



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2026 – 10:16 PM JST

PDB ID : 9WRZ / pdb_00009wrz
Title : Crystal structure of NUDIX hydrolase E83A mutant from *Limisphaera ngata-marikiensis* in complex with ITP
Authors : Wu, W.Q.; Li, Z.X.
Deposited on : 2025-09-12
Resolution : 3.10 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	:	1.8.5 (274361), CSD as541be (2020)
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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

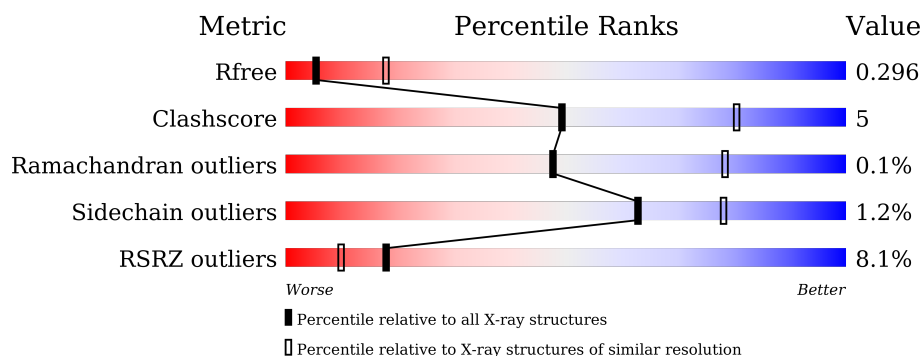
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	211	9% 81% 14% 5%
1	B	211	5% 84% 9% 7%
1	C	211	9% 77% 13% 9%
1	D	211	7% 82% 7% 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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ZN	C	302	-	-	-	X
3	ZN	D	302	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12285 atoms, of which 5997 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.

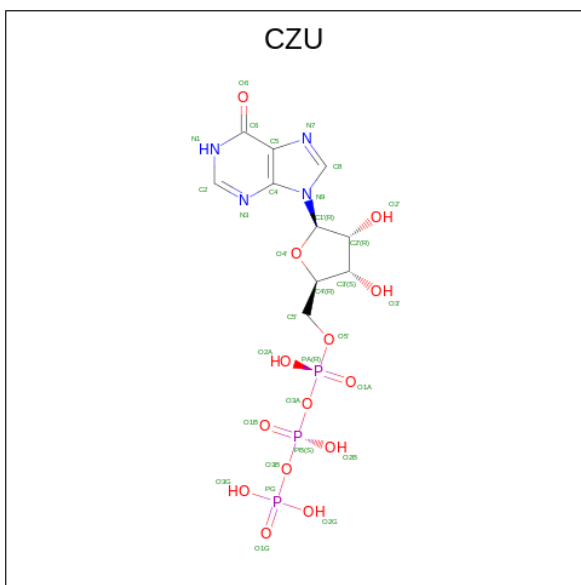
- Molecule 1 is a protein called NUDIX domain-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	201	Total	C	H	N	O	S	0	0	0
			3058	1005	1486	293	272	2			
1	B	196	Total	C	H	N	O	S	0	0	0
			3032	988	1490	288	264	2			
1	C	192	Total	C	H	N	O	S	0	0	0
			3012	976	1492	284	258	2			
1	D	190	Total	C	H	N	O	S	0	0	0
			2992	969	1485	282	254	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	ALA	GLU	engineered mutation	UNP A0A6M1RLF6
B	83	ALA	GLU	engineered mutation	UNP A0A6M1RLF6
C	83	ALA	GLU	engineered mutation	UNP A0A6M1RLF6
D	83	ALA	GLU	engineered mutation	UNP A0A6M1RLF6

- Molecule 2 is [(2 {R},3 {S},4 {R},5 {R})-3,4-bis(oxidanyl)-5-(6-oxidanylidene-1 {H}-purin-9-yl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl] phosphono hydrogen phosphate (CCD ID: CZU) (formula: C₁₀H₁₅N₄O₁₄P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 42	C 10	H 11	N 4	O 14	P 3	0	0
2	B	1	Total 42	C 10	H 11	N 4	O 14	P 3	0	0
2	C	1	Total 42	C 10	H 11	N 4	O 14	P 3	0	0
2	D	1	Total 42	C 10	H 11	N 4	O 14	P 3	0	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	7	Total O 7 7	0	0

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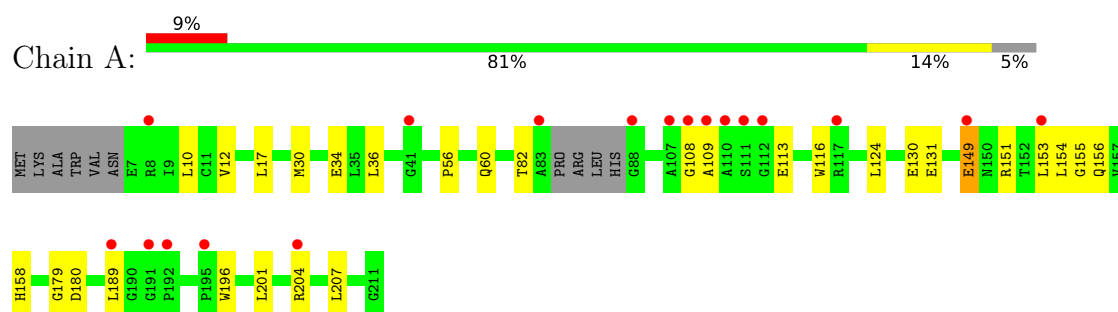
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	4	Total 4	O 4	0	0
4	C	7	Total 7	O 7	0	0
4	D	1	Total 1	O 1	0	0

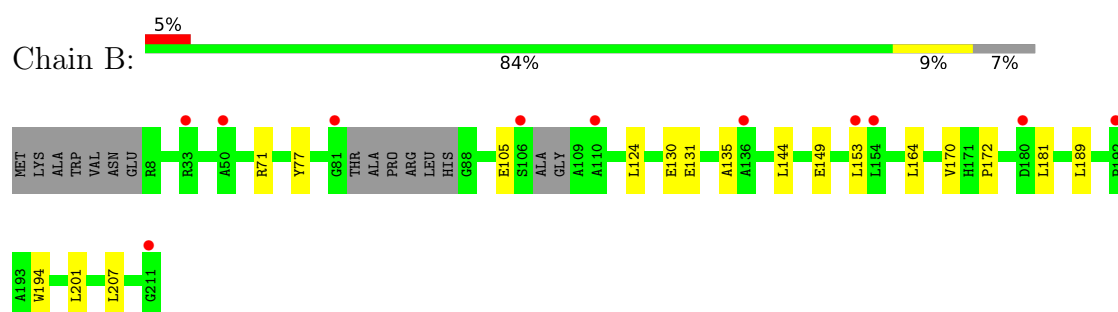
3 Residue-property plots [i](#)

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.

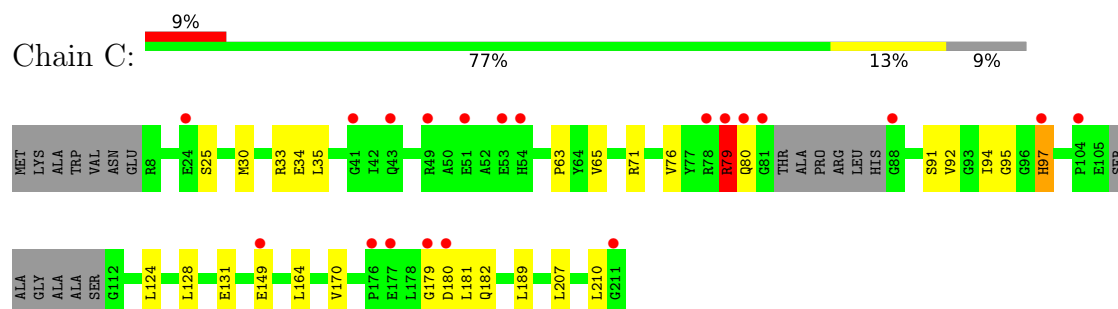
- Molecule 1: NUDIX domain-containing protein



