



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 07:41 PM UTC

PDB ID : 8TZ7 / pdb_00008tz7
EMDB ID : EMD-41736
Title : Cryo-EM structure of bovine concentrative nucleoside transporter 3 in complex with Molnupiravir, condition 1, INT1-INT1-INT1 conformation
Authors : Wright, N.J.; Lee, S.-Y.
Deposited on : 2023-08-26
Resolution : 3.00 Å(reported)
Based on initial model : 3TIJ

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

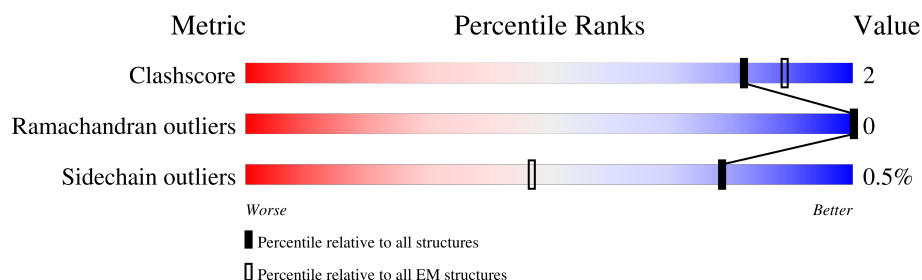
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	715	70% • 25%
1	B	715	69% 5% 25%
1	C	715	69% 5% 25%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24615 atoms, of which 12276 are hydrogens and 0 are deuteriums.

In the tables below, 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 Sodium/nucleoside cotransporter.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	533	Total	C	H	N	O	S	0	0
			8076	2688	4023	638	698	29		
1	B	533	Total	C	H	N	O	S	0	0
			8076	2688	4023	638	698	29		
1	C	533	Total	C	H	N	O	S	0	0
			8076	2688	4023	638	698	29		

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MET	-	initiating methionine	UNP F1MGR1
A	-13	ASP	-	expression tag	UNP F1MGR1
A	-12	TYR	-	expression tag	UNP F1MGR1
A	-11	LYS	-	expression tag	UNP F1MGR1
A	-10	ASP	-	expression tag	UNP F1MGR1
A	-9	ASP	-	expression tag	UNP F1MGR1
A	-8	ASP	-	expression tag	UNP F1MGR1
A	-7	ASP	-	expression tag	UNP F1MGR1
A	-6	LYS	-	expression tag	UNP F1MGR1
A	-5	LEU	-	expression tag	UNP F1MGR1
A	-4	GLU	-	expression tag	UNP F1MGR1
A	-3	ALA	-	expression tag	UNP F1MGR1
A	-2	THR	-	expression tag	UNP F1MGR1
A	-1	MET	-	expression tag	UNP F1MGR1
A	0	ALA	-	expression tag	UNP F1MGR1
A	698	SER	-	expression tag	UNP F1MGR1
A	699	ASN	-	expression tag	UNP F1MGR1
A	700	SER	-	expression tag	UNP F1MGR1
B	-14	MET	-	initiating methionine	UNP F1MGR1
B	-13	ASP	-	expression tag	UNP F1MGR1
B	-12	TYR	-	expression tag	UNP F1MGR1
B	-11	LYS	-	expression tag	UNP F1MGR1
B	-10	ASP	-	expression tag	UNP F1MGR1
B	-9	ASP	-	expression tag	UNP F1MGR1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	ASP	-	expression tag	UNP F1MGR1
B	-7	ASP	-	expression tag	UNP F1MGR1
B	-6	LYS	-	expression tag	UNP F1MGR1
B	-5	LEU	-	expression tag	UNP F1MGR1
B	-4	GLU	-	expression tag	UNP F1MGR1
B	-3	ALA	-	expression tag	UNP F1MGR1
B	-2	THR	-	expression tag	UNP F1MGR1
B	-1	MET	-	expression tag	UNP F1MGR1
B	0	ALA	-	expression tag	UNP F1MGR1
B	698	SER	-	expression tag	UNP F1MGR1
B	699	ASN	-	expression tag	UNP F1MGR1
B	700	SER	-	expression tag	UNP F1MGR1
C	-14	MET	-	initiating methionine	UNP F1MGR1
C	-13	ASP	-	expression tag	UNP F1MGR1
C	-12	TYR	-	expression tag	UNP F1MGR1
C	-11	LYS	-	expression tag	UNP F1MGR1
C	-10	ASP	-	expression tag	UNP F1MGR1
C	-9	ASP	-	expression tag	UNP F1MGR1
C	-8	ASP	-	expression tag	UNP F1MGR1
C	-7	ASP	-	expression tag	UNP F1MGR1
C	-6	LYS	-	expression tag	UNP F1MGR1
C	-5	LEU	-	expression tag	UNP F1MGR1
C	-4	GLU	-	expression tag	UNP F1MGR1
C	-3	ALA	-	expression tag	UNP F1MGR1
C	-2	THR	-	expression tag	UNP F1MGR1
C	-1	MET	-	expression tag	UNP F1MGR1
C	0	ALA	-	expression tag	UNP F1MGR1
C	698	SER	-	expression tag	UNP F1MGR1
C	699	ASN	-	expression tag	UNP F1MGR1
C	700	SER	-	expression tag	UNP F1MGR1

- Molecule 2 is N-hydroxy-5'-O-(2-methylpropanoyl)cytidine (CCD ID: XMO) (formula: $C_{13}H_{19}N_3O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total 42	C 13	H 19	N 3	O 7	0
2	B	1	Total 42	C 13	H 19	N 3	O 7	0
2	C	1	Total 42	C 13	H 19	N 3	O 7	0

- Molecule 3 is 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (CCD ID: LBN) (formula: $C_{42}H_{82}NO_8P$).

