



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:11 PM UTC

PDB ID : 3UXV / pdb_00003uxv
Title : Crystal Structure of 7-cyano-7-deazaguanine reductase, QueF from *Vibrio cholerae* complexed with NADP and PreQ
Authors : Kim, Y.; Zhou, M.; Gu, M.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2011-12-05
Resolution : 1.56 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

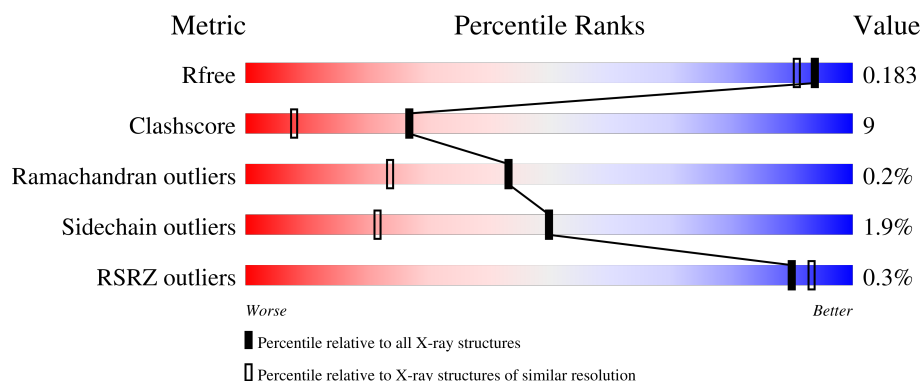
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.56 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	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	290	73% 13% • 12%
1	B	290	79% 10% • 11%
1	C	290	% 80% 9% 11%
1	D	290	74% 12% • 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	302	-	-	X	-
2	EDO	D	302	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10034 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 NADPH-dependent 7-cyano-7-deazaguanine reductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	Se	0	24	0
			2254	1396	403	443	6	6			
1	B	259	Total	C	N	O	S	Se	0	17	0
			2224	1380	394	437	6	7			
1	C	259	Total	C	N	O	S	Se	0	19	0
			2247	1395	400	439	6	7			
1	D	254	Total	C	N	O	S	Se	0	25	0
			2259	1403	400	444	6	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP C3LTF1
A	-1	ASN	-	expression tag	UNP C3LTF1
A	0	ALA	-	expression tag	UNP C3LTF1
A	194	ALA	CYS	engineered mutation	UNP C3LTF1
B	-2	SER	-	expression tag	UNP C3LTF1
B	-1	ASN	-	expression tag	UNP C3LTF1
B	0	ALA	-	expression tag	UNP C3LTF1
B	194	ALA	CYS	engineered mutation	UNP C3LTF1
C	-2	SER	-	expression tag	UNP C3LTF1
C	-1	ASN	-	expression tag	UNP C3LTF1
C	0	ALA	-	expression tag	UNP C3LTF1
C	194	ALA	CYS	engineered mutation	UNP C3LTF1
D	-2	SER	-	expression tag	UNP C3LTF1
D	-1	ASN	-	expression tag	UNP C3LTF1
D	0	ALA	-	expression tag	UNP C3LTF1
D	194	ALA	CYS	engineered mutation	UNP C3LTF1

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



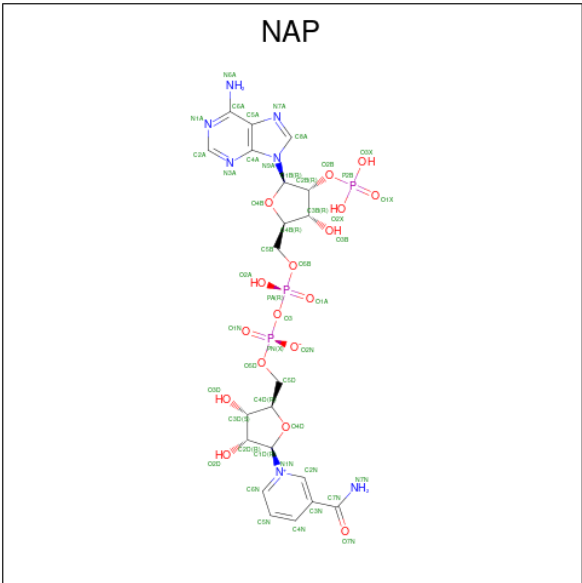
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

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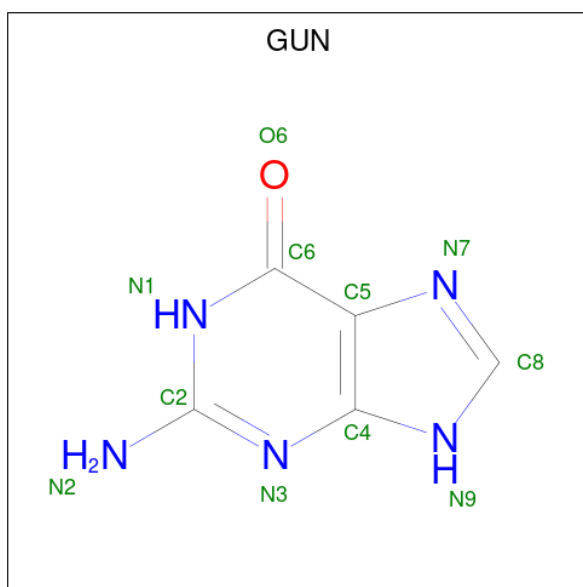
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	1
			78	30	10	32	6		
4	D	1	Total	C	N	O	P	0	1
			80	30	12	32	6		

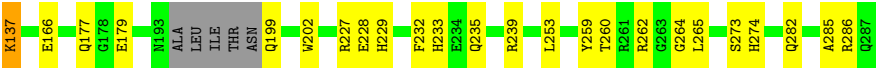
- Molecule 5 is GUANINE (CCD ID: GUN) (formula: C₅H₅N₅O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			11	5	5	1		
5	C	1	Total	C	N	O	0	0
			11	5	5	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	210	Total	O	0	0
			210	210		
6	B	194	Total	O	0	0
			194	194		
6	C	204	Total	O	0	0
			204	204		
6	D	224	Total	O	0	0
			224	224		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.37Å 71.39Å 71.36Å 109.89° 119.61° 99.46°	Depositor
Resolution (Å)	30.96 – 1.56 30.96 – 1.56	Depositor EDS
% Data completeness (in resolution range)	94.7 (30.96-1.56) 94.4 (30.96-1.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 1.56Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_920)	Depositor
R, R_{free}	0.161 , 0.189 0.156 , 0.183	Depositor DCC
R_{free} test set	7151 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.478 for l,-h-k-l,h 0.015 for -h-k-l,l,k 0.016 for k,h,-h-k-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	10034	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.32% 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: EDO, GUN, GOL, 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	0.89	2/2296 (0.1%)	0.95	0/3107
1	B	0.92	1/2266 (0.0%)	0.99	2/3070 (0.1%)
1	C	0.88	0/2289	0.96	0/3101
1	D	0.90	0/2300	0.95	3/3114 (0.1%)
All	All	0.90	3/9151 (0.0%)	0.96	5/12392 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	249	GLN	CA-C	6.24	1.57	1.53
1	A	99	LYS	C-O	-5.34	1.18	1.24
1	A	249	GLN	C-O	-5.03	1.21	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111	ALA	N-CA-C	6.07	117.90	111.28
1	D	95	SER	N-CA-C	5.61	117.48	111.36
1	D	199	GLN	CA-C-N	-5.36	114.46	120.14
1	D	199	GLN	C-N-CA	-5.36	114.46	120.14
1	B	196	ILE	N-CA-C	5.05	116.23	111.48

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	2254	0	2127	54	0
1	B	2224	0	2109	37	0
1	C	2247	0	2139	24	0
1	D	2259	0	2140	57	0
2	A	4	0	6	11	0
2	D	4	0	6	11	0
3	A	6	0	8	1	0
3	B	6	0	8	1	0
3	D	18	0	24	6	0
4	B	78	0	36	6	0
4	D	80	0	38	7	0
5	B	11	0	5	0	0
5	C	11	0	5	0	0
6	A	210	0	0	12	0
6	B	194	0	0	3	0
6	C	204	0	0	4	0
6	D	224	0	0	5	0
All	All	10034	0	8651	165	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 9.

