



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:05 PM UTC

PDB ID : 7YB1 / pdb_00007yb1
Title : Crystal Structure of anthrol reductase (CbAR) in complex with NADP+
Authors : Hou, X.D.; Rao, Y.J.
Deposited on : 2022-06-28
Resolution : 3.30 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

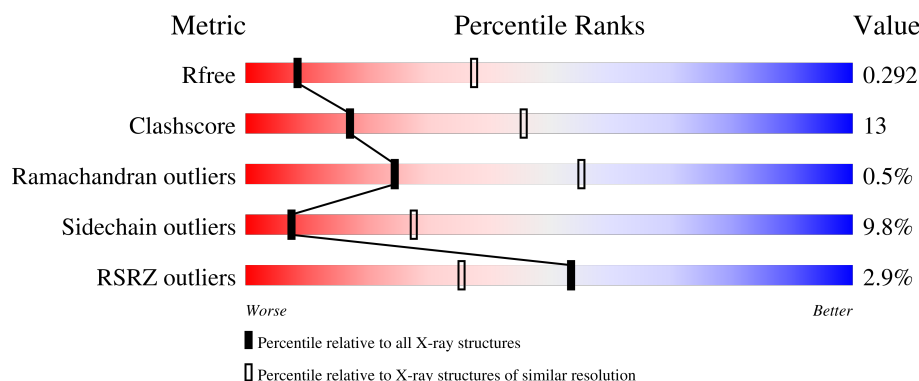
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	279	3% 65% 23% • 9%
1	B	279	3% 58% 27% 5% 11%
1	C	279	4% 59% 24% 6% 11%
1	D	279	% 66% 23% • 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7730 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 Versicolorin reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	251	Total	C	N	O	S	0	0	0
			1893	1189	342	358	4			
1	A	255	Total	C	N	O	S	0	0	0
			1926	1211	348	363	4			
1	B	248	Total	C	N	O	S	0	0	0
			1848	1158	333	353	4			
1	C	248	Total	C	N	O	S	0	0	0
			1854	1164	333	353	4			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	MET	-	initiating methionine	UNP A0A2G5I2X5
D	0	ALA	-	expression tag	UNP A0A2G5I2X5
D	269	ALA	-	expression tag	UNP A0A2G5I2X5
D	270	LEU	-	expression tag	UNP A0A2G5I2X5
D	271	GLU	-	expression tag	UNP A0A2G5I2X5
D	272	HIS	-	expression tag	UNP A0A2G5I2X5
D	273	HIS	-	expression tag	UNP A0A2G5I2X5
D	274	HIS	-	expression tag	UNP A0A2G5I2X5
D	275	HIS	-	expression tag	UNP A0A2G5I2X5
D	276	HIS	-	expression tag	UNP A0A2G5I2X5
D	277	HIS	-	expression tag	UNP A0A2G5I2X5
A	-1	MET	-	initiating methionine	UNP A0A2G5I2X5
A	0	ALA	-	expression tag	UNP A0A2G5I2X5
A	269	ALA	-	expression tag	UNP A0A2G5I2X5
A	270	LEU	-	expression tag	UNP A0A2G5I2X5
A	271	GLU	-	expression tag	UNP A0A2G5I2X5
A	272	HIS	-	expression tag	UNP A0A2G5I2X5
A	273	HIS	-	expression tag	UNP A0A2G5I2X5
A	274	HIS	-	expression tag	UNP A0A2G5I2X5
A	275	HIS	-	expression tag	UNP A0A2G5I2X5
A	276	HIS	-	expression tag	UNP A0A2G5I2X5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	277	HIS	-	expression tag	UNP A0A2G5I2X5
B	-1	MET	-	initiating methionine	UNP A0A2G5I2X5
B	0	ALA	-	expression tag	UNP A0A2G5I2X5
B	269	ALA	-	expression tag	UNP A0A2G5I2X5
B	270	LEU	-	expression tag	UNP A0A2G5I2X5
B	271	GLU	-	expression tag	UNP A0A2G5I2X5
B	272	HIS	-	expression tag	UNP A0A2G5I2X5
B	273	HIS	-	expression tag	UNP A0A2G5I2X5
B	274	HIS	-	expression tag	UNP A0A2G5I2X5
B	275	HIS	-	expression tag	UNP A0A2G5I2X5
B	276	HIS	-	expression tag	UNP A0A2G5I2X5
B	277	HIS	-	expression tag	UNP A0A2G5I2X5
C	-1	MET	-	initiating methionine	UNP A0A2G5I2X5
C	0	ALA	-	expression tag	UNP A0A2G5I2X5
C	269	ALA	-	expression tag	UNP A0A2G5I2X5
C	270	LEU	-	expression tag	UNP A0A2G5I2X5
C	271	GLU	-	expression tag	UNP A0A2G5I2X5
C	272	HIS	-	expression tag	UNP A0A2G5I2X5
C	273	HIS	-	expression tag	UNP A0A2G5I2X5
C	274	HIS	-	expression tag	UNP A0A2G5I2X5
C	275	HIS	-	expression tag	UNP A0A2G5I2X5
C	276	HIS	-	expression tag	UNP A0A2G5I2X5
C	277	HIS	-	expression tag	UNP A0A2G5I2X5

- # NAP
-
- The chemical structure of Naproxen (NAP) is shown, featuring a naphthalene ring system. The structure includes a carboxylic acid group (COOH) and a propyl side chain. The stereochemistry is indicated by wedges and dashes at the chiral center (C10). The atoms are numbered from 1 to 14, with the carboxylic acid group labeled with 'O1A' through 'O1D' and the propyl side chain labeled with 'C15' through 'C18'.

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

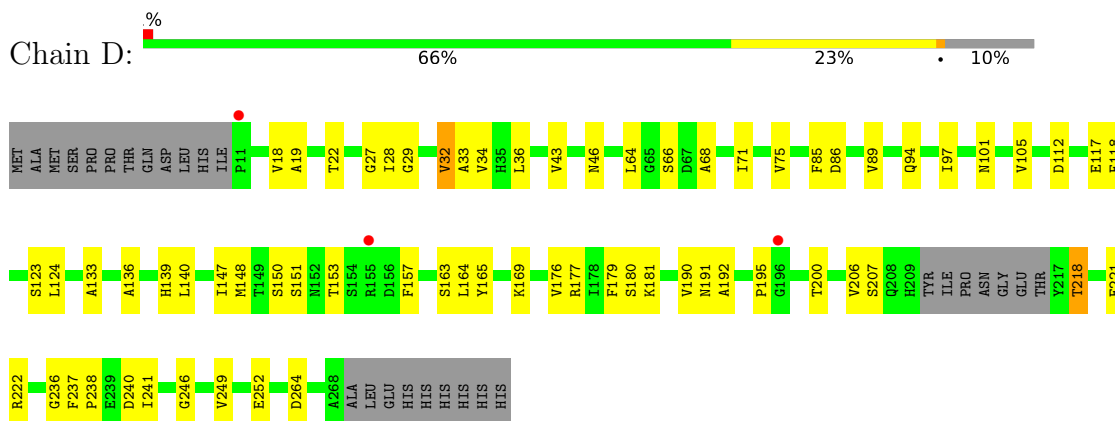
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	3	Total	O	0	0
			3	3		
3	A	9	Total	O	0	0
			9	9		
3	B	3	Total	O	0	0
			3	3		
3	C	2	Total	O	0	0
			2	2		

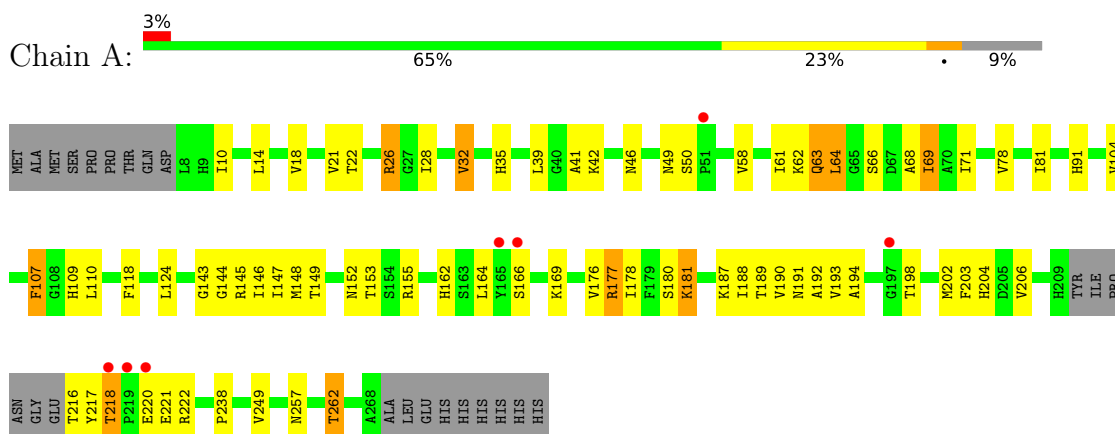
3 Residue-property plots

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.

