



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2021 – 10:12 AM JST

PDB ID : 7DBJ
Title : Crystal structure of human LDHB in complex with NADH, oxamate, and AXKO-0046
Authors : Sogabe, S.; Miwa, M.
Deposited on : 2020-10-20
Resolution : 1.55 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

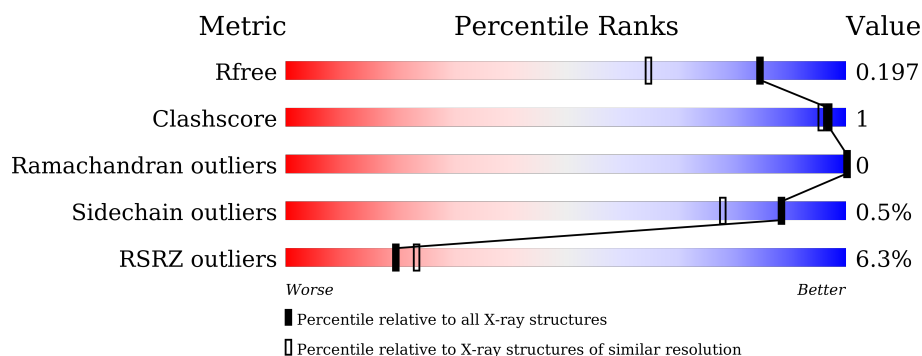
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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}	130704	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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	333	 7% 97%
1	B	333	 8% 96%
1	C	333	 6% 97%
1	D	333	 4% 96%

2 Entry composition ⓘ

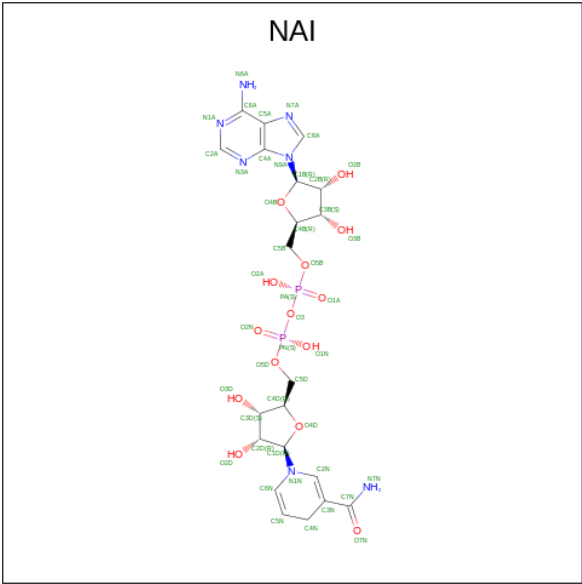
There are 6 unique types of molecules in this entry. The entry contains 11302 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-lactate dehydrogenase B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	1	0
			2564	1630	431	489	14			
1	B	333	Total	C	N	O	S	0	1	0
			2564	1630	431	489	14			
1	C	333	Total	C	N	O	S	0	0	0
			2561	1628	431	488	14			
1	D	333	Total	C	N	O	S	0	1	0
			2564	1630	431	489	14			

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).



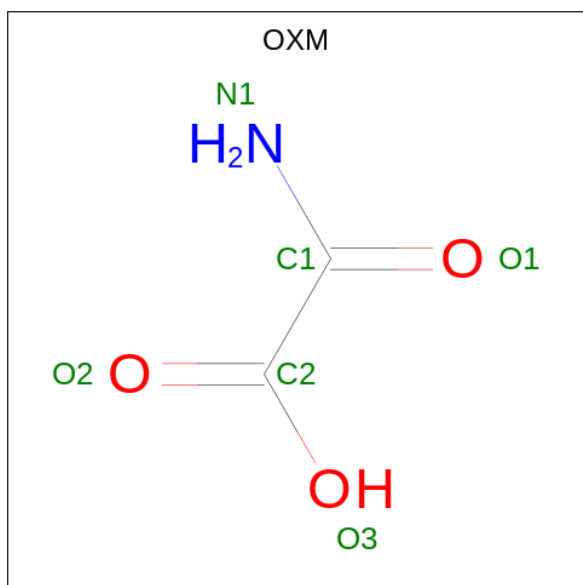
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is OXAMIC ACID (three-letter code: OXM) (formula: $C_2H_3NO_3$).



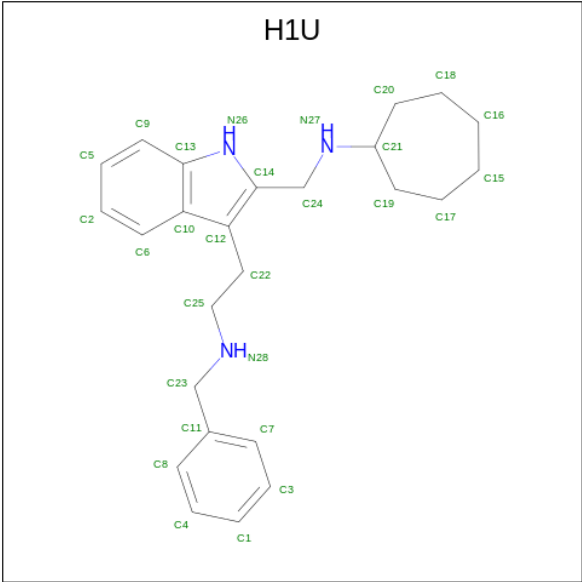
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			6	2	1	3		
3	B	1	Total	C	N	O	0	0
			6	2	1	3		
3	C	1	Total	C	N	O	0	0
			6	2	1	3		
3	D	1	Total	C	N	O	0	0
			6	2	1	3		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is N-[[3-[2-[(phenylmethyl)amino]ethyl]-1H-indol-2-yl]methyl]cycloheptanamine (three-letter code: H1U) (formula: C₂₅H₃₃N₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	N	0	0
			28	25	3		
5	D	1	Total	C	N	0	0
			28	25	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	183	Total	O	0	0
			183	183		
6	B	178	Total	O	0	0
			178	178		
6	C	207	Total	O	0	0
			207	207		
6	D	197	Total	O	0	0
			197	197		

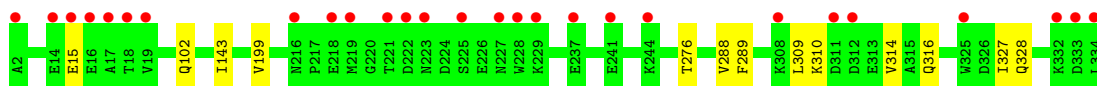
3 Residue-property plots [i](#)

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.

