



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:46 PM UTC

PDB ID : 6ARG / pdb_00006arg
Title : Aspergillus fumigatus Cytosolic Thiolase: Apo enzyme in complex with rubidium ions
Authors : Marshall, A.C.; Bond, C.S.; Bruning, J.B.
Deposited on : 2017-08-22
Resolution : 1.78 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

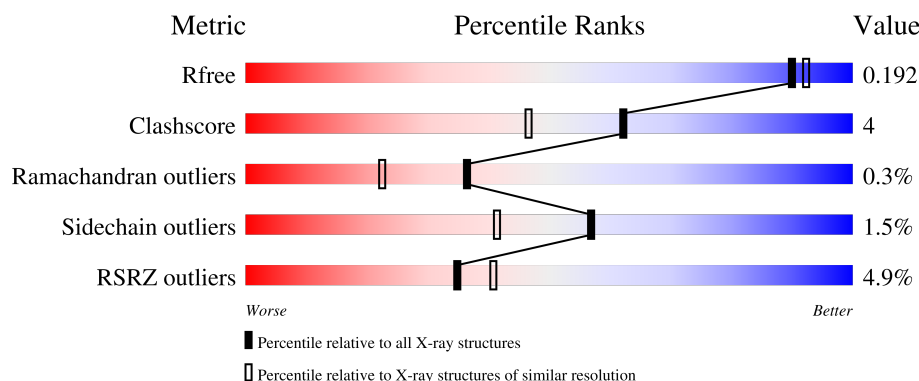
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	399	11% 85% 13% .
1	B	399	5% 91% 8% .
1	C	399	2% 92% 6% ..
1	D	399	2% 93% 5% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13089 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 Acetyl-CoA acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	6	0
			2860	1806	492	551	11			
1	B	396	Total	C	N	O	S	0	2	0
			2851	1793	494	552	12			
1	C	396	Total	C	N	O	S	0	8	0
			2877	1817	493	555	12			
1	D	395	Total	C	N	O	S	0	4	0
			2841	1790	488	551	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q4WCL5
B	0	GLY	-	expression tag	UNP Q4WCL5
C	0	GLY	-	expression tag	UNP Q4WCL5
D	0	GLY	-	expression tag	UNP Q4WCL5

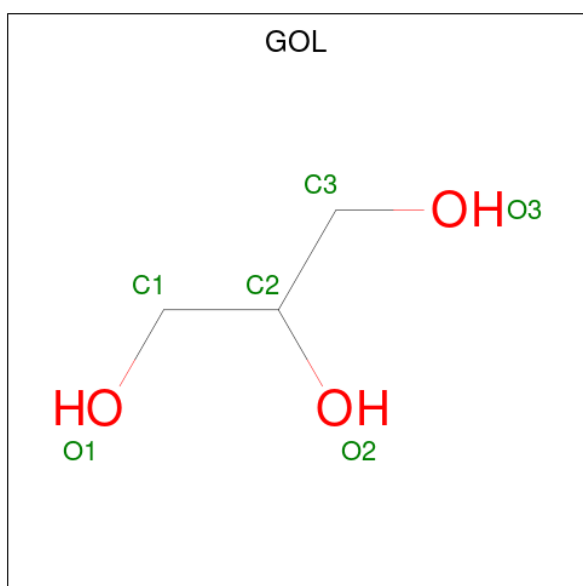
- Molecule 2 is RUBIDIUM ION (CCD ID: RB) (formula: Rb) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Rb	0	0
			3	3		
2	B	3	Total	Rb	0	0
			3	3		
2	C	3	Total	Rb	0	0
			3	3		
2	D	4	Total	Rb	0	0
			4	4		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	215	Total O 215 215	0	0
5	B	249	Total O 249 249	0	0
5	C	565	Total O 565 565	0	0

