



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:28 PM UTC

PDB ID : 7MES / pdb_00007mes
Title : Structure of ALDH4A1 complexed with trans-4-Hydroxy-D-proline
Authors : Bogner, A.N.; Stiers, K.M.; Tanner, J.J.
Deposited on : 2021-04-07
Resolution : 1.37 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

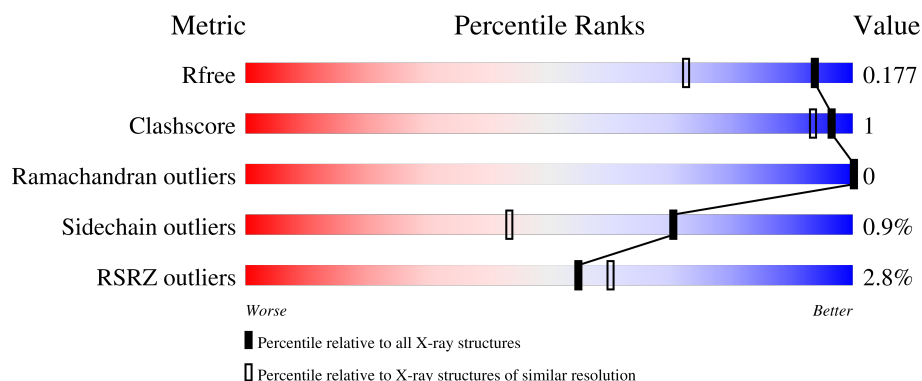
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

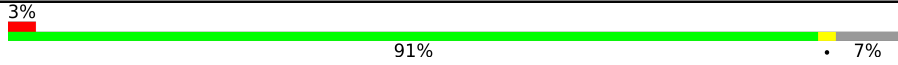
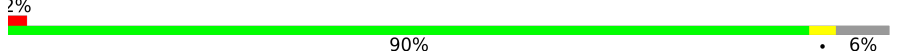
The reported resolution of this entry is 1.37 Å.

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	4403 (1.40-1.36)
Clashscore	190562	4528 (1.40-1.36)
Ramachandran outliers	187476	4459 (1.40-1.36)
Sidechain outliers	187428	4458 (1.40-1.36)
RSRZ outliers	180081	4399 (1.40-1.36)

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	563	
1	B	563	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8836 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 Delta-1-pyrroline-5-carboxylate dehydrogenase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	523	Total	C	N	O	S	0	7	0
			4002	2557	678	750	17			
1	B	527	Total	C	N	O	S	0	4	0
			4039	2576	692	754	17			

There are 48 discrepancies between the modelled and reference sequences:

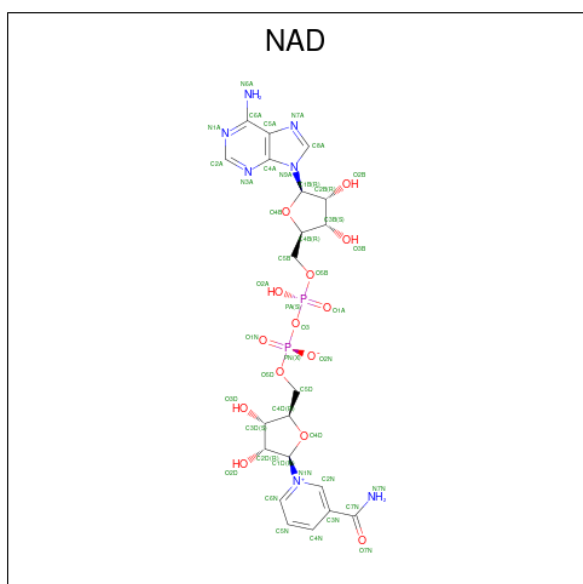
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q8CHT0
A	2	GLY	-	expression tag	UNP Q8CHT0
A	3	SER	-	expression tag	UNP Q8CHT0
A	4	SER	-	expression tag	UNP Q8CHT0
A	5	HIS	-	expression tag	UNP Q8CHT0
A	6	HIS	-	expression tag	UNP Q8CHT0
A	7	HIS	-	expression tag	UNP Q8CHT0
A	8	HIS	-	expression tag	UNP Q8CHT0
A	9	HIS	-	expression tag	UNP Q8CHT0
A	10	HIS	-	expression tag	UNP Q8CHT0
A	11	SER	-	expression tag	UNP Q8CHT0
A	12	SER	-	expression tag	UNP Q8CHT0
A	13	GLY	-	expression tag	UNP Q8CHT0
A	14	LEU	-	expression tag	UNP Q8CHT0
A	15	VAL	-	expression tag	UNP Q8CHT0
A	16	PRO	-	expression tag	UNP Q8CHT0
A	17	ARG	-	expression tag	UNP Q8CHT0
A	18	GLY	-	expression tag	UNP Q8CHT0
A	19	SER	-	expression tag	UNP Q8CHT0
A	20	HIS	-	expression tag	UNP Q8CHT0
A	21	MET	-	expression tag	UNP Q8CHT0
A	33	ALA	THR	conflict	UNP Q8CHT0
A	61	THR	MET	conflict	UNP Q8CHT0
A	468	LYS	GLN	conflict	UNP Q8CHT0
B	1	MET	-	expression tag	UNP Q8CHT0

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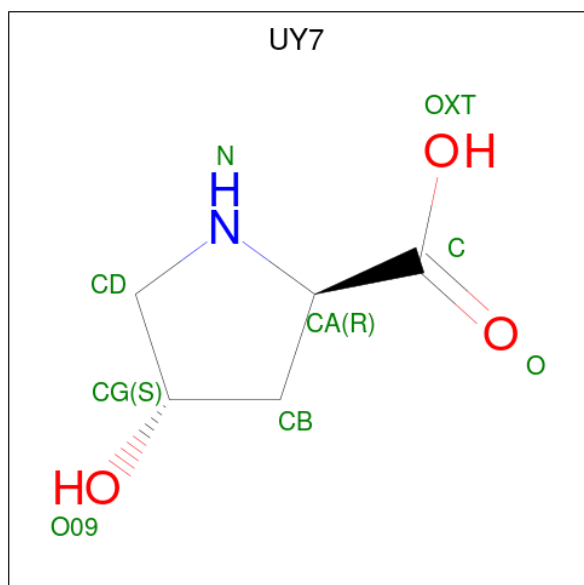
Chain	Residue	Modelled	Actual	Comment	Reference
B	2	GLY	-	expression tag	UNP Q8CHT0
B	3	SER	-	expression tag	UNP Q8CHT0
B	4	SER	-	expression tag	UNP Q8CHT0
B	5	HIS	-	expression tag	UNP Q8CHT0
B	6	HIS	-	expression tag	UNP Q8CHT0
B	7	HIS	-	expression tag	UNP Q8CHT0
B	8	HIS	-	expression tag	UNP Q8CHT0
B	9	HIS	-	expression tag	UNP Q8CHT0
B	10	HIS	-	expression tag	UNP Q8CHT0
B	11	SER	-	expression tag	UNP Q8CHT0
B	12	SER	-	expression tag	UNP Q8CHT0
B	13	GLY	-	expression tag	UNP Q8CHT0
B	14	LEU	-	expression tag	UNP Q8CHT0
B	15	VAL	-	expression tag	UNP Q8CHT0
B	16	PRO	-	expression tag	UNP Q8CHT0
B	17	ARG	-	expression tag	UNP Q8CHT0
B	18	GLY	-	expression tag	UNP Q8CHT0
B	19	SER	-	expression tag	UNP Q8CHT0
B	20	HIS	-	expression tag	UNP Q8CHT0
B	21	MET	-	expression tag	UNP Q8CHT0
B	33	ALA	THR	conflict	UNP Q8CHT0
B	61	THR	MET	conflict	UNP Q8CHT0
B	468	LYS	GLN	conflict	UNP Q8CHT0

