



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:27 PM UTC

PDB ID : 3QWH / pdb_00003qwh
Title : Crystal structure of the 17beta-hydroxysteroid dehydrogenase from *Cochliobolus lunatus* in complex with NADPH and kaempferol
Authors : Cassetta, A.; Lamba, D.; Krastanova, I.; Stojan, J.; Rizner, T.L.; Kristan, K.; Brunskole, M.
Deposited on : 2011-02-28
Resolution : 2.62 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

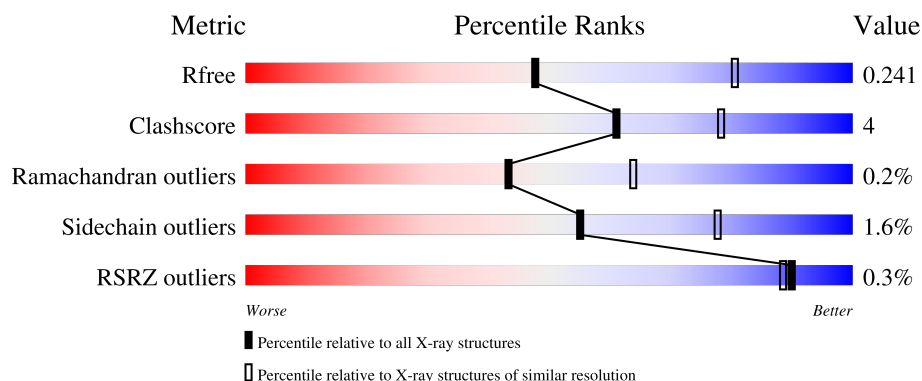
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	270	% 86% 10% .
1	B	270	90% 6% .
1	C	270	85% 10% 5%
1	D	270	86% 10% ..

2 Entry composition ⓘ

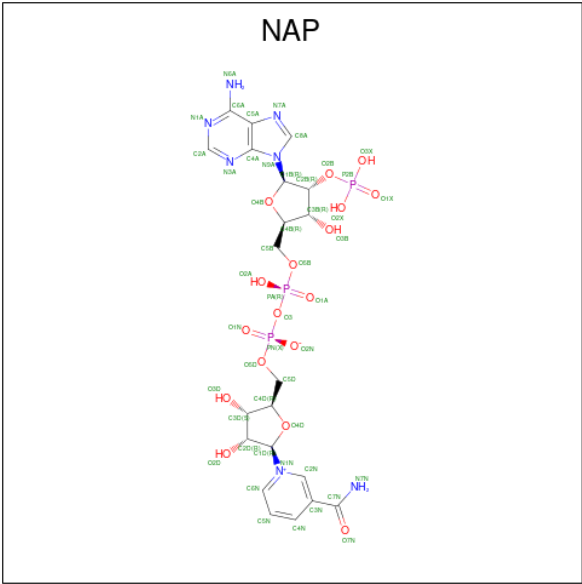
There are 5 unique types of molecules in this entry. The entry contains 8338 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 17beta-hydroxysteroid dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			1964	1236	353	372	3			
1	B	261	Total	C	N	O	S	0	0	0
			1971	1240	354	374	3			
1	C	257	Total	C	N	O	S	0	0	0
			1937	1216	350	368	3			
1	D	261	Total	C	N	O	S	0	0	0
			1971	1240	354	374	3			

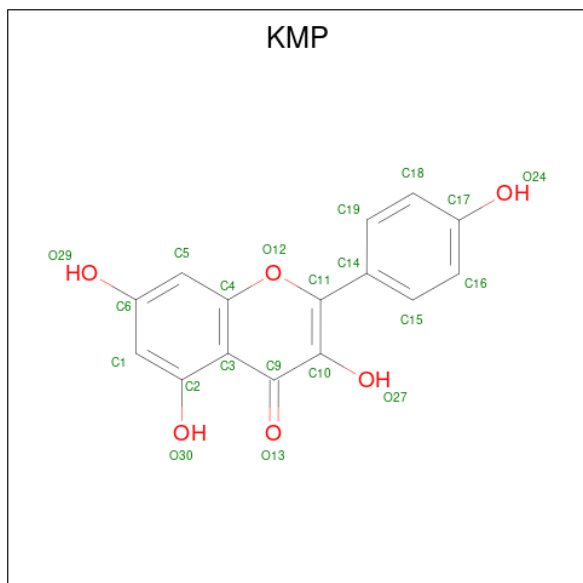
- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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

- Molecule 3 is 3,5,7-TRIHIDROXY-2-(4-HYDROXYPHENYL)-4H-CHROMEN-4-ONE (CCD ID: KMP) (formula: C₁₅H₁₀O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	15	6		
3	B	1	Total	C	O	0	0
			21	15	6		
3	D	1	Total	C	O	0	0
			21	15	6		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			7	4	3		

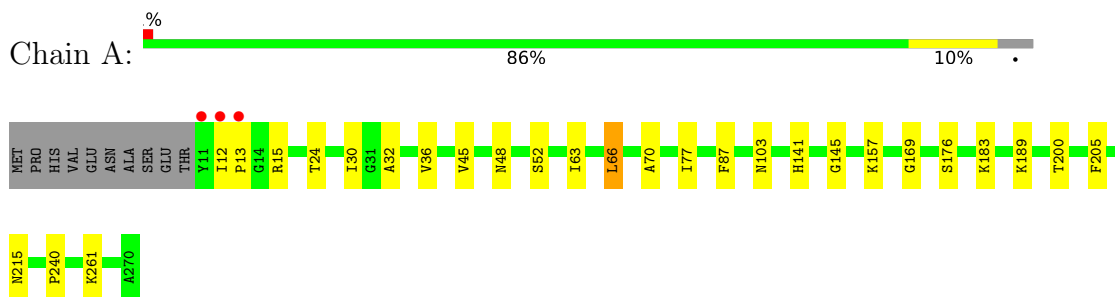
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	53	Total	O	0	0
			53	53		
5	B	70	Total	O	0	0
			70	70		
5	C	58	Total	O	0	0
			58	58		
5	D	52	Total	O	0	0
			52	52		

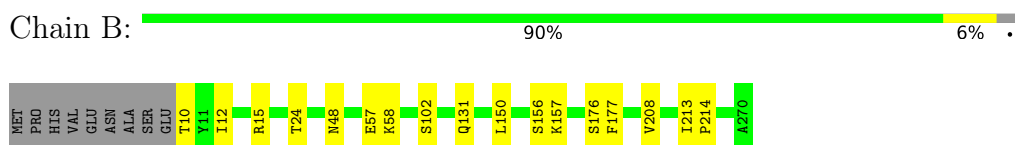
3 Residue-property plots

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.

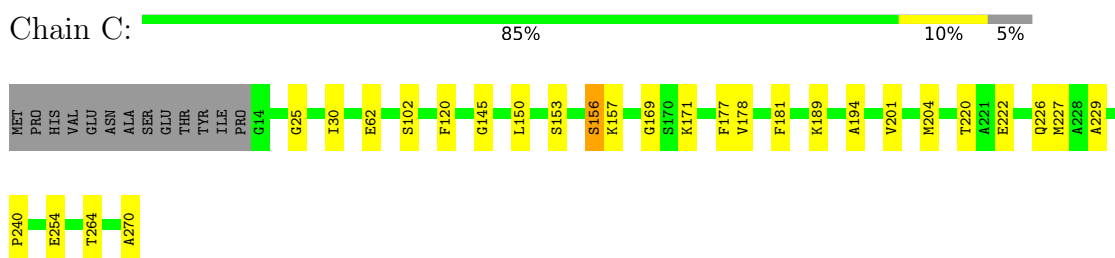
- Molecule 1: 17beta-hydroxysteroid dehydrogenase



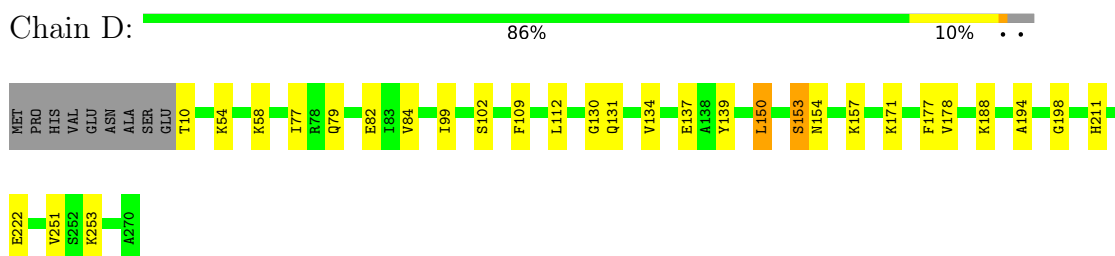
- Molecule 1: 17beta-hydroxysteroid dehydrogenase