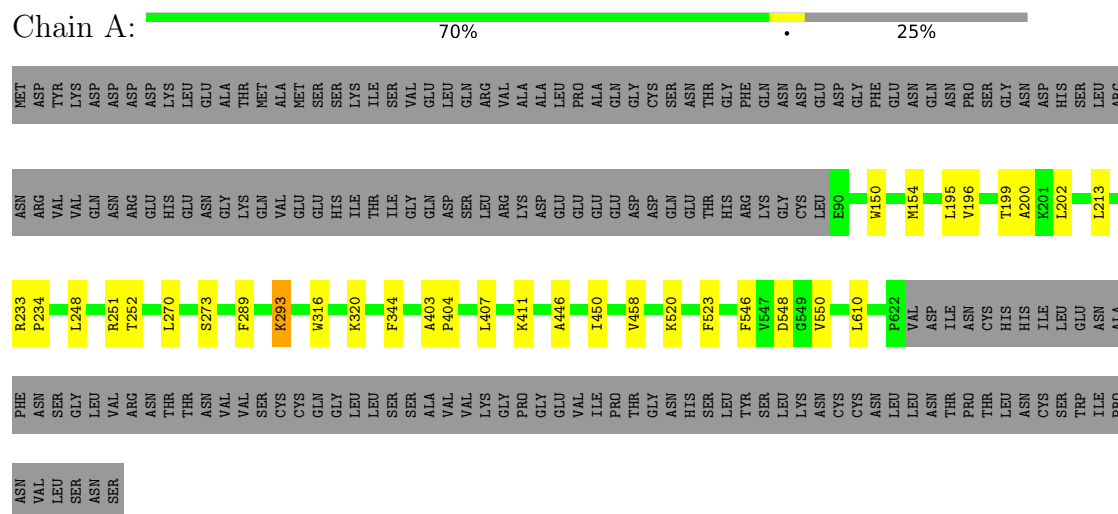


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	H	O	P	0
			87	28	50	8	1	
3	B	1	Total	C	H	O	P	0
			87	28	50	8	1	
3	C	1	Total	C	H	O	P	0
			87	28	50	8	1	

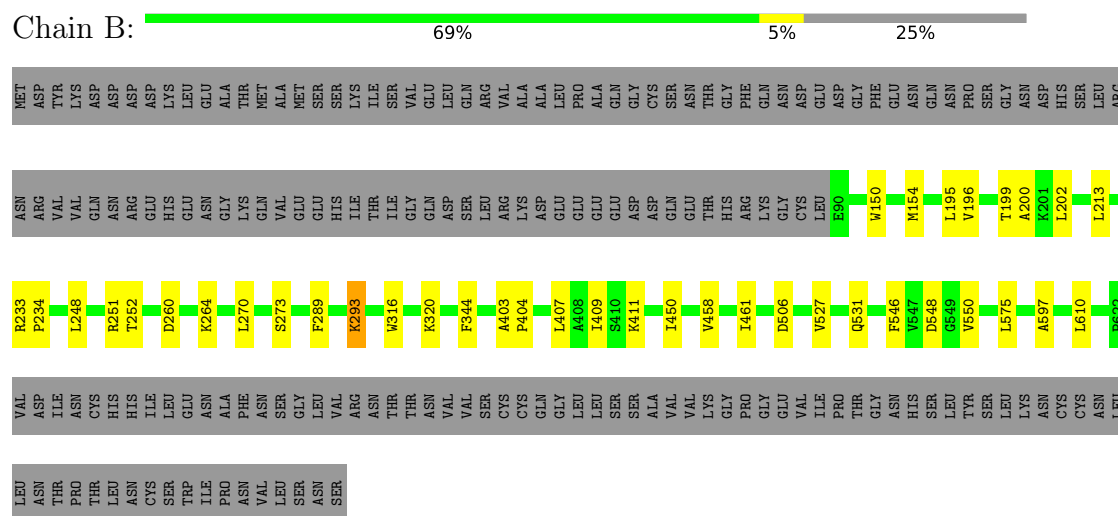
3 Residue-property plots

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. 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. 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: Sodium/nucleoside cotransporter



- Molecule 1: Sodium/nucleoside cotransporter



- Molecule 1: Sodium/nucleoside cotransporter



THR	CYS	R233	ASN	MET
LEU	HIS	P234	ARG	ASP
ASN	HIS		VAL	TYR
CYS	ILE	L248	VAL	LYS
SER	LEU		GLN	ASP
TRP	GLU	R251	ASN	ASP
PRO	ASN	T252	ARG	ASP
ASN	ALA		GLU	LYS
VAL	PHE	D260	HIS	LEU
LEU	ASN		GLU	GLU
SER	SER	K264	ASN	GLU
GLY	GLY		GLY	ALA
LEU	LEU	L270	LYS	THR
ASN	VAL		GLN	THR
SER	ARG	S273	VAL	MET
	ASN		GLU	ALA
	THR	V280	GLU	NET
	THR		HIS	SER
	ASN	F289	ILE	SER
	VAL		THR	LYS
	VAL	K293	ILE	SER
	CYS	W316	GLY	VAL
	CYS		GLN	GLU
	GLN	K320	ASP	LEU
	GLY		SER	GLN
	LEU	F344	LEU	ARG
	LEU		ARG	VAL
	SER	A403	LYS	ALA
	SER	P404	ASP	ALA
	VAL		GLU	LEU
	VAL	L407	GLU	PRO
	LYS	K411	GLU	ALA
	GLY		ASP	GLN
	PRO	I450	GLN	GLY
	GLY		GLU	THR
	GLU	V458	THR	GLY
	VAL		HIS	PHE
	ILE	K520	ARG	GLN
	THR	F523	LYS	ASN
	GLY		GLY	ASN
	ASN	V527	CYS	ASP
	HIS		LEU	GLU
	SER	Q531	E90	ASP
	LEU		W150	GLY
	TYR	F546	W154	PHE
	SER	V547	M154	GLU
	LEU	D548		ASN
	LYS	G549	L195	GLN
	ASN	V550	V196	ASN
	CYS			PRO
	CYS			SER
	CYS	L610	T199	GLY
	ASN		A200	GLY
	LEU	P622	K201	ASN
	LEU	VAL	L202	ASP
	ASN	ASP		HIS
	THR	ILE	L213	SER
	PRO	ASN		LEU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	127798	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