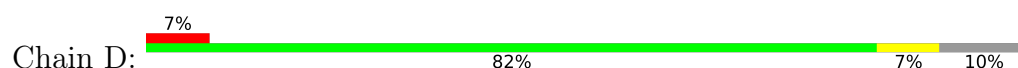
- Molecule 1: NUDIX domain-containing protein

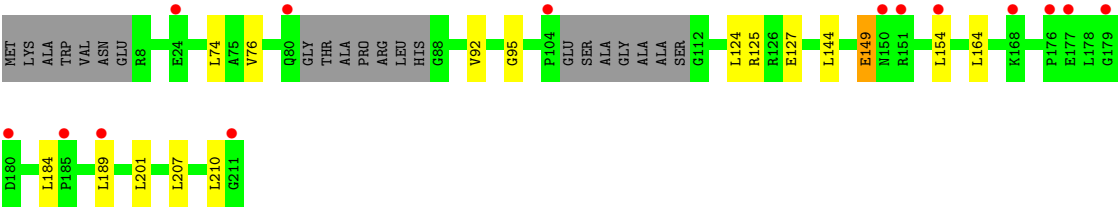


- Molecule 1: NUDIX domain-containing protein



- Molecule 1: NUDIX domain-containing protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	148.32Å 70.69Å 81.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.31 – 3.10 42.31 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (42.31-3.10) 99.6 (42.31-3.10)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.247 , 0.291 0.256 , 0.296	Depositor DCC
R_{free} test set	2000 reflections (8.41%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.823	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 27.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	12285	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.69 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.1922e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CZU, ZN

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	0.25	0/1621	0.50	0/2212
1	B	0.18	0/1590	0.35	0/2168
1	C	0.32	0/1568	0.65	5/2138 (0.2%)
1	D	0.19	0/1555	0.38	0/2121
All	All	0.24	0/6334	0.48	5/8639 (0.1%)

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	C	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	97	HIS	CB-CG-CD2	-11.79	115.88	131.20
1	C	97	HIS	CB-CG-ND1	10.00	137.70	122.70
1	C	79	ARG	N-CA-C	5.89	119.07	109.59
1	C	97	HIS	CA-CB-CG	5.84	119.64	113.80
1	C	79	ARG	CB-CA-C	-5.69	99.14	109.38

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	79	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	1572	1486	1536	22	0
1	B	1542	1490	1509	12	0
1	C	1520	1492	1489	19	0
1	D	1507	1485	1480	13	0
2	A	31	11	0	2	0
2	B	31	11	0	1	0
2	C	31	11	0	1	0
2	D	31	11	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	7	0	0	0	0
4	B	4	0	0	0	0
4	C	7	0	0	0	0
4	D	1	0	0	0	0
All	All	6288	5997	6014	66	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 5.

All (66) 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:196:TRP:CE3	1:A:204:ARG:HG2	2.32	0.65
1:C:76:VAL:HG22	1:C:92:VAL:HG12	1.79	0.64
1:B:105:GLU:HG3	1:D:125:ARG:HH21	1.65	0.61
1:A:131:GLU:OE2	2:A:301:CZU:O3B	2.19	0.60
1:A:149:GLU:HG3	1:A:201:LEU:HD23	1.82	0.59
1:A:189:LEU:HD13	1:A:207:LEU:HD11	1.83	0.59
1:D:149:GLU:CG	1:D:201:LEU:HD23	2.32	0.59
1:A:149:GLU:HG3	1:A:201:LEU:CD2	2.34	0.57
1:A:153:LEU:HD23	1:A:153:LEU:H	1.69	0.57
1:C:189:LEU:HD13	1:C:207:LEU:HD11	1.85	0.57
1:D:149:GLU:HG3	1:D:201:LEU:HD23	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:HIS:CE1	2:A:301:CZU:O2'	2.61	0.54
1:C:164:LEU:HD22	1:C:210:LEU:CD2	2.38	0.54
1:D:149:GLU:CD	1:D:201:LEU:HD23	2.32	0.53
1:C:65:VAL:O	1:C:65:VAL:HG23	2.09	0.53
1:B:144:LEU:HD11	1:B:164:LEU:HB2	1.90	0.53
1:B:153:LEU:HD23	1:B:153:LEU:H	1.75	0.51
1:D:76:VAL:HG22	1:D:92:VAL:HG12	1.92	0.51
1:D:124:LEU:HD23	1:D:124:LEU:C	2.35	0.51
1:C:124:LEU:C	1:C:124:LEU:HD23	2.36	0.51
1:B:124:LEU:C	1:B:124:LEU:HD23	2.36	0.51
1:D:144:LEU:HD11	1:D:164:LEU:HB2	1.94	0.49
1:D:95:GLY:HA2	1:D:127:GLU:HG2	1.93	0.49
1:D:74:LEU:HD11	1:D:210:LEU:CD1	2.43	0.49
1:C:164:LEU:HD13	1:C:210:LEU:HD21	1.95	0.48
1:C:131:GLU:OE2	2:C:301:CZU:O2B	2.31	0.48
1:B:189:LEU:HD13	1:B:207:LEU:HD11	1.96	0.48
1:A:196:TRP:HB3	1:A:204:ARG:HD2	1.96	0.47
1:D:189:LEU:HD13	1:D:207:LEU:HD11	1.96	0.47
1:C:71:ARG:HG3	1:C:170:VAL:HG13	1.96	0.47
1:A:60:GLN:HE21	1:A:158:HIS:CD2	2.32	0.47
1:A:124:LEU:C	1:A:124:LEU:HD23	2.40	0.46
1:C:30:MET:HE2	1:C:35:LEU:N	2.29	0.46
1:C:65:VAL:HG21	1:C:128:LEU:HD13	1.97	0.46
1:A:149:GLU:CG	1:A:201:LEU:HD23	2.46	0.46
1:A:149:GLU:OE1	1:A:155:GLY:HA3	2.16	0.45
1:B:201:LEU:C	1:B:201:LEU:HD23	2.41	0.45
1:C:181:LEU:HD23	1:C:182:GLN:N	2.32	0.45
1:D:154:LEU:HD22	1:D:154:LEU:H	1.82	0.45
1:B:77:TYR:HB3	1:B:181:LEU:HD12	1.99	0.45
1:A:149:GLU:HG2	1:A:151:ARG:H	1.82	0.45
1:B:201:LEU:HD23	1:B:201:LEU:O	2.17	0.44
1:C:33:ARG:HD2	1:C:33:ARG:N	2.31	0.44
1:A:56:PRO:HB3	1:A:156:GLN:HG2	1.99	0.44
1:A:108:GLY:O	1:A:109:ALA:HB3	2.17	0.44
1:A:179:GLY:O	1:A:180:ASP:C	2.61	0.43
1:A:10:LEU:HD21	1:A:116:TRP:CZ3	2.53	0.43
1:A:36:LEU:HB3	1:A:113:GLU:HG3	2.00	0.43
1:B:71:ARG:CZ	1:B:170:VAL:HG11	2.49	0.43
2:B:301:CZU:O3G	2:B:301:CZU:O1A	2.36	0.43
1:B:189:LEU:O	1:B:194:TRP:O	2.37	0.43
1:C:65:VAL:HG22	1:C:94:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LEU:HG	1:A:154:LEU:N	2.34	0.42
1:C:65:VAL:O	1:C:65:VAL:CG2	2.68	0.42
1:C:30:MET:HE3	1:C:34:GLU:HB3	2.02	0.41
1:D:76:VAL:HG21	1:D:184:LEU:HD12	2.02	0.41
1:A:130:GLU:HG3	1:A:131:GLU:HG3	2.02	0.41
1:B:130:GLU:HG3	1:B:131:GLU:HG3	2.02	0.41
1:C:79:ARG:HD2	1:C:91:SER:HB2	2.02	0.41
1:C:30:MET:CE	1:C:34:GLU:HB3	2.51	0.41
1:A:12:VAL:HG21	1:A:17:LEU:HD21	2.01	0.41
1:A:30:MET:CE	1:A:34:GLU:HG3	2.51	0.41
1:B:135:ALA:HB2	1:B:172:PRO:HB2	2.02	0.41
1:D:149:GLU:HG3	1:D:201:LEU:CD2	2.49	0.41
1:C:179:GLY:O	1:C:180:ASP:C	2.65	0.40
1:C:63:PRO:O	1:C:95:GLY:HA3	2.21	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	197/211 (93%)	190 (96%)	7 (4%)	0	100	100
1	B	190/211 (90%)	185 (97%)	5 (3%)	0	100	100
1	C	186/211 (88%)	179 (96%)	6 (3%)	1 (0%)	24	57
1	D	184/211 (87%)	178 (97%)	6 (3%)	0	100	100
All	All	757/844 (90%)	732 (97%)	24 (3%)	1 (0%)	48	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	25	SER