- Molecule 1: 17beta-hydroxysteroid dehydrogenase



- Molecule 1: 17beta-hydroxysteroid dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.95Å 116.64Å 70.24Å 90.00° 102.54° 90.00°	Depositor
Resolution (Å)	39.10 – 2.62 39.10 – 2.62	Depositor EDS
% Data completeness (in resolution range)	94.3 (39.10-2.62) 94.3 (39.10-2.62)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.98 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0094	Depositor
R, R_{free}	0.168 , 0.240 (Not available) , 0.241	Depositor DCC
R_{free} test set	1410 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8338	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% 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: KMP, PEG, 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	0.61	0/2003	0.85	0/2710
1	B	0.66	0/2010	0.88	1/2720 (0.0%)
1	C	0.63	0/1974	0.88	0/2669
1	D	0.61	0/2010	0.85	0/2720
All	All	0.63	0/7997	0.86	1/10819 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	208	VAL	N-CA-C	6.51	119.45	113.20

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	1964	0	1945	20	0
1	B	1971	0	1952	15	0
1	C	1937	0	1918	20	0
1	D	1971	0	1952	15	0
2	A	48	0	25	1	0
2	B	48	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	48	0	25	2	0
2	D	48	0	25	1	0
3	A	21	0	7	2	0
3	B	21	0	10	2	0
3	D	21	0	9	2	0
4	B	7	0	10	3	0
5	A	53	0	0	0	0
5	B	70	0	0	0	0
5	C	58	0	0	0	0
5	D	52	0	0	0	0
All	All	8338	0	7903	67	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 4.

All (67) 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)
3:A:272:KMP:O27	3:A:272:KMP:H15	1.77	0.82
1:C:157:LYS:HE3	1:D:157:LYS:HE3	1.65	0.78
3:B:272:KMP:H15	3:B:272:KMP:O27	1.84	0.76
1:B:57:GLU:HA	4:B:273:PEG:H21	1.70	0.72
1:A:157:LYS:HE3	1:B:157:LYS:HE3	1.71	0.72
3:D:272:KMP:H15	3:D:272:KMP:O27	1.89	0.71
1:D:102:SER:HB3	1:D:150:LEU:HD22	1.76	0.67
1:A:145:GLY:HA2	1:A:189:LYS:O	2.03	0.59
1:D:153:SER:HB3	1:D:171:LYS:HG3	1.87	0.57
1:A:261:LYS:HE2	1:C:264:THR:HB	1.85	0.57
1:B:57:GLU:HA	4:B:273:PEG:C2	2.34	0.57
1:C:169:GLY:HA3	1:D:177:PHE:CE1	2.39	0.57
1:B:10:THR:O	1:B:12:ILE:HD12	2.05	0.56
1:A:12:ILE:HB	1:A:15:ARG:HD3	1.87	0.56
1:D:130:GLY:O	1:D:134:VAL:HG23	2.06	0.55
1:C:181:PHE:CE1	1:D:112:LEU:HD13	2.43	0.54
1:B:57:GLU:HG2	4:B:273:PEG:H21	1.89	0.53
1:C:177:PHE:HB3	1:C:181:PHE:CE2	2.44	0.53
1:A:176:SER:OG	1:B:156:SER:O	2.28	0.52
1:B:131:GLN:HB3	1:B:150:LEU:HD13	1.93	0.50
1:D:79:GLN:HB2	1:D:82:GLU:HB2	1.93	0.50
1:A:87:PHE:HB3	1:A:141:HIS:CE1	2.47	0.49
1:C:220:THR:HG22	1:C:222:GLU:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:272:KMP:O27	3:A:272:KMP:C15	2.51	0.48
1:A:183:LYS:NZ	1:C:270:ALA:O	2.43	0.48
1:A:169:GLY:HA2	1:B:176:SER:HB2	1.96	0.48
1:A:200:THR:O	1:A:205:PHE:HB2	2.13	0.48
1:C:150:LEU:O	1:C:194:ALA:HA	2.15	0.47
1:D:139:TYR:CE1	1:D:188:LYS:HD3	2.50	0.47
1:C:25:GLY:HA3	2:C:271:NAP:H1B	1.97	0.47
1:D:178:VAL:HG11	1:D:194:ALA:HB2	1.96	0.47
1:C:30:ILE:HA	1:C:240:PRO:HB3	1.96	0.47
1:C:204:MET:HE1	2:C:271:NAP:H2D	1.96	0.46
1:A:63:ILE:HA	1:A:66:LEU:CD1	2.46	0.46
1:C:227:MET:HE2	1:C:227:MET:HB3	1.85	0.45
1:D:131:GLN:HB3	1:D:150:LEU:HD13	1.99	0.45
1:D:109:PHE:CE1	1:D:211:HIS:HB3	2.51	0.45
1:B:102:SER:CB	1:B:150:LEU:HD22	2.47	0.45
1:C:254:GLU:OE1	1:C:254:GLU:N	2.50	0.45
1:D:99:ILE:HG12	1:D:251:VAL:HB	1.99	0.45
1:D:77:ILE:HG12	2:D:271:NAP:H2A	1.99	0.44
1:A:63:ILE:HA	1:A:66:LEU:HD11	2.00	0.44
1:A:30:ILE:HB	2:A:271:NAP:H51N	1.99	0.44
1:A:32:ALA:O	1:A:36:VAL:HG23	2.18	0.43
3:B:272:KMP:O27	3:B:272:KMP:C15	2.58	0.43
1:C:178:VAL:HG11	1:C:194:ALA:HB2	1.98	0.43
1:D:154:ASN:CG	1:D:198:GLY:HA2	2.43	0.43
1:A:30:ILE:HA	1:A:240:PRO:HB3	2.01	0.43
1:A:169:GLY:HA3	1:B:177:PHE:CE1	2.54	0.43
1:C:153:SER:HB2	1:C:171:LYS:HG3	2.01	0.43
1:A:24:THR:HA	1:A:48:ASN:HB3	2.01	0.43
1:B:24:THR:HA	1:B:48:ASN:HB3	2.01	0.42
1:C:120:PHE:C	1:C:120:PHE:CD1	2.97	0.42
1:C:145:GLY:HA2	1:C:189:LYS:O	2.19	0.42
1:A:77:ILE:HG22	1:A:77:ILE:O	2.20	0.42
1:C:226:GLN:O	1:C:229:ALA:HB3	2.19	0.42
1:B:102:SER:HB3	1:B:150:LEU:HA	2.01	0.41
1:C:102:SER:HB3	1:C:150:LEU:HD22	2.02	0.41
1:A:45:VAL:O	1:A:70:ALA:HA	2.21	0.41
1:B:213:ILE:HA	1:B:214:PRO:HD2	1.93	0.41
1:D:84:VAL:HG22	1:D:137:GLU:CD	2.45	0.41
1:B:102:SER:HB3	1:B:150:LEU:HD22	2.03	0.41
1:C:153:SER:O	1:C:156:SER:HB2	2.21	0.40
1:A:12:ILE:O	1:A:15:ARG:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ILE:HA	1:A:13:PRO:HD3	1.89	0.40
1:B:12:ILE:HB	1:B:15:ARG:HD3	2.03	0.40
3:D:272:KMP:O27	3:D:272:KMP:C15	2.63	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	258/270 (96%)	248 (96%)	9 (4%)	1 (0%)	30	49
1	B	259/270 (96%)	249 (96%)	10 (4%)	0	100	100
1	C	255/270 (94%)	248 (97%)	6 (2%)	1 (0%)	30	49
1	D	259/270 (96%)	249 (96%)	10 (4%)	0	100	100
All	All	1031/1080 (96%)	994 (96%)	35 (3%)	2 (0%)	43	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	SER
1	C	201	VAL

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	207/216 (96%)	204 (99%)	3 (1%)	59	80
1	B	208/216 (96%)	207 (100%)	1 (0%)	81	91
1	C	204/216 (94%)	202 (99%)	2 (1%)	68	85
1	D	208/216 (96%)	201 (97%)	7 (3%)	32	58
All	All	827/864 (96%)	814 (98%)	13 (2%)	55	78

