



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:04 PM UTC

PDB ID : 2C2T / pdb_00002c2t
Title : Human Dihydrofolate Reductase Complexed With NADPH and 2,4-Diamino-5-((7,8-dicarbaundecaboran-7-yl)methyl)-6-methylpyrimidine, a novel boron containing, nonclassical Antifolate
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Deposited on : 2005-09-30
Resolution : 1.50 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

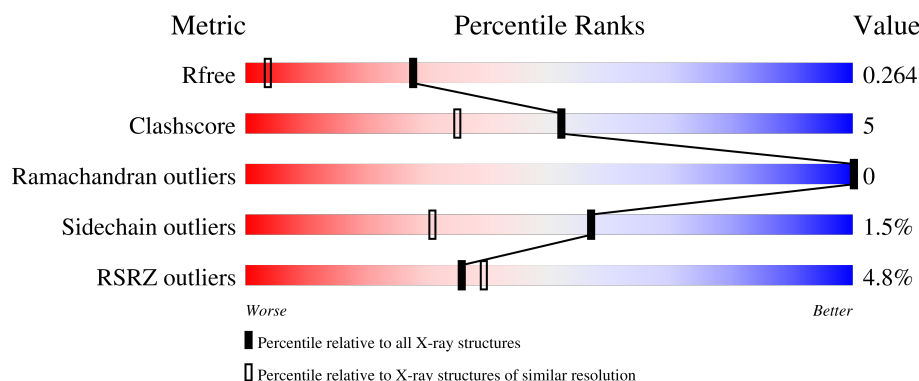
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	186	 5% 88% 11%
1	B	186	 4% 90% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	39B	A	1189[B]	X	-	-	-
3	39B	B	1189[B]	X	-	-	-

2 Entry composition [i](#)

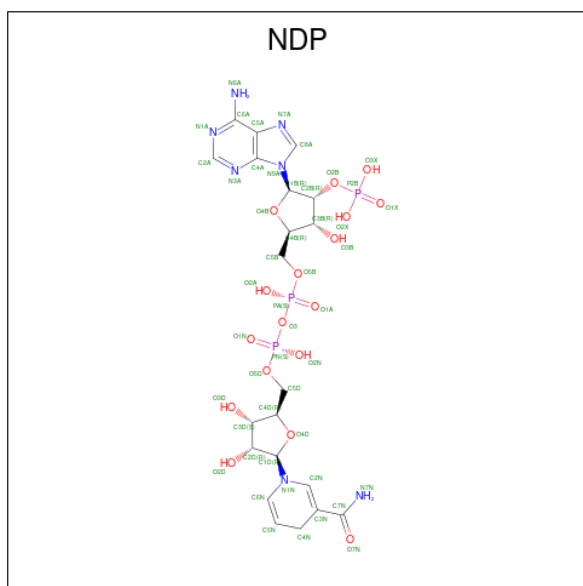
There are 5 unique types of molecules in this entry. The entry contains 3925 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DIHYDROFOLATE REDUCTASE.

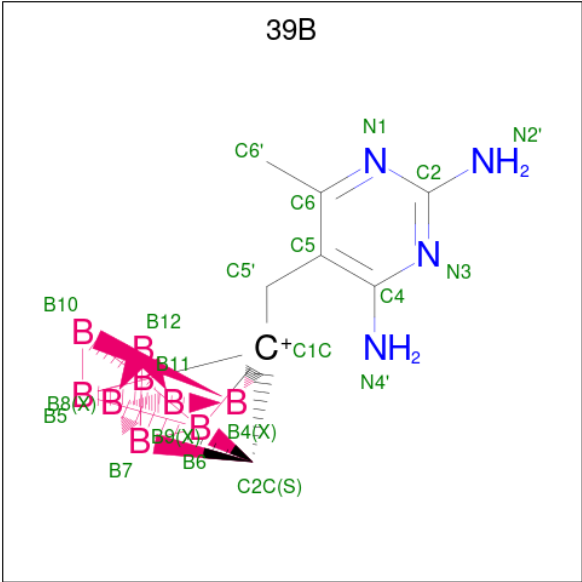
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	15	17	0
			1582	1022	264	289	7			
1	B	186	Total	C	N	O	S	27	11	0
			1550	994	257	291	8			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



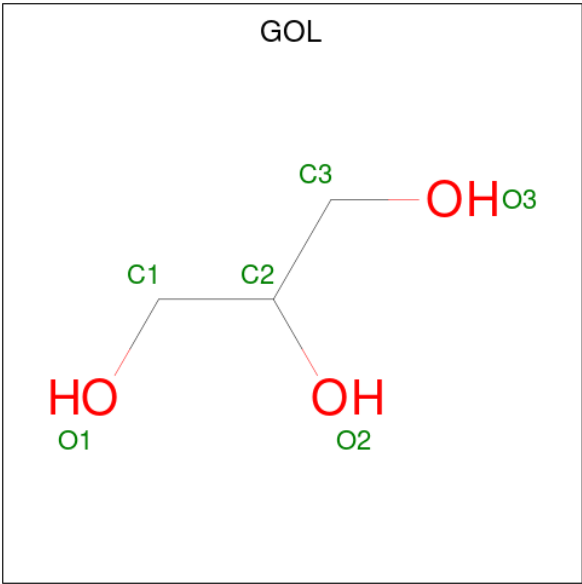
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is (S)-2,4-DIAMINO-5-((7,8-DICARBAUNDECABORAN-7-YL)METHYL)-6-METHYLPYRIMIDINE (CCD ID: 39B) (formula: $C_8H_9B_9N_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	B	C	N	0	1
			21	9	8	4		
3	A	1	Total	B	C	N	0	1
			21	9	8	4		
3	B	1	Total	B	C	N	0	1
			21	9	8	4		
3	B	1	Total	B	C	N	0	1
			21	9	8	4		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		

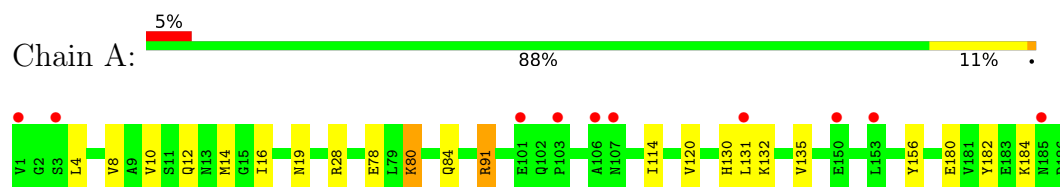
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	297	Total	O	0	8
			297	297		
5	B	310	Total	O	0	7
			310	310		

