



Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2026 – 04:20 PM EDT

PDB ID : 9Z11 / pdb_00009z11
Title : Crystal Structure of the Poly(Hexamethylene Adipamide) (Nylon66) Hydro-
lase Nyl50 in Complex with Butyrate at Room Temperature
Authors : Capra, N.; Meilleur, F.
Deposited on : 2025-11-03
Resolution : 2.00 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

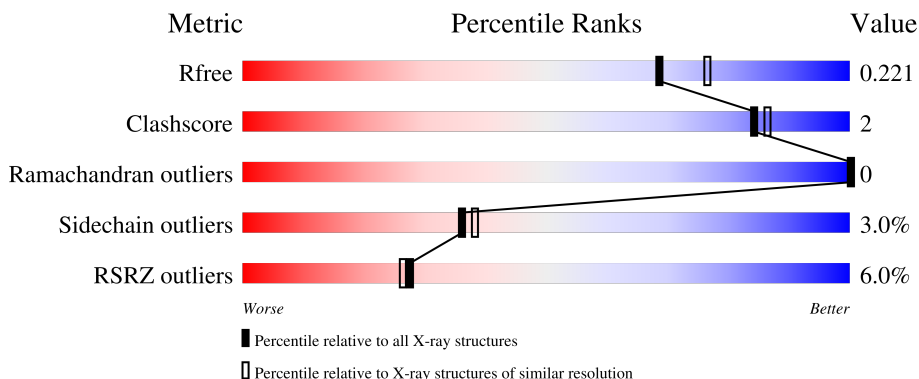
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	305	<div> <div>5%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div>..</div> </div> </div>
1	B	305	<div> <div>7%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>..</div> </div> </div>

2 Entry composition [i](#)

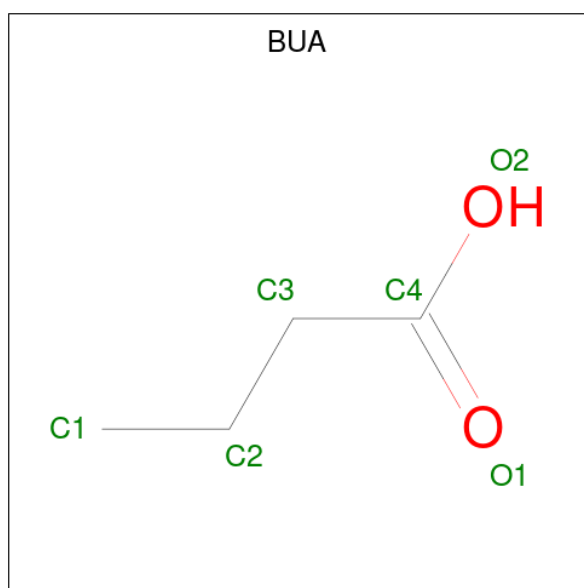
There are 3 unique types of molecules in this entry. The entry contains 4400 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Poly (Hexamethylene adipamide) hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	2	0
			2159	1345	379	420	15			
1	B	300	Total	C	N	O	S	0	2	0
			2158	1347	378	418	15			

- Molecule 2 is butanoic acid (CCD ID: BUA) (formula: $C_4H_8O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	4	2		
2	B	1	Total	C	O	0	0
			6	4	2		

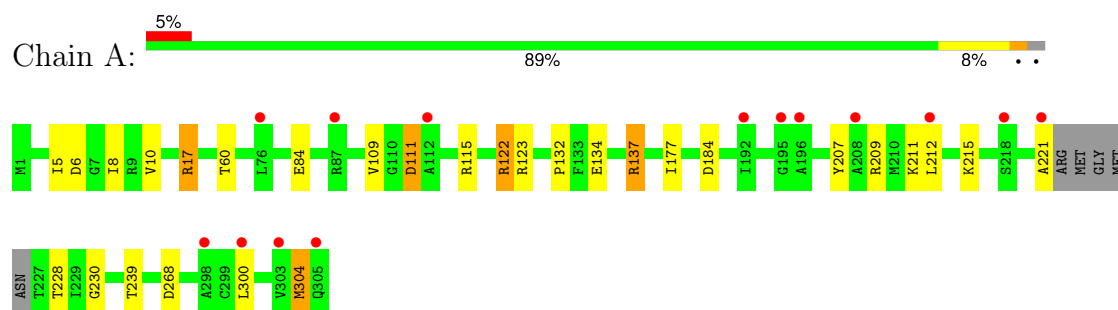
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	37	Total 37	O 37	0	0
3	B	34	Total 34	O 34	0	0

