	LYS	2.8
1	E	263	TRP	2.7
1	C	280	TYR	2.7
1	E	130	HIS	2.7
1	B	263	TRP	2.6
1	C	233	MET	2.6
1	G	232	HIS	2.6
1	A	262	LEU	2.6
1	A	266	LEU	2.5
1	G	131	ASP	2.5
1	D	231	VAL	2.5
1	G	69	GLU	2.5
1	D	232	HIS	2.5
1	C	228	SER	2.4
1	H	262	LEU	2.4
1	B	123	ASN	2.4
1	B	282	THR	2.4
1	D	266	LEU	2.4
1	D	263	TRP	2.4
1	E	265	THR	2.4
1	H	265	THR	2.4
1	H	282	THR	2.4
1	C	232	HIS	2.4
1	C	221	GLU	2.3
1	D	229	GLY	2.3
1	F	263	TRP	2.3
1	A	282	THR	2.3
1	A	69	GLU	2.2
1	B	233	MET	2.2
1	C	238	LYS	2.2
1	D	80	GLU	2.2
1	C	265	THR	2.2
1	C	101	GLN	2.2
1	C	123	ASN	2.2
1	C	264	THR	2.2
1	C	67	SER	2.1
1	B	265	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	265	THR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

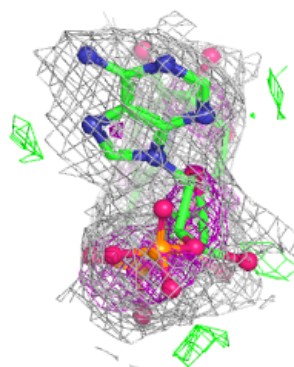
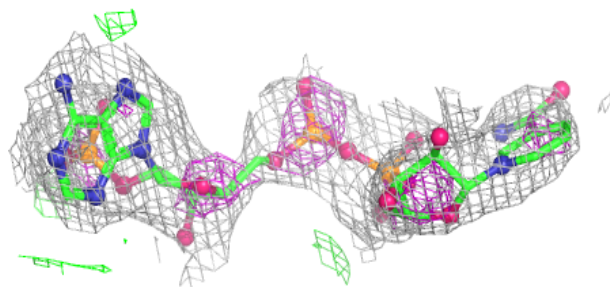
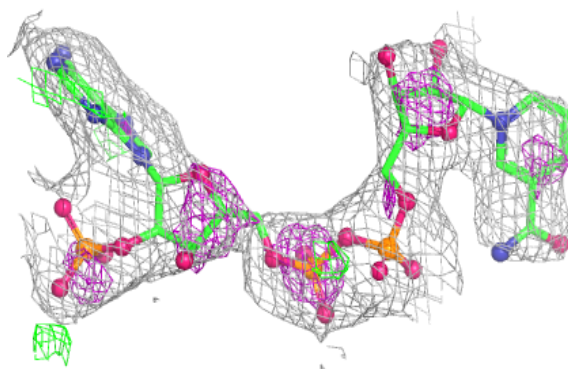
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAP	D	901	48/48	0.87	0.14	43,45,47,47	0
2	NAP	F	901	48/48	0.87	0.14	42,47,49,49	0
3	NN4	D	911	28/28	0.92	0.11	27,28,30,31	0
2	NAP	H	901	48/48	0.94	0.09	37,40,43,45	0
3	NN4	B	911	28/28	0.94	0.10	25,27,30,32	0
2	NAP	B	901	48/48	0.94	0.09	38,40,43,44	0
2	NAP	C	901	48/48	0.95	0.09	43,45,46,47	0
2	NAP	E	901	48/48	0.95	0.09	41,43,47,47	0
3	NN4	F	911	28/28	0.95	0.09	30,32,36,36	0
3	NN4	G	911	28/28	0.95	0.10	27,28,30,31	0
3	NN4	H	911	28/28	0.95	0.10	27,28,30,31	0
2	NAP	A	901	48/48	0.96	0.08	38,40,43,44	0
3	NN4	E	911	28/28	0.96	0.09	28,32,34,35	0
3	NN4	A	911	28/28	0.96	0.08	25,27,30,32	0
2	NAP	G	901	48/48	0.96	0.08	37,40,42,43	0
3	NN4	C	911	28/28	0.96	0.09	27,28,30,31	0