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



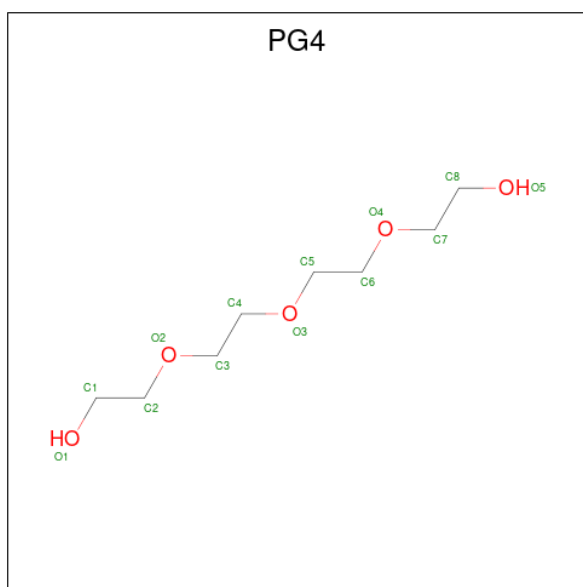
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is (4S)-4-hydroxy-D-proline (CCD ID: UY7) (formula: C₅H₉NO₃) (labeled as "Ligand of Interest" by depositor).



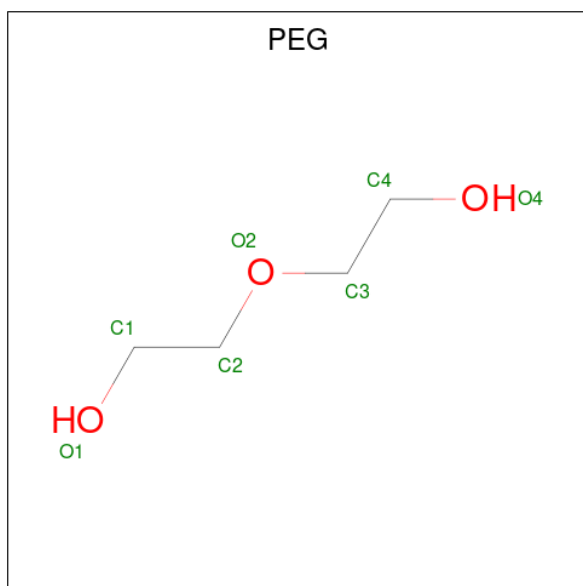
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	5	1	3		
3	A	1	Total	C	N	O	0	0
			9	5	1	3		
3	B	1	Total	C	N	O	0	0
			9	5	1	3		
3	B	1	Total	C	N	O	0	0
			9	5	1	3		

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



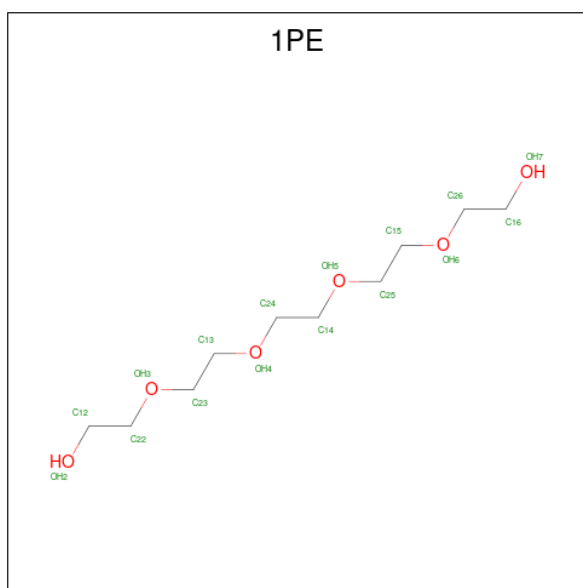
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



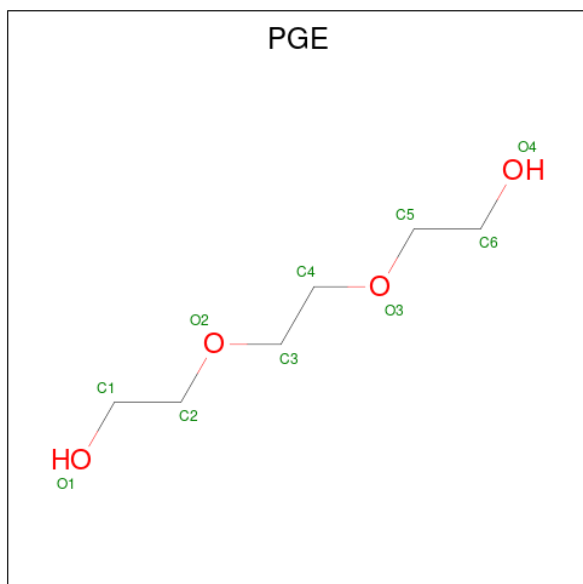
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			16	10	6		
6	B	1	Total	C	O	0	0
			16	10	6		

- Molecule 7 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			10	6	4		

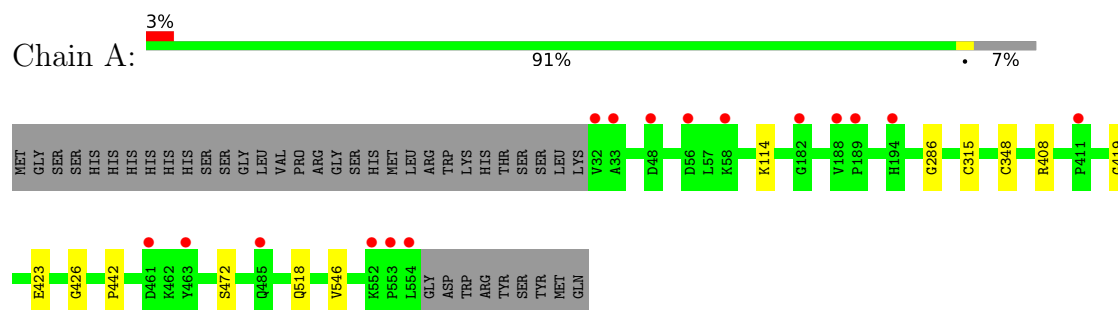
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	316	Total 316	O 316	0	0
8	B	321	Total 321	O 321	0	0