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	153/162 (94%)	151 (99%)	2 (1%)	61	77
1	B	151/162 (93%)	150 (99%)	1 (1%)	76	82
1	C	149/162 (92%)	146 (98%)	3 (2%)	48	72
1	D	148/162 (91%)	147 (99%)	1 (1%)	76	82
All	All	601/648 (93%)	594 (99%)	7 (1%)	63	78

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

Mol	Chain	Res	Type
1	A	82	THR
1	A	149	GLU
1	B	149	GLU
1	C	80	GLN
1	C	97	HIS
1	C	149	GLU
1	D	149	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	173	GLN
1	C	97	HIS
1	C	99	ASN
1	C	156	GLN
1	D	99	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	CZU	D	301	-	29,33,33	3.78	13 (44%)	44,52,52	2.21	12 (27%)
2	CZU	A	301	-	29,33,33	3.72	13 (44%)	44,52,52	2.21	15 (34%)
2	CZU	C	301	-	29,33,33	3.76	13 (44%)	44,52,52	2.27	12 (27%)
2	CZU	B	301	-	29,33,33	3.70	14 (48%)	44,52,52	2.12	13 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CZU	D	301	-	-	3/22/38/38	0/3/3/3
2	CZU	A	301	-	-	5/22/38/38	0/3/3/3
2	CZU	C	301	-	-	8/22/38/38	0/3/3/3
2	CZU	B	301	-	-	5/22/38/38	0/3/3/3

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	CZU	C2-N3	9.44	1.47	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	CZU	C2-N3	9.42	1.47	1.30
2	A	301	CZU	C2-N3	9.42	1.47	1.30
2	B	301	CZU	C2-N3	9.15	1.46	1.30
2	C	301	CZU	O4'-C1'	8.77	1.62	1.42
2	D	301	CZU	O4'-C1'	8.55	1.62	1.42
2	B	301	CZU	O4'-C1'	8.35	1.61	1.42
2	A	301	CZU	O4'-C1'	8.05	1.61	1.42
2	B	301	CZU	O4'-C4'	-7.97	1.27	1.45
2	A	301	CZU	O4'-C4'	-7.76	1.27	1.45
2	D	301	CZU	C2'-C1'	-7.55	1.29	1.53
2	A	301	CZU	C2'-C1'	-7.47	1.29	1.53
2	D	301	CZU	O4'-C4'	-7.47	1.28	1.45
2	C	301	CZU	O4'-C4'	-7.29	1.28	1.45
2	C	301	CZU	C2'-C1'	-7.16	1.30	1.53
2	B	301	CZU	C2'-C1'	-6.93	1.31	1.53
2	D	301	CZU	C4-N3	6.50	1.49	1.35
2	C	301	CZU	C4-N3	6.50	1.49	1.35
2	A	301	CZU	C4-N3	6.42	1.49	1.35
2	B	301	CZU	C4-N3	6.13	1.48	1.35
2	B	301	CZU	C2-N1	5.80	1.45	1.35
2	D	301	CZU	C2-N1	5.43	1.45	1.35
2	A	301	CZU	C2-N1	5.39	1.45	1.35
2	C	301	CZU	C2-N1	5.37	1.45	1.35
2	D	301	CZU	O2'-C2'	4.20	1.52	1.43
2	C	301	CZU	O2'-C2'	3.94	1.52	1.43
2	B	301	CZU	O2'-C2'	3.42	1.51	1.43
2	A	301	CZU	O2'-C2'	3.25	1.50	1.43
2	C	301	CZU	O3'-C3'	-3.05	1.35	1.43
2	D	301	CZU	O3'-C3'	-2.99	1.35	1.43
2	A	301	CZU	O6-C6	-2.86	1.18	1.23
2	A	301	CZU	O3'-C3'	-2.71	1.36	1.43
2	A	301	CZU	C5-N7	-2.56	1.34	1.39
2	C	301	CZU	C5-C6	2.51	1.53	1.44
2	B	301	CZU	O6-C6	-2.49	1.18	1.23
2	D	301	CZU	C5-N7	-2.49	1.34	1.39
2	C	301	CZU	O6-C6	-2.49	1.18	1.23
2	D	301	CZU	C5-C6	2.47	1.53	1.44
2	B	301	CZU	C6-N1	2.47	1.44	1.39
2	C	301	CZU	C5-N7	-2.46	1.34	1.39
2	B	301	CZU	C5-N7	-2.45	1.34	1.39
2	C	301	CZU	C6-N1	2.44	1.43	1.39
2	B	301	CZU	C5-C6	2.40	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	CZU	O6-C6	-2.38	1.19	1.23
2	D	301	CZU	C6-N1	2.29	1.43	1.39
2	B	301	CZU	O3'-C3'	-2.29	1.37	1.43
2	A	301	CZU	C5-C6	2.28	1.52	1.44
2	C	301	CZU	C8-N9	-2.19	1.32	1.37
2	A	301	CZU	C8-N9	-2.17	1.32	1.37
2	B	301	CZU	C4-N9	-2.12	1.32	1.38
2	A	301	CZU	C6-N1	2.09	1.43	1.39
2	B	301	CZU	C8-N9	-2.07	1.32	1.37
2	D	301	CZU	C8-N9	-2.06	1.33	1.37

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	CZU	C5-C6-N1	6.44	120.20	110.68
2	C	301	CZU	C5-C6-N1	6.39	120.13	110.68
2	D	301	CZU	C5-C6-N1	6.29	119.99	110.68
2	B	301	CZU	C5-C6-N1	5.97	119.51	110.68
2	C	301	CZU	N1-C2-N3	-5.14	119.89	125.57
2	B	301	CZU	N1-C2-N3	-5.13	119.90	125.57
2	D	301	CZU	N1-C2-N3	-5.02	120.03	125.57
2	A	301	CZU	N1-C2-N3	-4.87	120.19	125.57
2	D	301	CZU	C5-C4-N3	-4.83	120.05	127.26
2	C	301	CZU	C2-N3-C4	4.82	120.22	111.50
2	D	301	CZU	C2-N3-C4	4.78	120.16	111.50
2	C	301	CZU	C3'-C2'-C1'	4.75	110.45	101.43
2	C	301	CZU	C5-C4-N3	-4.65	120.33	127.26
2	A	301	CZU	C5-C4-N3	-4.50	120.55	127.26
2	A	301	CZU	C2-N3-C4	4.48	119.61	111.50
2	B	301	CZU	C2-N3-C4	4.22	119.13	111.50
2	A	301	CZU	C2-N1-C6	-3.94	119.74	125.03
2	D	301	CZU	C2-N1-C6	-3.88	119.82	125.03
2	C	301	CZU	C2-N1-C6	-3.86	119.85	125.03
2	D	301	CZU	C3'-C2'-C1'	3.66	108.37	101.43
2	A	301	CZU	C3'-C2'-C1'	3.61	108.28	101.43
2	C	301	CZU	PB-O3A-PA	-3.55	120.65	132.83
2	B	301	CZU	C5-C4-N3	-3.53	122.00	127.26
2	B	301	CZU	C2-N1-C6	-3.47	120.38	125.03
2	B	301	CZU	PB-O3A-PA	-3.44	121.03	132.83
2	B	301	CZU	C4-C5-N7	-3.10	105.81	110.72
2	C	301	CZU	C4-C5-N7	-3.08	105.85	110.72
2	D	301	CZU	PB-O3A-PA	-2.98	122.60	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	CZU	C4-C5-N7	-2.88	106.17	110.72
2	A	301	CZU	PB-O3B-PG	-2.77	123.32	132.83
2	D	301	CZU	PB-O3B-PG	-2.77	123.34	132.83
2	B	301	CZU	C6-C5-N7	2.61	135.11	130.25
2	C	301	CZU	C8-N7-C5	2.60	108.94	104.24
2	C	301	CZU	PB-O3B-PG	-2.55	124.06	132.83
2	B	301	CZU	C8-N7-C5	2.53	108.82	104.24
2	A	301	CZU	PB-O3A-PA	-2.47	124.35	132.83
2	D	301	CZU	C8-N7-C5	2.46	108.69	104.24
2	A	301	CZU	C4-C5-N7	-2.44	106.86	110.72
2	A	301	CZU	N9-C4-N3	2.43	132.61	126.94
2	A	301	CZU	C2'-C1'-N9	-2.43	106.32	113.22
2	B	301	CZU	PB-O3B-PG	-2.43	124.48	132.83
2	A	301	CZU	O2'-C2'-C3'	-2.41	104.02	111.82
2	B	301	CZU	N9-C8-N7	-2.39	108.88	113.39
2	A	301	CZU	C8-N7-C5	2.35	108.50	104.24
2	C	301	CZU	C6-C5-N7	2.33	134.58	130.25
2	A	301	CZU	O6-C6-C5	-2.31	120.47	126.60
2	D	301	CZU	O6-C6-C5	-2.26	120.61	126.60
2	B	301	CZU	O6-C6-C5	-2.25	120.62	126.60
2	D	301	CZU	N9-C4-N3	2.17	132.00	126.94
2	C	301	CZU	O6-C6-C5	-2.14	120.93	126.60
2	A	301	CZU	N9-C8-N7	-2.07	109.49	113.39
2	B	301	CZU	C2'-C3'-C4'	2.04	106.60	102.64

