



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 28, 2025 – 02:13 PM EDT

PDB ID : 9NO3 / pdb\_00009no3  
Title : The bifunctional arabinofuranosidase/xylosidase from metagenome of *Pseudacanthotermes militaris*.  
Authors : Gomes, B.M.; De Oliveira, G.S.; de Melo, V.S.; Rossini, N.O.; Dias, M.V.B.; Chambergo, F.S.  
Deposited on : 2025-03-07  
Resolution : 2.05 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](mailto: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>.

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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	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

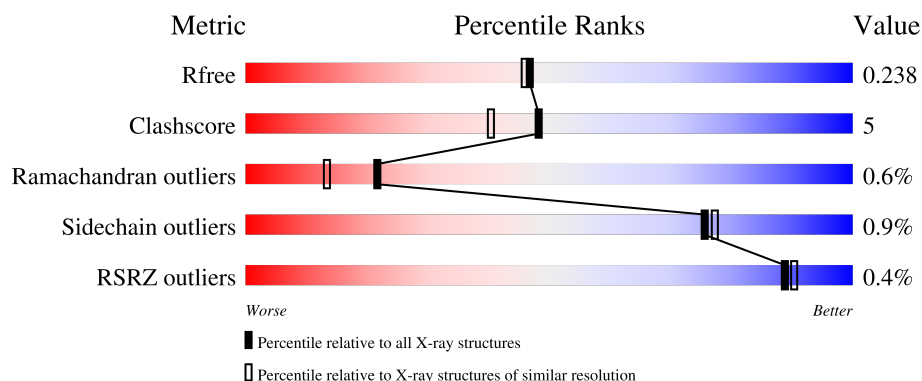
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*




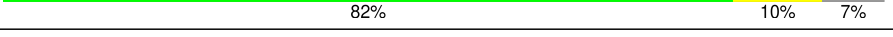
The reported resolution of this entry is 2.05 Å.

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))
$R_{free}$	164625	2096 (2.04-2.04)
Clashscore	180529	2229 (2.04-2.04)
Ramachandran outliers	177936	2217 (2.04-2.04)
Sidechain outliers	177891	2217 (2.04-2.04)
RSRZ outliers	164620	2096 (2.04-2.04)

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  $\geq 3$ , 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	506	 82% 11% 7%
1	B	506	 86% 13%
1	C	506	 87% 13%
1	D	506	 82% 10% 7%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16918 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 TerARA - arabinofuranosidase/xylosidase from metagenome of *Pseudacanthotermes militaris*.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	S	0	0	0
			3621	2309	602	692	18			
1	B	506	Total	C	N	O	S	0	1	0
			3888	2476	645	747	20			
1	C	506	Total	C	N	O	S	0	3	0
			3899	2483	645	750	21			
1	D	471	Total	C	N	O	S	0	1	0
			3617	2307	601	691	18			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		
2	B	3	Total	Ca	0	0
			3	3		
2	C	3	Total	Ca	0	0
			3	3		
2	D	2	Total	Ca	0	0
			2	2		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		
3	A	1	Total	C	N	O	0	0
			8	4	1	3		
3	D	1	Total	C	N	O	0	0
			8	4	1	3		
3	D	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

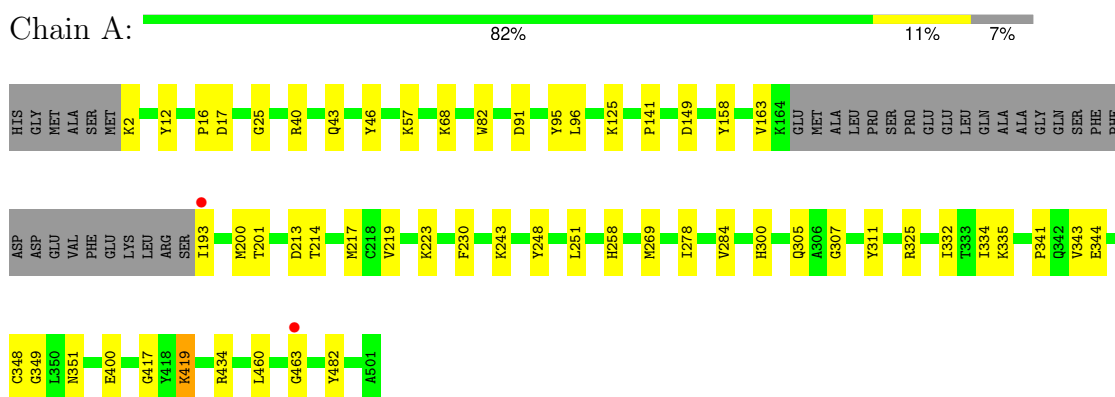
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	449	Total O 449 449	0	0
5	B	454	Total O 454 454	0	0
5	C	493	Total O 493 493	0	0
5	D	419	Total O 419 419	0	0

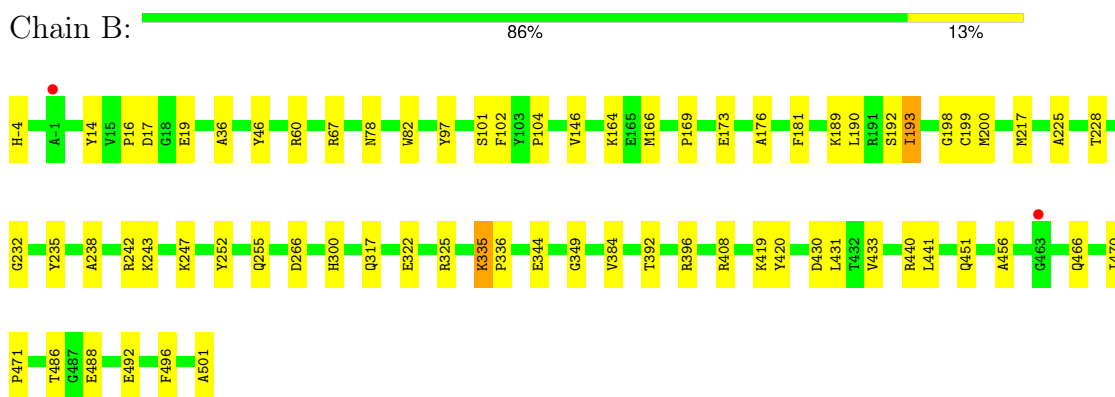
### 3 Residue-property plots

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.

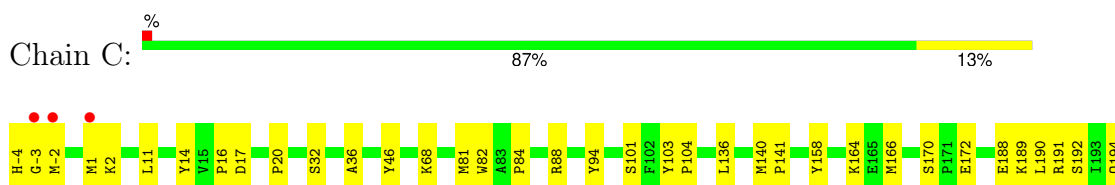
- Molecule 1: TerARA - arabinofuranosidase/xylosidase from metagenome of *Pseudacanthotermes militaris*.



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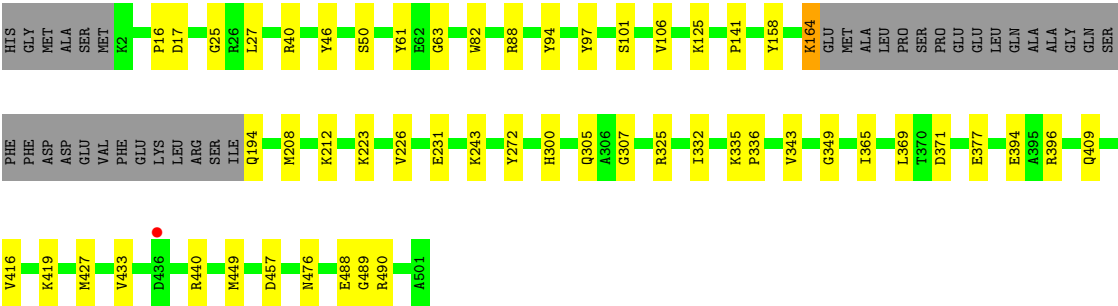
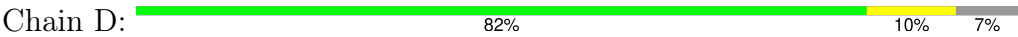


- Molecule 1: TerARA - arabinofuranosidase/xylosidase from metagenome of *Pseudacanthotermes militaris*.