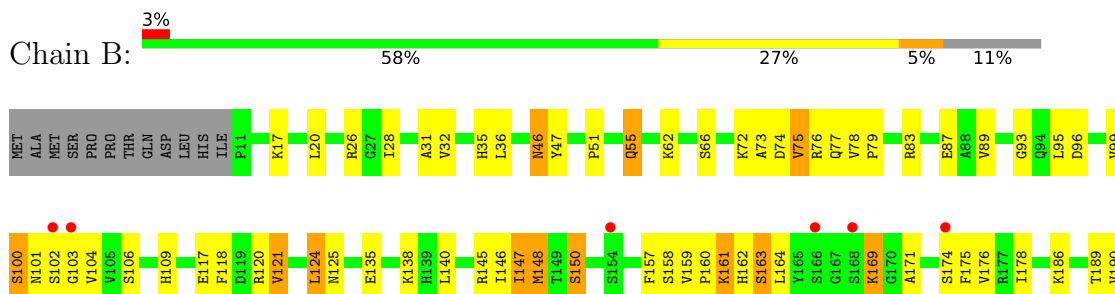
- Molecule 1: Versicolorin reductase



- Molecule 1: Versicolorin reductase

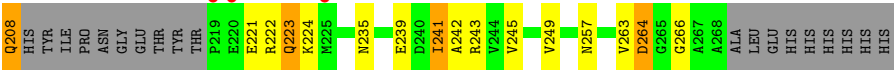
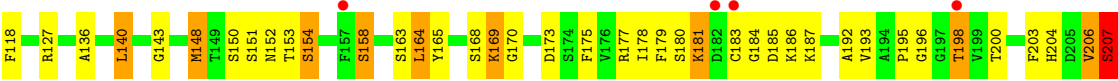


- Molecule 1: Versicolorin reductase





● Molecule 1: Versicolorin reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	124.62Å 124.62Å 134.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.66 – 3.30 23.66 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (23.66-3.30) 99.6 (23.66-3.30)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 3.30Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.206 , 0.285 0.225 , 0.292	Depositor DCC
R_{free} test set	887 reflections (5.38%)	wwPDB-VP
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 20.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	7730	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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

5.1 Standard geometry

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	1.08	0/1962	1.54	4/2653 (0.2%)
1	B	1.10	0/1880	1.57	7/2541 (0.3%)
1	C	1.11	0/1887	1.58	12/2550 (0.5%)
1	D	1.10	0/1928	1.52	2/2605 (0.1%)
All	All	1.10	0/7657	1.55	25/10349 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	207	SER	N-CA-C	-8.72	102.78	113.15
1	C	77	GLN	CA-C-N	8.32	125.48	120.24
1	C	77	GLN	C-N-CA	8.32	125.48	120.24
1	C	165	TYR	CA-C-N	6.71	129.59	120.54
1	C	165	TYR	C-N-CA	6.71	129.59	120.54
1	D	32	VAL	N-CA-C	-6.03	104.86	110.53
1	C	27	GLY	N-CA-C	5.69	117.13	111.21
1	B	124	LEU	N-CA-C	-5.45	106.68	113.55
1	B	77	GLN	CA-C-N	5.35	123.61	120.24
1	B	77	GLN	C-N-CA	5.35	123.61	120.24
1	C	266	GLY	N-CA-C	-5.33	107.68	115.63
1	B	109	HIS	CB-CA-C	5.32	119.10	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	39	LEU	N-CA-C	-5.22	106.69	113.16
1	A	262	THR	CB-CA-C	5.18	119.06	110.78
1	C	91	HIS	CA-CB-CG	-5.14	108.66	113.80
1	D	236	GLY	CA-C-O	-5.11	116.68	121.18
1	A	62	LYS	CA-C-N	5.08	127.39	120.54
1	A	62	LYS	C-N-CA	5.08	127.39	120.54
1	B	109	HIS	CA-CB-CG	5.08	118.88	113.80
1	C	31	ALA	N-CA-C	-5.06	106.96	113.23
1	C	30	ALA	N-CA-C	-5.03	107.31	113.50
1	A	152	ASN	N-CA-C	-5.01	107.01	113.23
1	C	153	THR	N-CA-C	-5.01	107.23	113.19
1	B	245	VAL	CA-C-N	5.00	126.44	120.13
1	B	245	VAL	C-N-CA	5.00	126.44	120.13

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	120	ARG	Sidechain

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	1926	0	1911	48	0
1	B	1848	0	1825	55	0
1	C	1854	0	1832	55	0
1	D	1893	0	1876	36	0
2	A	48	0	25	4	0
2	B	48	0	25	5	0
2	C	48	0	25	3	0
2	D	48	0	25	2	0
3	A	9	0	0	0	0
3	B	3	0	0	0	0
3	C	2	0	0	0	0
3	D	3	0	0	0	0
All	All	7730	0	7544	192	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 13.

