



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 07:40 AM UTC

PDB ID : 8B7P / pdb_00008b7p
Title : Crystal structure of an AA9 LPMO from *Aspergillus nidulans*, AnLPMOC
Authors : Males, A.; Rafael Fanchini Terrasan, C.; Davies, G.J.; Walton, P.H.
Deposited on : 2022-09-30
Resolution : 2.11 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
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

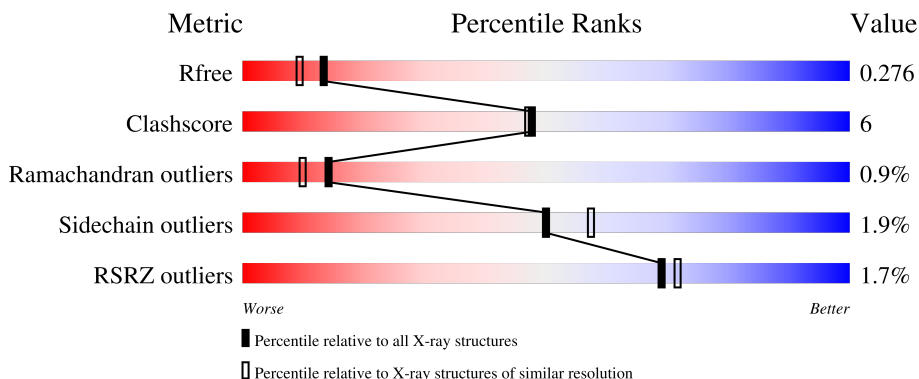
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	AAA	213	2% 89% 10%
1	BBB	213	% 87% 10%
1	CCC	213	2% 87% 12%
1	DDD	213	% 82% 17%

2 Entry composition [i](#)

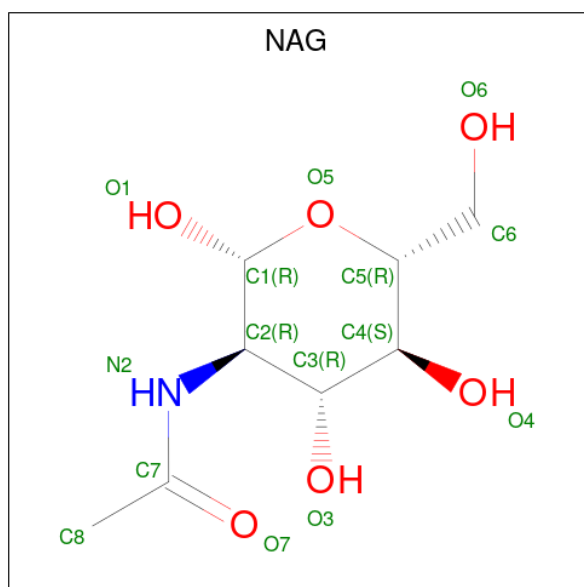
There are 4 unique types of molecules in this entry. The entry contains 12563 atoms, of which 5931 are hydrogens and 0 are deuteriums.

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 Endo-beta-1,4-glucanase D.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	213	Total	C	H	N	O	S	51	0	0
			3030	996	1464	256	311	3			
1	BBB	213	Total	C	H	N	O	S	51	1	0
			3043	1005	1464	256	315	3			
1	CCC	213	Total	C	H	N	O	S	49	1	0
			3062	1009	1480	259	311	3			
1	DDD	213	Total	C	H	N	O	S	49	0	0
			3046	1005	1467	257	314	3			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
2	BBB	1	Total	C	H	N	O	3	0
			28	8	14	1	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	CCC	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
2	DDD	1	Total	C	H	N	O	3	0
			28	8	14	1	5		

- Molecule 3 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	1	Total	Cu	0	0
			1	1		
3	BBB	1	Total	Cu	0	0
			1	1		
3	CCC	2	Total	Cu	0	0
			2	2		
3	DDD	2	Total	Cu	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	79	Total	O	0	0
			79	79		
4	BBB	67	Total	O	0	0
			67	67		
4	CCC	55	Total	O	0	2
			57	57		
4	DDD	61	Total	O	0	0
			61	61		

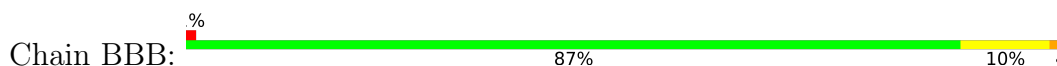
3 Residue-property plots [i](#)

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.

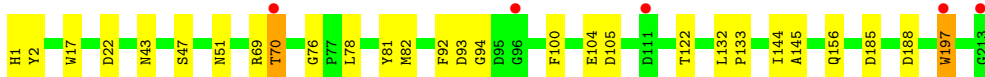
- Molecule 1: Endo-beta-1,4-glucanase D



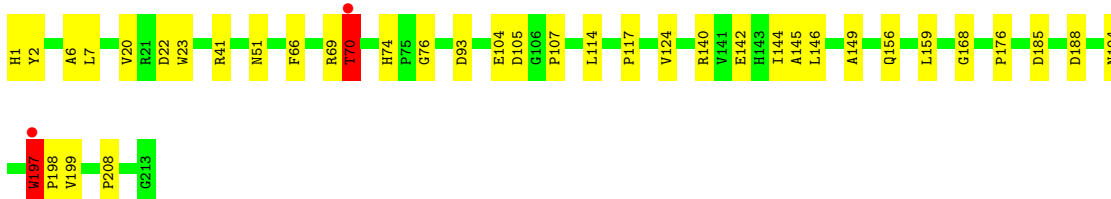
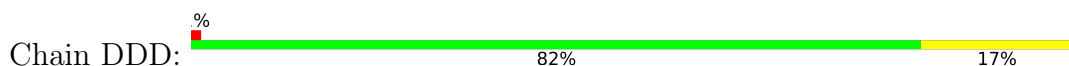
- Molecule 1: Endo-beta-1,4-glucanase D