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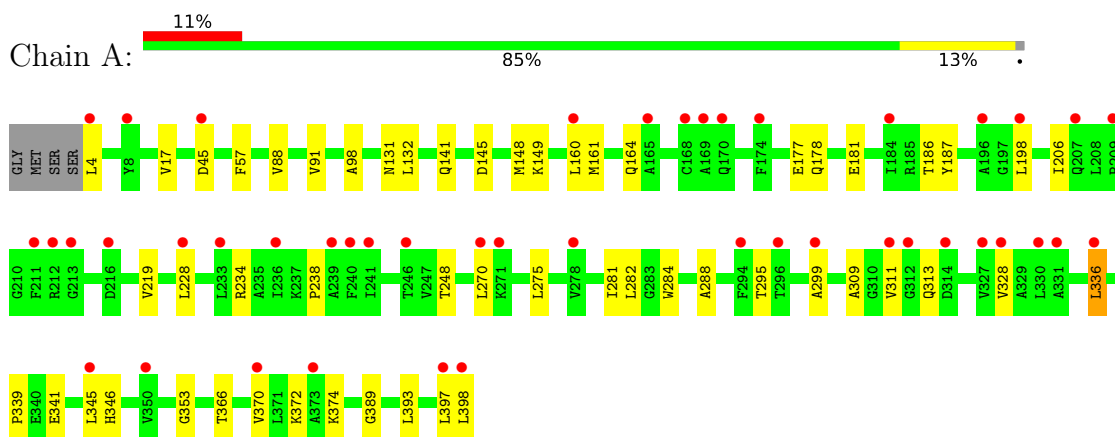
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	596	Total	O	0	0
			596	596		

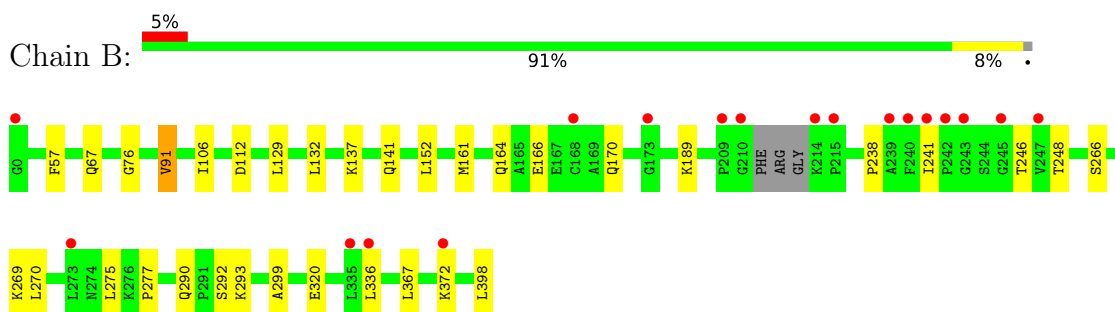
3 Residue-property plots [i](#)

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.

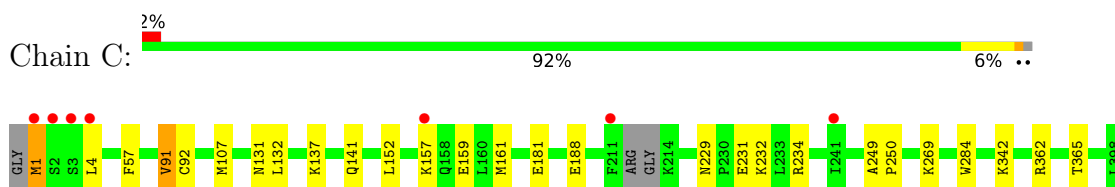
- Molecule 1: Acetyl-CoA acetyltransferase



- Molecule 1: Acetyl-CoA acetyltransferase

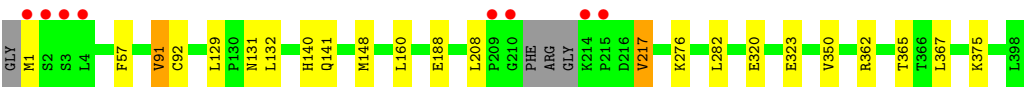


- Molecule 1: Acetyl-CoA acetyltransferase



- Molecule 1: Acetyl-CoA acetyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.26Å 105.37Å 110.26Å 90.00° 108.69° 90.00°	Depositor
Resolution (Å)	36.20 – 1.78 36.20 – 1.78	Depositor EDS
% Data completeness (in resolution range)	98.6 (36.20-1.78) 98.6 (36.20-1.78)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 1.78Å)	Xtriage
Refinement program	PHENIX dev_2686	Depositor
R, R_{free}	0.182 , 0.220 (Not available) , 0.192	Depositor DCC
R_{free} test set	7332 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	17.0	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13089	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.20	0/2923	0.41	0/3966
1	B	0.21	0/2900	0.42	0/3932
1	C	0.38	0/2944	0.54	0/3995
1	D	0.39	0/2896	0.55	0/3932
All	All	0.31	0/11663	0.48	0/15825

There are no bond length outliers.

There are no bond angle outliers.

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	2860	0	2923	41	0
1	B	2851	0	2913	25	0
1	C	2877	0	2953	22	0
1	D	2841	0	2891	15	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	4	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	C	12	0	16	1	0
4	D	6	0	8	0	0
5	A	215	0	0	7	0
5	B	249	0	0	6	0
5	C	565	0	0	8	2
5	D	596	0	0	2	1
All	All	13089	0	11704	95	2

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 4.