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: LBN, XMO

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	0.14	0/4164	0.31	0/5672
1	B	0.14	0/4164	0.31	0/5672
1	C	0.14	0/4164	0.31	0/5672
All	All	0.14	0/12492	0.31	0/17016

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	4053	4023	4023	19	0
1	B	4053	4023	4023	22	0
1	C	4053	4023	4023	22	0
2	A	23	19	0	1	0
2	B	23	19	0	1	0
2	C	23	19	0	1	0
3	A	37	50	0	0	0
3	B	37	50	0	0	0
3	C	37	50	0	0	0
All	All	12339	12276	12069	60	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 2.

All (60) 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)
2:A:801:XMO:O12	2:A:801:XMO:C11	1.68	1.24
2:C:801:XMO:C11	2:C:801:XMO:O12	1.68	1.22
2:B:801:XMO:C11	2:B:801:XMO:O12	1.68	1.16
1:B:458:VAL:HG21	1:C:450:ILE:HG12	1.88	0.55
1:C:248:LEU:O	1:C:252:THR:OG1	2.21	0.55
1:A:270:LEU:O	1:A:273:SER:OG	2.17	0.54
1:A:446:ALA:HB1	1:C:458:VAL:HG12	1.89	0.53
1:B:270:LEU:O	1:B:273:SER:OG	2.17	0.53
1:C:316:TRP:O	1:C:320:LYS:HG2	2.11	0.51
1:B:316:TRP:O	1:B:320:LYS:HG2	2.11	0.51
1:A:316:TRP:O	1:A:320:LYS:HG2	2.11	0.50
1:A:450:ILE:HG12	1:C:458:VAL:HG21	1.94	0.50
1:C:289:PHE:O	1:C:293:LYS:HB2	2.14	0.48
1:B:289:PHE:O	1:B:293:LYS:HB2	2.14	0.48
1:A:289:PHE:O	1:A:293:LYS:HB2	2.14	0.47
1:C:202:LEU:HD11	1:C:251:ARG:HH22	1.79	0.47
1:A:248:LEU:O	1:A:252:THR:OG1	2.22	0.47
1:B:202:LEU:HD11	1:B:251:ARG:HH22	1.79	0.47
1:C:213:LEU:HD12	1:C:610:LEU:HD22	1.97	0.47
1:B:213:LEU:HD12	1:B:610:LEU:HD22	1.97	0.47
1:C:546:PHE:HB3	1:C:548:ASP:O	2.15	0.46
1:A:202:LEU:HD11	1:A:251:ARG:HH22	1.79	0.46
1:B:548:ASP:C	1:B:550:VAL:H	2.23	0.46
1:A:195:LEU:O	1:A:199:THR:OG1	2.31	0.46
1:A:548:ASP:C	1:A:550:VAL:H	2.23	0.46
1:A:213:LEU:HD12	1:A:610:LEU:HD22	1.97	0.46
1:A:546:PHE:HB3	1:A:548:ASP:O	2.15	0.46
1:B:546:PHE:HB3	1:B:548:ASP:O	2.15	0.46
1:C:548:ASP:C	1:C:550:VAL:H	2.23	0.45
1:C:150:TRP:O	1:C:154:MET:HG2	2.17	0.45
1:C:270:LEU:O	1:C:273:SER:OG	2.17	0.45
1:B:195:LEU:O	1:B:199:THR:OG1	2.31	0.44
1:A:458:VAL:HG21	1:B:450:ILE:HG12	2.00	0.44
1:B:248:LEU:O	1:B:252:THR:OG1	2.21	0.44
1:A:150:TRP:O	1:A:154:MET:HG2	2.17	0.44
1:B:150:TRP:O	1:B:154:MET:HG2	2.17	0.43
1:C:233:ARG:HB3	1:C:234:PRO:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ARG:HB3	1:A:234:PRO:HD3	2.01	0.43
1:A:407:LEU:O	1:A:411:LYS:HG2	2.19	0.43
1:C:403:ALA:HB3	1:C:404:PRO:HD3	2.01	0.42
1:A:403:ALA:HB3	1:A:404:PRO:HD3	2.01	0.42
1:B:407:LEU:O	1:B:411:LYS:HG2	2.19	0.42
1:C:195:LEU:O	1:C:199:THR:OG1	2.31	0.42
1:B:233:ARG:HB3	1:B:234:PRO:HD3	2.01	0.42
1:C:407:LEU:O	1:C:411:LYS:HG2	2.19	0.42
1:B:403:ALA:HB3	1:B:404:PRO:HD3	2.01	0.42
1:C:196:VAL:O	1:C:200:ALA:HB3	2.20	0.41
1:B:506:ASP:OD1	1:B:506:ASP:N	2.53	0.41
1:A:446:ALA:O	1:C:458:VAL:HG11	2.21	0.41
1:B:461:ILE:HG13	1:C:280:VAL:HG21	2.02	0.41
1:B:260:ASP:O	1:B:264:LYS:HG2	2.21	0.41
1:A:196:VAL:O	1:A:200:ALA:HB3	2.20	0.41
1:B:196:VAL:O	1:B:200:ALA:HB3	2.21	0.41
1:A:520:LYS:O	1:A:523:PHE:O	2.40	0.40
1:C:520:LYS:O	1:C:523:PHE:O	2.40	0.40
1:B:527:VAL:O	1:B:531:GLN:HG2	2.21	0.40
1:B:575:LEU:HD11	1:B:597:ALA:HB1	2.03	0.40
1:C:260:ASP:O	1:C:264:LYS:HG2	2.21	0.40
1:C:527:VAL:O	1:C:531:GLN:HG2	2.21	0.40
1:B:409:ILE:HD11	1:B:610:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	531/715 (74%)	523 (98%)	8 (2%)	0	100	100
1	B	531/715 (74%)	523 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	531/715 (74%)	523 (98%)	8 (2%)	0	100	100
All	All	1593/2145 (74%)	1569 (98%)	24 (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 PDB entries followed by that with respect to all EM entries.

