



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2021 – 12:22 pm GMT

PDB ID : 6TO4
Title : Imine Reductase from Myxococcus stipitatus in complex with NADP+
Authors : Sharma, M.; Nestl, B.; Grogan, G.
Deposited on : 2019-12-11
Resolution : 2.29 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.24
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.24

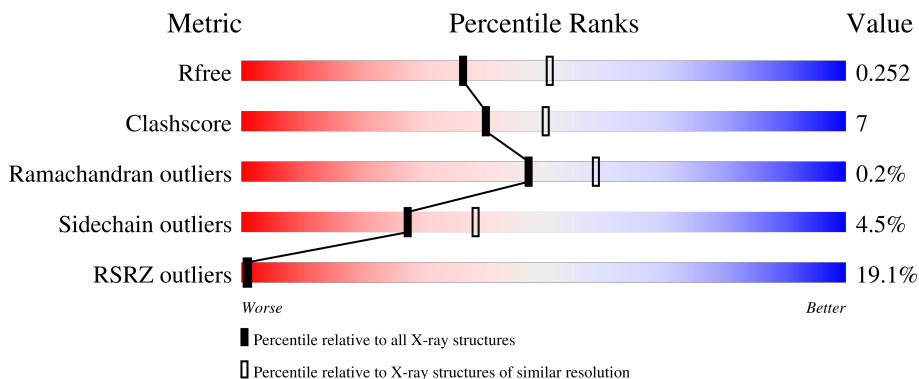
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	291	
1	B	291	
1	C	291	
1	D	291	

2 Entry composition [i](#)

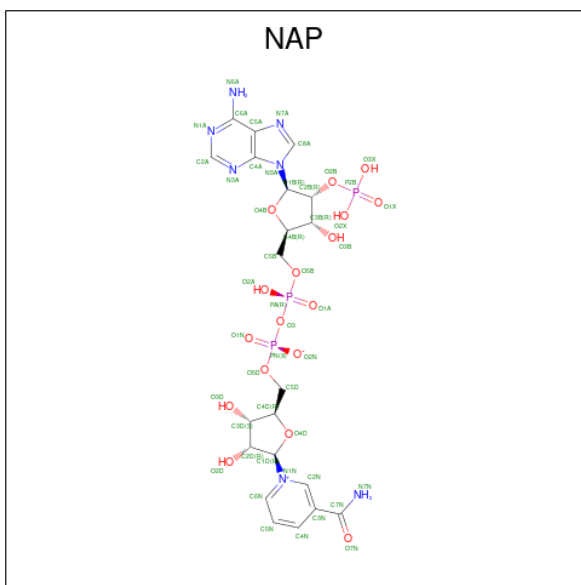
There are 3 unique types of molecules in this entry. The entry contains 8583 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Coenzyme F420-dependent NADP oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	291	Total 2154	C 1365	N 378	O 404	S 7	0	0	0
1	B	289	Total 2099	C 1322	N 371	O 400	S 6	0	0	0
1	C	290	Total 2132	C 1352	N 371	O 403	S 6	0	0	0
1	D	276	Total 1902	C 1191	N 343	O 362	S 6	0	0	0

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	C	1	48	21	7	17	3	0	0

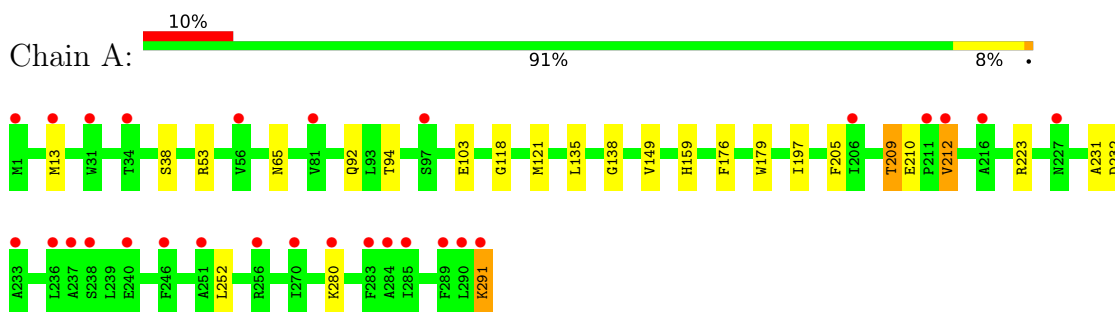
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	75	Total	O	0	0
			75	75		
3	B	18	Total	O	0	0
			18	18		
3	C	33	Total	O	0	0
			33	33		
3	D	26	Total	O	0	0
			26	26		

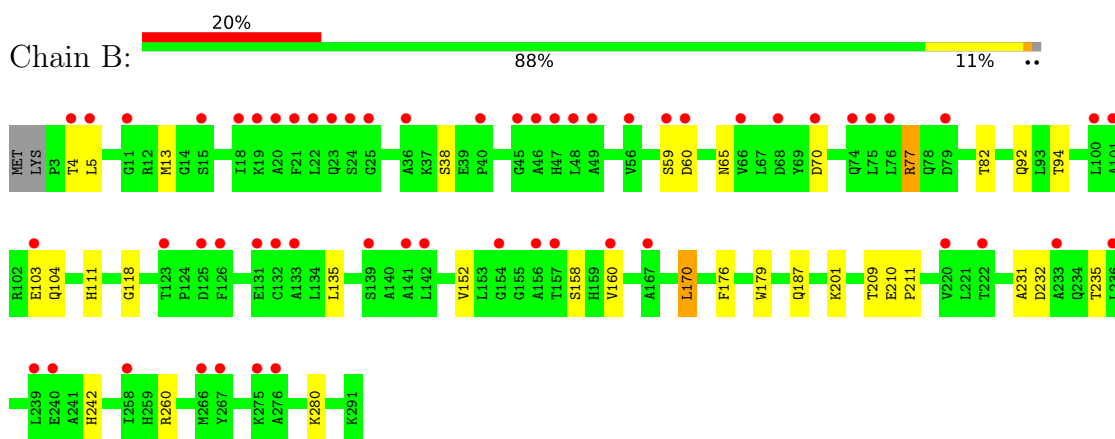
3 Residue-property plots [i](#)

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

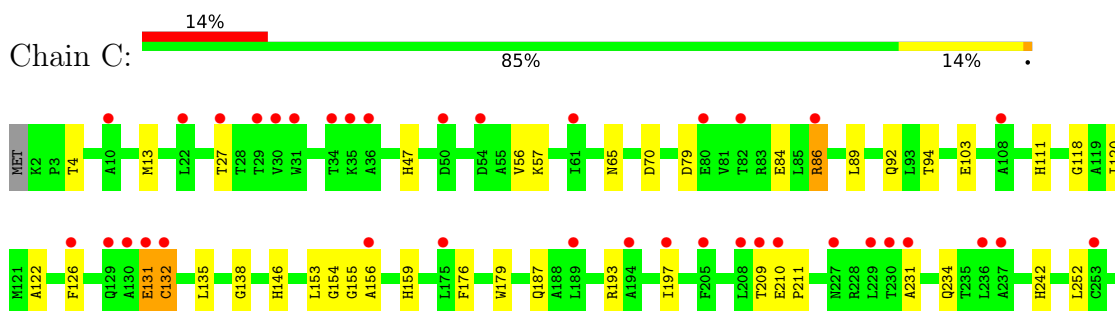
- Molecule 1: Coenzyme F420-dependent NADP oxidoreductase