All (192) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:VAL:HG22	1:B:147:ILE:HD13	1.58	0.85
2:C:301:NAP:O2N	2:C:301:NAP:N7N	2.10	0.84
1:C:164:LEU:HD12	1:C:164:LEU:O	1.81	0.81
1:A:202:MET:O	1:A:206:VAL:HG23	1.81	0.80
1:B:32:VAL:O	1:B:36:LEU:HG	1.87	0.74
1:C:118:PHE:HA	1:C:164:LEU:HD21	1.70	0.74
1:B:104:VAL:HG22	1:B:125:ASN:OD1	1.87	0.73
1:B:55:GLN:HE21	1:B:55:GLN:HA	1.53	0.72
1:C:105:VAL:HG21	1:C:206:VAL:HG21	1.72	0.72
1:A:204:HIS:O	1:A:222:ARG:NH1	2.24	0.70
1:D:117:GLU:HA	1:D:117:GLU:OE1	1.93	0.68
1:A:176:VAL:HG11	1:A:192:ALA:HB2	1.75	0.67
1:A:202:MET:HE1	2:A:301:NAP:H2D	1.75	0.67
1:A:143:GLY:HA2	1:A:187:LYS:O	1.93	0.67
1:C:193:VAL:O	1:C:195:PRO:HD3	1.95	0.67
1:B:20:LEU:HB2	1:B:95:LEU:HD11	1.77	0.67
1:A:26:ARG:HG3	2:A:301:NAP:H3B	1.75	0.66
1:A:194:ALA:HB3	1:A:262:THR:HA	1.78	0.66
1:C:198:THR:HG22	1:C:200:THR:HG23	1.77	0.66
1:A:63:GLN:HA	1:A:63:GLN:OE1	1.97	0.65
1:A:28:ILE:HA	1:A:238:PRO:HB3	1.78	0.65
1:C:28:ILE:HG12	1:C:198:THR:HG21	1.77	0.65
1:C:32:VAL:HG22	1:C:242:ALA:HA	1.80	0.64
1:C:223:GLN:HE21	1:C:235:ASN:ND2	1.96	0.64
1:B:147:ILE:HD11	1:B:249:VAL:HG12	1.79	0.63
1:C:80:GLU:OE1	1:C:83:ARG:NH2	2.33	0.62
1:D:75:VAL:HG23	1:D:124:LEU:HD12	1.81	0.62
1:C:136:ALA:O	1:C:140:LEU:HB2	2.00	0.61
1:D:33:ALA:HB1	1:D:43:VAL:HG11	1.83	0.61
1:C:206:VAL:C	1:C:208:GLN:H	2.09	0.61
1:A:218:THR:HG23	1:A:221:GLU:HG3	1.81	0.60
1:B:46:ASN:ND2	1:B:73:ALA:HB3	2.17	0.60
1:B:104:VAL:HG21	1:B:121:VAL:HA	1.82	0.60
1:C:207:SER:O	1:C:208:GLN:HB2	2.03	0.59
1:B:146:ILE:HB	1:B:190:VAL:HG22	1.85	0.58
1:C:28:ILE:HG21	1:C:241:ILE:HD12	1.85	0.58
1:C:168:SER:OG	1:C:169:LYS:HD3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:301:NAP:O5D	2:C:301:NAP:H2N	2.03	0.58
1:B:104:VAL:CG2	1:B:121:VAL:HA	2.33	0.58
1:B:104:VAL:HG13	1:B:124:LEU:HD23	1.86	0.58
1:B:207:SER:OG	1:B:222:ARG:NH1	2.37	0.57
1:C:28:ILE:CG2	1:C:241:ILE:HD12	2.35	0.57
1:B:147:ILE:HA	1:B:191:ASN:O	2.05	0.56
1:A:177:ARG:HB3	1:A:177:ARG:CZ	2.34	0.56
1:B:28:ILE:O	1:B:32:VAL:HG23	2.05	0.56
1:C:28:ILE:HD11	1:C:198:THR:HB	1.88	0.56
1:B:219:PRO:HG2	1:B:221:GLU:HB3	1.88	0.55
1:A:178:ILE:HG21	1:C:163:SER:N	2.22	0.55
1:C:26:ARG:HG3	2:C:301:NAP:H3B	1.89	0.54
1:C:203:PHE:HE2	1:C:223:GLN:HB2	1.72	0.54
1:A:61:ILE:O	1:A:64:LEU:HD12	2.08	0.54
1:B:103:GLY:HA2	2:B:301:NAP:H3D	1.89	0.54
1:D:118:PHE:HA	1:D:164:LEU:HD21	1.90	0.54
1:C:239:GLU:O	1:C:243:ARG:HG3	2.08	0.53
1:C:204:HIS:HA	1:C:207:SER:OG	2.08	0.53
1:A:14:LEU:HB2	1:A:41:ALA:HB2	1.90	0.53
1:B:32:VAL:HG11	1:B:245:VAL:HG11	1.90	0.53
1:D:252:GLU:OE1	1:D:252:GLU:N	2.40	0.52
1:B:46:ASN:HD21	1:B:73:ALA:HB3	1.72	0.52
1:D:136:ALA:O	1:D:140:LEU:HB2	2.09	0.52
1:C:178:ILE:O	1:C:181:LYS:HG2	2.10	0.52
1:A:118:PHE:HA	1:A:164:LEU:HD21	1.91	0.51
1:B:55:GLN:HA	1:B:55:GLN:NE2	2.23	0.51
1:C:193:VAL:HG21	1:C:241:ILE:HD11	1.92	0.51
1:A:69:ILE:HG21	1:A:91:HIS:CD2	2.45	0.51
1:D:28:ILE:HA	1:D:238:PRO:HB3	1.93	0.51
1:B:102:SER:HB2	1:B:124:LEU:HG	1.93	0.51
1:A:143:GLY:CA	1:A:187:LYS:O	2.59	0.51
1:A:178:ILE:CD1	1:C:158:SER:HA	2.42	0.50
1:B:62:LYS:HA	1:B:66:SER:O	2.12	0.50
1:C:31:ALA:HB1	1:C:239:GLU:HG3	1.93	0.50
1:C:150:SER:OG	1:C:169:LYS:HB3	2.11	0.50
2:B:301:NAP:O1N	2:B:301:NAP:N7N	2.44	0.50
1:C:203:PHE:CE2	1:C:223:GLN:HB2	2.46	0.50
1:D:22:THR:HA	1:D:46:ASN:HB3	1.94	0.50
1:A:109:HIS:O	1:A:110:LEU:C	2.54	0.50
1:D:237:PHE:O	1:D:240:ASP:HB2	2.11	0.50
1:A:28:ILE:CG1	1:A:198:THR:HG21	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:LEU:C	1:D:64:LEU:HD12	2.38	0.49
1:A:217:TYR:O	1:A:222:ARG:HD3	2.12	0.49
1:B:32:VAL:CG1	1:B:245:VAL:HG11	2.42	0.49
1:A:153:THR:O	1:A:166:SER:HB3	2.12	0.49
1:D:148:MET:O	1:D:192:ALA:HA	2.13	0.49
1:B:202:MET:HE1	2:B:301:NAP:H2D	1.94	0.49
1:C:152:ASN:ND2	1:C:264:ASP:OD1	2.43	0.49
1:B:35:HIS:NE2	1:B:243:ARG:HG2	2.28	0.49
1:C:32:VAL:O	1:C:36:LEU:HG	2.13	0.49
1:A:262:THR:HB	1:B:259:LYS:HE2	1.94	0.48
1:B:17:LYS:HA	1:B:96:ASP:OD2	2.13	0.48
1:B:74:ASP:C	1:B:76:ARG:N	2.68	0.48
1:C:208:GLN:HE21	1:C:208:GLN:HA	1.77	0.48
1:D:27:GLY:C	1:D:29:GLY:N	2.71	0.48
1:D:195:PRO:HB3	1:D:241:ILE:HG12	1.95	0.48
1:D:105:VAL:HG21	1:D:206:VAL:CG2	2.43	0.48
1:B:150:SER:HA	1:B:169:LYS:HB3	1.94	0.48
1:C:164:LEU:HD12	1:C:164:LEU:C	2.35	0.48
1:A:18:VAL:HA	1:A:42:LYS:O	2.14	0.48
1:D:43:VAL:O	1:D:68:ALA:HA	2.14	0.47
1:C:184:GLY:C	1:C:186:LYS:H	2.23	0.47
1:D:207:SER:HG	1:D:222:ARG:HE	1.61	0.47
1:B:74:ASP:C	1:B:76:ARG:H	2.23	0.47
1:B:102:SER:CB	1:B:124:LEU:HD11	2.45	0.47
1:B:121:VAL:HG21	1:B:164:LEU:HD22	1.97	0.47
1:B:162:HIS:O	1:B:164:LEU:N	2.48	0.47
1:C:113:VAL:HG11	1:C:164:LEU:HD22	1.97	0.47
1:D:179:PHE:HB3	1:D:190:VAL:HG21	1.96	0.47
1:A:50:SER:HB2	2:A:301:NAP:O2X	2.15	0.46
1:A:148:MET:O	1:A:192:ALA:HA	2.15	0.46
1:B:145:ARG:HG3	1:B:249:VAL:HA	1.98	0.46
1:A:149:THR:HG21	2:A:301:NAP:H4D	1.97	0.46
1:B:26:ARG:NH2	2:B:301:NAP:O3X	2.41	0.46
1:B:32:VAL:HG22	1:B:242:ALA:HA	1.97	0.46
1:C:206:VAL:C	1:C:208:GLN:N	2.72	0.46
1:D:28:ILE:O	1:D:32:VAL:HG23	2.16	0.46
1:D:200:THR:HG21	2:D:301:NAP:O2N	2.15	0.46
1:B:162:HIS:O	1:B:163:SER:C	2.58	0.46
1:C:51:PRO:HG2	1:C:52:THR:H	1.81	0.46
1:C:170:GLY:O	1:C:173:ASP:HB2	2.16	0.46
1:B:89:VAL:O	1:B:93:GLY:N	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:ILE:HD11	1:B:249:VAL:CG1	2.46	0.45
1:B:74:ASP:OD1	2:B:301:NAP:N6A	2.48	0.45
1:B:100:SER:HB3	1:B:148:MET:HA	1.98	0.45
1:D:150:SER:OG	1:D:151:SER:N	2.46	0.45
1:D:165:TYR:O	1:D:169:LYS:HG2	2.16	0.45
1:B:176:VAL:HG11	1:B:192:ALA:HB2	1.98	0.44
1:A:69:ILE:HD11	1:A:71:ILE:HD11	1.99	0.44
1:B:157:PHE:HZ	1:B:267:ALA:O	2.01	0.44
1:B:47:TYR:CE2	1:B:51:PRO:HB3	2.53	0.44
1:B:135:GLU:OE2	1:B:138:LYS:NZ	2.43	0.44
1:D:33:ALA:O	1:D:34:VAL:C	2.61	0.44
1:C:207:SER:OG	1:C:222:ARG:NH1	2.51	0.44
1:C:175:PHE:HB3	1:C:179:PHE:CE2	2.53	0.44
1:C:180:SER:HB2	1:C:257:ASN:OD1	2.19	0.43
1:C:186:LYS:O	1:C:187:LYS:C	2.61	0.43
1:A:177:ARG:CZ	1:A:177:ARG:CB	2.97	0.43
1:C:15:ASP:HA	1:C:40:GLY:O	2.18	0.43
1:A:107:PHE:CE1	1:A:162:HIS:ND1	2.86	0.43
1:B:31:ALA:O	1:B:35:HIS:HB2	2.17	0.43
1:B:117:GLU:O	1:B:121:VAL:HG13	2.19	0.43
1:B:118:PHE:HA	1:B:164:LEU:HD11	2.01	0.43
1:D:27:GLY:O	1:D:29:GLY:N	2.52	0.43
1:D:153:THR:HA	1:D:157:PHE:O	2.19	0.43
1:A:146:ILE:C	1:A:147:ILE:HD13	2.44	0.43
1:A:147:ILE:HA	1:A:191:ASN:O	2.18	0.43
1:A:181:LYS:H	1:A:181:LYS:HG2	1.48	0.43
1:D:176:VAL:HG11	1:D:192:ALA:HB2	2.01	0.43
1:A:145:ARG:HG3	1:A:249:VAL:O	2.18	0.43
1:B:78:VAL:N	1:B:79:PRO:CD	2.82	0.43
1:D:133:ALA:O	1:D:136:ALA:HB3	2.18	0.43
1:D:218:THR:HG23	1:D:221:GLU:CD	2.44	0.43
1:D:246:GLY:HA2	1:D:249:VAL:HG22	2.01	0.43
1:B:83:ARG:O	1:B:87:GLU:HG3	2.19	0.43
1:D:32:VAL:O	1:D:36:LEU:HG	2.18	0.42
1:A:61:ILE:HG21	1:A:68:ALA:HB2	2.01	0.42
1:C:21:VAL:HG12	1:C:24:SER:HB2	2.01	0.42
1:C:152:ASN:CG	1:C:196:GLY:HA2	2.45	0.42
1:D:147:ILE:HA	1:D:191:ASN:O	2.19	0.42
1:B:160:PRO:O	1:B:161:LYS:CB	2.67	0.42
1:A:58:VAL:HG13	1:A:68:ALA:HB3	2.00	0.42
1:B:148:MET:O	1:B:192:ALA:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:VAL:N	1:C:79:PRO:CD	2.82	0.42
1:D:105:VAL:HG21	1:D:206:VAL:HG22	2.00	0.42
1:A:146:ILE:O	1:A:190:VAL:HA	2.19	0.42
1:C:30:ALA:O	1:C:34:VAL:HG23	2.20	0.42
1:A:118:PHE:CZ	1:C:127:ARG:HA	2.55	0.42
1:A:61:ILE:HA	1:A:64:LEU:HD11	2.01	0.42
1:C:31:ALA:O	1:C:35:HIS:HB2	2.19	0.42
1:A:21:VAL:HG21	1:A:32:VAL:HG12	2.02	0.41
1:B:147:ILE:HD12	1:B:147:ILE:N	2.35	0.41
1:C:208:GLN:HA	1:C:208:GLN:NE2	2.35	0.41
1:D:86:ASP:OD1	1:D:139:HIS:NE2	2.53	0.41
1:D:150:SER:O	2:D:301:NAP:H6N	2.20	0.41
1:B:194:ALA:HB3	1:B:262:THR:HA	2.01	0.41
1:A:104:VAL:HG13	1:A:124:LEU:HD23	2.02	0.41
1:A:198:THR:O	1:A:203:PHE:HB2	2.21	0.41
1:D:18:VAL:HG23	1:D:94:GLN:HE21	1.85	0.41
1:D:85:PHE:O	1:D:89:VAL:HG23	2.20	0.41
1:A:35:HIS:O	1:A:39:LEU:HG	2.20	0.41
1:B:171:ALA:HB1	1:B:175:PHE:CZ	2.56	0.41
1:C:245:VAL:O	1:C:249:VAL:HG13	2.21	0.41
1:C:143:GLY:HA2	1:C:187:LYS:O	2.20	0.41
1:C:152:ASN:C	1:C:154:SER:H	2.28	0.41
1:C:169:LYS:HA	1:C:169:LYS:HD2	1.72	0.41
1:A:78:VAL:O	1:A:81:ILE:HB	2.21	0.41
1:A:144:GLY:O	1:A:188:ILE:HA	2.21	0.41
1:A:218:THR:CG2	1:A:221:GLU:HG3	2.49	0.41
1:D:19:ALA:HA	1:D:97:ILE:O	2.21	0.40
1:A:22:THR:HA	1:A:46:ASN:OD1	2.20	0.40
1:C:169:LYS:N	1:C:169:LYS:CD	2.82	0.40
1:A:257:ASN:HD22	1:B:232:LEU:HD11	1.86	0.40
1:C:184:GLY:C	1:C:186:LYS:N	2.77	0.40
1:C:148:MET:O	1:C:192:ALA:HA	2.21	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	251/279 (90%)	224 (89%)	27 (11%)	0	100	100
1	B	244/279 (88%)	227 (93%)	14 (6%)	3 (1%)	10	37
1	C	244/279 (88%)	216 (88%)	26 (11%)	2 (1%)	16	45
1	D	247/279 (88%)	227 (92%)	20 (8%)	0	100	100
All	All	986/1116 (88%)	894 (91%)	87 (9%)	5 (0%)	24	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	161	LYS
1	B	163	SER
1	C	183	CYS
1	B	75	VAL
1	C	51	PRO

