



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:11 AM UTC

PDB ID : 6TQ5 / pdb_00006tq5
Title : Alcohol dehydrogenase from *Candida magnoliae* DSMZ 70638 (ADHA): complex with NADP+
Authors : Rovida, S.; Aalbers, F.S.; Fraaije, M.W.; Mattevi, A.
Deposited on : 2019-12-16
Resolution : 1.60 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

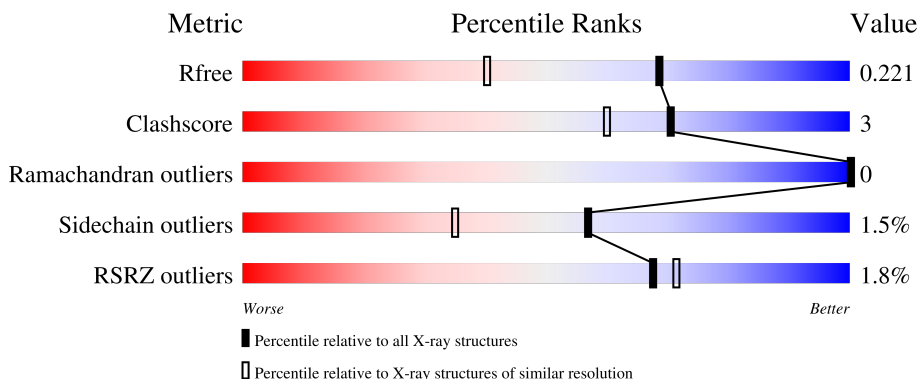
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

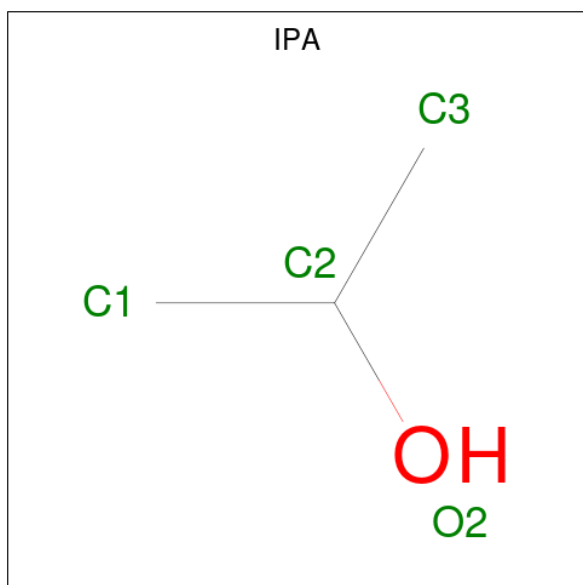
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	246	81% 15% ..
1	B	246	86% 11% .
1	C	246	4% 83% 13% ..
1	D	246	84% 13% ..

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			39	15	5	16	3		
2	D	1	Total	C	N	O	P	0	0
			39	15	5	16	3		

- Molecule 3 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	3	1		
3	C	1	Total	C	O	0	0
			4	3	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

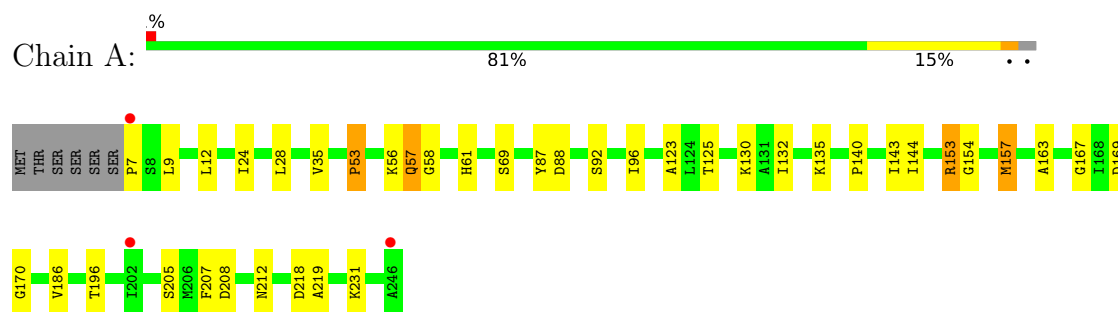
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	137	Total	O	0	0
			137	137		
5	B	143	Total	O	0	0
			143	143		
5	C	140	Total	O	0	0
			140	140		
5	D	139	Total	O	0	0
			139	139		

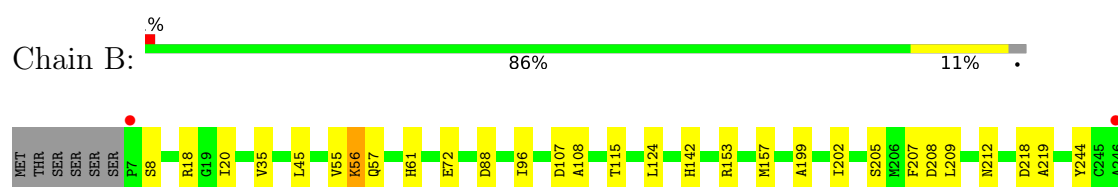
3 Residue-property plots

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.

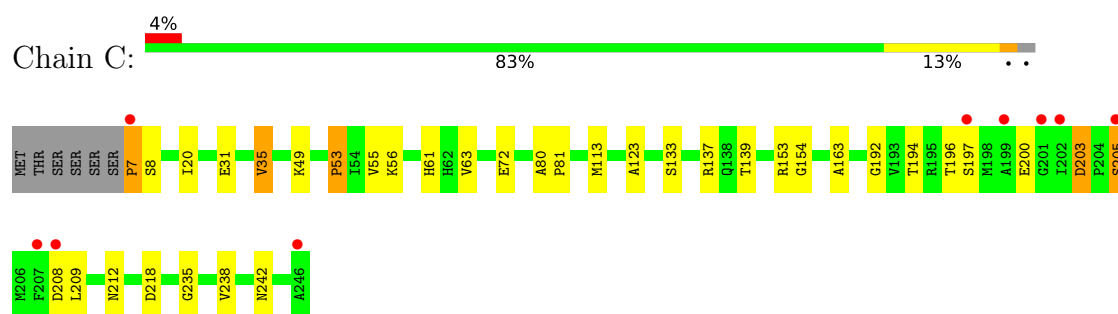
- Molecule 1: Enzyme subunit



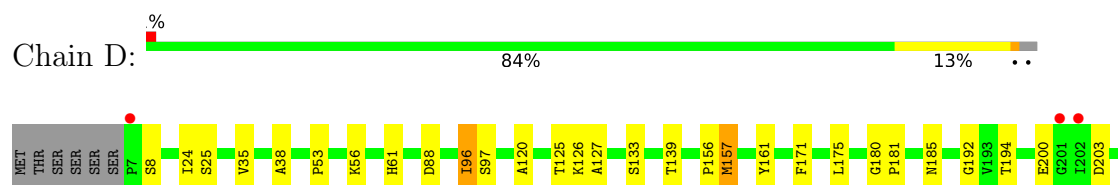
- Molecule 1: Enzyme subunit



- Molecule 1: Enzyme subunit



- Molecule 1: Enzyme subunit



F207				
D208				
V228				
T236				
A246				

4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	76.11Å 113.14Å 124.21Å 90.00° 94.04° 90.00°	Depositor
Resolution (Å)	83.55 – 1.60 83.55 – 1.60	Depositor EDS
% Data completeness (in resolution range)	97.3 (83.55-1.60) 97.3 (83.55-1.60)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.141 , 0.197 (Not available) , 0.221	Depositor DCC
R_{free} test set	6542 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	14.8	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7848	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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, GOL, IPA