- Molecule 1: Coenzyme F420-dependent NADP oxidoreductase



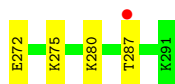
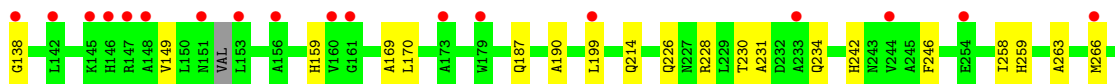
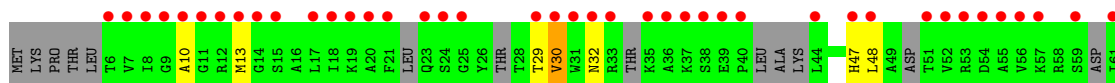
- Molecule 1: Coenzyme F420-dependent NADP oxidoreductase





● Molecule 1: Coenzyme F420-dependent NADP oxidoreductase

Chain D: 32% 79% 14% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	118.71Å 42.58Å 121.40Å 90.00° 110.37° 90.00°	Depositor
Resolution (Å)	49.32 – 2.29 49.27 – 2.29	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.32-2.29) 100.0 (49.27-2.29)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.29 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.212 , 0.239 0.223 , 0.252	Depositor DCC
R_{free} test set	2520 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	43.1	Xtrriage
Anisotropy	0.442	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.010 for l,-k,h	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8583	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% of the height of the origin peak. No significant pseudotranslation is detected.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAP

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	0.53	0/2188	0.66	0/2972
1	B	0.48	0/2131	0.63	0/2904
1	C	0.52	0/2166	0.64	0/2949
1	D	0.50	0/1921	0.64	0/2611
All	All	0.51	0/8406	0.64	0/11436

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2154	0	2144	26	0
1	B	2099	0	2036	25	0
1	C	2132	0	2094	52	0
1	D	1902	0	1740	36	0
2	A	48	0	25	0	0
2	B	48	0	25	0	0
2	C	48	0	25	2	0
3	A	75	0	0	1	0
3	B	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	33	0	0	1	0
3	D	26	0	0	4	0
All	All	8583	0	8089	119	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 7.