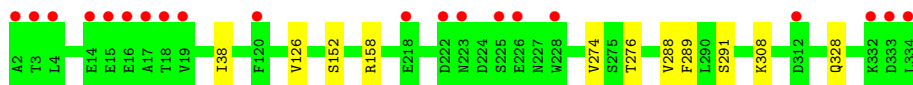
- Molecule 1: L-lactate dehydrogenase B chain



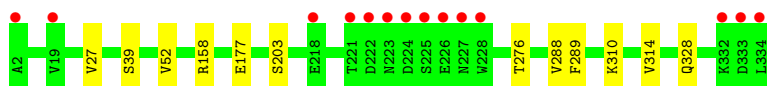
- Molecule 1: L-lactate dehydrogenase B chain



- Molecule 1: L-lactate dehydrogenase B chain



- Molecule 1: L-lactate dehydrogenase B chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.39Å 137.58Å 84.91Å 90.00° 109.26° 90.00°	Depositor
Resolution (Å)	43.50 – 1.55 43.46 – 1.55	Depositor EDS
% Data completeness (in resolution range)	98.9 (43.50-1.55) 99.0 (43.46-1.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.8.0266	Depositor
R, R_{free}	0.170 , 0.192 0.179 , 0.197	Depositor DCC
R_{free} test set	9146 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	21.4	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11302	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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: EDO, H1U, OXM, NAI

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	0.77	0/2608	0.81	2/3534 (0.1%)
1	B	0.75	0/2608	0.78	0/3534
1	C	0.75	0/2602	0.79	1/3526 (0.0%)
1	D	0.75	0/2608	0.79	1/3534 (0.0%)
All	All	0.76	0/10426	0.79	4/14128 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	ARG	NE-CZ-NH2	-8.07	116.27	120.30
1	C	158	ARG	NE-CZ-NH1	-7.54	116.53	120.30
1	A	175	MET	CG-SD-CE	-7.02	88.97	100.20
1	D	158	ARG	NE-CZ-NH1	-6.51	117.05	120.30

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	2564	0	2635	4	0
1	B	2564	0	2635	6	0
1	C	2561	0	2630	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2564	0	2635	5	0
2	A	44	0	27	0	0
2	B	44	0	27	0	0
2	C	44	0	27	0	0
2	D	44	0	27	0	0
3	A	6	0	2	0	0
3	B	6	0	2	0	0
3	C	6	0	2	0	0
3	D	6	0	2	0	0
4	A	4	0	6	0	0
4	B	4	0	6	1	0
4	C	8	0	12	2	0
4	D	12	0	18	0	0
5	C	28	0	0	0	0
5	D	28	0	0	0	0
6	A	183	0	0	0	0
6	B	178	0	0	0	0
6	C	207	0	0	0	0
6	D	197	0	0	0	0
All	All	11302	0	10693	20	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 (20) 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:288:VAL:HA	1:A:328:GLN:HE22	1.64	0.61
1:C:288:VAL:HA	1:C:328:GLN:HE22	1.66	0.60
1:D:288:VAL:HA	1:D:328:GLN:HE22	1.71	0.56
1:B:309:LEU:HB2	1:B:314:VAL:HG22	1.90	0.54
1:B:288:VAL:HA	1:B:328:GLN:HE22	1.73	0.52
1:B:143:ILE:HD13	1:B:327:ILE:HG21	1.95	0.47
1:A:38:ILE:HG13	4:B:403:EDO:H22	1.96	0.47
1:B:199:VAL:HG22	1:B:316:GLN:HG3	1.97	0.46
1:D:276:THR:O	1:D:289:PHE:HA	2.16	0.46
1:A:176:ALA:HB1	1:A:181:ILE:O	2.17	0.45
1:D:203:SER:HB3	1:D:310:LYS:HG3	1.99	0.44
1:C:38:ILE:HG13	4:C:605:EDO:H11	1.99	0.44
1:A:215:LEU:CD2	1:C:308:LYS:HE2	2.47	0.44
1:C:276:THR:O	1:C:289:PHE:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:LYS:O	1:B:314:VAL:HG23	2.20	0.42
1:B:276:THR:O	1:B:289:PHE:HA	2.20	0.41
4:C:605:EDO:H12	1:D:39:SER:HA	2.03	0.41
1:C:274:VAL:O	1:C:291:SER:HA	2.21	0.40
1:C:126:VAL:HG21	1:C:152:SER:HB2	2.03	0.40
1:D:27:VAL:HG22	1:D:52:VAL:CG1	2.51	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	332/333 (100%)	323 (97%)	9 (3%)	0	100	100
1	B	332/333 (100%)	322 (97%)	10 (3%)	0	100	100
1	C	331/333 (99%)	321 (97%)	10 (3%)	0	100	100
1	D	332/333 (100%)	323 (97%)	9 (3%)	0	100	100
All	All	1327/1332 (100%)	1289 (97%)	38 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	290/289 (100%)	288 (99%)	2 (1%)	84	69
1	B	290/289 (100%)	288 (99%)	2 (1%)	84	69
1	C	289/289 (100%)	289 (100%)	0	100	100
1	D	290/289 (100%)	288 (99%)	2 (1%)	84	69
All	All	1159/1156 (100%)	1153 (100%)	6 (0%)	88	78

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

Mol	Chain	Res	Type
1	A	16	GLU
1	A	312	ASP
1	B	15	GLU
1	B	102	GLN
1	D	177	GLU
1	D	314	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	328	GLN
1	B	21	ASN
1	B	328	GLN
1	C	21	ASN
1	C	328	GLN
1	D	21	ASN
1	D	102	GLN
1	D	328	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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

17 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OXM	B	402	-	2,5,5	0.46	0	2,6,6	0.88	0
4	EDO	D	606	-	3,3,3	0.05	0	2,2,2	0.17	0
4	EDO	B	403	-	3,3,3	0.08	0	2,2,2	0.35	0
5	H1U	C	601	-	29,31,31	1.10	1 (3%)	28,40,40	1.58	2 (7%)
4	EDO	D	604	-	3,3,3	0.12	0	2,2,2	0.16	0
3	OXM	D	603	-	2,5,5	0.34	0	2,6,6	0.97	0
4	EDO	C	604	-	3,3,3	0.12	0	2,2,2	0.13	0
4	EDO	D	605	-	3,3,3	0.04	0	2,2,2	0.17	0
2	NAI	B	401	-	42,48,48	0.56	0	47,73,73	0.87	1 (2%)
3	OXM	A	402	-	2,5,5	0.31	0	2,6,6	0.82	0
3	OXM	C	603	-	2,5,5	0.10	0	2,6,6	0.76	0
4	EDO	A	403	-	3,3,3	0.11	0	2,2,2	0.06	0
2	NAI	A	401	-	42,48,48	0.57	0	47,73,73	0.99	3 (6%)
2	NAI	C	602	-	42,48,48	0.60	0	47,73,73	0.96	3 (6%)
4	EDO	C	605	-	3,3,3	0.04	0	2,2,2	0.35	0
5	H1U	D	601	-	29,31,31	1.03	2 (6%)	28,40,40	1.17	3 (10%)
2	NAI	D	602	-	42,48,48	0.57	0	47,73,73	0.82	1 (2%)