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	1.75	20/1830 (1.1%)	1.43	13/2487 (0.5%)
1	B	1.63	13/1823 (0.7%)	1.36	11/2477 (0.4%)
1	C	1.64	18/1815 (1.0%)	1.42	7/2468 (0.3%)
1	D	1.67	16/1794 (0.9%)	1.34	5/2439 (0.2%)
All	All	1.67	67/7262 (0.9%)	1.39	36/9871 (0.4%)

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	SER	CB-OG	-10.82	1.20	1.42
1	B	88	ASP	CG-OD2	8.68	1.41	1.25
1	D	246	ALA	C-O	8.37	1.40	1.23
1	A	157	MET	CB-CG	7.92	1.76	1.52
1	C	212	ASN	C-N	-7.33	1.24	1.32
1	D	96	ILE	CA-CB	7.27	1.64	1.54
1	C	55	VAL	N-CA	-7.18	1.38	1.46
1	D	120	ALA	C-O	-7.12	1.15	1.24
1	D	236	THR	N-CA	-6.95	1.36	1.45
1	D	126	LYS	C-O	-6.91	1.16	1.24
1	B	142	HIS	N-CA	-6.86	1.37	1.46
1	A	219	ALA	N-CA	-6.86	1.38	1.46
1	C	72	GLU	C-O	6.77	1.32	1.24
1	B	8	SER	C-O	-6.53	1.16	1.24
1	A	132	ILE	CA-CB	6.45	1.62	1.54
1	D	25	SER	N-CA	-6.29	1.38	1.46
1	D	88	ASP	CG-OD1	6.28	1.37	1.25
1	B	20	ILE	CA-CB	6.26	1.62	1.54
1	C	163	ALA	C-O	6.16	1.31	1.24
1	D	97	SER	CB-OG	-6.13	1.29	1.42
1	B	219	ALA	C-O	6.08	1.31	1.24
1	C	218	ASP	CG-OD1	6.06	1.36	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	96	ILE	CA-CB	6.01	1.62	1.54
1	D	161	TYR	N-CA	-5.91	1.39	1.46
1	C	113	MET	C-O	5.84	1.30	1.24
1	C	7	PRO	N-CA	-5.84	1.38	1.47
1	A	207	PHE	N-CA	-5.81	1.38	1.45
1	C	238	VAL	CA-CB	5.80	1.60	1.53
1	B	108	ALA	C-O	5.79	1.31	1.24
1	D	24	ILE	CA-C	5.77	1.59	1.52
1	B	45	LEU	C-O	-5.75	1.17	1.24
1	A	12	LEU	CA-C	5.75	1.59	1.52
1	C	242	ASN	CG-OD1	5.75	1.34	1.23
1	D	38	ALA	CA-C	-5.73	1.45	1.52
1	D	185	ASN	C-O	5.67	1.30	1.23
1	A	144	ILE	N-CA	5.65	1.53	1.46
1	B	115	THR	N-CA	-5.63	1.39	1.46
1	A	88	ASP	CG-OD2	5.57	1.35	1.25
1	A	130	LYS	C-O	5.53	1.30	1.24
1	A	125	THR	C-O	5.52	1.30	1.24
1	B	218	ASP	CA-C	5.49	1.59	1.52
1	B	207	PHE	N-CA	-5.49	1.39	1.45
1	B	124	LEU	CB-CG	-5.44	1.42	1.53
1	D	125	THR	C-O	-5.44	1.17	1.24
1	A	208	ASP	CA-C	-5.43	1.47	1.53
1	C	197	SER	CA-C	5.42	1.60	1.52
1	D	203	ASP	C-O	5.39	1.29	1.24
1	A	212	ASN	CA-CB	5.34	1.59	1.52
1	A	9	LEU	C-O	-5.32	1.16	1.23
1	C	209	LEU	N-CA	5.26	1.55	1.45
1	C	163	ALA	CA-C	5.22	1.59	1.52
1	A	169	ASP	C-N	5.22	1.40	1.33
1	C	205	SER	C-O	-5.20	1.17	1.24
1	B	72	GLU	CD-OE1	5.19	1.35	1.25
1	C	123	ALA	C-O	5.19	1.30	1.24
1	D	207	PHE	N-CA	-5.16	1.39	1.45
1	D	127	ALA	C-O	-5.15	1.18	1.24
1	B	199	ALA	N-CA	-5.14	1.40	1.46
1	A	123	ALA	C-O	5.12	1.30	1.24
1	A	205	SER	C-O	-5.12	1.17	1.24
1	C	235	GLY	C-O	5.10	1.30	1.24
1	A	163	ALA	CA-C	5.09	1.59	1.52
1	A	92	SER	CA-CB	-5.09	1.46	1.52
1	C	35	VAL	C-O	5.05	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153	ARG	N-CA	5.04	1.52	1.46
1	C	8	SER	N-CA	5.03	1.52	1.46
1	C	139	THR	CA-CB	5.02	1.60	1.54

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	55	VAL	N-CA-C	7.52	120.12	112.90
1	D	157	MET	CG-SD-CE	-7.35	84.74	100.90
1	C	133	SER	CA-CB-OG	-6.82	97.45	111.10
1	D	246	ALA	CA-C-O	-6.57	101.28	121.00
1	D	208	ASP	CA-C-O	-6.47	114.33	121.58
1	B	208	ASP	CA-C-O	-6.45	114.84	122.13
1	A	157	MET	CG-SD-CE	6.29	114.73	100.90
1	B	56	LYS	N-CA-C	-6.09	98.34	108.75
1	B	18	ARG	NE-CZ-NH1	-5.99	115.51	121.50
1	A	154	GLY	N-CA-C	5.85	118.66	111.93
1	A	196	THR	N-CA-C	5.79	117.40	109.18
1	B	56	LYS	CA-CB-CG	5.74	125.59	114.10
1	C	212	ASN	O-C-N	-5.72	116.27	122.79
1	B	18	ARG	NE-CZ-NH2	5.71	124.33	119.20
1	A	24	ILE	N-CA-C	-5.68	104.97	110.42
1	A	7	PRO	CA-C-N	-5.64	115.28	122.77
1	A	7	PRO	C-N-CA	-5.64	115.28	122.77
1	A	28	LEU	N-CA-C	-5.63	105.22	111.36
1	A	208	ASP	CA-C-O	-5.62	115.78	122.13
1	B	205	SER	N-CA-C	5.59	119.20	112.38
1	B	209	LEU	N-CA-C	5.57	117.70	109.62
1	A	157	MET	CB-CG-SD	-5.46	96.31	112.70
1	B	88	ASP	CB-CG-OD1	-5.35	106.10	118.40
1	C	212	ASN	CA-C-N	-5.34	114.26	122.69
1	C	212	ASN	C-N-CA	-5.34	114.26	122.69
1	C	200	GLU	N-CA-C	-5.32	101.11	109.25
1	A	167	GLY	O-C-N	5.30	127.28	122.19
1	B	107	ASP	N-CA-C	5.22	116.97	111.28
1	C	208	ASP	N-CA-CB	-5.21	103.54	110.57
1	D	207	PHE	CA-C-O	5.19	127.84	121.56
1	A	87	TYR	N-CA-C	5.18	118.06	109.46
1	A	53	PRO	CB-CA-C	-5.16	104.63	111.23
1	A	170	GLY	O-C-N	5.16	127.14	122.19
1	C	137	ARG	NE-CZ-NH1	-5.15	116.35	121.50
1	B	56	LYS	CB-CA-C	-5.13	99.53	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	133	SER	CA-CB-OG	-5.12	100.85	111.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1797	0	1813	14	0
1	B	1781	0	1808	9	0
1	C	1773	0	1791	17	0
1	D	1761	0	1775	11	0
2	A	40	0	19	0	0
2	B	39	0	18	0	0
2	C	39	0	18	0	0
2	D	39	0	18	0	0
3	A	4	0	8	0	0
3	C	4	0	8	3	0
4	C	6	0	7	1	0
4	D	6	0	8	2	0
5	A	137	0	0	2	1
5	B	143	0	0	3	0
5	C	140	0	0	2	0
5	D	139	0	0	3	0
All	All	7848	0	7291	49	1