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	416/608 (68%)	414 (100%)	2 (0%)	81	89
1	B	416/608 (68%)	414 (100%)	2 (0%)	81	89
1	C	416/608 (68%)	414 (100%)	2 (0%)	81	89
All	All	1248/1824 (68%)	1242 (100%)	6 (0%)	78	89

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	293	LYS
1	A	344	PHE
1	B	293	LYS
1	B	344	PHE
1	C	293	LYS
1	C	344	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	444	GLN
1	B	444	GLN
1	C	444	GLN

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 ⓘ

6 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	XMO	A	801	-	24,24,24	4.71	14 (58%)	31,34,34	1.16	4 (12%)
3	LBN	C	802	-	36,36,51	1.39	4 (11%)	39,41,59	1.00	2 (5%)
2	XMO	B	801	-	24,24,24	4.72	14 (58%)	31,34,34	1.16	4 (12%)
2	XMO	C	801	-	24,24,24	4.72	15 (62%)	31,34,34	1.16	4 (12%)
3	LBN	A	802	-	36,36,51	1.39	5 (13%)	39,41,59	1.00	2 (5%)
3	LBN	B	802	-	36,36,51	1.38	4 (11%)	39,41,59	1.00	2 (5%)

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	XMO	A	801	-	-	0/13/31/31	0/2/2/2
3	LBN	C	802	-	-	10/38/38/55	-
2	XMO	B	801	-	-	0/13/31/31	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	XMO	C	801	-	-	0/13/31/31	0/2/2/2
3	LBN	A	802	-	-	10/38/38/55	-
3	LBN	B	802	-	-	10/38/38/55	-

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	XMO	O12-C11	11.56	1.68	1.42
2	A	801	XMO	O12-C11	11.52	1.68	1.42
2	C	801	XMO	O12-C11	11.51	1.68	1.42
2	B	801	XMO	C10-C11	-7.62	1.29	1.53
2	A	801	XMO	C10-C11	-7.61	1.29	1.53
2	C	801	XMO	C10-C11	-7.61	1.29	1.53
2	A	801	XMO	C16-N17	7.34	1.45	1.32
2	C	801	XMO	C16-N17	7.34	1.45	1.32
2	B	801	XMO	C16-N17	7.31	1.45	1.32
2	C	801	XMO	O06-C04	7.20	1.48	1.33
2	B	801	XMO	O06-C04	7.18	1.48	1.33
2	A	801	XMO	O06-C04	7.14	1.48	1.33
2	C	801	XMO	C18-N17	7.01	1.50	1.36
2	A	801	XMO	C18-N17	6.98	1.50	1.36
2	B	801	XMO	C18-N17	6.97	1.50	1.36
2	B	801	XMO	C14-C15	6.24	1.49	1.35
2	C	801	XMO	C14-C15	6.22	1.49	1.35
2	A	801	XMO	C14-C15	6.20	1.49	1.35
2	B	801	XMO	O12-C08	-5.97	1.31	1.45
2	A	801	XMO	O12-C08	-5.96	1.31	1.45
2	C	801	XMO	O12-C08	-5.94	1.31	1.45
3	C	802	LBN	P1-O4	4.70	1.65	1.50
3	B	802	LBN	P1-O4	4.68	1.65	1.50
3	A	802	LBN	P1-O4	4.68	1.65	1.50
2	B	801	XMO	C18-N13	4.41	1.49	1.40
2	A	801	XMO	C18-N13	4.40	1.49	1.40
2	C	801	XMO	C18-N13	4.39	1.49	1.40
2	A	801	XMO	C15-C16	4.28	1.50	1.41
2	C	801	XMO	C15-C16	4.27	1.50	1.41
2	A	801	XMO	O23-C09	-4.23	1.32	1.43
2	C	801	XMO	O23-C09	-4.23	1.32	1.43
2	B	801	XMO	C15-C16	4.22	1.50	1.41
2	B	801	XMO	O23-C09	-4.21	1.32	1.43
2	B	801	XMO	C16-N20	3.88	1.44	1.35
2	A	801	XMO	C16-N20	3.87	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	XMO	C16-N20	3.82	1.44	1.35
2	B	801	XMO	O19-C18	-3.64	1.16	1.23
2	A	801	XMO	O19-C18	-3.61	1.17	1.23
2	C	801	XMO	O19-C18	-3.61	1.17	1.23
2	B	801	XMO	C14-N13	3.46	1.46	1.38
2	A	801	XMO	C14-N13	3.44	1.46	1.38
2	C	801	XMO	C14-N13	3.43	1.46	1.38
3	C	802	LBN	O7-C34	3.19	1.43	1.34
3	A	802	LBN	O7-C34	3.17	1.43	1.34
3	B	802	LBN	O7-C34	3.16	1.43	1.34
3	A	802	LBN	O5-C25	2.70	1.41	1.33
3	C	802	LBN	O5-C25	2.70	1.41	1.33
3	B	802	LBN	O5-C25	2.68	1.41	1.33
2	A	801	XMO	C09-C10	2.48	1.60	1.53
2	C	801	XMO	C09-C10	2.45	1.60	1.53
2	B	801	XMO	C09-C10	2.43	1.60	1.53
3	A	802	LBN	P1-O1	2.22	1.67	1.60
3	B	802	LBN	P1-O1	2.19	1.67	1.60
3	C	802	LBN	P1-O1	2.19	1.67	1.60
3	A	802	LBN	O5-C3	-2.01	1.40	1.45
2	C	801	XMO	O05-C04	-2.00	1.16	1.21