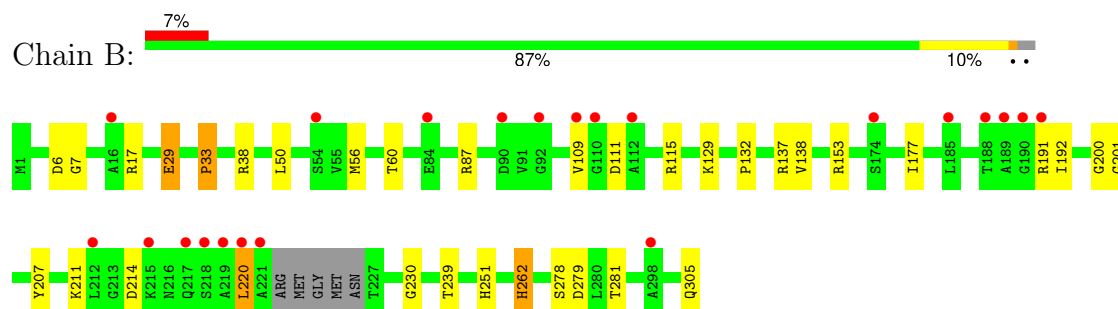
3 Residue-property plots [i](#)

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

- Molecule 1: Poly (Hexamethylene adipamide) hydrolase



- Molecule 1: Poly (Hexamethylene adipamide) hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.88Å 96.48Å 105.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.41 – 2.00 28.41 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.8 (28.41-2.00) 95.1 (28.41-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0431	Depositor
R, R_{free}	0.168 , 0.217 0.176 , 0.221	Depositor DCC
R_{free} test set	1863 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 60.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4400	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% 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: BUA

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	1.01	1/2188 (0.0%)	1.44	15/2968 (0.5%)
1	B	1.01	1/2190 (0.0%)	1.42	18/2971 (0.6%)
All	All	1.01	2/4378 (0.0%)	1.43	33/5939 (0.6%)

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	2
1	B	0	4
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	ARG	NE-CZ	5.67	1.39	1.33
1	B	192	ILE	C-O	-5.10	1.19	1.24

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	ARG	NE-CZ-NH2	-9.83	110.36	119.20
1	B	281	THR	CA-CB-OG1	-8.47	96.90	109.60
1	A	221	ALA	CA-C-O	-8.35	106.61	120.80
1	A	6	ASP	CA-CB-CG	8.07	120.67	112.60
1	B	279	ASP	CB-CA-C	-6.97	97.29	110.67
1	B	279	ASP	CA-CB-CG	6.81	119.41	112.60
1	B	305	GLN	CA-C-O	-6.43	109.87	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	305	GLN	N-CA-CB	6.37	121.32	110.50
1	B	132	PRO	CB-CA-C	6.07	118.93	110.98
1	B	200	GLY	CA-C-N	-5.99	116.96	123.30
1	B	200	GLY	C-N-CA	-5.99	116.96	123.30
1	B	38	ARG	N-CA-CB	-5.83	102.57	110.67
1	A	109	VAL	N-CA-CB	5.79	120.94	111.44
1	A	304	MET	CB-CA-C	-5.67	100.99	110.81
1	A	184	ASP	CA-CB-CG	5.57	118.17	112.60
1	B	239	THR	CA-CB-OG1	-5.55	101.27	109.60
1	B	201	GLY	CA-C-O	-5.51	115.15	119.83
1	B	111	ASP	CA-CB-CG	5.50	118.10	112.60
1	B	6	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	123	ARG	CD-NE-CZ	5.44	132.02	124.40
1	B	262	HIS	CA-CB-CG	5.44	119.24	113.80
1	A	10	VAL	CA-C-N	5.42	125.34	121.65
1	A	10	VAL	C-N-CA	5.42	125.34	121.65
1	A	123	ARG	CG-CD-NE	5.37	123.81	112.00
1	A	132	PRO	CB-CA-C	5.35	118.36	111.46
1	A	134	GLU	CB-CG-CD	-5.33	103.53	112.60
1	B	109	VAL	N-CA-CB	5.29	119.96	111.23
1	B	214	ASP	CA-CB-CG	5.22	117.82	112.60
1	B	138	VAL	N-CA-CB	-5.19	102.22	111.92
1	A	111	ASP	CA-C-N	5.17	127.92	120.38
1	A	111	ASP	C-N-CA	5.17	127.92	120.38
1	B	305	GLN	CB-CA-C	-5.12	100.37	110.10
1	A	239	THR	CA-CB-OG1	-5.11	101.93	109.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	ARG	Sidechain
1	A	209	ARG	Sidechain
1	B	137	ARG	Sidechain
1	B	17	ARG	Sidechain
1	B	191	ARG	Sidechain
1	B	87	ARG	Sidechain