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 3.

All (49) 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:A:157:MET:CG	1:A:157:MET:CB	1.76	1.63
1:A:153:ARG:HD2	5:D:409:HOH:O	1.56	1.05
5:B:521:HOH:O	1:C:153:ARG:HD2	1.64	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:VAL:H	1:A:61:HIS:HD2	1.19	0.91
1:D:35:VAL:H	1:D:61:HIS:HD2	1.23	0.86
1:B:35:VAL:H	1:B:61:HIS:HD2	1.25	0.84
1:A:157:MET:CB	1:A:157:MET:SD	2.66	0.83
1:C:35:VAL:H	1:C:61:HIS:HD2	1.24	0.80
1:A:135:LYS:HE2	5:A:438:HOH:O	1.90	0.71
1:C:35:VAL:H	1:C:61:HIS:CD2	2.09	0.68
1:D:35:VAL:H	1:D:61:HIS:CD2	2.11	0.61
1:C:203:ASP:OD1	1:C:205:SER:OG	2.17	0.59
1:D:96:ILE:HD11	5:D:462:HOH:O	2.01	0.59
1:D:56:LYS:HE3	4:D:302:GOL:O2	2.04	0.58
1:A:35:VAL:H	1:A:61:HIS:CD2	2.11	0.56
1:B:35:VAL:H	1:B:61:HIS:CD2	2.15	0.55
1:C:31:GLU:O	3:C:302:IPA:H32	2.09	0.53
1:C:49:LYS:HD3	1:C:63:VAL:HG13	1.91	0.53
1:C:192:GLY:O	1:C:194[A]:THR:HG23	2.08	0.53
1:C:31:GLU:O	3:C:302:IPA:C3	2.58	0.52
1:C:53:PRO:O	1:C:61:HIS:HE1	1.92	0.51
1:C:80:ALA:HB1	5:C:410:HOH:O	2.10	0.51
1:A:157:MET:CG	1:A:157:MET:CA	2.81	0.49
1:B:153:ARG:HG3	1:C:153:ARG:NH2	2.29	0.47
1:C:154:GLY:HA2	5:C:423:HOH:O	2.15	0.47
1:B:212:ASN:ND2	5:B:401:HOH:O	2.48	0.46
1:C:194[B]:THR:HG23	1:C:196:THR:HG23	1.97	0.46
1:B:96[B]:ILE:HD13	1:B:96[B]:ILE:HA	1.56	0.46
1:B:153:ARG:HG3	1:C:153:ARG:CZ	2.45	0.46
1:A:157:MET:HB3	1:A:157:MET:HE2	1.98	0.45
1:D:156:PRO:C	1:D:157:MET:HG2	2.42	0.45
1:A:157:MET:HB3	1:A:157:MET:CE	2.47	0.45
1:A:140:PRO:HD2	1:A:231[B]:LYS:HG2	1.99	0.44
1:C:56:LYS:HD2	3:C:302:IPA:H33	1.98	0.44
1:A:53:PRO:O	1:A:61:HIS:HE1	2.00	0.44
1:C:81:PRO:HB2	4:C:303:GOL:H31	1.99	0.43
1:D:171:PHE:CE2	1:D:175:LEU:HD11	2.53	0.43
1:D:192:GLY:O	1:D:194:THR:HG23	2.18	0.43
1:B:153:ARG:HD3	1:B:244:TYR:CZ	2.54	0.43
1:C:20:ILE:HD11	1:C:194[B]:THR:HG21	2.00	0.42
1:A:57:GLN:HG2	1:A:58:GLY:N	2.35	0.42
1:D:53:PRO:O	1:D:61:HIS:HE1	2.03	0.42
1:B:96[B]:ILE:HG23	1:B:96[B]:ILE:HD12	1.70	0.42
1:D:139:THR:HG23	5:D:432:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96[B]:ILE:HD13	5:B:434:HOH:O	2.20	0.41
1:D:180:GLY:N	1:D:181:PRO:CD	2.84	0.41
1:A:218:ASP:CG	5:A:414:HOH:O	2.64	0.40
1:A:143:ILE:O	1:A:186:VAL:HA	2.21	0.40
1:D:8:SER:HA	4:D:302:GOL:O3	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:536:HOH:O	5:A:536:HOH:O[2_555]	0.68	1.52

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	243/246 (99%)	235 (97%)	8 (3%)	0	100	100
1	B	242/246 (98%)	237 (98%)	5 (2%)	0	100	100
1	C	241/246 (98%)	234 (97%)	7 (3%)	0	100	100
1	D	238/246 (97%)	231 (97%)	7 (3%)	0	100	100
All	All	964/984 (98%)	937 (97%)	27 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	194/195 (100%)	192 (99%)	2 (1%)	68	50
1	B	193/195 (99%)	189 (98%)	4 (2%)	47	23
1	C	192/195 (98%)	189 (98%)	3 (2%)	55	33
1	D	189/195 (97%)	187 (99%)	2 (1%)	65	46
All	All	768/780 (98%)	757 (99%)	11 (1%)	57	38

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LYS
1	A	57	GLN
1	B	56	LYS
1	B	57	GLN
1	B	157	MET
1	B	202	ILE
1	C	7	PRO
1	C	53	PRO
1	C	203	ASP
1	D	200	GLU
1	D	228	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	142	HIS
1	A	242	ASN
1	B	61	HIS
1	B	212	ASN
1	B	242	ASN
1	C	57	GLN
1	C	61	HIS
1	C	212	ASN
1	C	242	ASN
1	D	57	GLN
1	D	61	HIS
1	D	65	GLN
1	D	212	ASN

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Mol	Chain	Res	Type
1	D	242	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	IPA	A	302	-	3,3,3	0.98	0	3,3,3	1.18	0
3	IPA	C	302	-	3,3,3	0.84	0	3,3,3	1.91	1 (33%)
2	NAP	B	301	-	42,42,52	1.79	9 (21%)	60,65,80	2.19	20 (33%)
4	GOL	D	302	-	5,5,5	0.50	0	5,5,5	1.87	2 (40%)
2	NAP	D	301	-	42,42,52	1.65	7 (16%)	60,65,80	2.05	20 (33%)
2	NAP	C	301	-	42,42,52	2.07	9 (21%)	60,65,80	2.15	15 (25%)
4	GOL	C	303	-	5,5,5	1.95	2 (40%)	5,5,5	2.85	2 (40%)
2	NAP	A	301	-	42,43,52	1.51	5 (11%)	62,67,80	2.52	18 (29%)