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	LBN	O7-C34-C35	3.63	119.33	111.48
3	A	802	LBN	O7-C34-C35	3.62	119.31	111.48
3	C	802	LBN	O7-C34-C35	3.61	119.28	111.48
2	C	801	XMO	O06-C04-C02	2.92	119.14	111.52
2	A	801	XMO	O06-C04-C02	2.92	119.14	111.52
2	B	801	XMO	O06-C04-C02	2.92	119.14	111.52
3	C	802	LBN	O5-C25-C26	2.66	119.94	111.83
3	A	802	LBN	O5-C25-C26	2.65	119.92	111.83
3	B	802	LBN	O5-C25-C26	2.65	119.91	111.83
2	B	801	XMO	C09-C10-C11	2.51	106.20	101.46
2	A	801	XMO	C09-C10-C11	2.48	106.15	101.46
2	C	801	XMO	C09-C10-C11	2.48	106.15	101.46
2	C	801	XMO	C14-C15-C16	2.27	119.73	117.00
2	B	801	XMO	C14-C15-C16	2.26	119.72	117.00
2	A	801	XMO	C14-C15-C16	2.24	119.69	117.00
2	C	801	XMO	O06-C04-O05	-2.06	120.38	124.14
2	B	801	XMO	O06-C04-O05	-2.05	120.38	124.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	XMO	O06-C04-O05	-2.04	120.42	124.14

There are no chirality outliers.

All (30) torsion outliers are listed below:

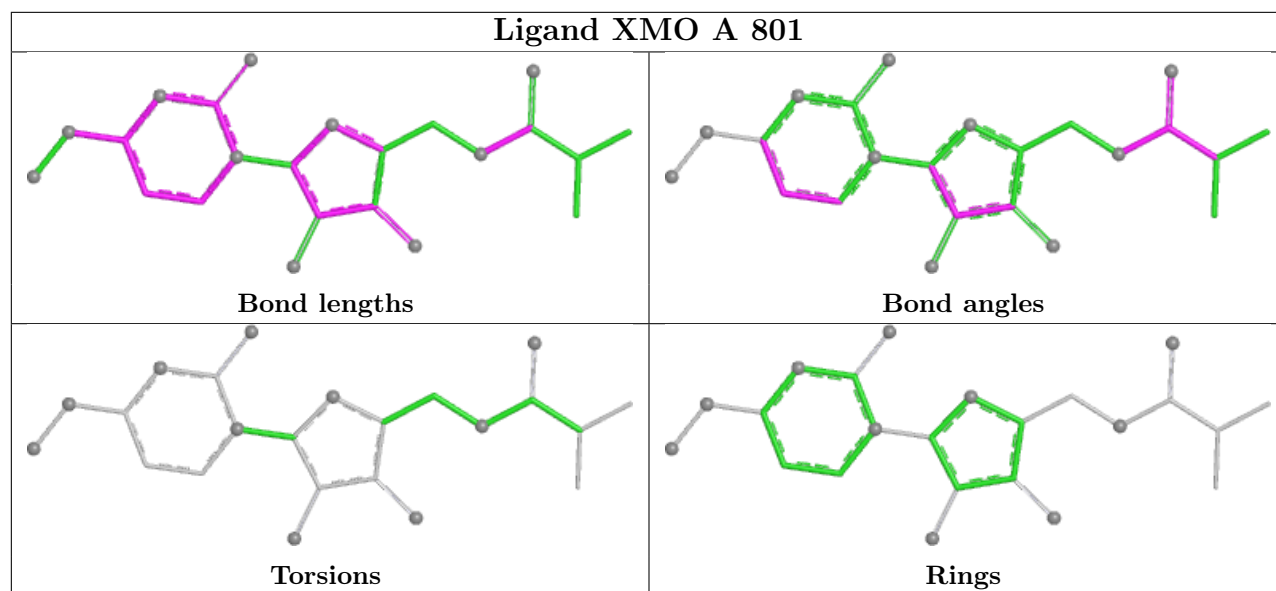
Mol	Chain	Res	Type	Atoms
3	A	802	LBN	O8-C34-O7-C2
3	B	802	LBN	O8-C34-O7-C2
3	C	802	LBN	O8-C34-O7-C2
3	A	802	LBN	C35-C34-O7-C2
3	B	802	LBN	C35-C34-O7-C2
3	C	802	LBN	C35-C34-O7-C2
3	A	802	LBN	C26-C25-O5-C3
3	B	802	LBN	C26-C25-O5-C3
3	C	802	LBN	C26-C25-O5-C3
3	A	802	LBN	O6-C25-O5-C3
3	B	802	LBN	O6-C25-O5-C3
3	C	802	LBN	O6-C25-O5-C3
3	B	802	LBN	C11-C14-C17-C20
3	C	802	LBN	C11-C14-C17-C20
3	A	802	LBN	C11-C14-C17-C20
3	A	802	LBN	C14-C11-C8-C5
3	B	802	LBN	C14-C11-C8-C5
3	C	802	LBN	C14-C11-C8-C5
3	A	802	LBN	C34-C35-C36-C37
3	B	802	LBN	C34-C35-C36-C37
3	C	802	LBN	C34-C35-C36-C37
3	A	802	LBN	C20-C22-C23-C24
3	B	802	LBN	C20-C22-C23-C24
3	C	802	LBN	C20-C22-C23-C24
3	B	802	LBN	C17-C20-C22-C23
3	C	802	LBN	C17-C20-C22-C23
3	A	802	LBN	C17-C20-C22-C23
3	A	802	LBN	C42-C5-C8-C11
3	B	802	LBN	C42-C5-C8-C11
3	C	802	LBN	C42-C5-C8-C11

