



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:07 AM UTC

PDB ID : 7ZG3 / pdb_00007zg3
Title : Structure of the mouse 8-oxoguanine DNA Glycosylase mOGG1 in complex with ligand TH011228
Authors : Davies, J.R.; Scaletti, E.; Stenmark, P.
Deposited on : 2022-04-01
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

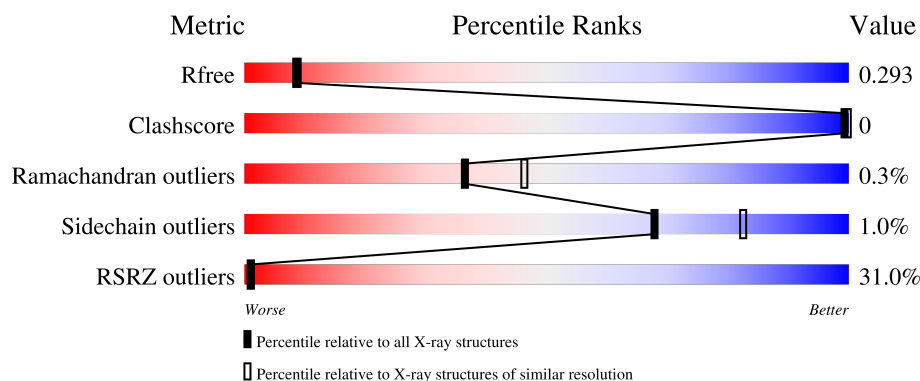
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	318	39% 95%
1	B	318	42% 95%
1	C	318	9% 96%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7375 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.

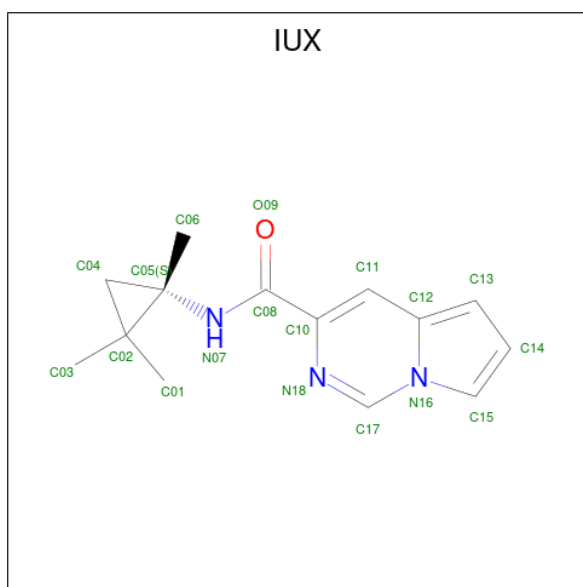
- Molecule 1 is a protein called N-glycosylase/DNA lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	0	0
			2316	1485	410	410	11			
1	B	308	Total	C	N	O	S	0	0	0
			2402	1535	431	425	11			
1	C	310	Total	C	N	O	S	0	0	0
			2448	1561	443	433	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	GLY	-	expression tag	UNP O08760
A	10	HIS	SER	conflict	UNP O08760
B	8	GLY	-	expression tag	UNP O08760
B	10	HIS	SER	conflict	UNP O08760
C	8	GLY	-	expression tag	UNP O08760
C	10	HIS	SER	conflict	UNP O08760

- Molecule 2 is {N}-[(1 {S})-1,2,2-trimethylcyclopropyl]pyrrolo[1,2-c]pyrimidine-3-carboxamide (CCD ID: IUX) (formula: C₁₄H₁₇N₃O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			18	14	3	1		
2	B	1	Total	C	N	O	0	0
			18	14	3	1		
2	C	1	Total	C	N	O	0	0
			18	14	3	1		

- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ni	0	0
			1	1		

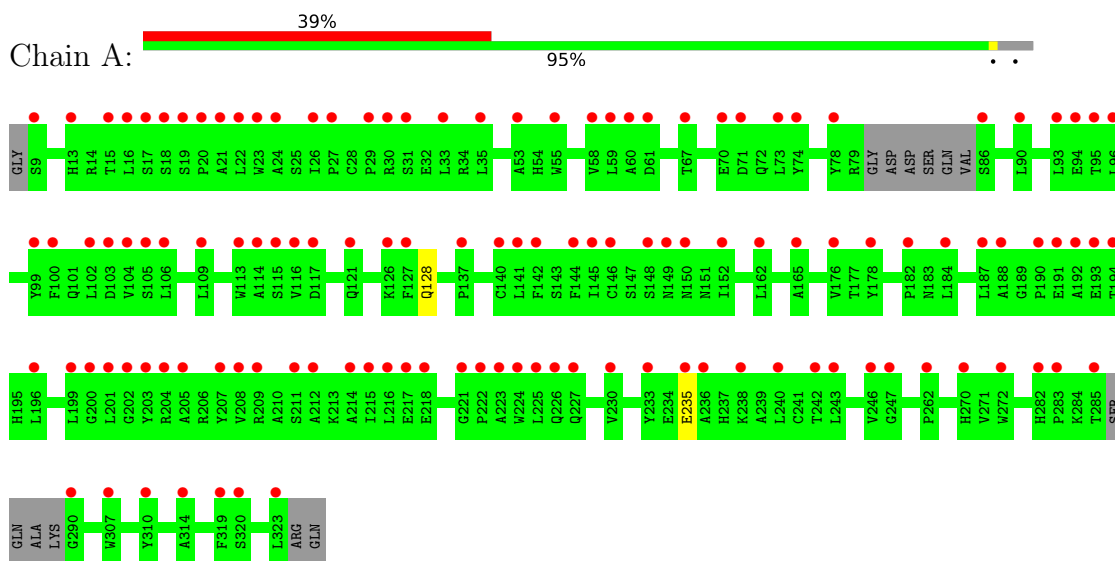
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	31	Total	O	0	0
			31	31		
4	B	36	Total	O	0	0
			36	36		
4	C	87	Total	O	0	0
			87	87		

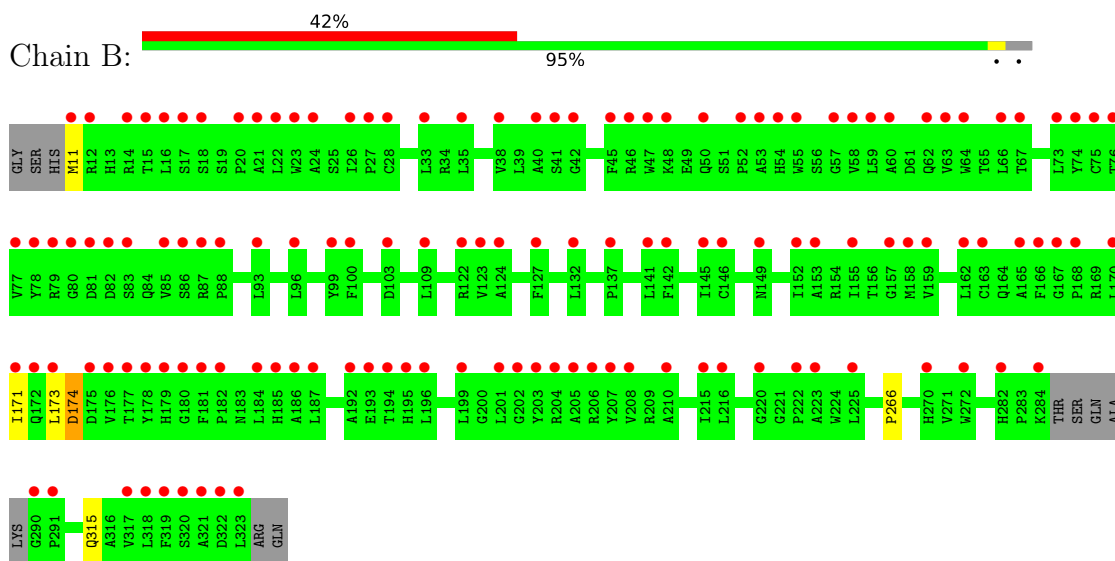
3 Residue-property plots

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.