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
3	OXM	B	402	-	-	0/0/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	D	606	-	-	1/1/1/1	-
4	EDO	B	403	-	-	1/1/1/1	-
5	H1U	C	601	-	-	3/8/21/21	0/4/4/4
4	EDO	D	604	-	-	0/1/1/1	-
3	OXM	D	603	-	-	0/0/4/4	-
4	EDO	C	604	-	-	1/1/1/1	-
4	EDO	D	605	-	-	0/1/1/1	-
2	NAI	B	401	-	-	4/25/72/72	0/5/5/5
3	OXM	A	402	-	-	0/0/4/4	-
3	OXM	C	603	-	-	0/0/4/4	-
4	EDO	A	403	-	-	0/1/1/1	-
2	NAI	A	401	-	-	4/25/72/72	0/5/5/5
2	NAI	C	602	-	-	4/25/72/72	0/5/5/5
4	EDO	C	605	-	-	1/1/1/1	-
5	H1U	D	601	-	-	2/8/21/21	0/4/4/4
2	NAI	D	602	-	-	4/25/72/72	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	601	H1U	C22-C12	-3.49	1.46	1.52
5	D	601	H1U	C22-C12	-3.11	1.46	1.52
5	D	601	H1U	C19-C21	2.13	1.55	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	601	H1U	C22-C12-C14	-7.17	122.26	127.30
5	D	601	H1U	C22-C12-C14	-3.38	124.92	127.30
2	A	401	NAI	PN-O3-PA	-3.09	122.22	132.83
2	C	602	NAI	PN-O3-PA	-2.94	122.75	132.83
2	B	401	NAI	PN-O3-PA	-2.93	122.77	132.83
2	A	401	NAI	C1D-N1N-C2N	-2.60	116.78	121.11
2	D	602	NAI	PN-O3-PA	-2.55	124.08	132.83
2	A	401	NAI	C5A-C6A-N6A	2.38	123.97	120.35
5	C	601	H1U	C5-C9-C13	-2.27	116.82	120.08
2	C	602	NAI	O4D-C1D-C2D	-2.25	101.74	106.64
5	D	601	H1U	C24-N27-C21	2.17	117.25	114.14
5	D	601	H1U	C23-C11-C8	-2.16	116.44	120.91
2	C	602	NAI	C1D-N1N-C2N	-2.05	117.69	121.11

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	601	H1U	C10-C12-C22-C25
5	C	601	H1U	C14-C12-C22-C25
5	C	601	H1U	C12-C22-C25-N28
5	D	601	H1U	C10-C12-C22-C25
5	D	601	H1U	C14-C12-C22-C25
2	C	602	NAI	C2D-C1D-N1N-C2N
2	A	401	NAI	C2D-C1D-N1N-C2N
2	B	401	NAI	C2D-C1D-N1N-C2N
2	A	401	NAI	O4D-C1D-N1N-C2N
2	B	401	NAI	O4D-C1D-N1N-C2N
2	D	602	NAI	C2D-C1D-N1N-C2N
2	C	602	NAI	O4D-C1D-N1N-C2N
4	C	605	EDO	O1-C1-C2-O2
2	D	602	NAI	O4D-C1D-N1N-C2N
4	B	403	EDO	O1-C1-C2-O2
4	D	606	EDO	O1-C1-C2-O2
2	B	401	NAI	O4B-C4B-C5B-O5B
2	D	602	NAI	C2D-C1D-N1N-C6N
4	C	604	EDO	O1-C1-C2-O2
2	A	401	NAI	O4B-C4B-C5B-O5B
2	C	602	NAI	O4B-C4B-C5B-O5B
2	D	602	NAI	O4B-C4B-C5B-O5B
2	A	401	NAI	C2D-C1D-N1N-C6N
2	B	401	NAI	C2D-C1D-N1N-C6N
2	C	602	NAI	C2D-C1D-N1N-C6N

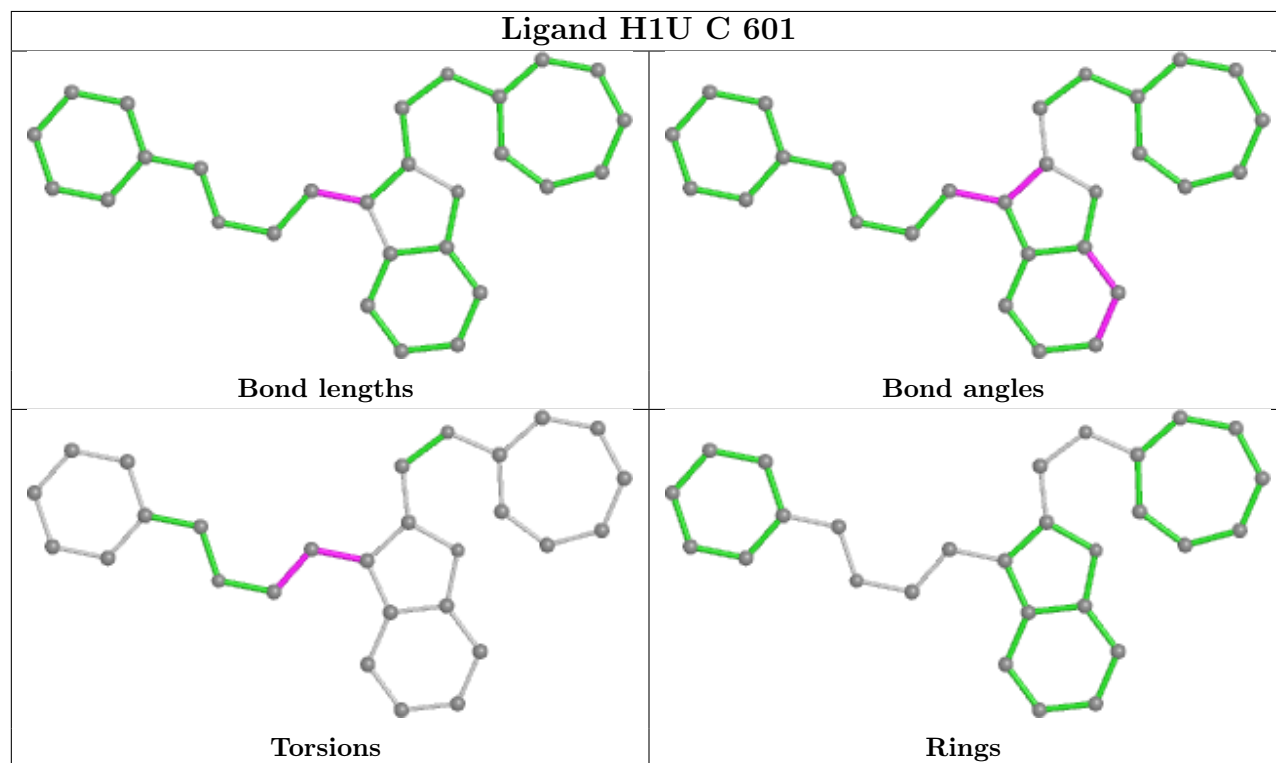
There are no ring outliers.