All (165) 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:64:LEU:HD22	1:B:265:LEU:HD23	1.35	1.07
6:A:727:HOH:O	1:B:66[B]:GLU:HG2	1.73	0.86
1:B:64:LEU:HD22	1:B:265:LEU:CD2	2.05	0.85
1:D:91:ASN:HD21	3:D:304:GOL:H12	1.42	0.85
1:D:232:PHE:HD2	1:D:235[A]:GLN:NE2	1.77	0.83
1:C:66[B]:GLU:HG2	6:C:689:HOH:O	1.80	0.81
1:D:66[B]:GLU:HG3	6:D:289:HOH:O	1.83	0.79
1:B:268:ASN:HD21	1:B:287:GLN:HE22	1.30	0.75
1:D:232:PHE:HD2	1:D:235[A]:GLN:HE22	1.32	0.74
1:D:232:PHE:CD2	1:D:235[A]:GLN:NE2	2.55	0.74
1:B:191:LYS:HE2	1:B:200:PRO:HB3	1.71	0.72
1:A:286:ARG:HB2	2:A:302:EDO:H21	1.70	0.72
1:C:191:LYS:HE2	1:C:200:PRO:HB3	1.72	0.71
6:C:689:HOH:O	1:D:260[A]:THR:HG21	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:ARG:HB2	2:D:302:EDO:H12	1.73	0.70
1:B:133[B]:THR:HG22	6:B:379:HOH:O	1.91	0.70
1:A:107:GLN:NE2	6:A:728:HOH:O	2.23	0.69
1:D:262:ARG:HG3	4:D:301[B]:NAP:H1D	1.74	0.69
1:A:260[A]:THR:HG21	6:A:727:HOH:O	1.93	0.68
1:C:227[B]:ARG:HG3	6:C:354:HOH:O	1.93	0.68
4:B:301[B]:NAP:O3X	4:B:301[B]:NAP:H52N	1.93	0.67
1:D:285:ALA:N	2:D:302:EDO:H21	2.09	0.67
1:A:285:ALA:N	2:A:302:EDO:H12	2.10	0.66
1:A:232:PHE:HB2	1:A:235:GLN:CD	2.21	0.66
1:A:228[B]:GLU:O	1:A:229[B]:HIS:HB2	1.96	0.66
1:C:227[B]:ARG:NH1	1:D:107:GLN:OE1	2.30	0.65
1:D:91:ASN:HD21	3:D:304:GOL:C1	2.07	0.65
1:A:274:HIS:HB3	3:A:303:GOL:O2	1.98	0.63
1:D:202:TRP:HB2	1:D:260[B]:THR:CG2	2.28	0.63
1:D:82[B]:GLU:HG3	1:D:137:LYS:HZ1	1.64	0.62
1:B:191:LYS:HD3	1:B:227[B]:ARG:CG	2.30	0.62
1:B:258:ARG:HA	1:B:268:ASN:HD22	1.63	0.61
1:C:233:HIS:HD2	1:C:267[B]:ILE:HG22	1.63	0.61
1:C:96:LYS:HB2	4:D:301[A]:NAP:H2D	1.81	0.61
1:D:48:LEU:HD11	1:D:235[B]:GLN:HE22	1.65	0.61
1:D:66[B]:GLU:HG2	1:D:264:GLY:HA3	1.83	0.61
1:B:99:LYS:HZ3	4:B:301[A]:NAP:H51N	1.66	0.61
1:D:232:PHE:HB2	1:D:235[A]:GLN:CD	2.26	0.61
1:A:286:ARG:CB	2:A:302:EDO:H21	2.30	0.60
1:A:201:ASP:OD2	1:A:262[A]:ARG:HD2	2.02	0.60
1:B:96:LYS:HB2	4:B:301[A]:NAP:H2D	1.83	0.60
1:C:191:LYS:HD3	1:C:227[A]:ARG:HG2	1.84	0.59
1:D:285:ALA:H	2:D:302:EDO:H21	1.67	0.59
1:A:107:GLN:OE1	1:B:227[B]:ARG:NH1	2.36	0.58
1:D:286:ARG:CB	2:D:302:EDO:H12	2.32	0.58
1:A:182:SER:OG	1:A:210:HIS:HD2	1.86	0.58
1:D:91:ASN:ND2	3:D:304:GOL:H12	2.17	0.58
1:A:227[B]:ARG:NH2	1:B:107:GLN:OE1	2.37	0.58
1:D:44:ASN:CB	1:D:235[B]:GLN:HG3	2.34	0.58
1:D:202:TRP:HB2	1:D:260[B]:THR:HG21	1.85	0.58
1:C:139:LEU:HD13	2:D:302:EDO:H22	1.86	0.57
1:D:227:ARG:NH2	6:D:817:HOH:O	2.10	0.57
1:A:232:PHE:HB2	1:A:235:GLN:OE1	2.04	0.57
1:B:191:LYS:HD3	1:B:227[A]:ARG:CG	2.35	0.57
1:D:260[B]:THR:HG23	6:D:339:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229[A]:HIS:HB3	6:A:827:HOH:O	2.06	0.56
1:A:285:ALA:H	2:A:302:EDO:H12	1.70	0.56
1:D:274:HIS:HB3	3:D:303:GOL:H11	1.87	0.56
2:A:302:EDO:H11	1:B:139:LEU:HD13	1.87	0.55
1:B:64:LEU:CD2	1:B:265:LEU:HD23	2.22	0.55
1:A:229[A]:HIS:ND1	1:A:231[A]:GLU:OE2	2.39	0.54
1:A:228[B]:GLU:O	1:A:229[B]:HIS:CB	2.55	0.54
1:C:99:LYS:HZ3	4:D:301[A]:NAP:H51N	1.73	0.54
1:D:274:HIS:HB3	3:D:303:GOL:C1	2.37	0.54
1:B:191:LYS:HD3	1:B:227[B]:ARG:HG2	1.89	0.54
1:B:191:LYS:HD3	1:B:227[B]:ARG:HG3	1.89	0.54
1:A:180[A]:GLU:OE1	1:A:210:HIS:HE1	1.90	0.54
1:C:263:GLY:HA3	4:D:301[B]:NAP:N3A	2.23	0.54
1:D:51:SER:OG	1:D:53:THR:HG23	2.08	0.54
1:D:286:ARG:HE	2:D:302:EDO:H12	1.73	0.54
1:C:193:ASN:HB3	1:C:198:ASN:HA	1.89	0.53
1:A:106:ASN:O	1:B:227[B]:ARG:NH1	2.38	0.53
1:C:233:HIS:HD2	1:C:267[B]:ILE:CG2	2.19	0.53
1:D:262:ARG:CG	4:D:301[B]:NAP:H1D	2.39	0.53
1:A:99:LYS:NZ	1:A:103:ASN:HD21	2.07	0.52
1:B:263:GLY:HA3	4:B:301[B]:NAP:N3A	2.25	0.52
1:A:178:GLY:HA3	1:A:213:LYS:HB3	1.92	0.52
1:D:51:SER:HG	1:D:53:THR:HG23	1.75	0.52
1:D:286:ARG:HE	2:D:302:EDO:C1	2.23	0.52
6:A:455:HOH:O	1:B:73:LYS:HE3	2.10	0.51
1:D:82[A]:GLU:HG2	6:D:476:HOH:O	2.10	0.51
1:D:96:LYS:HB2	4:D:301[B]:NAP:H2D	1.93	0.51
1:A:286:ARG:H	2:A:302:EDO:C2	2.24	0.51
1:D:286:ARG:H	2:D:302:EDO:C1	2.24	0.51
1:C:228:GLU:HG3	6:C:787:HOH:O	2.10	0.51
1:D:99[B]:LYS:NZ	1:D:103:ASN:HD21	2.09	0.51
1:D:66[B]:GLU:CG	1:D:264:GLY:HA3	2.41	0.50
1:A:233:HIS:HB3	1:A:259:TYR:CE2	2.46	0.50
1:A:166[A]:GLU:O	1:A:225:SER:HB2	2.12	0.50
1:B:268:ASN:ND2	1:B:287:GLN:HE22	2.06	0.49
1:B:191:LYS:HD3	1:B:227[A]:ARG:HG2	1.94	0.49
1:D:44:ASN:OD1	1:D:235[A]:GLN:NE2	2.45	0.49
1:C:62:TRP:CE2	1:C:267[B]:ILE:HG13	2.48	0.49
1:B:201[B]:ASP:CG	1:B:233:HIS:HE2	2.20	0.48
1:D:44:ASN:HB3	1:D:235[B]:GLN:HG3	1.95	0.48
1:D:51:SER:OG	1:D:53:THR:CG2	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:ASP:CG	1:C:233:HIS:HE1	2.21	0.48
1:A:286:ARG:HE	2:A:302:EDO:C2	2.26	0.48
1:D:233:HIS:HB3	1:D:259:TYR:CE2	2.48	0.48
1:D:202:TRP:HB2	1:D:260[B]:THR:HG22	1.95	0.48
1:B:279:ASN:HD21	1:C:145[B]:GLU:CD	2.22	0.47
1:D:262:ARG:HD3	4:D:301[B]:NAP:O1X	2.14	0.47
1:D:232:PHE:HD2	1:D:235[A]:GLN:CD	2.21	0.47
1:A:44[A]:ASN:CG	1:A:235:GLN:HE21	2.22	0.47
1:A:44[B]:ASN:CG	1:A:235:GLN:HG2	2.40	0.47
1:A:99:LYS:HZ3	1:A:103:ASN:HD21	1.62	0.47
1:D:179[B]:GLU:H	1:D:179[B]:GLU:CD	2.22	0.47
1:A:224:VAL:O	1:A:227[B]:ARG:HB2	2.15	0.47
1:C:48:LEU:HD21	1:C:239[B]:ARG:HD2	1.97	0.47
1:D:229:HIS:NE2	1:D:239[B]:ARG:NE	2.63	0.46
1:C:195:LEU:HD12	1:C:232:PHE:CE1	2.50	0.46
1:A:31:TYR:CZ	1:A:33:PRO:HG3	2.50	0.46
1:A:180[A]:GLU:OE1	1:A:210:HIS:CE1	2.68	0.46
1:C:191:LYS:HD3	1:C:227[A]:ARG:CG	2.44	0.46
1:B:191:LYS:HD3	1:B:227[A]:ARG:HG3	1.93	0.45
1:D:166:GLU:HA	1:D:228:GLU:HB2	1.98	0.45
1:A:262[A]:ARG:HG3	6:A:741:HOH:O	2.16	0.45
1:B:280:HIS:CE1	6:B:465:HOH:O	2.69	0.45
1:B:267[A]:ILE:HG13	1:B:268:ASN:N	2.28	0.45
1:A:286:ARG:H	2:A:302:EDO:C1	2.30	0.45
6:A:690:HOH:O	1:B:99:LYS:HD2	2.15	0.45
2:A:302:EDO:C1	1:B:139:LEU:HD13	2.46	0.44
1:C:57:GLN:HG3	1:C:275:GLN:O	2.18	0.44
1:B:133[B]:THR:HG23	6:B:384:HOH:O	2.17	0.44
1:A:44[A]:ASN:CB	1:A:235:GLN:HG2	2.47	0.44
1:A:44[A]:ASN:ND2	1:A:235:GLN:HE21	2.16	0.44
1:A:282:GLN:HG2	6:A:644:HOH:O	2.17	0.44
1:C:233:HIS:CD2	1:C:267[B]:ILE:CG2	3.01	0.44
1:D:137:LYS:HZ3	1:D:137:LYS:HB2	1.83	0.44
1:A:192:SER:HB3	6:A:827:HOH:O	2.18	0.44
1:A:233:HIS:HD2	1:A:267[B]:ILE:HD12	1.83	0.44
1:D:35:LEU:O	1:D:97:SER:HB2	2.18	0.43
1:A:44[B]:ASN:CB	1:A:235:GLN:HG2	2.49	0.43
1:A:138:SER:OG	1:A:140[B]:ASN:ND2	2.51	0.43
1:D:107:GLN:NE2	6:D:789:HOH:O	2.51	0.43
1:B:69:TRP:CE2	1:B:116:VAL:HG21	2.54	0.43
1:D:202:TRP:O	1:D:260[B]:THR:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:LYS:HE2	1:A:142:TYR:OH	2.18	0.43
1:A:232:PHE:HD2	1:A:235:GLN:HE22	1.66	0.43
1:A:286:ARG:HE	2:A:302:EDO:H21	1.84	0.43
1:B:151:GLN:HE22	1:C:282[A]:GLN:NE2	2.17	0.42
1:D:253:LEU:H	1:D:273:SER:HG	1.66	0.42
1:D:50:LEU:HD23	1:D:50:LEU:HA	1.72	0.42
1:A:262[B]:ARG:HD3	4:B:301[B]:NAP:O1X	2.19	0.42
1:A:140[B]:ASN:N	1:A:140[B]:ASN:HD22	2.18	0.42
1:D:44:ASN:HB2	1:D:235[B]:GLN:HG3	2.01	0.42
1:D:82[B]:GLU:HG3	1:D:137:LYS:NZ	2.34	0.42
1:D:286:ARG:CG	2:D:302:EDO:H12	2.50	0.42
1:B:164:ASN:OD1	1:B:164:ASN:C	2.63	0.41
1:A:286:ARG:HG3	2:A:302:EDO:H11	2.03	0.41
1:B:151:GLN:HE21	1:C:148:VAL:HG12	1.85	0.41
1:D:282:GLN:HG2	3:D:305:GOL:O3	2.20	0.41
1:B:268:ASN:HD21	1:B:287:GLN:NE2	2.05	0.41
1:A:191:LYS:O	1:A:227[B]:ARG:HA	2.21	0.41
1:A:239[B]:ARG:HE	1:A:243:ASP:CG	2.28	0.41
1:B:127:CYS:HA	3:B:302:GOL:H2	2.03	0.41
1:A:265:LEU:HD23	1:A:265:LEU:N	2.35	0.41
1:D:99[B]:LYS:HZ3	1:D:103:ASN:HD21	1.68	0.41
1:A:274:HIS:CE1	6:A:351:HOH:O	2.74	0.41
1:D:286:ARG:H	2:D:302:EDO:C2	2.33	0.41
1:A:249:GLN:HG2	6:A:708:HOH:O	2.21	0.41
1:C:139:LEU:HD13	2:D:302:EDO:C2	2.50	0.41
1:A:274:HIS:HE1	6:A:351:HOH:O	2.04	0.40
1:A:262[A]:ARG:NH1	1:B:66[A]:GLU:OE2	2.48	0.40
1:A:96:LYS:HB2	4:B:301[B]:NAP:H2D	2.03	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	275/290 (95%)	263 (96%)	8 (3%)	4 (2%)	8	1
1	B	274/290 (94%)	272 (99%)	2 (1%)	0	100	100
1	C	277/290 (96%)	271 (98%)	6 (2%)	0	100	100
1	D	275/290 (95%)	269 (98%)	6 (2%)	0	100	100
All	All	1101/1160 (95%)	1075 (98%)	22 (2%)	4 (0%)	43	13