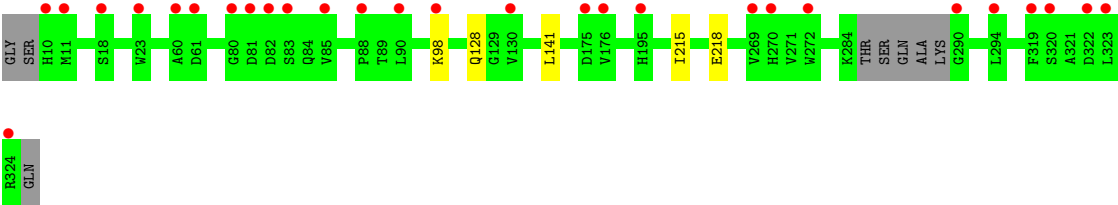
- Molecule 1: N-glycosylase/DNA lyase



- Molecule 1: N-glycosylase/DNA lyase



- Molecule 1: N-glycosylase/DNA lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.79Å 81.32Å 169.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.95 – 2.30 84.95 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (84.95-2.30) 99.9 (84.95-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.276 , 0.307 (Not available) , 0.293	Depositor DCC
R_{free} test set	2577 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	57.3	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7375	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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: IUX, NI

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	0.52	0/2382	0.76	0/3254
1	B	0.54	0/2471	0.79	0/3373
1	C	0.53	0/2518	0.77	0/3431
All	All	0.53	0/7371	0.77	0/10058

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 [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	2316	0	2185	0	0
1	B	2402	0	2305	2	0
1	C	2448	0	2377	1	0
2	A	18	0	0	0	0
2	B	18	0	0	0	0
2	C	18	0	0	0	0
3	A	1	0	0	0	0
4	A	31	0	0	0	0
4	B	36	0	0	0	0
4	C	87	0	0	0	0
All	All	7375	0	6867	3	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 0.

All (3) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:PRO:HD2	1:B:315:GLN:HE22	1.68	0.58
1:C:141:LEU:HD21	1:C:215:ILE:HD11	1.95	0.48
1:B:173:LEU:O	1:B:174:ASP:C	2.63	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	26/318 (8%)	25 (96%)	1 (4%)	0	100	100
1	B	91/318 (29%)	86 (94%)	4 (4%)	1 (1%)	11	13
1	C	249/318 (78%)	242 (97%)	7 (3%)	0	100	100
All	All	366/954 (38%)	353 (96%)	12 (3%)	1 (0%)	36	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	174	ASP

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	228/266 (86%)	226 (99%)	2 (1%)	70	84
1	B	244/266 (92%)	242 (99%)	2 (1%)	73	86
1	C	254/266 (96%)	251 (99%)	3 (1%)	63	79
All	All	726/798 (91%)	719 (99%)	7 (1%)	68	82

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	235	GLU
1	B	11	MET
1	B	171	ILE
1	C	98	LYS
1	C	128	GLN
1	C	218	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	119	HIS
1	A	282	HIS
1	B	50	GLN
1	B	62	GLN
1	B	68	GLN
1	B	108	GLN
1	B	219	GLN
1	B	226	GLN
1	B	282	HIS
1	B	315	GLN
1	C	68	GLN
1	C	112	HIS
1	C	119	HIS
1	C	219	GLN
1	C	226	GLN
1	C	276	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](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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	IUX	C	401	-	18,20,20	3.11	8 (44%)	17,32,32	1.83	5 (29%)
2	IUX	A	401	-	18,20,20	3.23	9 (50%)	17,32,32	1.82	5 (29%)
2	IUX	B	401	-	18,20,20	3.35	9 (50%)	17,32,32	1.83	5 (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	IUX	C	401	-	-	0/8/21/21	0/3/3/3
2	IUX	A	401	-	-	0/8/21/21	0/3/3/3
2	IUX	B	401	-	-	0/8/21/21	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	IUX	C08-N07	8.20	1.45	1.34
2	A	401	IUX	C08-N07	7.86	1.45	1.34
2	C	401	IUX	C08-N07	7.62	1.44	1.34
2	B	401	IUX	C10-C08	6.36	1.60	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	IUX	C10-C08	6.13	1.60	1.48
2	C	401	IUX	C10-C08	5.91	1.60	1.48
2	B	401	IUX	C17-N16	5.63	1.43	1.37
2	A	401	IUX	C17-N16	5.22	1.42	1.37
2	C	401	IUX	C17-N16	5.03	1.42	1.37
2	A	401	IUX	C17-N18	4.72	1.39	1.30
2	B	401	IUX	C17-N18	4.65	1.39	1.30
2	C	401	IUX	C17-N18	4.60	1.39	1.30
2	B	401	IUX	C11-C12	2.59	1.46	1.39
2	A	401	IUX	C11-C12	2.56	1.46	1.39
2	B	401	IUX	C04-C05	2.53	1.56	1.50
2	A	401	IUX	C04-C05	2.52	1.56	1.50
2	C	401	IUX	C11-C12	2.43	1.46	1.39
2	C	401	IUX	C04-C05	2.34	1.56	1.50
2	A	401	IUX	C15-C14	2.33	1.42	1.37
2	B	401	IUX	C15-C14	2.32	1.42	1.37
2	C	401	IUX	C15-C14	2.29	1.42	1.37
2	B	401	IUX	C06-C05	2.28	1.56	1.52
2	A	401	IUX	C06-C05	2.18	1.55	1.52
2	A	401	IUX	C04-C02	2.16	1.56	1.50
2	B	401	IUX	C04-C02	2.11	1.56	1.50
2	C	401	IUX	C04-C02	2.10	1.56	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	IUX	O09-C08-N07	-3.66	118.18	124.35
2	B	401	IUX	O09-C08-N07	-3.56	118.35	124.35
2	A	401	IUX	O09-C08-N07	-3.55	118.36	124.35
2	C	401	IUX	N16-C17-N18	-3.01	119.52	124.61
2	B	401	IUX	N16-C17-N18	-2.99	119.55	124.61
2	A	401	IUX	N16-C17-N18	-2.94	119.65	124.61
2	B	401	IUX	C11-C10-N18	-2.91	118.52	122.63
2	A	401	IUX	C11-C10-N18	-2.89	118.53	122.63
2	C	401	IUX	C11-C10-N18	-2.79	118.68	122.63
2	B	401	IUX	O09-C08-C10	-2.09	115.92	121.15
2	C	401	IUX	C13-C12-C11	2.08	134.12	126.76
2	A	401	IUX	C13-C12-C11	2.05	134.03	126.76
2	B	401	IUX	C13-C12-C11	2.04	133.97	126.76
2	A	401	IUX	O09-C08-C10	-2.03	116.06	121.15
2	C	401	IUX	O09-C08-C10	-2.03	116.07	121.15