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	LEU
1	A	103	ASN
1	A	215	ASN
1	B	58	LYS
1	C	62	GLU
1	C	156	SER
1	D	10	THR
1	D	54	LYS
1	D	58	LYS
1	D	150	LEU
1	D	153	SER
1	D	222	GLU
1	D	253	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	HIS
1	B	37	HIS
1	B	223	GLN
1	B	226	GLN
1	B	237	ASN
1	B	241	GLN
1	C	103	ASN
1	D	37	HIS

5.3.3 RNA ⓘ

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](#)

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	$\# Z > 2$
2	NAP	B	271	-	50,52,52	1.71	8 (16%)	71,80,80	1.58	12 (16%)
3	KMP	B	272	-	23,23,23	1.69	4 (17%)	34,34,34	1.64	6 (17%)
2	NAP	C	271	-	50,52,52	1.86	9 (18%)	71,80,80	1.56	11 (15%)
3	KMP	D	272	-	23,23,23	1.69	4 (17%)	34,34,34	1.47	5 (14%)
4	PEG	B	273	-	6,6,6	0.59	0	5,5,5	0.20	0
2	NAP	D	271	-	50,52,52	1.66	6 (12%)	71,80,80	1.72	12 (16%)
3	KMP	A	272	-	23,23,23	1.49	4 (17%)	34,34,34	1.62	4 (11%)
2	NAP	A	271	-	50,52,52	1.76	7 (14%)	71,80,80	1.65	13 (18%)

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	271	-	-	1/35/67/67	0/5/5/5
3	KMP	B	272	-	-	0/4/4/4	0/3/3/3
2	NAP	C	271	-	-	5/35/67/67	0/5/5/5
3	KMP	D	272	-	-	0/4/4/4	0/3/3/3
4	PEG	B	273	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	D	271	-	-	3/35/67/67	0/5/5/5
3	KMP	A	272	-	-	0/4/4/4	0/3/3/3
2	NAP	A	271	-	-	3/35/67/67	0/5/5/5

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	271	NAP	O7N-C7N	6.20	1.35	1.24
2	A	271	NAP	C2N-N1N	6.18	1.41	1.35
2	C	271	NAP	C2N-N1N	6.13	1.41	1.35
2	B	271	NAP	O7N-C7N	6.07	1.35	1.24
2	A	271	NAP	O7N-C7N	6.07	1.35	1.24
2	C	271	NAP	O7N-C7N	5.81	1.34	1.24
2	B	271	NAP	C2N-N1N	5.73	1.41	1.35
3	D	272	KMP	C10-C11	5.40	1.41	1.36
2	D	271	NAP	C2N-N1N	5.31	1.40	1.35
3	B	272	KMP	C10-C11	4.84	1.41	1.36
2	A	271	NAP	PN-O3	4.78	1.64	1.59
2	B	271	NAP	O4D-C1D	4.54	1.46	1.40
2	C	271	NAP	PN-O3	4.41	1.64	1.59
3	D	272	KMP	C14-C11	-4.12	1.41	1.47
3	A	272	KMP	C14-C11	-4.11	1.41	1.47
3	B	272	KMP	C14-C11	-4.08	1.41	1.47
3	A	272	KMP	C10-C11	3.99	1.40	1.36
2	C	271	NAP	PA-O3	3.97	1.63	1.59
2	D	271	NAP	O4D-C1D	3.88	1.46	1.40
2	C	271	NAP	C5A-N7A	-3.31	1.33	1.39
2	D	271	NAP	PN-O3	3.12	1.62	1.59
2	B	271	NAP	C5A-N7A	-2.89	1.33	1.39
2	C	271	NAP	C4A-N9A	-2.78	1.31	1.37
3	B	272	KMP	C3-C9	-2.71	1.39	1.46
2	A	271	NAP	C5A-N7A	-2.62	1.34	1.39
2	D	271	NAP	C5A-N7A	-2.56	1.34	1.39
3	D	272	KMP	C3-C9	-2.51	1.40	1.46
2	C	271	NAP	O4D-C1D	2.50	1.44	1.40
2	B	271	NAP	C6N-N1N	2.48	1.41	1.35
3	B	272	KMP	C10-C9	-2.47	1.39	1.46
2	C	271	NAP	C6N-N1N	2.46	1.40	1.35
2	A	271	NAP	C6N-N1N	2.40	1.40	1.35
2	D	271	NAP	C6N-N1N	2.36	1.40	1.35
2	B	271	NAP	C3N-C7N	2.35	1.54	1.50
3	A	272	KMP	C3-C9	-2.31	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	271	NAP	O4D-C1D	2.28	1.43	1.40
2	B	271	NAP	PA-O3	2.21	1.61	1.59
2	A	271	NAP	C3N-C7N	2.17	1.53	1.50
2	B	271	NAP	C4A-N9A	-2.14	1.33	1.37
3	D	272	KMP	C10-C9	-2.13	1.40	1.46
3	A	272	KMP	C10-C9	-2.08	1.40	1.46
2	C	271	NAP	P2B-O2X	2.02	1.62	1.54

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	272	KMP	O12-C11-C14	5.87	119.09	110.87
2	D	271	NAP	C5A-C4A-N3A	-5.53	119.10	126.72
3	B	272	KMP	O12-C11-C14	5.47	118.53	110.87
2	C	271	NAP	C2B-C1B-N9A	-5.02	105.49	113.75
2	A	271	NAP	C5A-C4A-N3A	-4.95	119.90	126.72
3	A	272	KMP	C14-C11-C10	-4.82	120.86	128.44
2	A	271	NAP	C2B-C1B-N9A	-4.79	105.87	113.75
2	B	271	NAP	C5A-C4A-N3A	-4.77	120.14	126.72
2	B	271	NAP	N3A-C2A-N1A	-4.72	121.44	128.58
3	B	272	KMP	C14-C11-C10	-4.69	121.06	128.44
2	D	271	NAP	N3A-C2A-N1A	-4.67	121.51	128.58
3	D	272	KMP	O12-C11-C14	4.65	117.38	110.87
2	C	271	NAP	N3A-C2A-N1A	-4.52	121.74	128.58
2	A	271	NAP	N3A-C2A-N1A	-4.47	121.82	128.58
2	D	271	NAP	C2B-C1B-N9A	-4.44	106.45	113.75
2	C	271	NAP	C5A-C4A-N3A	-4.19	120.94	126.72
2	D	271	NAP	O4B-C1B-N9A	4.02	115.81	108.09
3	D	272	KMP	C14-C11-C10	-3.98	122.19	128.44
2	D	271	NAP	C2A-N3A-C4A	3.92	121.39	111.83
2	C	271	NAP	N9A-C8A-N7A	-3.80	108.55	113.94
2	D	271	NAP	N9A-C8A-N7A	-3.69	108.70	113.94
2	B	271	NAP	N9A-C8A-N7A	-3.66	108.74	113.94
2	D	271	NAP	N3A-C4A-N9A	3.66	133.39	127.17
2	A	271	NAP	N3A-C4A-N9A	3.65	133.38	127.17
2	A	271	NAP	O4B-C1B-N9A	3.62	115.04	108.09
2	B	271	NAP	C2B-C1B-N9A	-3.61	107.81	113.75
2	B	271	NAP	N3A-C4A-N9A	3.61	133.31	127.17
2	B	271	NAP	C2A-N3A-C4A	3.49	120.36	111.83
2	A	271	NAP	C2A-N3A-C4A	3.42	120.18	111.83
2	D	271	NAP	C5A-N7A-C8A	3.36	108.72	103.45
2	C	271	NAP	N3A-C4A-N9A	3.32	132.81	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	271	NAP	C4A-N9A-C8A	3.27	109.17	105.74
2	D	271	NAP	C4A-C5A-N7A	-3.26	106.85	110.58
2	A	271	NAP	N9A-C8A-N7A	-3.12	109.51	113.94
2	B	271	NAP	C4A-N9A-C8A	3.02	108.91	105.74
2	C	271	NAP	C2A-N3A-C4A	2.95	119.04	111.83
2	B	271	NAP	C6N-N1N-C2N	-2.84	119.46	121.88
2	C	271	NAP	C5A-N7A-C8A	2.83	107.90	103.45
3	B	272	KMP	C2-C3-C4	2.81	120.09	117.41
2	B	271	NAP	C5A-N7A-C8A	2.79	107.84	103.45
2	A	271	NAP	C5A-N7A-C8A	2.78	107.82	103.45
2	A	271	NAP	O4B-C1B-C2B	-2.75	101.85	106.59
2	C	271	NAP	C6N-N1N-C2N	-2.69	119.59	121.88
2	A	271	NAP	O4B-C4B-C5B	-2.69	100.72	109.33
3	D	272	KMP	C2-C3-C4	2.67	119.96	117.41
2	A	271	NAP	C4A-C5A-N7A	-2.67	107.53	110.58
3	B	272	KMP	C11-C10-C9	-2.63	119.65	121.52
3	A	272	KMP	O12-C4-C5	2.62	119.55	115.83
3	B	272	KMP	O12-C4-C5	2.60	119.52	115.83
3	D	272	KMP	C11-C10-C9	-2.57	119.68	121.52
2	A	271	NAP	C4A-N9A-C8A	2.55	108.41	105.74
2	D	271	NAP	C5B-C4B-C3B	-2.53	106.09	115.21
3	A	272	KMP	C2-C3-C4	2.52	119.82	117.41
2	D	271	NAP	C4A-N9A-C8A	2.36	108.22	105.74
3	D	272	KMP	O12-C4-C5	2.35	119.16	115.83
2	B	271	NAP	C4A-C5A-N7A	-2.29	107.97	110.58
2	B	271	NAP	O2A-PA-O3	2.19	113.19	107.27
2	A	271	NAP	C6N-N1N-C2N	-2.15	120.05	121.88
2	C	271	NAP	C4A-C5A-N7A	-2.14	108.14	110.58
3	B	272	KMP	C3-C9-C10	2.12	119.88	116.88
2	B	271	NAP	O4B-C1B-C2B	-2.07	103.02	106.59
2	D	271	NAP	C5D-C4D-C3D	-2.05	107.84	115.21
2	C	271	NAP	O4B-C1B-N9A	2.03	111.99	108.09