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	204/225 (91%)	185 (91%)	19 (9%)	8	30
1	B	194/225 (86%)	171 (88%)	23 (12%)	5	20
1	C	195/225 (87%)	170 (87%)	25 (13%)	4	18
1	D	200/225 (89%)	189 (94%)	11 (6%)	19	48
All	All	793/900 (88%)	715 (90%)	78 (10%)	7	28

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	66	SER

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Mol	Chain	Res	Type
1	D	71	ILE
1	D	101	ASN
1	D	112	ASP
1	D	123	SER
1	D	163	SER
1	D	177	ARG
1	D	180	SER
1	D	181	LYS
1	D	218	THR
1	D	264	ASP
1	A	10	ILE
1	A	26	ARG
1	A	32	VAL
1	A	49	ASN
1	A	63	GLN
1	A	64	LEU
1	A	66	SER
1	A	69	ILE
1	A	107	PHE
1	A	155	ARG
1	A	169	LYS
1	A	177	ARG
1	A	180	SER
1	A	181	LYS
1	A	189	THR
1	A	193	VAL
1	A	216	THR
1	A	218	THR
1	A	220	GLU
1	B	46	ASN
1	B	55	GLN
1	B	72	LYS
1	B	75	VAL
1	B	100	SER
1	B	101	ASN
1	B	106	SER
1	B	121	VAL
1	B	140	LEU
1	B	147	ILE
1	B	148	MET
1	B	150	SER
1	B	158	SER

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Mol	Chain	Res	Type
1	B	159	VAL
1	B	169	LYS
1	B	174	SER
1	B	178	ILE
1	B	186	LYS
1	B	189	THR
1	B	220	GLU
1	B	238	PRO
1	B	241	ILE
1	B	263	VAL
1	C	14	LEU
1	C	46	ASN
1	C	64	LEU
1	C	80	GLU
1	C	100	SER
1	C	140	LEU
1	C	148	MET
1	C	151	SER
1	C	154	SER
1	C	158	SER
1	C	164	LEU
1	C	169	LYS
1	C	177	ARG
1	C	181	LYS
1	C	185	ASP
1	C	198	THR
1	C	206	VAL
1	C	207	SER
1	C	208	GLN
1	C	221	GLU
1	C	223	GLN
1	C	224	LYS
1	C	241	ILE
1	C	263	VAL
1	C	264	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	142	ASN
1	D	162	HIS
1	A	35	HIS

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Mol	Chain	Res	Type
1	A	223	GLN
1	A	228	HIS
1	A	235	ASN
1	B	49	ASN
1	B	55	GLN
1	B	162	HIS
1	C	35	HIS
1	C	53	HIS
1	C	204	HIS
1	C	208	GLN
1	C	235	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	A	301	-	50,52,52	2.57	22 (44%)	71,80,80	2.08	19 (26%)
2	NAP	C	301	-	50,52,52	2.12	18 (36%)	71,80,80	2.51	27 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAP	B	301	-	50,52,52	2.08	20 (40%)	71,80,80	2.36	26 (36%)
2	NAP	D	301	-	50,52,52	2.36	27 (54%)	71,80,80	2.05	20 (28%)

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	A	301	-	-	9/35/67/67	0/5/5/5
2	NAP	C	301	-	-	5/35/67/67	0/5/5/5
2	NAP	B	301	-	-	5/35/67/67	0/5/5/5
2	NAP	D	301	-	-	11/35/67/67	0/5/5/5