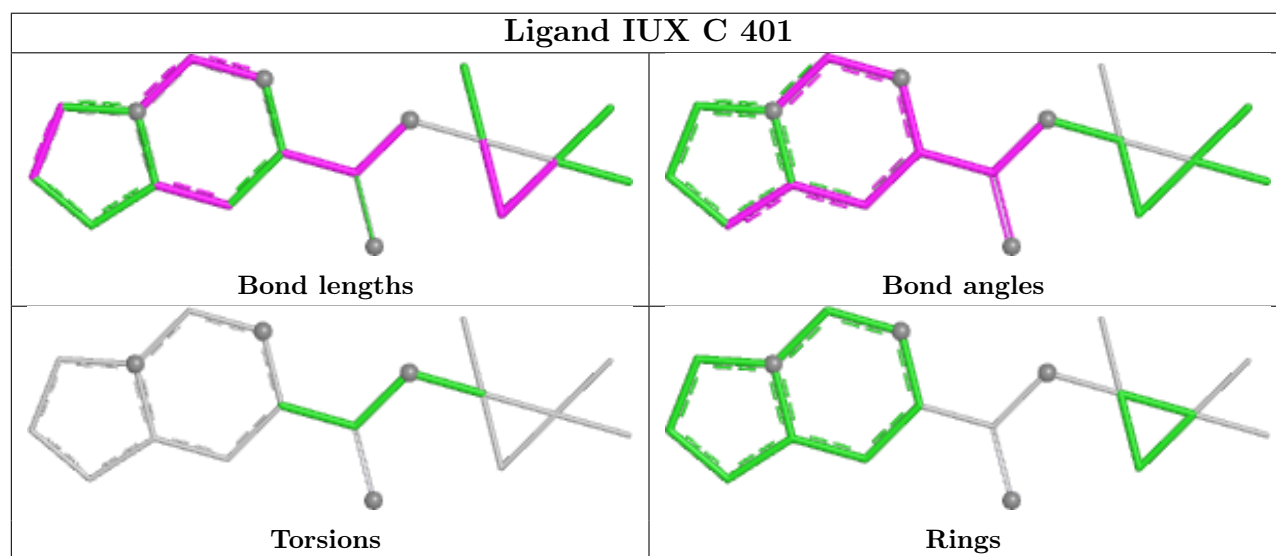
There are no chirality outliers.