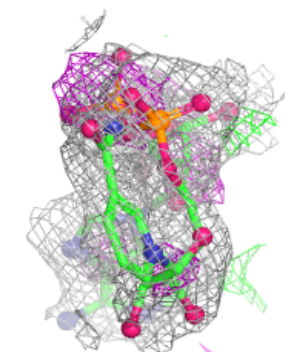
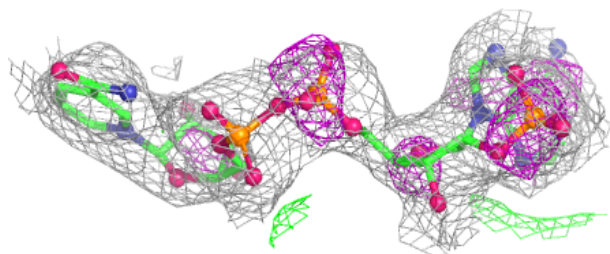
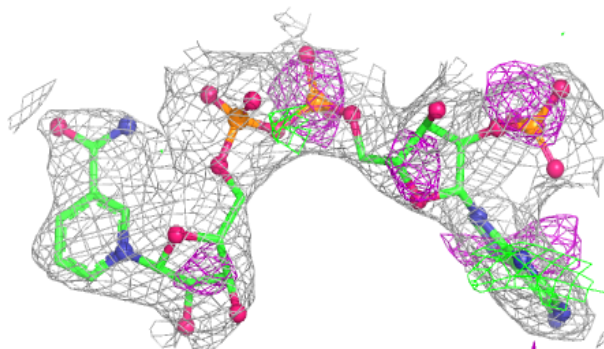
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP D 901:

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

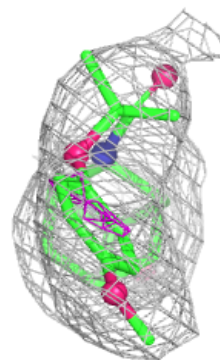
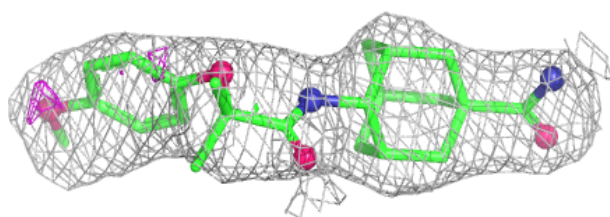
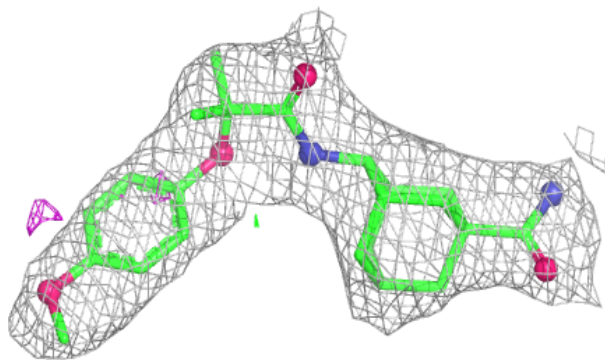
**Electron density around NAP F 901:**