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	271	NAP	C5D-O5D-PN-O3
2	A	271	NAP	C5D-O5D-PN-O2N
2	D	271	NAP	C3B-C4B-C5B-O5B
2	D	271	NAP	O4B-C4B-C5B-O5B
2	C	271	NAP	PN-O3-PA-O1A

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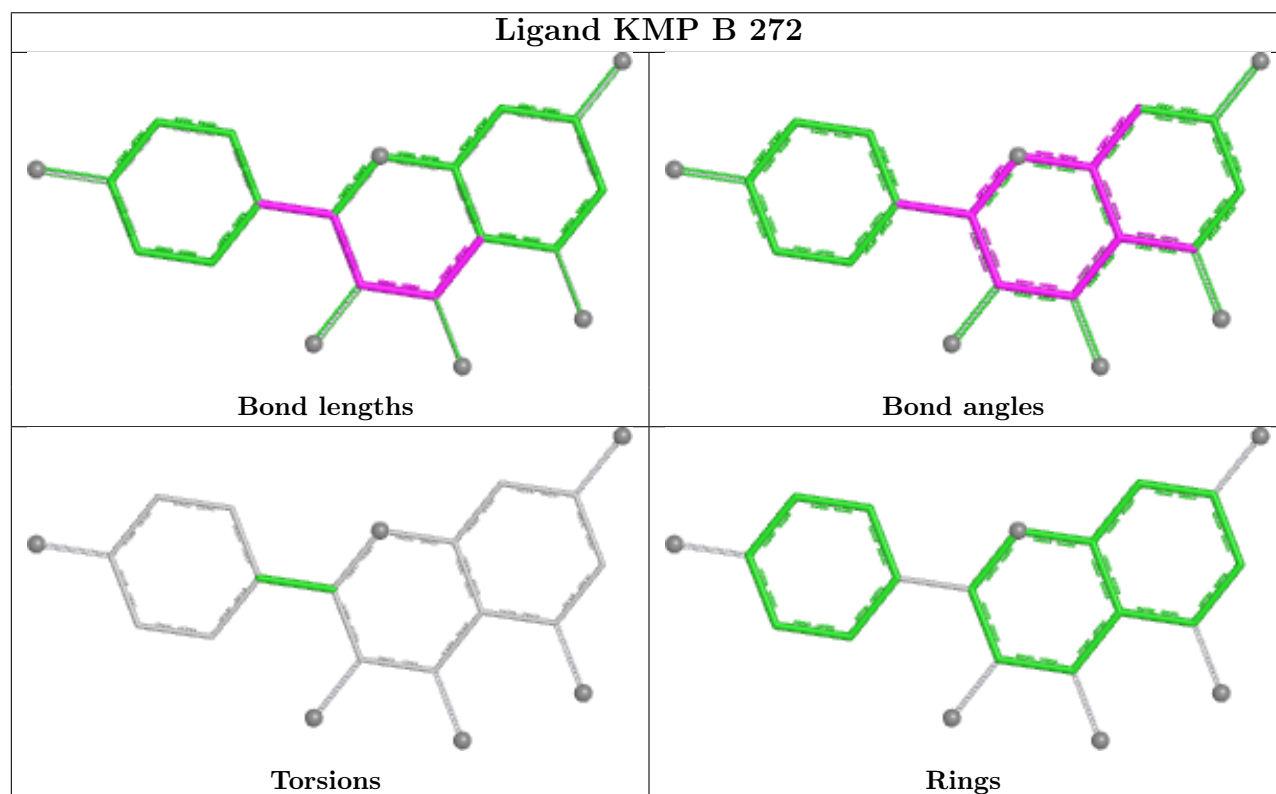
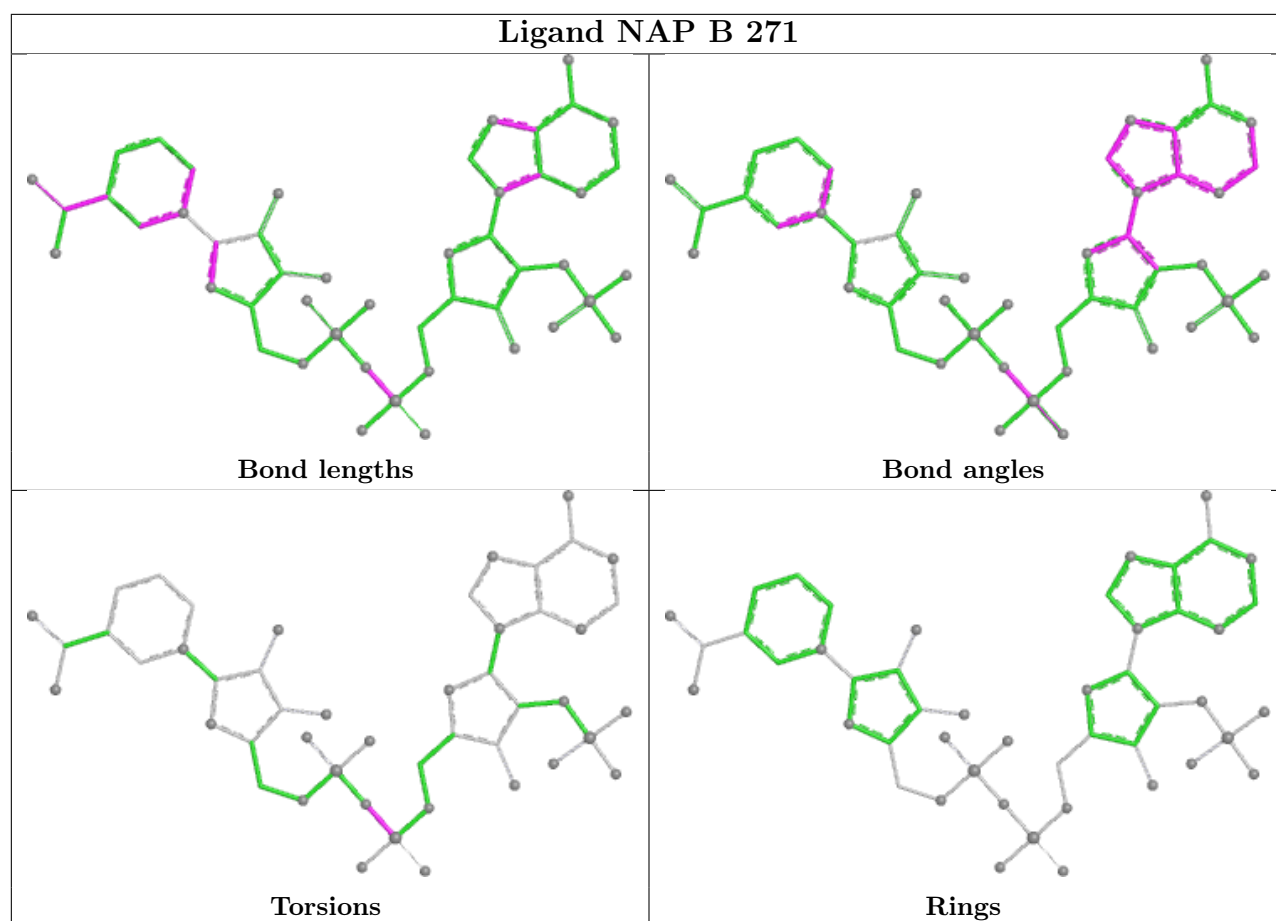
Mol	Chain	Res	Type	Atoms
2	C	271	NAP	O4D-C4D-C5D-O5D
4	B	273	PEG	C1-C2-O2-C3
4	B	273	PEG	O1-C1-C2-O2
2	D	271	NAP	O4D-C4D-C5D-O5D
2	C	271	NAP	PN-O3-PA-O2A
2	C	271	NAP	O4D-C1D-N1N-C2N
2	C	271	NAP	O4D-C1D-N1N-C6N
2	B	271	NAP	PN-O3-PA-O2A
2	A	271	NAP	PA-O3-PN-O2N