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	NAP	PN-O3	-7.37	1.51	1.59
2	A	301	NAP	PA-O3	-6.70	1.52	1.59
2	D	301	NAP	PA-O3	-5.11	1.54	1.59
2	D	301	NAP	PN-O3	-4.57	1.54	1.59
2	C	301	NAP	C8A-N9A	-4.28	1.30	1.37
2	A	301	NAP	C8A-N9A	-4.26	1.30	1.37
2	C	301	NAP	PN-O3	-4.15	1.55	1.59
2	C	301	NAP	C4A-N9A	-4.08	1.29	1.37
2	D	301	NAP	C4A-N9A	-4.04	1.29	1.37
2	A	301	NAP	O7N-C7N	-3.92	1.16	1.24
2	B	301	NAP	C5A-N7A	-3.90	1.32	1.39
2	B	301	NAP	O7N-C7N	-3.80	1.17	1.24
2	A	301	NAP	C4A-N9A	-3.77	1.29	1.37
2	A	301	NAP	C3N-C7N	-3.75	1.45	1.50
2	B	301	NAP	C8A-N9A	-3.68	1.31	1.37
2	D	301	NAP	O7N-C7N	-3.61	1.17	1.24
2	A	301	NAP	P2B-O2X	-3.54	1.41	1.54
2	B	301	NAP	C4A-N9A	-3.53	1.30	1.37
2	D	301	NAP	P2B-O2B	-3.48	1.53	1.59
2	D	301	NAP	C8A-N9A	-3.45	1.31	1.37
2	D	301	NAP	C5A-N7A	-3.45	1.32	1.39
2	C	301	NAP	O7N-C7N	-3.38	1.17	1.24
2	A	301	NAP	C5A-N7A	-3.37	1.32	1.39
2	D	301	NAP	O4B-C4B	-3.28	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	NAP	P2B-O2X	-3.26	1.42	1.54
2	A	301	NAP	O4D-C4D	-3.19	1.37	1.45
2	C	301	NAP	C5A-N7A	-3.17	1.33	1.39
2	B	301	NAP	C5A-C4A	3.13	1.44	1.39
2	C	301	NAP	O4B-C4B	-3.07	1.38	1.45
2	B	301	NAP	O4B-C4B	-3.07	1.38	1.45
2	B	301	NAP	PN-O3	-3.06	1.56	1.59
2	A	301	NAP	P2B-O3X	-3.03	1.43	1.54
2	B	301	NAP	P2B-O2X	-2.99	1.43	1.54
2	C	301	NAP	O4D-C4D	-2.97	1.38	1.45
2	A	301	NAP	PA-O2A	-2.97	1.41	1.55
2	B	301	NAP	P2B-O3X	-2.93	1.43	1.54
2	D	301	NAP	C2N-N1N	-2.88	1.31	1.35
2	D	301	NAP	P2B-O3X	-2.80	1.44	1.54
2	D	301	NAP	C3N-C7N	-2.79	1.46	1.50
2	A	301	NAP	P2B-O2B	-2.77	1.54	1.59
2	A	301	NAP	C3B-C4B	-2.76	1.46	1.53
2	A	301	NAP	C5A-C4A	2.75	1.44	1.39
2	C	301	NAP	C3B-C4B	-2.75	1.46	1.53
2	D	301	NAP	O4D-C4D	-2.73	1.38	1.45
2	B	301	NAP	PA-O1A	-2.72	1.41	1.50
2	B	301	NAP	C2N-N1N	-2.72	1.32	1.35
2	A	301	NAP	C2N-C3N	-2.70	1.34	1.39
2	C	301	NAP	PA-O2A	-2.69	1.42	1.55
2	B	301	NAP	PN-O2N	-2.67	1.43	1.55
2	A	301	NAP	C2N-N1N	-2.67	1.32	1.35
2	B	301	NAP	PA-O3	-2.64	1.56	1.59
2	A	301	NAP	O4B-C4B	-2.63	1.39	1.45
2	A	301	NAP	PN-O1N	-2.62	1.41	1.50
2	D	301	NAP	P2B-O1X	-2.60	1.42	1.50
2	C	301	NAP	P2B-O1X	-2.60	1.42	1.50
2	C	301	NAP	P2B-O3X	-2.59	1.45	1.54
2	D	301	NAP	C3B-C4B	-2.56	1.46	1.53
2	D	301	NAP	PN-O1N	-2.53	1.42	1.50
2	B	301	NAP	P2B-O1X	-2.53	1.42	1.50
2	D	301	NAP	C7N-N7N	-2.51	1.28	1.33
2	C	301	NAP	C3D-C4D	-2.50	1.46	1.53
2	C	301	NAP	P2B-O2B	-2.50	1.55	1.59
2	D	301	NAP	C5A-C4A	2.48	1.43	1.39
2	B	301	NAP	C2B-C1B	-2.44	1.47	1.53
2	C	301	NAP	C5A-C6A	2.43	1.47	1.41
2	D	301	NAP	P2B-O2X	-2.39	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	NAP	C5A-C6A	2.38	1.47	1.41
2	D	301	NAP	C2B-C1B	-2.38	1.47	1.53
2	D	301	NAP	C5A-C6A	2.30	1.47	1.41
2	D	301	NAP	PA-O2A	-2.29	1.44	1.55
2	D	301	NAP	O4D-C1D	-2.26	1.37	1.40
2	C	301	NAP	C2A-N1A	-2.26	1.29	1.33
2	D	301	NAP	C4N-C3N	-2.26	1.36	1.39
2	D	301	NAP	C3B-C2B	-2.24	1.48	1.53
2	B	301	NAP	C6N-N1N	-2.23	1.30	1.35
2	B	301	NAP	PA-O2A	-2.23	1.45	1.55
2	C	301	NAP	PN-O1N	-2.22	1.43	1.50
2	A	301	NAP	PA-O5B	-2.19	1.50	1.59
2	B	301	NAP	O4D-C4D	-2.17	1.40	1.45
2	D	301	NAP	C3D-C4D	-2.16	1.47	1.53
2	D	301	NAP	C6N-N1N	-2.13	1.30	1.35
2	D	301	NAP	PN-O5D	-2.13	1.51	1.59
2	C	301	NAP	PA-O1A	-2.12	1.43	1.50
2	A	301	NAP	C7N-N7N	-2.09	1.29	1.33
2	A	301	NAP	C2B-C1B	-2.09	1.48	1.53
2	B	301	NAP	C4N-C3N	-2.08	1.36	1.39
2	A	301	NAP	C3D-C4D	-2.07	1.47	1.53

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	NAP	C3N-C7N-N7N	6.29	125.49	117.74
2	A	301	NAP	O4B-C1B-C2B	-6.17	95.96	106.59
2	B	301	NAP	C5A-C4A-N3A	-6.10	118.31	126.72
2	B	301	NAP	C3N-C7N-N7N	6.09	125.24	117.74
2	C	301	NAP	C4D-O4D-C1D	5.90	115.33	109.92
2	C	301	NAP	C5A-C4A-N3A	-5.71	118.86	126.72
2	A	301	NAP	C5A-C4A-N3A	-5.60	119.01	126.72
2	C	301	NAP	O3D-C3D-C4D	-5.43	95.49	111.08
2	C	301	NAP	C4A-C5A-N7A	-5.37	104.44	110.58
2	C	301	NAP	O2B-P2B-O1X	-5.24	90.64	109.33
2	D	301	NAP	O3D-C3D-C4D	-5.05	96.56	111.08
2	B	301	NAP	O2B-P2B-O1X	-5.00	91.53	109.33
2	D	301	NAP	C5A-C4A-N3A	-4.97	119.88	126.72
2	A	301	NAP	C4A-C5A-N7A	-4.74	105.16	110.58
2	B	301	NAP	O4B-C1B-C2B	-4.68	98.54	106.59
2	C	301	NAP	O3B-C3B-C4B	-4.61	97.85	111.08
2	B	301	NAP	N3A-C4A-N9A	4.61	135.00	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	NAP	C4A-C5A-N7A	-4.36	105.60	110.58
2	C	301	NAP	C2A-N3A-C4A	4.31	122.35	111.83
2	B	301	NAP	C4D-O4D-C1D	4.22	113.79	109.92
2	A	301	NAP	N3A-C4A-N9A	4.21	134.33	127.17
2	B	301	NAP	O4B-C1B-N9A	4.16	116.07	108.09
2	D	301	NAP	O2B-P2B-O1X	-4.15	94.55	109.33
2	B	301	NAP	O3D-C3D-C4D	-4.11	99.29	111.08
2	D	301	NAP	O4B-C1B-N9A	4.05	115.86	108.09
2	A	301	NAP	O3B-C3B-C4B	-4.03	99.51	111.08
2	C	301	NAP	C6A-C5A-N7A	4.02	139.84	132.09
2	B	301	NAP	C2A-N3A-C4A	3.97	121.54	111.83
2	B	301	NAP	O7N-C7N-N7N	-3.97	116.88	122.62
2	D	301	NAP	C3N-C7N-N7N	3.96	122.62	117.74
2	B	301	NAP	C4A-C5A-N7A	-3.90	106.12	110.58
2	A	301	NAP	N3A-C2A-N1A	-3.83	122.78	128.58
2	C	301	NAP	O7N-C7N-C3N	-3.75	115.01	119.60
2	A	301	NAP	C2B-C1B-N9A	-3.72	107.62	113.75
2	D	301	NAP	C2A-N3A-C4A	3.66	120.76	111.83
2	D	301	NAP	O4B-C1B-C2B	-3.65	100.30	106.59
2	C	301	NAP	N3A-C2A-N1A	-3.64	123.07	128.58
2	D	301	NAP	N3A-C2A-N1A	-3.57	123.17	128.58
2	A	301	NAP	C2A-N3A-C4A	3.53	120.44	111.83
2	C	301	NAP	N3A-C4A-N9A	3.47	133.07	127.17
2	A	301	NAP	O2A-PA-O3	-3.47	97.90	107.27
2	A	301	NAP	C4A-N9A-C8A	3.43	109.34	105.74
2	B	301	NAP	C2B-C1B-N9A	-3.43	108.11	113.75
2	C	301	NAP	C4A-N9A-C8A	3.35	109.26	105.74
2	D	301	NAP	N3A-C4A-N9A	3.34	132.84	127.17
2	B	301	NAP	N3A-C2A-N1A	-3.30	123.59	128.58
2	C	301	NAP	C5A-N7A-C8A	3.23	108.52	103.45
2	D	301	NAP	C6A-C5A-N7A	3.16	138.18	132.09
2	A	301	NAP	C2A-N1A-C6A	3.16	123.92	118.73
2	A	301	NAP	O2N-PN-O1N	3.10	126.85	112.44
2	C	301	NAP	C6N-N1N-C2N	-3.06	119.28	121.88
2	D	301	NAP	C6N-N1N-C1D	-3.06	113.73	119.73
2	A	301	NAP	C5A-N7A-C8A	2.99	108.14	103.45
2	C	301	NAP	N9A-C8A-N7A	-2.99	109.70	113.94
2	D	301	NAP	O3B-C3B-C4B	-2.96	102.58	111.08
2	C	301	NAP	O3-PN-O1N	-2.96	101.80	110.70
2	A	301	NAP	C6A-C5A-N7A	2.95	137.78	132.09
2	B	301	NAP	O2X-P2B-O2B	2.86	116.99	105.85
2	B	301	NAP	O3X-P2B-O1X	2.79	121.70	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	NAP	O3-PN-O1N	-2.75	102.44	110.70
2	B	301	NAP	O3-PN-O1N	2.71	118.87	110.70
2	D	301	NAP	C2A-N1A-C6A	2.66	123.10	118.73
2	A	301	NAP	O3D-C3D-C4D	-2.64	103.50	111.08
2	D	301	NAP	C5A-N7A-C8A	2.63	107.58	103.45
2	B	301	NAP	O4B-C4B-C5B	-2.62	100.94	109.33
2	A	301	NAP	O3-PA-O1A	2.58	118.45	110.70
2	B	301	NAP	O3B-C3B-C2B	-2.57	103.99	111.19
2	D	301	NAP	C4A-N9A-C8A	2.56	108.43	105.74
2	C	301	NAP	O3X-P2B-O1X	2.56	120.80	110.83
2	C	301	NAP	O2A-PA-O3	2.52	114.09	107.27
2	C	301	NAP	O4B-C1B-C2B	-2.52	102.25	106.59
2	B	301	NAP	C6A-C5A-N7A	2.51	136.93	132.09
2	D	301	NAP	C2N-N1N-C1D	2.51	124.67	119.13
2	C	301	NAP	O2N-PN-O3	2.50	114.03	107.27
2	B	301	NAP	O3B-C3B-C4B	-2.50	103.91	111.08
2	C	301	NAP	O2N-PN-O1N	2.43	123.74	112.44
2	C	301	NAP	O7N-C7N-N7N	-2.43	119.11	122.62
2	B	301	NAP	C5A-N7A-C8A	2.37	107.18	103.45
2	B	301	NAP	O3-PA-O1A	2.30	117.62	110.70
2	B	301	NAP	C2A-N1A-C6A	2.29	122.49	118.73
2	A	301	NAP	N9A-C8A-N7A	-2.29	110.69	113.94
2	A	301	NAP	P2B-O2B-C2B	-2.24	117.46	123.43
2	D	301	NAP	O2N-PN-O1N	2.21	122.74	112.44
2	B	301	NAP	C2D-C3D-C4D	2.21	106.88	102.61
2	D	301	NAP	O7N-C7N-N7N	-2.21	119.42	122.62
2	C	301	NAP	C5B-C4B-C3B	-2.14	107.51	115.21
2	B	301	NAP	C4A-N9A-C8A	2.13	107.98	105.74
2	C	301	NAP	O5D-C5D-C4D	2.11	116.19	108.99
2	B	301	NAP	O2N-PN-O5D	-2.09	98.11	107.57
2	C	301	NAP	C5A-C4A-N9A	2.07	108.07	105.81
2	D	301	NAP	P2B-O2B-C2B	-2.06	117.94	123.43
2	C	301	NAP	C5D-C4D-C3D	-2.01	107.97	115.21