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	2159	0	2174	11	0
1	B	2158	0	2181	9	0
2	A	6	0	7	0	0
2	B	6	0	7	0	0
3	A	37	0	0	0	0
3	B	34	0	0	0	0
All	All	4400	0	4369	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 2.

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:137:ARG:HG3	1:A:137:ARG:HH11	1.20	1.02
1:A:137:ARG:HG3	1:A:137:ARG:NH1	1.96	0.72
1:A:17:ARG:NH2	1:A:111:ASP:OD2	2.24	0.71
1:A:207:TYR:CZ	1:A:211:LYS:HD2	2.28	0.68
1:B:207:TYR:CZ	1:B:211:LYS:HD2	2.35	0.61
1:A:137:ARG:HH11	1:A:137:ARG:CG	2.05	0.61
1:A:177:ILE:HD13	1:A:230:GLY:HA3	1.85	0.58
1:B:220:LEU:HD12	1:B:220:LEU:N	2.22	0.55
1:B:220:LEU:HD12	1:B:220:LEU:H	1.73	0.52
1:B:33:PRO:HB2	1:B:50[B]:LEU:HD22	1.91	0.52
1:B:7:GLY:HA3	1:B:29:GLU:HG3	1.92	0.51
1:A:137:ARG:NH1	1:A:137:ARG:CG	2.69	0.50
1:B:177:ILE:HD13	1:B:230:GLY:HA3	1.99	0.45
1:A:84:GLU:OE1	1:A:122:ARG:NH2	2.52	0.43
1:B:251:HIS:ND1	1:B:262:HIS:HE1	2.18	0.41
1:A:300:LEU:O	1:A:304:MET:HG2	2.20	0.41
1:B:56:MET:HE2	1:B:56:MET:HB2	1.97	0.41
1:A:228:THR:O	1:A:268:ASP:HA	2.22	0.41
1:A:5:ILE:HB	1:A:8:ILE:HD12	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 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	297/305 (97%)	290 (98%)	7 (2%)	0	100	100
1	B	297/305 (97%)	287 (97%)	10 (3%)	0	100	100
All	All	594/610 (97%)	577 (97%)	17 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	219/222 (99%)	214 (98%)	5 (2%)	44	49
1	B	219/222 (99%)	211 (96%)	8 (4%)	30	30
All	All	438/444 (99%)	425 (97%)	13 (3%)	36	38

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	THR
1	A	115	ARG
1	A	137	ARG
1	A	212	LEU
1	A	215	LYS
1	B	29	GLU
1	B	33	PRO
1	B	60	THR

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Mol	Chain	Res	Type
1	B	115	ARG
1	B	129	LYS
1	B	153	ARG
1	B	220	LEU
1	B	278	SER

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

Mol	Chain	Res	Type
1	B	252	ASN
1	B	262	HIS

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 ⓘ

2 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	BUA	A	401	-	5,5,5	1.24	0	5,5,5	1.28	0
2	BUA	B	401	-	5,5,5	1.36	1 (20%)	5,5,5	1.74	1 (20%)

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	BUA	A	401	-	-	3/3/3/3	-
2	BUA	B	401	-	-	1/3/3/3	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	BUA	C3-C4	2.04	1.55	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	BUA	O2-C4-C3	2.39	121.55	114.00

There are no chirality outliers.