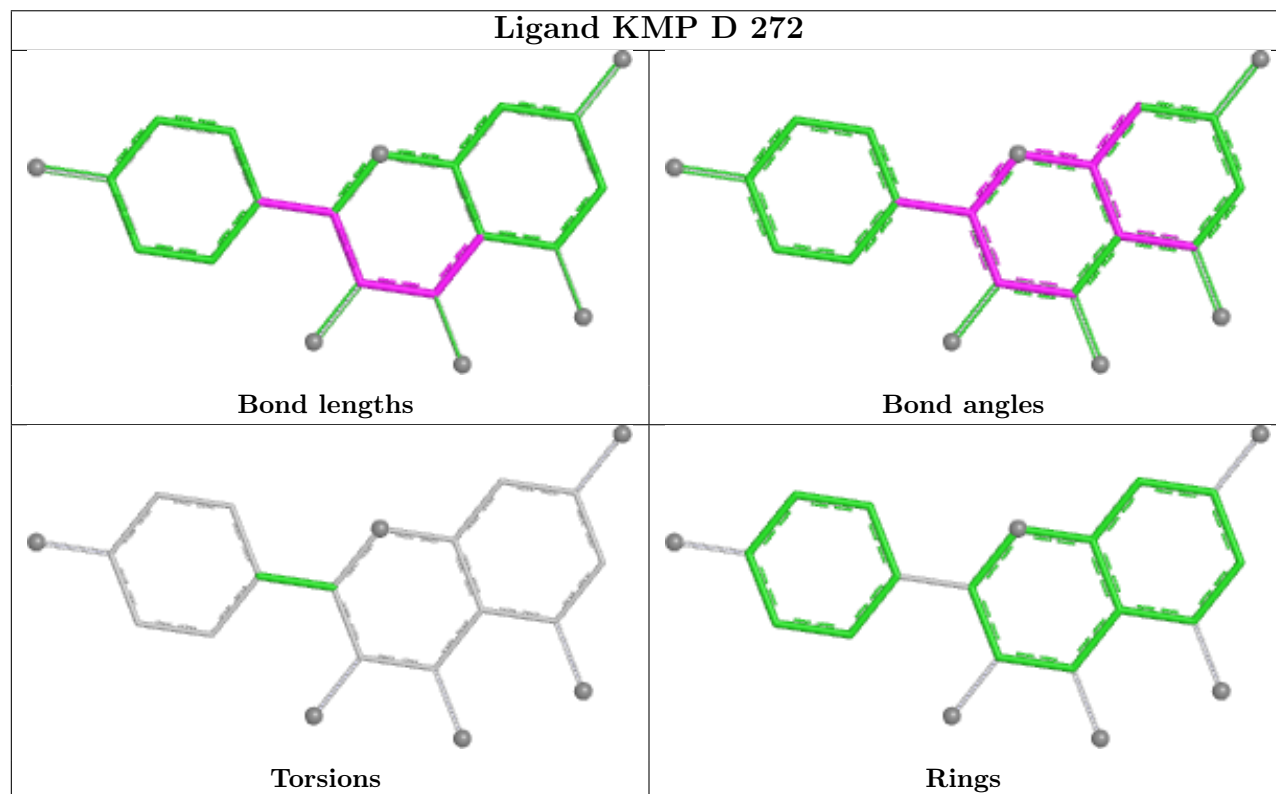
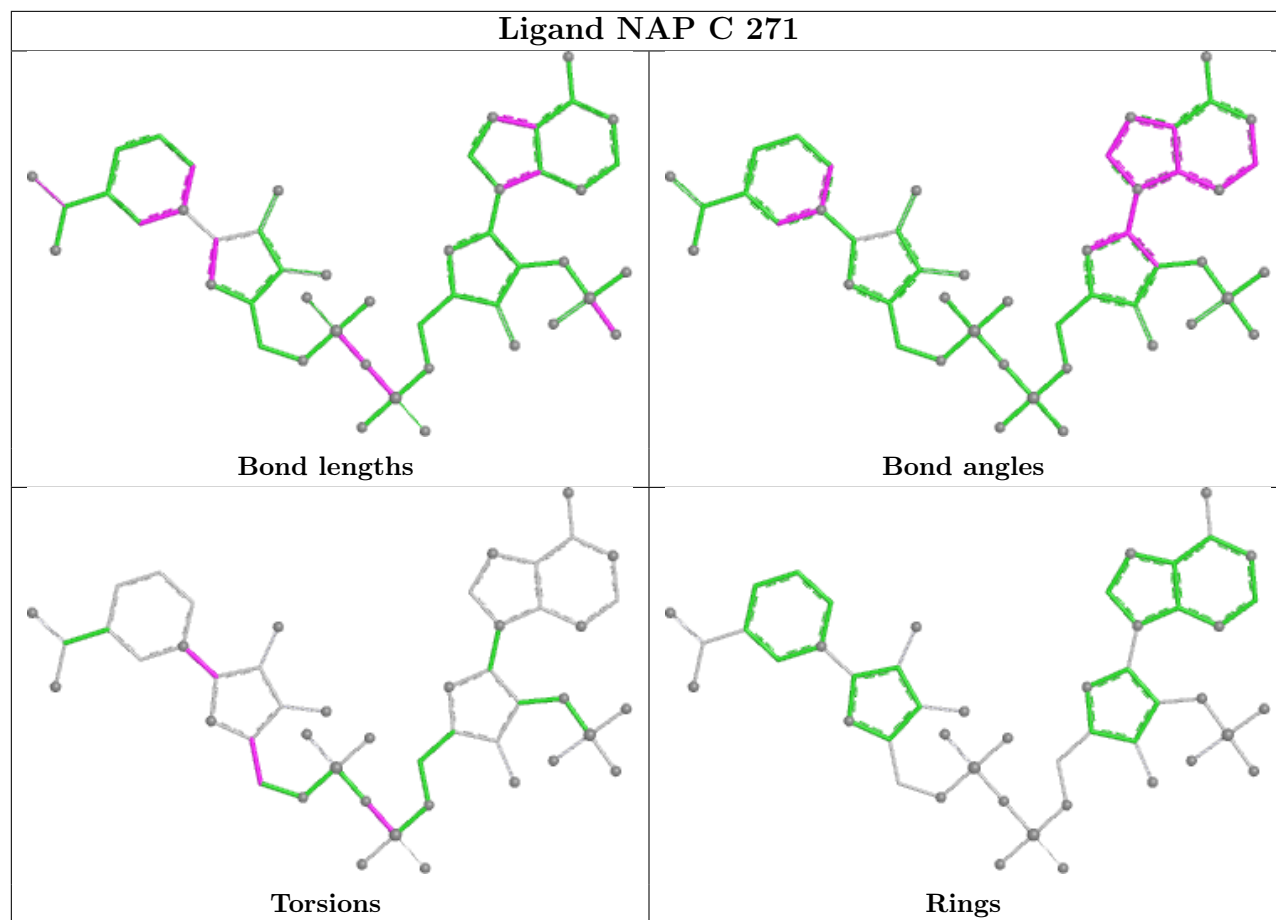
There are no ring outliers.