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	B	301	-	-	3/27/56/67	0/4/4/5
4	GOL	D	302	-	-	2/4/4/4	-
2	NAP	D	301	-	-	4/27/56/67	0/4/4/5
2	NAP	C	301	-	-	4/27/56/67	0/4/4/5
4	GOL	C	303	-	-	1/4/4/4	-
2	NAP	A	301	-	-	3/27/59/67	0/4/4/5

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	NAP	PN-O3	7.88	1.68	1.59
2	C	301	NAP	PA-O3	5.89	1.65	1.59
2	A	301	NAP	PA-O3	4.99	1.64	1.59
2	B	301	NAP	P2B-O2B	4.83	1.68	1.59
2	D	301	NAP	P2B-O2B	4.76	1.67	1.59
2	A	301	NAP	C4A-N9A	-4.11	1.29	1.37
2	B	301	NAP	C5A-C4A	4.10	1.46	1.39
2	B	301	NAP	PN-O3	4.03	1.63	1.59
2	D	301	NAP	O4D-C1D	3.97	1.52	1.43
2	C	301	NAP	P2B-O2B	3.95	1.66	1.59
2	D	301	NAP	C5A-C6A	3.91	1.51	1.41
2	A	301	NAP	C5A-C4A	3.75	1.45	1.39
2	D	301	NAP	C5A-C4A	3.54	1.45	1.39
2	C	301	NAP	C4A-N9A	-3.44	1.30	1.37
2	B	301	NAP	O4D-C1D	3.28	1.50	1.43
2	B	301	NAP	C2A-N3A	3.28	1.39	1.33
2	D	301	NAP	C8A-N7A	3.27	1.38	1.31
2	D	301	NAP	PA-O3	3.26	1.63	1.59
2	B	301	NAP	PA-O3	3.12	1.62	1.59
2	C	301	NAP	C5A-C4A	2.97	1.44	1.39
4	C	303	GOL	O1-C1	2.95	1.54	1.42
2	C	301	NAP	C8A-N7A	2.82	1.37	1.31
2	B	301	NAP	O4D-C4D	2.82	1.49	1.44
2	B	301	NAP	C8A-N7A	2.70	1.36	1.31
2	C	301	NAP	C4A-N3A	2.57	1.39	1.34
2	B	301	NAP	C5A-C6A	2.31	1.47	1.41
2	A	301	NAP	P2B-O2B	2.28	1.63	1.59
2	C	301	NAP	PN-O1N	2.23	1.58	1.50
4	C	303	GOL	O3-C3	-2.22	1.33	1.42
2	D	301	NAP	C1D-C2D	2.16	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	NAP	C2A-N3A	2.15	1.37	1.33
2	C	301	NAP	O4D-C1D	2.11	1.48	1.43

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	NAP	O4D-C1D-N1N	-10.95	93.13	110.57
2	D	301	NAP	O4D-C1D-C2D	-9.84	88.81	105.76
2	B	301	NAP	O4D-C1D-C2D	-7.45	92.92	105.76
2	C	301	NAP	C4A-N9A-C8A	6.46	112.53	105.74
2	A	301	NAP	C4A-N9A-C8A	6.30	112.35	105.74
2	B	301	NAP	N3A-C2A-N1A	-5.99	119.52	128.58
2	C	301	NAP	C5A-C4A-N3A	-5.91	118.58	126.72
4	C	303	GOL	O2-C2-C3	-5.10	88.08	109.18
2	A	301	NAP	O4B-C4B-C3B	5.07	115.22	105.15
2	C	301	NAP	O4D-C1D-C2D	-4.94	97.25	105.76
2	C	301	NAP	N3A-C4A-N9A	4.84	135.40	127.17
2	A	301	NAP	N9A-C8A-N7A	-4.76	107.18	113.94
2	C	301	NAP	N9A-C8A-N7A	-4.66	107.33	113.94
2	C	301	NAP	O5D-C5D-C4D	-4.00	95.38	108.99
2	A	301	NAP	C4A-C5A-N7A	-3.88	106.15	110.58
2	B	301	NAP	C4A-N9A-C8A	3.78	109.70	105.74
2	B	301	NAP	O3-PA-O1A	-3.72	99.52	110.70
2	A	301	NAP	O2D-C2D-C1D	3.60	122.47	110.10
2	B	301	NAP	C2B-C1B-N9A	-3.52	107.97	113.75
2	B	301	NAP	C2A-N1A-C6A	3.36	124.25	118.73
2	A	301	NAP	O2A-PA-O1A	3.31	127.85	112.44
2	A	301	NAP	C5A-C4A-N3A	-3.30	122.18	126.72
2	B	301	NAP	C6A-C5A-C4A	-3.22	112.78	117.18
2	B	301	NAP	O2N-PN-O3	-3.22	98.58	107.27
2	A	301	NAP	C4B-O4B-C1B	-3.21	102.37	109.47
2	C	301	NAP	C4A-C5A-N7A	-3.19	106.93	110.58
2	B	301	NAP	N3A-C4A-N9A	3.19	132.59	127.17
2	A	301	NAP	C5A-N7A-C8A	3.15	108.41	103.45
2	C	301	NAP	C2A-N3A-C4A	3.14	119.50	111.83
2	C	301	NAP	C2B-C1B-N9A	-3.13	108.59	113.75
2	B	301	NAP	C2A-N3A-C4A	3.13	119.47	111.83
4	D	302	GOL	O1-C1-C2	-3.11	96.39	110.38
2	C	301	NAP	O3-PN-O1N	-3.04	101.57	110.70
2	B	301	NAP	O2B-P2B-O1X	-3.03	98.53	109.33
2	D	301	NAP	O3-PN-O1N	-2.93	101.89	110.70
2	A	301	NAP	O4D-C4D-C3D	-2.92	99.36	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	NAP	C2B-C1B-N9A	-2.83	109.09	113.75
2	B	301	NAP	C5A-C4A-N9A	-2.83	102.73	105.81
2	A	301	NAP	O2A-PA-O3	-2.82	99.64	107.27
2	D	301	NAP	N3A-C4A-N9A	2.82	131.96	127.17
2	A	301	NAP	N3A-C4A-N9A	2.82	131.96	127.17
2	D	301	NAP	O2A-PA-O3	-2.80	99.70	107.27
4	C	303	GOL	O2-C2-C1	2.76	120.61	109.18
2	D	301	NAP	C5A-C4A-N3A	-2.74	122.94	126.72
2	D	301	NAP	O4D-C4D-C3D	-2.60	102.23	104.63
2	C	301	NAP	C4B-O4B-C1B	-2.56	103.81	109.47
2	D	301	NAP	C2A-N3A-C4A	2.56	118.08	111.83
2	B	301	NAP	O2N-PN-O1N	2.56	124.34	112.44
2	C	301	NAP	O4B-C4B-C3B	2.55	110.21	105.15
2	A	301	NAP	C6A-C5A-N7A	2.52	136.95	132.09
3	C	302	IPA	O2-C2-C1	2.51	126.44	110.28
2	B	301	NAP	O2A-PA-O3	2.48	113.97	107.27
2	C	301	NAP	O2N-PN-O1N	2.47	123.95	112.44
2	D	301	NAP	O3-PA-O1A	2.45	118.08	110.70
2	A	301	NAP	O5B-PA-O1A	-2.45	99.23	108.94
2	D	301	NAP	O2N-PN-O5D	2.42	118.54	107.57
2	D	301	NAP	C4A-N9A-C8A	2.41	108.27	105.74
2	C	301	NAP	C5A-N7A-C8A	2.39	107.21	103.45
2	A	301	NAP	C2B-C1B-N9A	-2.38	109.83	113.75
2	D	301	NAP	O2B-P2B-O1X	-2.38	100.86	109.33
2	D	301	NAP	O3X-P2B-O2B	-2.28	96.95	105.85
2	D	301	NAP	C3B-C2B-C1B	-2.28	98.45	102.81
2	C	301	NAP	N3A-C2A-N1A	-2.27	125.15	128.58
2	D	301	NAP	O2N-PN-O3	2.24	113.33	107.27
2	A	301	NAP	C4D-O4D-C1D	2.22	113.24	108.63
2	B	301	NAP	O4D-C4D-C3D	-2.22	102.58	104.63
2	D	301	NAP	C6A-C5A-C4A	-2.22	114.15	117.18
2	D	301	NAP	O2D-C2D-C3D	2.22	115.79	111.43
2	D	301	NAP	N3A-C2A-N1A	-2.18	125.28	128.58
2	B	301	NAP	O5D-C5D-C4D	-2.17	101.59	108.99
2	B	301	NAP	C5A-C6A-N6A	-2.17	117.91	123.29
2	D	301	NAP	O2A-PA-O1A	2.17	122.54	112.44
2	D	301	NAP	O3X-P2B-O2X	2.12	115.75	107.80
2	B	301	NAP	N6A-C6A-N1A	2.09	123.03	118.38
4	D	302	GOL	O2-C2-C1	-2.07	100.59	109.18
2	A	301	NAP	O2B-C2B-C1B	2.05	117.27	110.05
2	B	301	NAP	O2X-P2B-O2B	-2.02	97.98	105.85
2	B	301	NAP	O2X-P2B-O1X	2.01	118.67	110.83