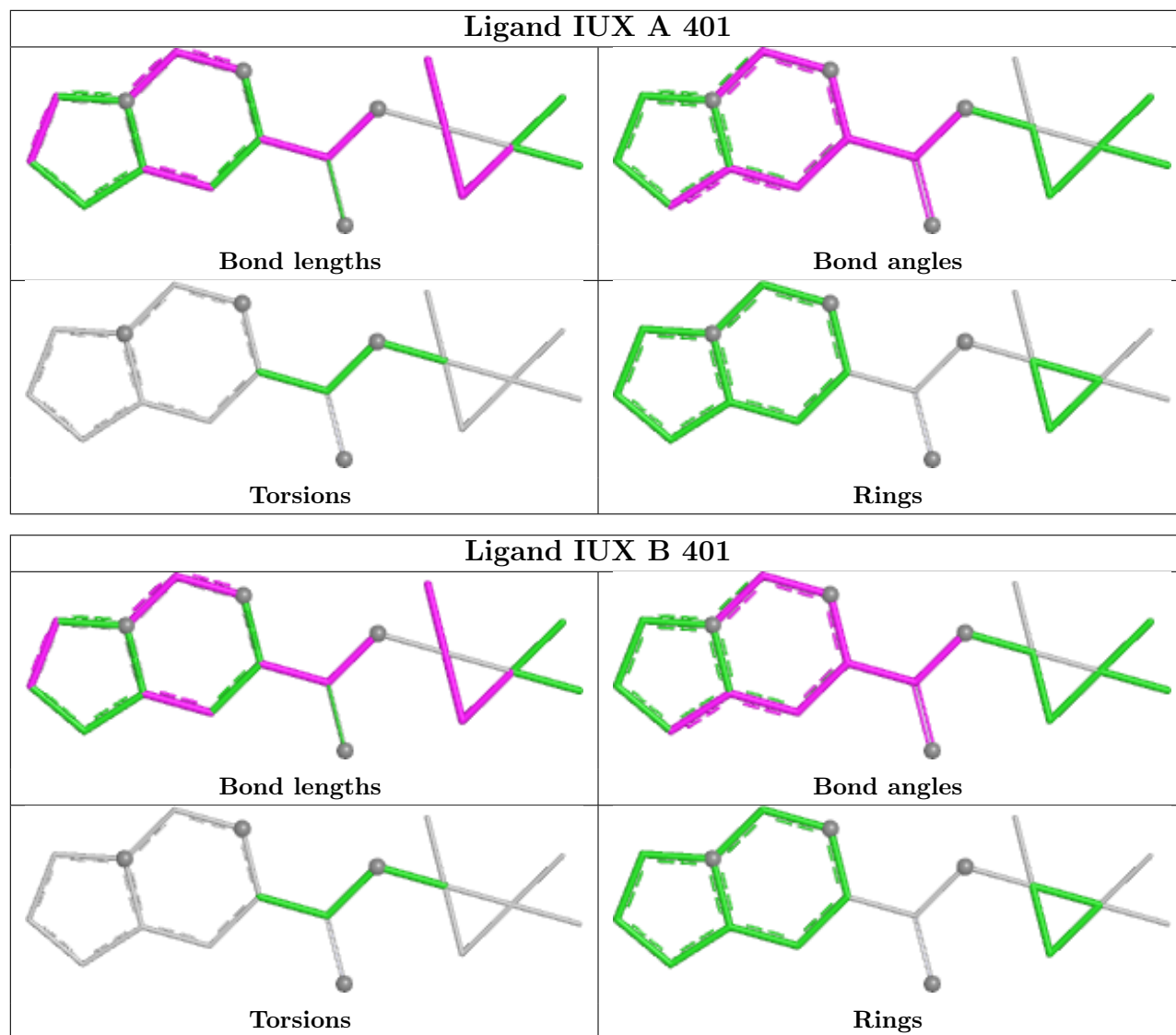
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	305/318 (95%)	1.87	125 (40%) 0 0	50, 76, 108, 119	0
1	B	308/318 (96%)	1.87	133 (43%) 0 0	44, 76, 104, 116	0
1	C	310/318 (97%)	0.86	28 (9%) 15 16	36, 53, 82, 101	0
All	All	923/954 (96%)	1.53	286 (30%) 1 1	36, 69, 102, 119	0