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	301	NAP	C5B-O5B-PA-O1A
2	D	301	NAP	C5B-O5B-PA-O2A
2	D	301	NAP	C5B-O5B-PA-O3
2	D	301	NAP	C5D-O5D-PN-O1N

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Mol	Chain	Res	Type	Atoms
2	A	301	NAP	C5B-O5B-PA-O3
2	A	301	NAP	PN-O3-PA-O5B
2	A	301	NAP	C5D-O5D-PN-O3
2	A	301	NAP	C5D-O5D-PN-O1N
2	B	301	NAP	O4D-C4D-C5D-O5D
2	C	301	NAP	O4D-C4D-C5D-O5D
2	D	301	NAP	O4D-C4D-C5D-O5D
2	A	301	NAP	C3B-C4B-C5B-O5B
2	B	301	NAP	C3D-C4D-C5D-O5D
2	C	301	NAP	C3D-C4D-C5D-O5D
2	A	301	NAP	O4B-C4B-C5B-O5B
2	D	301	NAP	O4B-C4B-C5B-O5B
2	D	301	NAP	C3B-C4B-C5B-O5B
2	D	301	NAP	C3D-C4D-C5D-O5D
2	D	301	NAP	PN-O3-PA-O5B
2	B	301	NAP	PN-O3-PA-O1A
2	B	301	NAP	C2B-O2B-P2B-O1X
2	D	301	NAP	C5D-O5D-PN-O3
2	D	301	NAP	C5D-O5D-PN-O2N
2	A	301	NAP	C5B-O5B-PA-O1A
2	A	301	NAP	C5D-O5D-PN-O2N
2	C	301	NAP	PN-O3-PA-O1A
2	C	301	NAP	PN-O3-PA-O2A
2	A	301	NAP	O4D-C4D-C5D-O5D
2	C	301	NAP	C2B-O2B-P2B-O1X
2	B	301	NAP	PN-O3-PA-O2A

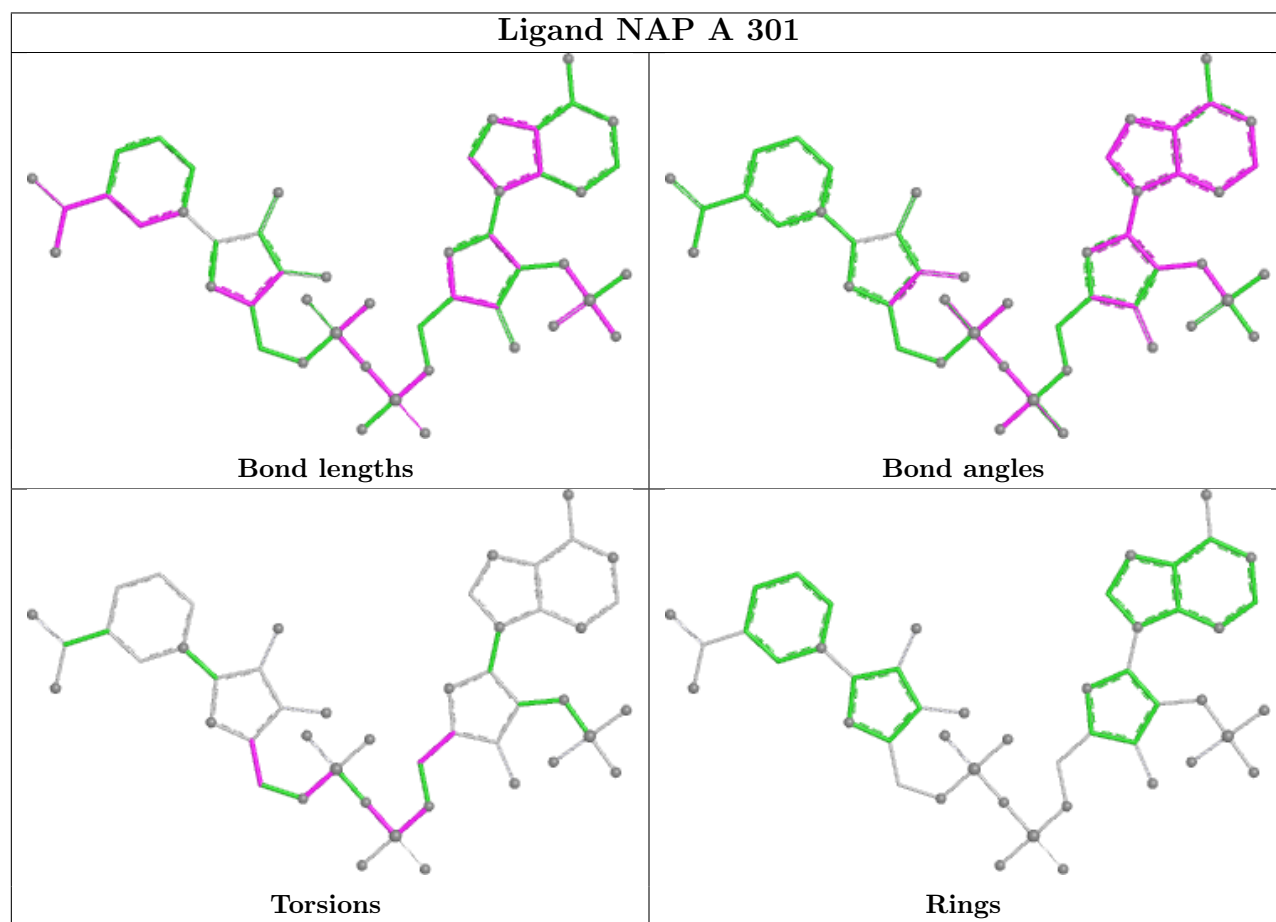
There are no ring outliers.