All (119) 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:C:132:CYS:O	1:C:156:ALA:HB3	1.33	1.25
1:C:132:CYS:CB	1:C:154:GLY:HA3	1.67	1.22
1:C:132:CYS:CB	1:C:154:GLY:CA	2.20	1.20
1:C:132:CYS:SG	1:C:154:GLY:HA3	1.91	1.11
1:C:132:CYS:SG	1:C:153:LEU:O	2.12	1.08
1:D:10:ALA:HB3	1:D:32:ASN:HD22	1.12	1.08
1:C:132:CYS:SG	1:C:154:GLY:CA	2.43	1.07
1:C:132:CYS:HB3	1:C:154:GLY:HA3	1.27	1.06
1:C:56:VAL:HG12	1:C:84:GLU:HG3	1.44	0.97
1:C:132:CYS:O	1:C:156:ALA:CB	2.15	0.95
1:C:57:LYS:CG	1:C:84:GLU:OE2	2.15	0.94
1:D:10:ALA:HB3	1:D:32:ASN:ND2	1.87	0.90
1:C:132:CYS:HB3	1:C:154:GLY:CA	1.92	0.87
1:A:149:VAL:HG23	3:A:461:HOH:O	1.76	0.85
1:A:179:TRP:HE1	1:D:242:HIS:HD2	1.25	0.84
1:B:4:THR:HG23	1:B:59:SER:HA	1.60	0.83
1:C:132:CYS:CB	1:C:154:GLY:HA2	2.08	0.82
1:C:132:CYS:SG	1:C:154:GLY:HA2	2.20	0.81
1:A:176:PHE:CE2	1:D:266:MET:CE	2.66	0.79
1:C:132:CYS:HB2	1:C:154:GLY:CA	2.14	0.78
1:A:176:PHE:CE2	1:D:266:MET:HE2	2.18	0.78
1:C:86:ARG:HH21	1:C:111:HIS:HA	1.49	0.78
1:A:210:GLU:OE2	1:D:214:GLN:NE2	2.17	0.77
1:B:242:HIS:HD2	1:C:179:TRP:HE1	1.32	0.74
1:C:132:CYS:HG	1:C:154:GLY:CA	1.98	0.74
1:A:176:PHE:CZ	1:D:266:MET:HE2	2.23	0.73
1:B:179:TRP:HE1	1:C:242:HIS:HD2	1.37	0.71
1:D:10:ALA:CB	1:D:32:ASN:HD22	1.95	0.71
1:D:149:VAL:HG23	3:D:311:HOH:O	1.88	0.71
1:C:56:VAL:CG1	1:C:84:GLU:HG3	2.20	0.69
1:D:13:MET:HB3	1:D:65:ASN:HD21	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:VAL:HG22	1:B:160:VAL:O	1.93	0.69
1:C:132:CYS:HB2	1:C:154:GLY:HA2	1.72	0.68
1:B:232:ASP:H	1:B:235:THR:HG23	1.59	0.68
1:C:252:LEU:C	1:C:252:LEU:HD23	2.15	0.67
1:C:132:CYS:HG	1:C:153:LEU:C	1.97	0.67
1:B:170:LEU:HD13	1:C:197:ILE:HD12	1.77	0.66
1:D:73:ASP:O	1:D:77:ARG:HB2	1.97	0.64
1:C:56:VAL:HG12	1:C:84:GLU:CG	2.22	0.63
1:A:176:PHE:CE2	1:D:266:MET:HE1	2.31	0.63
1:D:69:TYR:O	1:D:70:ASP:CB	2.45	0.63
1:C:4:THR:HG22	1:C:27:THR:OG1	2.00	0.61
1:C:210:GLU:N	1:C:211:PRO:CD	2.63	0.61
1:C:131:GLU:HA	1:C:131:GLU:OE1	1.98	0.61
1:B:170:LEU:HD13	1:C:197:ILE:CD1	2.31	0.61
1:A:291:LYS:HE2	1:A:291:LYS:C	2.21	0.61
1:C:252:LEU:HD23	1:C:252:LEU:O	2.01	0.61
1:D:29:THR:O	1:D:47:HIS:O	2.18	0.61
1:C:209:THR:O	1:C:209:THR:HG23	2.02	0.59
1:B:160:VAL:HG21	1:B:170:LEU:HD22	1.84	0.58
1:A:209:THR:O	1:A:212:VAL:HG12	2.03	0.58
1:B:160:VAL:HG21	1:B:170:LEU:CD2	2.34	0.57
1:C:92:GLN:HE21	1:C:94:THR:H	1.51	0.57
1:B:4:THR:CG2	1:B:59:SER:HA	2.33	0.56
1:B:231:ALA:HA	1:B:235:THR:HG21	1.85	0.56
1:B:210:GLU:HB3	1:B:211:PRO:HD3	1.87	0.56
1:C:13:MET:HB3	1:C:65:ASN:HD21	1.71	0.55
1:D:92:GLN:HE21	1:D:94:THR:H	1.55	0.54
1:B:13:MET:HB3	1:B:65:ASN:HD21	1.71	0.54
1:B:92:GLN:HE21	1:B:94:THR:H	1.56	0.54
1:B:232:ASP:H	1:B:235:THR:CG2	2.19	0.54
1:C:132:CYS:HB3	1:C:154:GLY:C	2.28	0.54
1:D:111:HIS:HE1	3:D:323:HOH:O	1.90	0.54
1:D:272:GLU:HG3	3:D:316:HOH:O	2.07	0.53
1:A:92:GLN:HE21	1:A:94:THR:H	1.53	0.53
1:A:197:ILE:HD11	1:D:169:ALA:HB3	1.90	0.53
1:A:176:PHE:CZ	1:D:266:MET:CE	2.91	0.53
1:D:246:PHE:HZ	1:D:266:MET:HE3	1.74	0.53
1:D:82:THR:HG22	1:D:107:TRP:HZ2	1.74	0.52
1:C:122:ALA:O	2:C:301:NAP:H4N	2.10	0.52
1:B:176:PHE:CD1	1:C:187:GLN:HB3	2.46	0.51
1:A:13:MET:HB3	1:A:65:ASN:HD21	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:ARG:NH2	1:B:103:GLU:OE2	2.44	0.49
1:B:82:THR:HG21	1:B:111:HIS:CD2	2.48	0.49
1:A:291:LYS:HD3	1:D:190:ALA:HB1	1.95	0.49
1:C:132:CYS:O	1:C:156:ALA:CA	2.60	0.49
1:D:263:ALA:HA	1:D:266:MET:CE	2.42	0.49
1:D:138:GLY:O	1:D:159:HIS:HE1	1.96	0.49
1:B:4:THR:HG23	1:B:60:ASP:H	1.78	0.48
1:C:47:HIS:HB3	3:C:431:HOH:O	2.12	0.48
1:B:231:ALA:HB2	1:B:280:LYS:O	2.13	0.48
1:C:138:GLY:O	1:C:159:HIS:HE1	1.96	0.48
1:D:29:THR:O	1:D:30:VAL:HG23	2.14	0.48
1:D:111:HIS:CE1	3:D:323:HOH:O	2.65	0.48
1:A:197:ILE:HD13	1:D:170:LEU:HG	1.96	0.47
1:B:4:THR:C	1:B:5:LEU:HD12	2.35	0.47
1:C:86:ARG:NH2	1:C:111:HIS:HA	2.25	0.47
1:C:120:ILE:O	2:C:301:NAP:H5N	2.14	0.47
1:C:132:CYS:HG	1:C:154:GLY:HA2	1.67	0.46
1:A:138:GLY:O	1:A:159:HIS:HE1	1.99	0.46
1:A:176:PHE:CD1	1:D:187:GLN:HB3	2.51	0.46
1:A:223:ARG:NH1	1:A:232:ASP:OD1	2.49	0.46
1:C:252:LEU:C	1:C:252:LEU:CD2	2.84	0.45
1:C:132:CYS:O	1:C:156:ALA:N	2.49	0.45
1:A:231:ALA:HB2	1:A:280:LYS:O	2.17	0.45
1:D:226:GLN:OE1	1:D:228:ARG:NH1	2.50	0.45
1:C:231:ALA:HB2	1:C:280:LYS:O	2.18	0.44
1:A:205:PHE:O	1:A:209:THR:HB	2.16	0.44
1:C:118:GLY:HA2	1:C:135:LEU:O	2.18	0.44
1:C:132:CYS:CB	1:C:154:GLY:C	2.83	0.44
1:A:291:LYS:HG3	1:D:258:ILE:HA	2.00	0.44
1:B:187:GLN:HB3	1:C:176:PHE:CD1	2.52	0.43
1:D:118:GLY:HA2	1:D:135:LEU:O	2.17	0.43
1:B:82:THR:CG2	1:B:111:HIS:CD2	3.01	0.43
1:A:291:LYS:HB2	1:D:259:HIS:H	1.82	0.43
1:C:132:CYS:HB2	1:C:155:GLY:N	2.34	0.43
1:B:118:GLY:HA2	1:B:135:LEU:O	2.19	0.42
1:D:231:ALA:HB2	1:D:280:LYS:O	2.19	0.42
1:A:118:GLY:HA2	1:A:135:LEU:O	2.19	0.42
1:C:210:GLU:N	1:C:211:PRO:HD3	2.33	0.42
1:D:266:MET:HE3	1:D:266:MET:HB2	1.75	0.42
1:C:86:ARG:HH21	1:C:111:HIS:CA	2.25	0.42
1:C:89:LEU:HD22	1:C:146:HIS:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:VAL:O	1:B:160:VAL:CG2	2.65	0.42
1:C:132:CYS:HB2	1:C:155:GLY:H	1.84	0.41
1:D:263:ALA:HA	1:D:266:MET:HE3	2.02	0.41
1:A:121:MET:HA	1:A:121:MET:HE3	2.02	0.41
1:A:252:LEU:O	1:A:252:LEU:HD23	2.21	0.40
1:A:176:PHE:HE2	1:D:266:MET:CE	2.25	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	289/291 (99%)	285 (99%)	4 (1%)	0	100	100
1	B	287/291 (99%)	281 (98%)	6 (2%)	0	100	100
1	C	288/291 (99%)	280 (97%)	8 (3%)	0	100	100
1	D	258/291 (89%)	251 (97%)	5 (2%)	2 (1%)	19	23
All	All	1122/1164 (96%)	1097 (98%)	23 (2%)	2 (0%)	47	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	30	VAL
1	D	70	ASP

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	213/230 (93%)	207 (97%)	6 (3%)	43	60
1	B	202/230 (88%)	192 (95%)	10 (5%)	24	34
1	C	207/230 (90%)	198 (96%)	9 (4%)	29	40
1	D	164/230 (71%)	154 (94%)	10 (6%)	18	25
All	All	786/920 (85%)	751 (96%)	35 (4%)	27	39