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

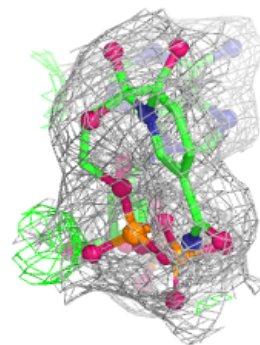
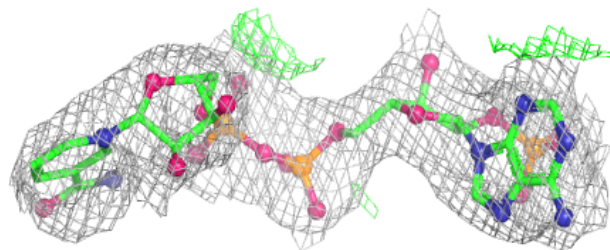
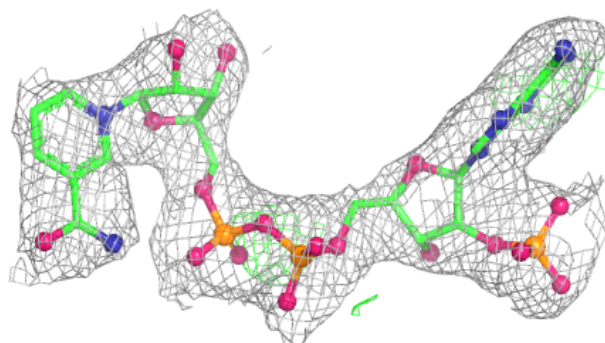


Electron density around NN4 D 911:

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

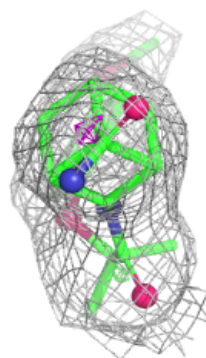
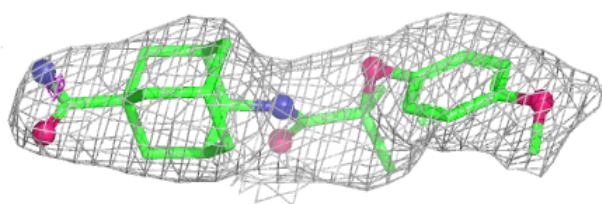
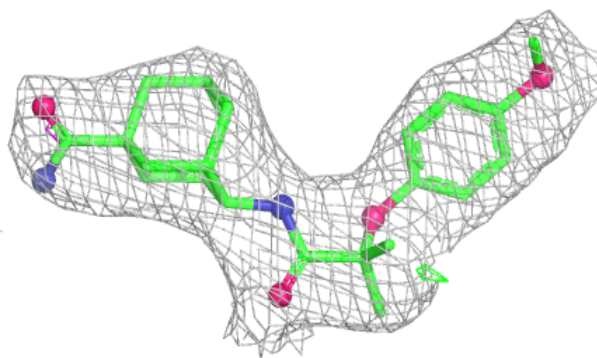
**Electron density around NAP H 901:**

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

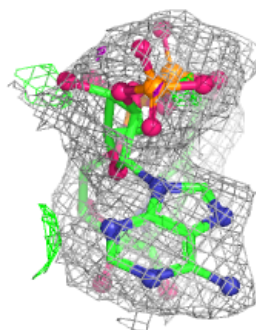
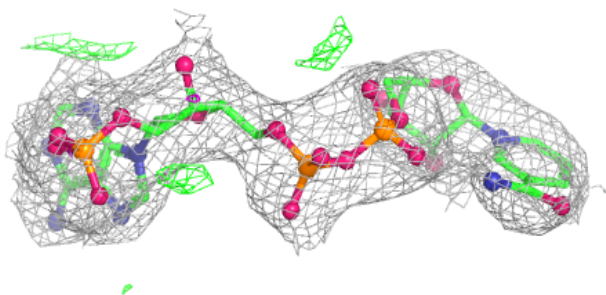
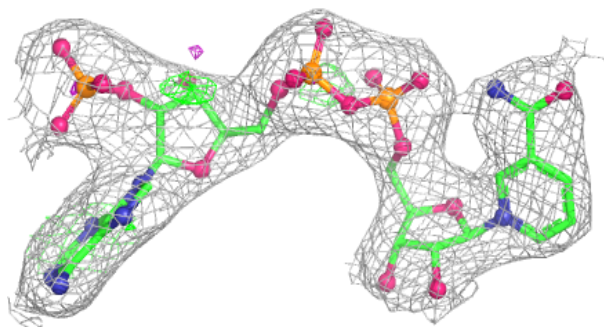


Electron density around NN4 B 911:

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

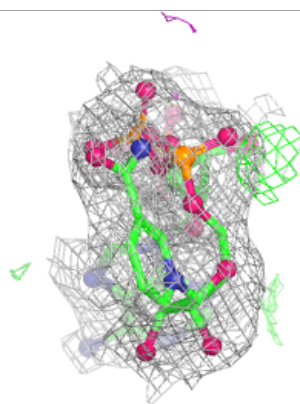
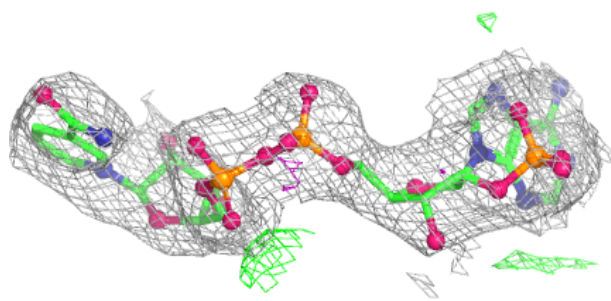
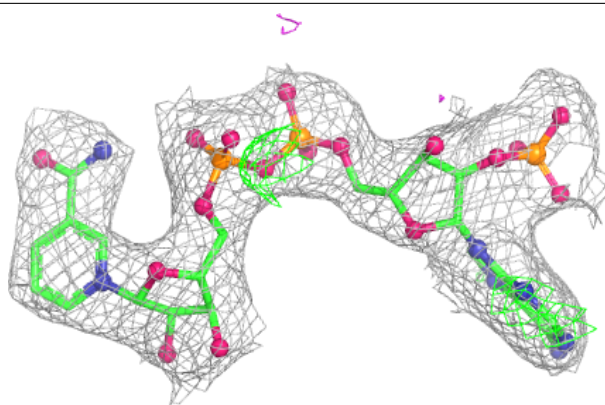
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and green (positive)

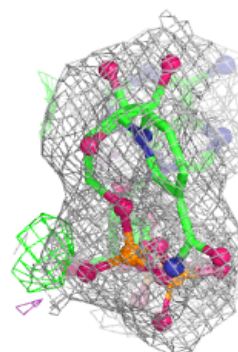
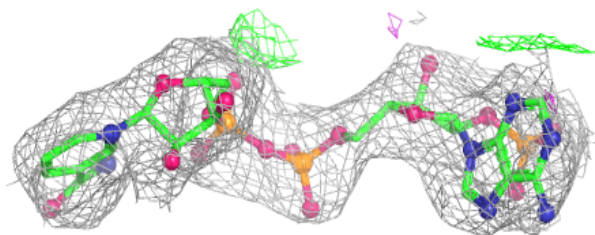
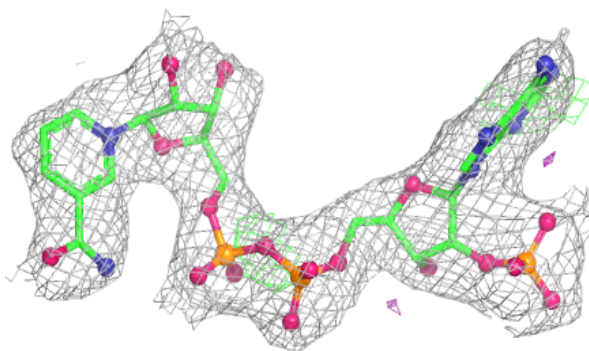


Electron density around NAP C 901:

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

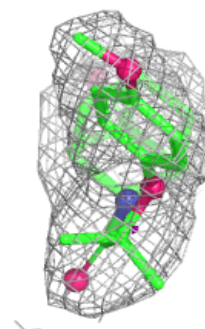
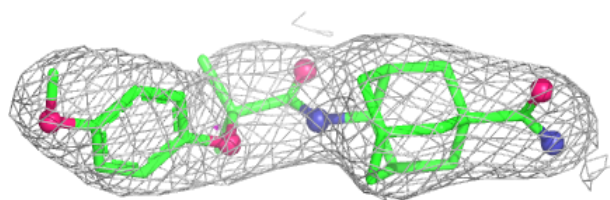
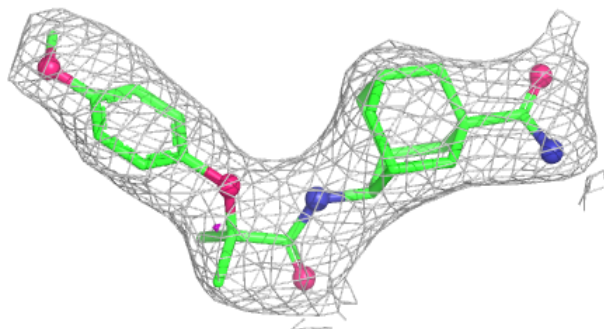
**Electron density around NAP E 901:**

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

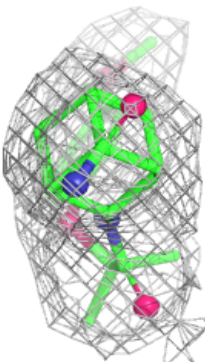
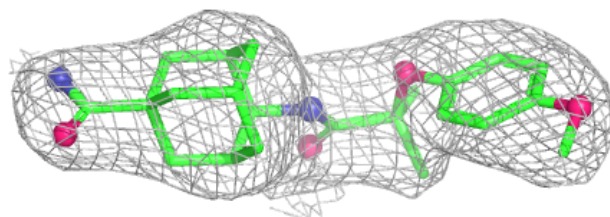
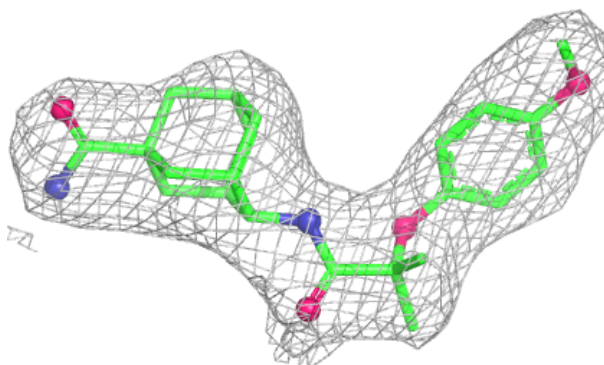


Electron density around NN4 F 911:

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

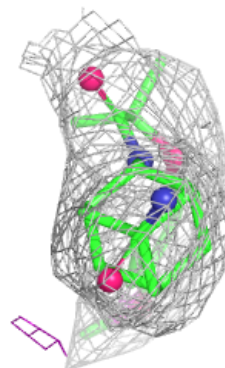
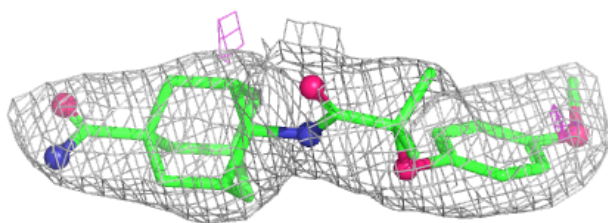
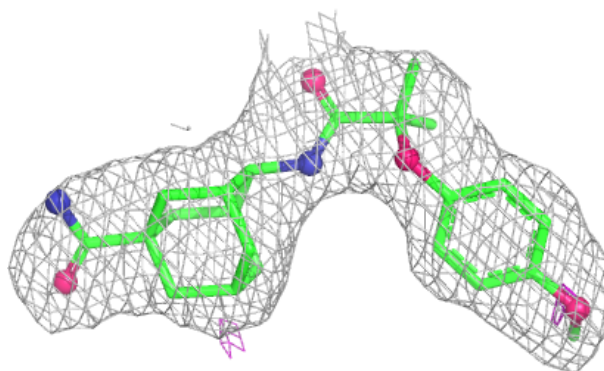
**Electron density around NN4 G 911:**

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and green (positive)