● Molecule 1: TerARA - arabinofuranosidase/xylosidase from metagenome of *Pseudacanthotermes militaris*.



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.37Å 85.77Å 90.60Å 77.34° 68.05° 63.76°	Depositor
Resolution (Å)	44.94 – 2.05 44.94 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.2 (44.94-2.05) 97.2 (44.94-2.05)	Depositor EDS
$R_{merge}$	0.41	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.26 (at 2.05Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.178 , 0.238 0.177 , 0.238	Depositor DCC
$R_{free}$ test set	5824 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 52.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.069 for h,h-k,h-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16918	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CA, TRS

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	0.33	0/3724	0.54	2/5065 (0.0%)
1	B	0.34	0/3998	0.56	2/5436 (0.0%)
1	C	0.33	0/4018	0.55	2/5461 (0.0%)
1	D	0.32	0/3723	0.53	2/5064 (0.0%)
All	All	0.33	0/15463	0.54	8/21026 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	419	LYS	CA-C-N	6.58	133.54	121.70
1	B	419	LYS	C-N-CA	6.58	133.54	121.70
1	D	419	LYS	CA-C-N	6.39	133.21	121.70
1	D	419	LYS	C-N-CA	6.39	133.21	121.70
1	A	419	LYS	CA-C-N	6.17	132.80	121.70
1	A	419	LYS	C-N-CA	6.17	132.80	121.70
1	C	419	LYS	CA-C-N	5.47	131.55	121.70
1	C	419	LYS	C-N-CA	5.47	131.55	121.70

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	3621	0	3432	35	0
1	B	3888	0	3680	45	0
1	C	3899	0	3698	40	0
1	D	3617	0	3430	38	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	2	0	0	0	0
3	A	16	0	24	3	0
3	D	16	0	24	1	0
4	B	18	0	24	0	0
4	C	18	0	24	0	0
5	A	449	0	0	8	0
5	B	454	0	0	13	0
5	C	493	0	0	6	0
5	D	419	0	0	15	1
All	All	16918	0	14336	159	1