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	229[A]	HIS
1	A	229[B]	HIS
1	A	227[A]	ARG
1	A	227[B]	ARG

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	250/249 (100%)	246 (98%)	4 (2%)	55	28
1	B	247/249 (99%)	241 (98%)	6 (2%)	43	15
1	C	249/249 (100%)	244 (98%)	5 (2%)	48	20
1	D	251/249 (101%)	245 (98%)	6 (2%)	43	15
All	All	997/996 (100%)	976 (98%)	21 (2%)	50	19

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

Mol	Chain	Res	Type
1	A	137	LYS
1	A	193	ASN
1	A	227[A]	ARG
1	A	227[B]	ARG
1	B	53	THR
1	B	201[A]	ASP
1	B	201[B]	ASP

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Mol	Chain	Res	Type
1	B	231	GLU
1	B	267[A]	ILE
1	B	267[B]	ILE
1	C	44	ASN
1	C	228	GLU
1	C	231	GLU
1	C	262	ARG
1	C	265	LEU
1	D	51	SER
1	D	107	GLN
1	D	137	LYS
1	D	177	GLN
1	D	265[A]	LEU
1	D	265[B]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	72	GLN
1	A	103	ASN
1	A	106	ASN
1	A	210	HIS
1	A	235	GLN
1	B	151	GLN
1	B	230	ASN
1	B	268	ASN
1	B	274	HIS
1	B	280	HIS
1	C	44	ASN
1	C	103	ASN
1	C	177	GLN
1	C	198	ASN
1	C	230	ASN
1	C	233	HIS
1	C	274	HIS
1	C	275	GLN
1	D	37	GLN
1	D	57	GLN
1	D	91	ASN
1	D	103	ASN
1	D	106	ASN