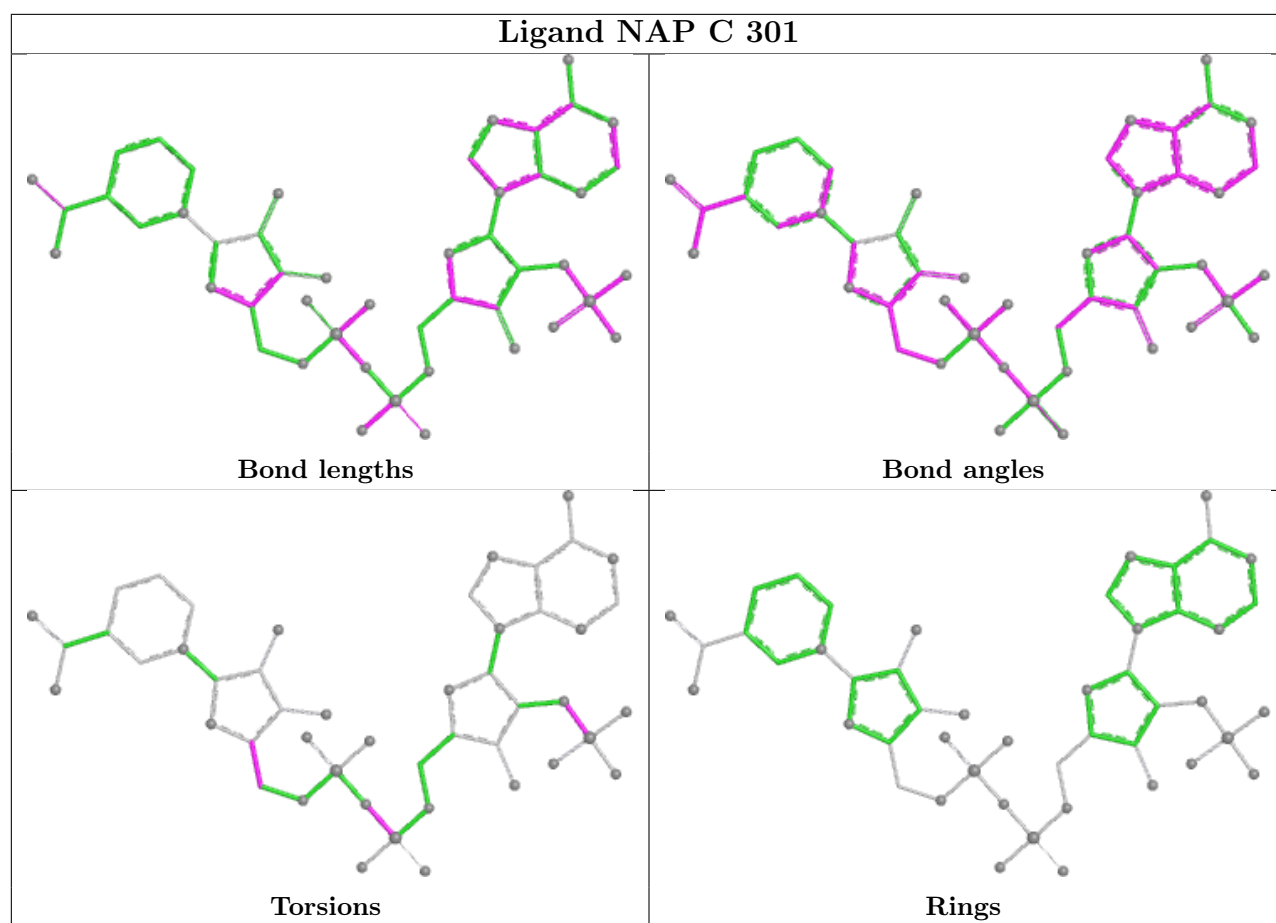
4 monomers are involved in 14 short contacts:

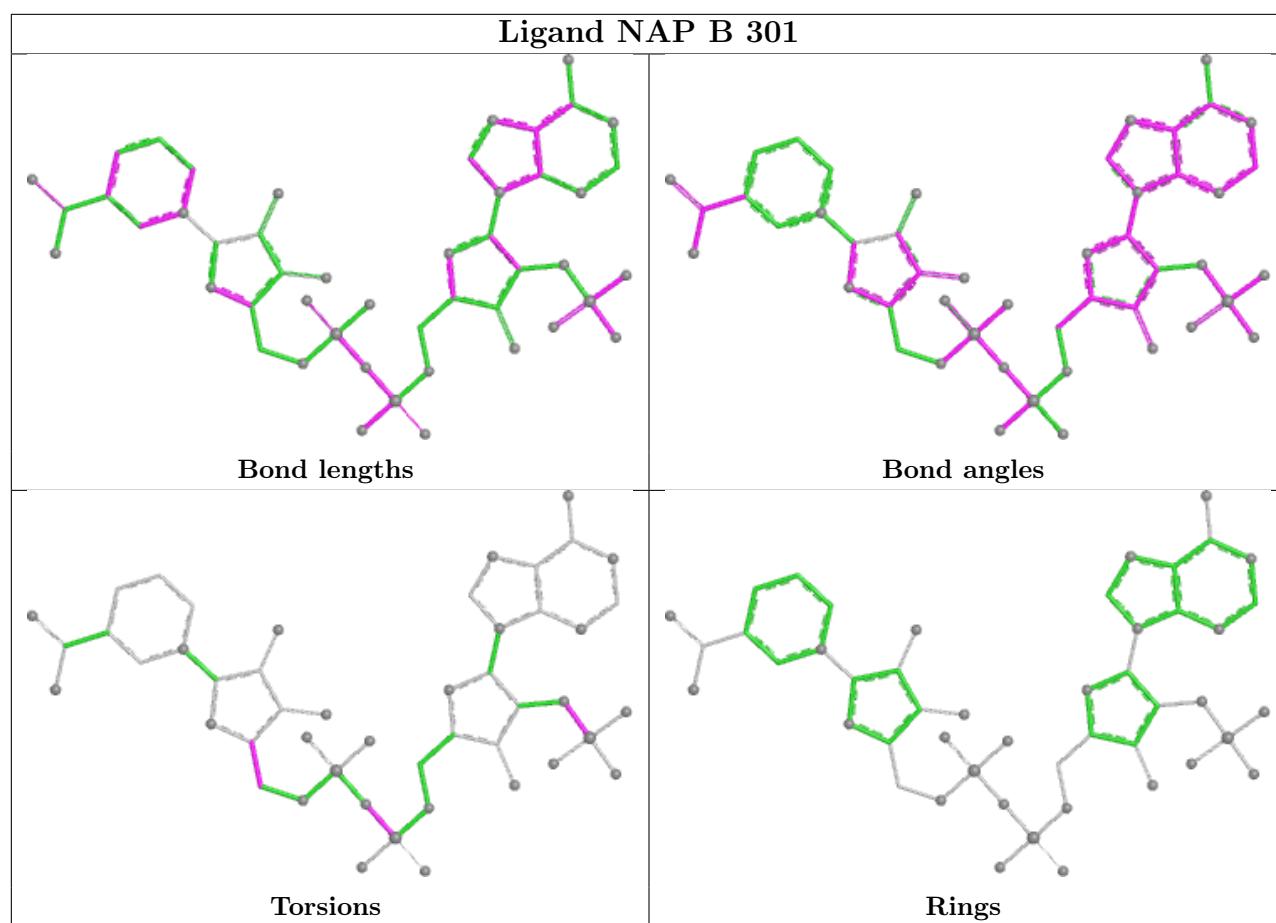
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	NAP	4	0
2	C	301	NAP	3	0
2	B	301	NAP	5	0
2	D	301	NAP	2	0

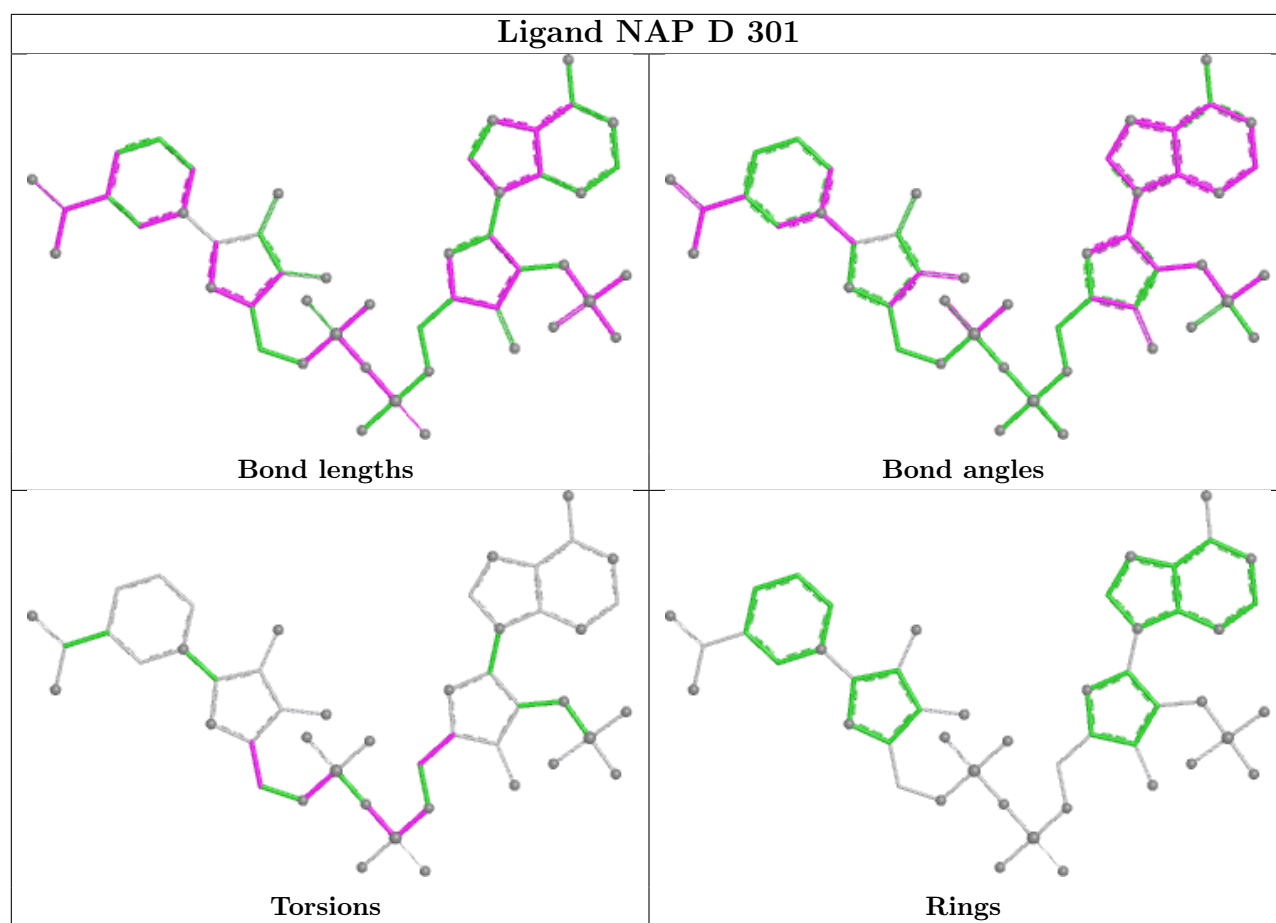
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	255/279 (91%)	0.23	7 (2%) 56 37	9, 13, 28, 37	0
1	B	248/279 (88%)	0.29	9 (3%) 46 31	7, 15, 39, 56	0
1	C	248/279 (88%)	0.40	10 (4%) 42 28	8, 16, 37, 65	0
1	D	251/279 (89%)	0.14	3 (1%) 76 58	9, 14, 37, 51	0
All	All	1002/1116 (89%)	0.26	29 (2%) 53 35	7, 15, 34, 65	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	102	SER	5.9
1	C	225	MET	3.5
1	C	157	PHE	3.3
1	C	219	PRO	3.1
1	A	220	GLU	3.0
1	C	49	ASN	2.9
1	B	219	PRO	2.9
1	C	29	GLY	2.7
1	C	198	THR	2.7
1	B	154	SER	2.6
1	A	197	GLY	2.6
1	B	103	GLY	2.5
1	C	24	SER	2.5
1	B	228	HIS	2.5
1	C	183	CYS	2.4
1	A	219	PRO	2.4
1	A	165	TYR	2.4
1	A	166	SER	2.2
1	C	220	GLU	2.2
1	A	51	PRO	2.2
1	D	155	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	174	SER	2.2
1	C	182	ASP	2.1
1	A	218	THR	2.1
1	B	166	SER	2.1
1	D	196	GLY	2.1
1	D	11	PRO	2.1
1	B	168	SER	2.0
1	B	225	MET	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](#)