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 (159) 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:D:226:VAL:HA	1:D:231:GLU:HG3	1.52	0.92
1:C:-2:MET:HB3	1:C:359:GLY:HA3	1.60	0.83
1:D:305:GLN:NE2	1:D:307:GLY:O	2.14	0.79
1:A:305:GLN:NE2	1:A:307:GLY:O	2.22	0.72
3:A:604:TRS:H12	5:A:722:HOH:O	1.90	0.72
1:B:466:GLN:OE1	5:B:701:HOH:O	2.07	0.70
1:B:431:LEU:HD13	1:B:470:ILE:HD12	1.74	0.70
1:D:377:GLU:OE1	5:D:701:HOH:O	2.12	0.66
1:B:501:ALA:O	5:B:704:HOH:O	2.14	0.66
1:B:232:GLY:O	5:B:703:HOH:O	2.13	0.66
1:A:243:LYS:HE3	1:A:248:TYR:CZ	2.31	0.65
1:B:164:LYS:HE3	1:B:166:MET:HE3	1.77	0.65
1:B:471:PRO:O	5:B:702:HOH:O	2.13	0.65
1:B:456:ALA:HB2	1:B:470:ILE:HG12	1.78	0.65
1:D:427:MET:HA	1:D:427:MET:HE3	1.79	0.64
1:B:200:MET:HE1	1:B:217:MET:HG3	1.78	0.64
1:A:17:ASP:OD2	3:A:604:TRS:O3	2.16	0.63
1:A:91:ASP:OD2	1:A:95:TYR:OH	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:ARG:NH1	5:B:711:HOH:O	2.32	0.63
1:C:-2:MET:SD	5:C:1138:HOH:O	2.56	0.62
1:C:164:LYS:NZ	1:C:377:GLU:OE2	2.30	0.62
1:B:392:THR:HG21	1:B:408:ARG:HD2	1.81	0.61
1:C:392:THR:HG21	1:C:408:ARG:HD2	1.82	0.61
1:D:164:LYS:NZ	5:D:714:HOH:O	2.34	0.60
1:A:40:ARG:NH1	5:A:716:HOH:O	2.36	0.59
1:A:17:ASP:HA	1:A:300:HIS:HB3	1.84	0.58
1:A:2:LYS:N	5:A:715:HOH:O	2.36	0.58
1:C:231:GLU:OE2	5:C:701:HOH:O	2.16	0.58
1:A:68:LYS:NZ	5:A:706:HOH:O	2.32	0.58
1:C:-3:GLY:O	1:C:-2:MET:HG2	2.04	0.58
1:A:258:HIS:CE1	1:A:284:VAL:HB	2.39	0.57
1:B:199:CYS:C	1:B:200:MET:HE2	2.30	0.57
1:A:163:VAL:HG12	1:A:223:LYS:HD2	1.85	0.57
1:D:377:GLU:HA	5:D:875:HOH:O	2.04	0.56
1:C:1:MET:HE2	1:C:2:LYS:NZ	2.20	0.56
1:C:396:ARG:NH1	5:C:719:HOH:O	2.39	0.56
1:A:46:TYR:OH	1:A:82:TRP:O	2.21	0.55
1:B:181:PHE:HD2	1:B:181:PHE:H	1.55	0.55
1:A:141:PRO:HA	1:A:158:TYR:CD2	2.42	0.54
1:B:451:GLN:NE2	5:B:722:HOH:O	2.41	0.54
1:D:16:PRO:HB3	1:D:325:ARG:HB2	1.88	0.54
1:D:212:LYS:NZ	5:D:721:HOH:O	2.41	0.54
1:C:431:LEU:HD13	1:C:470:ILE:HD12	1.91	0.53
1:B:384:VAL:CG1	1:D:25:GLY:HA3	2.39	0.53
1:B:16:PRO:HB3	1:B:325:ARG:HB2	1.91	0.53
1:D:394:GLU:CD	1:D:396:ARG:HH21	2.13	0.52
1:A:40:ARG:HG2	1:A:43:GLN:HG2	1.90	0.52
1:D:40:ARG:NH2	5:D:725:HOH:O	2.43	0.52
1:D:223:LYS:HE2	5:D:861:HOH:O	2.10	0.51
1:A:57:LYS:NZ	1:A:351:ASN:O	2.44	0.51
1:B:17:ASP:HA	1:B:300:HIS:HB3	1.90	0.51
1:C:1:MET:HE2	1:C:2:LYS:HZ3	1.76	0.51
1:C:-4:HIS:O	5:C:702:HOH:O	2.19	0.51
1:D:272:TYR:O	5:D:702:HOH:O	2.19	0.51
1:C:16:PRO:HB3	1:C:325:ARG:HB2	1.92	0.50
1:D:369:LEU:HD12	1:D:416:VAL:HG22	1.93	0.50
1:A:201:THR:OG1	1:A:269:MET:HG2	2.12	0.50
1:D:335:LYS:HB3	1:D:336:PRO:HD2	1.94	0.50
1:C:140:MET:HB2	1:C:194:GLN:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:ALA:O	1:B:228:THR:OG1	2.25	0.49
1:D:365:ILE:HB	5:D:711:HOH:O	2.11	0.49
1:D:440:ARG:NH1	5:D:729:HOH:O	2.45	0.49
1:A:213:ASP:OD1	1:A:214:THR:N	2.46	0.49
1:B:102:PHE:CZ	1:B:169:PRO:HG3	2.47	0.49
1:C:-2:MET:HB3	1:C:359:GLY:CA	2.39	0.49
1:B:488:GLU:OE1	5:B:705:HOH:O	2.19	0.48
1:C:-2:MET:HB2	1:C:360:SER:O	2.13	0.48
1:C:396:ARG:HG3	5:C:719:HOH:O	2.12	0.48
1:D:332:ILE:HG22	1:D:343:VAL:HG11	1.95	0.48
1:D:457:ASP:O	5:D:703:HOH:O	2.20	0.48
1:B:247:LYS:NZ	1:B:266:ASP:OD2	2.39	0.48
3:A:604:TRS:H11	5:A:817:HOH:O	2.12	0.48
1:D:17:ASP:HA	1:D:300:HIS:HB3	1.94	0.47
1:D:106:VAL:HG23	1:D:141:PRO:HB3	1.97	0.47
1:A:335:LYS:HZ3	1:A:341:PRO:HG2	1.79	0.47
1:C:17:ASP:HA	1:C:300:HIS:HB3	1.96	0.47
1:C:409:GLN:NE2	1:C:490:ARG:HH11	2.13	0.47
1:A:16:PRO:HB3	1:A:325:ARG:HB2	1.95	0.47
1:C:408:ARG:HA	1:C:492:GLU:HG2	1.97	0.47
1:B:104:PRO:HG3	1:B:192:SER:HB2	1.96	0.46
1:B:200:MET:CE	1:B:217:MET:HG3	2.46	0.46
1:C:368:HIS:HB3	1:C:417:GLY:HA3	1.97	0.46
1:A:344:GLU:OE1	1:A:419:LYS:NZ	2.40	0.46
1:B:46:TYR:OH	1:B:82:TRP:O	2.28	0.46
1:B:396:ARG:HD3	5:B:766:HOH:O	2.15	0.46
1:C:170:SER:OG	1:C:172:GLU:HG2	2.15	0.46
1:A:332:ILE:HG22	1:A:343:VAL:HG11	1.97	0.46
1:B:97:TYR:CD1	1:B:146[A]:VAL:HG21	2.51	0.45
1:D:490:ARG:NH2	5:D:722:HOH:O	2.41	0.45
1:D:476:ASN:ND2	5:D:736:HOH:O	2.49	0.45
1:C:265:SER:HB2	1:C:272:TYR:HA	1.98	0.45
1:B:344:GLU:OE2	1:B:420:TYR:OH	2.24	0.45
1:A:311:TYR:OH	5:A:701:HOH:O	2.19	0.45
1:B:486:THR:HG23	5:B:807:HOH:O	2.16	0.45
1:A:125:LYS:HB2	1:A:125:LYS:HE2	1.74	0.45
1:D:488:GLU:HG2	1:D:489:GLY:H	1.82	0.45
1:B:14:TYR:CE1	1:B:36:ALA:HB2	2.51	0.45
1:C:190:LEU:HD23	1:C:190:LEU:HA	1.73	0.44
1:D:449:MET:HE3	1:D:449:MET:HB3	1.73	0.44
1:A:269:MET:HE3	1:A:269:MET:HB2	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:GLY:HA3	1:C:384:VAL:CG1	2.47	0.44
1:B:430:ASP:O	1:B:496:PHE:HA	2.17	0.44
1:C:104:PRO:HG2	1:C:192:SER:HB2	1.99	0.44
1:A:219:VAL:HG13	1:A:230:PHE:CE2	2.51	0.44
1:A:434:ARG:NH1	5:A:740:HOH:O	2.51	0.44
1:D:243:LYS:HA	1:D:243:LYS:HD2	1.74	0.44
1:B:60:ARG:NH2	5:B:735:HOH:O	2.49	0.44
1:C:46:TYR:CZ	1:C:81:MET:HB3	2.52	0.44
1:B:199:CYS:HB2	1:B:235:TYR:CD1	2.53	0.44
1:B:78:ASN:HB2	1:B:176:ALA:HB1	1.98	0.44
3:D:604:TRS:H11	5:D:758:HOH:O	2.17	0.44
1:D:125:LYS:HB2	1:D:125:LYS:HE2	1.76	0.43
1:D:40:ARG:HB2	5:D:858:HOH:O	2.18	0.43
1:B:238:ALA:O	1:B:252:TYR:HA	2.18	0.43
1:C:141:PRO:HA	1:C:158:TYR:CD1	2.54	0.43
1:D:371:ASP:HB2	5:D:764:HOH:O	2.18	0.43
1:B:173:GLU:HA	5:B:1027:HOH:O	2.17	0.43
1:D:97:TYR:OH	1:D:208:MET:HE3	2.18	0.43
1:A:12:TYR:CZ	1:A:400:GLU:HG3	2.53	0.43
1:C:11:LEU:O	1:C:326:GLN:NE2	2.52	0.43
1:B:317:GLN:OE1	1:B:322:GLU:HA	2.19	0.43
1:D:61:TYR:CZ	1:D:63:GLY:HA2	2.54	0.42
1:B:67:ARG:NH1	5:B:743:HOH:O	2.52	0.42
1:D:141:PRO:HA	1:D:158:TYR:CD1	2.54	0.42
1:D:194:GLN:O	1:D:194:GLN:HG2	2.18	0.42
1:D:409:GLN:HB3	1:D:490:ARG:HH12	1.85	0.42
1:A:251:LEU:HD21	1:A:278:ILE:HD12	2.02	0.42
1:D:27:LEU:O	1:D:50:SER:HA	2.19	0.42
1:A:348:CYS:SG	5:A:968:HOH:O	2.44	0.42
1:B:198:GLY:O	1:B:200:MET:HE3	2.20	0.42
1:C:14:TYR:CE1	1:C:36:ALA:HB2	2.54	0.42
1:A:200:MET:HE3	1:A:200:MET:HB3	1.82	0.42
1:B:189:LYS:O	1:B:193:ILE:HD13	2.20	0.41
1:B:441:LEU:HD12	1:B:441:LEU:HA	1.92	0.41
1:C:404:LEU:HD12	1:C:405:HIS:N	2.35	0.41
1:B:440:ARG:HE	1:B:440:ARG:HB3	1.54	0.41
1:C:16:PRO:HG2	1:C:32[B]:SER:OG	2.20	0.41
1:C:103:TYR:HA	1:C:104:PRO:HD3	1.92	0.41
1:A:217:MET:HE2	1:A:217:MET:HB3	1.95	0.41
1:B:335:LYS:HB3	1:B:336:PRO:HD2	2.03	0.41
1:C:68:LYS:HG2	1:C:81:MET:HE2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:ARG:HD3	1:D:94:TYR:CE1	2.55	0.41
1:B:433:VAL:HA	1:B:492:GLU:O	2.20	0.41
1:C:46:TYR:OH	1:C:82:TRP:O	2.35	0.41
1:C:20:PRO:HD2	1:C:242:ARG:HH21	1.86	0.41
1:A:43:GLN:O	1:A:68:LYS:NZ	2.53	0.41
1:C:457:ASP:HB2	5:C:957:HOH:O	2.21	0.41
1:C:458:LEU:HD21	1:C:491:LEU:HD13	2.03	0.41
1:D:409:GLN:OE1	1:D:490:ARG:NH1	2.54	0.41
1:A:12:TYR:CG	1:A:400:GLU:HB2	2.56	0.41
1:B:189:LYS:NZ	5:B:724:HOH:O	2.54	0.41
1:B:19:GLU:OE1	1:B:242:ARG:NH2	2.47	0.40
1:B:243:LYS:HA	1:B:243:LYS:HD2	1.67	0.40
1:C:88:ARG:HD3	1:C:94:TYR:CE2	2.56	0.40
1:C:188:GLU:OE2	1:C:191:ARG:NH1	2.55	0.40
1:C:238:ALA:O	1:C:252:TYR:HA	2.21	0.40
1:A:149:ASP:OD2	1:A:248:TYR:OH	2.37	0.40
1:A:417:GLY:HA3	1:A:482:TYR:CD2	2.57	0.40
1:D:46:TYR:OH	1:D:82:TRP:O	2.24	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:995:HOH:O	5:D:1086:HOH:O[1_655]	2.16	0.04

## 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	468/506 (92%)	446 (95%)	20 (4%)	2 (0%)	30 23
1	B	505/506 (100%)	486 (96%)	16 (3%)	3 (1%)	22 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	507/506 (100%)	479 (94%)	24 (5%)	4 (1%)	16	9
1	D	468/506 (92%)	451 (96%)	15 (3%)	2 (0%)	30	23
All	All	1948/2024 (96%)	1862 (96%)	75 (4%)	11 (1%)	22	13

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	349	GLY
1	B	349	GLY
1	C	189	LYS
1	A	463	GLY
1	C	349	GLY
1	B	101	SER
1	C	101	SER
1	D	349	GLY
1	B	255	GLN
1	D	101	SER
1	C	84	PRO

### 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	371/399 (93%)	367 (99%)	4 (1%)	70	71
1	B	399/399 (100%)	395 (99%)	4 (1%)	73	74
1	C	402/399 (101%)	398 (99%)	4 (1%)	73	74
1	D	371/399 (93%)	369 (100%)	2 (0%)	86	88
All	All	1543/1596 (97%)	1529 (99%)	14 (1%)	75	77

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	LEU

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Mol	Chain	Res	Type
1	A	193	ILE
1	A	334	ILE
1	A	460	LEU
1	B	-4	HIS
1	B	190	LEU
1	B	193	ILE
1	B	335	LYS
1	C	136	LEU
1	C	166	MET
1	C	458	LEU
1	C	491	LEU
1	D	164	LYS
1	D	433	VAL

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

Mol	Chain	Res	Type
1	A	267	GLN
1	A	388	GLN
1	A	409	GLN
1	B	267	GLN
1	B	451	GLN
1	C	409	GLN
1	C	451	GLN
1	D	388	GLN
1	D	424	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.