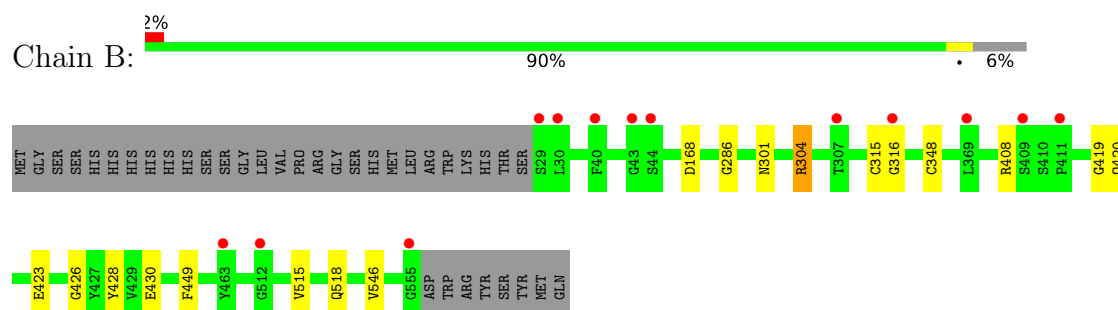
3 Residue-property plots [i](#)

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

- Molecule 1: Delta-1-pyrroline-5-carboxylate dehydrogenase, mitochondrial



- Molecule 1: Delta-1-pyrroline-5-carboxylate dehydrogenase, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.74Å 94.11Å 131.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.55 – 1.37 76.55 – 1.37	Depositor EDS
% Data completeness (in resolution range)	99.3 (76.55-1.37) 99.9 (76.55-1.37)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 1.37Å)	Xtriage
Refinement program	PHENIX 1.19.1	Depositor
R, R_{free}	0.161 , 0.172 (Not available) , 0.177	Depositor DCC
R_{free} test set	10979 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	16.2	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 35.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8836	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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: NAD, PEG, 1PE, UY7, PGE, PG4

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	0.23	0/4122	0.48	0/5606
1	B	0.22	0/4150	0.47	0/5640
All	All	0.23	0/8272	0.47	0/11246

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4002	0	3918	8	0
1	B	4039	0	3969	10	0
2	A	23	0	12	0	0
2	B	23	0	12	0	0
3	A	18	0	0	0	0
3	B	18	0	0	0	0
4	A	13	0	18	1	0
5	A	14	0	20	1	0
5	B	7	0	10	1	0
6	A	16	0	22	0	0
6	B	16	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	10	0	14	0	0
8	A	316	0	0	1	0
8	B	321	0	0	0	0
All	All	8836	0	8017	16	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 1.

All (16) 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:408:ARG:NH2	1:A:419:GLY:O	2.26	0.67
1:A:472:SER:HA	5:A:605:PEG:H21	1.85	0.58
1:B:408:ARG:NH2	1:B:419:GLY:O	2.40	0.53
1:B:423:GLU:HA	1:B:426:GLY:O	2.08	0.53
1:B:301:ASN:O	1:B:304:ARG:HG2	2.09	0.52
1:A:423:GLU:HA	1:A:426:GLY:O	2.11	0.50
1:A:546:VAL:HG11	1:B:518:GLN:HA	1.96	0.47
1:B:286:GLY:O	1:B:315:CYS:HA	2.15	0.47
1:A:114:LYS:NZ	8:A:703:HOH:O	2.46	0.46
1:B:428:TYR:HB3	5:B:605:PEG:H22	1.97	0.46
1:A:518:GLN:HA	1:B:546:VAL:HG11	1.99	0.45
1:A:286:GLY:O	1:A:315:CYS:HA	2.16	0.45
1:A:442:PRO:HG3	4:A:604:PG4:H11	2.00	0.44
1:B:316:GLY:HA2	1:B:348[B]:CYS:HB3	1.99	0.44
1:B:420:GLN:HB2	1:B:430:GLU:CD	2.45	0.41
1:B:168:ASP:HB3	1:B:515:VAL:HB	2.02	0.41

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	528/563 (94%)	518 (98%)	10 (2%)	0	100	100
1	B	387/563 (69%)	380 (98%)	7 (2%)	0	100	100
All	All	915/1126 (81%)	898 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	41/461 (9%)	39 (95%)	2 (5%)	22	2
1	B	281/461 (61%)	279 (99%)	2 (1%)	76	52
All	All	322/922 (35%)	318 (99%)	4 (1%)	70	33

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	348[A]	CYS
1	A	348[B]	CYS
1	B	304	ARG
1	B	449	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	297	GLN
1	B	363	GLN

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](#)

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	$\# Z > 2$
5	PEG	A	605	-	6,6,6	0.12	0	5,5,5	0.11	0
7	PGE	B	604	-	9,9,9	0.29	0	8,8,8	0.33	0
3	UY7	A	602	-	9,9,9	1.33	2 (22%)	10,12,12	1.61	2 (20%)
3	UY7	B	603	-	9,9,9	1.05	1 (11%)	10,12,12	1.55	2 (20%)
3	UY7	A	603	-	9,9,9	0.81	0	10,12,12	1.16	0
4	PG4	A	604	-	12,12,12	0.14	0	11,11,11	0.61	0
5	PEG	B	605	-	6,6,6	0.09	0	5,5,5	0.10	0
2	NAD	A	601	-	25,25,48	1.37	3 (12%)	37,38,73	1.50	7 (18%)
5	PEG	A	606	-	6,6,6	0.14	0	5,5,5	0.05	0
6	1PE	B	606	-	15,15,15	0.13	0	14,14,14	0.15	0
3	UY7	B	602	-	9,9,9	1.46	2 (22%)	10,12,12	1.67	3 (30%)
6	1PE	A	607	-	15,15,15	0.12	0	14,14,14	0.16	0
2	NAD	B	601	-	25,25,48	1.25	2 (8%)	37,38,73	1.49	6 (16%)

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
5	PEG	A	605	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PGE	B	604	-	-	1/7/7/7	-
3	UY7	A	602	-	-	2/4/13/13	0/1/1/1
3	UY7	B	603	-	-	0/4/13/13	0/1/1/1
3	UY7	A	603	-	-	0/4/13/13	0/1/1/1
4	PG4	A	604	-	-	1/10/10/10	-
5	PEG	B	605	-	-	1/4/4/4	-
2	NAD	A	601	-	-	2/10/26/62	0/3/3/5
5	PEG	A	606	-	-	1/4/4/4	-
6	1PE	B	606	-	-	1/13/13/13	-
3	UY7	B	602	-	-	0/4/13/13	0/1/1/1
6	1PE	A	607	-	-	0/13/13/13	-
2	NAD	B	601	-	-	1/10/26/62	0/3/3/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	NAD	PA-O5B	3.87	1.72	1.60
2	B	601	NAD	PA-O5B	3.41	1.71	1.60
3	B	602	UY7	CA-C	3.02	1.60	1.52
3	A	602	UY7	CA-C	2.93	1.60	1.52
2	A	601	NAD	C8A-N9A	2.20	1.41	1.37
2	B	601	NAD	C3B-C4B	2.10	1.58	1.53
3	B	603	UY7	OXT-C	-2.08	1.24	1.30
2	A	601	NAD	C5A-C4A	2.03	1.42	1.39
3	B	602	UY7	OXT-C	-2.02	1.24	1.30
3	A	602	UY7	OXT-C	-2.00	1.24	1.30