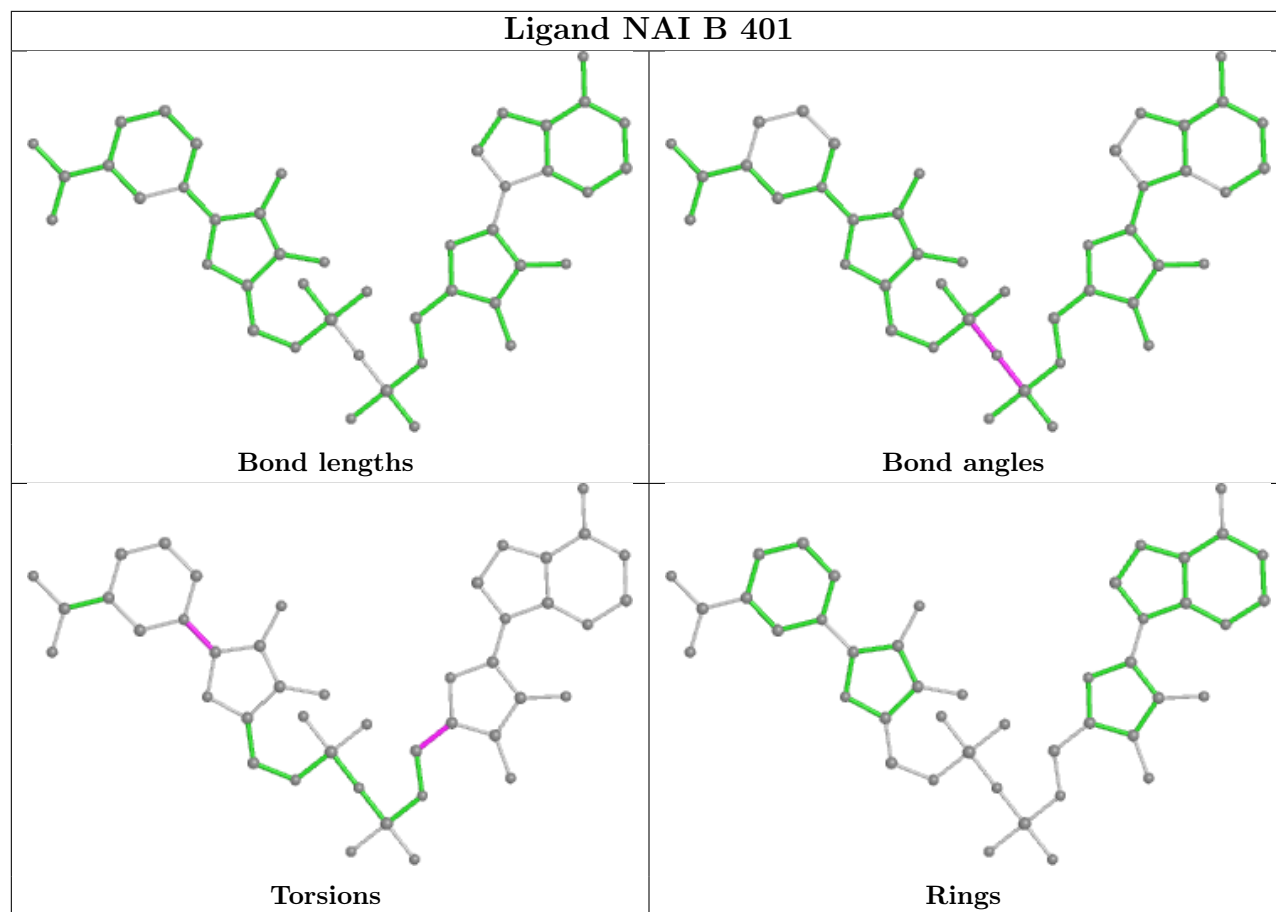
2 monomers are involved in 3 short contacts:

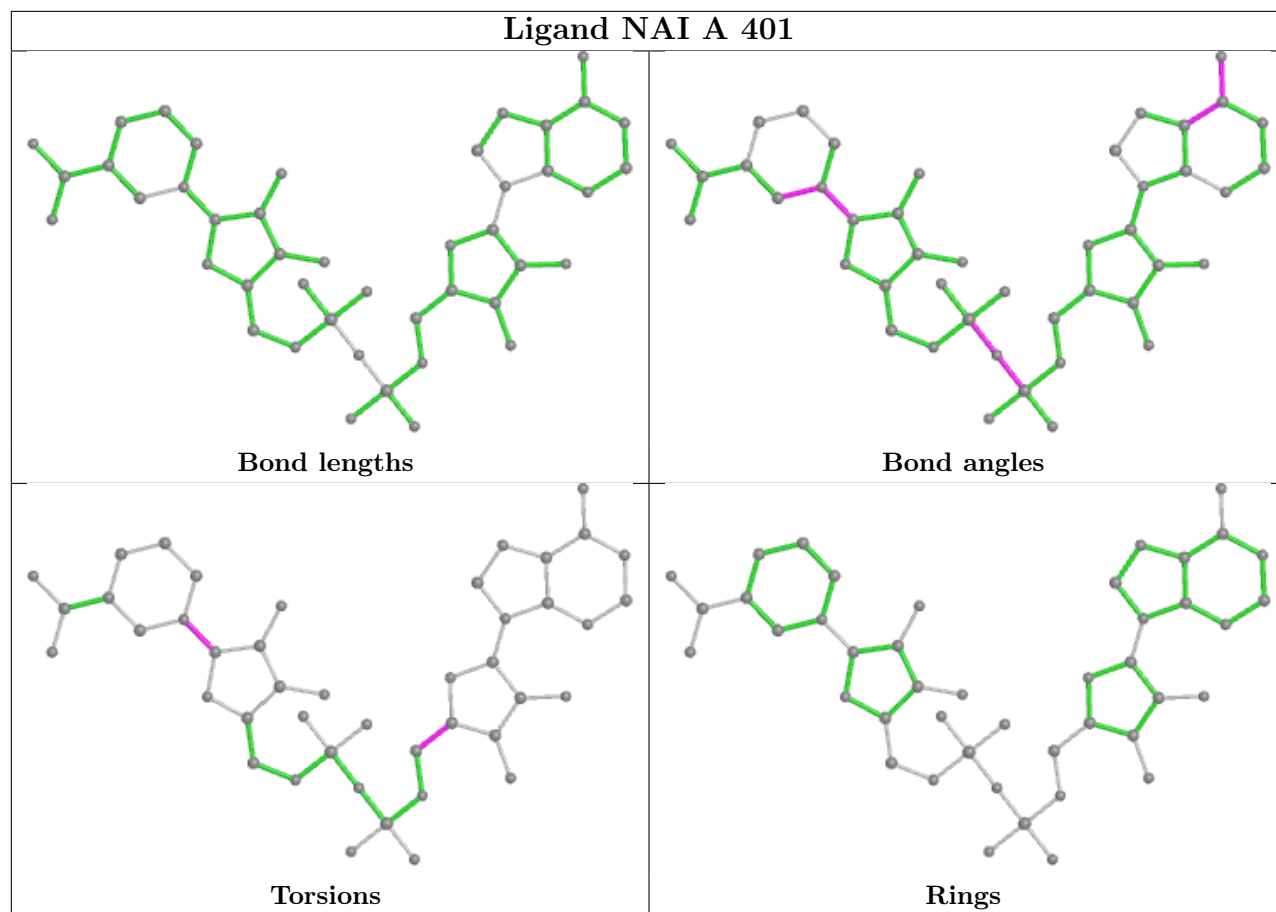
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	403	EDO	1	0
4	C	605	EDO	2	0