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Mol	Chain	Res	Type
1	D	251	GLN
1	D	274	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 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	$\# Z > 2$
4	NAP	B	301[A]	-	42,42,52	1.05	2 (4%)	60,65,80	1.89	14 (23%)
3	GOL	D	304	-	5,5,5	0.70	0	5,5,5	1.53	1 (20%)
2	EDO	A	302	-	3,3,3	0.90	0	2,2,2	1.22	0
3	GOL	A	303	-	5,5,5	0.63	0	5,5,5	1.18	0
5	GUN	C	300	-	12,12,12	1.45	2 (16%)	15,17,17	2.51	9 (60%)
3	GOL	B	302	-	5,5,5	0.45	0	5,5,5	0.79	0
2	EDO	D	302	-	3,3,3	0.82	0	2,2,2	1.18	0
4	NAP	D	301[B]	-	42,43,52	0.97	2 (4%)	62,67,80	1.77	10 (16%)
3	GOL	D	303	-	5,5,5	0.35	0	5,5,5	0.94	0
4	NAP	D	301[A]	-	42,43,52	0.95	3 (7%)	62,67,80	1.85	16 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAP	B	301[B]	-	42,42,52	1.05	3 (7%)	60,65,80	1.98	15 (25%)
3	GOL	D	305	-	5,5,5	0.41	0	5,5,5	0.82	0
5	GUN	B	300	-	12,12,12	1.41	2 (16%)	15,17,17	2.54	8 (53%)

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
4	NAP	B	301[A]	-	-	5/27/56/67	0/4/4/5
3	GOL	D	304	-	-	4/4/4/4	-
2	EDO	A	302	-	-	1/1/1/1	-
3	GOL	A	303	-	-	2/4/4/4	-
5	GUN	C	300	-	-	-	0/2/2/2
3	GOL	B	302	-	-	2/4/4/4	-
2	EDO	D	302	-	-	1/1/1/1	-
4	NAP	D	301[B]	-	-	11/27/59/67	0/4/4/5
3	GOL	D	303	-	-	0/4/4/4	-
4	NAP	D	301[A]	-	-	9/27/59/67	0/4/4/5
4	NAP	B	301[B]	-	-	6/27/56/67	0/4/4/5
3	GOL	D	305	-	-	1/4/4/4	-
5	GUN	B	300	-	-	-	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	300	GUN	C6-N1	-3.34	1.32	1.38
5	C	300	GUN	C6-N1	-3.01	1.33	1.38
4	B	301[B]	NAP	PN-O3	2.49	1.62	1.59
4	B	301[A]	NAP	C8A-N7A	2.48	1.36	1.31
4	D	301[B]	NAP	PN-O3	2.13	1.61	1.59
5	C	300	GUN	C2-N3	2.10	1.38	1.33
4	B	301[B]	NAP	C8A-N9A	-2.10	1.34	1.37
4	D	301[A]	NAP	C8A-N7A	2.10	1.35	1.31
5	B	300	GUN	C2-N3	2.08	1.38	1.33
4	B	301[A]	NAP	O4B-C1B	2.06	1.46	1.42
4	D	301[A]	NAP	C5A-N7A	-2.05	1.35	1.39
4	B	301[B]	NAP	C5A-N7A	-2.03	1.35	1.39
4	D	301[A]	NAP	C8A-N9A	-2.03	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	301[B]	NAP	C8A-N7A	2.01	1.35	1.31

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	301[B]	NAP	N3A-C2A-N1A	-6.50	118.74	128.58
4	B	301[B]	NAP	N3A-C2A-N1A	-6.48	118.78	128.58
4	D	301[A]	NAP	N3A-C2A-N1A	-6.29	119.07	128.58
4	B	301[A]	NAP	N3A-C2A-N1A	-6.20	119.19	128.58
4	D	301[B]	NAP	C5A-C4A-N3A	-6.10	118.32	126.72
4	B	301[A]	NAP	C5A-C4A-N3A	-5.30	119.42	126.72
4	B	301[B]	NAP	C5A-C4A-N3A	-5.16	119.61	126.72
5	B	300	GUN	N9-C4-N3	5.11	132.20	125.99
4	D	301[A]	NAP	C5A-C4A-N3A	-4.69	120.26	126.72
5	C	300	GUN	N9-C4-N3	4.66	131.66	125.99
4	D	301[B]	NAP	C2A-N3A-C4A	4.49	122.79	111.83
4	B	301[B]	NAP	O5D-C5D-C4D	4.26	123.51	108.99
4	D	301[B]	NAP	N3A-C4A-N9A	4.23	134.37	127.17
4	B	301[B]	NAP	N9A-C8A-N7A	-3.95	108.33	113.94
4	B	301[A]	NAP	C2A-N3A-C4A	3.94	121.45	111.83
4	B	301[B]	NAP	C2A-N3A-C4A	3.93	121.44	111.83
4	B	301[B]	NAP	O4D-C4D-C3D	-3.93	101.00	104.63
4	D	301[A]	NAP	N9A-C8A-N7A	-3.89	108.41	113.94
5	C	300	GUN	C2-N3-C4	3.76	119.99	113.36
4	B	301[B]	NAP	N3A-C4A-N9A	3.75	133.54	127.17
4	B	301[A]	NAP	N9A-C8A-N7A	-3.73	108.64	113.94
4	D	301[A]	NAP	C2A-N3A-C4A	3.66	120.77	111.83
5	B	300	GUN	C2-N3-C4	3.55	119.63	113.36
4	B	301[A]	NAP	N3A-C4A-N9A	3.50	133.11	127.17
4	D	301[A]	NAP	N3A-C4A-N9A	3.41	132.97	127.17
4	D	301[A]	NAP	C4A-N9A-C8A	3.37	109.27	105.74
4	B	301[B]	NAP	C4A-N9A-C8A	3.30	109.20	105.74
5	B	300	GUN	C8-N7-C5	3.27	108.80	104.38
5	C	300	GUN	N9-C8-N7	-3.25	109.21	112.98
5	B	300	GUN	N9-C8-N7	-3.24	109.22	112.98
4	D	301[A]	NAP	C4D-O4D-C1D	-3.20	102.00	108.63
5	C	300	GUN	C2-N1-C6	-3.15	119.41	125.11
4	D	301[B]	NAP	N9A-C8A-N7A	-3.12	109.51	113.94
5	C	300	GUN	C8-N7-C5	3.06	108.51	104.38
4	D	301[A]	NAP	C2A-N1A-C6A	2.89	123.48	118.73
4	D	301[A]	NAP	C5A-N7A-C8A	2.81	107.87	103.45
4	D	301[A]	NAP	C2B-C1B-N9A	-2.80	109.14	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	301[B]	NAP	C5A-N7A-C8A	2.80	107.85	103.45
4	B	301[B]	NAP	C1D-C2D-C3D	2.80	106.11	101.63
4	B	301[A]	NAP	O2B-P2B-O1X	-2.79	99.38	109.33
5	B	300	GUN	C2-N1-C6	-2.78	120.06	125.11
4	B	301[A]	NAP	C5A-N7A-C8A	2.72	107.72	103.45
5	B	300	GUN	C4-C5-N7	-2.65	106.03	110.17
4	B	301[B]	NAP	O2X-P2B-O2B	2.64	116.14	105.85
4	B	301[A]	NAP	O3X-P2B-O2B	2.62	116.07	105.85
5	C	300	GUN	C4-C5-N7	-2.62	106.07	110.17
5	C	300	GUN	C5-C6-N1	2.62	119.91	113.25
5	B	300	GUN	C5-C6-N1	2.61	119.90	113.25
4	D	301[B]	NAP	C5A-N7A-C8A	2.59	107.52	103.45
4	B	301[A]	NAP	C4A-N9A-C8A	2.57	108.44	105.74
4	B	301[B]	NAP	C5D-C4D-C3D	2.54	124.37	115.21
4	D	301[A]	NAP	C4A-C5A-N7A	-2.51	107.71	110.58
4	D	301[B]	NAP	C4A-C5A-N7A	-2.50	107.72	110.58
4	B	301[A]	NAP	C4A-C5A-N7A	-2.48	107.75	110.58
4	B	301[B]	NAP	C4A-C5A-N7A	-2.46	107.78	110.58
5	B	300	GUN	C6-C5-N7	2.41	134.67	130.29
4	B	301[A]	NAP	P2B-O2B-C2B	-2.41	117.00	123.43
5	C	300	GUN	C5-C4-N9	2.30	109.46	106.17
4	D	301[A]	NAP	O3X-P2B-O2B	2.30	114.79	105.85
4	D	301[A]	NAP	P2B-O2B-C2B	-2.29	117.33	123.43
4	B	301[B]	NAP	C2A-N1A-C6A	2.26	122.44	118.73
4	B	301[A]	NAP	C1D-C2D-C3D	2.24	105.21	101.63
4	D	301[A]	NAP	O2B-P2B-O1X	-2.22	101.41	109.33
4	B	301[B]	NAP	C2B-C1B-N9A	-2.18	110.16	113.75
4	D	301[B]	NAP	C4D-O4D-C1D	-2.12	104.23	108.63
4	D	301[B]	NAP	O2X-P2B-O2B	2.11	114.08	105.85
4	D	301[A]	NAP	O3B-C3B-C2B	-2.11	105.27	111.19
4	D	301[B]	NAP	C4A-N9A-C8A	2.10	107.94	105.74
4	B	301[A]	NAP	O4B-C4B-C5B	2.08	115.99	109.33
4	B	301[A]	NAP	O3B-C3B-C2B	-2.04	105.47	111.19
4	D	301[A]	NAP	O4B-C1B-N9A	2.04	112.01	108.09
3	D	304	GOL	C3-C2-C1	-2.03	104.33	111.80
5	C	300	GUN	C6-C5-N7	2.01	133.95	130.29