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	NAD	O2A-PA-O1A	4.80	129.53	110.83
2	A	601	NAD	O2A-PA-O1A	4.55	128.56	110.83
2	B	601	NAD	O2A-PA-O5B	-3.55	97.40	106.67
2	A	601	NAD	O3-PA-O1A	-3.41	97.57	110.83
2	A	601	NAD	O5B-PA-O1A	-2.96	98.45	106.44
2	B	601	NAD	O3-PA-O2A	-2.91	96.90	107.80
3	B	602	UY7	O-C-CA	-2.84	113.11	122.26
3	B	603	UY7	O-C-CA	-2.81	113.21	122.26
2	A	601	NAD	C4A-N9A-C1B	-2.66	120.41	126.63
3	A	602	UY7	O-C-CA	-2.62	113.81	122.26
2	A	601	NAD	O3-PA-O2A	2.58	117.49	107.80
3	B	602	UY7	O09-CG-CD	-2.54	105.11	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	NAD	C4A-N9A-C1B	-2.43	120.94	126.63
3	A	602	UY7	O09-CG-CD	-2.43	105.34	110.30
2	A	601	NAD	C1B-N9A-C8A	2.40	132.42	127.09
2	B	601	NAD	C1B-N9A-C8A	2.15	131.86	127.09
3	B	602	UY7	OXT-C-CA	2.12	120.69	113.51
2	B	601	NAD	O3-PA-O1A	2.09	118.97	110.83
3	B	603	UY7	CB-CG-CD	2.02	105.41	103.16
2	A	601	NAD	O3B-C3B-C4B	-2.00	105.33	111.08

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	NAD	C5B-O5B-PA-O1A
7	B	604	PGE	O3-C5-C6-O4
4	A	604	PG4	C1-C2-O2-C3
2	A	601	NAD	C2B-C1B-N9A-C8A
5	A	605	PEG	C4-C3-O2-C2
5	A	606	PEG	C1-C2-O2-C3
5	B	605	PEG	C4-C3-O2-C2
3	A	602	UY7	OXT-C-CA-CB
2	B	601	NAD	C2B-C1B-N9A-C8A
3	A	602	UY7	O-C-CA-CB
6	B	606	1PE	C12-C22-OH3-C23

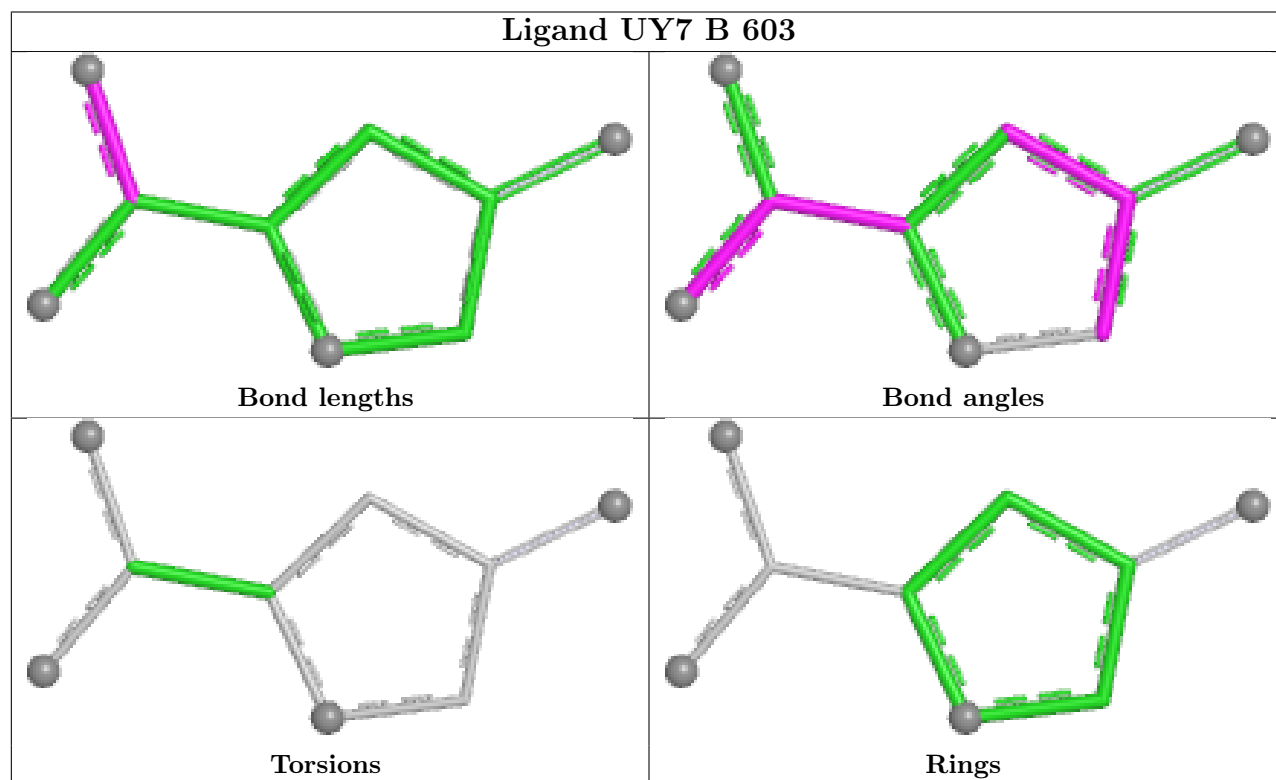
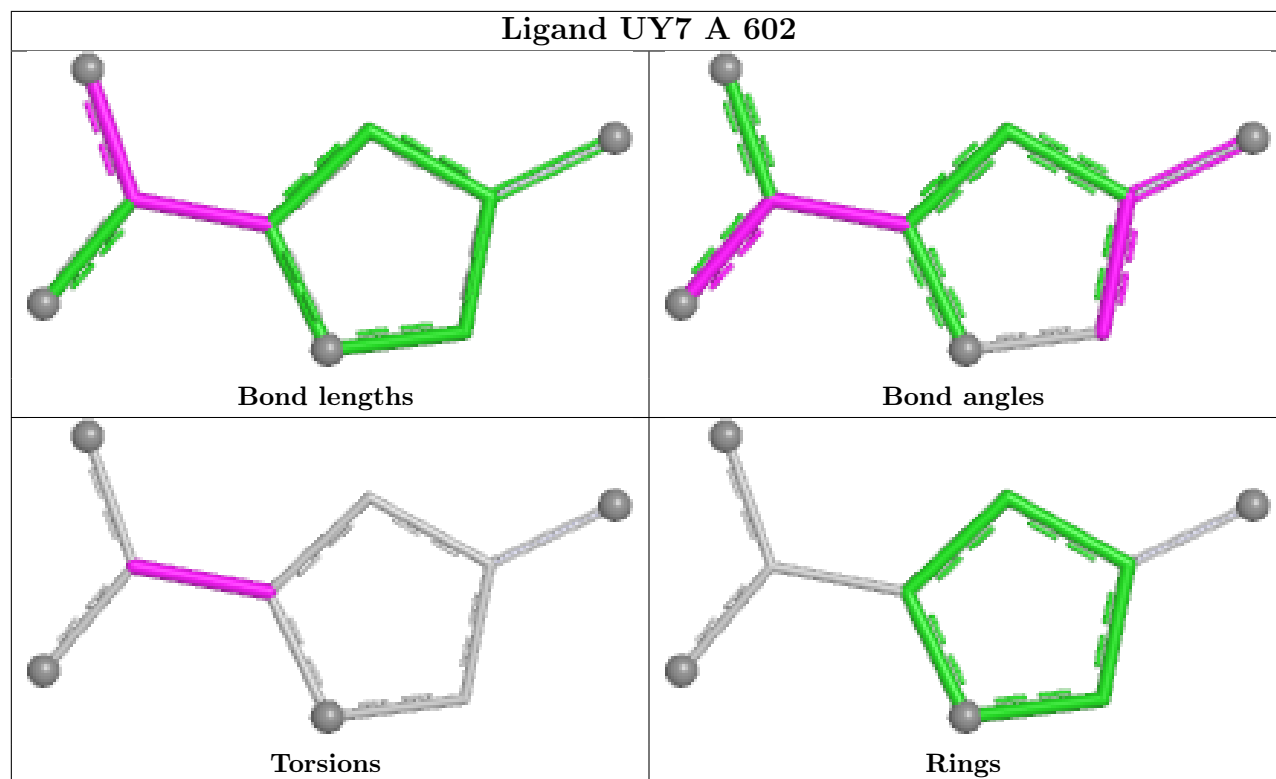
There are no ring outliers.