There are no chirality outliers.

All (17) torsion outliers are listed below:

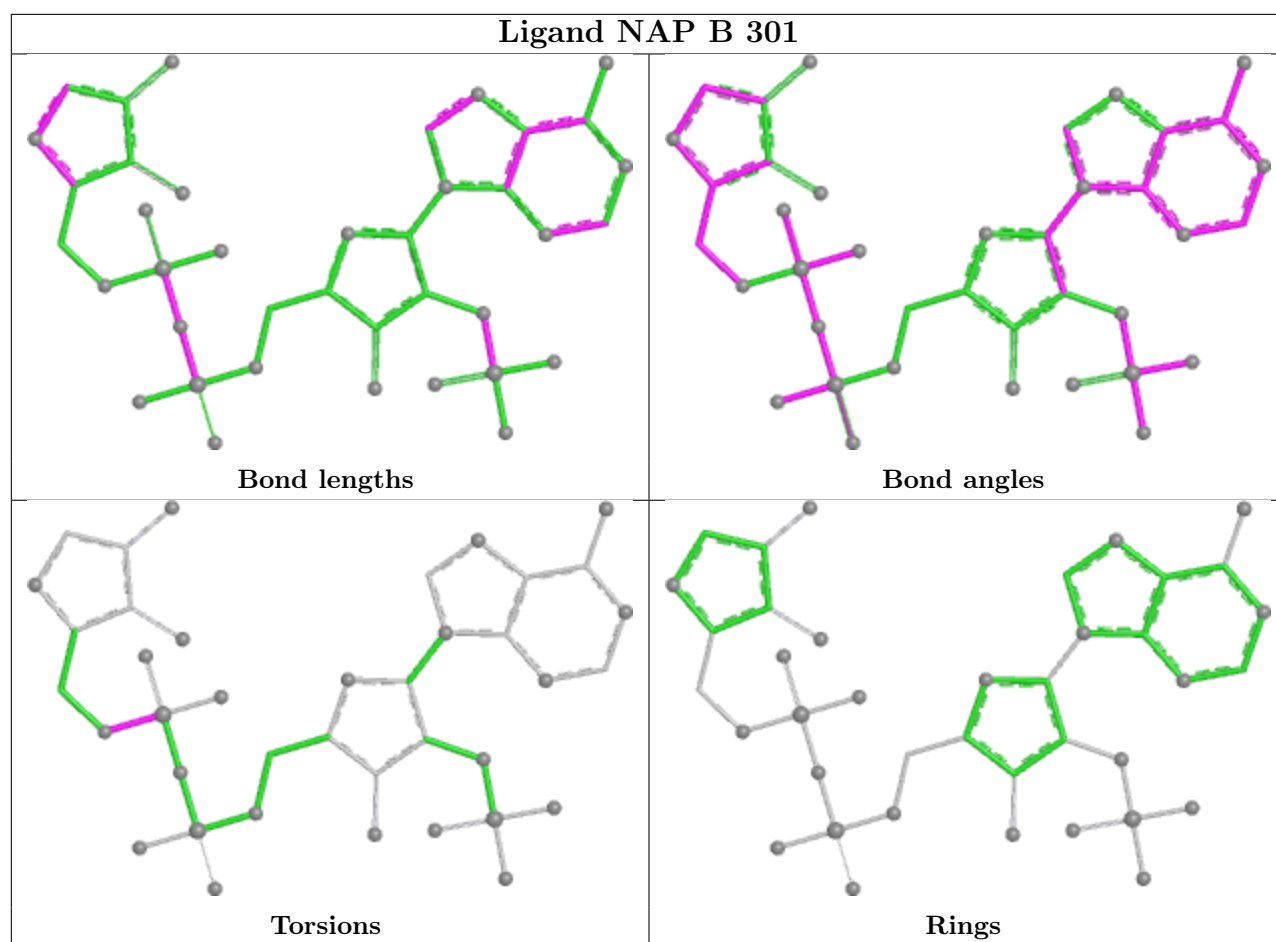
Mol	Chain	Res	Type	Atoms
2	A	301	NAP	C5D-O5D-PN-O3
2	A	301	NAP	C5D-O5D-PN-O2N
2	B	301	NAP	C5D-O5D-PN-O3
2	B	301	NAP	C5D-O5D-PN-O1N
2	C	301	NAP	C5D-O5D-PN-O3
2	C	301	NAP	C5D-O5D-PN-O1N
2	C	301	NAP	C5D-O5D-PN-O2N
2	D	301	NAP	C5D-O5D-PN-O3
2	D	301	NAP	C5D-O5D-PN-O2N
4	D	302	GOL	O1-C1-C2-C3
4	C	303	GOL	O1-C1-C2-O2
4	D	302	GOL	O1-C1-C2-O2
2	A	301	NAP	C5D-O5D-PN-O1N
2	B	301	NAP	C5D-O5D-PN-O2N
2	D	301	NAP	C5D-O5D-PN-O1N
2	C	301	NAP	C2B-O2B-P2B-O3X
2	D	301	NAP	C2B-O2B-P2B-O2X