- Molecule 1: Endo-beta-1,4-glucanase D



- Molecule 1: Endo-beta-1,4-glucanase D



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	47.90Å 64.38Å 76.24Å 86.46° 85.54° 68.21°	Depositor
Resolution (Å)	75.96 – 2.11 75.96 – 2.11	Depositor EDS
% Data completeness (in resolution range)	80.4 (75.96-2.11) 79.7 (75.96-2.11)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.213 , 0.273 0.216 , 0.276	Depositor DCC
R_{free} test set	1947 reflections (3.34%)	wwPDB-VP
Wilson B-factor (Å ²)	16.6	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 27.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.098 for -h,-h+k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12563	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.25% 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: HIC, NAG, CU

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	AAA	1.10	0/1604	1.38	5/2206 (0.2%)
1	BBB	1.08	0/1622	1.39	7/2234 (0.3%)
1	CCC	1.09	0/1625	1.37	5/2234 (0.2%)
1	DDD	1.09	2/1619 (0.1%)	1.44	8/2228 (0.4%)
All	All	1.09	2/6470 (0.0%)	1.39	25/8902 (0.3%)

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	AAA	0	2
1	CCC	0	1
1	DDD	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	DDD	74	HIS	CE1-NE2	5.04	1.37	1.32
1	DDD	117	PRO	C-O	-5.03	1.17	1.24

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DDD	70	THR	CB-CA-C	9.53	129.39	110.42
1	DDD	70	THR	CA-CB-OG1	-8.57	96.75	109.60
1	BBB	70	THR	CB-CA-C	7.40	125.14	110.42
1	AAA	70	THR	CB-CA-C	6.53	123.42	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	70	THR	CB-CA-C	6.21	122.78	110.42
1	DDD	69	ARG	N-CA-CB	6.07	119.04	110.24
1	DDD	105	ASP	CB-CA-C	-5.92	99.06	109.71
1	BBB	198	PRO	N-CA-C	-5.82	101.07	110.55
1	BBB	110	THR	CA-C-N	5.61	128.58	120.79
1	BBB	110	THR	C-N-CA	5.61	128.58	120.79
1	CCC	104	GLU	CA-C-N	5.48	132.01	122.81
1	CCC	104	GLU	C-N-CA	5.48	132.01	122.81
1	DDD	104	GLU	CA-C-N	5.43	132.47	122.92
1	DDD	104	GLU	C-N-CA	5.43	132.47	122.92
1	AAA	69	ARG	O-C-N	5.22	129.14	123.13
1	BBB	69	ARG	CA-C-N	5.15	131.37	121.54
1	BBB	69	ARG	C-N-CA	5.15	131.37	121.54
1	AAA	69	ARG	CA-C-N	5.12	131.31	121.54
1	AAA	69	ARG	C-N-CA	5.12	131.31	121.54
1	AAA	93	ASP	CA-CB-CG	5.09	117.69	112.60
1	CCC	69	ARG	CA-C-N	5.07	131.23	121.54
1	CCC	69	ARG	C-N-CA	5.07	131.23	121.54
1	BBB	198	PRO	N-CA-CB	5.02	107.53	103.36
1	DDD	69	ARG	CA-C-N	5.01	131.10	121.54
1	DDD	69	ARG	C-N-CA	5.01	131.10	121.54

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	196	TYR	Peptide
1	AAA	197	TRP	Peptide
1	CCC	122	THR	Peptide
1	DDD	197	TRP	Peptide

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	AAA	1566	1464	1447	11	0
1	BBB	1579	1464	1450	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CCC	1582	1480	1465	11	0
1	DDD	1579	1467	1454	25	0
2	AAA	14	14	13	0	0
2	BBB	14	14	13	0	0
2	CCC	14	14	13	0	0
2	DDD	14	14	13	0	0
3	AAA	1	0	0	0	0
3	BBB	1	0	0	0	0
3	CCC	2	0	0	0	0
3	DDD	2	0	0	0	0
4	AAA	79	0	0	3	0
4	BBB	67	0	0	3	0
4	CCC	57	0	0	0	0
4	DDD	61	0	0	2	0
All	All	6632	5931	5868	68	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 6.