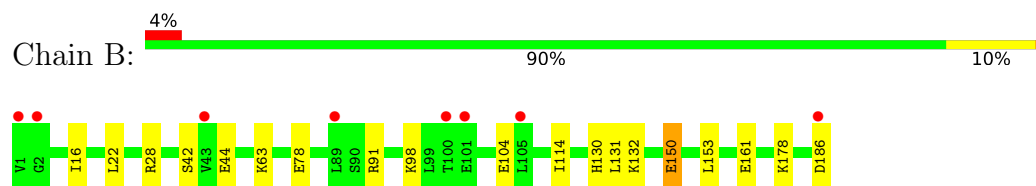
3 Residue-property plots [i](#)

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: DIHYDROFOLATE REDUCTASE



• Molecule 1: DIHYDROFOLATE REDUCTASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	87.63Å 94.35Å 96.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.50 20.00 – 1.50	Depositor EDS
% Data completeness (in resolution range)	98.1 (20.00-1.50) 98.0 (20.00-1.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.158 , 0.213 (Not available) , 0.264	Depositor DCC
R_{free} test set	3168 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	17.7	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 60.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3925	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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: 39B, GOL, NDP

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	1.07	3/1679 (0.2%)	0.78	1/2264 (0.0%)
1	B	1.38	6/1623 (0.4%)	1.21	8/2190 (0.4%)
All	All	1.23	9/3302 (0.3%)	1.02	9/4454 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	44	GLU	CB-CG	30.44	2.43	1.52
1	B	28	ARG	CD-NE	-29.80	1.04	1.46
1	A	91	ARG	CD-NE	-22.93	1.14	1.46
1	A	28	ARG	CD-NE	-19.20	1.19	1.46
1	B	63	LYS	CB-CG	-15.99	1.04	1.52
1	B	150	GLU	CB-CG	-15.00	1.07	1.52
1	A	80	LYS	CB-CG	-14.53	1.08	1.52
1	B	161	GLU	CG-CD	-7.39	1.33	1.52
1	B	78	GLU	CG-CD	5.03	1.64	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	150	GLU	CB-CG-CD	32.60	168.03	112.60
1	B	28	ARG	CD-NE-CZ	17.10	148.34	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	28	ARG	CG-CD-NE	17.01	149.42	112.00
1	B	150	GLU	CA-CB-CG	11.50	137.11	114.10
1	B	63	LYS	CA-CB-CG	9.29	132.68	114.10
1	B	44	GLU	CA-CB-CG	-8.46	97.17	114.10
1	B	161	GLU	CB-CG-CD	5.90	122.63	112.60
1	B	91	ARG	CB-CG-CD	-5.79	97.98	111.30
1	A	91	ARG	CG-CD-NE	5.15	123.32	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	91	ARG	Sidechain

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5.2 Torsion angles [i](#)

5.2.1 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	201/186 (108%)	198 (98%)	3 (2%)	0	100	100
1	B	195/186 (105%)	193 (99%)	2 (1%)	0	100	100
All	All	396/372 (106%)	391 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.2.2 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	185/168 (110%)	185 (100%)	0	100	100
1	B	179/168 (106%)	174 (97%)	5 (3%)	38	11
All	All	364/336 (108%)	359 (99%)	5 (1%)	57	33

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	42	SER
1	B	114	ILE
1	B	131	LEU
1	B	150	GLU
1	B	186	ASP

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

Mol	Chain	Res	Type
1	A	5	ASN
1	A	126	ASN
1	A	127	HIS
1	A	130	HIS
1	A	140	GLN
1	B	5	ASN
1	B	29	ASN
1	B	64	ASN

5.2.3 RNA ⓘ

There are no RNA molecules in this entry.

5.3 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.4 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.5 Ligand geometry

7 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	39B	B	1189[B]	-	26,36,36	1.31	3 (11%)	76,109,109	2.31	9 (11%)
2	NDP	A	1187	-	51,52,52	1.17	4 (7%)	71,80,80	1.54	14 (19%)
2	NDP	B	1187	-	51,52,52	1.34	7 (13%)	71,80,80	1.55	13 (18%)
4	GOL	B	1190	-	5,5,5	0.72	0	5,5,5	0.37	0
3	39B	B	1188[A]	-	26,36,36	1.31	3 (11%)	76,109,109	2.30	9 (11%)
3	39B	A	1189[B]	-	26,36,36	1.45	3 (11%)	76,109,109	2.25	5 (6%)
3	39B	A	1188[A]	-	26,36,36	1.47	3 (11%)	76,109,109	2.26	5 (6%)

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	39B	B	1189[B]	-	1/1/11/11	2/5/300/300	0/1/16/16
2	NDP	A	1187	-	-	4/34/77/77	0/5/5/5
2	NDP	B	1187	-	-	3/34/77/77	0/5/5/5
4	GOL	B	1190	-	-	4/4/4/4	-
3	39B	B	1188[A]	-	-	1/5/300/300	0/1/16/16
3	39B	A	1188[A]	-	-	2/5/300/300	0/1/16/16
3	39B	A	1189[B]	-	1/1/11/11	2/5/300/300	0/1/16/16

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1187	NDP	O7N-C7N	5.21	1.36	1.24
3	A	1188[A]	39B	C6-N1	5.09	1.41	1.34
3	A	1189[B]	39B	C6-N1	5.09	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1187	NDP	O7N-C7N	4.65	1.35	1.24
3	B	1188[A]	39B	C6-N1	4.21	1.40	1.34
3	B	1189[B]	39B	C6-N1	4.21	1.40	1.34
3	A	1188[A]	39B	B7-B6	-3.41	1.75	1.86
3	A	1189[B]	39B	B7-B6	-3.39	1.75	1.86
3	B	1189[B]	39B	B7-B6	-3.37	1.75	1.86
3	B	1188[A]	39B	B7-B6	-3.20	1.75	1.86
2	B	1187	NDP	C2A-N1A	3.09	1.39	1.33
2	B	1187	NDP	C2A-N3A	2.86	1.39	1.33
2	B	1187	NDP	PA-O3	2.50	1.62	1.59
2	A	1187	NDP	C2A-N1A	2.48	1.38	1.33
2	A	1187	NDP	C5A-N7A	-2.47	1.34	1.39
2	B	1187	NDP	PN-O3	2.41	1.62	1.59
2	B	1187	NDP	C5A-N7A	-2.41	1.34	1.39
2	A	1187	NDP	C2A-N3A	2.37	1.38	1.33
3	A	1188[A]	39B	C5-C4	2.13	1.44	1.41
3	A	1189[B]	39B	C5-C4	2.13	1.44	1.41
3	B	1188[A]	39B	C5-C4	2.07	1.44	1.41
3	B	1189[B]	39B	C5-C4	2.07	1.44	1.41
2	B	1187	NDP	C8A-N7A	2.06	1.35	1.31