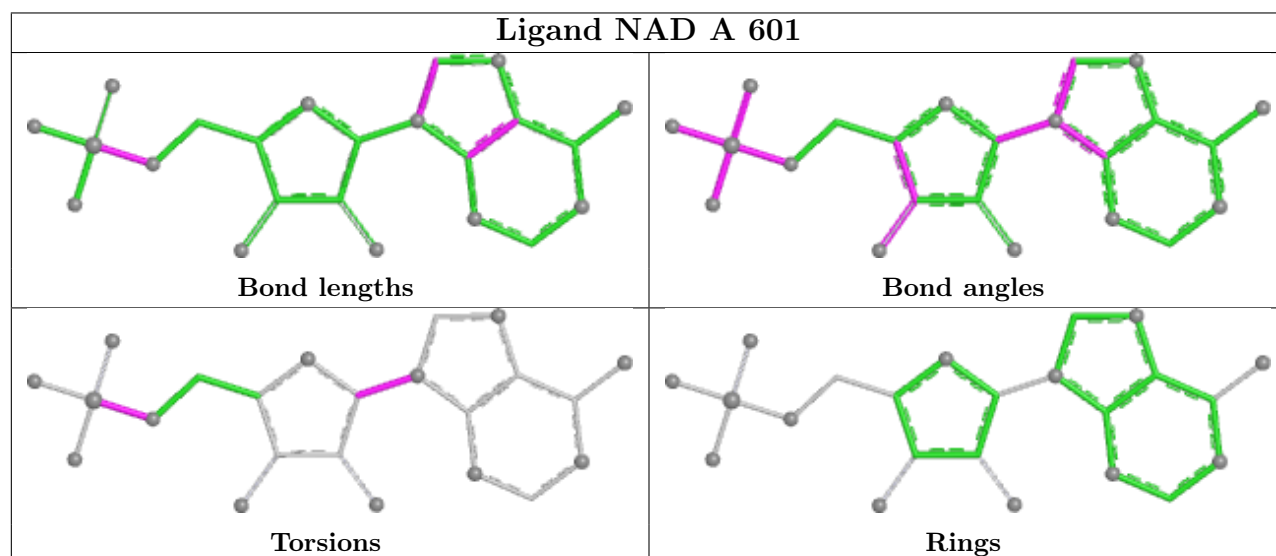
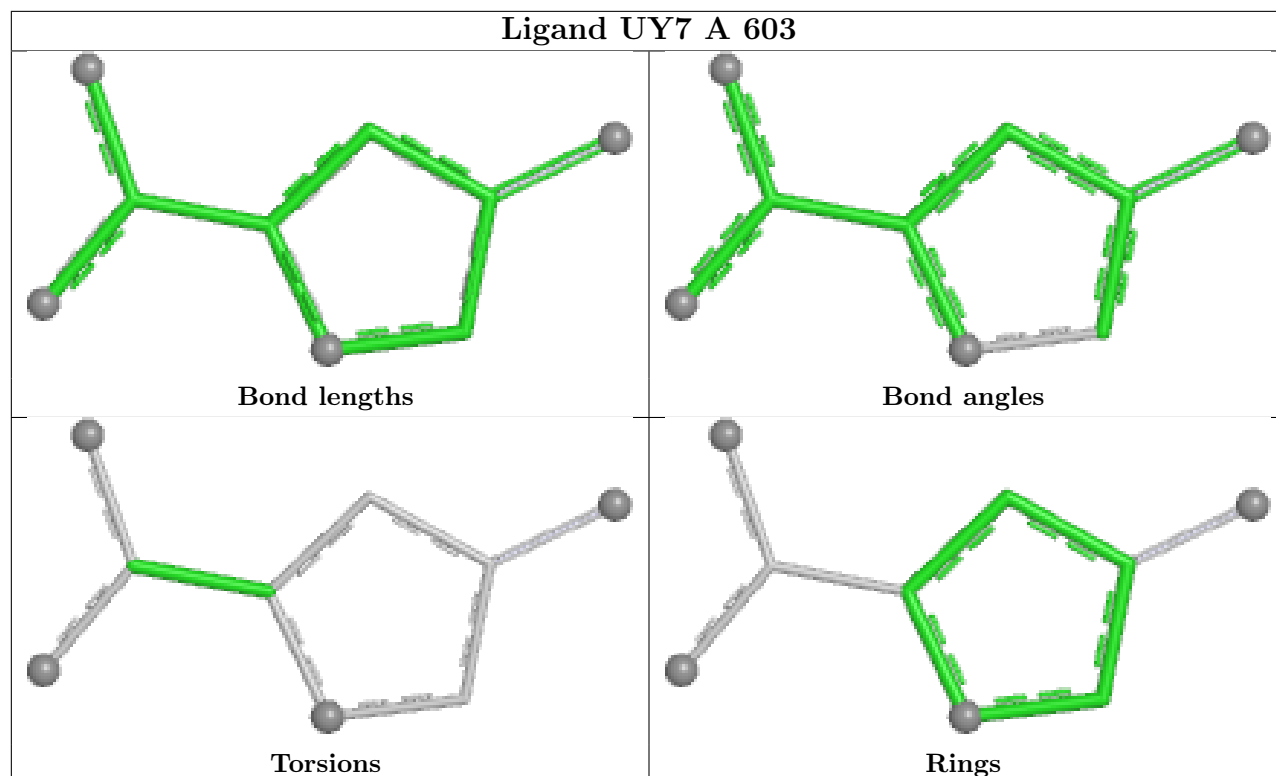
3 monomers are involved in 3 short contacts:

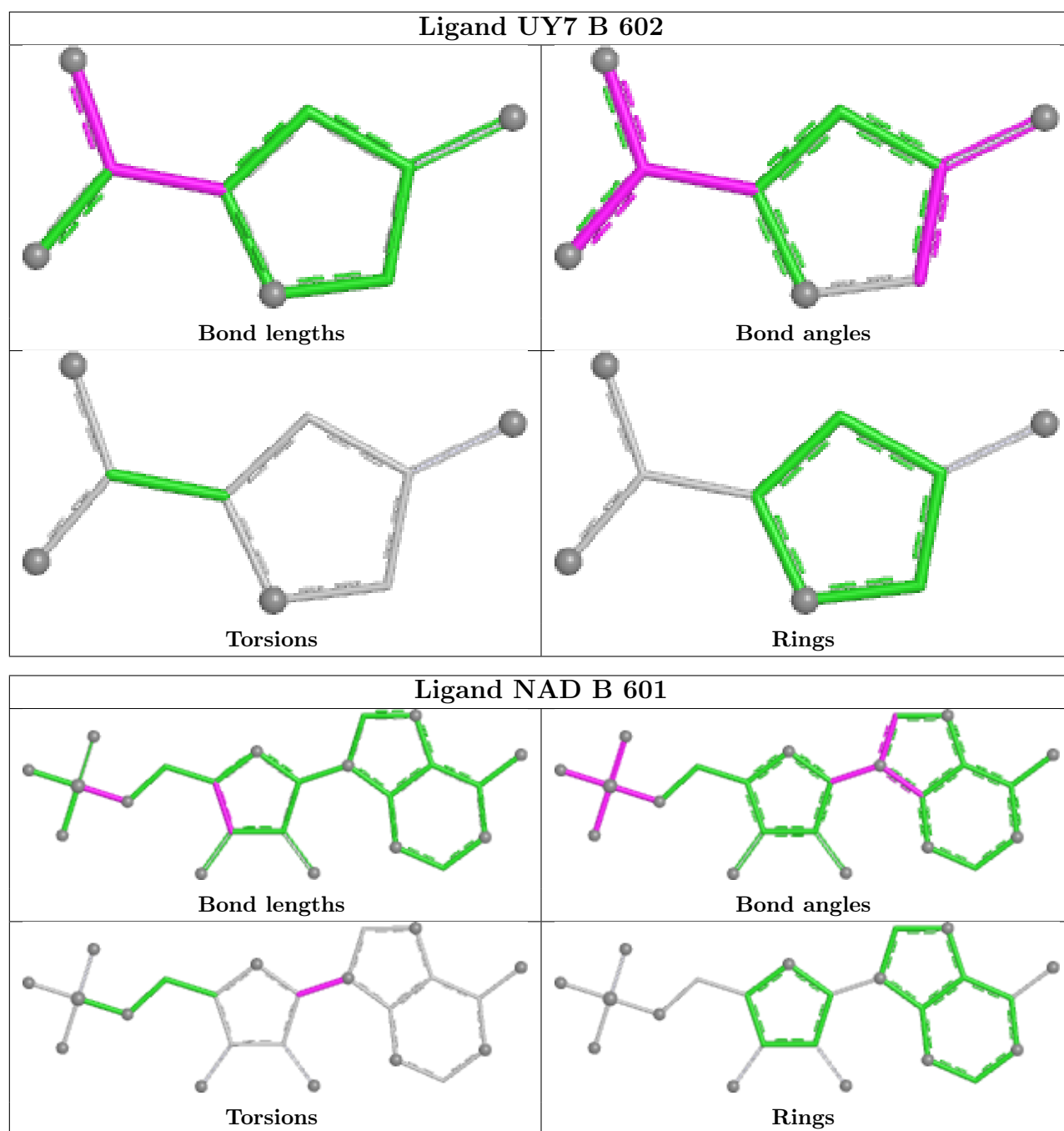
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	605	PEG	1	0
4	A	604	PG4	1	0
5	B	605	PEG	1	0

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	523/563 (92%)	0.15	16 (3%)	51 57	10, 17, 29, 47	7 (1%)
1	B	527/563 (93%)	0.28	13 (2%)	58 64	12, 18, 33, 42	4 (0%)
All	All	1050/1126 (93%)	0.21	29 (2%)	55 60	10, 17, 31, 47	11 (1%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	32	VAL	4.0
1	B	555	GLY	3.7
1	B	30	LEU	3.6
1	A	188	VAL	3.4
1	B	29	SER	3.4
1	A	463	TYR	3.1
1	A	553	PRO	3.1
1	A	552	LYS	3.1
1	A	411	PRO	2.7
1	A	554	LEU	2.6
1	A	33	ALA	2.6
1	A	58	LYS	2.5
1	A	182	GLY	2.5
1	A	48	ASP	2.5
1	A	461	ASP	2.5
1	B	44	SER	2.4
1	B	316	GLY	2.4
1	A	189	PRO	2.3
1	B	411	PRO	2.3
1	A	56	ASP	2.3
1	B	369	LEU	2.2
1	A	194	HIS	2.2
1	A	485	GLN	2.2
1	B	43	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	512	GLY	2.2
1	B	307	THR	2.1
1	B	409	SER	2.1
1	B	463	TYR	2.1
1	B	40	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

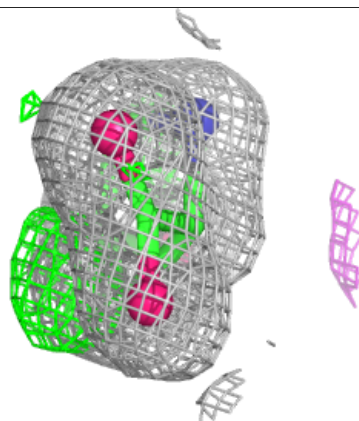
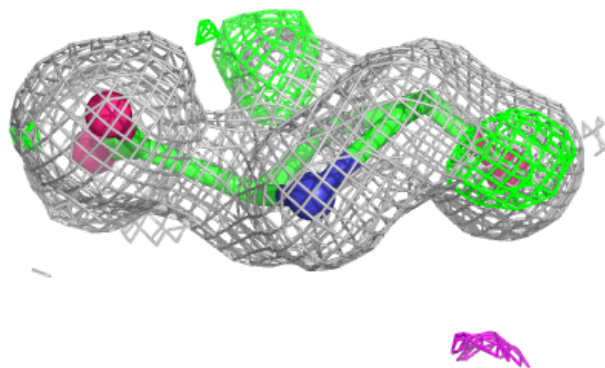
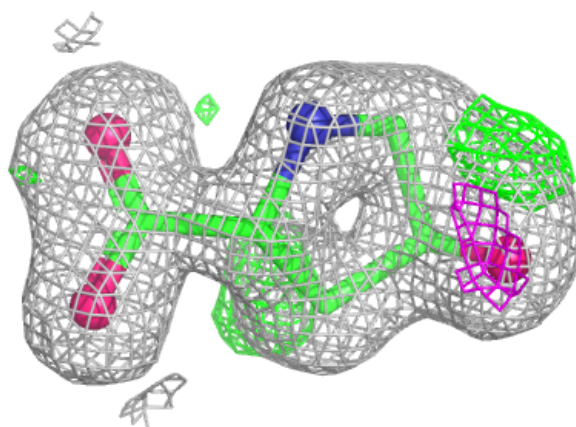
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PEG	B	605	7/7	0.83	0.14	29,33,36,40	0
7	PGE	B	604	10/10	0.84	0.14	29,34,38,38	0
4	PG4	A	604	13/13	0.86	0.13	29,33,38,40	0
5	PEG	A	606	7/7	0.86	0.14	30,31,38,40	0
5	PEG	A	605	7/7	0.88	0.12	25,27,37,39	0
3	UY7	B	602	9/9	0.92	0.09	18,20,21,23	9
3	UY7	A	603	9/9	0.92	0.12	12,17,23,23	9
6	1PE	A	607	16/16	0.93	0.10	24,27,30,30	0
6	1PE	B	606	16/16	0.94	0.09	23,26,28,30	0
2	NAD	A	601	23/44	0.94	0.08	15,17,24,36	0
3	UY7	A	602	9/9	0.95	0.07	16,17,19,22	9
3	UY7	B	603	9/9	0.95	0.08	17,21,27,29	9
2	NAD	B	601	23/44	0.95	0.07	15,16,30,31	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.