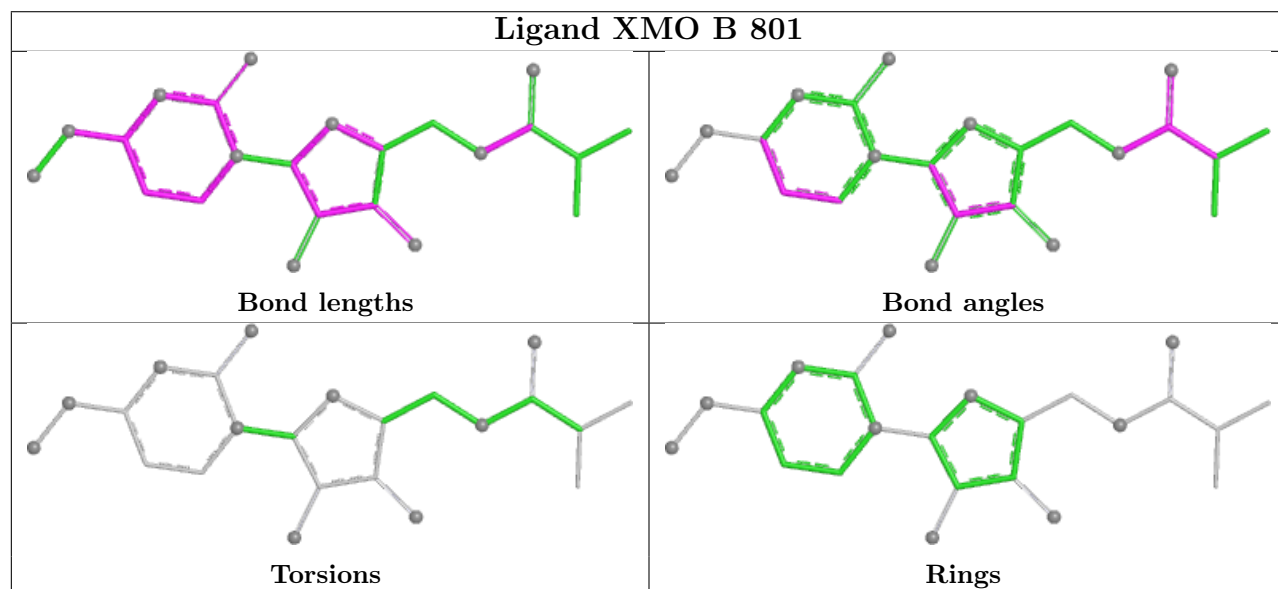
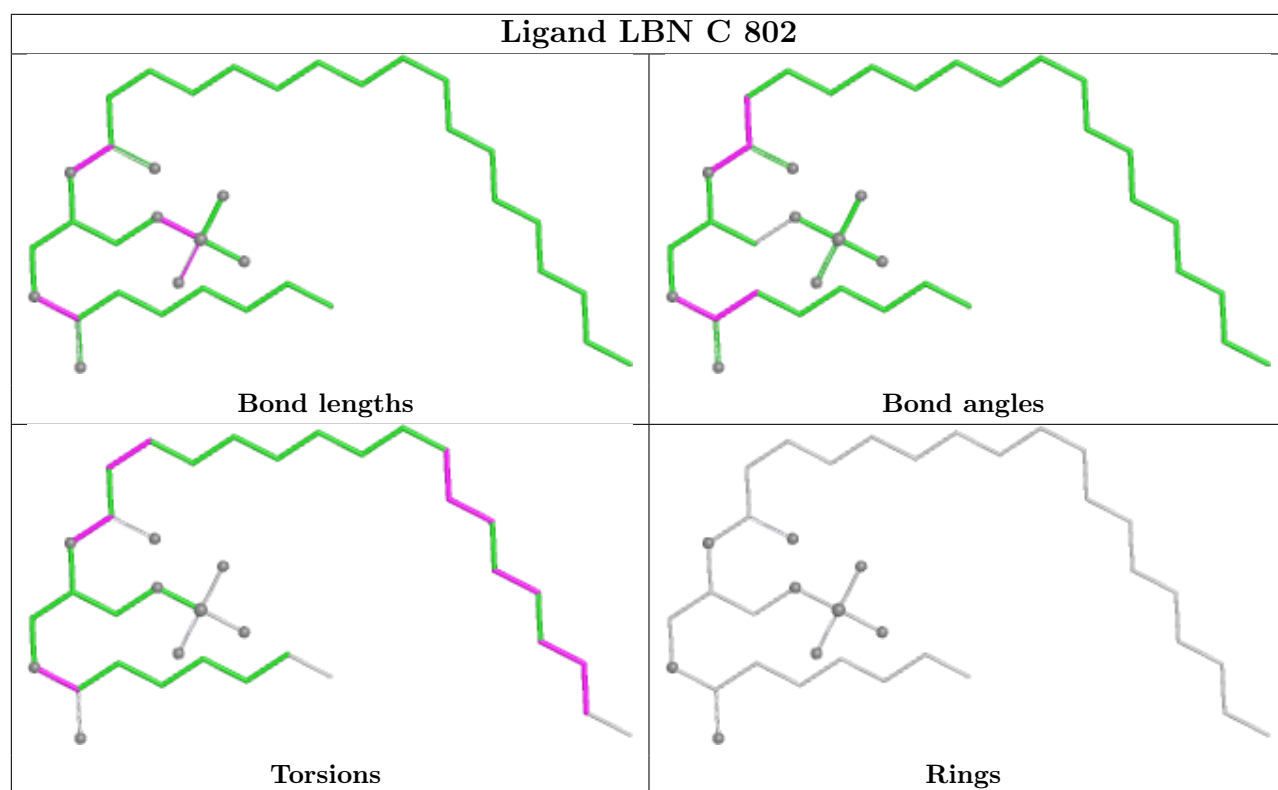
There are no ring outliers.