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1188[A]	39B	B8-B7-B6	16.05	107.42	91.02
3	A	1189[B]	39B	B8-B7-B6	16.02	107.39	91.02
3	B	1189[B]	39B	B8-B7-B6	15.77	107.13	91.02
3	B	1188[A]	39B	B8-B7-B6	15.74	107.11	91.02
3	A	1188[A]	39B	B6-B7-C2C	8.93	59.68	54.90
3	A	1189[B]	39B	B6-B7-C2C	8.89	59.66	54.90
3	B	1188[A]	39B	B6-B7-C2C	8.65	59.53	54.90
3	B	1189[B]	39B	B6-B7-C2C	8.63	59.52	54.90
2	A	1187	NDP	N3A-C2A-N1A	-5.74	119.89	128.58
2	B	1187	NDP	N3A-C2A-N1A	-5.25	120.63	128.58
3	B	1188[A]	39B	C2-N1-C6	4.50	120.46	116.79
3	B	1189[B]	39B	C2-N1-C6	4.50	120.46	116.79
2	A	1187	NDP	C6N-N1N-C2N	4.03	123.63	119.32
2	B	1187	NDP	N9A-C8A-N7A	-3.82	108.51	113.94
2	B	1187	NDP	C5A-C4A-N3A	-3.63	121.72	126.72
2	A	1187	NDP	N9A-C8A-N7A	-3.60	108.83	113.94
2	B	1187	NDP	C5A-N7A-C8A	3.59	109.09	103.45
2	B	1187	NDP	C3N-C7N-N7N	3.57	124.00	117.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1187	NDP	C5A-C4A-N3A	-3.31	122.16	126.72
3	A	1188[A]	39B	B8-B7-B11	3.28	108.33	103.71
3	B	1189[B]	39B	B8-B7-B11	3.28	108.32	103.71
2	B	1187	NDP	C6N-N1N-C2N	3.22	122.76	119.32
3	B	1188[A]	39B	B8-B7-B11	3.20	108.20	103.71
3	A	1189[B]	39B	B8-B7-B11	3.08	108.04	103.71
2	A	1187	NDP	C1D-N1N-C2N	-3.08	116.07	121.14
2	A	1187	NDP	C5A-N7A-C8A	3.01	108.18	103.45
2	A	1187	NDP	C3N-C7N-N7N	2.80	122.64	117.67
2	B	1187	NDP	C3N-C2N-N1N	-2.75	119.17	123.20
3	B	1188[A]	39B	C6'-C6-C5	2.73	125.94	122.31
3	B	1189[B]	39B	C6'-C6-C5	2.73	125.94	122.31
2	B	1187	NDP	C2A-N3A-C4A	2.70	118.43	111.83
2	B	1187	NDP	C4A-C5A-N7A	-2.59	107.62	110.58
2	A	1187	NDP	C2A-N3A-C4A	2.59	118.16	111.83
2	B	1187	NDP	C1D-N1N-C2N	-2.57	116.91	121.14
2	A	1187	NDP	C2A-N1A-C6A	2.54	122.90	118.73
3	A	1188[A]	39B	B8-B7-B12	2.38	60.16	56.04
3	B	1189[B]	39B	B8-B7-B12	2.35	60.09	56.04
3	B	1188[A]	39B	B8-B7-B12	2.28	59.98	56.04
2	B	1187	NDP	N3A-C4A-N9A	2.27	131.03	127.17
3	A	1189[B]	39B	B8-B7-B12	2.24	59.91	56.04
2	B	1187	NDP	O7N-C7N-C3N	-2.24	116.69	120.90
2	A	1187	NDP	N3A-C4A-N9A	2.23	130.97	127.17
3	A	1188[A]	39B	C2-N1-C6	2.17	118.56	116.79
3	A	1189[B]	39B	C2-N1-C6	2.17	118.56	116.79
2	A	1187	NDP	O3-PN-O1N	-2.15	104.24	110.70
3	B	1188[A]	39B	N4'-C4-N3	-2.12	114.17	117.03
3	B	1189[B]	39B	N4'-C4-N3	-2.12	114.17	117.03
2	A	1187	NDP	C6A-C5A-C4A	2.10	120.05	117.18
2	A	1187	NDP	C3N-C2N-N1N	-2.07	120.17	123.20
2	B	1187	NDP	O2A-PA-O3	2.04	112.80	107.27
2	A	1187	NDP	O2A-PA-O3	2.02	112.74	107.27
3	B	1188[A]	39B	C5-C4-N3	2.02	125.02	121.33
3	B	1189[B]	39B	C5-C4-N3	2.02	125.02	121.33
3	B	1188[A]	39B	N3-C2-N1	-2.00	122.41	125.48
3	B	1189[B]	39B	N3-C2-N1	-2.00	122.41	125.48

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1189[B]	39B	C2C

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Mol	Chain	Res	Type	Atom
3	B	1189[B]	39B	C2C

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1189[B]	39B	C2C-C1C-C5'-C5
3	A	1189[B]	39B	B5-C1C-C5'-C5
3	B	1189[B]	39B	C2C-C1C-C5'-C5
4	B	1190	GOL	O1-C1-C2-C3
4	B	1190	GOL	O1-C1-C2-O2
2	A	1187	NDP	PA-O3-PN-O5D
2	B	1187	NDP	PA-O3-PN-O5D
4	B	1190	GOL	O2-C2-C3-O3
3	A	1188[A]	39B	B6-C1C-C5'-C5
3	B	1189[B]	39B	B4-C1C-C5'-C5
2	A	1187	NDP	C4D-C5D-O5D-PN
2	B	1187	NDP	C4D-C5D-O5D-PN
2	B	1187	NDP	O4D-C1D-N1N-C2N
2	A	1187	NDP	O4D-C1D-N1N-C2N
4	B	1190	GOL	C1-C2-C3-O3
2	A	1187	NDP	C2N-C3N-C7N-N7N
3	A	1188[A]	39B	C2C-C1C-C5'-C5
3	B	1188[A]	39B	C2C-C1C-C5'-C5