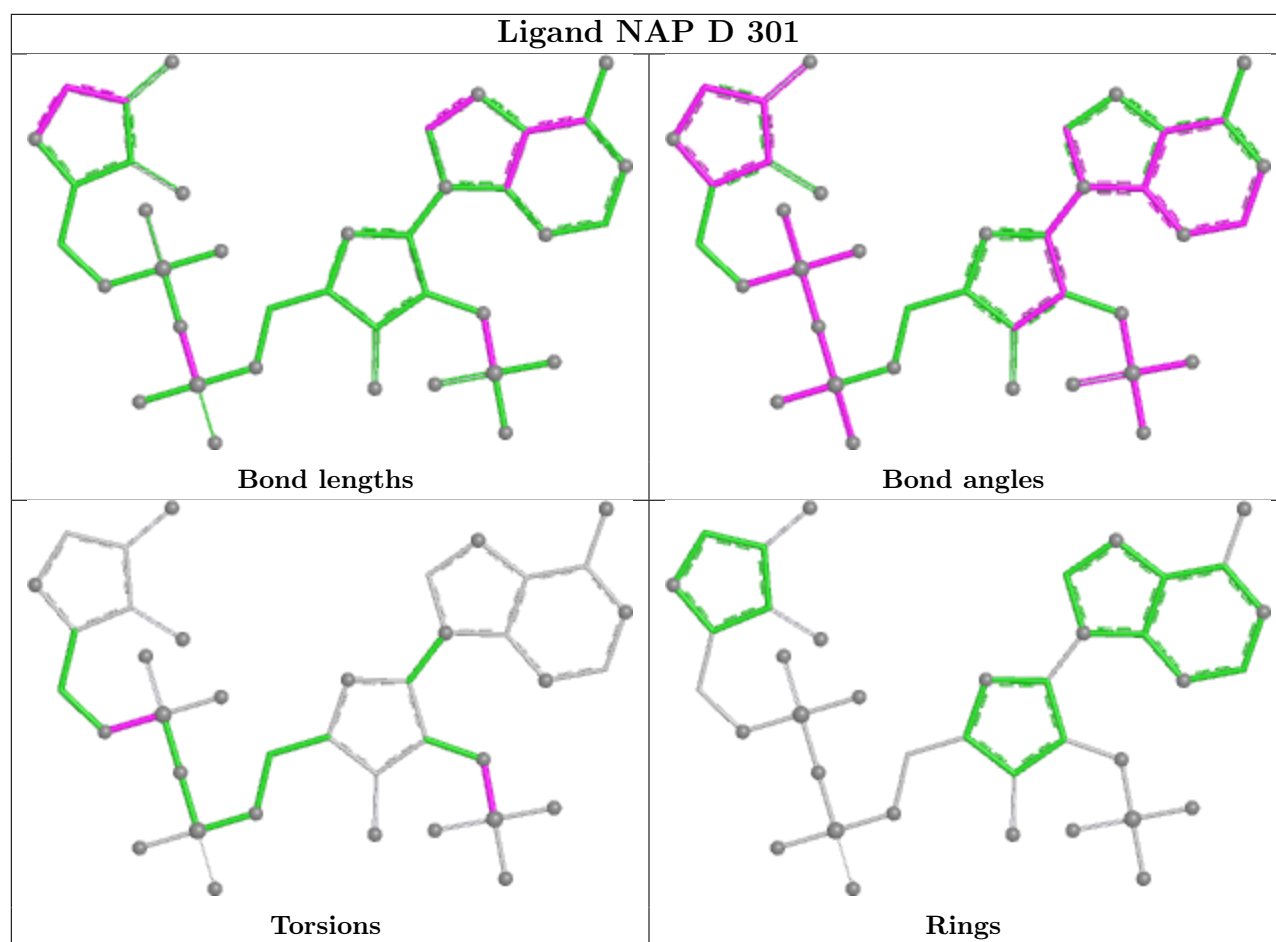
There are no ring outliers.

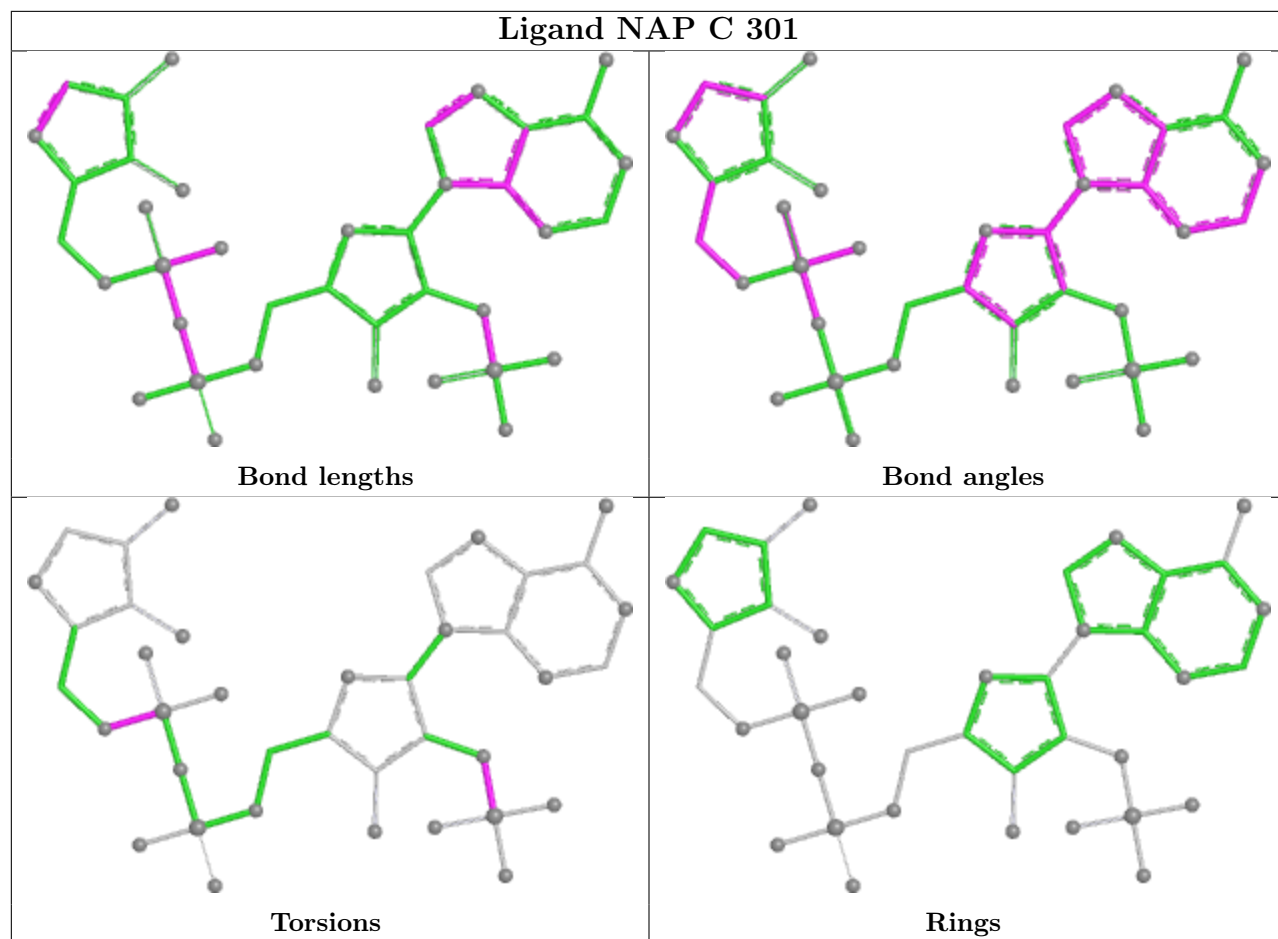
3 monomers are involved in 6 short contacts:

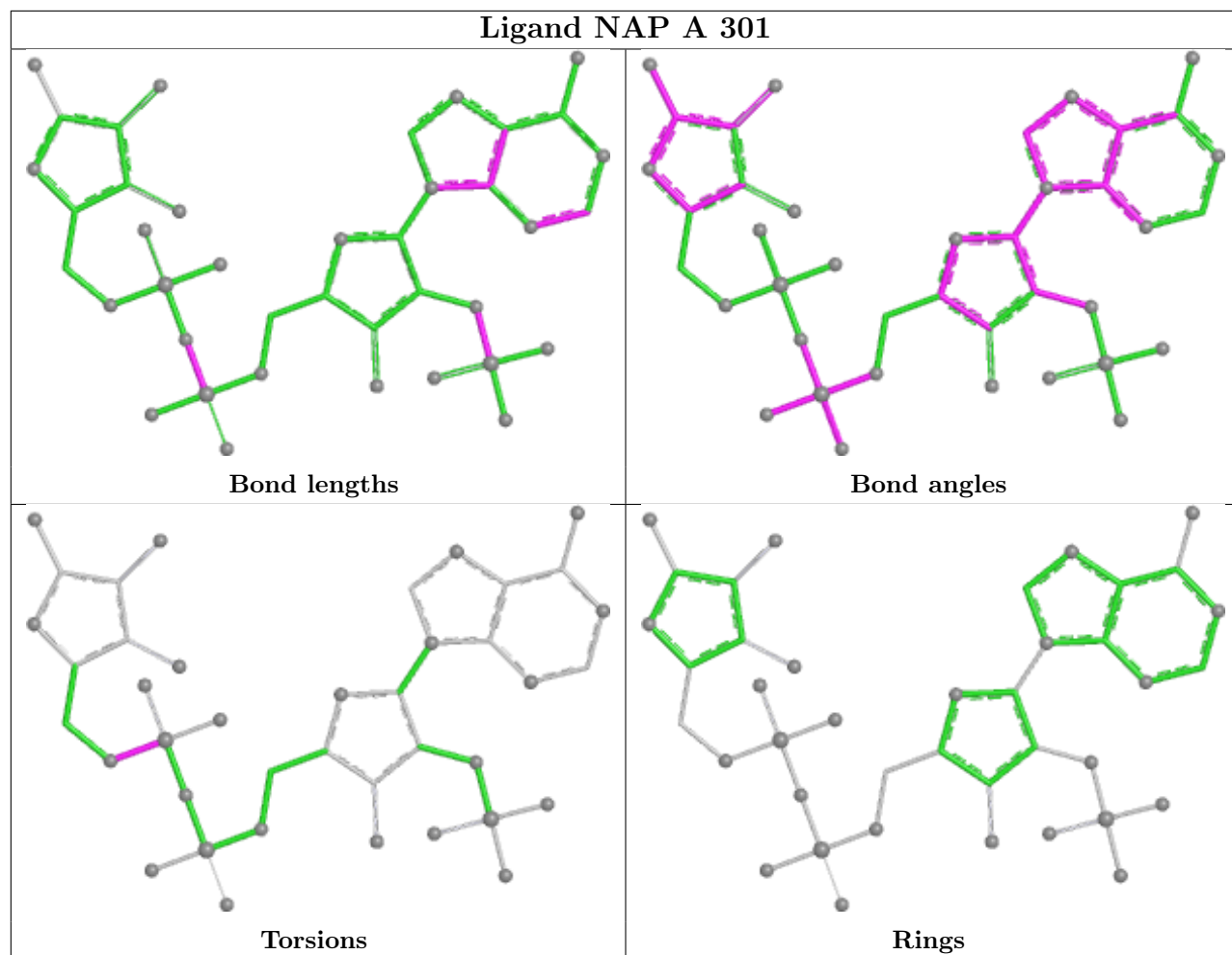
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	302	IPA	3	0
4	D	302	GOL	2	0
4	C	303	GOL	1	0

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 ⓘ

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	240/246 (97%)	-0.55	3 (1%) 75 79	7, 13, 32, 53	5 (2%)
1	B	240/246 (97%)	-0.44	2 (0%) 82 86	8, 16, 35, 52	4 (1%)
1	C	240/246 (97%)	-0.37	9 (3%) 44 46	9, 15, 42, 83	3 (1%)
1	D	240/246 (97%)	-0.45	3 (1%) 75 79	10, 16, 38, 54	0
All	All	960/984 (97%)	-0.45	17 (1%) 67 71	7, 15, 36, 83	12 (1%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	PRO	5.2
1	D	7	PRO	5.2
1	C	201	GLY	4.6
1	C	7	PRO	4.2
1	C	202	ILE	3.9
1	B	7	PRO	3.4
1	C	199	ALA	3.1
1	C	246	ALA	2.9
1	A	246	ALA	2.8
1	C	197	SER	2.6
1	B	246	ALA	2.6
1	C	205	SER	2.4
1	C	208	ASP	2.1
1	A	202	ILE	2.1
1	D	201	GLY	2.1
1	D	202	ILE	2.1
1	C	207	PHE	2.1

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

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](#)

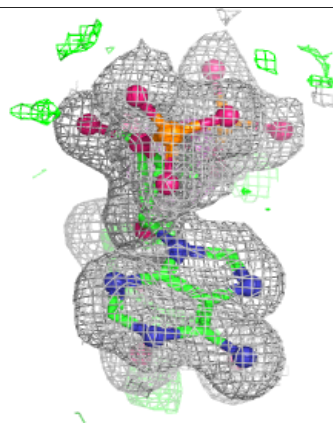
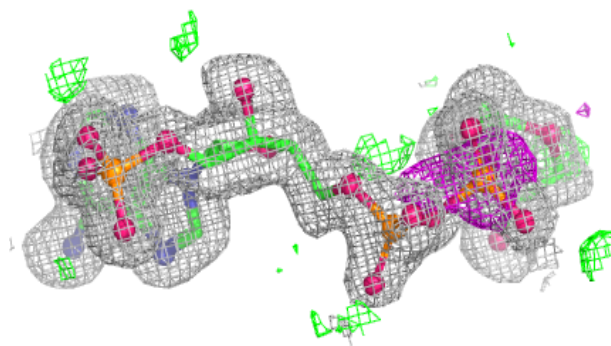
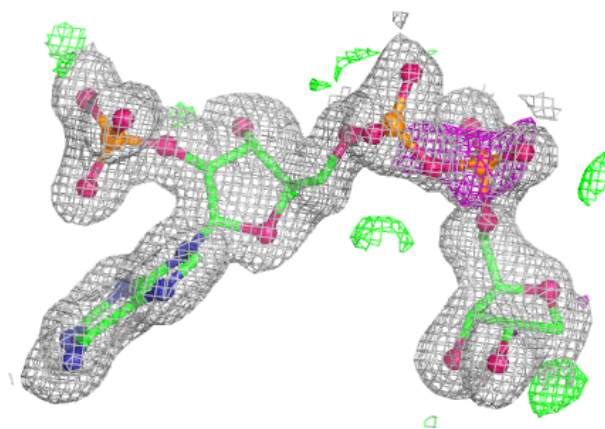
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	GOL	C	303	6/6	0.80	0.14	26,27,34,48	0
3	IPA	C	302	4/4	0.88	0.14	27,29,29,36	0
4	GOL	D	302	6/6	0.91	0.10	27,37,46,51	0
3	IPA	A	302	4/4	0.92	0.19	29,29,31,38	0
2	NAP	C	301	39/48	0.96	0.07	17,24,41,44	0
2	NAP	B	301	39/48	0.98	0.05	16,18,23,25	0
2	NAP	A	301	40/48	0.98	0.04	10,15,20,34	0
2	NAP	D	301	39/48	0.99	0.04	14,19,25,27	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.