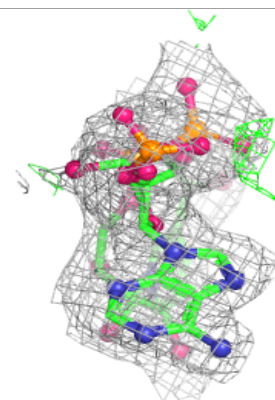
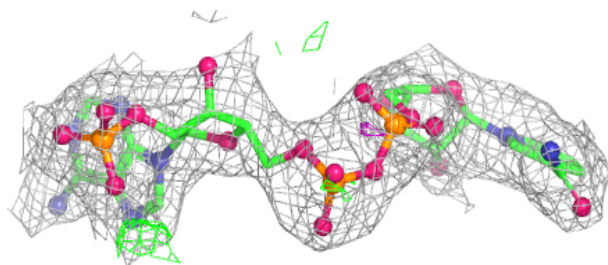
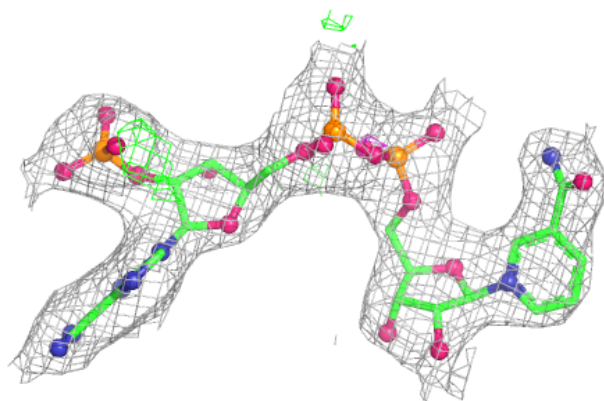
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAP	D	301	48/48	0.95	0.09	12,13,15,16	0
2	NAP	A	301	48/48	0.95	0.09	10,11,13,14	0
2	NAP	C	301	48/48	0.95	0.09	12,15,17,17	0
2	NAP	B	301	48/48	0.96	0.09	10,12,14,15	0

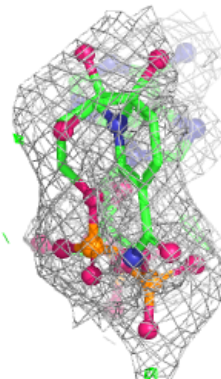
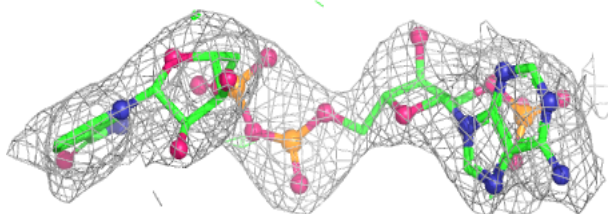
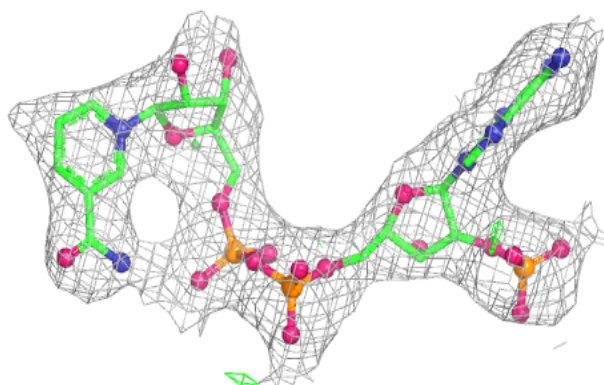
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP D 301:

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

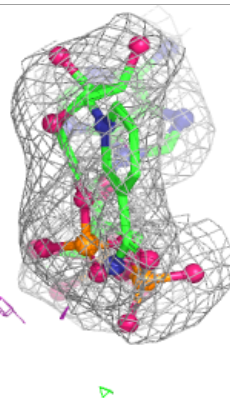
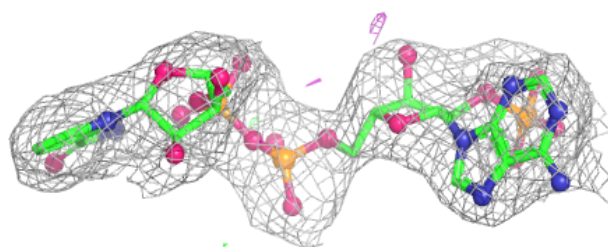
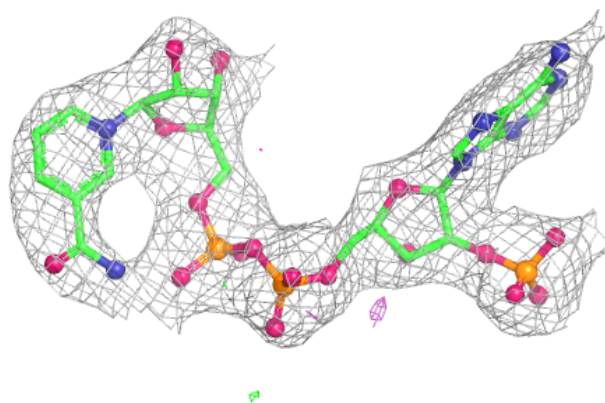
**Electron density around NAP A 301:**

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

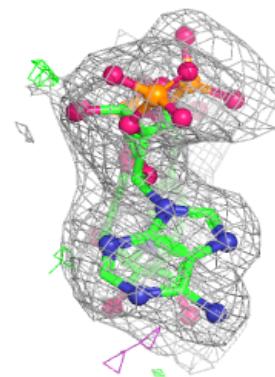
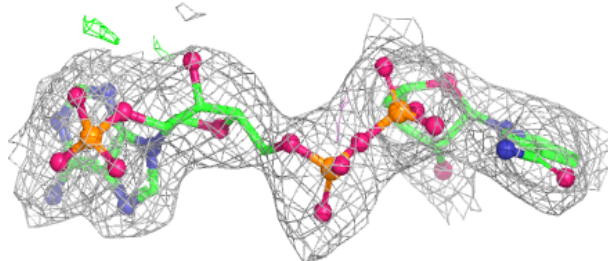
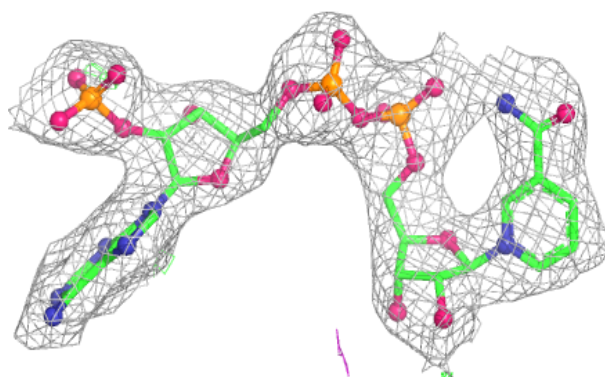


Electron density around NAP C 301:

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

**Electron density around NAP B 301:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.