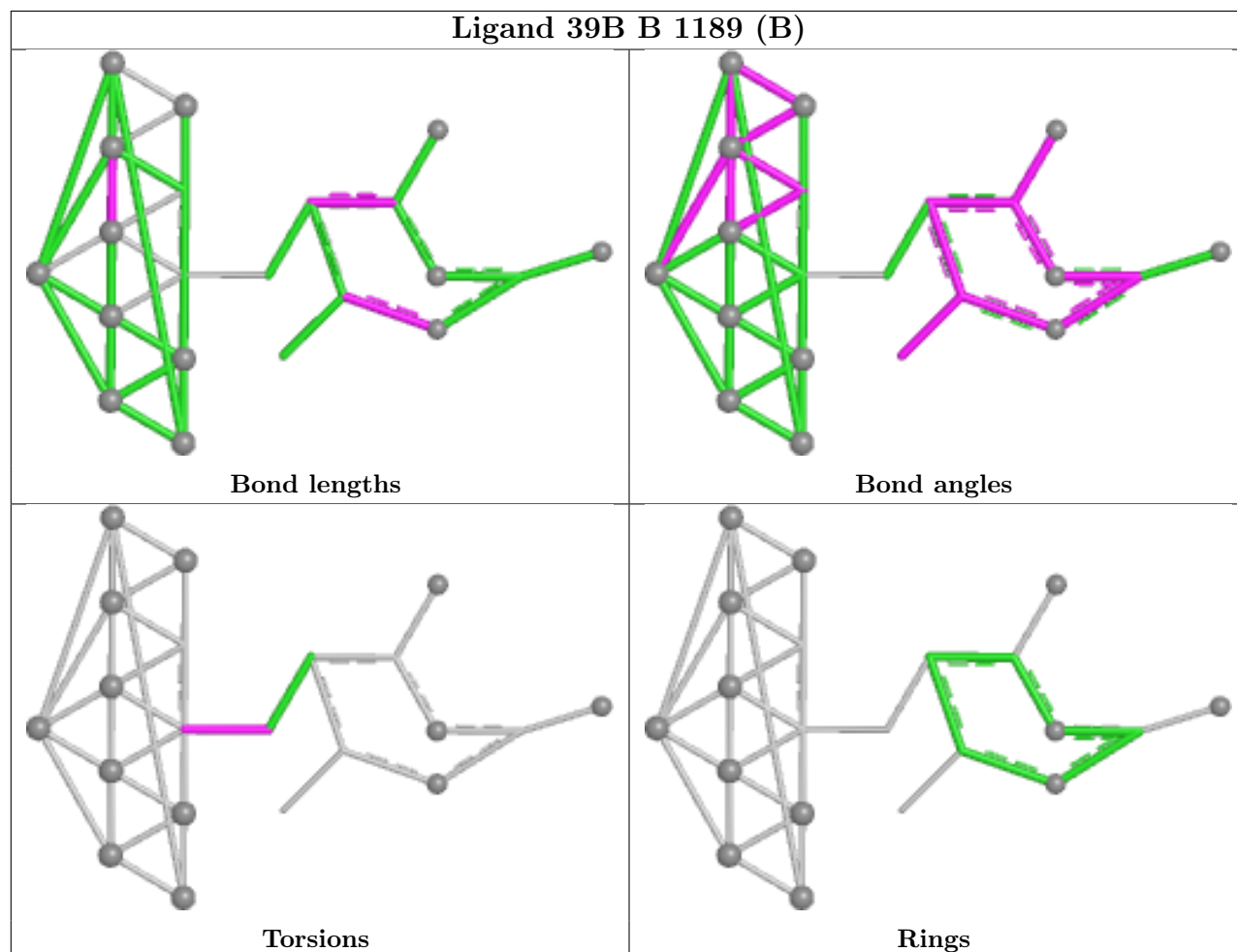
There are no ring outliers.

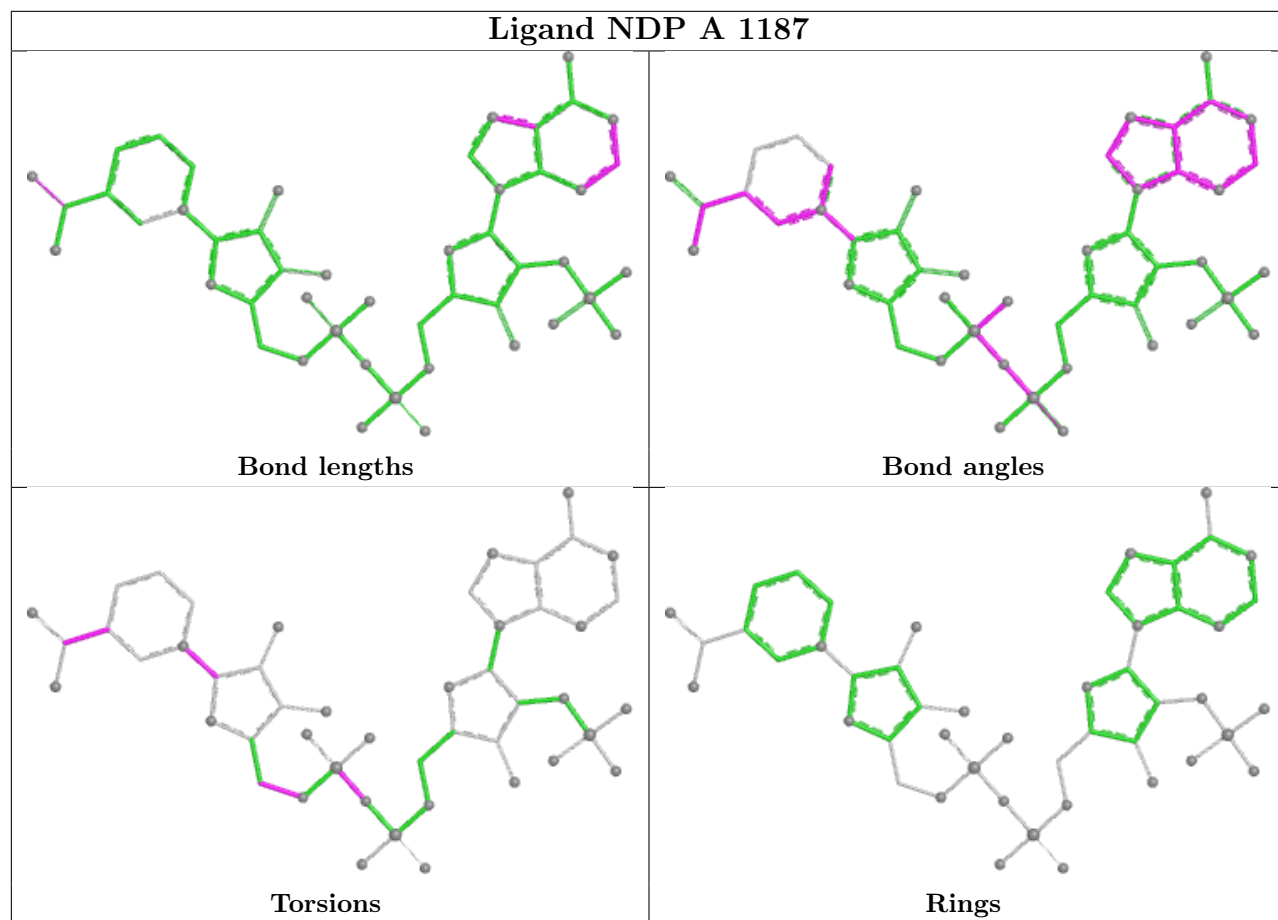
6 monomers are involved in 11 short contacts:

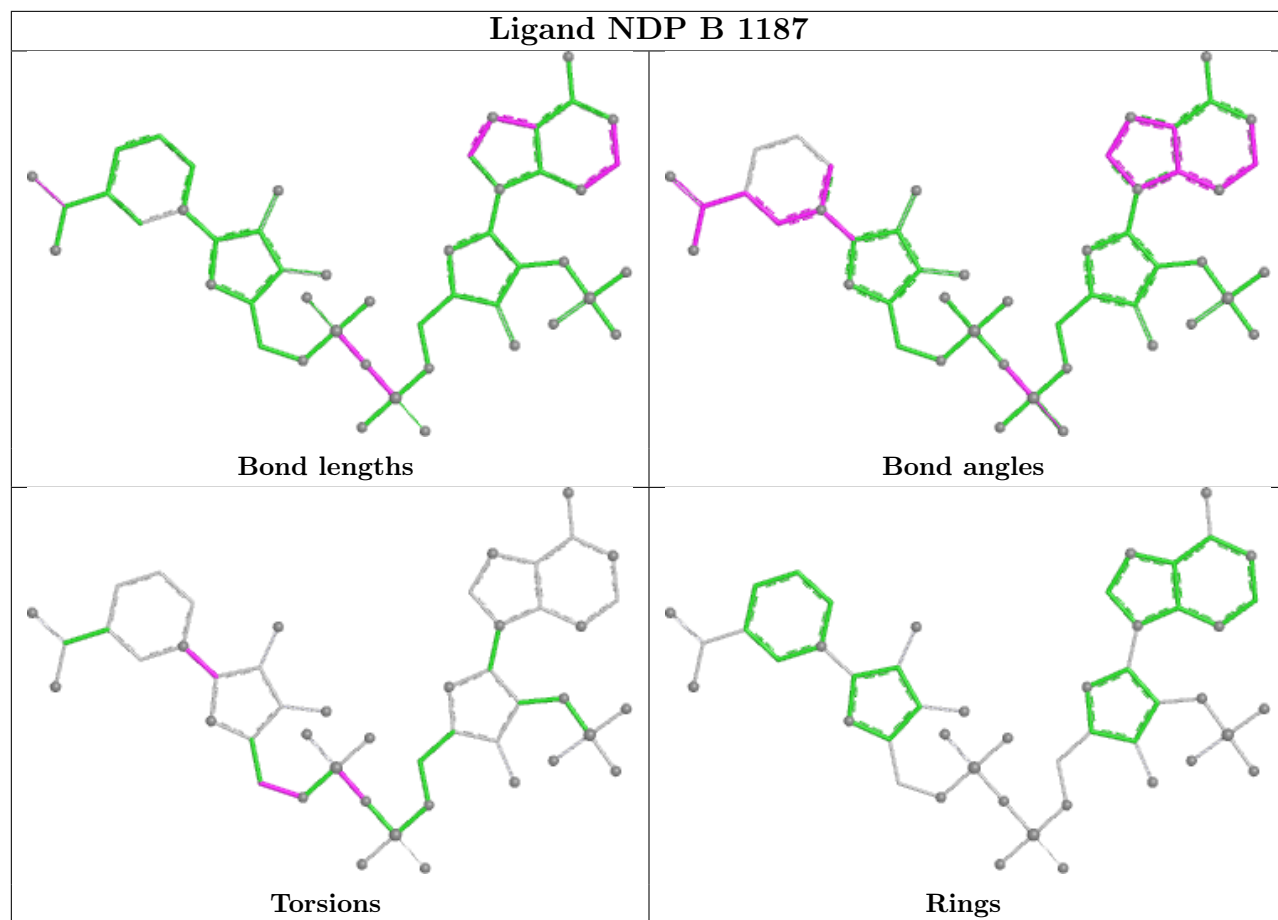
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1189[B]	39B	1	0
2	A	1187	NDP	2	0
2	B	1187	NDP	3	0
3	B	1188[A]	39B	4	0
3	A	1189[B]	39B	1	0
3	A	1188[A]	39B	3	0

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

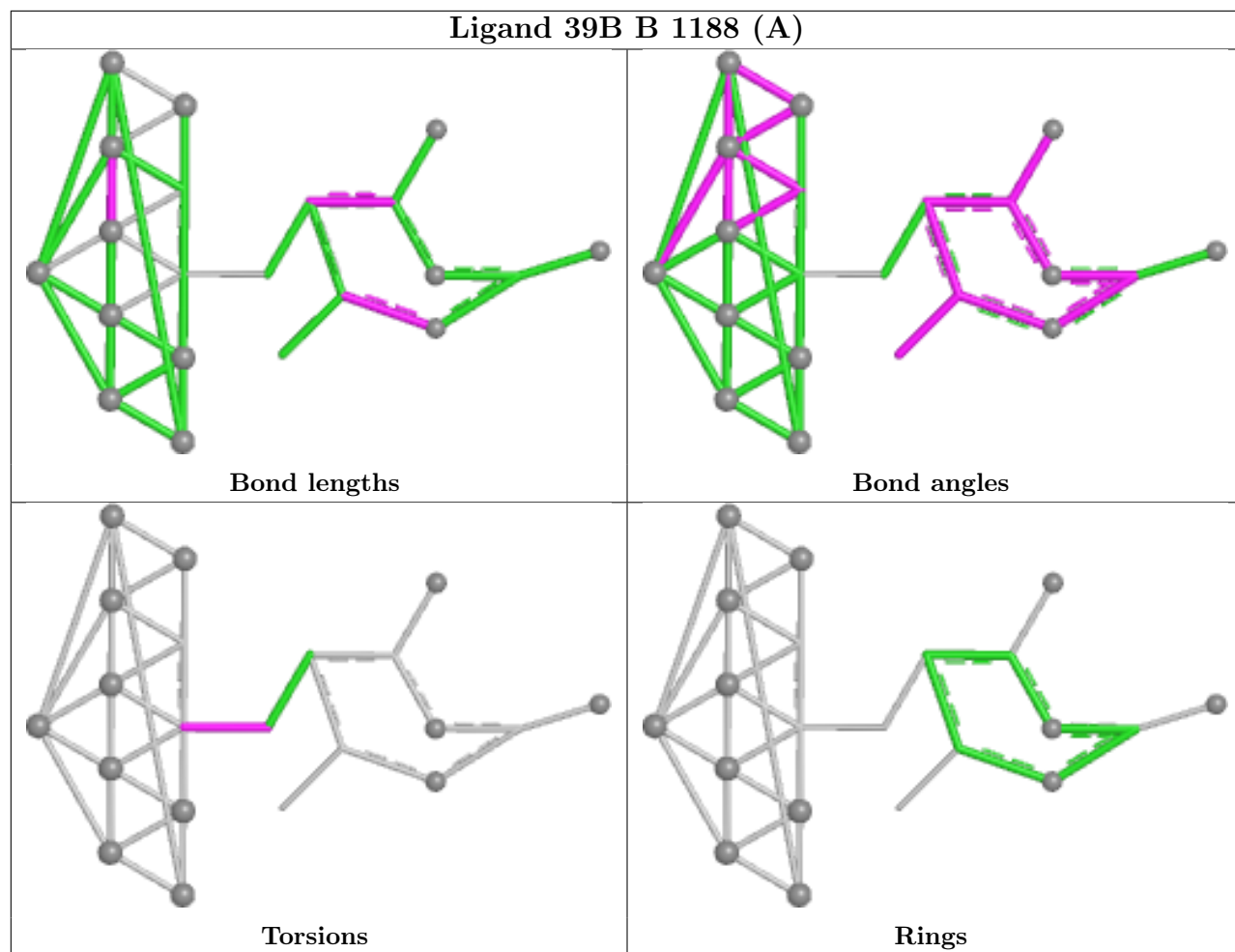
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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