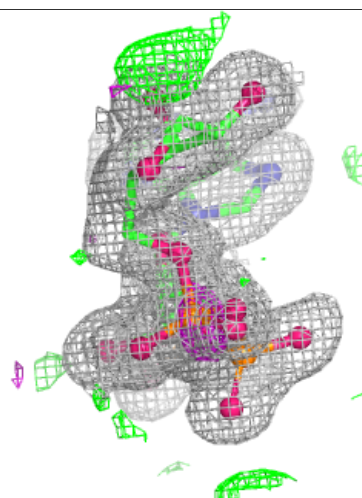
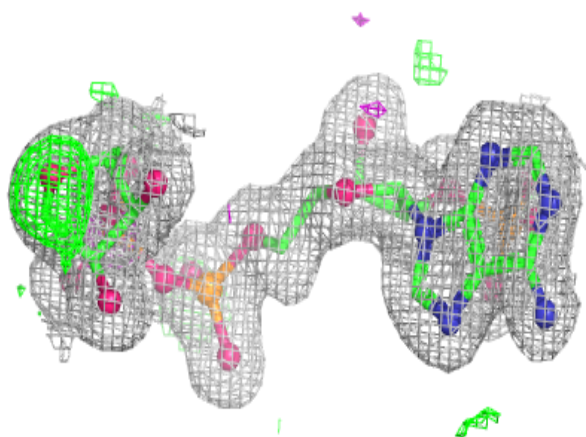
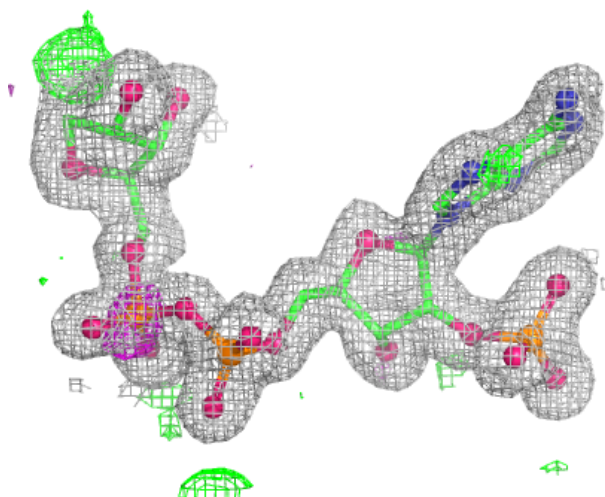
Electron density around NAP C 301:

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



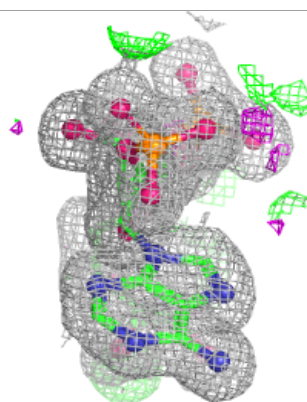
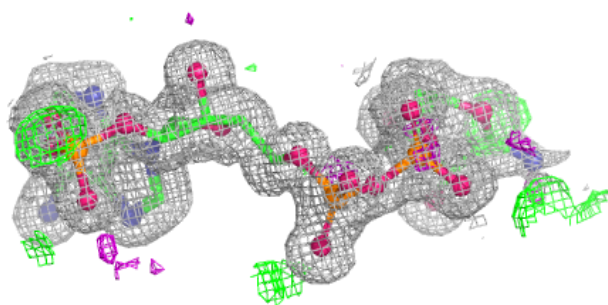
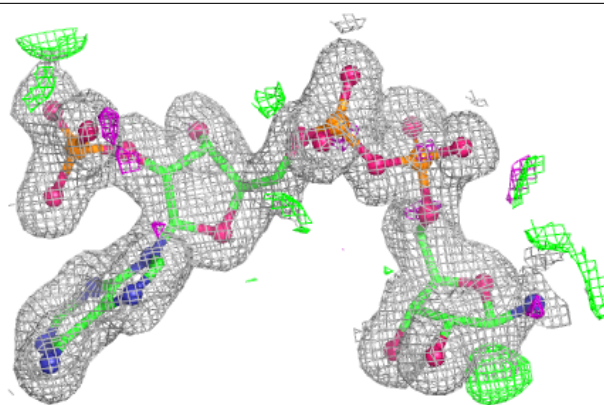
Electron density around NAP B 301:

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

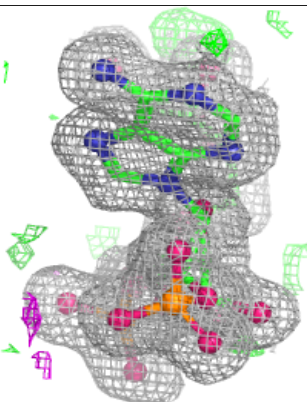
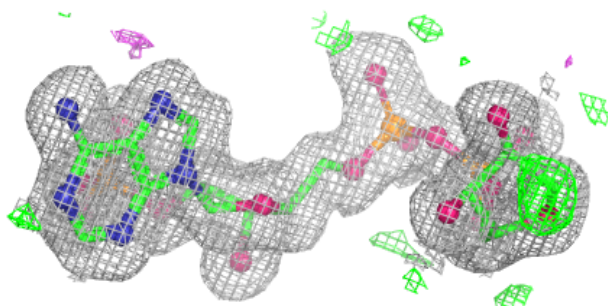
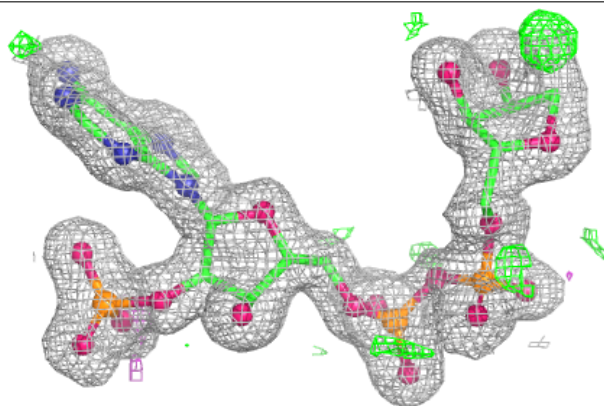


Electron density around NAP A 301:

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

**Electron density around NAP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.