## 5.6 Ligand geometry

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 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	$\# Z  > 2$
4	GOL	B	604	-	5,5,5	1.03	0	5,5,5	0.95	0
3	TRS	A	604	-	7,7,7	0.57	0	9,9,9	0.78	0
3	TRS	A	603	-	7,7,7	0.31	0	9,9,9	0.50	0
4	GOL	B	603	-	5,5,5	0.61	0	5,5,5	1.48	1 (20%)
4	GOL	C	601	-	5,5,5	0.87	0	5,5,5	1.03	0
4	GOL	B	605	-	5,5,5	1.11	0	5,5,5	0.93	0
3	TRS	D	601	-	7,7,7	0.40	0	9,9,9	0.80	0
3	TRS	D	604	-	7,7,7	0.36	0	9,9,9	1.05	0
4	GOL	C	605	-	5,5,5	1.05	0	5,5,5	1.03	0
4	GOL	C	604	-	5,5,5	1.02	0	5,5,5	0.99	0

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
4	GOL	B	604	-	-	3/4/4/4	-
3	TRS	A	604	-	-	9/9/9/9	-
3	TRS	A	603	-	-	4/9/9/9	-
4	GOL	B	603	-	-	2/4/4/4	-
4	GOL	C	601	-	-	2/4/4/4	-
4	GOL	B	605	-	-	0/4/4/4	-
3	TRS	D	601	-	-	1/9/9/9	-
3	TRS	D	604	-	-	3/9/9/9	-
4	GOL	C	605	-	-	0/4/4/4	-
4	GOL	C	604	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	603	GOL	C3-C2-C1	-2.48	102.72	111.80

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	603	TRS	C2-C-C1-O1
3	A	603	TRS	C3-C-C1-O1
3	A	603	TRS	N-C-C1-O1
3	A	604	TRS	C2-C-C1-O1
3	A	604	TRS	C2-C-C3-O3
4	B	603	GOL	O1-C1-C2-O2
4	B	604	GOL	C1-C2-C3-O3
4	B	603	GOL	O1-C1-C2-C3
4	C	601	GOL	C1-C2-C3-O3
4	B	604	GOL	O2-C2-C3-O3
3	A	604	TRS	C3-C-C1-O1
3	A	604	TRS	C1-C-C2-O2
3	A	604	TRS	C1-C-C3-O3
3	D	604	TRS	C1-C-C3-O3
4	B	604	GOL	O1-C1-C2-O2
3	A	604	TRS	C3-C-C2-O2
3	A	604	TRS	N-C-C3-O3
3	D	604	TRS	N-C-C3-O3
3	D	604	TRS	C2-C-C3-O3
4	C	601	GOL	O2-C2-C3-O3
3	A	604	TRS	N-C-C1-O1
3	A	604	TRS	N-C-C2-O2
3	A	603	TRS	C1-C-C2-O2
3	D	601	TRS	C2-C-C3-O3

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	604	TRS	3	0
3	D	604	TRS	1	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	472/506 (93%)	-0.41	2 (0%) 89 90	9, 19, 35, 62	0
1	B	506/506 (100%)	-0.45	2 (0%) 89 90	9, 19, 34, 56	1 (0%)
1	C	506/506 (100%)	-0.47	3 (0%) 85 88	8, 19, 34, 62	3 (0%)
1	D	471/506 (93%)	-0.33	1 (0%) 92 93	11, 22, 39, 63	1 (0%)
All	All	1955/2024 (96%)	-0.42	8 (0%) 89 90	8, 20, 36, 63	5 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	193	ILE	3.3
1	C	-2	MET	3.0
1	B	463	GLY	3.0
1	A	463	GLY	2.6
1	C	-3	GLY	2.5
1	B	-1	ALA	2.4
1	D	436	ASP	2.4
1	C	1	MET	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 ⓘ

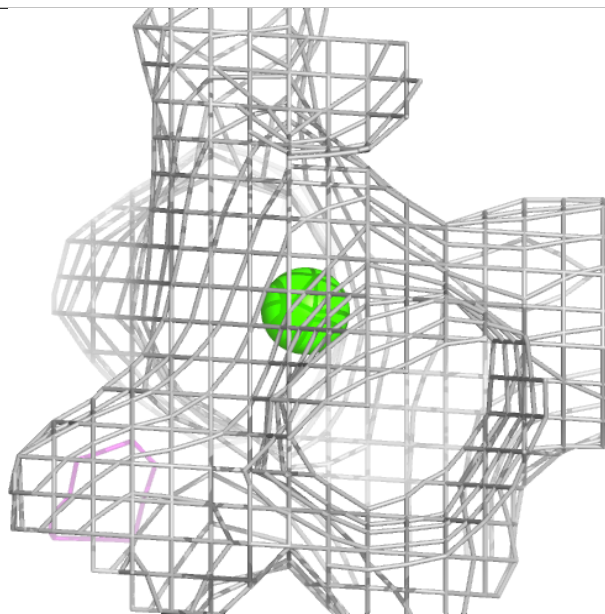
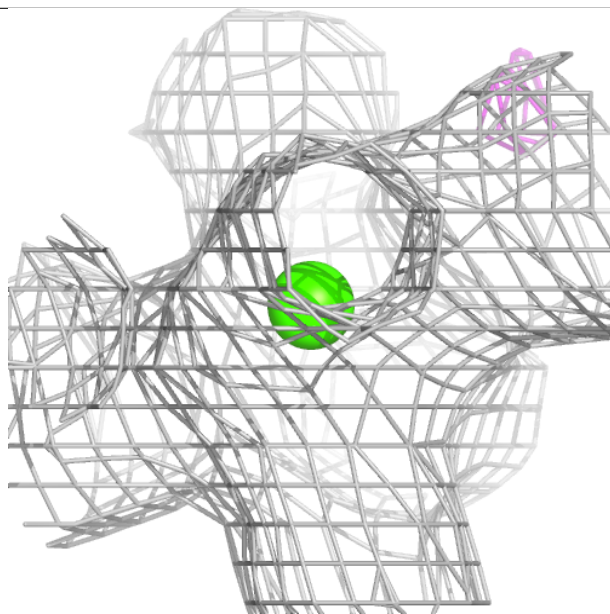
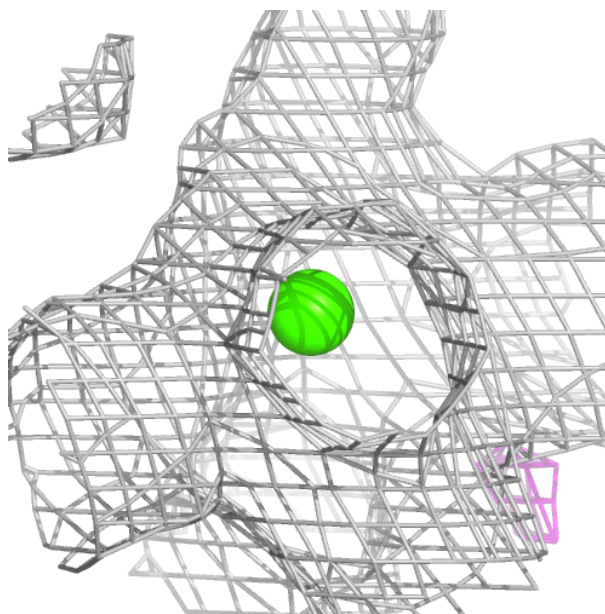
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	B	604	6/6	0.85	0.12	20,24,28,30	0
3	TRS	D	604	8/8	0.87	0.10	19,24,25,28	0
3	TRS	A	603	8/8	0.87	0.11	19,21,26,33	0
4	GOL	B	605	6/6	0.88	0.09	31,36,39,40	0
4	GOL	C	601	6/6	0.88	0.10	41,42,43,44	0
4	GOL	C	604	6/6	0.90	0.08	18,24,26,26	0
4	GOL	B	603	6/6	0.91	0.09	18,20,24,26	0
3	TRS	D	601	8/8	0.93	0.08	16,19,24,24	0
3	TRS	A	604	8/8	0.94	0.07	17,21,28,29	0
2	CA	C	606	1/1	0.95	0.07	55,55,55,55	0
4	GOL	C	605	6/6	0.95	0.06	12,16,19,20	0
2	CA	B	606	1/1	0.97	0.06	46,46,46,46	0
2	CA	A	601	1/1	0.97	0.09	26,26,26,26	0
2	CA	B	601	1/1	0.97	0.08	27,27,27,27	0
2	CA	C	602	1/1	0.98	0.09	23,23,23,23	0
2	CA	B	602	1/1	0.99	0.05	24,24,24,24	0
2	CA	C	603	1/1	0.99	0.05	28,28,28,28	0
2	CA	A	602	1/1	0.99	0.05	29,29,29,29	0
2	CA	D	602	1/1	0.99	0.07	28,28,28,28	0
2	CA	D	603	1/1	0.99	0.05	25,25,25,25	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.