All (68) 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:BBB:197:TRP:CG	1:BBB:198:PRO:HD3	1.88	1.08
1:DDD:197:TRP:CG	1:DDD:198:PRO:HD3	2.01	0.96
1:BBB:197:TRP:CD1	1:BBB:198:PRO:HD3	2.01	0.96
1:DDD:197:TRP:CD2	1:DDD:198:PRO:HD3	2.13	0.84
1:BBB:194:ASN:CG	1:BBB:197:TRP:HB2	2.07	0.80
1:BBB:197:TRP:CG	1:BBB:198:PRO:CD	2.67	0.78
1:AAA:70:THR:HB	4:AAA:412:HOH:O	1.88	0.73
1:BBB:70:THR:HB	4:BBB:443:HOH:O	1.87	0.72
1:BBB:114:LEU:HD11	1:BBB:200:PRO:HG2	1.70	0.72
1:DDD:194:ASN:CG	1:DDD:197:TRP:HB2	2.18	0.68
1:BBB:194:ASN:ND2	1:BBB:197:TRP:HB2	2.14	0.62
1:BBB:197:TRP:CB	1:BBB:198:PRO:CD	2.78	0.61
1:DDD:194:ASN:ND2	1:DDD:197:TRP:HB2	2.16	0.60
1:BBB:134:ASP:OD2	4:BBB:401:HOH:O	2.16	0.59
1:DDD:107:PRO:HB2	1:DDD:114:LEU:HG	1.84	0.59
1:BBB:197:TRP:CD1	1:BBB:198:PRO:CD	2.81	0.59
1:BBB:3:VAL:HG22	1:BBB:69:ARG:HB3	1.84	0.59
1:DDD:145:ALA:HB3	1:DDD:156:GLN:HB2	1.86	0.56
1:DDD:197:TRP:CB	1:DDD:198:PRO:CD	2.84	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:197:TRP:O	1:CCC:197:TRP:HE3	1.90	0.55
1:DDD:114:LEU:HD13	1:DDD:199:VAL:HG13	1.90	0.54
1:BBB:185:ASP:HB3	1:BBB:188:ASP:OD1	2.08	0.53
1:DDD:7:LEU:HD13	1:DDD:20:VAL:CG2	2.40	0.52
1:DDD:7:LEU:HD13	1:DDD:20:VAL:HG22	1.90	0.52
1:BBB:24:THR:HB	1:BBB:44:LYS:HD2	1.92	0.52
1:DDD:197:TRP:HB3	1:DDD:198:PRO:CD	2.40	0.51
1:CCC:132:LEU:HD12	1:CCC:133:PRO:HD2	1.92	0.51
1:BBB:197:TRP:HB3	1:BBB:198:PRO:CD	2.41	0.51
1:BBB:123:ASN:OD1	1:BBB:123:ASN:C	2.53	0.51
1:CCC:185:ASP:HB3	1:CCC:188:ASP:OD1	2.12	0.50
1:DDD:168:GLY:HA2	4:DDD:440:HOH:O	2.12	0.50
1:DDD:197:TRP:CG	1:DDD:198:PRO:CD	2.86	0.50
1:DDD:197:TRP:CB	1:DDD:198:PRO:HD3	2.41	0.49
1:DDD:142:GLU:HB2	1:DDD:159:LEU:HD23	1.93	0.49
1:CCC:76:GLY:HA3	1:CCC:144:ILE:O	2.13	0.49
1:DDD:76:GLY:HA3	1:DDD:144:ILE:O	2.12	0.48
1:BBB:88:ASP:HB3	4:BBB:441:HOH:O	2.12	0.48
1:DDD:6:ALA:O	1:DDD:66:PHE:HA	2.14	0.48
1:AAA:198:PRO:HG2	4:AAA:401:HOH:O	2.14	0.47
1:AAA:88:ASP:HB3	4:AAA:458:HOH:O	2.14	0.47
1:BBB:197:TRP:HB3	1:BBB:198:PRO:HD2	1.98	0.46
1:DDD:176:PRO:HG2	1:DDD:208:PRO:HB2	1.98	0.46
1:CCC:82:MET:HB2	1:CCC:100:PHE:CZ	2.51	0.45
1:DDD:185:ASP:HB3	1:DDD:188:ASP:OD1	2.16	0.45
1:CCC:78:LEU:H	1:CCC:105:ASP:HB2	1.82	0.45
1:DDD:41:ARG:NH1	1:DDD:93:ASP:O	2.46	0.45
1:AAA:77:PRO:HG3	1:AAA:203:TYR:CE2	2.51	0.45
1:DDD:140:ARG:NH2	1:DDD:159:LEU:CD2	2.80	0.44
1:DDD:188:ASP:HB3	4:DDD:451:HOH:O	2.16	0.44
1:BBB:49:ASN:OD1	1:BBB:49:ASN:C	2.60	0.44
1:CCC:47:SER:O	1:CCC:93:ASP:HA	2.17	0.44
1:AAA:140:ARG:NH2	1:AAA:159:LEU:HD21	2.32	0.44
1:BBB:145:ALA:HB3	1:BBB:156:GLN:HB2	1.99	0.44
1:DDD:140:ARG:NH2	1:DDD:159:LEU:HD22	2.33	0.43
1:AAA:78:LEU:O	1:AAA:104:GLU:HA	2.18	0.42
1:AAA:3:VAL:HG22	1:AAA:69:ARG:HB3	2.01	0.42
1:DDD:146:LEU:HA	1:DDD:149:ALA:HB2	2.00	0.42
1:DDD:22:ASP:OD1	1:DDD:23:TRP:N	2.52	0.42
1:AAA:142:GLU:HB2	1:AAA:159:LEU:HD23	2.01	0.42
1:CCC:17:TRP:CE3	1:CCC:22:ASP:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:47:SER:O	1:BBB:93:ASP:HA	2.19	0.41
1:CCC:145:ALA:HB3	1:CCC:156:GLN:HB2	2.01	0.41
1:AAA:82:MET:HA	1:AAA:138:LEU:O	2.20	0.41
1:AAA:21:ARG:HD3	1:AAA:46:ALA:O	2.21	0.41
1:AAA:22:ASP:OD1	1:AAA:23:TRP:N	2.53	0.41
1:BBB:86:PRO:HD2	1:BBB:92:PHE:CD1	2.56	0.41
1:CCC:92:PHE:CZ	1:CCC:94:GLY:HA2	2.56	0.40
1:CCC:81:TYR:HA	1:CCC:100:PHE:O	2.22	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	AAA	211/213 (99%)	195 (92%)	15 (7%)	1 (0%)	24	22
1	BBB	212/213 (100%)	200 (94%)	10 (5%)	2 (1%)	14	10
1	CCC	212/213 (100%)	197 (93%)	13 (6%)	2 (1%)	14	10
1	DDD	211/213 (99%)	199 (94%)	9 (4%)	3 (1%)	9	5
All	All	846/852 (99%)	791 (94%)	47 (6%)	8 (1%)	14	10

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	197	TRP
1	DDD	197	TRP
1	CCC	51	ASN
1	DDD	51	ASN
1	DDD	70	THR
1	CCC	43	ASN
1	AAA	198	PRO