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	A	53	ARG
1	A	103	GLU
1	A	209	THR
1	A	212	VAL
1	A	291	LYS
1	B	38	SER
1	B	70	ASP
1	B	77	ARG
1	B	104	GLN
1	B	152	VAL
1	B	158	SER
1	B	170	LEU
1	B	201	LYS
1	B	209	THR
1	B	260	ARG
1	C	70	ASP
1	C	79	ASP
1	C	86	ARG
1	C	103	GLU
1	C	126	PHE
1	C	131	GLU
1	C	132	CYS
1	C	193	ARG
1	C	234	GLN
1	D	48	LEU
1	D	69	TYR
1	D	77	ARG
1	D	95	SER
1	D	103	GLU

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Mol	Chain	Res	Type
1	D	199	LEU
1	D	230	THR
1	D	234	GLN
1	D	275	LYS
1	D	287	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	92	GLN
1	A	146	HIS
1	A	159	HIS
1	B	65	ASN
1	B	92	GLN
1	B	111	HIS
1	B	242	HIS
1	C	65	ASN
1	C	92	GLN
1	C	146	HIS
1	C	159	HIS
1	C	242	HIS
1	D	32	ASN
1	D	47	HIS
1	D	65	ASN
1	D	92	GLN
1	D	104	GLN
1	D	110	GLN
1	D	146	HIS
1	D	159	HIS
1	D	242	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAP	C	301	-	45,52,52	1.57	10 (22%)	56,80,80	1.28	7 (12%)
2	NAP	B	301	-	45,52,52	1.55	13 (28%)	56,80,80	1.35	8 (14%)
2	NAP	A	301	-	45,52,52	1.80	14 (31%)	56,80,80	1.21	7 (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
2	NAP	C	301	-	-	6/31/67/67	0/5/5/5
2	NAP	B	301	-	-	5/31/67/67	0/5/5/5
2	NAP	A	301	-	-	6/31/67/67	0/5/5/5

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	NAP	P2B-O2X	-3.20	1.42	1.54
2	A	301	NAP	P2B-O3X	-3.10	1.42	1.54
2	A	301	NAP	PN-O2N	-2.95	1.41	1.55
2	C	301	NAP	P2B-O2X	-2.82	1.44	1.54
2	A	301	NAP	PA-O2A	-2.82	1.42	1.55
2	C	301	NAP	P2B-O3X	-2.80	1.44	1.54
2	A	301	NAP	O7N-C7N	-2.78	1.18	1.24
2	C	301	NAP	O7N-C7N	-2.77	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	NAP	C4A-N3A	-2.74	1.31	1.35
2	B	301	NAP	P2B-O3X	-2.71	1.44	1.54
2	B	301	NAP	P2B-O2X	-2.71	1.44	1.54
2	B	301	NAP	O7N-C7N	-2.60	1.19	1.24
2	A	301	NAP	PA-O1A	-2.60	1.41	1.50
2	A	301	NAP	P2B-O2B	-2.60	1.54	1.59
2	A	301	NAP	C4A-N3A	-2.57	1.32	1.35
2	B	301	NAP	PN-O2N	-2.50	1.43	1.55
2	C	301	NAP	C2D-C1D	-2.45	1.50	1.53
2	A	301	NAP	C2N-N1N	-2.44	1.32	1.35
2	C	301	NAP	PA-O2A	-2.43	1.43	1.55
2	B	301	NAP	PA-O2A	-2.40	1.44	1.55
2	B	301	NAP	P2B-O2B	-2.40	1.54	1.59
2	A	301	NAP	PN-O1N	-2.40	1.42	1.50
2	C	301	NAP	O4D-C4D	-2.34	1.39	1.45
2	A	301	NAP	O4B-C4B	-2.33	1.39	1.45
2	A	301	NAP	C5A-N7A	-2.26	1.31	1.39
2	C	301	NAP	PN-O2N	-2.21	1.44	1.55
2	B	301	NAP	C2D-C1D	-2.21	1.50	1.53
2	A	301	NAP	C2D-C1D	-2.15	1.50	1.53
2	B	301	NAP	C4A-N3A	-2.15	1.32	1.35
2	C	301	NAP	P2B-O2B	-2.12	1.55	1.59
2	B	301	NAP	P2B-O1X	-2.05	1.43	1.50
2	A	301	NAP	O4B-C1B	-2.04	1.38	1.41
2	B	301	NAP	C5A-N7A	-2.03	1.32	1.39
2	C	301	NAP	C2N-N1N	-2.03	1.32	1.35
2	B	301	NAP	PN-O1N	-2.02	1.43	1.50
2	B	301	NAP	C2N-N1N	-2.01	1.32	1.35
2	B	301	NAP	PA-O1A	-2.01	1.43	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	NAP	N3A-C2A-N1A	-3.64	122.99	128.68
2	B	301	NAP	N3A-C2A-N1A	-3.33	123.47	128.68
2	B	301	NAP	C3N-C7N-N7N	3.10	121.47	117.75
2	A	301	NAP	O3B-C3B-C4B	-2.87	102.76	111.05
2	C	301	NAP	N3A-C2A-N1A	-2.79	124.31	128.68
2	C	301	NAP	C3N-C7N-N7N	2.69	120.98	117.75
2	C	301	NAP	O4D-C1D-C2D	-2.67	103.03	106.93
2	C	301	NAP	O3B-C3B-C4B	-2.58	103.60	111.05
2	B	301	NAP	O4B-C1B-C2B	-2.52	102.22	106.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	NAP	O7N-C7N-N7N	-2.45	119.10	122.58
2	C	301	NAP	C4A-C5A-N7A	-2.43	106.86	109.40
2	A	301	NAP	O4B-C1B-C2B	-2.41	102.40	106.59
2	A	301	NAP	C4A-C5A-N7A	-2.36	106.94	109.40
2	B	301	NAP	O7N-C7N-C3N	-2.30	116.88	119.63
2	A	301	NAP	C3N-C7N-N7N	2.26	120.47	117.75
2	B	301	NAP	O3X-P2B-O2X	2.17	115.94	107.64
2	B	301	NAP	C1B-N9A-C4A	-2.14	122.87	126.64
2	B	301	NAP	C5N-C4N-C3N	-2.12	117.83	120.34
2	A	301	NAP	C2A-N1A-C6A	2.10	122.35	118.75
2	C	301	NAP	O4B-C1B-C2B	-2.07	103.00	106.59
2	B	301	NAP	C3B-C2B-C1B	-2.05	99.03	102.89
2	A	301	NAP	O2N-PN-O1N	2.01	122.19	112.24

There are no chirality outliers.