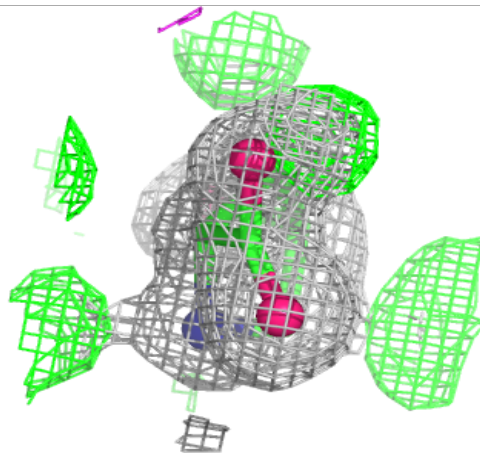
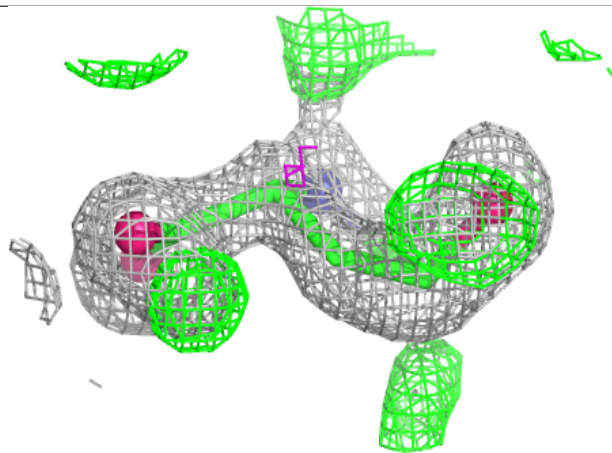
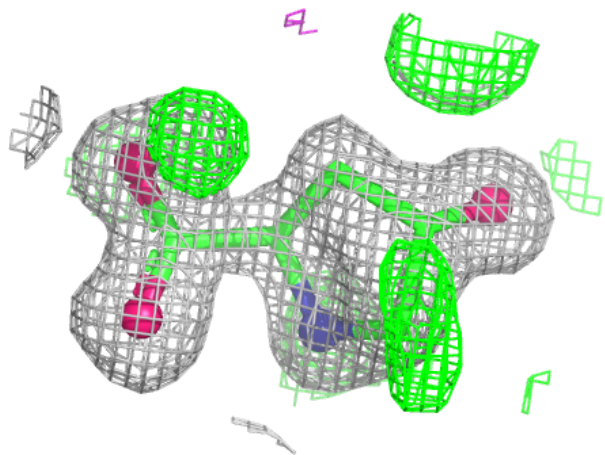
Electron density around UY7 B 602:

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



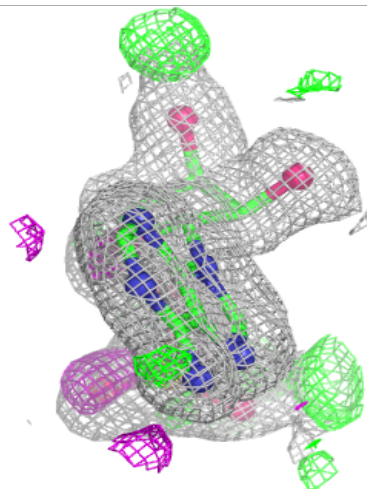
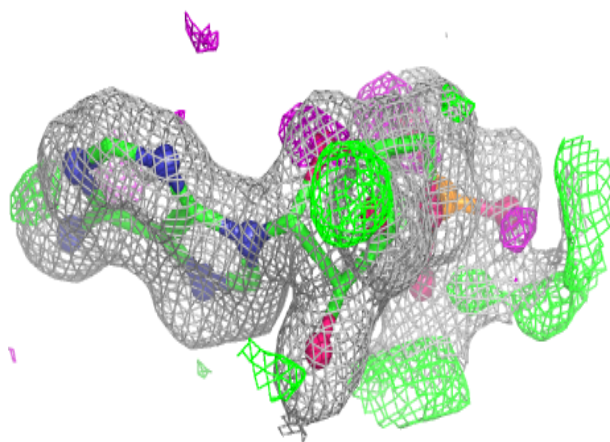
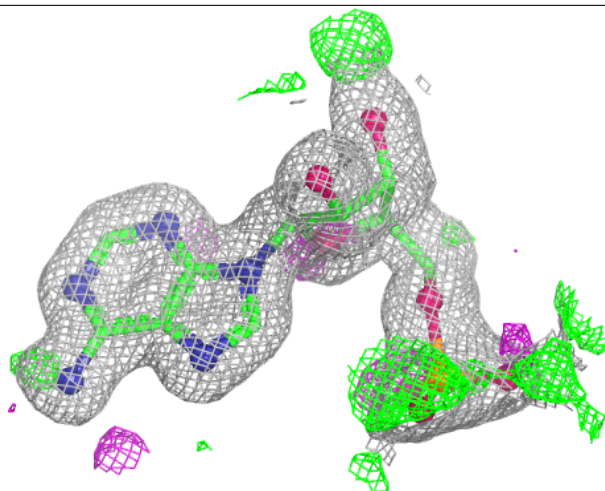
Electron density around UY7 A 603:

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



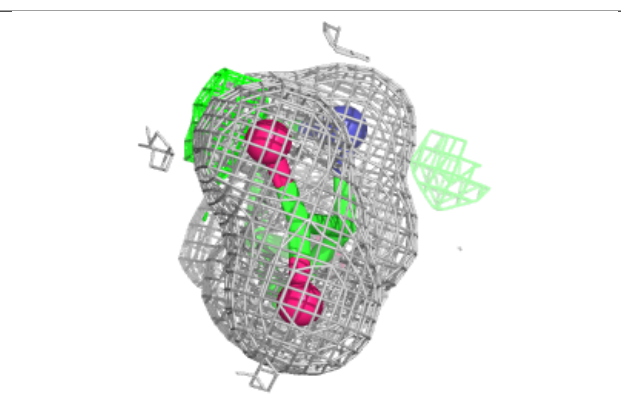
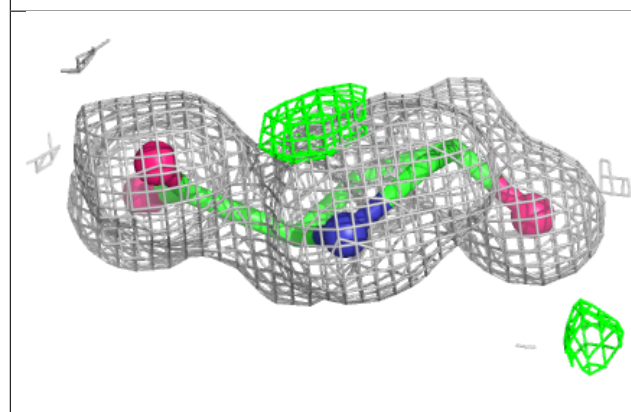
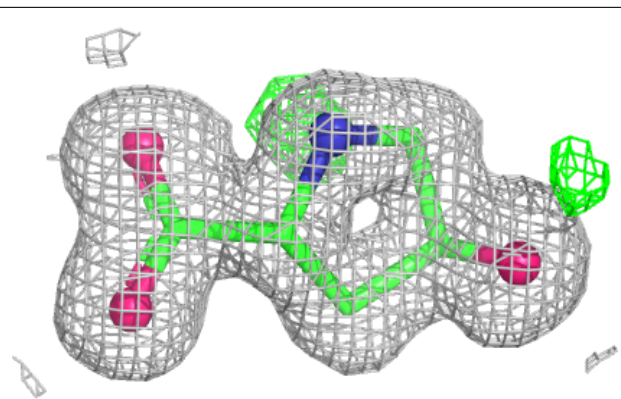
Electron density around NAD A 601:

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



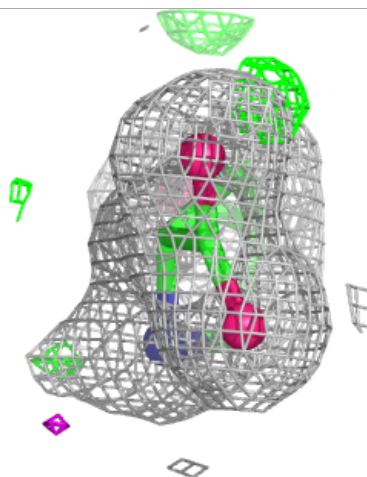
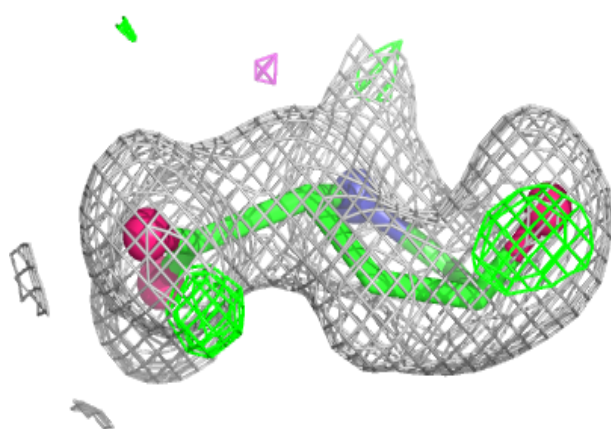
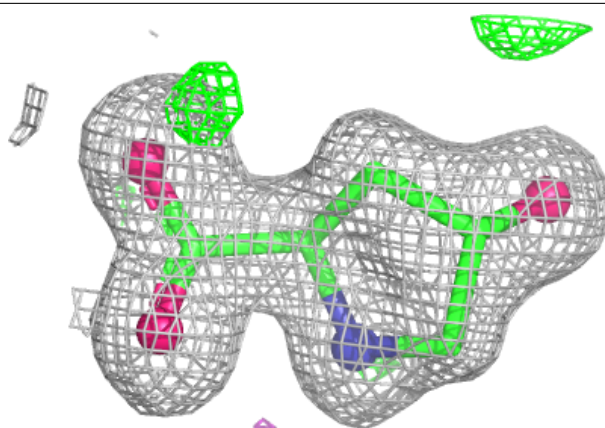
Electron density around UY7 A 602:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



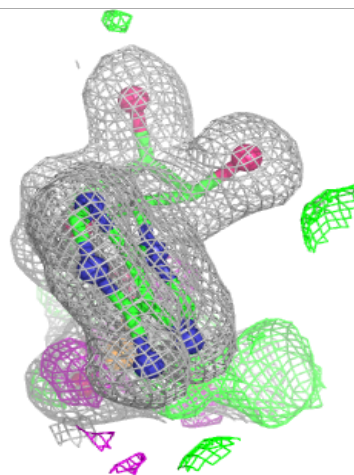
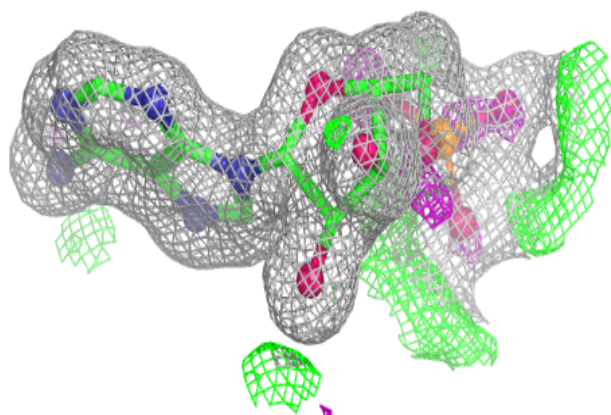
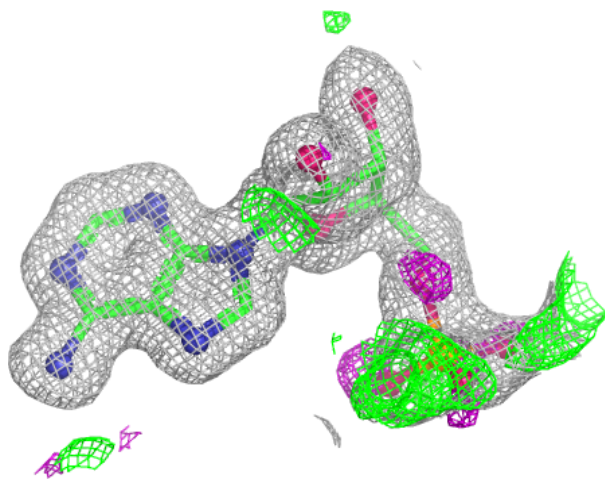
Electron density around UY7 B 603:

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



Electron density around NAD B 601:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.