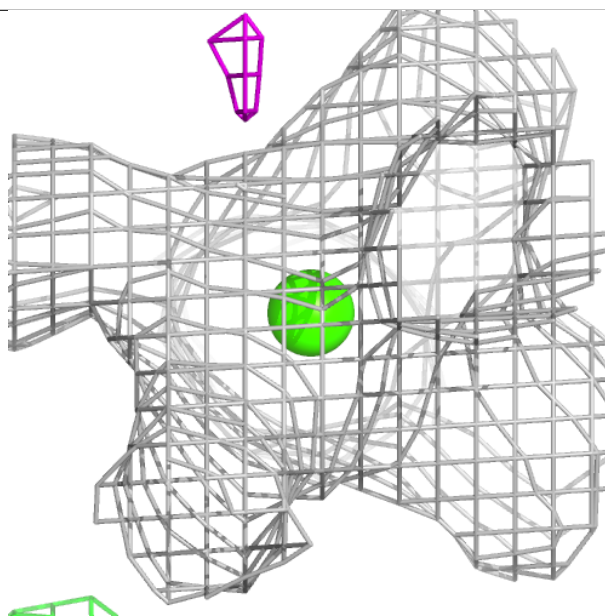
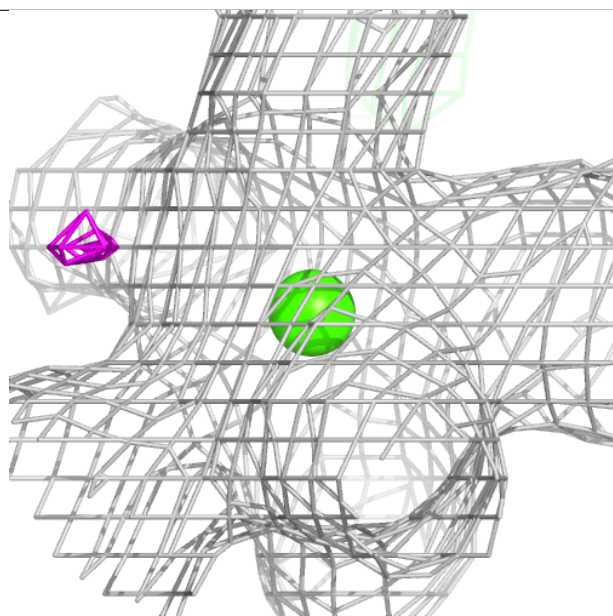
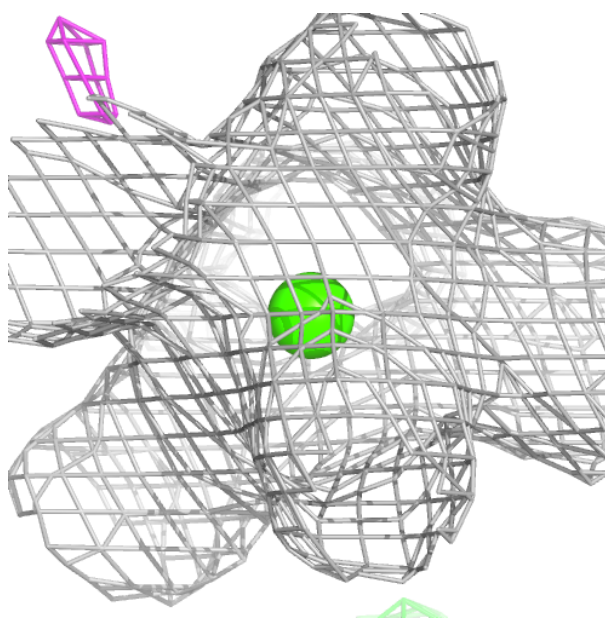
**Electron density around CA C 606:**

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



**Electron density around CA B 606:**

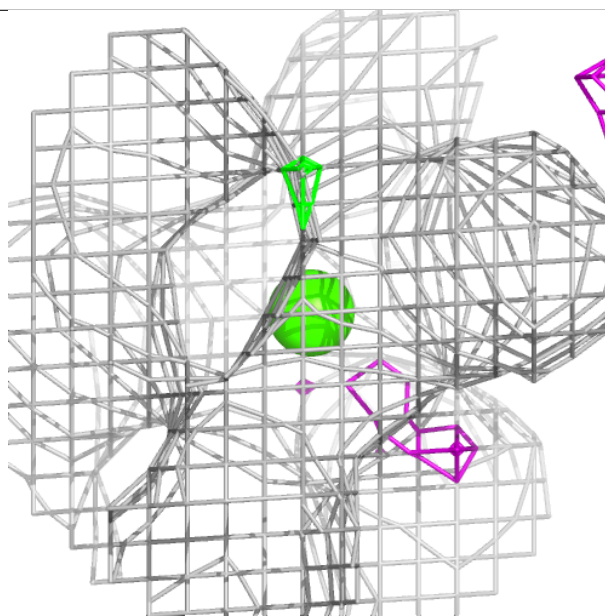
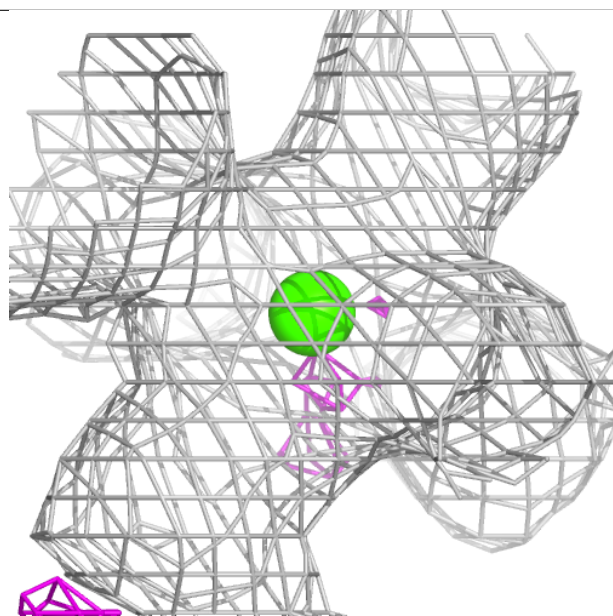
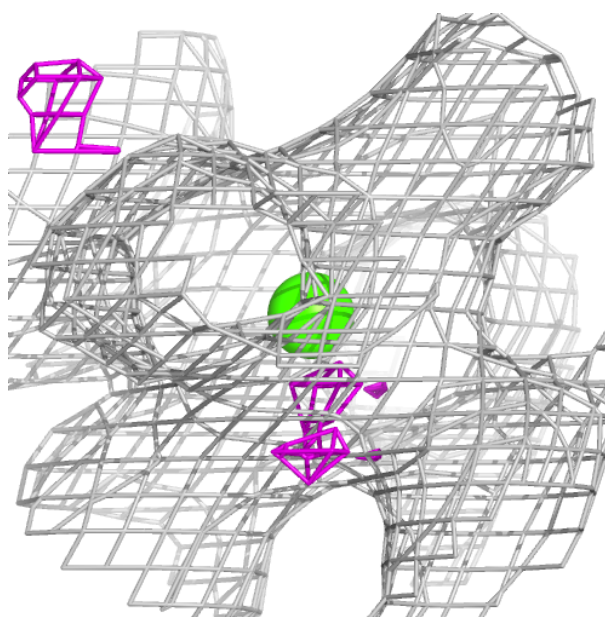
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CA A 601:**