All (17) torsion outliers are listed below:

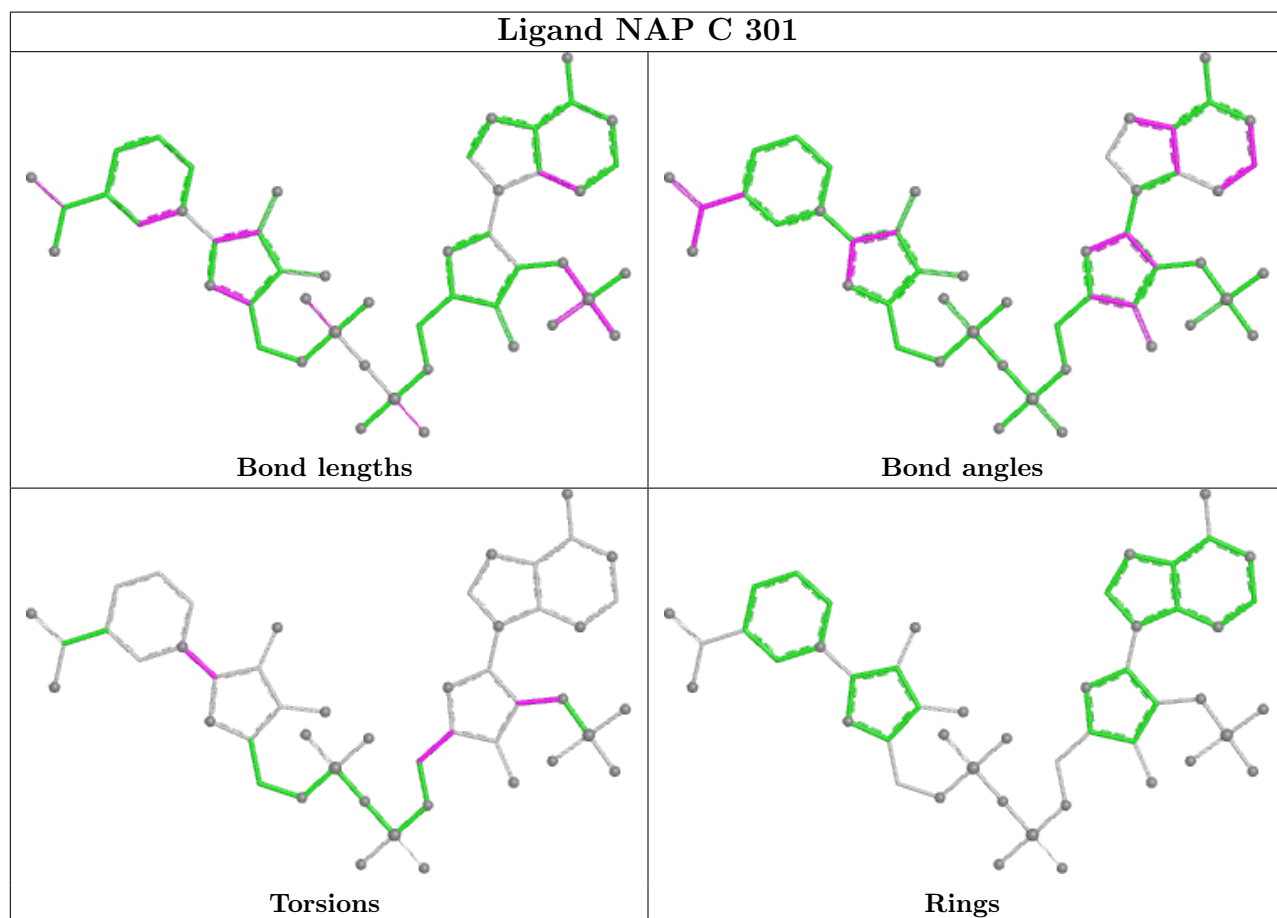
Mol	Chain	Res	Type	Atoms
2	A	301	NAP	O4D-C1D-N1N-C2N
2	B	301	NAP	O4D-C1D-N1N-C2N
2	C	301	NAP	O4D-C1D-N1N-C2N
2	A	301	NAP	C2B-O2B-P2B-O2X
2	A	301	NAP	C5D-O5D-PN-O3
2	B	301	NAP	C2B-O2B-P2B-O2X
2	A	301	NAP	O4B-C4B-C5B-O5B
2	A	301	NAP	C5D-O5D-PN-O1N
2	C	301	NAP	C1B-C2B-O2B-P2B
2	C	301	NAP	C3B-C2B-O2B-P2B
2	A	301	NAP	C2D-C1D-N1N-C6N
2	B	301	NAP	C2B-O2B-P2B-O3X
2	B	301	NAP	C5D-O5D-PN-O3
2	C	301	NAP	C2D-C1D-N1N-C2N
2	C	301	NAP	C2D-C1D-N1N-C6N
2	B	301	NAP	O4B-C4B-C5B-O5B
2	C	301	NAP	O4B-C4B-C5B-O5B

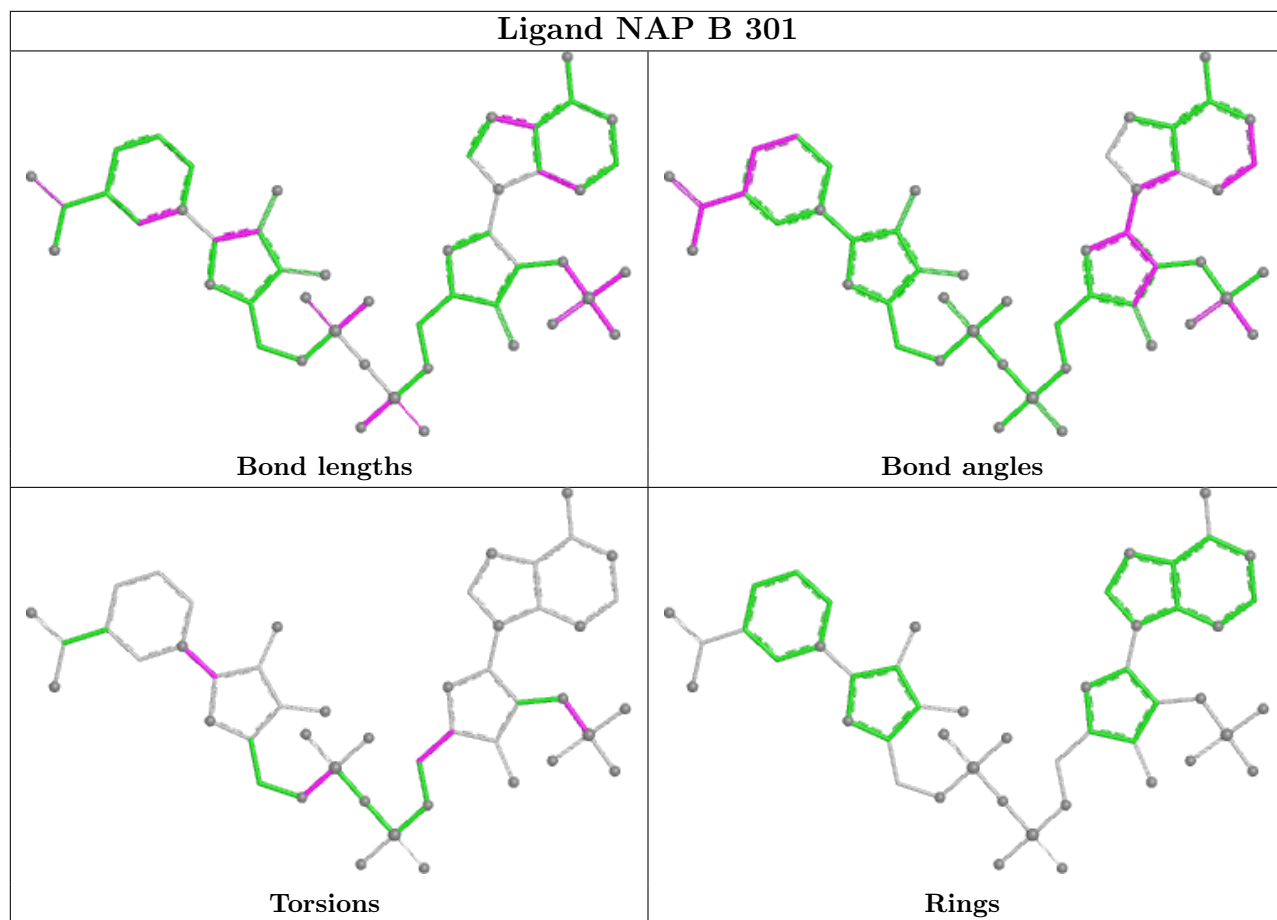
There are no ring outliers.