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

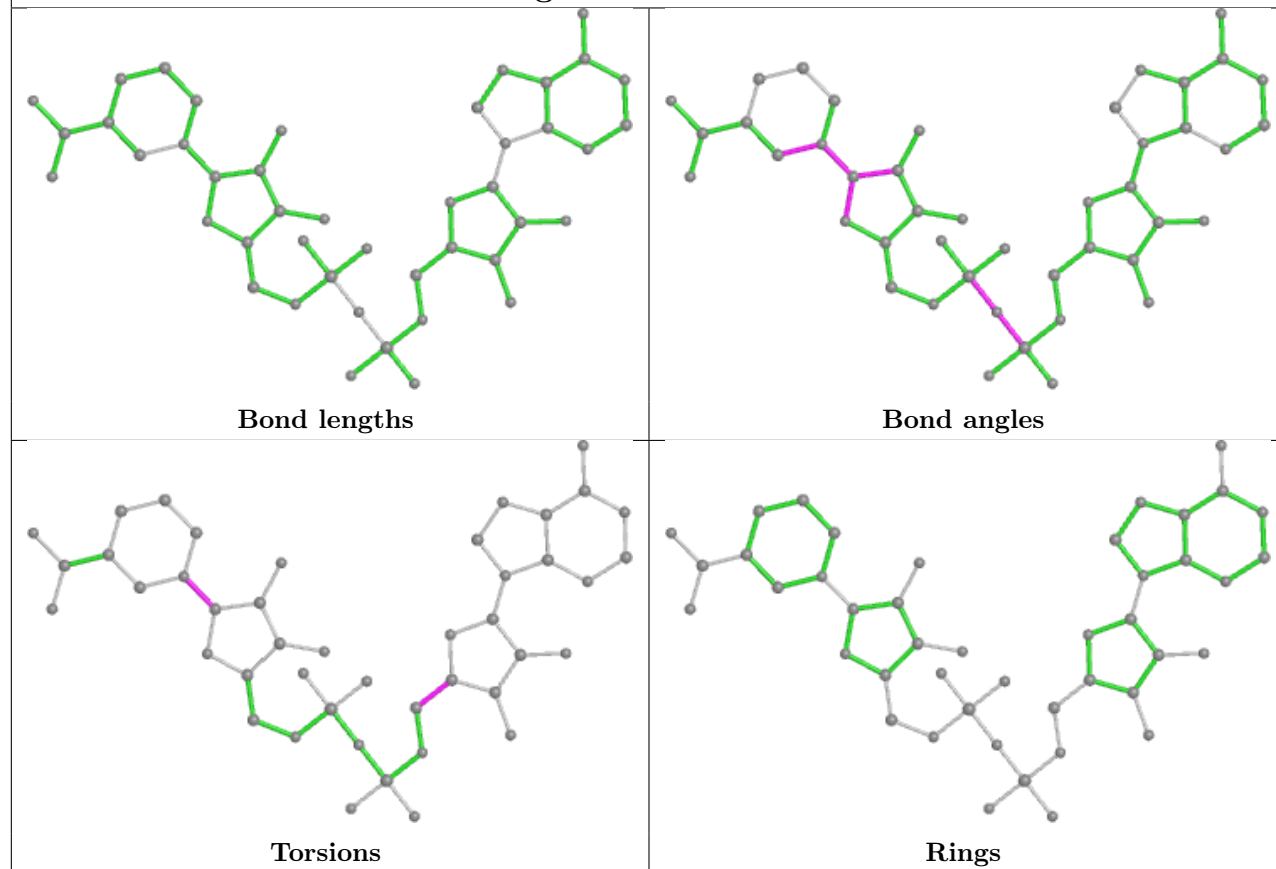
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