All (95) 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:B:372:LYS:NZ	5:B:502:HOH:O	2.11	0.83
1:B:299:ALA:HA	1:B:336:LEU:HD21	1.64	0.80
1:C:1:MET:HA	1:C:4:LEU:HD12	1.65	0.79
1:B:137:LYS:NZ	5:B:503:HOH:O	2.11	0.78
1:A:4:LEU:N	5:A:501:HOH:O	2.18	0.75
1:C:269:LYS:NZ	5:C:503:HOH:O	2.20	0.73
1:C:4:LEU:HB3	1:C:107:MET:HE3	1.71	0.73
1:C:181:GLU:OE2	1:C:234:ARG:NH2	2.22	0.72
1:B:170:GLN:O	5:B:501:HOH:O	2.11	0.69
1:A:206:ILE:N	5:A:502:HOH:O	2.27	0.68
1:A:148:MET:HE3	1:D:140:HIS:CE1	2.29	0.67
1:D:208:LEU:HB2	1:D:217:VAL:HG13	1.76	0.66
1:C:188:GLU:OE2	5:C:502:HOH:O	2.12	0.66
1:A:161:MET:HE3	1:B:67:GLN:HE22	1.63	0.62
1:A:181:GLU:OE1	1:A:234:ARG:NH1	2.34	0.60
1:A:270:LEU:HD12	1:A:275:LEU:HB2	1.82	0.60
1:B:290[A]:GLN:HB2	1:B:293:LYS:HG3	1.83	0.59
1:A:313:GLN:NE2	1:A:336:LEU:O	2.30	0.59
1:B:76:GLY:O	5:B:504:HOH:O	2.17	0.59
1:B:112:ASP:HB3	1:B:269:LYS:HG3	1.85	0.58
1:A:346:HIS:ND1	1:A:370:VAL:HG22	2.18	0.58
1:D:375:LYS:NZ	5:D:509:HOH:O	2.38	0.57
1:B:290[B]:GLN:HB3	1:B:293:LYS:HG3	1.86	0.57
1:A:145:ASP:HB3	1:A:148:MET:HE2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:ASN:CG	1:C:232:LYS:HG3	2.32	0.54
1:A:187:TYR:HB3	1:A:228:LEU:HD22	1.89	0.54
1:A:132:LEU:HD21	1:C:141:GLN:HG3	1.89	0.54
1:B:170:GLN:HG2	5:B:703:HOH:O	2.06	0.54
1:D:131:ASN:N	1:D:131:ASN:OD1	2.42	0.53
1:C:342:LYS:NZ	5:C:501:HOH:O	2.10	0.53
1:D:188:GLU:OE1	5:D:501:HOH:O	2.19	0.52
1:A:148:MET:HE1	1:D:140:HIS:H	1.74	0.51
1:A:148:MET:HE1	1:D:140:HIS:N	2.25	0.51
1:A:282:LEU:HB3	1:A:309:ALA:HB1	1.93	0.51
1:A:45:ASP:OD1	1:A:45:ASP:N	2.41	0.50
1:A:219:VAL:N	5:A:502:HOH:O	2.45	0.49
1:B:320:GLU:HG3	1:B:367:LEU:HB2	1.95	0.49
1:B:141:GLN:HG3	1:D:132:LEU:HD21	1.95	0.49
1:B:129:LEU:HD21	1:D:129:LEU:HD21	1.95	0.48
1:A:178:GLN:O	5:A:503:HOH:O	2.20	0.48
1:B:132:LEU:HD21	1:D:141:GLN:HG3	1.96	0.48
1:D:320:GLU:HG3	1:D:367:LEU:HB2	1.94	0.48
1:A:299:ALA:HA	1:A:336:LEU:HD21	1.95	0.48
1:A:282:LEU:HD23	1:A:311:VAL:HG21	1.95	0.48
1:A:339:PRO:HB2	1:A:341[B]:GLU:HG2	1.96	0.48
1:A:145:ASP:HB3	1:A:148:MET:CE	2.44	0.47
1:A:219:VAL:O	5:A:502:HOH:O	2.19	0.47
1:A:397:LEU:HD12	1:A:398:LEU:H	1.79	0.47
1:A:141:GLN:HG3	1:C:132:LEU:HD21	1.97	0.47
1:B:166:GLU:HG2	1:B:241:ILE:HD12	1.97	0.47
1:A:160:LEU:O	1:A:164:GLN:NE2	2.48	0.46
1:B:238:PRO:HA	1:B:248:THR:HG22	1.97	0.46
1:A:284:TRP:HB3	1:A:393:LEU:HD23	1.97	0.46
1:C:157:LYS:HD2	1:C:159:GLU:OE1	2.16	0.46