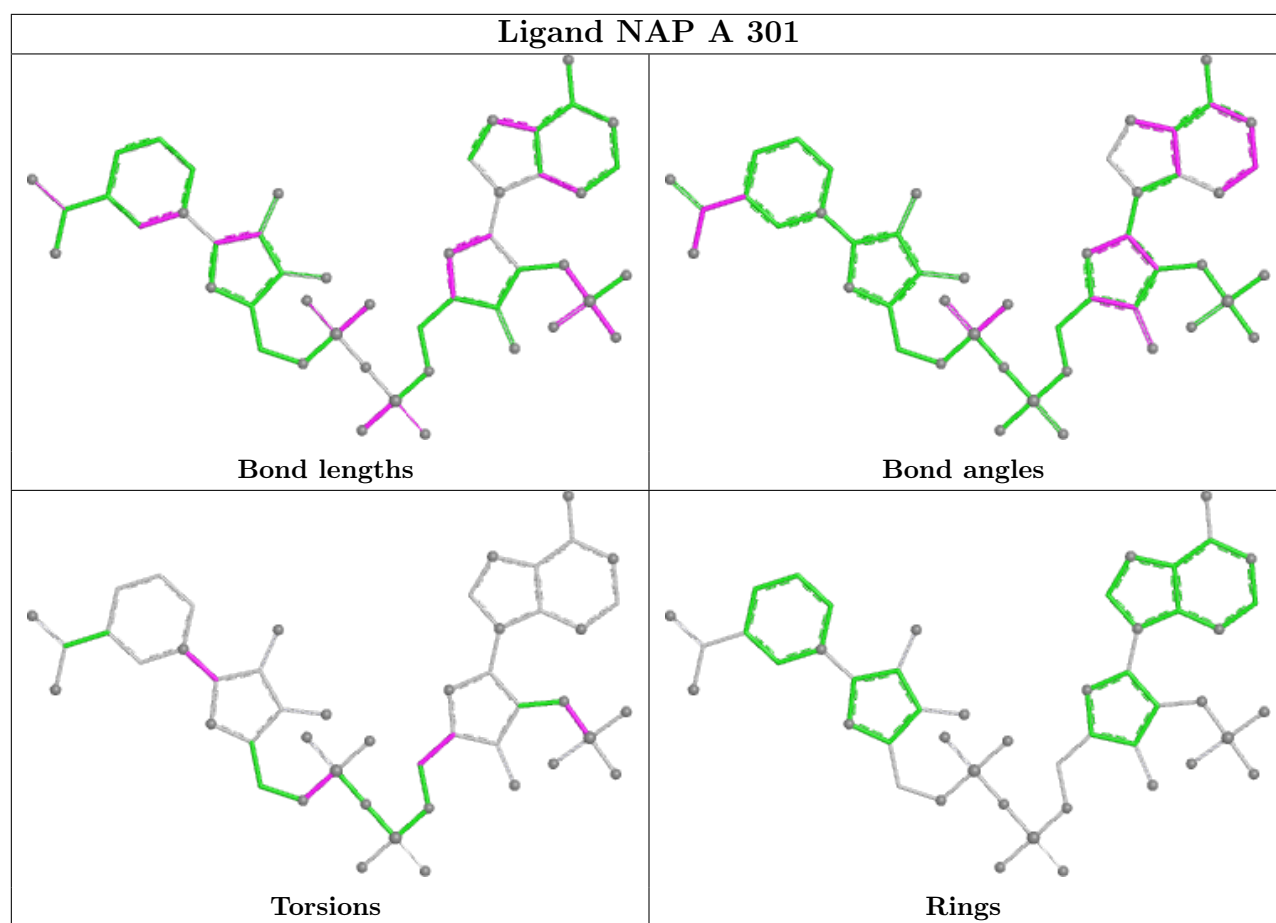
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	NAP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

6 Fit of model and data

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	291/291 (100%)	1.11	28 (9%) 8 10	31, 43, 77, 98	0
1	B	289/291 (99%)	1.37	57 (19%) 1 1	33, 58, 83, 100	0
1	C	290/291 (99%)	1.22	40 (13%) 2 4	34, 49, 70, 80	0
1	D	276/291 (94%)	1.93	94 (34%) 0 0	35, 63, 101, 124	0
All	All	1146/1164 (98%)	1.40	219 (19%) 1 1	31, 52, 91, 124	0