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	CZU	C5'-O5'-PA-O1A
2	B	301	CZU	PB-O3B-PG-O3G
2	C	301	CZU	PB-O3A-PA-O5'
2	D	301	CZU	C3'-C4'-C5'-O5'
2	A	301	CZU	C3'-C4'-C5'-O5'
2	A	301	CZU	O4'-C4'-C5'-O5'
2	C	301	CZU	C3'-C4'-C5'-O5'
2	C	301	CZU	O4'-C4'-C5'-O5'
2	D	301	CZU	O4'-C4'-C5'-O5'
2	B	301	CZU	PA-O3A-PB-O3B
2	C	301	CZU	PB-O3B-PG-O1G
2	A	301	CZU	C5'-O5'-PA-O3A
2	C	301	CZU	PG-O3B-PB-O2B

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Mol	Chain	Res	Type	Atoms
2	A	301	CZU	C5'-O5'-PA-O2A
2	D	301	CZU	C4'-C5'-O5'-PA
2	B	301	CZU	O4'-C4'-C5'-O5'
2	C	301	CZU	PB-O3B-PG-O2G
2	C	301	CZU	PB-O3B-PG-O3G
2	B	301	CZU	PA-O3A-PB-O1B
2	C	301	CZU	PG-O3B-PB-O1B
2	B	301	CZU	PB-O3B-PG-O1G

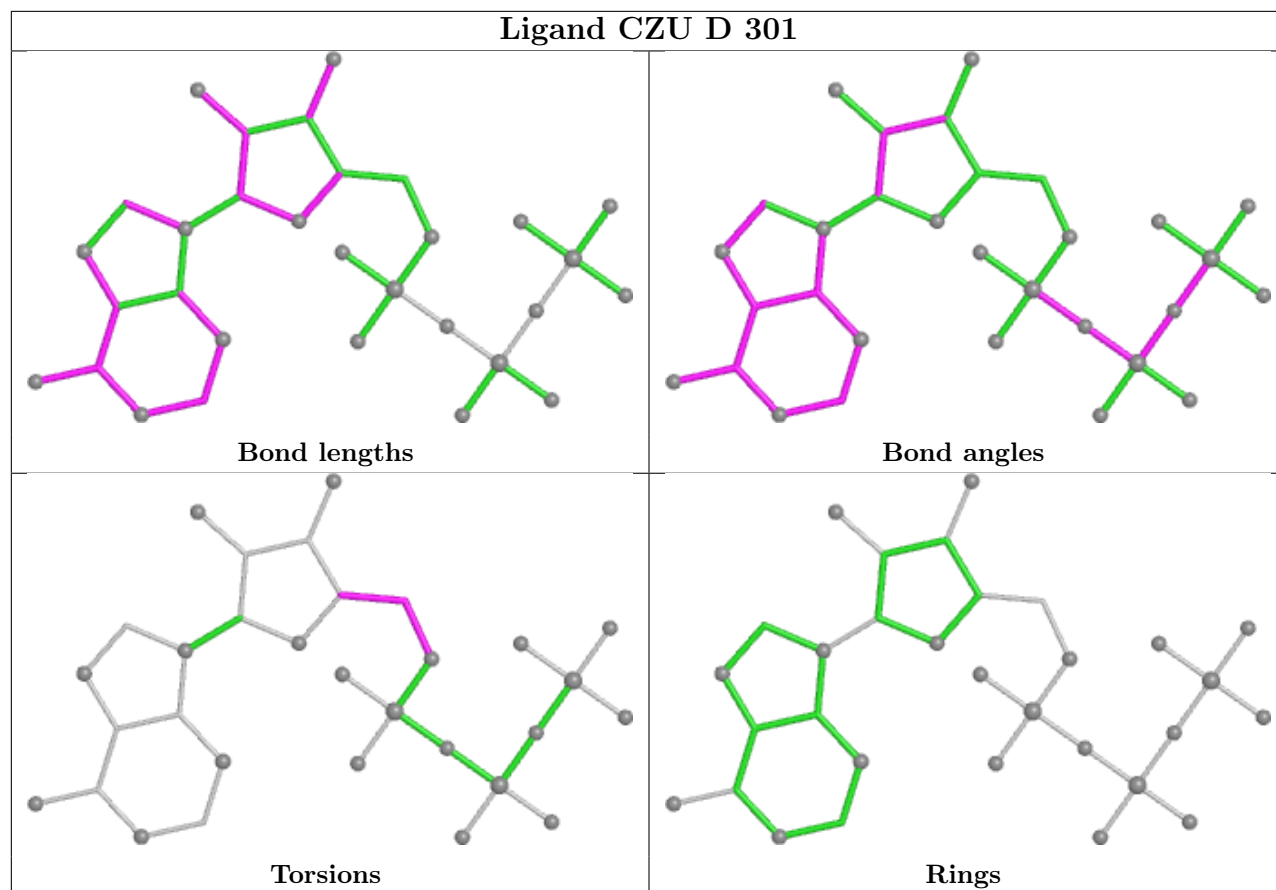
There are no ring outliers.

3 monomers are involved in 4 short contacts:

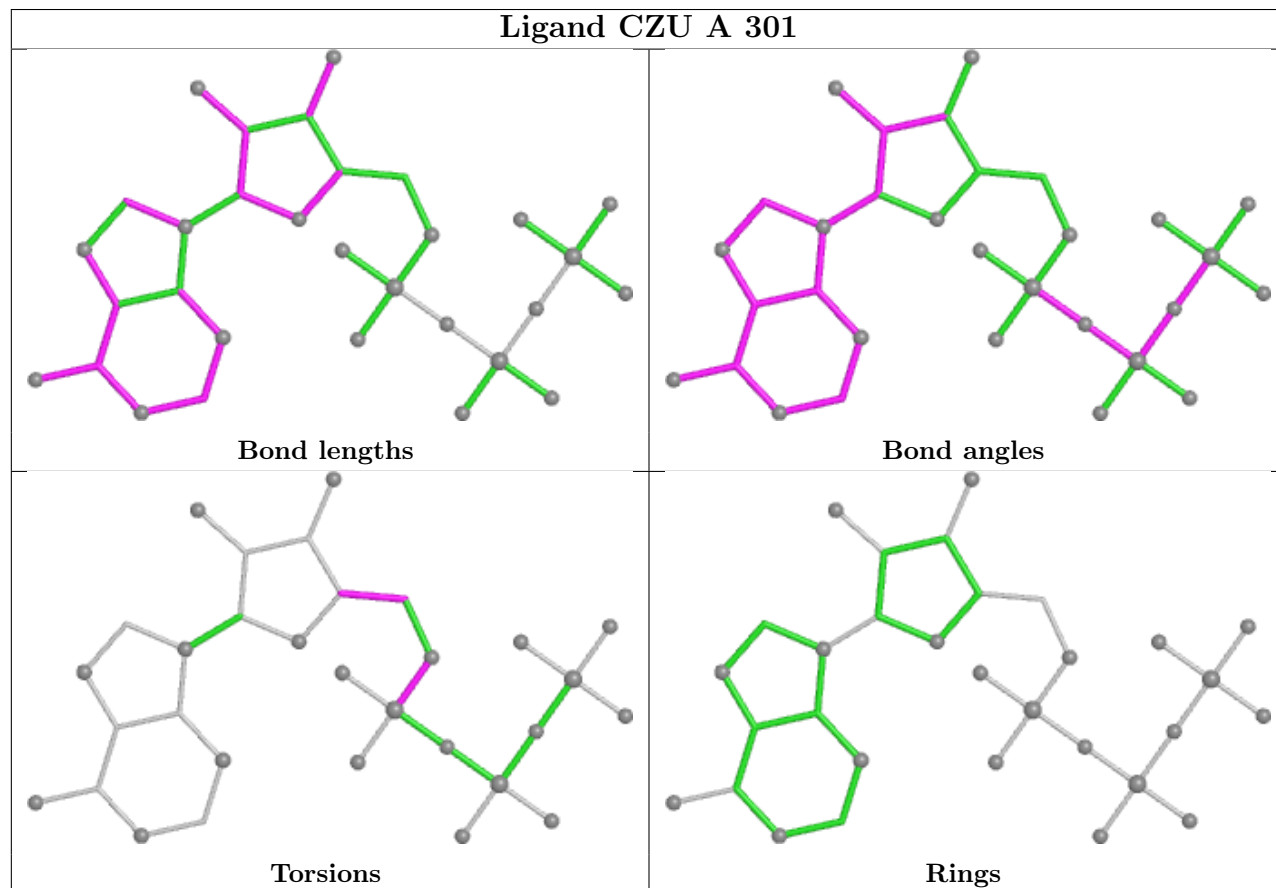
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	CZU	2	0
2	C	301	CZU	1	0
2	B	301	CZU	1	0

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.