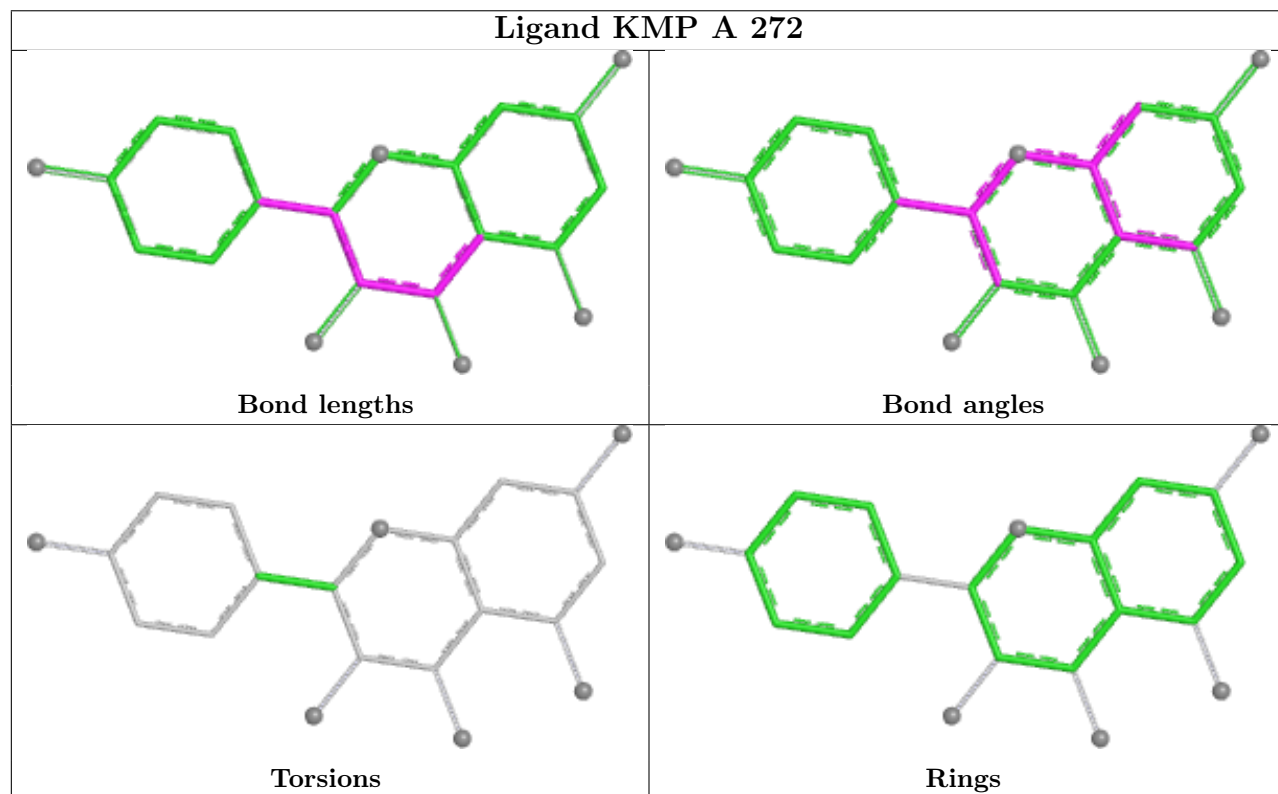
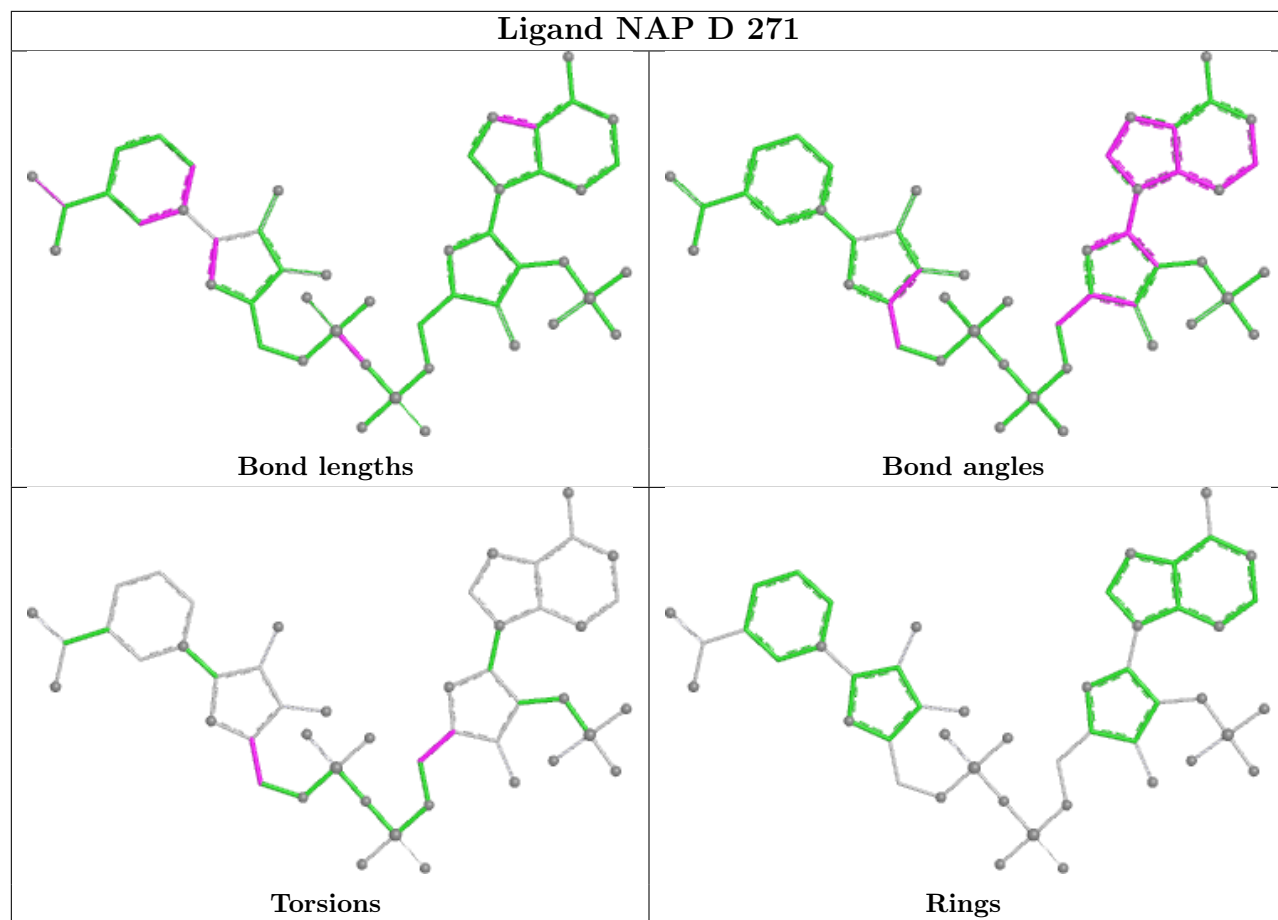
7 monomers are involved in 13 short contacts:

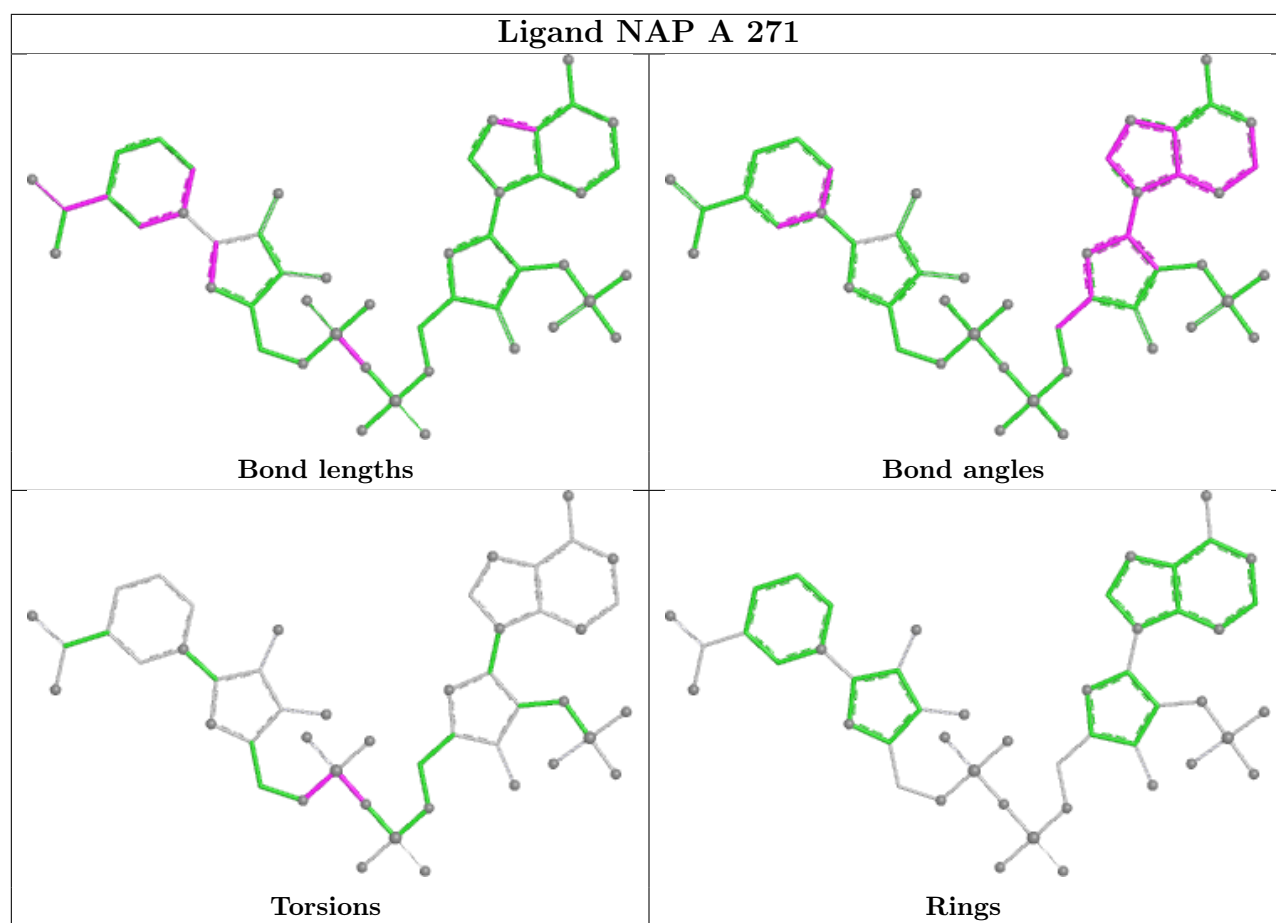
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	272	KMP	2	0
2	C	271	NAP	2	0
3	D	272	KMP	2	0
4	B	273	PEG	3	0
2	D	271	NAP	1	0
3	A	272	KMP	2	0
2	A	271	NAP	1	0

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	260/270 (96%)	-0.33	3 (1%) 76 73	31, 38, 57, 68	0
1	B	261/270 (96%)	-0.33	0 100 100	31, 38, 56, 72	0
1	C	257/270 (95%)	-0.33	0 100 100	29, 38, 55, 66	0
1	D	261/270 (96%)	-0.29	0 100 100	30, 39, 58, 69	0
All	All	1039/1080 (96%)	-0.32	3 (0%) 90 88	29, 38, 57, 72	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	12	ILE	2.5
1	A	11	TYR	2.2
1	A	13	PRO	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](#)

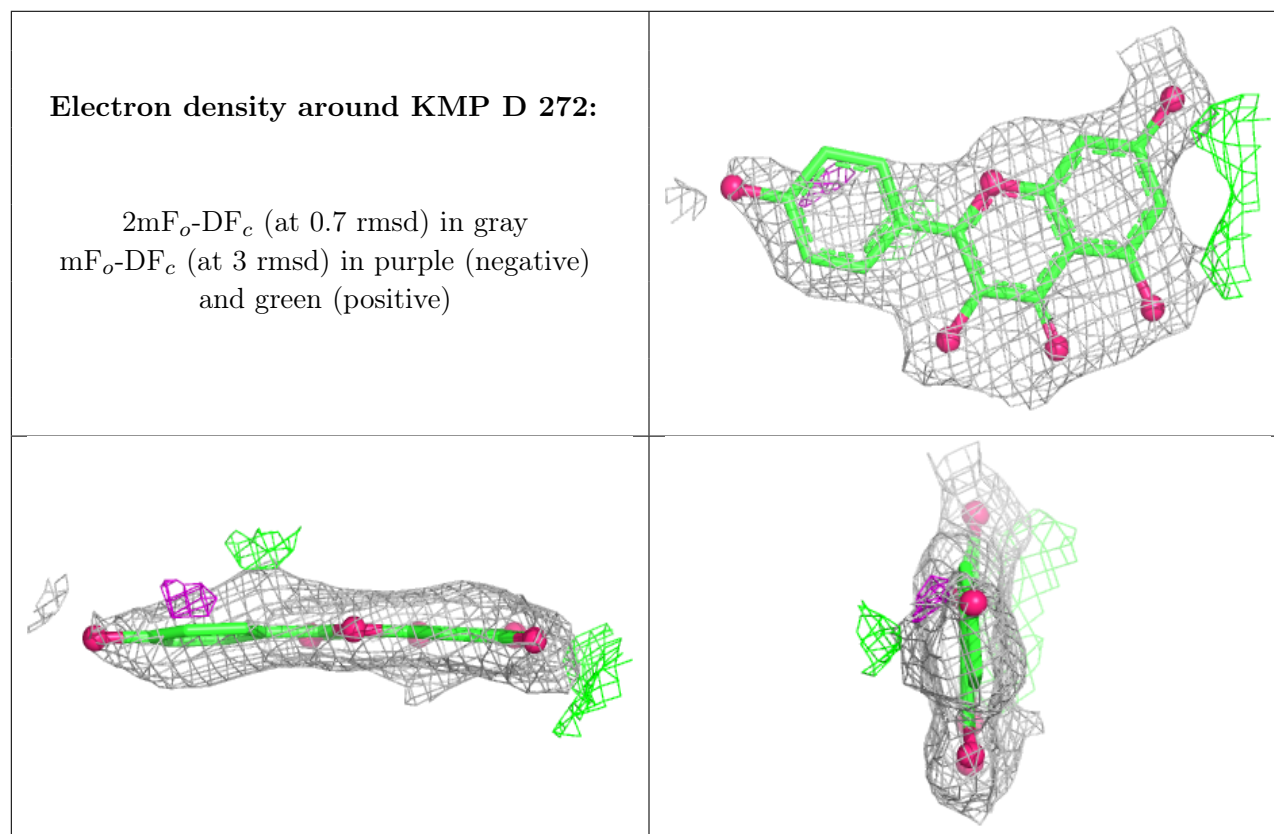
There are no oligosaccharides in this entry.

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.

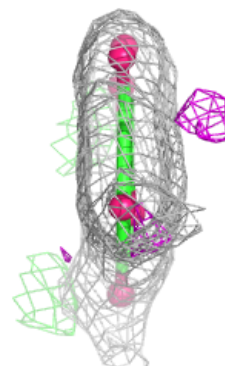
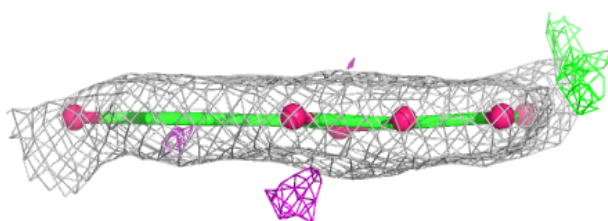
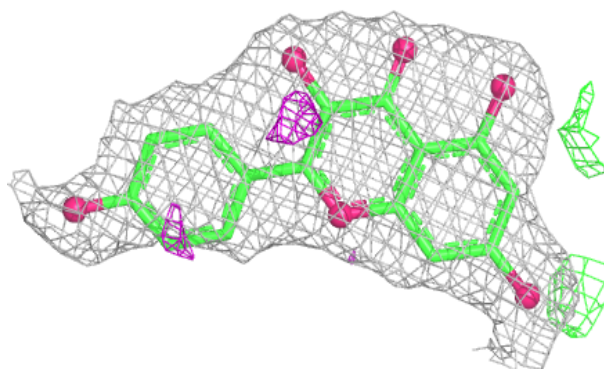
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PEG	B	273	7/7	0.79	0.17	52,55,57,57	0
3	KMP	D	272	21/21	0.84	0.14	45,50,54,54	21
3	KMP	B	272	21/21	0.87	0.12	50,53,60,61	0
3	KMP	A	272	21/21	0.88	0.14	54,58,60,60	21
2	NAP	B	271	48/48	0.97	0.06	26,30,34,35	0
2	NAP	D	271	48/48	0.97	0.06	24,28,32,33	0
2	NAP	A	271	48/48	0.97	0.06	24,29,30,31	0
2	NAP	C	271	48/48	0.98	0.05	21,29,31,31	0