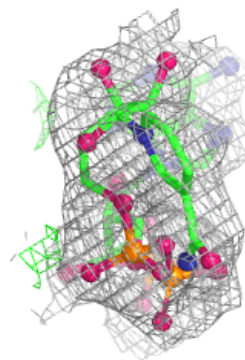
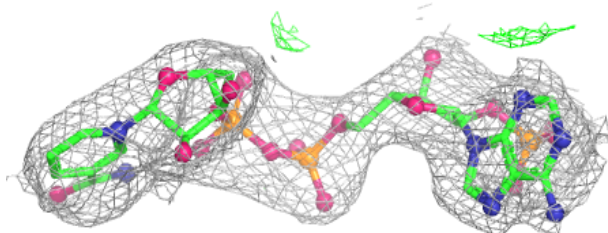
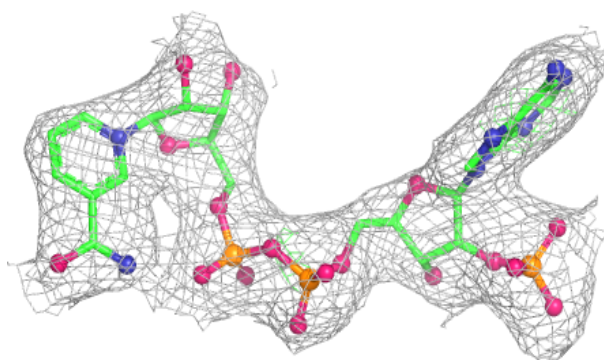


Electron density around NN4 H 911:

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

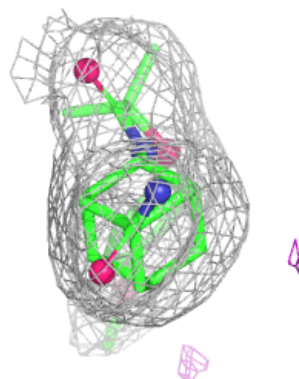
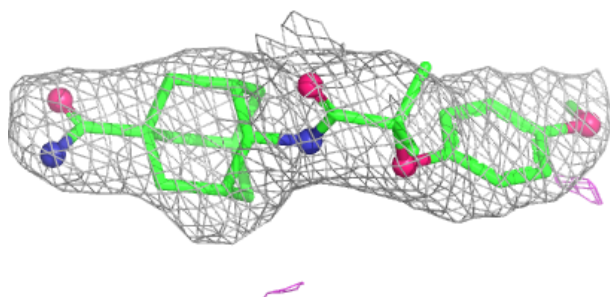
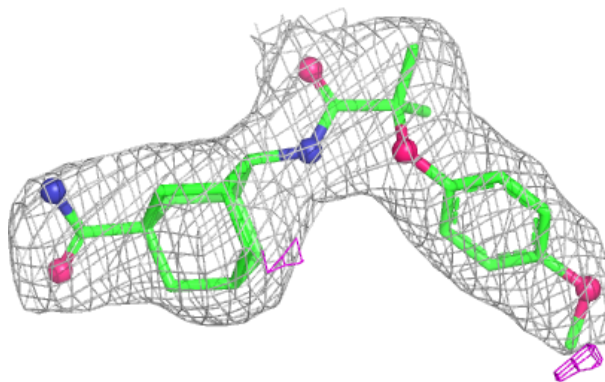
**Electron density around NAP A 901:**