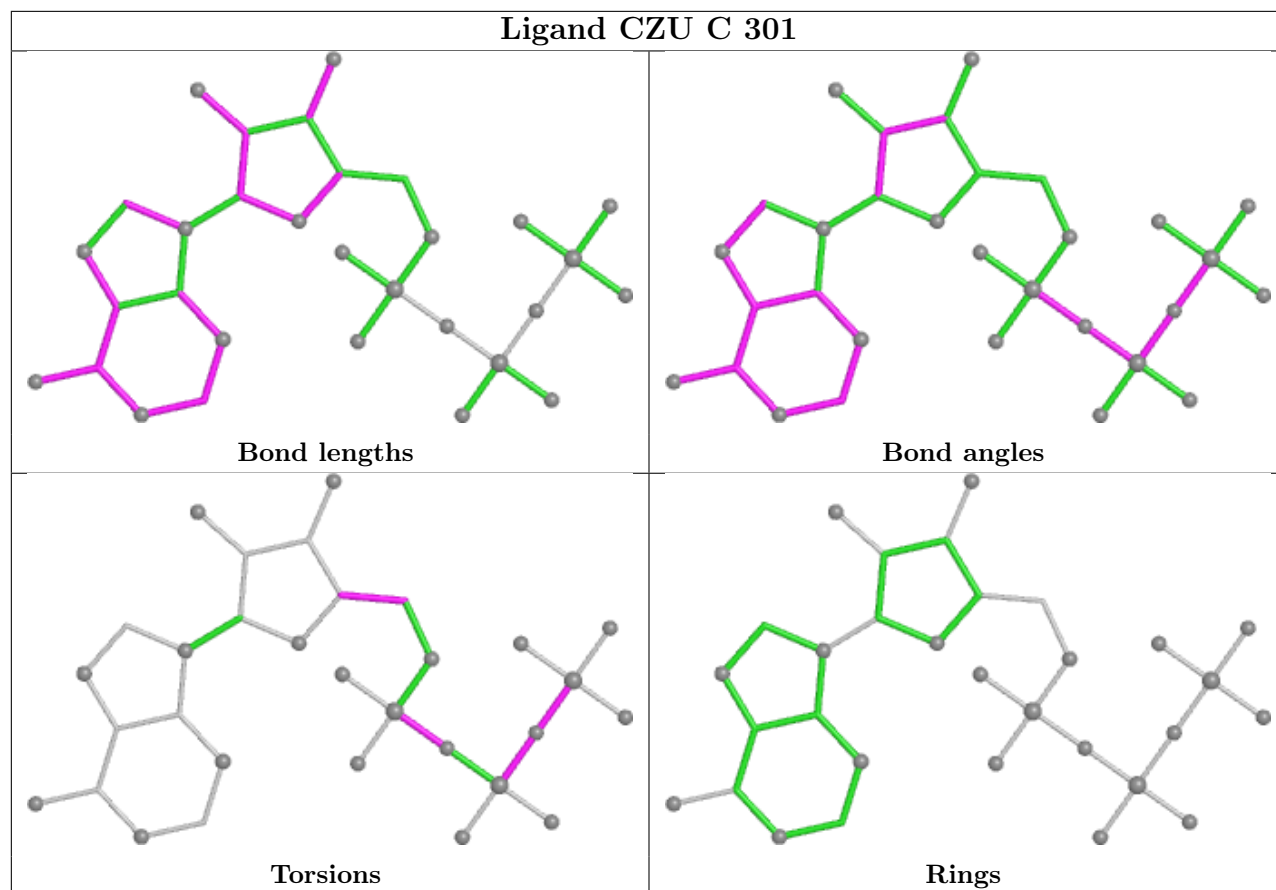
Ligand CZU D 301



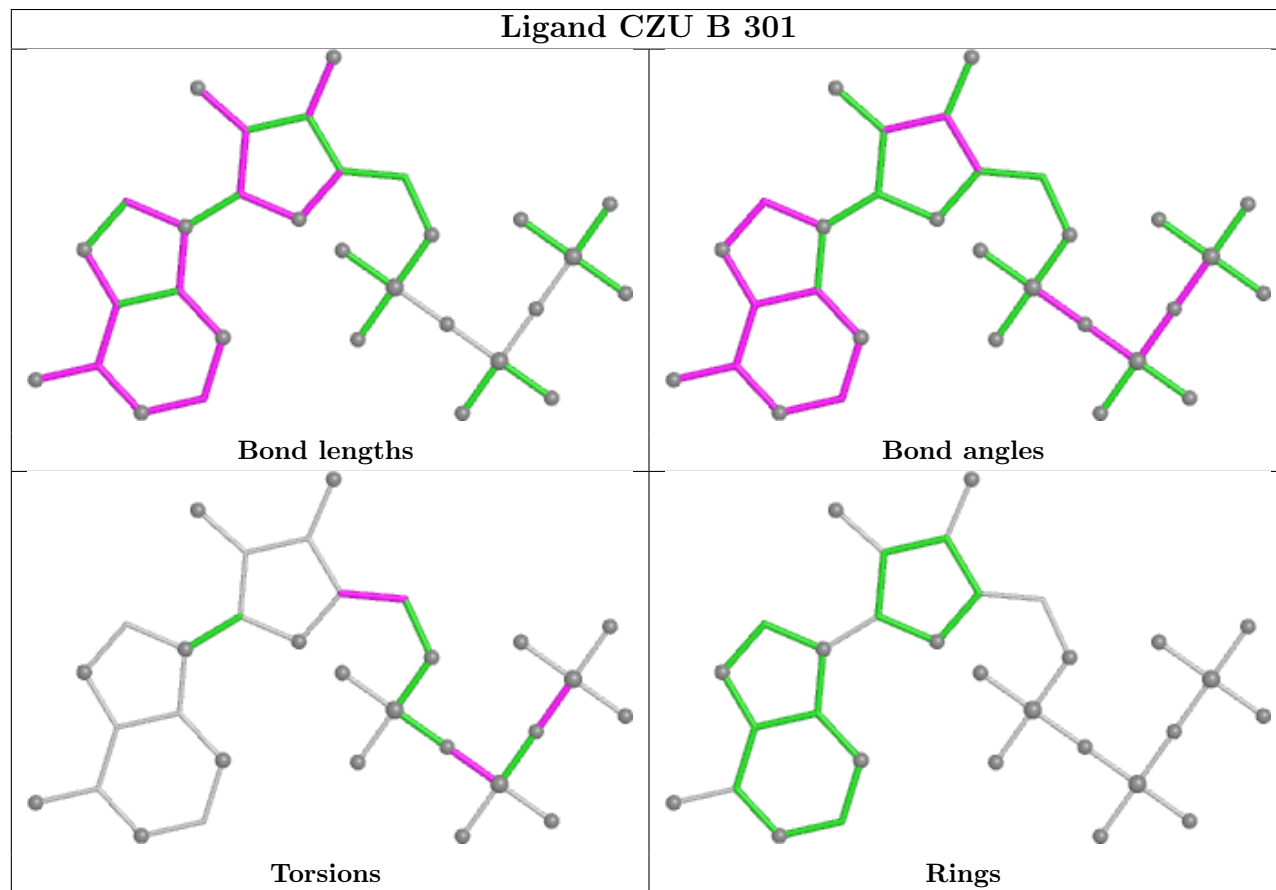
Ligand CZU A 301



Ligand CZU C 301



Ligand CZU B 301



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	201/211 (95%)	0.74	18 (8%) 15 8	20, 33, 53, 83	0
1	B	196/211 (92%)	0.62	11 (5%) 30 16	19, 32, 54, 81	0
1	C	192/211 (90%)	0.67	20 (10%) 11 6	17, 34, 59, 93	0
1	D	190/211 (90%)	0.60	14 (7%) 20 11	21, 33, 53, 68	0
All	All	779/844 (92%)	0.66	63 (8%) 18 10	17, 33, 54, 93	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	153	LEU	4.8
1	C	177	GLU	4.5
1	A	109	ALA	4.2
1	C	88	GLY	3.9
1	A	108	GLY	3.8
1	A	110	ALA	3.7
1	D	150	ASN	3.5
1	A	88	GLY	3.4
1	C	180	ASP	3.3
1	C	80	GLN	3.2
1	C	97	HIS	3.1
1	D	211	GLY	3.1
1	B	136	ALA	3.1
1	A	41	GLY	3.1
1	B	180	ASP	3.1
1	B	81	GLY	3.0
1	B	192	PRO	2.9
1	A	8	ARG	2.9
1	A	192	PRO	2.9
1	D	24	GLU	2.9
1	C	49	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	111	SER	2.8
1	C	179	GLY	2.8
1	A	83	ALA	2.8
1	B	50	ALA	2.7
1	B	153	LEU	2.6
1	C	24	GLU	2.6
1	D	154	LEU	2.6
1	B	211	GLY	2.5
1	C	81	GLY	2.5
1	A	107	ALA	2.5
1	A	149	GLU	2.5
1	C	53	GLU	2.5
1	A	204	ARG	2.5
1	C	104	PRO	2.4
1	C	51	GLU	2.4
1	B	106	SER	2.4
1	A	189	LEU	2.4
1	A	191	GLY	2.3
1	B	110	ALA	2.3
1	D	151	ARG	2.3
1	C	54	HIS	2.3
1	C	149	GLU	2.3
1	D	177	GLU	2.3
1	D	189	LEU	2.3
1	B	33	ARG	2.3
1	B	154	LEU	2.2
1	C	211	GLY	2.2
1	D	179	GLY	2.2
1	D	185	PRO	2.2
1	C	78	ARG	2.2
1	C	176	PRO	2.2
1	D	168	LYS	2.2
1	A	195	PRO	2.1
1	D	180	ASP	2.1
1	D	80	GLN	2.1
1	A	112	GLY	2.1
1	C	43	GLN	2.1
1	C	41	GLY	2.1
1	D	176	PRO	2.1
1	C	79	ARG	2.0
1	D	104	PRO	2.0
1	A	117	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

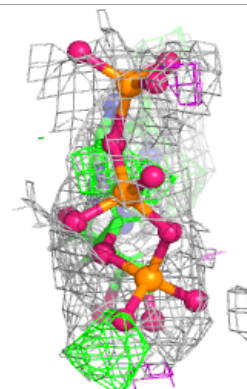
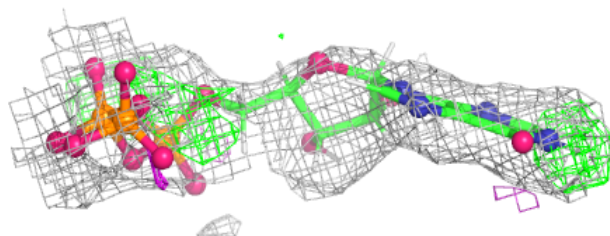
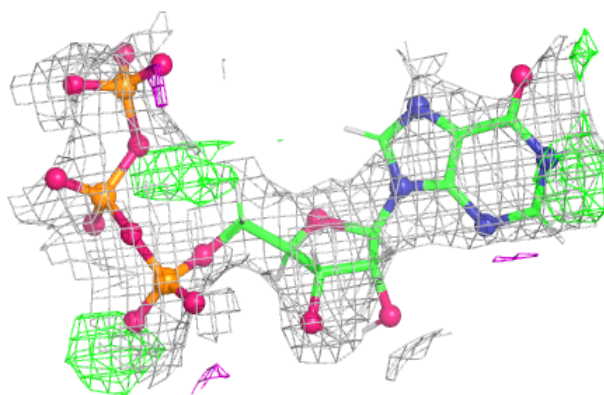
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CZU	C	301	31/31	0.61	0.24	44,64,79,99	0
2	CZU	D	301	31/31	0.68	0.19	47,65,80,97	0
2	CZU	B	301	31/31	0.74	0.20	28,41,78,83	0
3	ZN	C	302	1/1	0.77	0.49	30,30,30,30	0
2	CZU	A	301	31/31	0.78	0.17	40,54,76,88	0
3	ZN	D	302	1/1	0.79	0.50	30,30,30,30	0
3	ZN	B	302	1/1	0.86	0.42	30,30,30,30	0
3	ZN	A	302	1/1	0.93	0.09	89,89,89,89	0

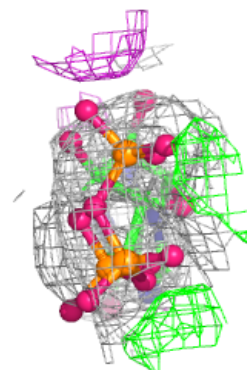
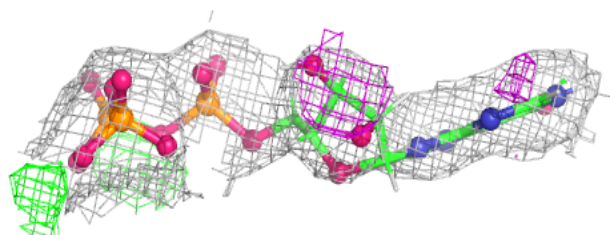
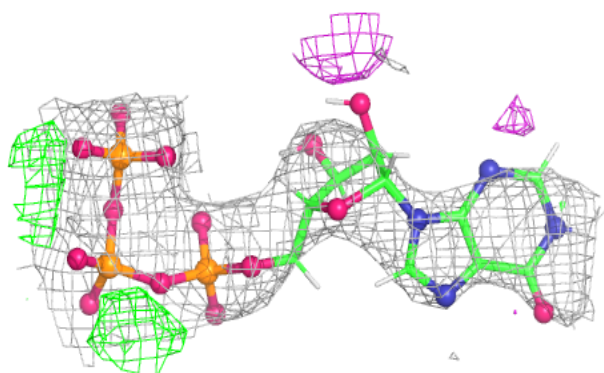
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CZU C 301:

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

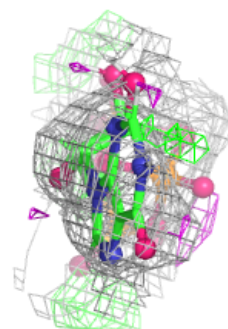
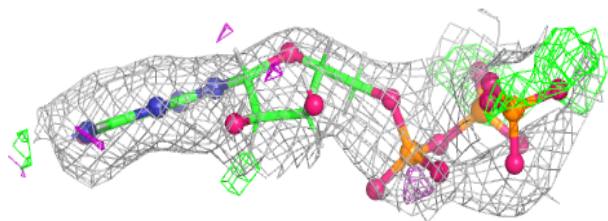
**Electron density around CZU D 301:**