All (286) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	201	LEU	5.5
1	A	217	GLU	5.3
1	B	82	ASP	4.9
1	B	11	MET	4.8
1	A	142	PHE	4.7
1	B	53	ALA	4.4
1	A	203	TYR	4.4
1	B	26	ILE	4.3
1	B	321	ALA	4.3
1	B	22	LEU	4.2
1	B	77	VAL	4.2
1	B	73	LEU	4.1
1	A	215	ILE	4.1
1	B	205	ALA	4.1
1	A	320	SER	4.0
1	B	208	VAL	4.0
1	B	319	PHE	4.0
1	A	224	TRP	4.0
1	B	16	LEU	3.9
1	B	64	TRP	3.9
1	A	216	LEU	3.9
1	A	18	SER	3.8
1	B	176	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	165	ALA	3.8
1	B	167	GLY	3.8
1	A	323	LEU	3.8
1	B	162	LEU	3.8
1	B	170	LEU	3.8
1	B	180	GLY	3.7
1	C	82	ASP	3.7
1	B	168	PRO	3.7
1	B	187	LEU	3.6
1	A	188	ALA	3.6
1	A	191	GLU	3.6
1	A	149	ASN	3.6
1	C	11	MET	3.6
1	B	85	VAL	3.6
1	B	81	ASP	3.6
1	A	290	GLY	3.5
1	B	38	VAL	3.5
1	B	45	PHE	3.5
1	A	96	LEU	3.4
1	A	184	LEU	3.4
1	B	173	LEU	3.4
1	B	322	ASP	3.4
1	A	74	TYR	3.4
1	B	159	VAL	3.4
1	A	114	ALA	3.4
1	B	54	HIS	3.4
1	B	163	CYS	3.4
1	A	100	PHE	3.3
1	C	319	PHE	3.3
1	A	246	VAL	3.3
1	A	201	LEU	3.3
1	B	158	MET	3.2
1	A	282	HIS	3.2
1	B	222	PRO	3.2
1	B	15	THR	3.2
1	C	10	HIS	3.2
1	B	171	ILE	3.2
1	B	166	PHE	3.2
1	B	55	TRP	3.2
1	A	190	PRO	3.2
1	B	52	PRO	3.2
1	A	104	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	16	LEU	3.1
1	A	90	LEU	3.1
1	A	115	SER	3.1
1	B	172	GLN	3.1
1	C	85	VAL	3.1
1	A	20	PRO	3.1
1	A	307	TRP	3.1
1	A	214	ALA	3.1
1	A	141	LEU	3.1
1	B	199	LEU	3.1
1	B	74	TYR	3.0
1	A	148	SER	3.0
1	B	149	ASN	3.0
1	A	187	LEU	3.0
1	B	206	ARG	3.0
1	A	117	ASP	3.0
1	A	207	TYR	3.0
1	B	145	ILE	3.0
1	A	86	SER	3.0
1	C	290	GLY	3.0
1	A	192	ALA	3.0
1	B	165	ALA	3.0
1	C	176	VAL	3.0
1	B	195	HIS	3.0
1	A	194	THR	2.9
1	B	177	THR	2.9
1	B	220	GLY	2.9
1	A	319	PHE	2.9
1	B	23	TRP	2.9
1	A	223	ALA	2.9
1	C	323	LEU	2.9
1	B	87	ARG	2.9
1	A	285	THR	2.9
1	A	17	SER	2.9
1	B	78	TYR	2.9
1	A	102	LEU	2.9
1	B	60	ALA	2.9
1	B	196	LEU	2.9
1	A	230	VAL	2.9
1	A	193	GLU	2.9
1	B	18	SER	2.9
1	B	153	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	123	VAL	2.9
1	A	145	ILE	2.9
1	A	152	ILE	2.9
1	B	132	LEU	2.8
1	B	272	TRP	2.8
1	A	67	THR	2.8
1	B	14	ARG	2.8
1	B	155	ILE	2.8
1	A	146	CYS	2.8
1	B	28	CYS	2.8
1	A	211	SER	2.8
1	B	42	GLY	2.8
1	B	96	LEU	2.8
1	A	247	GLY	2.8
1	B	182	PRO	2.8
1	A	93	LEU	2.8
1	B	99	TYR	2.8
1	B	203	TYR	2.8
1	B	40	ALA	2.8
1	B	175	ASP	2.7
1	A	19	SER	2.7
1	A	196	LEU	2.7
1	A	236	ALA	2.7
1	C	81	ASP	2.7
1	B	59	LEU	2.7
1	B	216	LEU	2.7
1	B	152	ILE	2.7
1	B	86	SER	2.7
1	A	21	ALA	2.7
1	B	223	ALA	2.7
1	A	116	VAL	2.7
1	B	80	GLY	2.7
1	B	290	GLY	2.7
1	B	27	PRO	2.7
1	A	73	LEU	2.7
1	B	66	LEU	2.7
1	A	15	THR	2.6
1	C	80	GLY	2.6
1	B	109	LEU	2.6
1	B	323	LEU	2.6
1	B	291	PRO	2.6
1	B	320	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	270	HIS	2.6
1	A	59	LEU	2.6
1	A	23	TRP	2.6
1	B	21	ALA	2.6
1	B	47	TRP	2.6
1	A	176	VAL	2.6
1	B	58	VAL	2.6
1	B	76	THR	2.6
1	B	83	SER	2.6
1	B	93	LEU	2.6
1	B	63	VAL	2.6
1	A	205	ALA	2.5
1	B	207	TYR	2.5
1	A	70	GLU	2.5
1	A	150	ASN	2.5
1	A	126	LYS	2.5
1	C	272	TRP	2.5
1	A	208	VAL	2.5
1	A	53	ALA	2.5
1	A	29	PRO	2.5
1	B	146	CYS	2.5
1	B	181	PHE	2.5
1	A	26	ILE	2.5
1	C	294	LEU	2.5
1	B	192	ALA	2.5
1	A	227	GLN	2.5
1	C	23	TRP	2.4
1	A	22	LEU	2.4
1	A	233	TYR	2.4
1	A	262	PRO	2.4
1	B	79	ARG	2.4
1	B	127	PHE	2.4
1	B	178	TYR	2.4
1	A	13	HIS	2.4
1	B	282	HIS	2.4
1	A	209	ARG	2.4
1	B	122	ARG	2.4
1	B	100	PHE	2.4
1	B	12	ARG	2.4
1	C	324	ARG	2.4
1	B	20	PRO	2.4
1	B	57	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	95	THR	2.4
1	C	83	SER	2.4
1	C	320	SER	2.4
1	A	225	LEU	2.4
1	B	33	LEU	2.4
1	B	225	LEU	2.4
1	C	90	LEU	2.4
1	A	178	TYR	2.3
1	B	202	GLY	2.3
1	C	98	LYS	2.3
1	A	9	SER	2.3
1	B	35	LEU	2.3
1	A	78	TYR	2.3
1	B	48	LYS	2.3
1	A	31	SER	2.3
1	B	184	LEU	2.3
1	B	318	LEU	2.3
1	A	182	PRO	2.3
1	A	272	TRP	2.3
1	B	124	ALA	2.3
1	A	242	THR	2.3
1	B	17	SER	2.3
1	A	94	GLU	2.3
1	A	58	VAL	2.3
1	A	127	PHE	2.3
1	A	199	LEU	2.3
1	B	141	LEU	2.3
1	B	157	GLY	2.3
1	A	30	ARG	2.3
1	A	99	TYR	2.3
1	A	212	ALA	2.3
1	C	60	ALA	2.3
1	A	226	GLN	2.3
1	B	50	GLN	2.3
1	A	162	LEU	2.2
1	A	240	LEU	2.2
1	B	103	ASP	2.2
1	A	222	PRO	2.2
1	A	221	GLY	2.2
1	A	121	GLN	2.2
1	B	215	ILE	2.2
1	B	142	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	27	PRO	2.2
1	B	185	HIS	2.2
1	B	186	ALA	2.2
1	A	144	PHE	2.2
1	B	193	GLU	2.2
1	A	105	SER	2.2
1	A	113	TRP	2.2
1	A	33	LEU	2.2
1	A	35	LEU	2.2
1	B	204	ARG	2.2
1	A	61	ASP	2.2
1	A	71	ASP	2.2
1	C	269	VAL	2.2
1	A	235	GLU	2.2
1	B	284	LYS	2.2
1	A	140	CYS	2.2
1	B	24	ALA	2.2
1	A	204	ARG	2.1
1	A	106	LEU	2.1
1	A	243	LEU	2.1
1	A	60	ALA	2.1
1	B	41	SER	2.1
1	B	67	THR	2.1
1	B	194	THR	2.1
1	B	210	ALA	2.1
1	A	109	LEU	2.1
1	B	62	GLN	2.1
1	B	88	PRO	2.1
1	B	137	PRO	2.1
1	A	200	GLY	2.1
1	B	75	CYS	2.1
1	A	310	TYR	2.1
1	C	175	ASP	2.1
1	A	270	HIS	2.1
1	A	283	PRO	2.1
1	C	88	PRO	2.1
1	C	130	VAL	2.1
1	A	24	ALA	2.1
1	A	218	GLU	2.1
1	A	103	ASP	2.1
1	C	61	ASP	2.1
1	C	195	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	55	TRP	2.1
1	B	46	ARG	2.1
1	A	238	LYS	2.0
1	C	18	SER	2.0
1	C	270	HIS	2.0
1	C	322	ASP	2.0
1	B	317	VAL	2.0
1	A	202	GLY	2.0
1	A	314	ALA	2.0
1	B	179	HIS	2.0
1	A	137	PRO	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](#)