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	302	GOL	O1-C1-C2-C3

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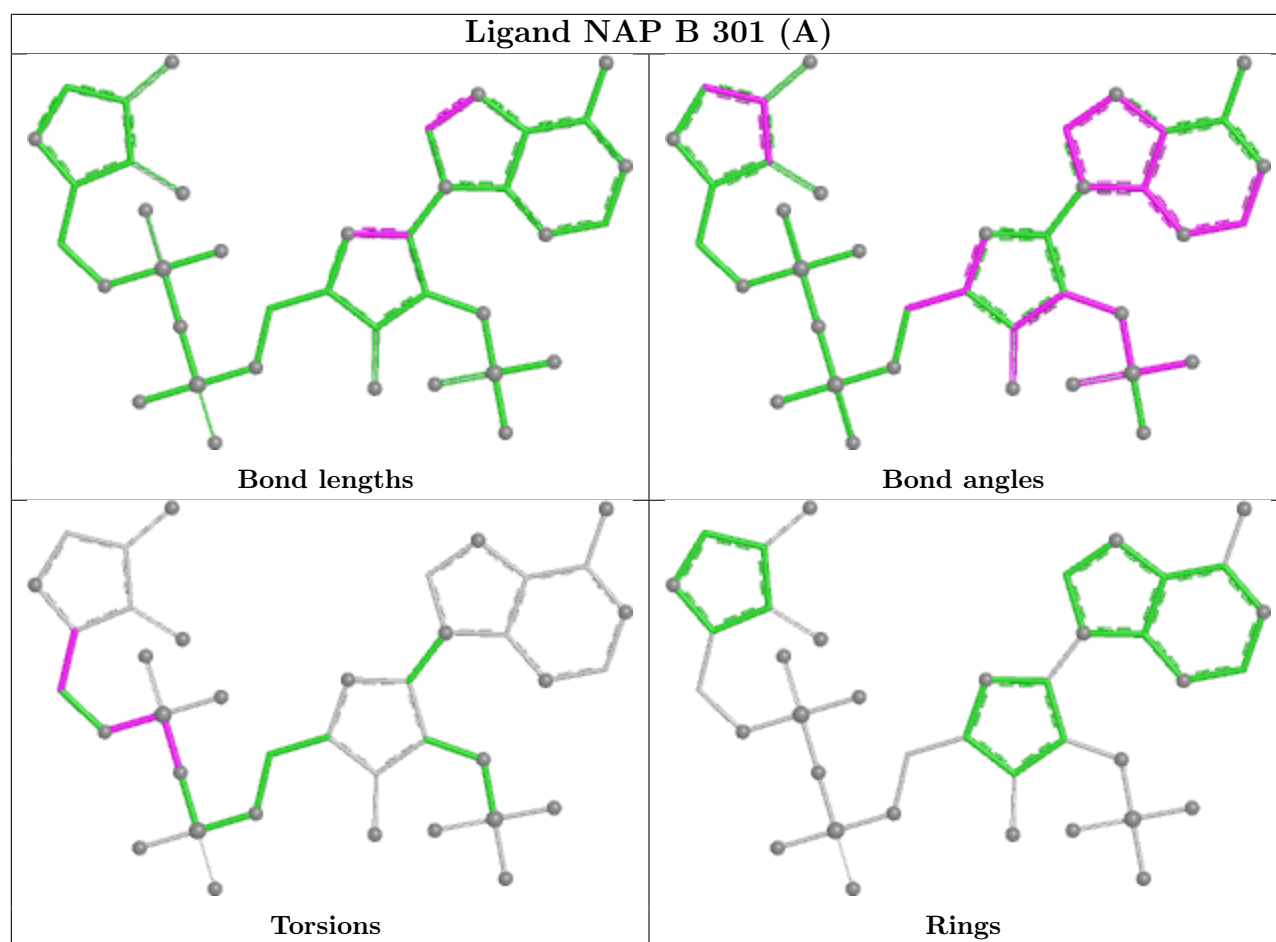
Mol	Chain	Res	Type	Atoms
3	D	304	GOL	O1-C1-C2-C3
3	D	304	GOL	C1-C2-C3-O3
4	B	301[A]	NAP	C5D-O5D-PN-O3
4	B	301[A]	NAP	C5D-O5D-PN-O2N
4	B	301[B]	NAP	PA-O3-PN-O5D
4	B	301[B]	NAP	O4D-C4D-C5D-O5D
4	D	301[A]	NAP	O4B-C4B-C5B-O5B
4	D	301[A]	NAP	C5D-O5D-PN-O1N
4	D	301[A]	NAP	O4D-C4D-C5D-O5D
4	D	301[B]	NAP	O4B-C4B-C5B-O5B
4	D	301[B]	NAP	C5D-O5D-PN-O3
4	D	301[B]	NAP	C5D-O5D-PN-O1N
4	B	301[A]	NAP	O4D-C4D-C5D-O5D
4	B	301[B]	NAP	C3D-C4D-C5D-O5D
4	D	301[A]	NAP	C3D-C4D-C5D-O5D
4	D	301[B]	NAP	C3B-C4B-C5B-O5B
4	D	301[B]	NAP	O4D-C4D-C5D-O5D
4	D	301[A]	NAP	C3B-C4B-C5B-O5B
3	A	303	GOL	O1-C1-C2-C3
3	B	302	GOL	O1-C1-C2-O2
3	D	304	GOL	O1-C1-C2-O2
3	D	304	GOL	O2-C2-C3-O3
4	B	301[A]	NAP	C3D-C4D-C5D-O5D
4	D	301[B]	NAP	C3D-C4D-C5D-O5D
4	B	301[A]	NAP	PA-O3-PN-O5D
4	B	301[B]	NAP	PN-O3-PA-O5B
4	D	301[A]	NAP	PA-O3-PN-O2N
4	B	301[B]	NAP	C5D-O5D-PN-O2N
4	D	301[A]	NAP	C5D-O5D-PN-O3
4	D	301[A]	NAP	C5D-O5D-PN-O2N
4	D	301[B]	NAP	C5D-O5D-PN-O2N
3	D	305	GOL	C1-C2-C3-O3
4	D	301[A]	NAP	PA-O3-PN-O1N
4	D	301[B]	NAP	PA-O3-PN-O2N
2	A	302	EDO	O1-C1-C2-O2
2	D	302	EDO	O1-C1-C2-O2
3	A	303	GOL	O1-C1-C2-O2
4	B	301[B]	NAP	C2B-O2B-P2B-O1X
4	D	301[B]	NAP	C2B-O2B-P2B-O1X
4	D	301[B]	NAP	PA-O3-PN-O1N
4	D	301[B]	NAP	C2B-O2B-P2B-O3X