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



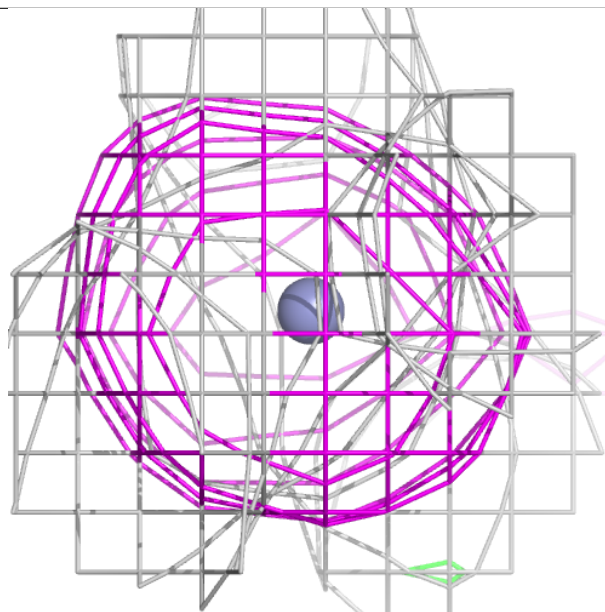
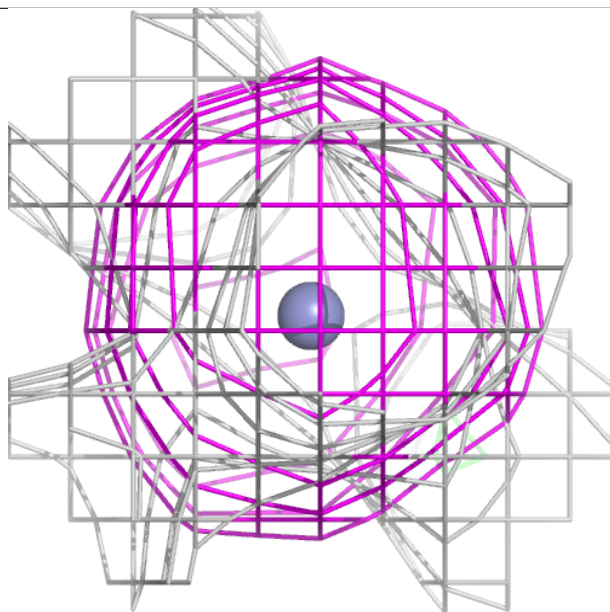
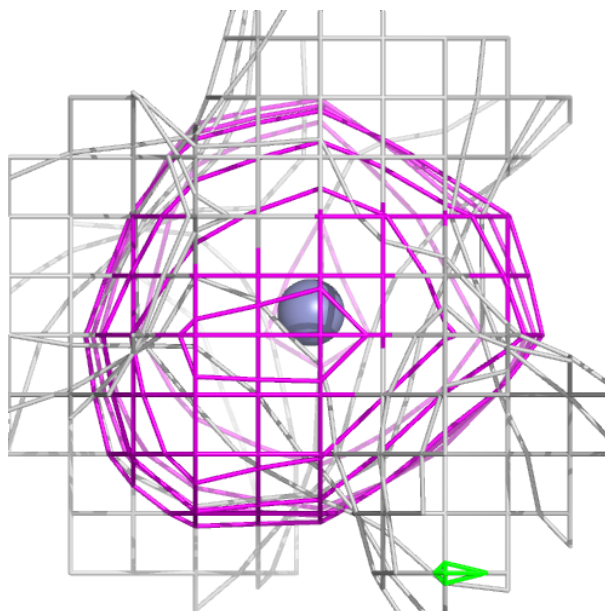
Electron density around CZU B 301:

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



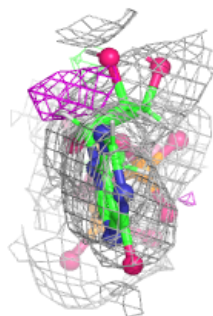
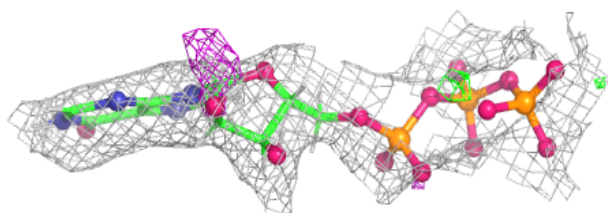
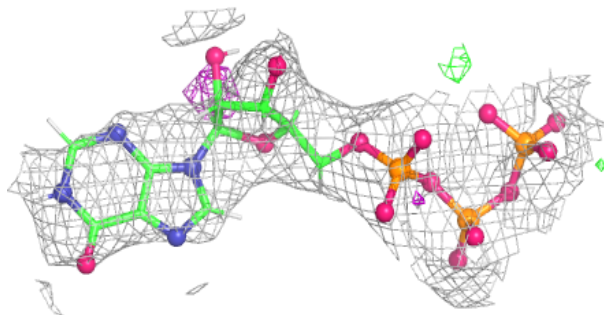
Electron density around ZN C 302:

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



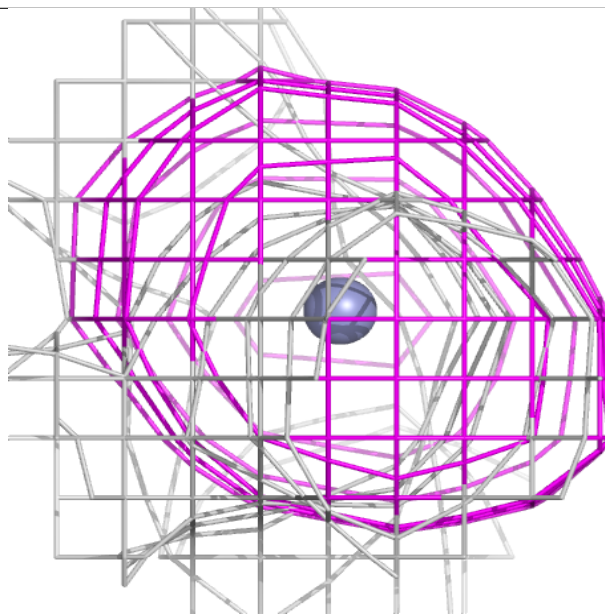
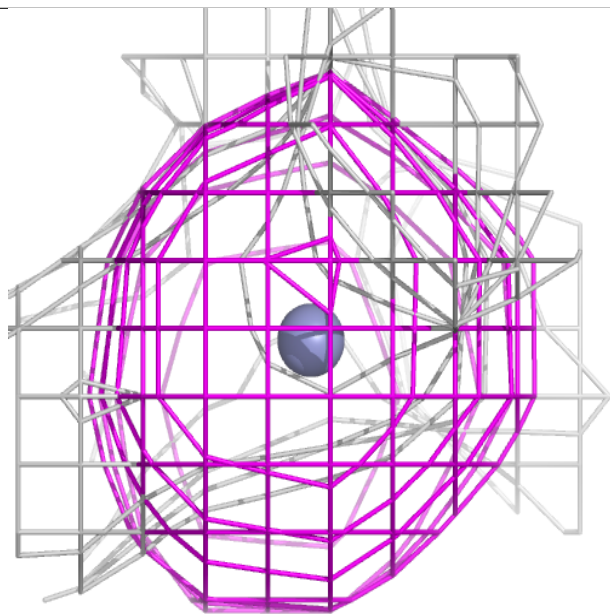
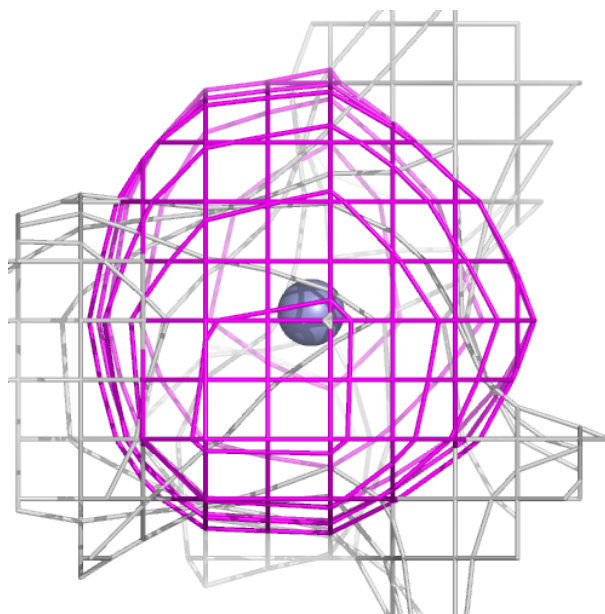
Electron density around CZU A 301:

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



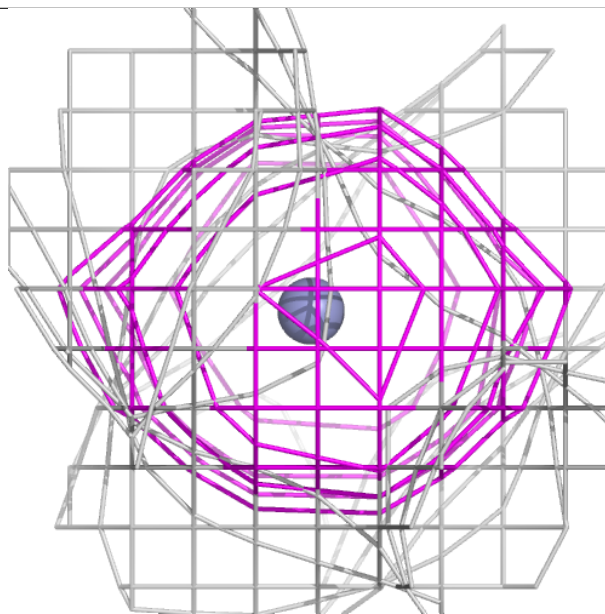
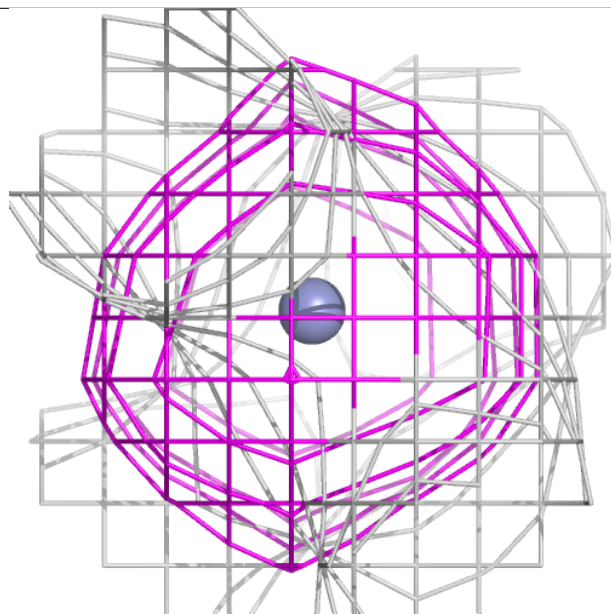
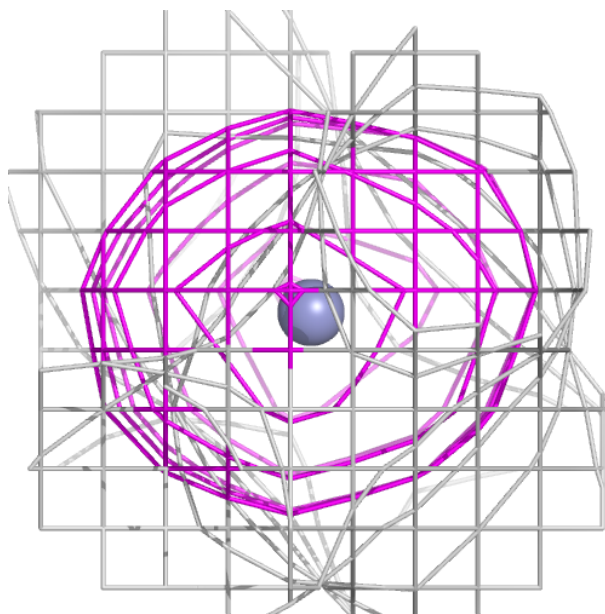
Electron density around ZN D 302:

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



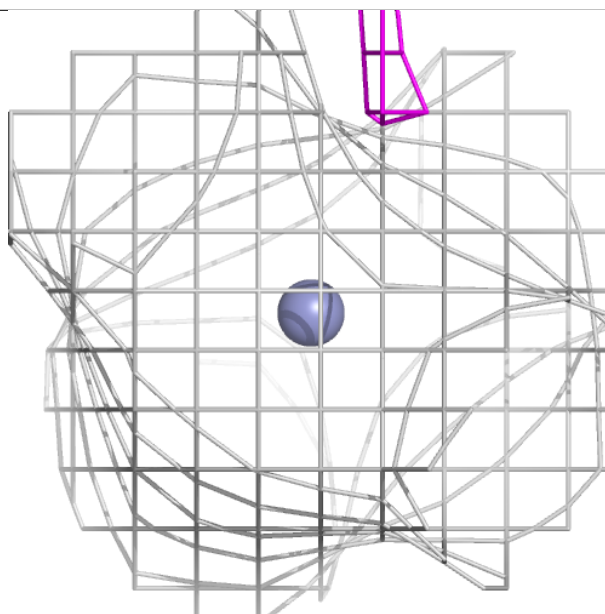
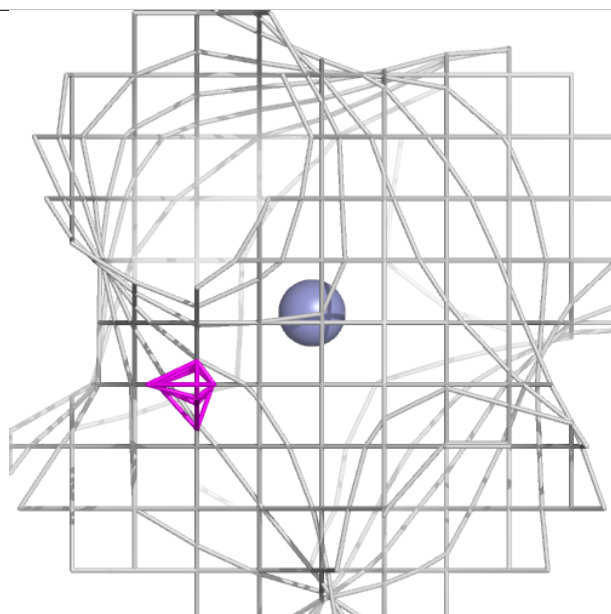
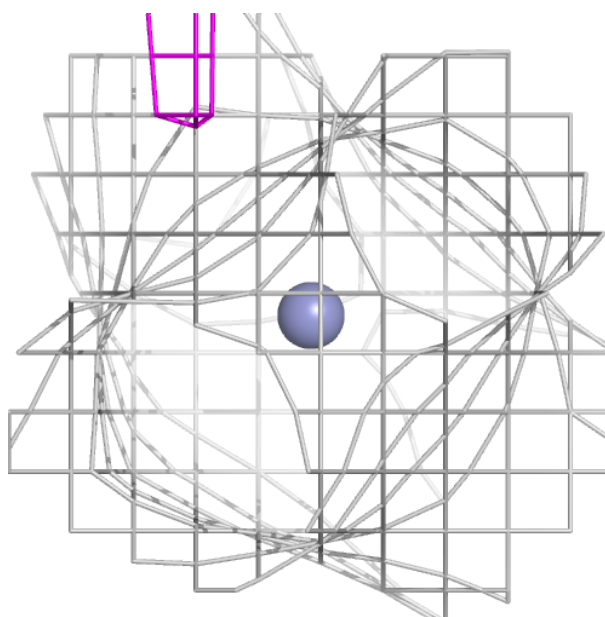
Electron density around ZN B 302:

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



Electron density around ZN A 302:

$2mF_o-DF_c$ (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.