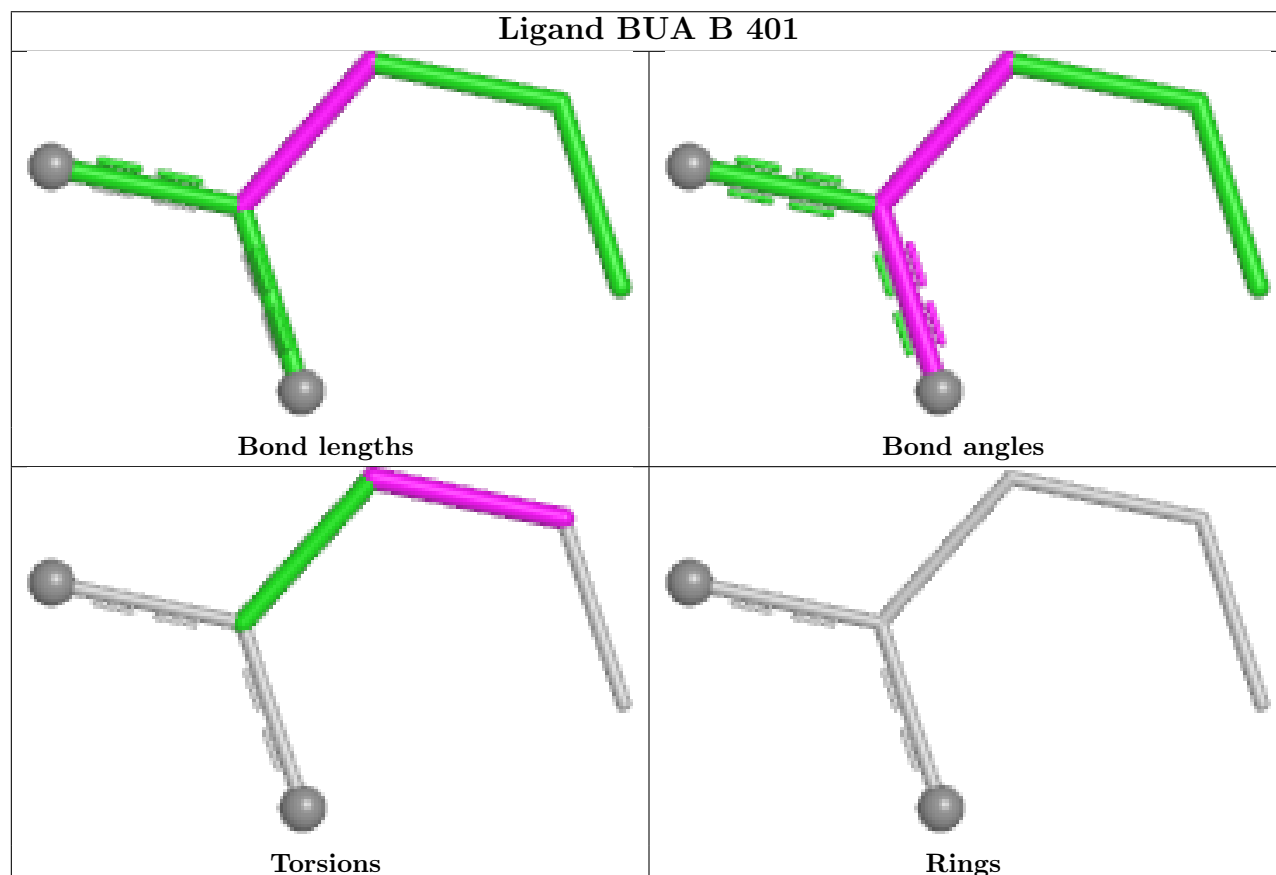
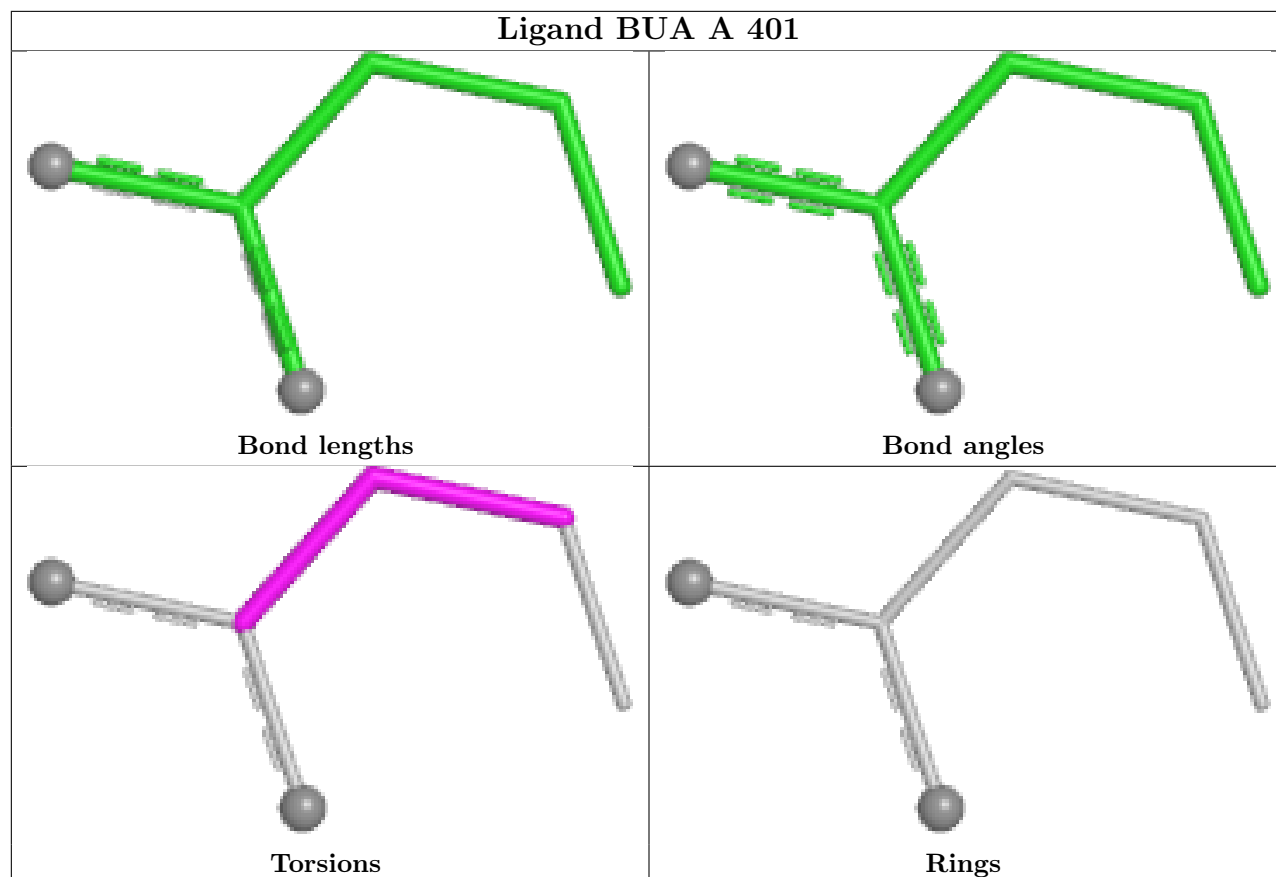
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	BUA	C1-C2-C3-C4
2	B	401	BUA	C1-C2-C3-C4
2	A	401	BUA	C2-C3-C4-O2
2	A	401	BUA	C2-C3-C4-O1