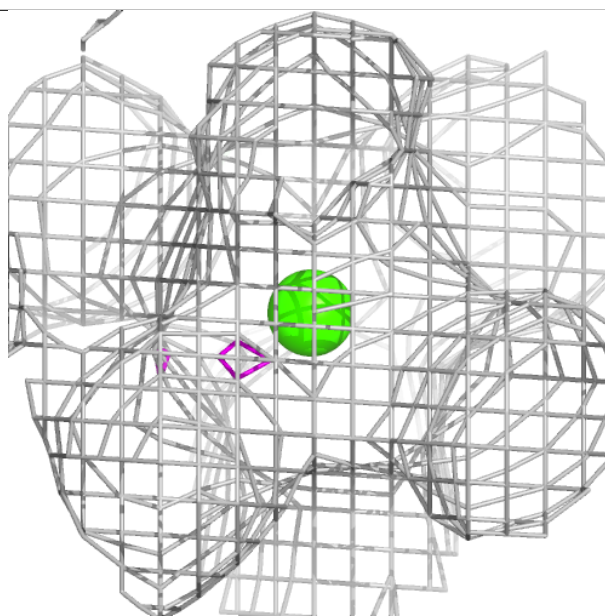
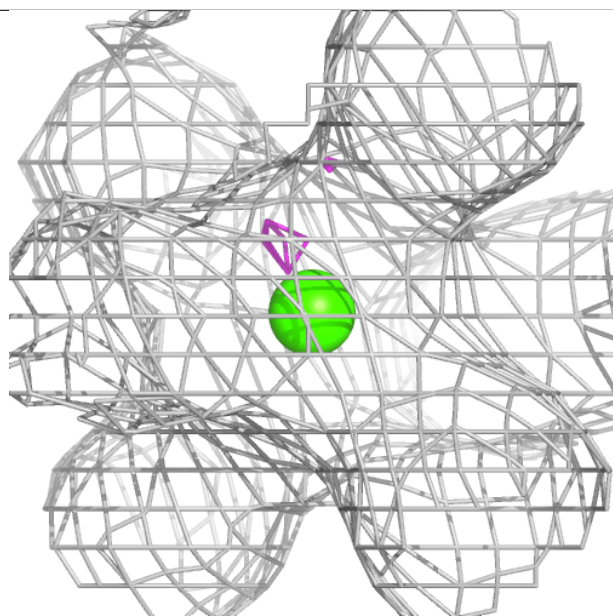
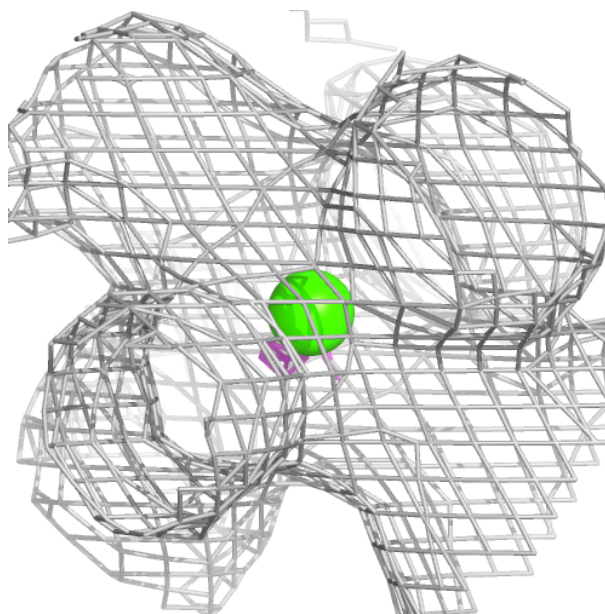
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





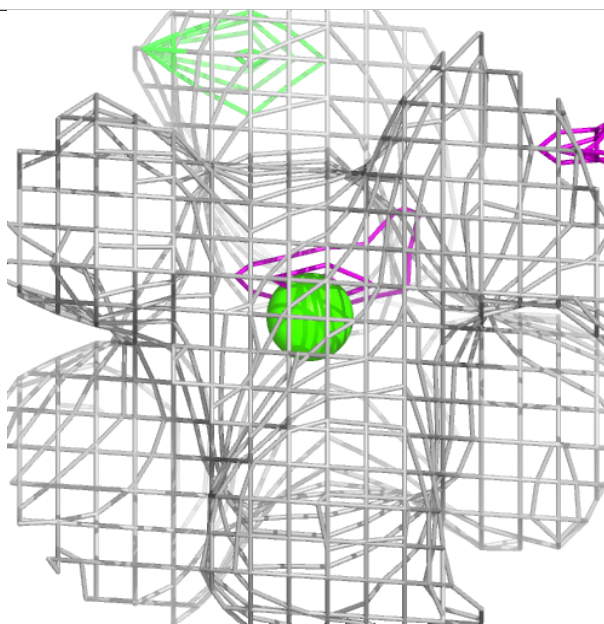
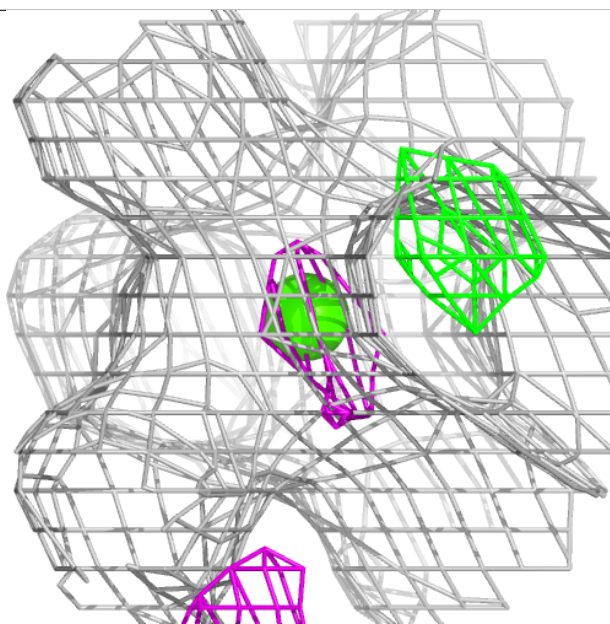
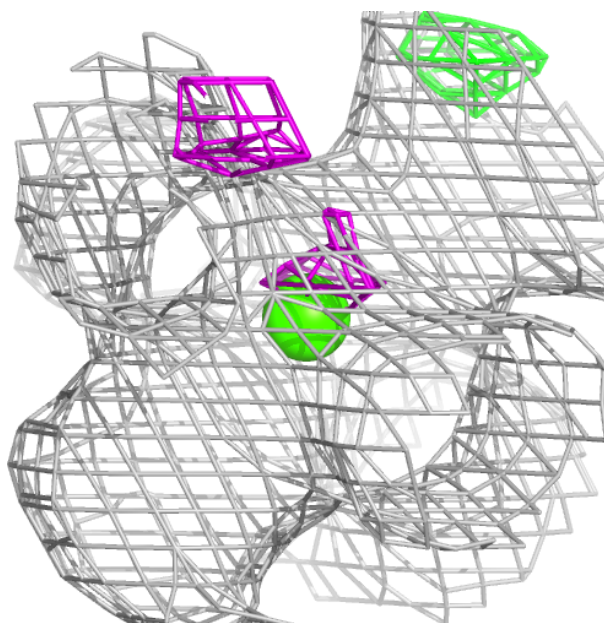
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and green (positive)