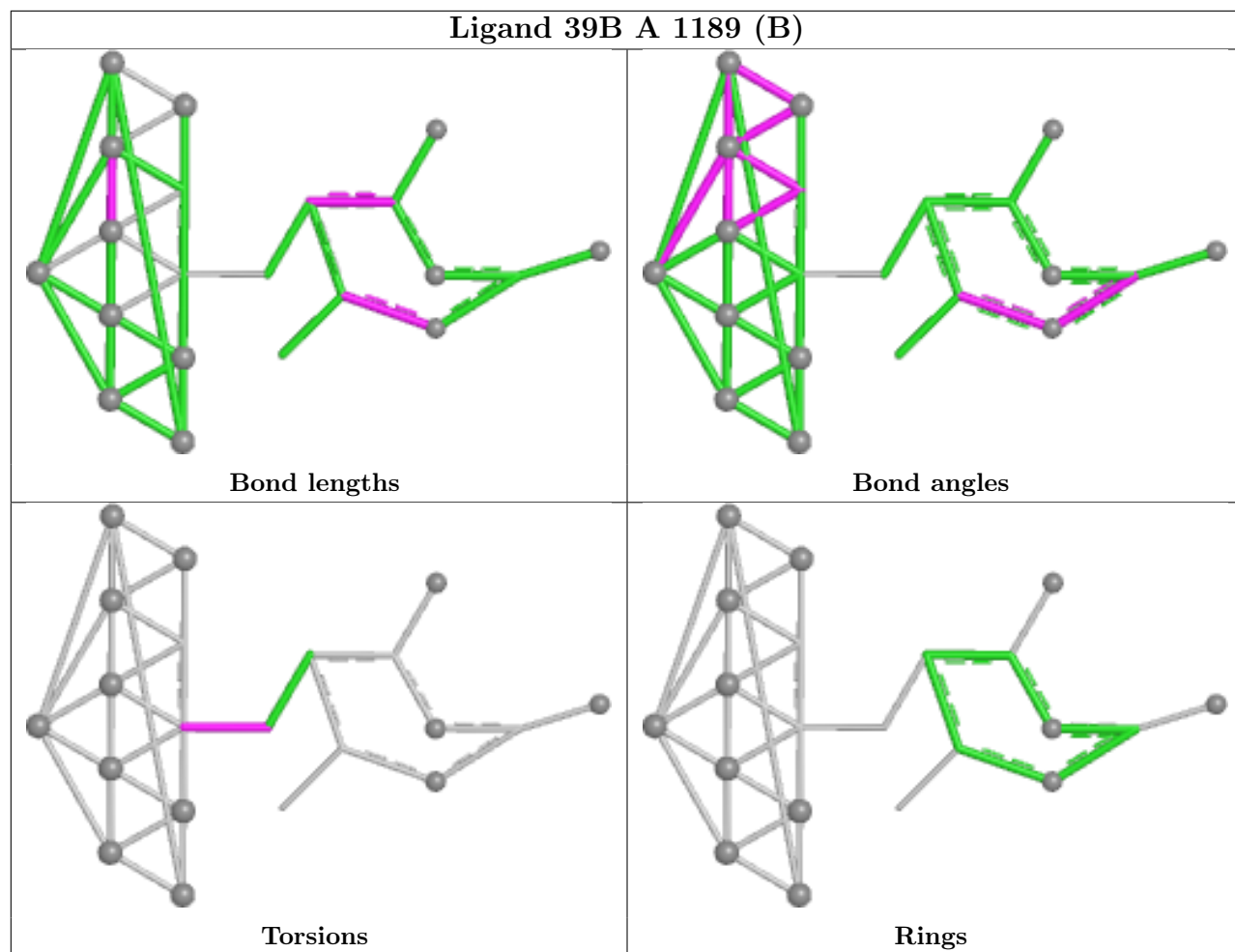


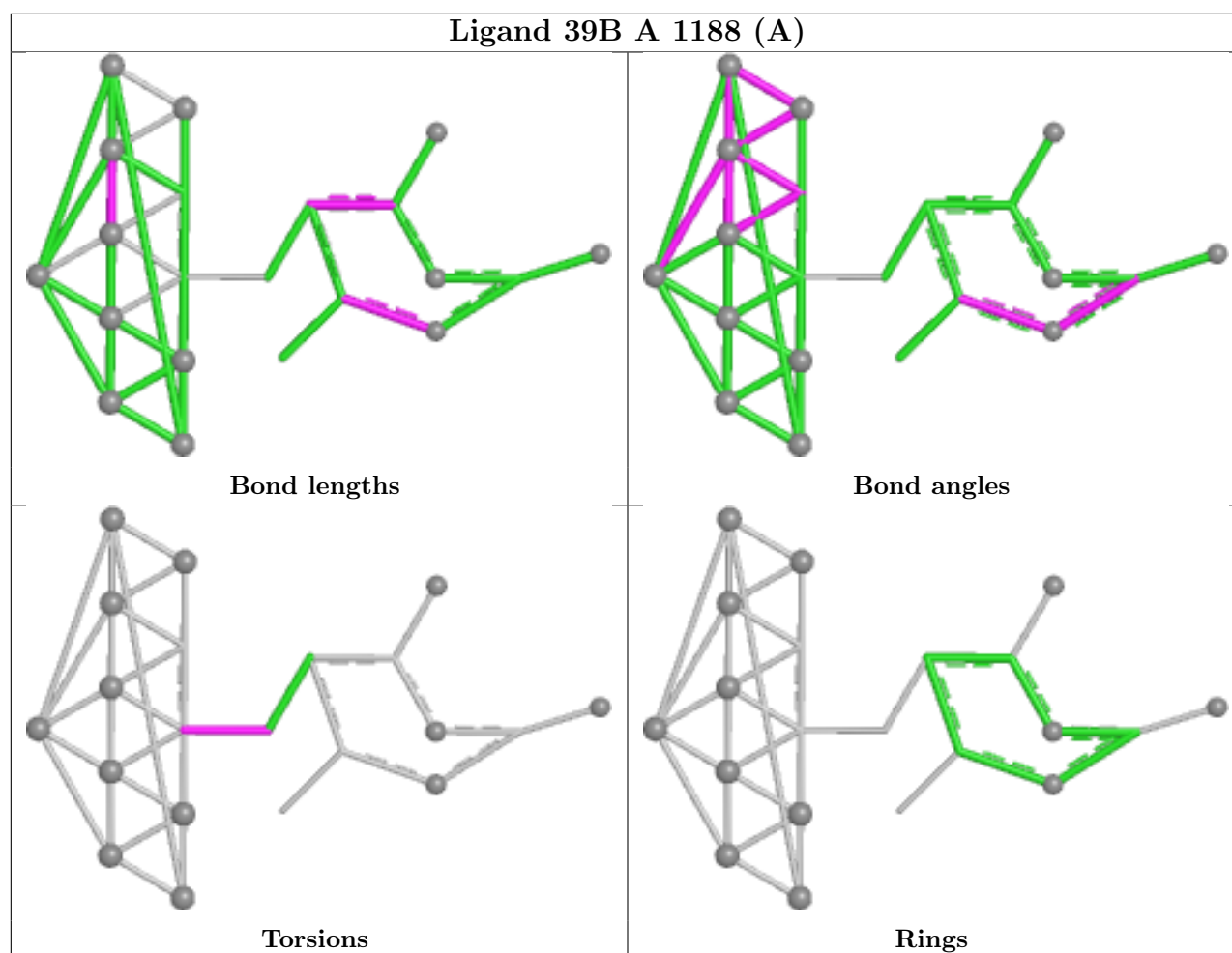


Ligand 39B B 1188 (A)



Ligand 39B A 1189 (B)





5.6 Other polymers [i](#)

There are no such residues in this entry.

5.7 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	186/186 (100%)	0.36	10 (5%) 31 34	8, 19, 30, 37	21 (11%)
1	B	186/186 (100%)	0.62	8 (4%) 40 44	10, 21, 30, 36	18 (9%)
All	All	372/372 (100%)	0.49	18 (4%) 35 39	8, 20, 31, 37	39 (10%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	VAL	5.1
1	B	2	GLY	4.6
1	A	103	PRO	4.6
1	A	3	SER	4.0
1	A	106	ALA	4.0
1	B	186	ASP	3.7
1	A	1	VAL	3.6
1	A	153	LEU	3.3
1	A	131	LEU	2.7
1	A	150	GLU	2.7
1	B	100	THR	2.7
1	B	101	GLU	2.5
1	A	107	ASN	2.4
1	B	89	LEU	2.4
1	A	101	GLU	2.4
1	B	105	LEU	2.3
1	A	185	ASN	2.2