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Mol	Chain	Res	Type
1	BBB	70	THR

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	AAA	159/165 (96%)	157 (99%)	2 (1%)	61	69
1	BBB	161/165 (98%)	157 (98%)	4 (2%)	42	47
1	CCC	161/165 (98%)	158 (98%)	3 (2%)	50	57
1	DDD	161/165 (98%)	158 (98%)	3 (2%)	50	57
All	All	642/660 (97%)	630 (98%)	12 (2%)	50	57

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	2	TYR
1	AAA	151	THR
1	BBB	2	TYR
1	BBB	90	SER
1	BBB	123	ASN
1	BBB	159	LEU
1	CCC	2	TYR
1	CCC	70	THR
1	CCC	197	TRP
1	DDD	2	TYR
1	DDD	70	THR
1	DDD	124	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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$
1	HIC	BBB	1	1,3	10,11,12	0.82	1 (10%)	9,14,16	1.02	1 (11%)
1	HIC	DDD	1	1,3	10,11,12	0.66	0	9,14,16	1.19	1 (11%)
1	HIC	CCC	1	1,3	10,11,12	0.61	0	9,14,16	1.37	2 (22%)
1	HIC	AAA	1	1,3	10,11,12	0.55	0	9,14,16	1.17	1 (11%)

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
1	HIC	BBB	1	1,3	-	1/5/6/8	0/1/1/1
1	HIC	DDD	1	1,3	-	3/5/6/8	0/1/1/1
1	HIC	CCC	1	1,3	-	1/5/6/8	0/1/1/1
1	HIC	AAA	1	1,3	-	1/5/6/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	1	HIC	CD2-NE2	2.20	1.40	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DDD	1	HIC	CD2-NE2-CE1	-3.02	105.52	106.71
1	BBB	1	HIC	CD2-NE2-CE1	-2.60	105.68	106.71
1	AAA	1	HIC	CD2-NE2-CE1	-2.58	105.69	106.71
1	CCC	1	HIC	CZ-NE2-CD2	-2.27	123.05	126.03
1	CCC	1	HIC	NE2-CE1-ND1	-2.11	111.85	112.66

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AAA	1	HIC	O-C-CA-CB
1	BBB	1	HIC	O-C-CA-CB
1	CCC	1	HIC	O-C-CA-CB
1	DDD	1	HIC	O-C-CA-CB
1	DDD	1	HIC	C-CA-CB-CG
1	DDD	1	HIC	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 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	NAG	DDD	301	1	14,14,15	1.12	0	17,19,21	1.35	2 (11%)
2	NAG	CCC	301	1	14,14,15	0.61	0	17,19,21	1.30	2 (11%)
2	NAG	AAA	301	1	14,14,15	0.76	0	17,19,21	1.20	0
2	NAG	BBB	301	1	14,14,15	1.39	2 (14%)	17,19,21	2.43	5 (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	NAG	DDD	301	1	-	0/6/23/26	0/1/1/1
2	NAG	CCC	301	1	-	0/6/23/26	0/1/1/1
2	NAG	AAA	301	1	-	0/6/23/26	0/1/1/1
2	NAG	BBB	301	1	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	301	NAG	C1-C2	3.23	1.56	1.52
2	BBB	301	NAG	C2-N2	2.12	1.49	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	301	NAG	C2-N2-C7	6.90	132.14	122.90
2	BBB	301	NAG	O7-C7-N2	3.97	129.00	121.98
2	CCC	301	NAG	C8-C7-N2	-3.04	111.07	116.12
2	BBB	301	NAG	O7-C7-C8	-2.92	116.86	122.05
2	BBB	301	NAG	O5-C1-C2	2.87	115.73	111.29
2	DDD	301	NAG	O5-C1-C2	2.47	115.11	111.29
2	CCC	301	NAG	O7-C7-N2	2.19	125.85	121.98
2	DDD	301	NAG	C1-O5-C5	2.17	115.09	112.19
2	BBB	301	NAG	C1-C2-N2	2.15	113.82	110.43

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	BBB	301	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	AAA	212/213 (99%)	0.02	4 (1%) 66 69	8, 16, 23, 34	0
1	BBB	212/213 (99%)	0.15	3 (1%) 73 76	10, 17, 26, 54	1 (0%)
1	CCC	212/213 (99%)	0.21	5 (2%) 59 62	9, 18, 27, 55	1 (0%)
1	DDD	212/213 (99%)	0.07	2 (0%) 81 83	9, 16, 24, 50	0
All	All	848/852 (99%)	0.12	14 (1%) 69 71	8, 17, 26, 55	2 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	197	TRP	7.6
1	DDD	197	TRP	6.8
1	BBB	197	TRP	6.1
1	AAA	111	ASP	4.1
1	AAA	197	TRP	3.8
1	AAA	70	THR	3.3
1	BBB	70	THR	3.2
1	CCC	213	GLY	3.0
1	DDD	70	THR	2.9
1	BBB	213	GLY	2.7
1	CCC	111	ASP	2.6
1	CCC	70	THR	2.4
1	AAA	159	LEU	2.3
1	CCC	96	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	HIC	AAA	1	11/12	0.93	0.09	16,17,18,19	0
1	HIC	BBB	1	11/12	0.93	0.09	16,20,22,23	0
1	HIC	CCC	1	11/12	0.94	0.07	12,12,14,15	0
1	HIC	DDD	1	11/12	0.95	0.06	13,13,14,14	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