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 [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	300/305 (98%)	0.25	14 (4%) 36 35	13, 27, 52, 76	1 (0%)
1	B	300/305 (98%)	0.25	22 (7%) 21 19	15, 27, 54, 76	1 (0%)
All	All	600/610 (98%)	0.25	36 (6%) 27 26	13, 27, 54, 76	2 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	112	ALA	4.2
1	B	54	SER	3.3
1	A	112	ALA	3.2
1	A	218	SER	3.2
1	B	190	GLY	3.0
1	B	217	GLN	3.0
1	B	188	THR	3.0
1	B	84	GLU	3.0
1	B	218	SER	2.9
1	B	109	VAL	2.9
1	A	303	VAL	2.8
1	B	191	ARG	2.8
1	A	298	ALA	2.7
1	B	298	ALA	2.6
1	B	189	ALA	2.6
1	A	305	GLN	2.5
1	A	300	LEU	2.5
1	B	185	LEU	2.5
1	B	212	LEU	2.5
1	A	221	ALA	2.5
1	B	219	ALA	2.5
1	A	192	ILE	2.5
1	B	90	ASP	2.4
1	B	110	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	221	ALA	2.4
1	A	196	ALA	2.4
1	B	215	LYS	2.4
1	A	76	LEU	2.3
1	B	16	ALA	2.3
1	A	212	LEU	2.3
1	B	174	SER	2.2
1	A	195	GLY	2.1
1	B	92	GLY	2.1
1	B	220	LEU	2.1
1	A	87	ARG	2.1
1	A	208	ALA	2.1