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

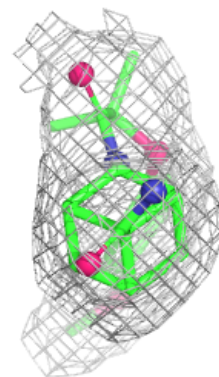
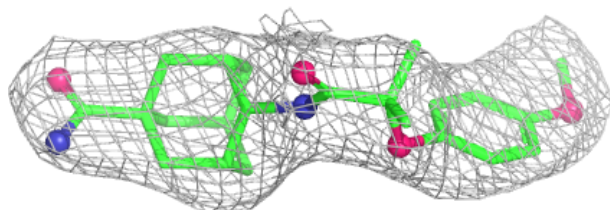
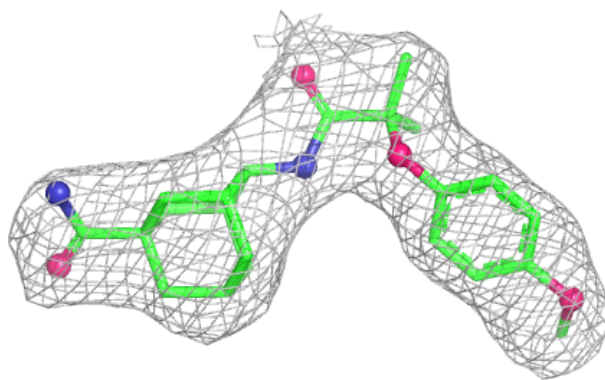


Electron density around NN4 E 911:

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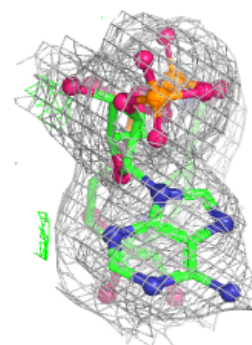
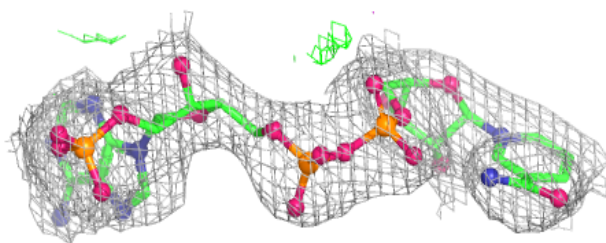
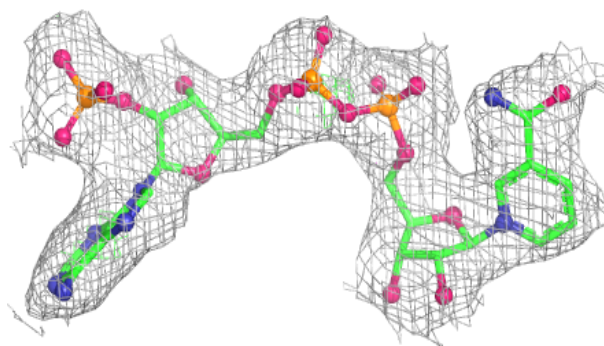
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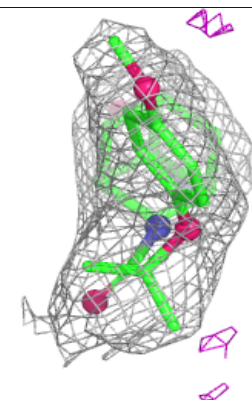
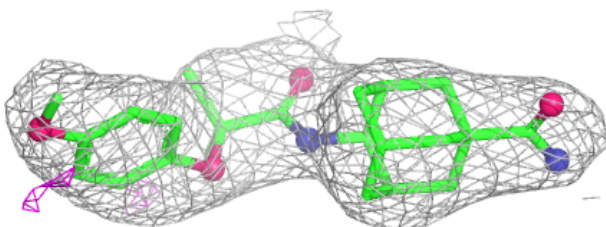
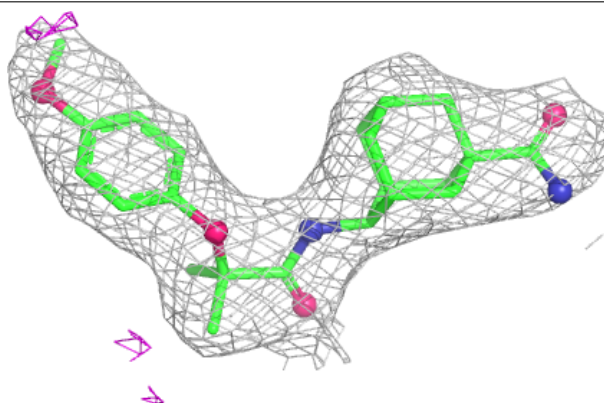


Electron density around NAP G 901:

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 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.