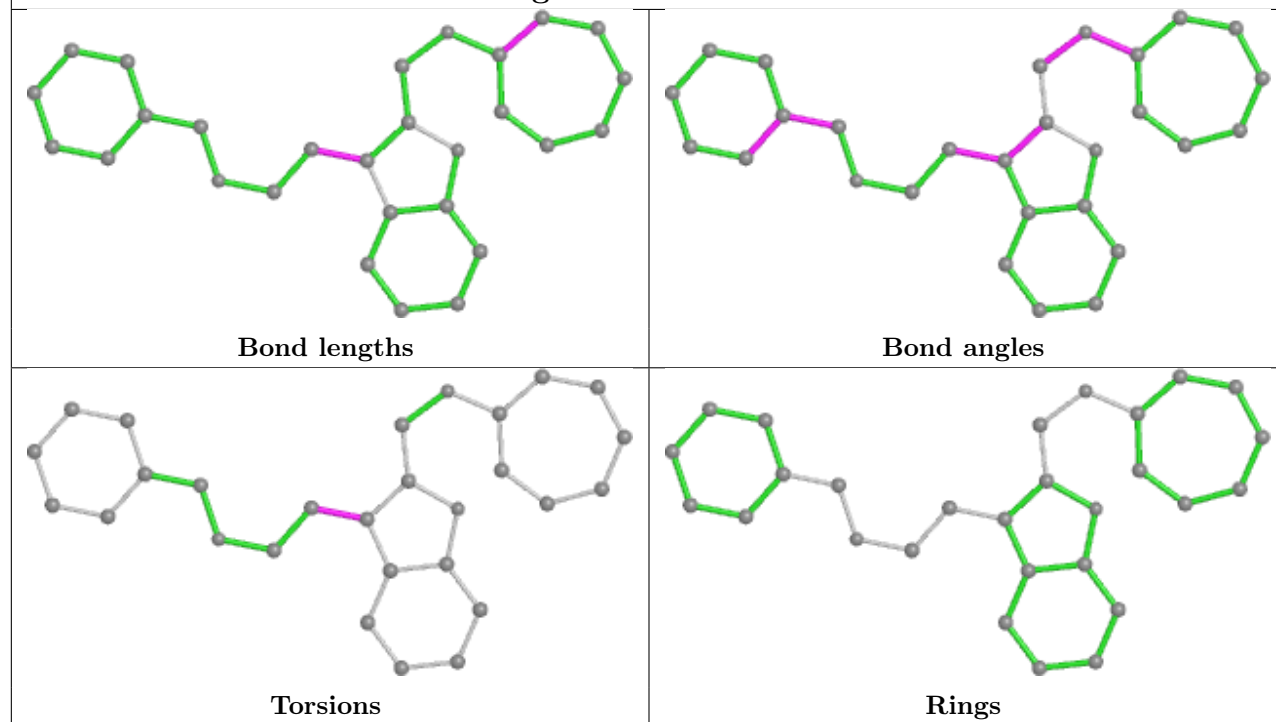


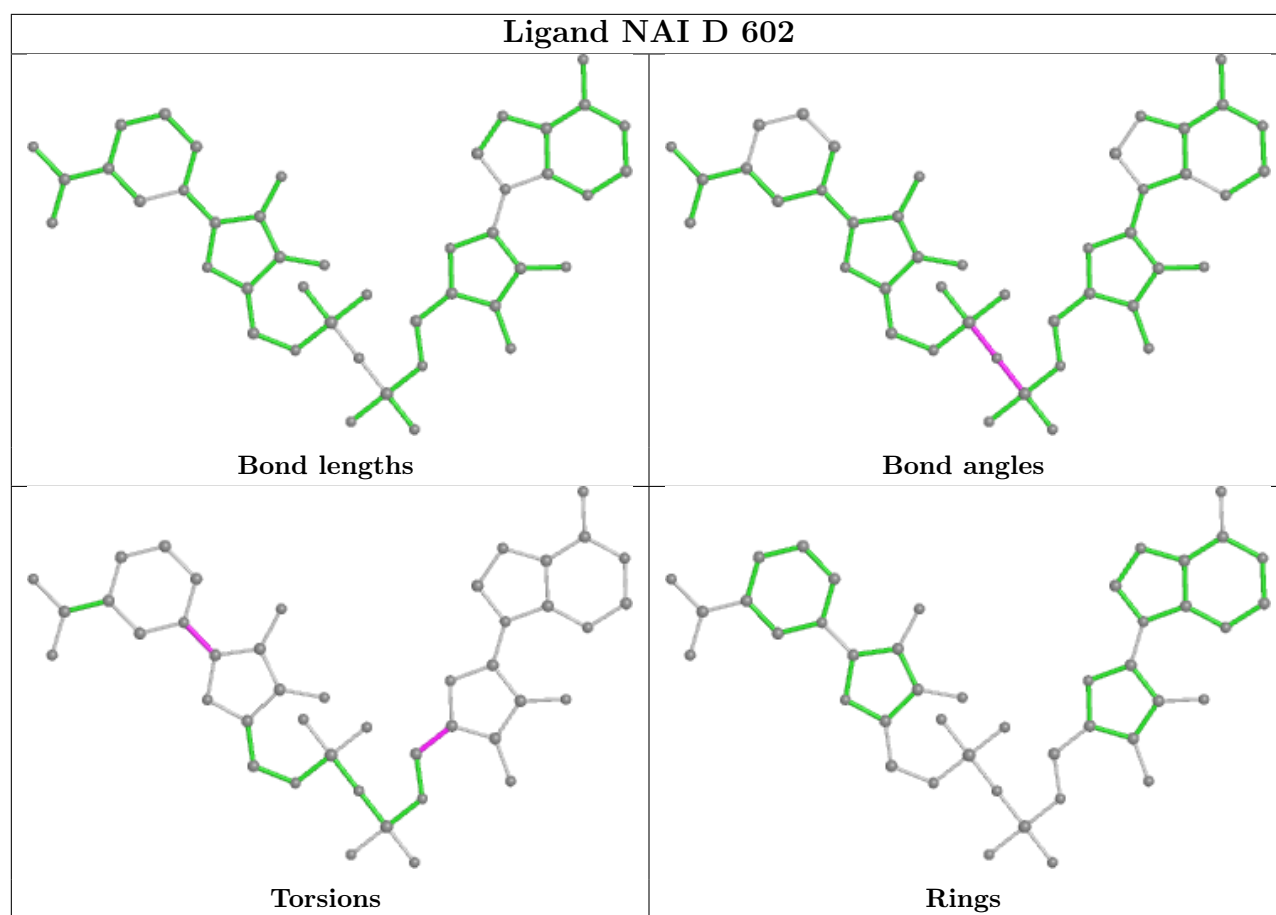


Ligand NAI C 602



Ligand H1U D 601





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	333/333 (100%)	0.28	23 (6%)	16 20	18, 23, 35, 43	0
1	B	333/333 (100%)	0.30	27 (8%)	12 14	18, 26, 40, 47	0
1	C	333/333 (100%)	0.24	20 (6%)	21 25	17, 22, 33, 42	0
1	D	333/333 (100%)	0.21	14 (4%)	36 41	18, 24, 36, 48	0
All	All	1332/1332 (100%)	0.26	84 (6%)	20 23	17, 23, 37, 48	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	17	ALA	12.7
1	A	334	LEU	9.5
1	A	17	ALA	8.9
1	A	120	PHE	7.9
1	B	334	LEU	7.8
1	C	334	LEU	7.3
1	C	18	THR	7.1
1	A	18	THR	5.9
1	A	223	ASN	5.9
1	D	223	ASN	5.8
1	D	2	ALA	5.6
1	C	223	ASN	5.6
1	A	14	GLU	5.5
1	A	222	ASP	5.4
1	C	333	ASP	5.2
1	D	334	LEU	5.2
1	C	2	ALA	5.1
1	C	15	GLU	5.0
1	A	333	ASP	4.7
1	A	16	GLU	4.6
1	B	19	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	223	ASN	4.5
1	C	120	PHE	4.4
1	C	16	GLU	4.3
1	B	14	GLU	4.3
1	D	333	ASP	4.3
1	A	15	GLU	4.2
1	B	18	THR	4.1
1	C	222	ASP	3.9
1	D	222	ASP	3.9
1	B	16	GLU	3.9
1	B	333	ASP	3.9
1	C	14	GLU	3.9
1	D	227	ASN	3.7
1	D	332	LYS	3.6
1	B	222	ASP	3.6
1	A	332	LYS	3.5
1	B	17	ALA	3.4
1	B	2	ALA	3.4
1	C	332	LYS	3.4
1	B	311	ASP	3.4
1	C	225	SER	3.3
1	D	225	SER	3.3
1	B	225	SER	3.2
1	A	218	GLU	3.1
1	A	330	ASP	3.1
1	D	221	THR	3.1
1	D	218	GLU	3.1
1	B	227	ASN	3.0
1	C	19	VAL	3.0
1	D	19	VAL	3.0
1	A	112	GLN	2.9
1	B	15	GLU	2.9
1	A	19	VAL	2.8
1	D	224	ASP	2.7
1	B	221	THR	2.6
1	B	237	GLU	2.6
1	A	2	ALA	2.6
1	A	228	TRP	2.6
1	A	225	SER	2.6
1	A	227	ASN	2.5
1	B	218	GLU	2.5
1	B	325	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	332	LYS	2.5
1	C	218	GLU	2.4
1	B	228	TRP	2.4
1	B	229	LYS	2.4
1	A	285	GLU	2.3
1	B	312	ASP	2.3
1	B	244	LYS	2.3
1	B	241	GLU	2.3
1	B	219	MET	2.3
1	D	228	TRP	2.3
1	D	226	GLU	2.2
1	C	4	LEU	2.2
1	C	312	ASP	2.2
1	B	308	LYS	2.2
1	A	312	ASP	2.1
1	C	228	TRP	2.1
1	C	3	THR	2.1
1	B	216	ASN	2.1
1	A	226	GLU	2.0
1	A	261	ILE	2.0
1	C	226	GLU	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 monosaccharides 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.