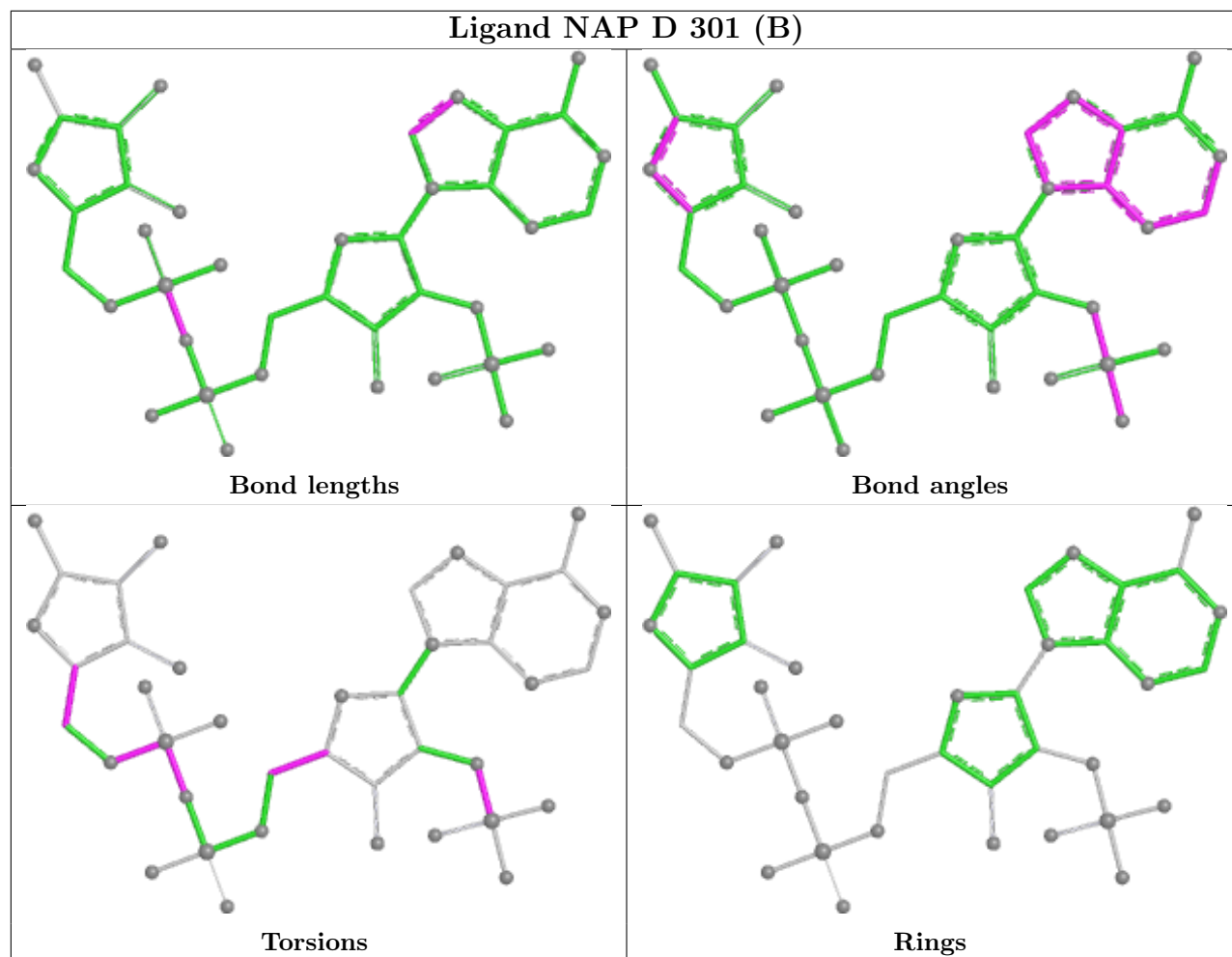
There are no ring outliers.

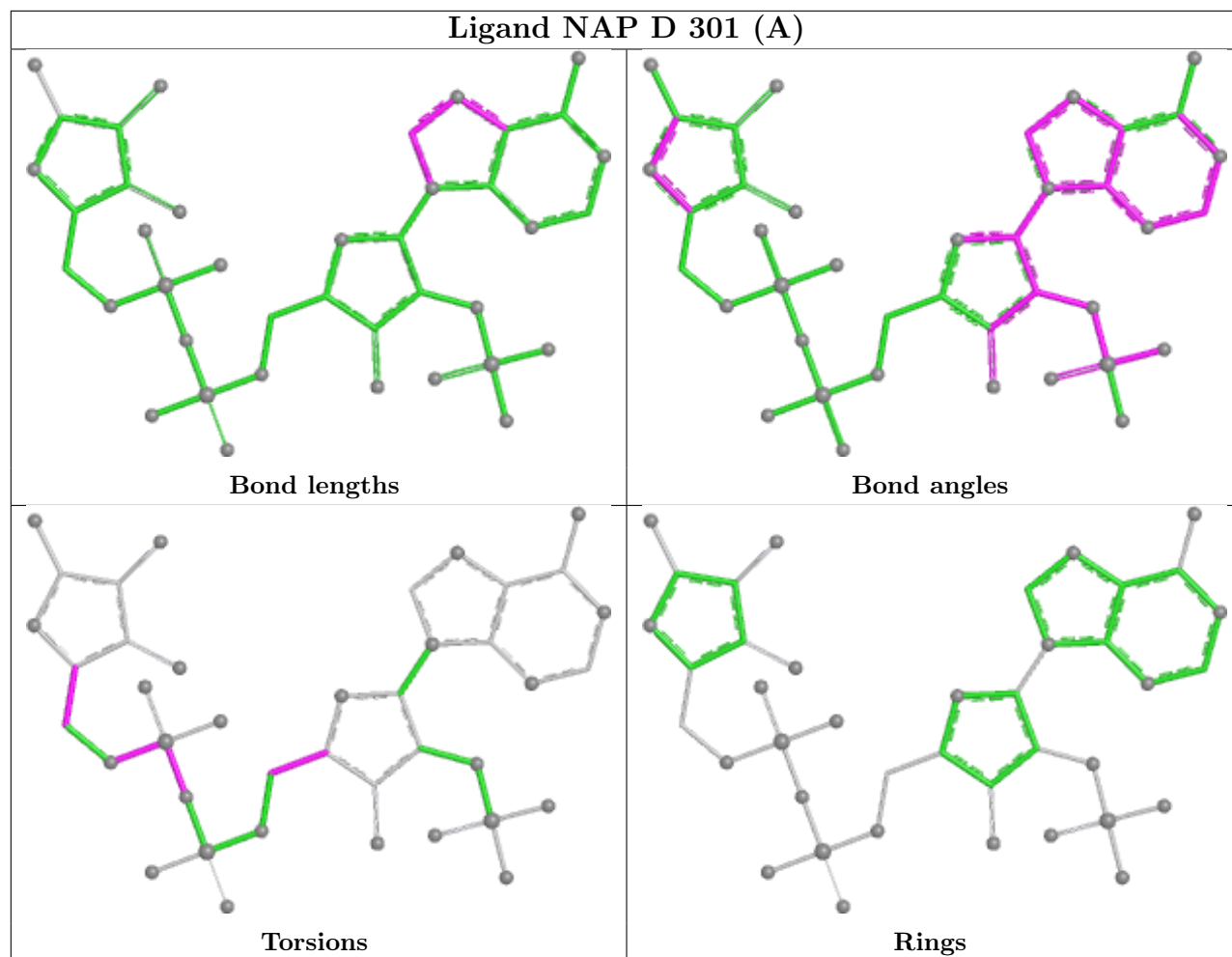
11 monomers are involved in 43 short contacts:

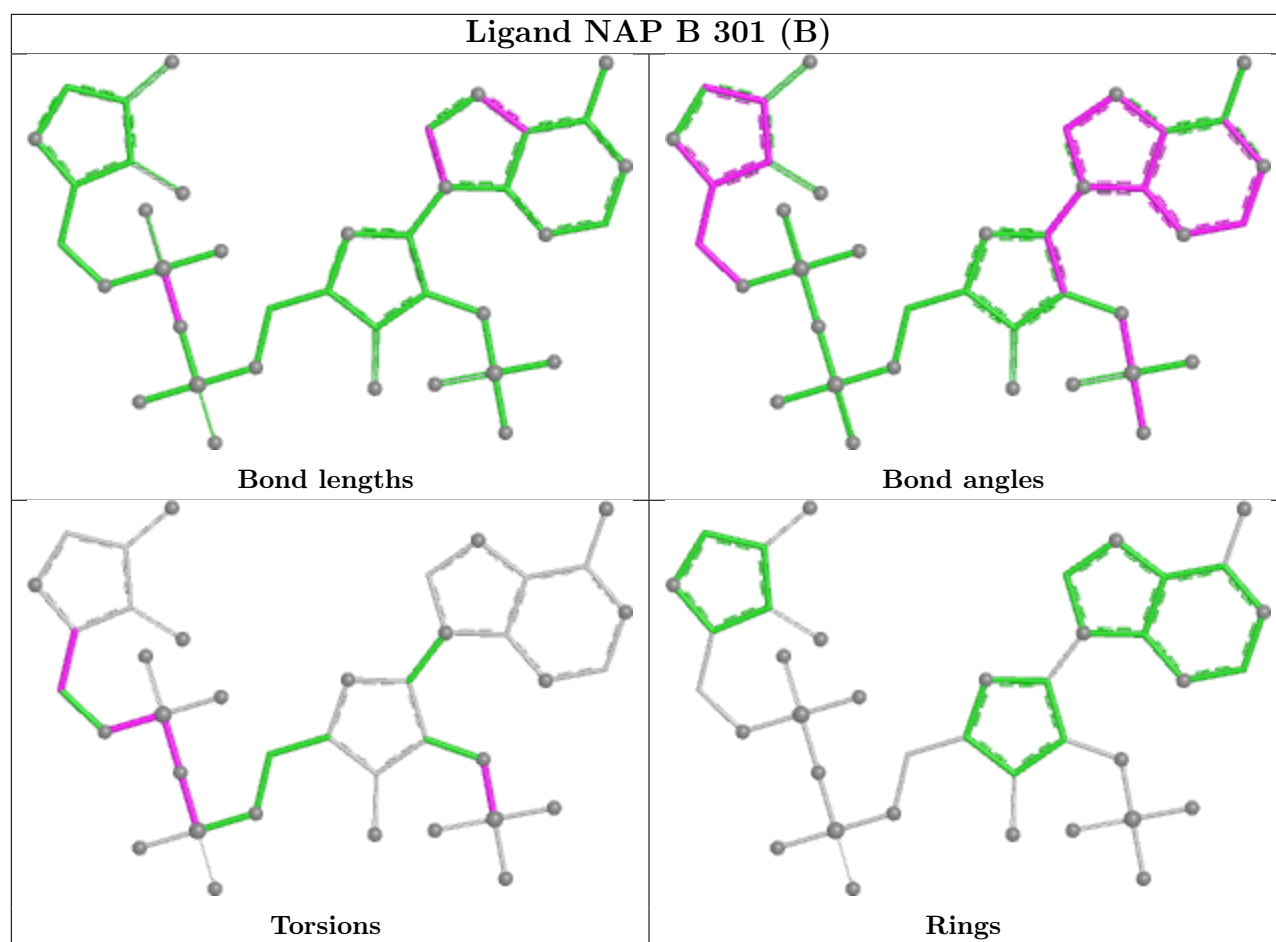
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	301[A]	NAP	2	0
3	D	304	GOL	3	0
2	A	302	EDO	11	0
3	A	303	GOL	1	0
3	B	302	GOL	1	0
2	D	302	EDO	11	0
4	D	301[B]	NAP	5	0
3	D	303	GOL	2	0
4	D	301[A]	NAP	2	0
4	B	301[B]	NAP	4	0
3	D	305	GOL	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/290 (86%)	-1.13	0 100 100	7, 18, 36, 69	29 (11%)
1	B	255/290 (87%)	-1.16	1 (0%) 88 92	7, 17, 37, 61	24 (9%)
1	C	255/290 (87%)	-1.16	2 (0%) 82 87	7, 17, 34, 57	31 (12%)
1	D	250/290 (86%)	-1.14	0 100 100	7, 18, 42, 69	30 (12%)
All	All	1010/1160 (87%)	-1.15	3 (0%) 90 93	7, 18, 38, 69	114 (11%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	195	LEU	4.5
1	C	195	LEU	4.5
1	C	197	THR	2.1

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](#)

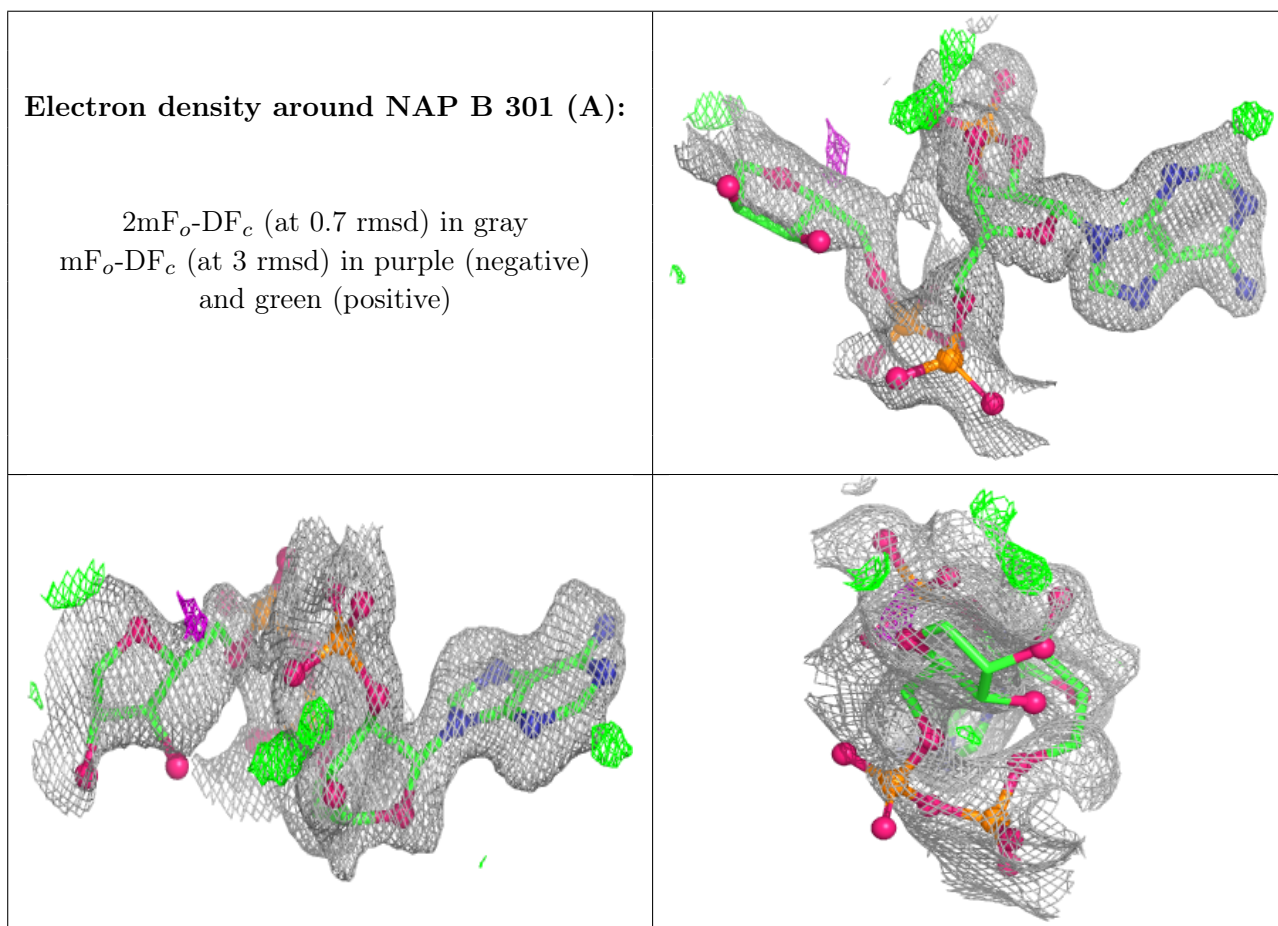
There are no oligosaccharides in this entry.

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.