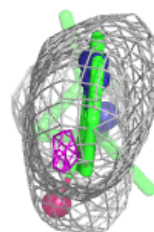
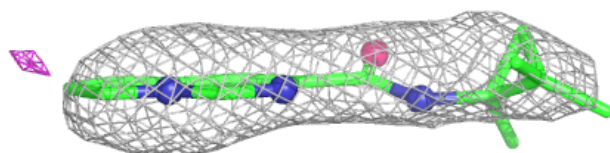
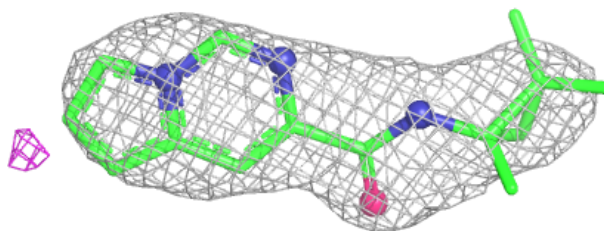
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	IUX	A	401	18/18	0.88	0.18	71,72,77,77	0
2	IUX	B	401	18/18	0.89	0.20	71,73,81,81	0
2	IUX	C	401	18/18	0.92	0.12	48,49,53,53	0
3	NI	A	402	1/1	0.96	0.12	47,47,47,47	0