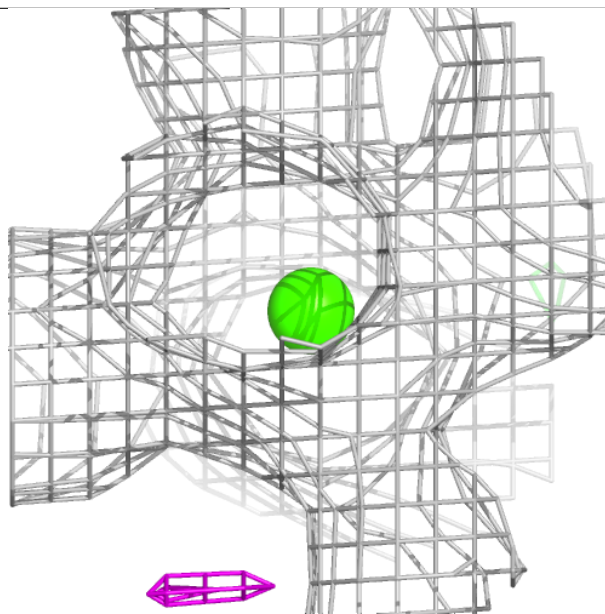
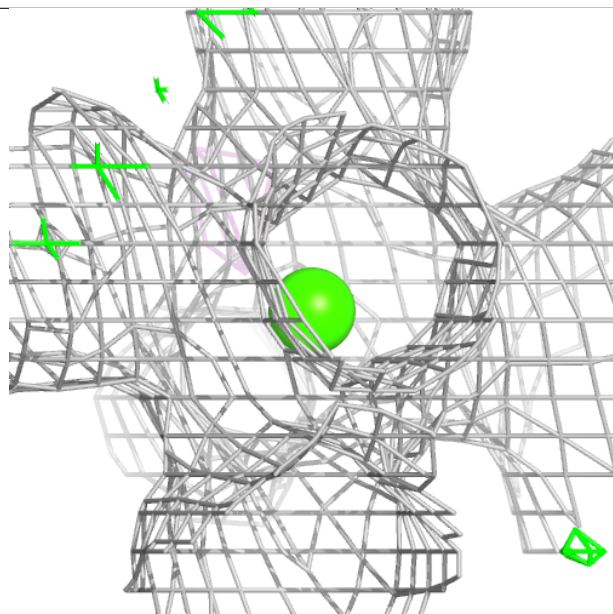
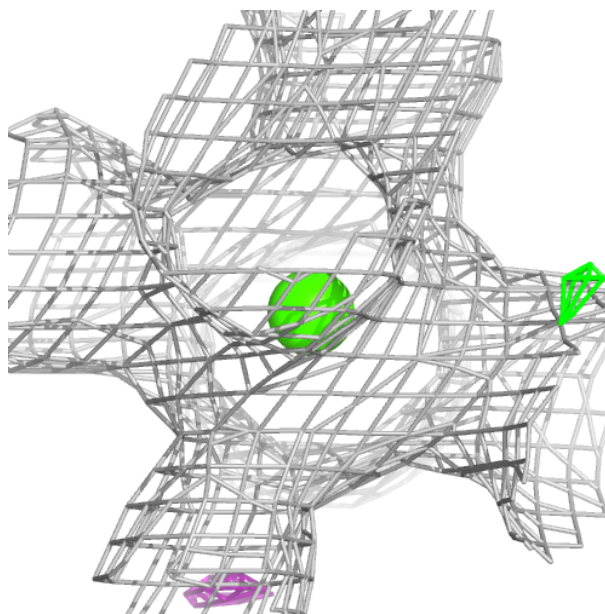
**Electron density around CA C 602:**

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



**Electron density around CA B 602:**

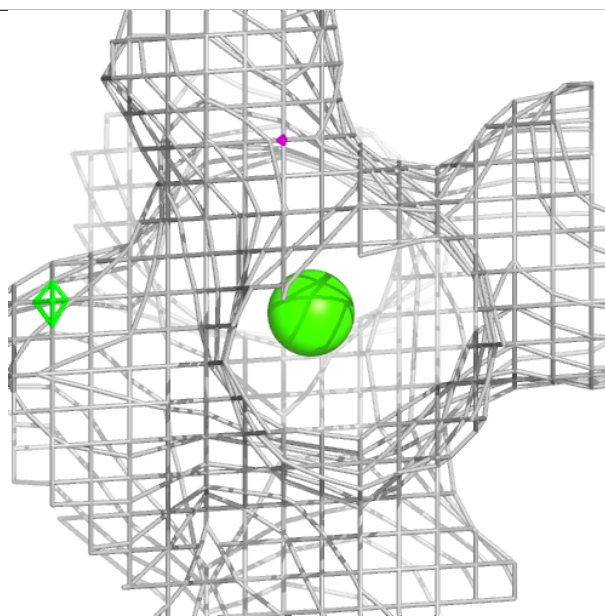
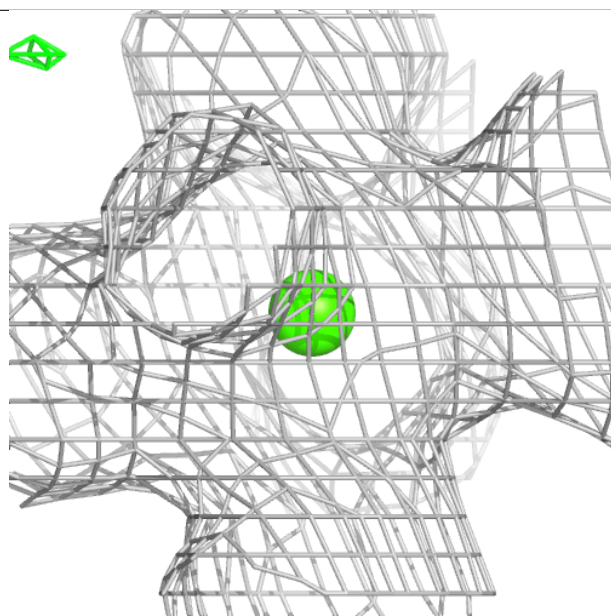
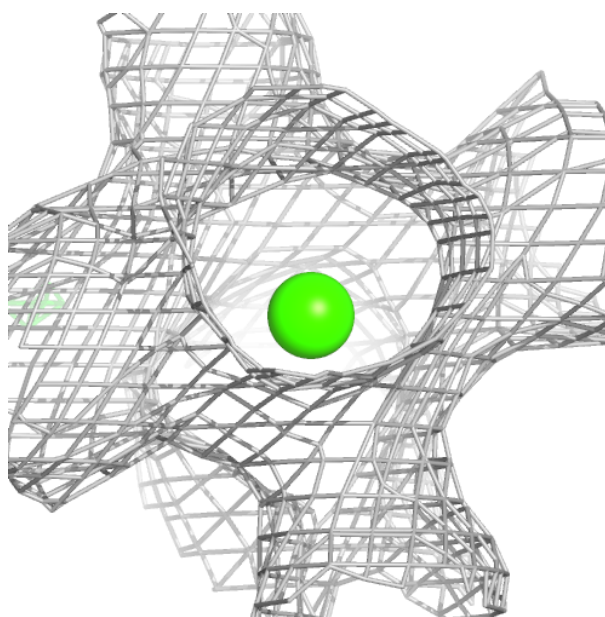
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





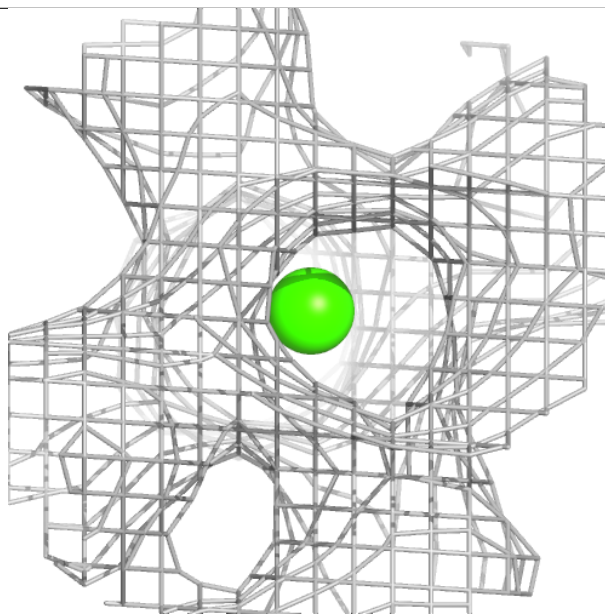
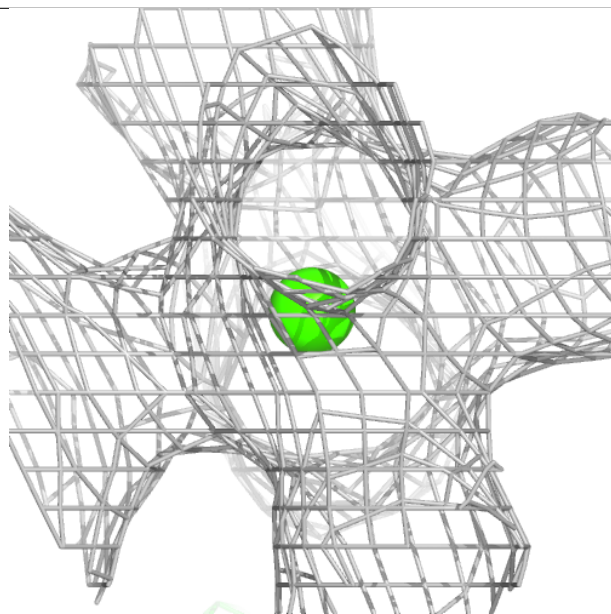
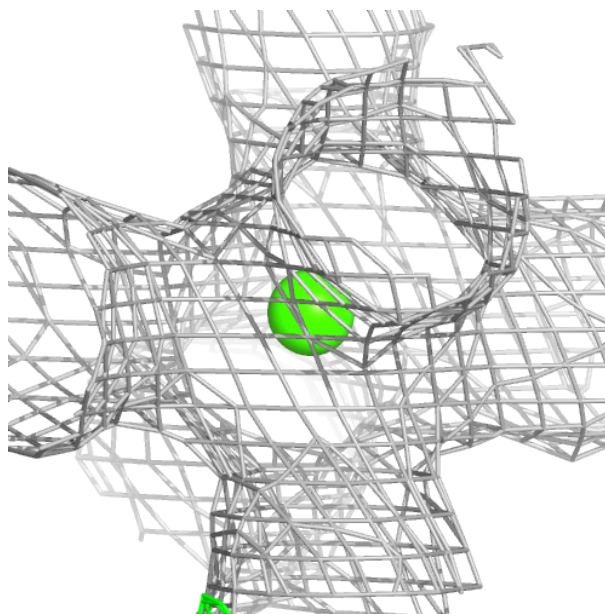
**Electron density around CA C 603:**