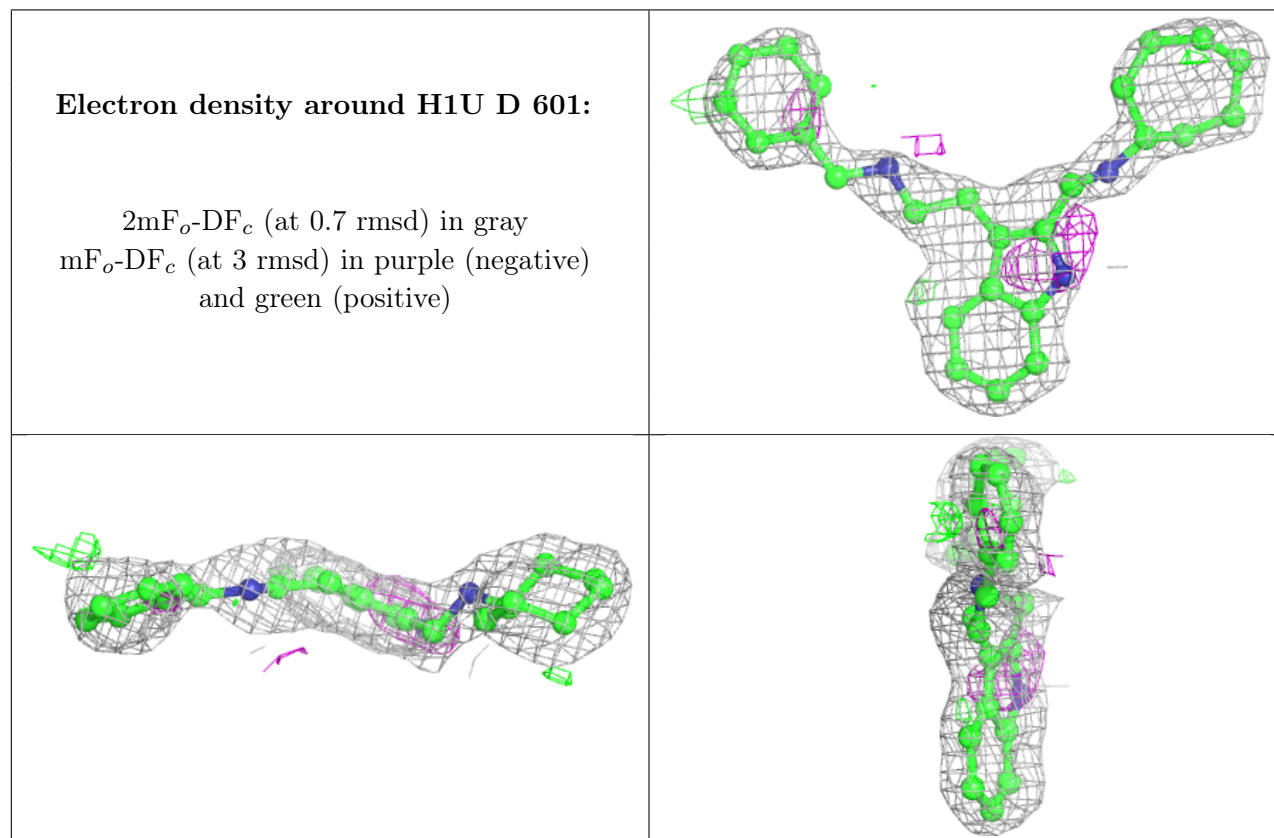
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	H1U	D	601	28/28	0.67	0.18	32,39,42,43	0
5	H1U	C	601	28/28	0.77	0.18	27,37,39,40	0

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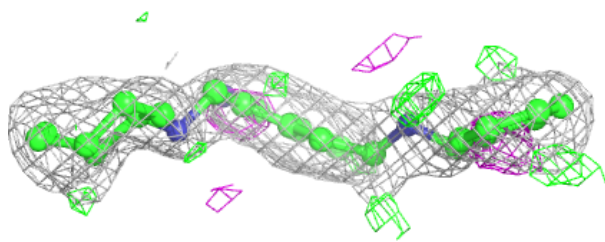
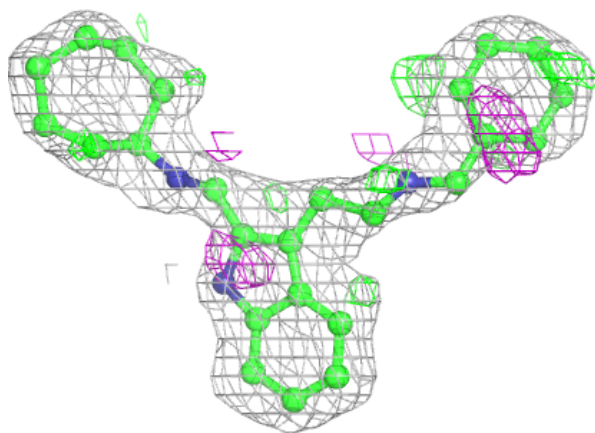
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	D	606	4/4	0.77	0.27	41,41,41,42	0
4	EDO	B	403	4/4	0.82	0.15	37,38,39,40	0
4	EDO	D	604	4/4	0.87	0.12	33,34,34,34	0
4	EDO	C	605	4/4	0.87	0.13	37,37,38,39	0
4	EDO	C	604	4/4	0.90	0.11	34,39,39,40	0
4	EDO	A	403	4/4	0.93	0.22	36,37,37,38	0
4	EDO	D	605	4/4	0.94	0.10	34,36,36,37	0
2	NAI	B	401	44/44	0.96	0.09	22,25,28,29	0
2	NAI	D	602	44/44	0.96	0.10	20,23,29,30	0
3	OXM	A	402	6/6	0.96	0.08	21,23,25,25	0
2	NAI	A	401	44/44	0.96	0.09	20,24,29,30	0
3	OXM	B	402	6/6	0.97	0.07	27,27,28,28	0
3	OXM	C	603	6/6	0.97	0.09	20,22,23,23	0
3	OXM	D	603	6/6	0.97	0.07	25,26,27,27	0
2	NAI	C	602	44/44	0.97	0.09	18,22,27,29	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.