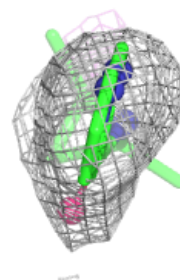
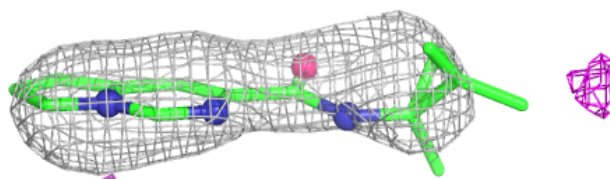
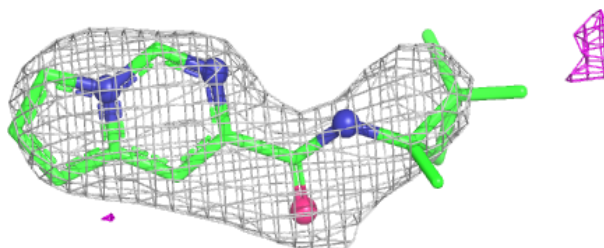
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around IUX A 401:

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

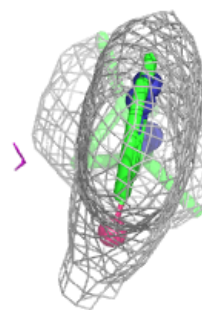
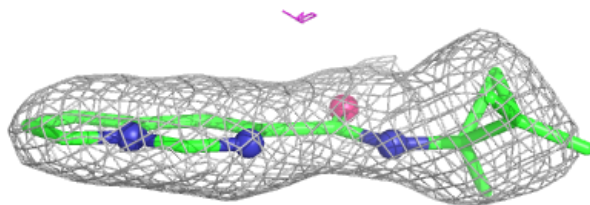
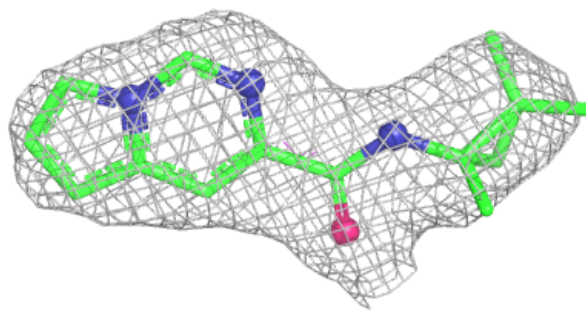
**Electron density around IUX B 401:**

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



Electron density around IUX C 401:

$2mF_o-DF_c$ (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.