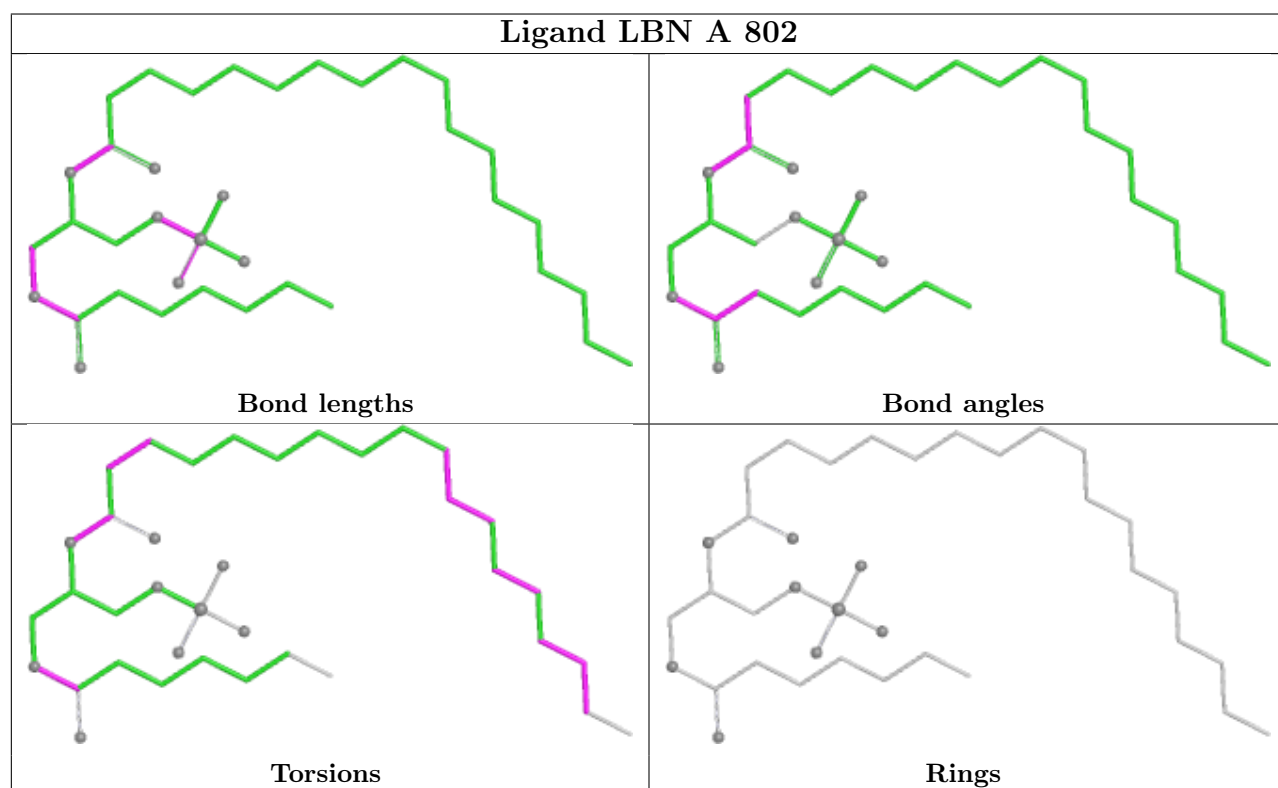
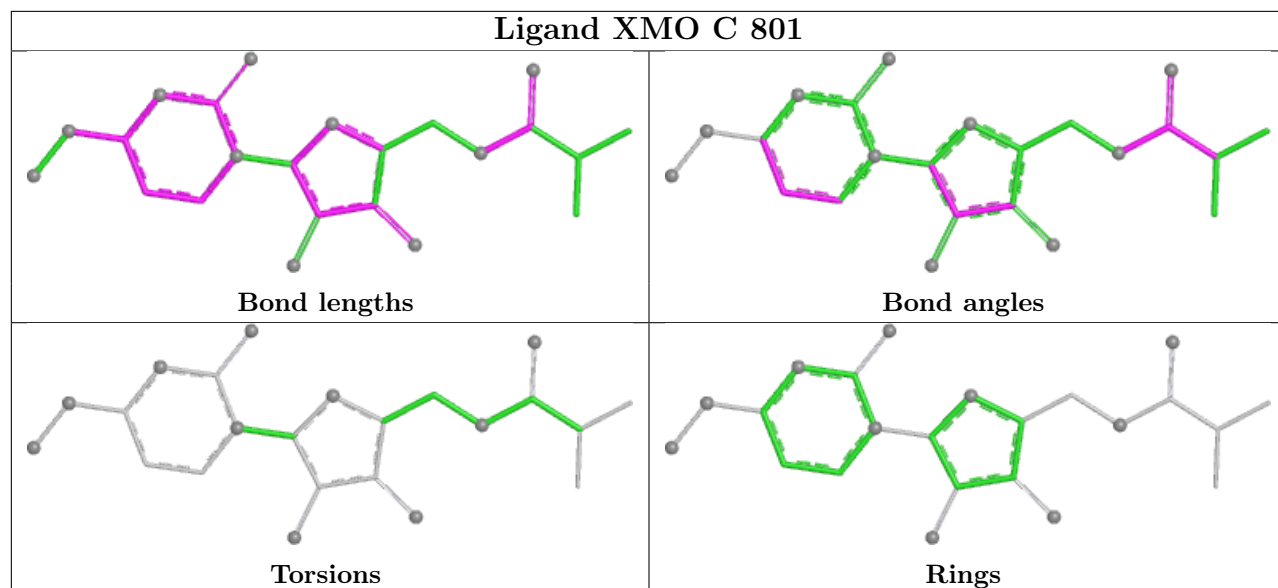
3 monomers are involved in 3 short contacts:

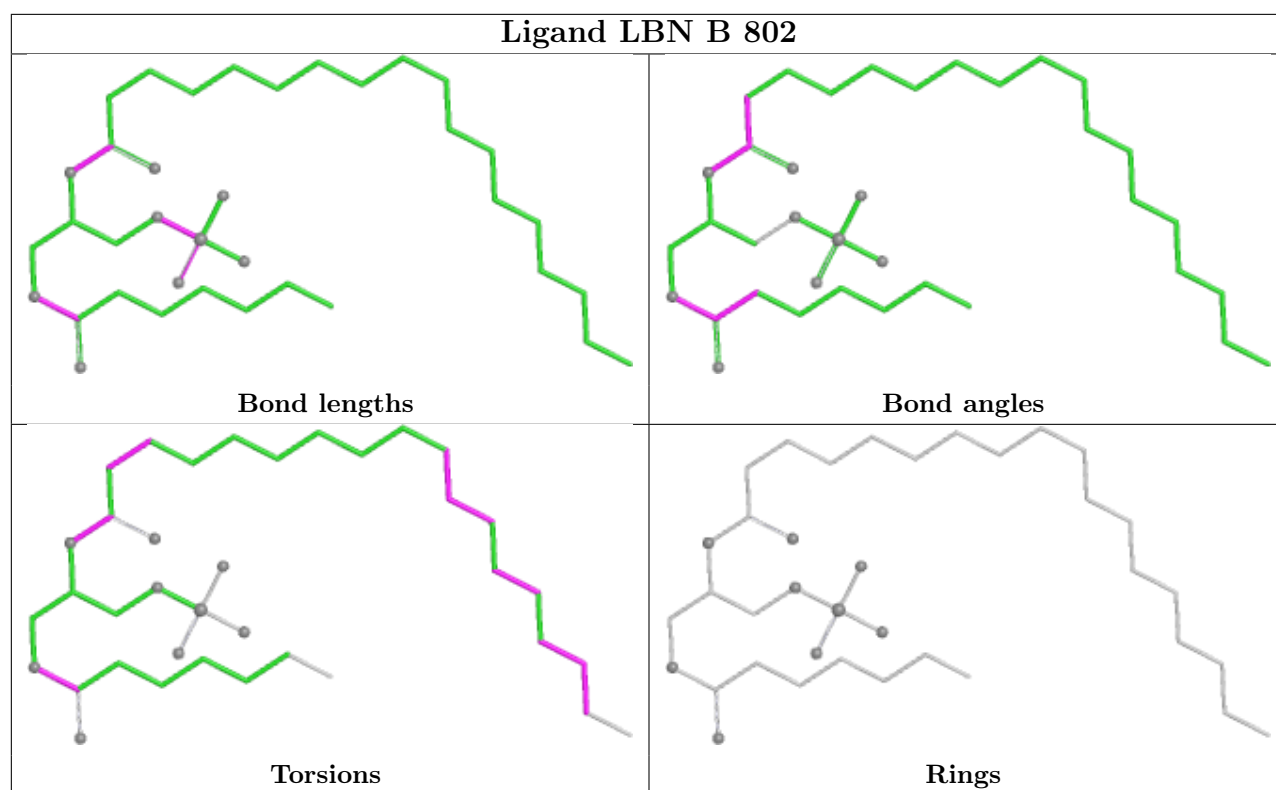
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	XMO	1	0
2	B	801	XMO	1	0
2	C	801	XMO	1	0

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 Map visualisation

This section contains visualisations of the EMDB entry EMD-41736. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit ⓘ

This section was not generated.