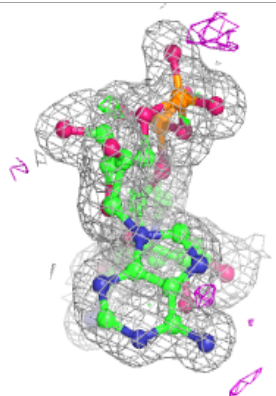
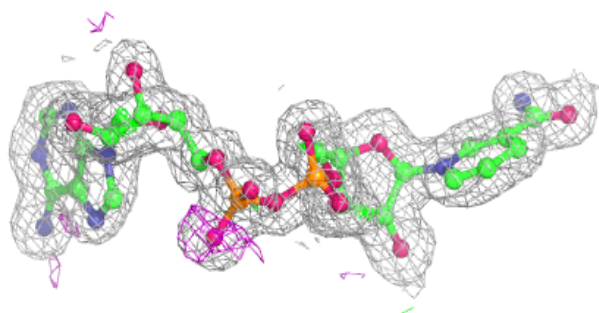
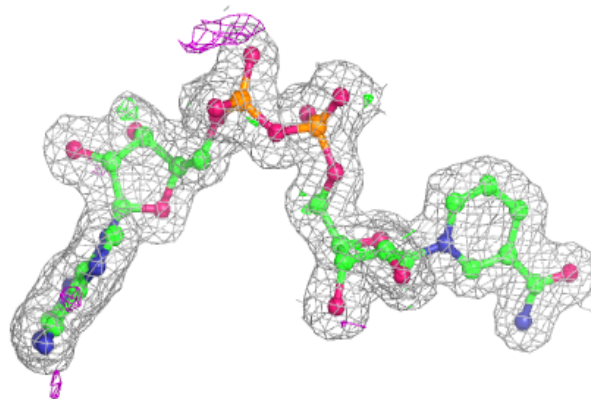
Electron density around H1U C 601:

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

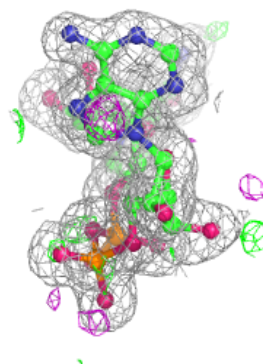
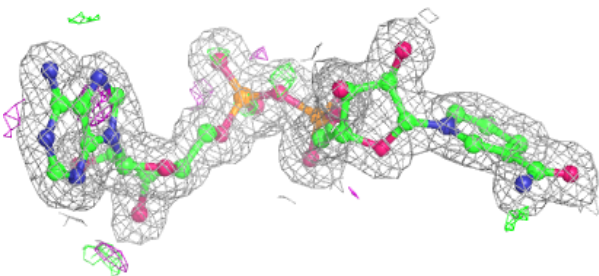
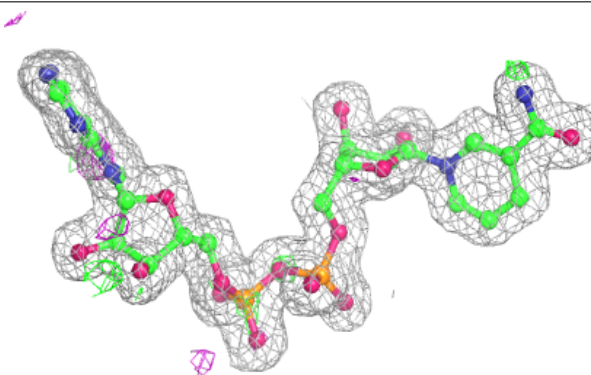


Electron density around NAI B 401:

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

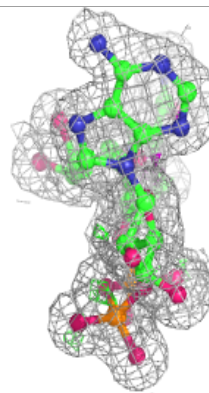
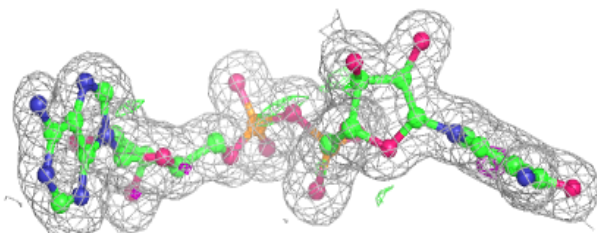
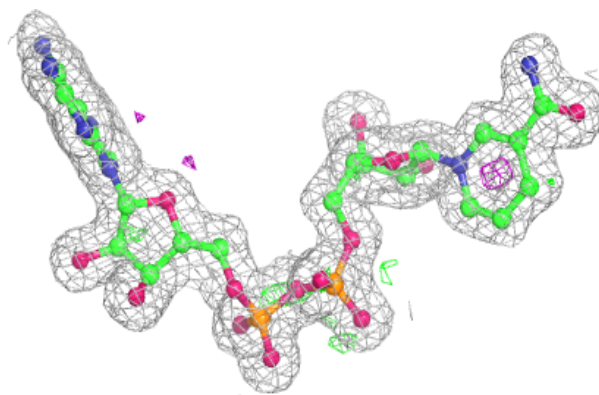
**Electron density around NAI D 602:**

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

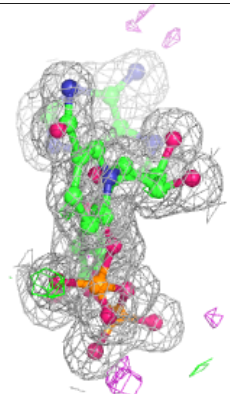
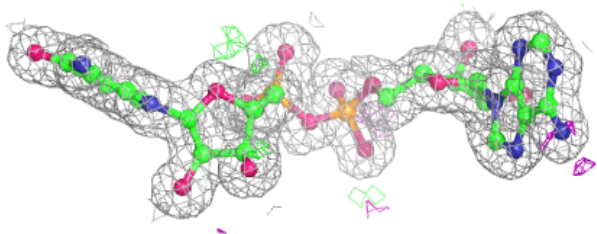
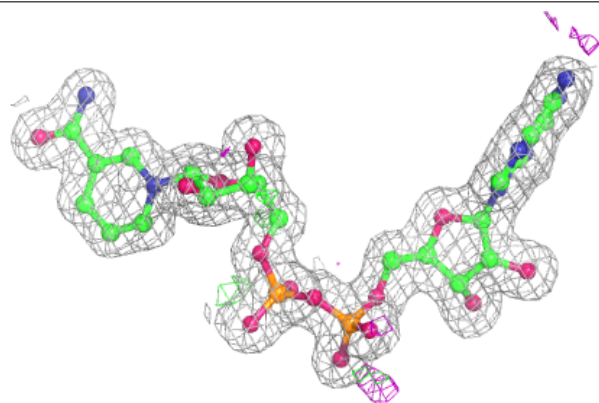


Electron density around NAI A 401:

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

**Electron density around NAI C 602:**

$2mF_o-DF_c$ (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.