All (219) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	24	SER	10.8
1	D	56	VAL	10.1
1	D	10	ALA	9.9
1	C	132	CYS	9.8
1	C	131	GLU	9.3
1	A	236	LEU	8.6
1	D	153	LEU	8.3
1	D	29	THR	8.2
1	D	59	SER	8.1
1	D	85	LEU	8.1
1	D	52	VAL	7.8
1	D	156	ALA	7.6
1	B	23	GLN	7.1
1	D	44	LEU	6.6
1	D	75	LEU	6.5
1	D	40	PRO	6.4
1	B	25	GLY	6.3
1	D	13	MET	5.6
1	D	38	SER	5.6
1	B	4	THR	5.6
1	D	31	TRP	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	132	CYS	5.4
1	D	123	THR	5.4
1	D	36	ALA	5.3
1	B	18	ILE	5.2
1	D	9	GLY	5.1
1	D	18	ILE	5.0
1	B	59	SER	4.9
1	C	130	ALA	4.8
1	B	156	ALA	4.8
1	D	37	LYS	4.8
1	D	11	GLY	4.7
1	C	194	ALA	4.5
1	D	142	LEU	4.5
1	D	81	VAL	4.5
1	D	20	ALA	4.5
1	B	21	PHE	4.5
1	D	30	VAL	4.4
1	C	236	LEU	4.4
1	D	7	VAL	4.4
1	D	138	GLY	4.4
1	D	133	ALA	4.4
1	A	211	PRO	4.3
1	D	15	SER	4.2
1	D	48	LEU	4.2
1	D	32	ASN	4.1
1	D	19	LYS	4.1
1	D	63	VAL	4.1
1	B	48	LEU	4.0
1	C	231	ALA	4.0
1	D	161	GLY	3.9
1	B	36	ALA	3.9
1	A	233	ALA	3.9
1	D	6	THR	3.8
1	A	290	LEU	3.8
1	B	60	ASP	3.8
1	C	126	PHE	3.8
1	D	25	GLY	3.7
1	C	61	ILE	3.7
1	B	19	LYS	3.7
1	C	27	THR	3.7
1	B	40	PRO	3.6
1	D	77	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	35	LYS	3.5
1	C	290	LEU	3.5
1	B	139	SER	3.5
1	B	74	GLN	3.5
1	D	94	THR	3.3
1	A	251	ALA	3.3
1	D	199	LEU	3.3
1	D	73	ASP	3.3
1	D	51	THR	3.3
1	D	179	TRP	3.3
1	D	173	ALA	3.3
1	B	22	LEU	3.3
1	D	127	ILE	3.3
1	D	121	MET	3.3
1	B	68	ASP	3.3
1	A	284	ALA	3.3
1	B	126	PHE	3.3
1	D	12	ARG	3.2
1	A	246	PHE	3.2
1	D	254	GLU	3.2
1	C	34	THR	3.2
1	D	53	ARG	3.2
1	D	74	GLN	3.1
1	A	237	ALA	3.1
1	C	209	THR	3.1
1	C	82	THR	3.1
1	D	21	PHE	3.1
1	D	33	ARG	3.1
1	A	291	LYS	3.1
1	B	49	ALA	3.1
1	D	128	GLY	3.0
1	C	257	ASN	3.0
1	C	197	ILE	3.0
1	C	189	LEU	3.0
1	D	86	ARG	3.0
1	D	146	HIS	3.0
1	B	125	ASP	2.9
1	D	126	PHE	2.9
1	C	205	PHE	2.9
1	C	30	VAL	2.9
1	D	65	ASN	2.9
1	C	208	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	95	SER	2.9
1	C	227	ASN	2.8
1	B	133	ALA	2.8
1	C	237	ALA	2.8
1	D	23	GLN	2.8
1	B	160	VAL	2.8
1	C	35	LYS	2.8
1	A	238	SER	2.7
1	B	220	VAL	2.7
1	B	24	SER	2.7
1	C	50	ASP	2.7
1	B	276	ALA	2.7
1	D	83	ARG	2.7
1	B	236	LEU	2.7
1	B	233	ALA	2.7
1	A	216	ALA	2.6
1	A	289	PHE	2.6
1	B	15	SER	2.6
1	A	227	ASN	2.6
1	D	109	ARG	2.6
1	D	17	LEU	2.6
1	D	93	LEU	2.6
1	A	212	VAL	2.6
1	D	148	ALA	2.6
1	D	105	GLU	2.6
1	B	142	LEU	2.6
1	B	45	GLY	2.6
1	D	71	THR	2.5
1	D	54	ASP	2.5
1	A	285	ILE	2.5
1	D	147	ARG	2.5
1	C	129	GLN	2.5
1	A	256	ARG	2.5
1	D	98	PRO	2.5
1	B	56	VAL	2.4
1	D	160	VAL	2.4
1	D	8	ILE	2.4
1	B	5	LEU	2.4
1	C	10	ALA	2.4
1	D	132	CYS	2.4
1	B	154	GLY	2.4
1	D	287	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	69	TYR	2.3
1	C	253	CYS	2.3
1	B	11	GLY	2.3
1	A	34	THR	2.3
1	B	157	THR	2.3
1	C	86	ARG	2.3
1	A	206	ILE	2.3
1	B	75	LEU	2.3
1	D	151	ASN	2.3
1	C	230	THR	2.3
1	D	61	ILE	2.3
1	B	141	ALA	2.3
1	D	125	ASP	2.3
1	C	22	LEU	2.3
1	D	39	GLU	2.3
1	B	258	ILE	2.3
1	B	76	LEU	2.3
1	B	100	LEU	2.3
1	D	82	THR	2.3
1	B	131	GLU	2.2
1	B	46	ALA	2.2
1	D	14	GLY	2.2
1	C	80	GLU	2.2
1	C	29	THR	2.2
1	D	266	MET	2.2
1	B	267	TYR	2.2
1	B	20	ALA	2.2
1	C	210	GLU	2.2
1	D	111	HIS	2.2
1	B	103	GLU	2.2
1	B	101	ALA	2.2
1	C	54	ASP	2.2
1	D	55	ALA	2.2
1	B	240	GLU	2.2
1	A	1	MET	2.2
1	A	81	VAL	2.1
1	B	275	LYS	2.1
1	A	280	LYS	2.1
1	D	62	ILE	2.1
1	D	107	TRP	2.1
1	A	56	VAL	2.1
1	B	167	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	108	ALA	2.1
1	C	274	VAL	2.1
1	A	13	MET	2.1
1	B	47	HIS	2.1
1	D	114	ASP	2.1
1	A	240	GLU	2.1
1	C	31	TRP	2.1
1	B	66	VAL	2.1
1	B	70	ASP	2.1
1	B	266	MET	2.1
1	B	123	THR	2.1
1	D	122	ALA	2.1
1	D	233	ALA	2.1
1	D	244	VAL	2.1
1	A	270	ILE	2.0
1	D	145	LYS	2.0
1	C	36	ALA	2.0
1	C	156	ALA	2.0
1	A	97	SER	2.0
1	A	31	TRP	2.0
1	B	79	ASP	2.0
1	D	57	LYS	2.0
1	B	239	LEU	2.0
1	C	175	LEU	2.0
1	C	229	LEU	2.0
1	B	222	THR	2.0
1	D	47	HIS	2.0
1	A	283	PHE	2.0
1	D	115	TYR	2.0
1	D	76	LEU	2.0