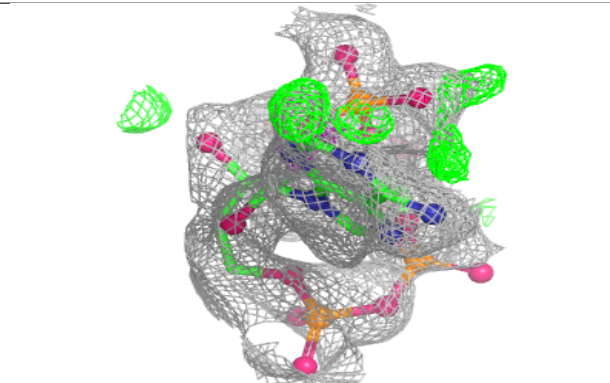
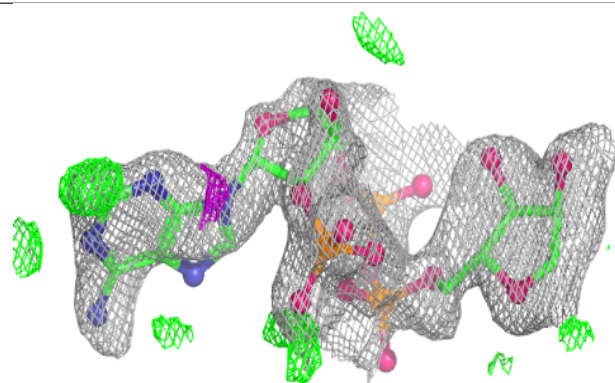
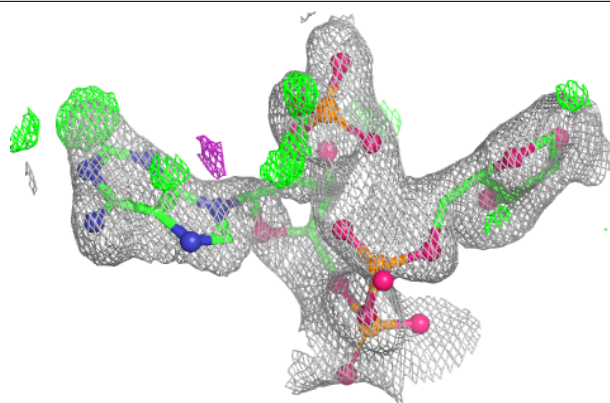
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	D	303	6/6	0.97	0.06	41,43,44,52	0
3	GOL	B	302	6/6	0.98	0.05	45,49,51,55	0
3	GOL	A	303	6/6	0.98	0.06	47,48,55,61	0
3	GOL	D	305	6/6	0.98	0.05	38,47,48,50	0
4	NAP	B	301[A]	39/48	0.98	0.04	22,30,46,51	39
4	NAP	B	301[B]	39/48	0.98	0.04	21,30,46,46	39
4	NAP	D	301[A]	40/48	0.98	0.05	18,31,47,49	40
4	NAP	D	301[B]	40/48	0.98	0.05	18,32,46,48	40
5	GUN	C	300	11/11	0.98	0.04	9,18,23,24	11
2	EDO	D	302	4/4	0.99	0.12	16,21,25,30	0
2	EDO	A	302	4/4	0.99	0.07	17,19,24,29	0
5	GUN	B	300	11/11	0.99	0.04	9,20,24,24	11
3	GOL	D	304	6/6	0.99	0.05	27,40,41,42	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.

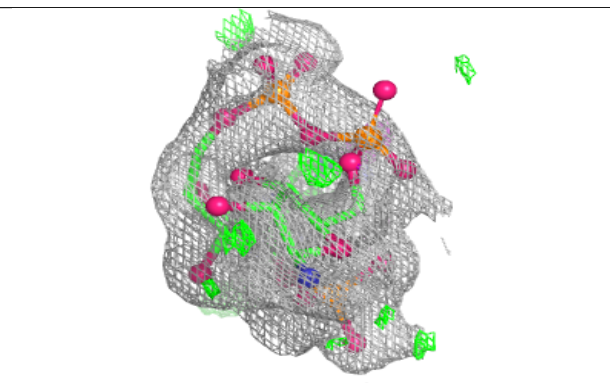
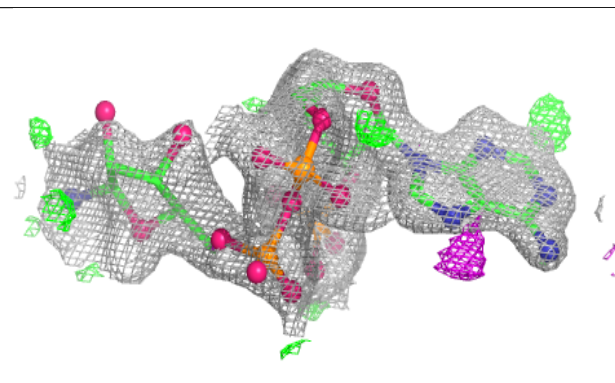
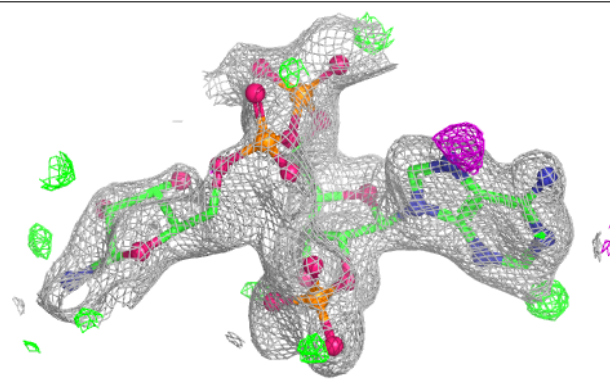


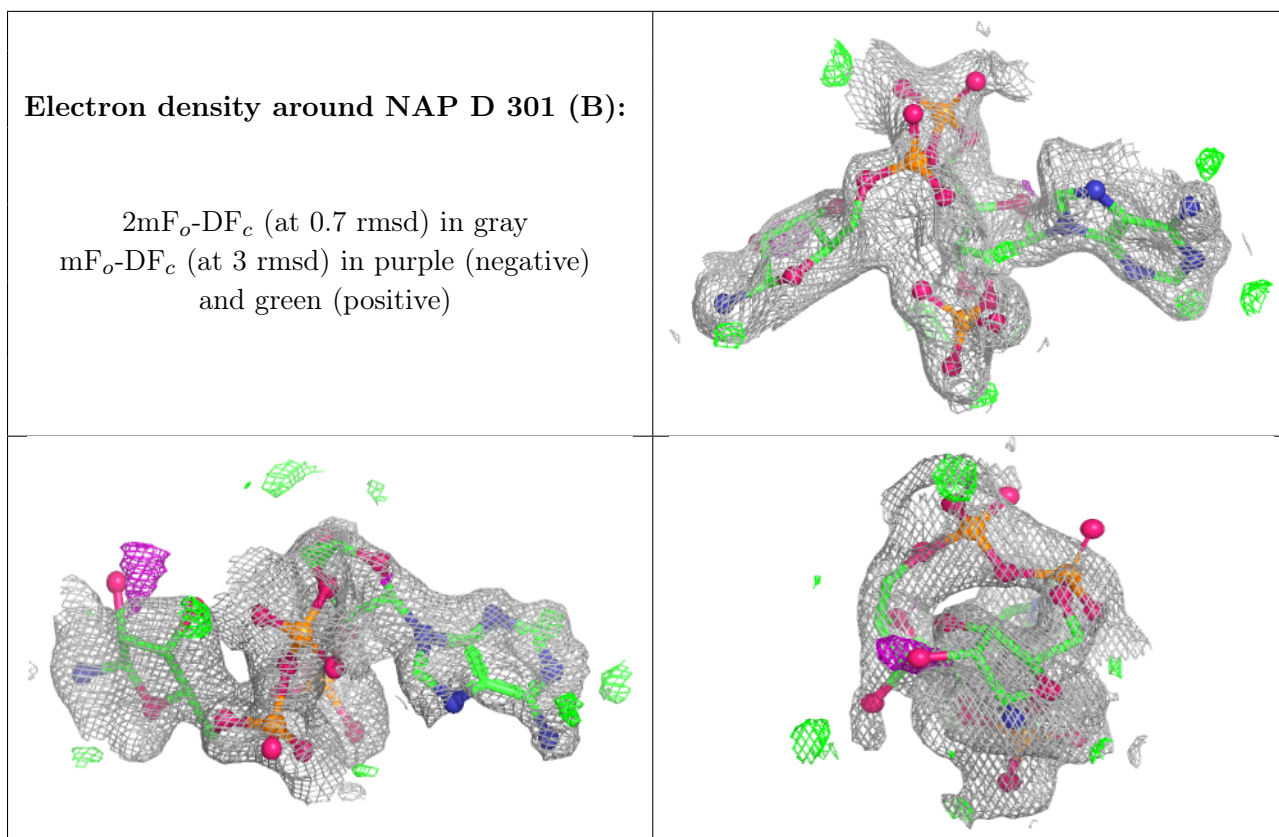
Electron density around NAP B 301 (B):

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

**Electron density around NAP D 301 (A):**

$2mF_o-DF_c$ (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.