1	B	43	VAL	2.2

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](#)

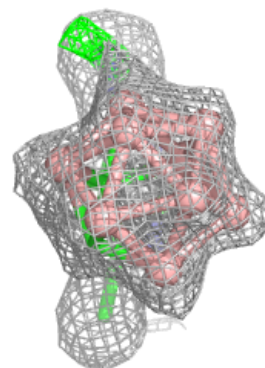
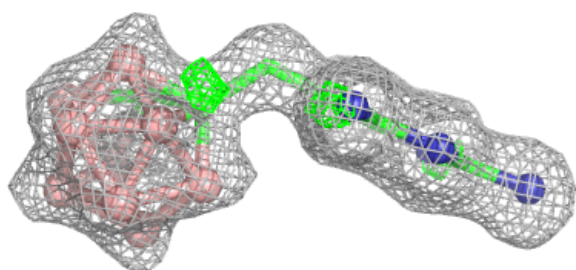
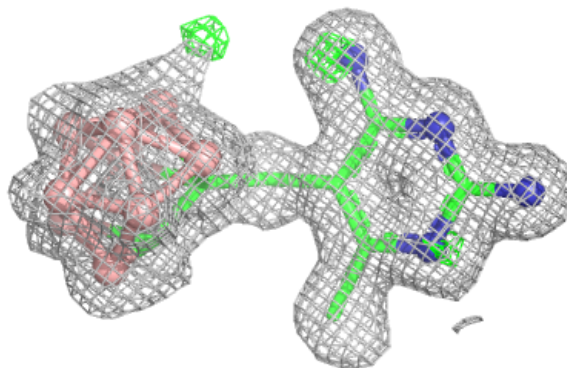
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	B	1190	6/6	0.75	0.16	35,36,38,38	0
3	39B	A	1188[A]	21/21	0.94	0.09	16,19,21,22	21
3	39B	B	1188[A]	21/21	0.95	0.08	19,21,22,23	21
3	39B	B	1189[B]	21/21	0.95	0.07	19,21,22,22	21
3	39B	A	1189[B]	21/21	0.95	0.09	16,19,21,22	21
2	NDP	B	1187	48/48	0.96	0.07	15,20,26,29	0
2	NDP	A	1187	48/48	0.98	0.06	15,19,23,25	0

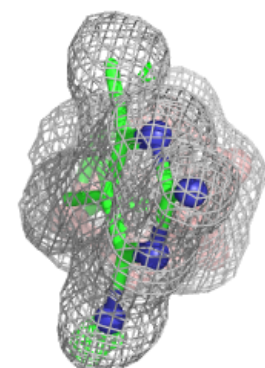
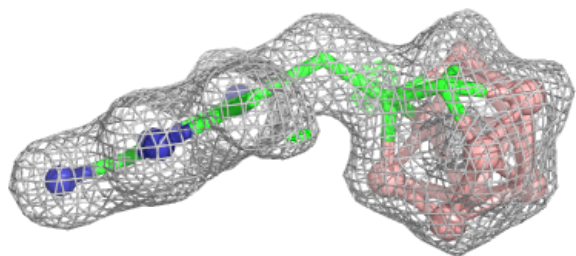
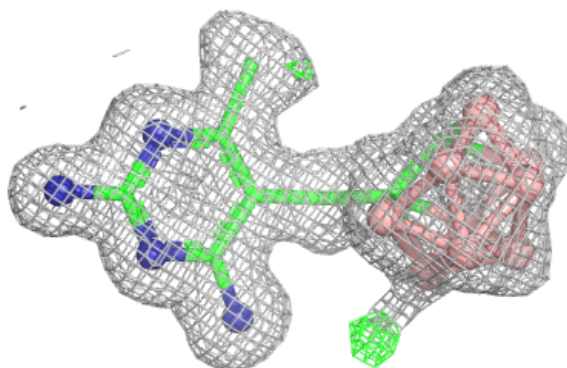
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 39B A 1188 (A):