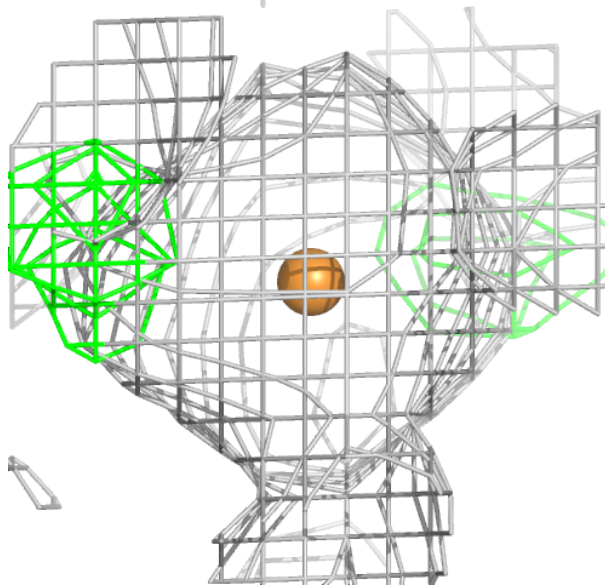
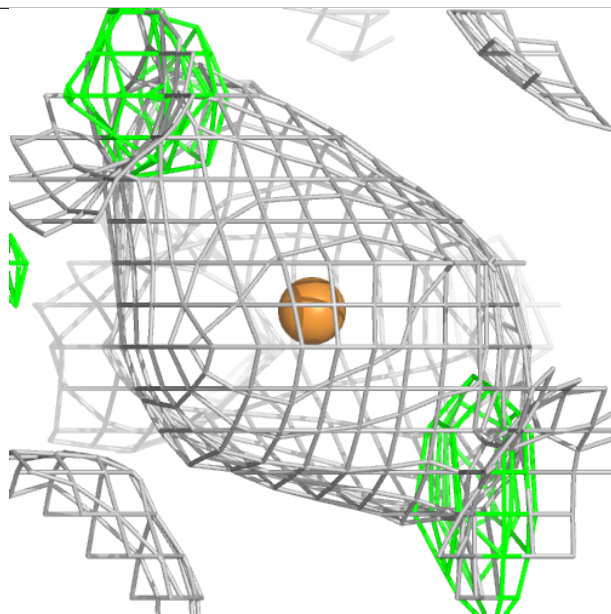
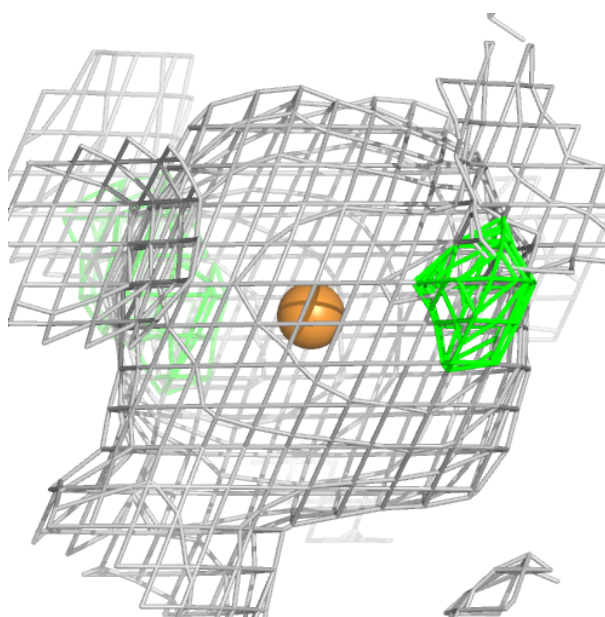
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	NAG	BBB	301	14/15	0.79	0.12	22,25,26,27	3
2	NAG	AAA	301	14/15	0.85	0.12	25,26,28,29	3
2	NAG	DDD	301	14/15	0.87	0.11	23,26,27,28	3
2	NAG	CCC	301	14/15	0.89	0.10	22,25,30,30	3
3	CU	DDD	303	1/1	0.95	0.06	49,49,49,49	0
3	CU	CCC	303	1/1	0.97	0.08	51,51,51,51	0
3	CU	AAA	302	1/1	0.98	0.02	16,16,16,16	0
3	CU	BBB	302	1/1	0.99	0.02	19,19,19,19	0
3	CU	DDD	302	1/1	0.99	0.02	19,19,19,19	0
3	CU	CCC	302	1/1	0.99	0.02	17,17,17,17	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.