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



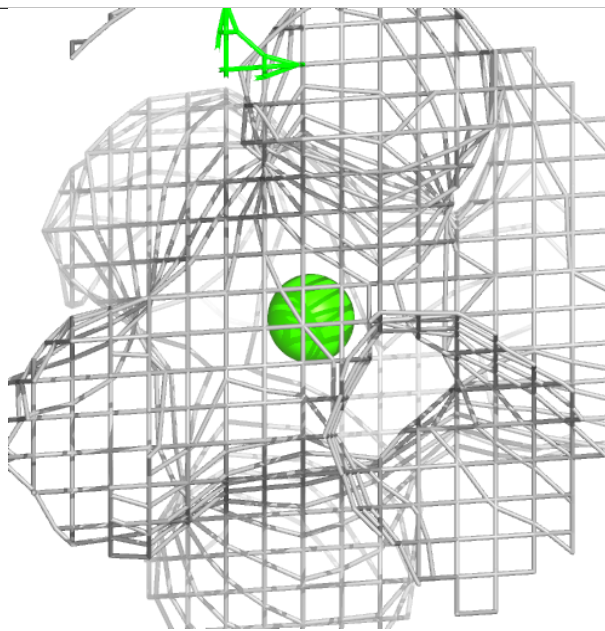
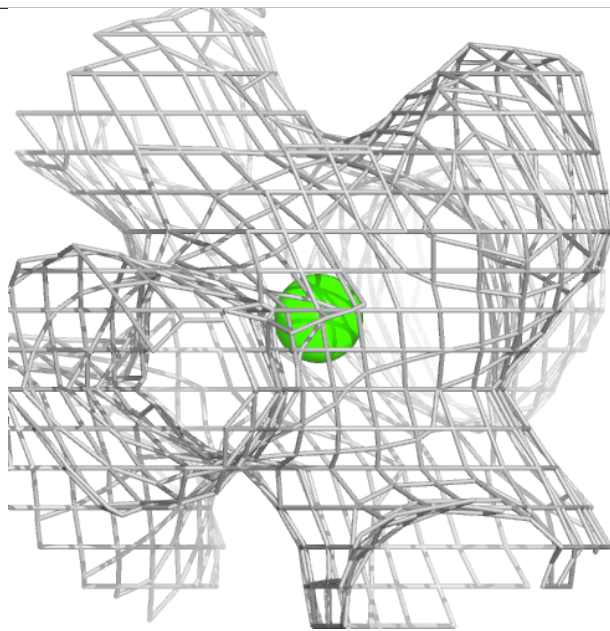
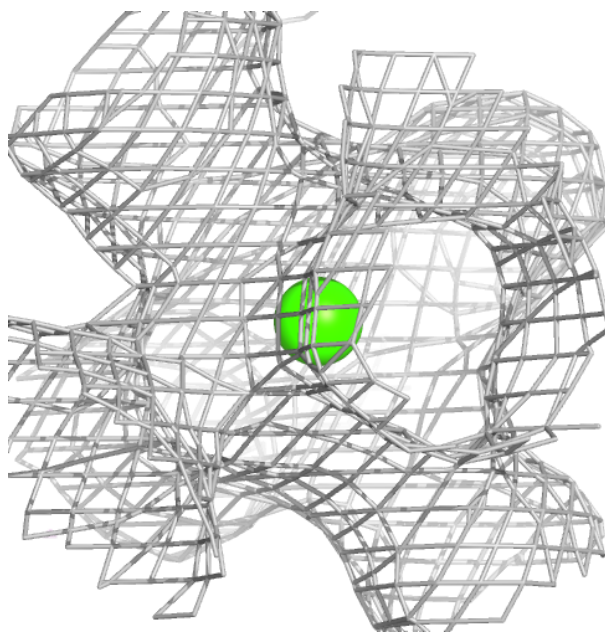
**Electron density around CA A 602:**

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



**Electron density around CA D 602:**

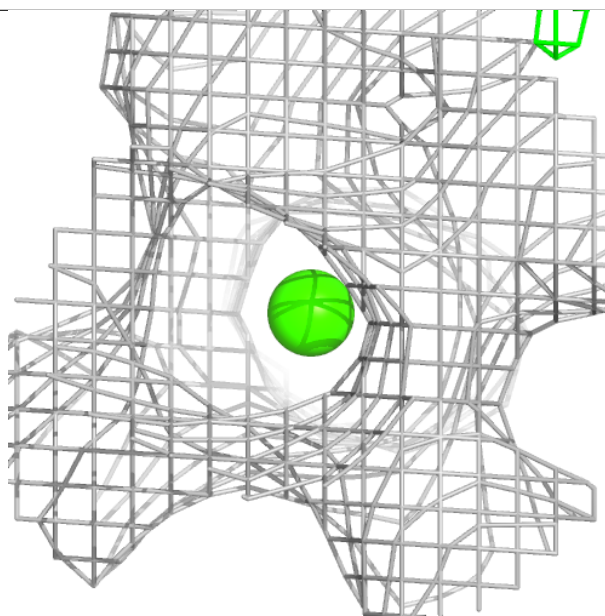
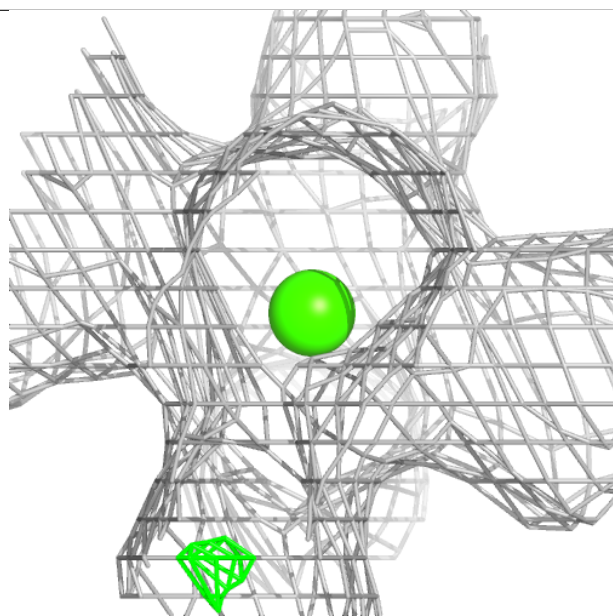
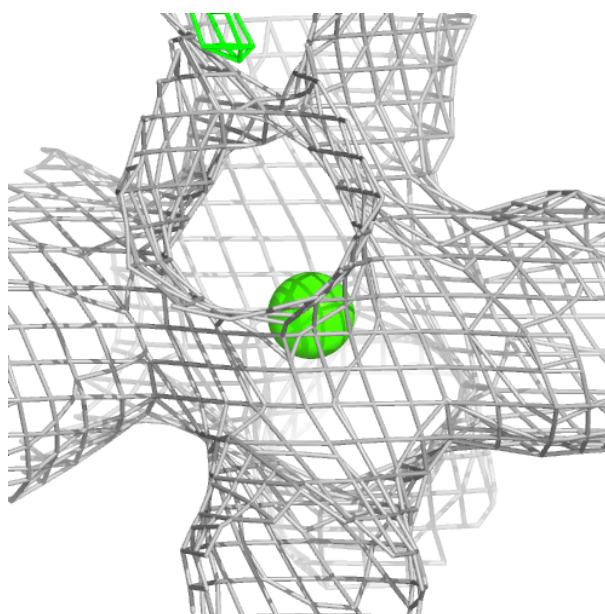
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CA D 603:**

$2mF_o-DF_c$  (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.