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

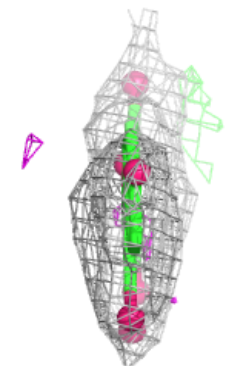
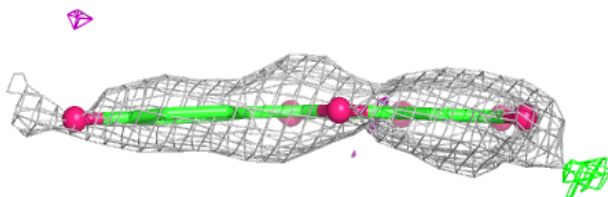
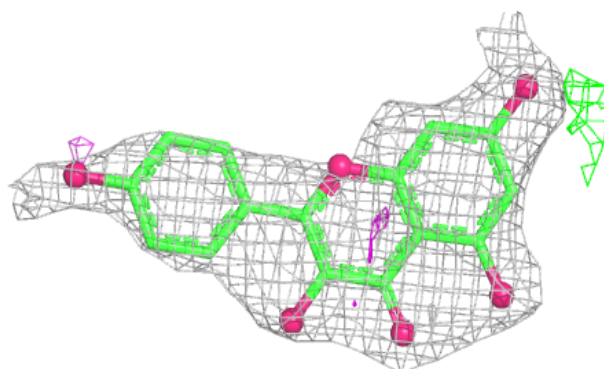


Electron density around KMP B 272:

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

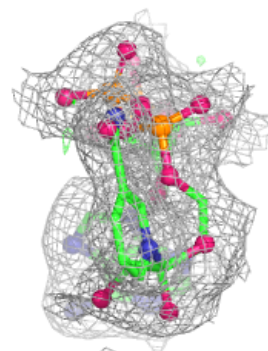
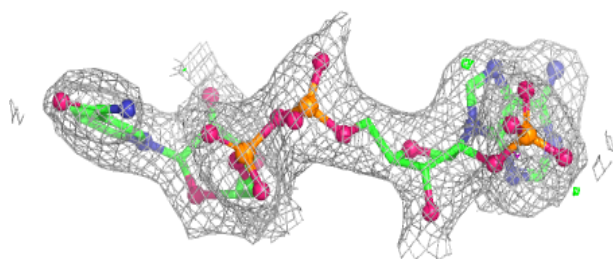
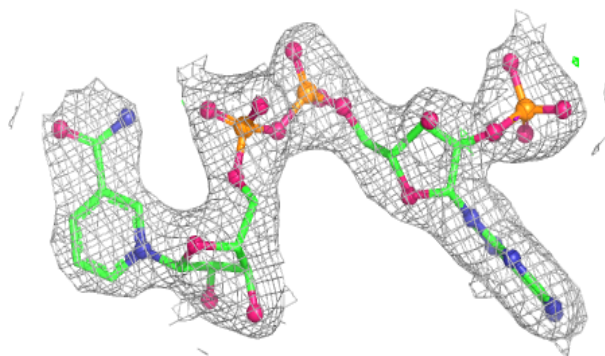
**Electron density around KMP A 272:**

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

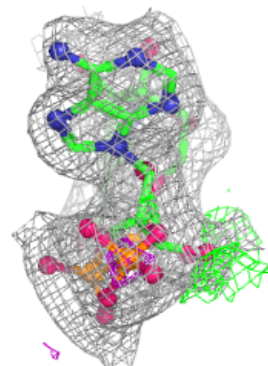
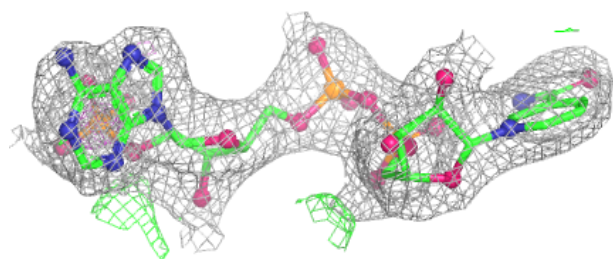
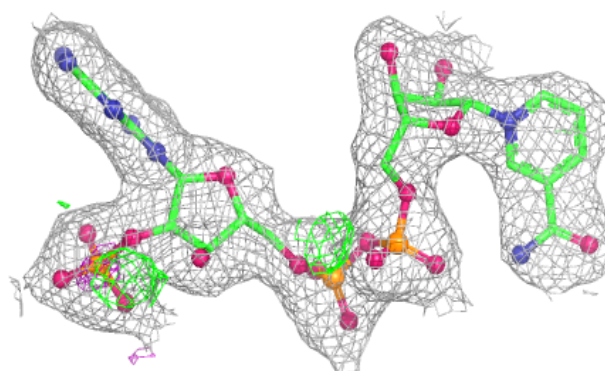


Electron density around NAP B 271:

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

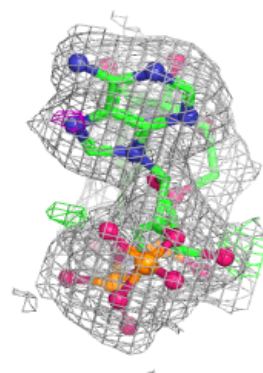
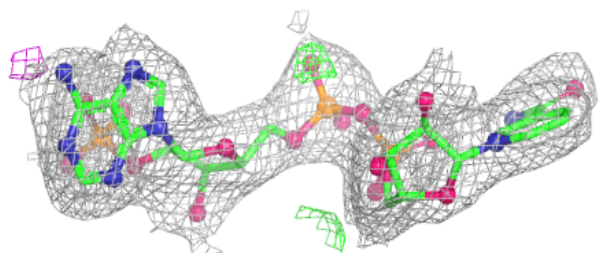
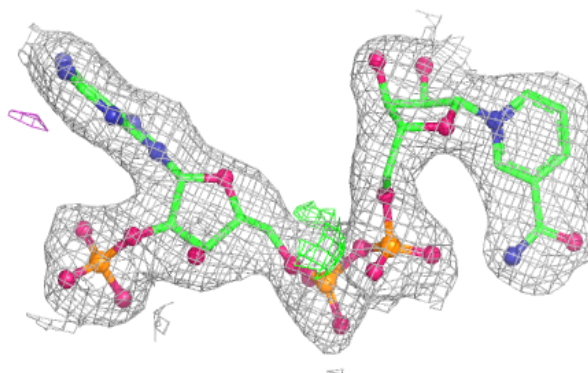
**Electron density around NAP D 271:**

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

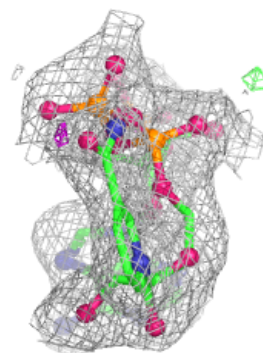
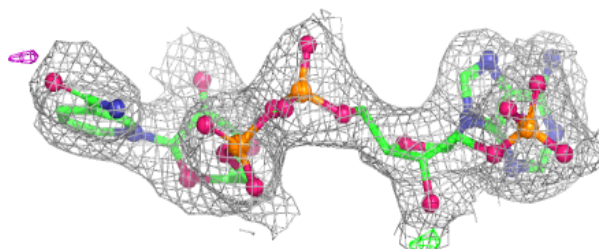
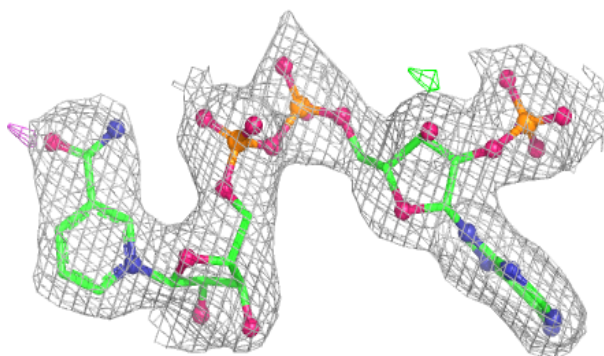


Electron density around NAP A 271:

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

**Electron density around NAP C 271:**

$2mF_o-DF_c$ (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.