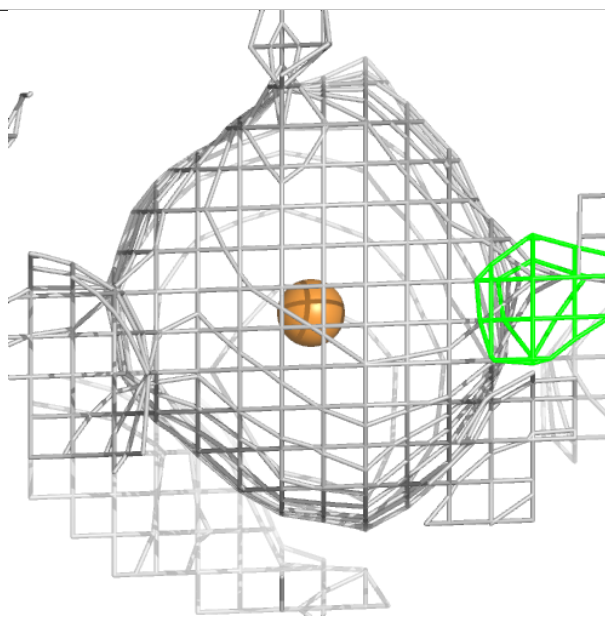
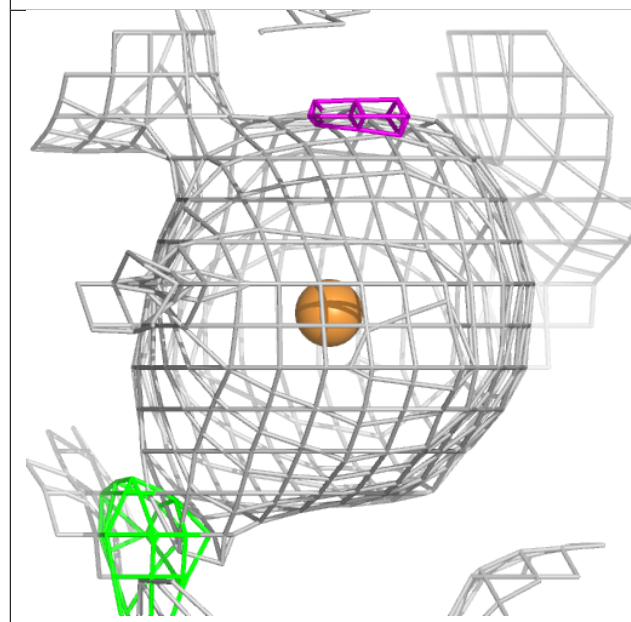
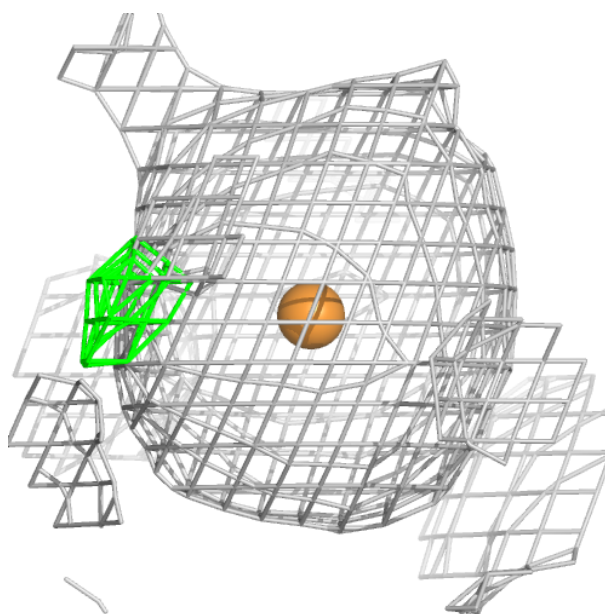
Electron density around CU DDD 303:

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



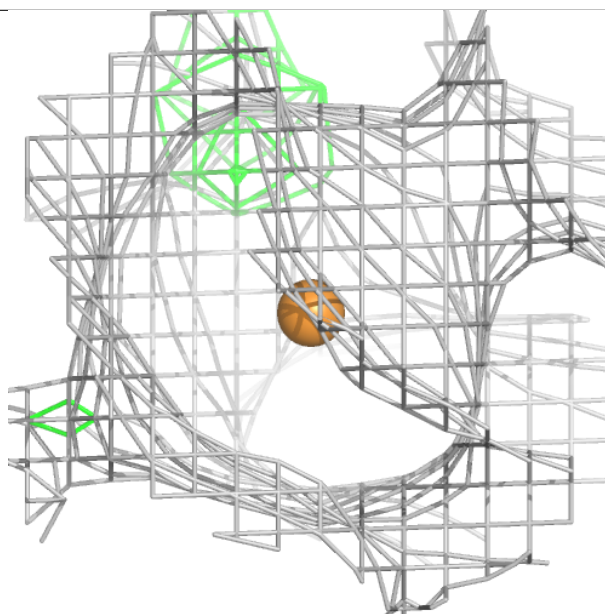
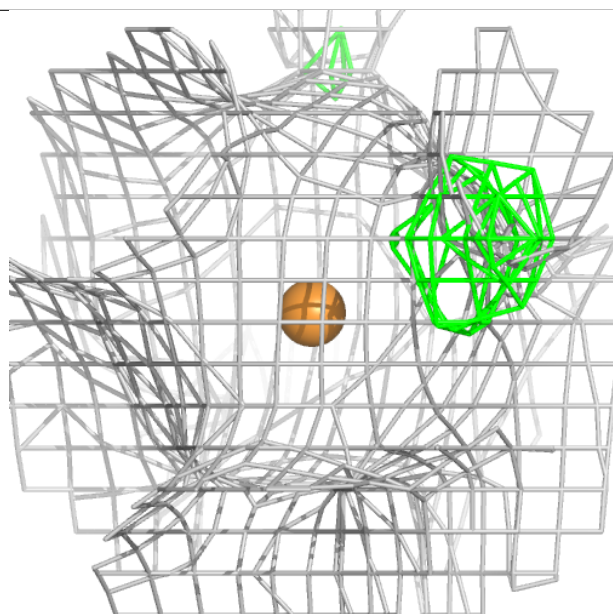
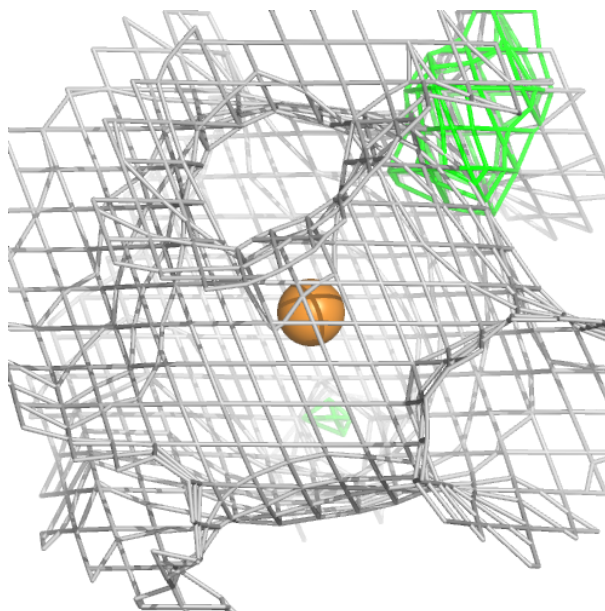
Electron density around CU CCC 303:

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and green (positive)



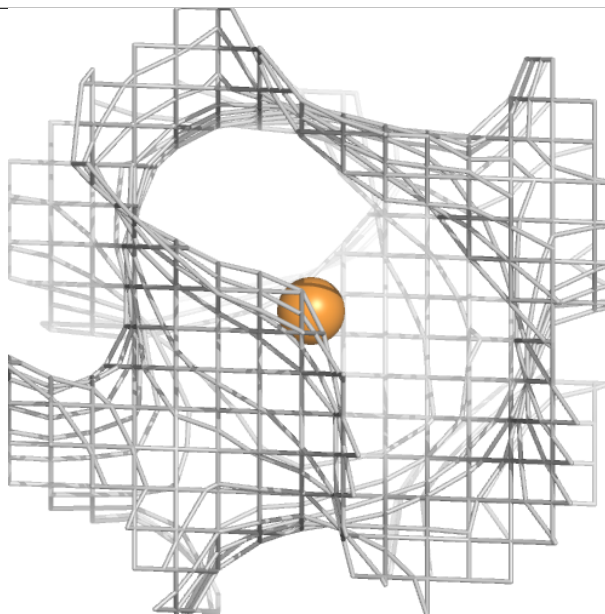
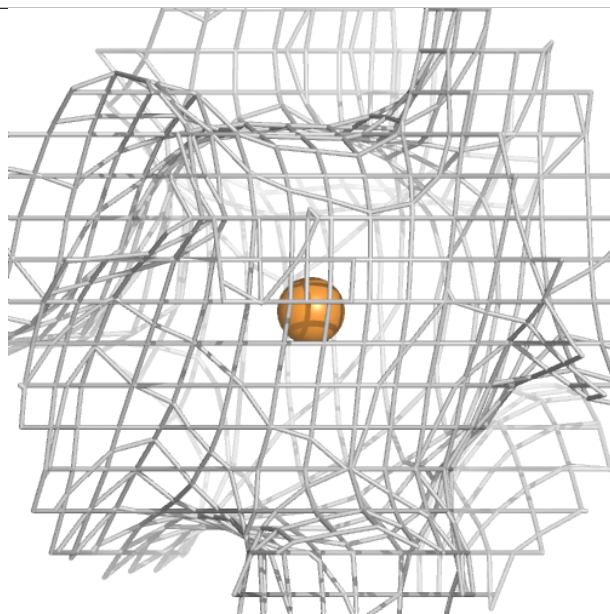
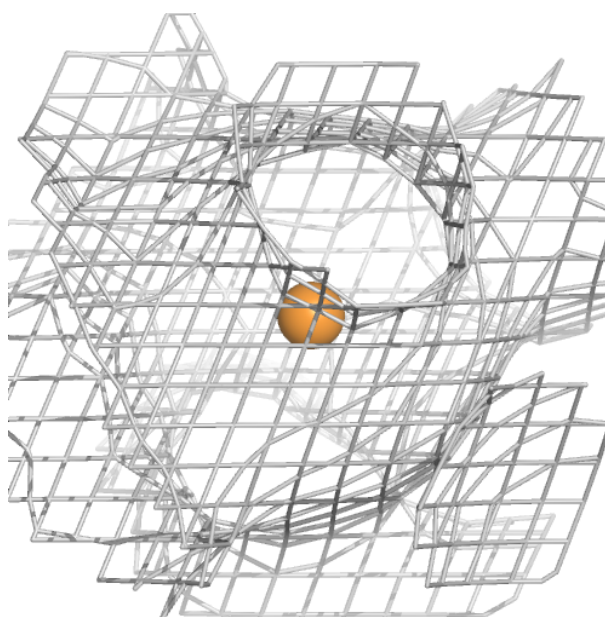
Electron density around CU AAA 302:

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and green (positive)