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

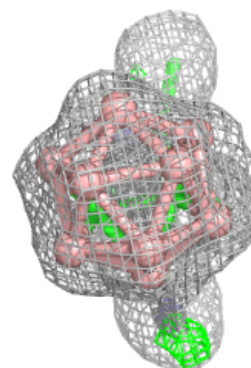
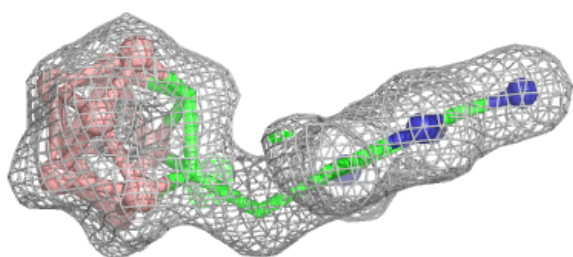
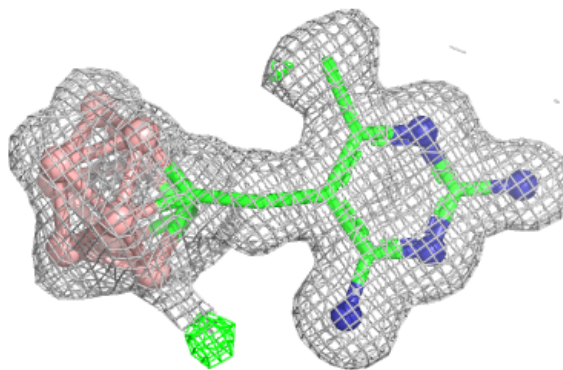
**Electron density around 39B B 1188 (A):**

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

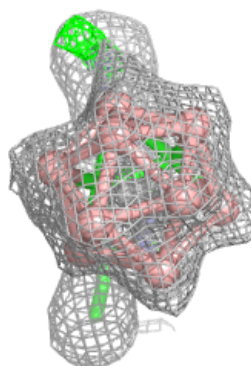
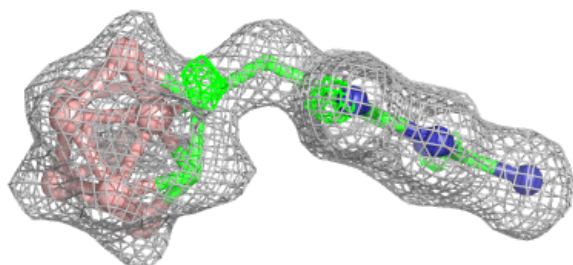
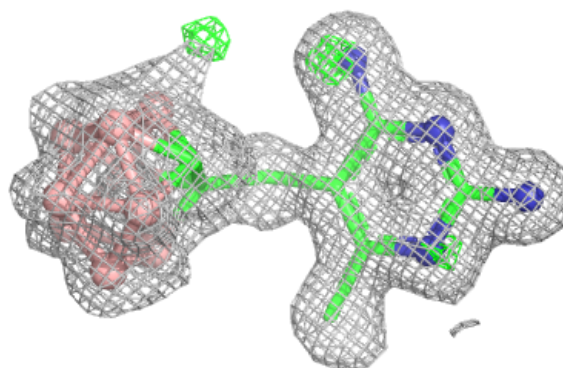


Electron density around 39B B 1189 (B):

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

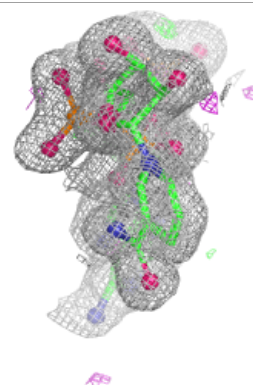
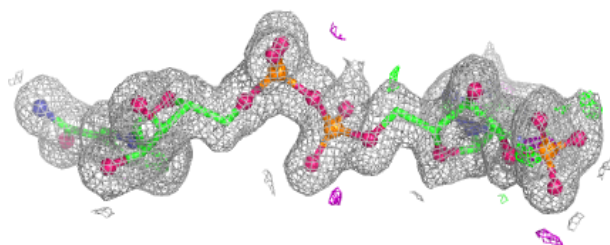
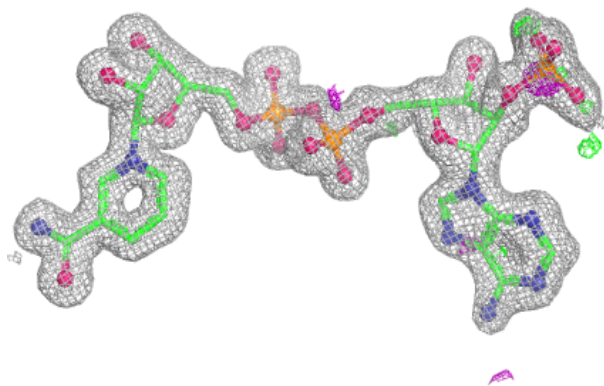
**Electron density around 39B A 1189 (B):**

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

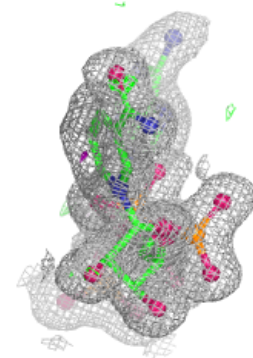
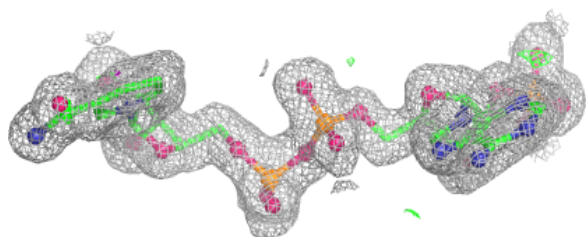
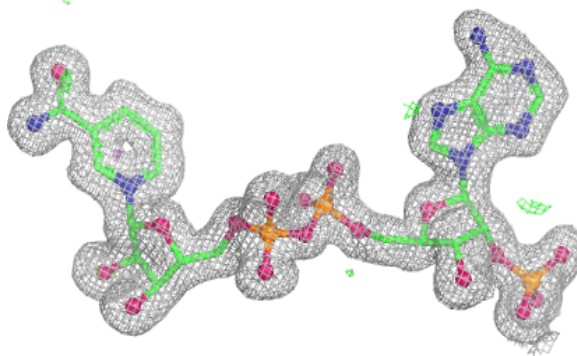


Electron density around NDP B 1187:

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

**Electron density around NDP A 1187:**

$2mF_o-DF_c$ (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.