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

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

6.3 Carbohydrates [\(i\)](#)

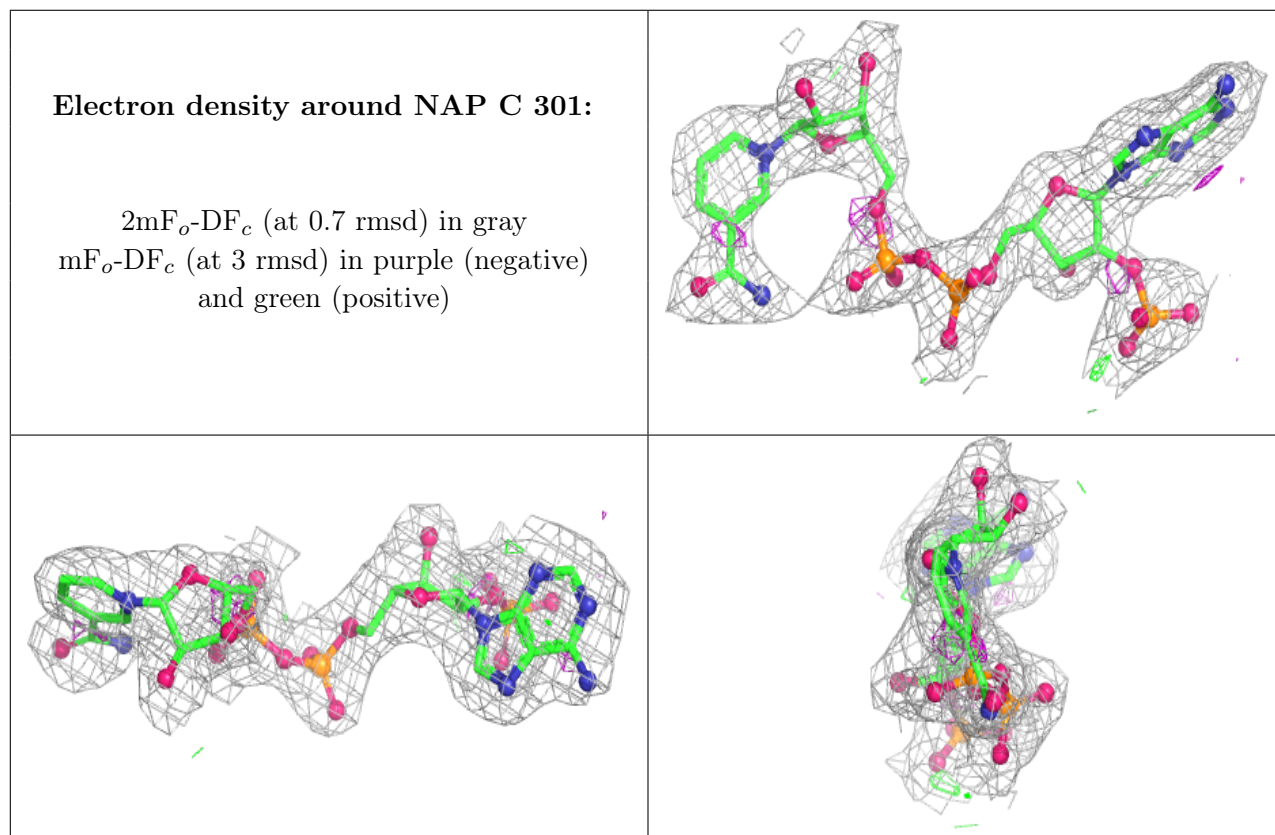
There are no monosaccharides in this entry.

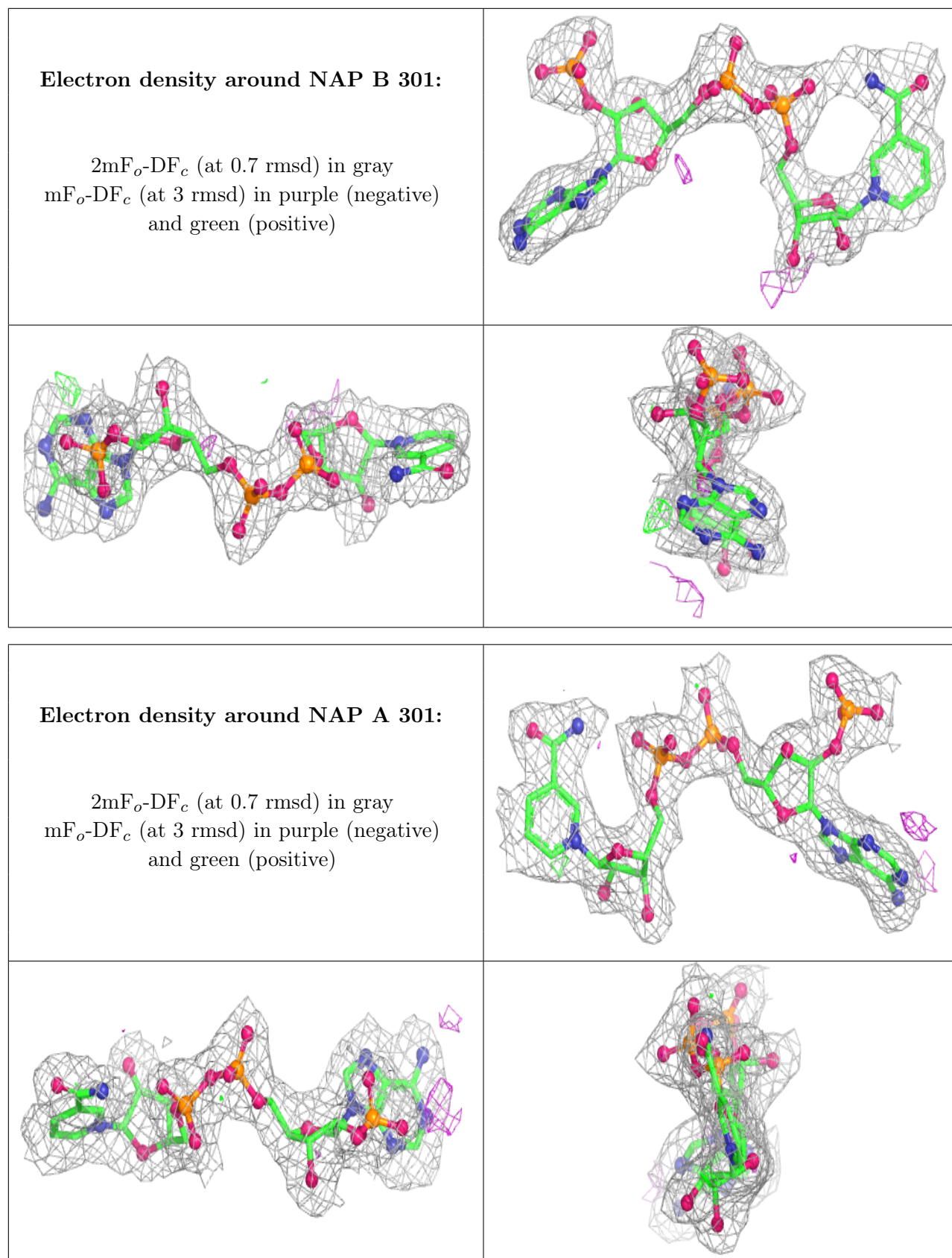
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	C	301	48/48	0.84	0.21	36,43,49,51	0
2	NAP	B	301	48/48	0.87	0.20	42,52,59,64	0
2	NAP	A	301	48/48	0.93	0.17	28,32,36,38	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.