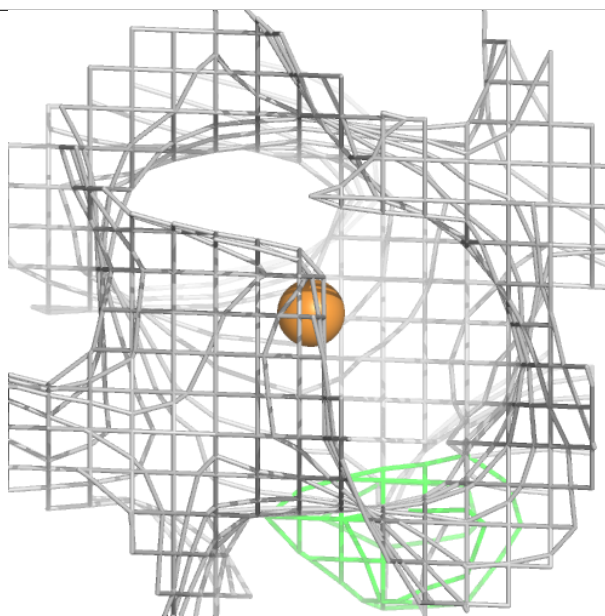
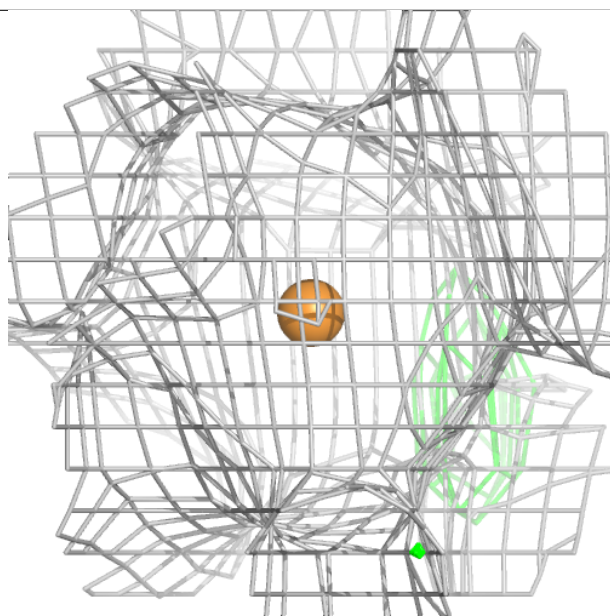
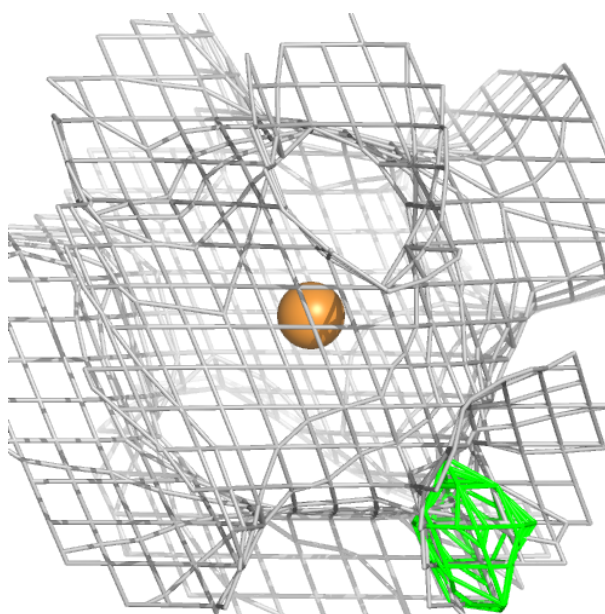
Electron density around CU BBB 302:

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and green (positive)



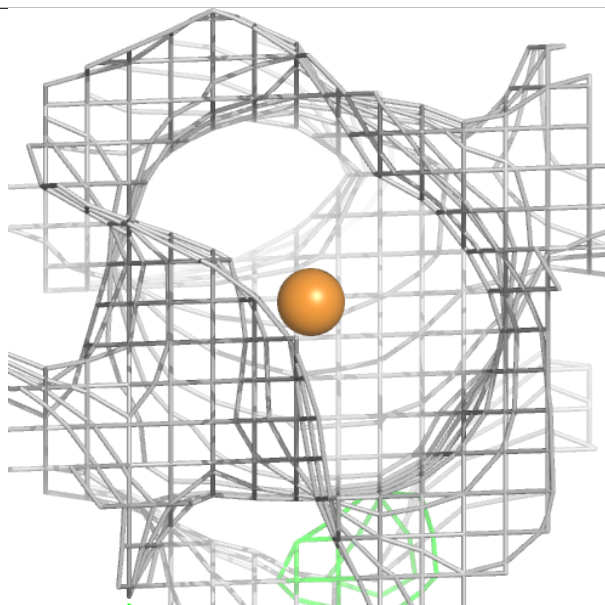
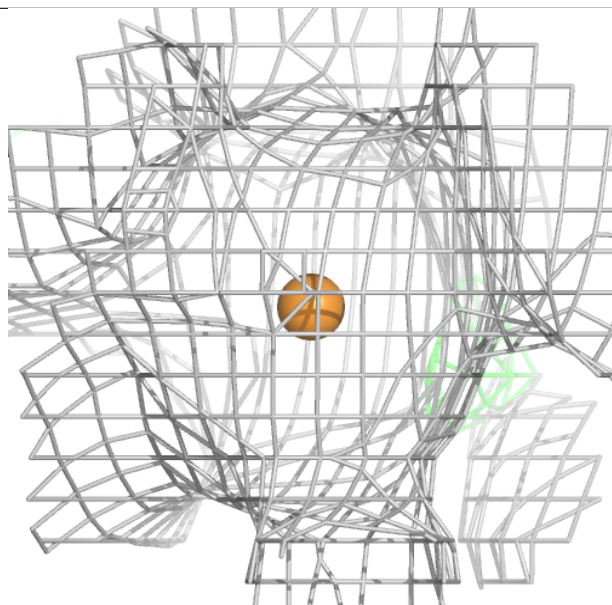
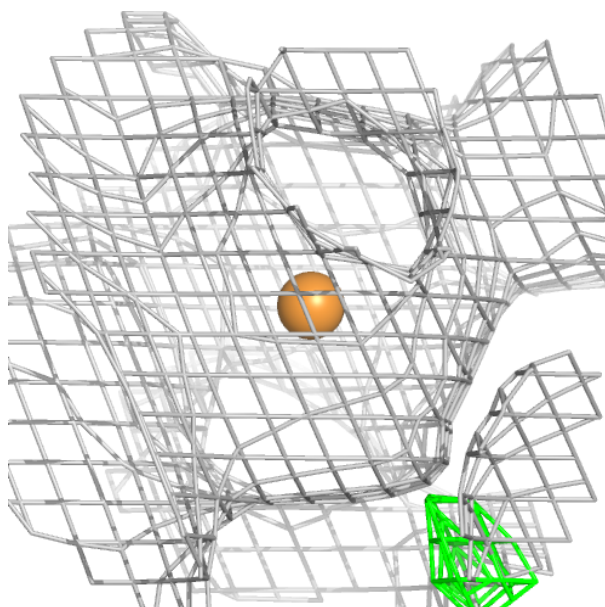
Electron density around CU DDD 302:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CU CCC 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 ⓘ

There are no such residues in this entry.