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](#)

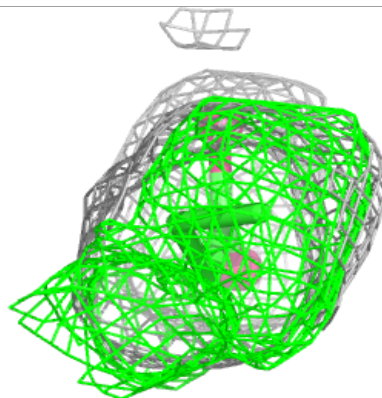
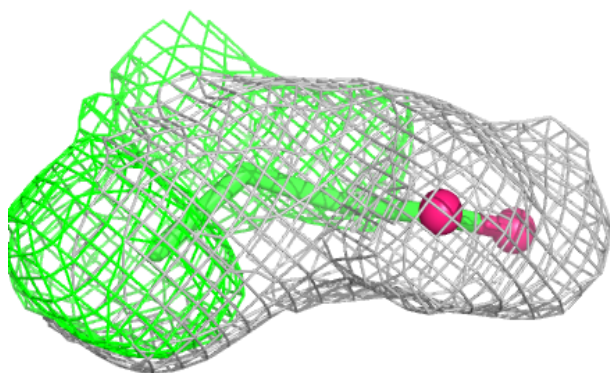
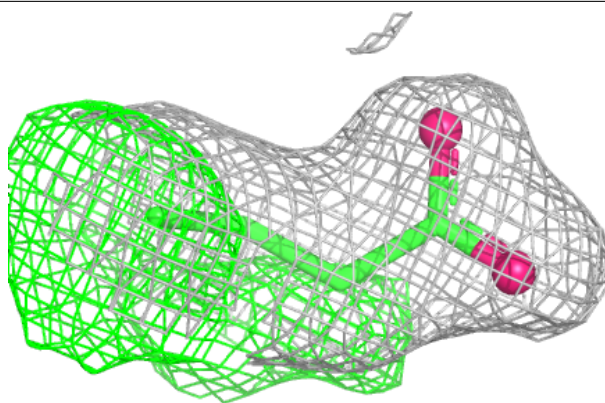
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BUA	B	401	6/6	0.62	0.22	49,52,61,61	0
2	BUA	A	401	6/6	0.74	0.17	42,54,60,63	0

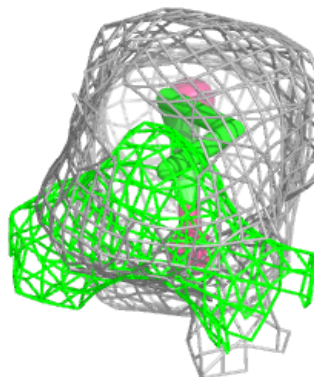
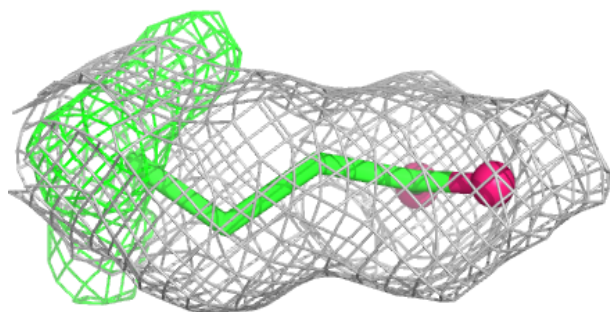
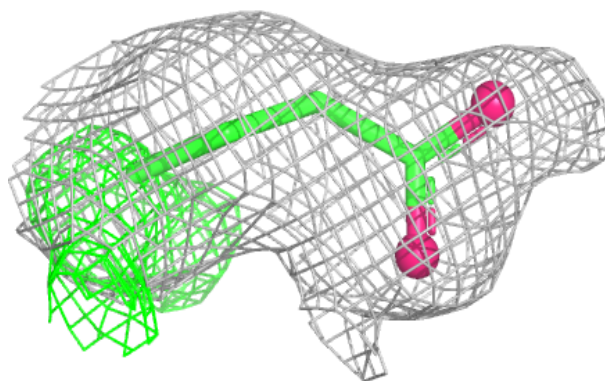
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BUA 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 BUA 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.