1:C:4:LEU:HD13	1:C:107:MET:HE1	1.97	0.46
4:C:406:GOL:H32	5:C:523:HOH:O	2.16	0.45
1:B:166:GLU:O	1:B:170:GLN:HG3	2.17	0.45
1:C:362:ARG:O	1:C:365[B]:THR:HG22	2.16	0.45
1:D:1:MET:HG2	1:D:282:LEU:O	2.16	0.45
1:D:148:MET:HE3	1:D:160:LEU:HD11	1.98	0.45
1:B:164:GLN:CD	1:B:292:SER:HA	2.42	0.45
1:A:17:VAL:HG11	1:A:353:GLY:HA3	2.00	0.44
1:C:152:LEU:HA	1:C:161:MET:HE2	1.99	0.44
1:D:362:ARG:O	1:D:365[B]:THR:HG22	2.18	0.44
1:A:295:THR:HB	1:A:328:VAL:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:N	5:C:520:HOH:O	2.49	0.43
1:C:1:MET:HE2	1:C:284:TRP:CZ3	2.53	0.43
1:B:152:LEU:HA	1:B:161:MET:HE2	1.99	0.43
1:C:1:MET:HE2	1:C:284:TRP:HZ3	1.82	0.43
1:C:161:MET:HE1	5:C:789:HOH:O	2.17	0.43
1:C:249:ALA:HB3	1:C:250:PRO:HD3	2.00	0.43
1:B:270:LEU:HD12	1:B:275:LEU:HB2	2.01	0.43
1:A:206:ILE:O	5:A:502:HOH:O	2.21	0.42
1:C:157:LYS:HB2	1:C:159:GLU:HB2	2.00	0.42
1:A:281:ILE:HG23	1:A:393:LEU:HD21	2.02	0.42
1:A:346:HIS:CE1	1:A:370:VAL:HA	2.54	0.42
1:A:288:ALA:HA	1:A:389:GLY:HA2	2.02	0.42
1:B:290[A]:GLN:H	1:B:290[A]:GLN:CD	2.28	0.41
1:A:88:VAL:HG21	1:A:98:ALA:HB2	2.03	0.41
1:A:345:LEU:HD13	1:A:374:LYS:HE2	2.03	0.41
1:A:238:PRO:HA	1:A:248:THR:HG22	2.02	0.41
1:C:181:GLU:HG3	5:C:979:HOH:O	2.20	0.41
1:A:149[A]:LYS:NZ	5:A:510:HOH:O	2.34	0.41
1:A:177:GLU:OE2	1:A:177:GLU:N	2.54	0.41
1:B:106:ILE:HG23	1:B:266:SER:HB3	2.02	0.41
1:A:4:LEU:HD23	1:A:4:LEU:HA	1.83	0.41
1:A:131:ASN:OD1	1:A:131:ASN:N	2.54	0.41
1:B:166:GLU:OE2	1:B:246:THR:OG1	2.29	0.41
1:C:137:LYS:NZ	5:C:529:HOH:O	2.53	0.41
1:A:366:THR:O	1:A:370:VAL:HG23	2.21	0.40
1:D:323:GLU:HB3	1:D:350:VAL:HG23	2.03	0.40
1:A:187:TYR:CD1	1:A:228:LEU:HB2	2.56	0.40
1:B:277:PRO:HB2	1:B:398:LEU:HD12	2.03	0.40
1:B:189:LYS:NZ	5:B:524:HOH:O	2.53	0.40

All (2) 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:C:921:HOH:O	5:D:837:HOH:O[1_455]	2.14	0.06
5:C:510:HOH:O	5:C:704:HOH:O[2_547]	2.16	0.04

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	399/399 (100%)	390 (98%)	8 (2%)	1 (0%)	36	22
1	B	394/399 (99%)	381 (97%)	12 (3%)	1 (0%)	36	22
1	C	400/399 (100%)	393 (98%)	6 (2%)	1 (0%)	36	22
1	D	395/399 (99%)	387 (98%)	7 (2%)	1 (0%)	36	22
All	All	1588/1596 (100%)	1551 (98%)	33 (2%)	4 (0%)	36	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	91	VAL
1	A	91	VAL
1	C	91	VAL
1	D	91	VAL

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	295/298 (99%)	290 (98%)	5 (2%)	53	36
1	B	295/298 (99%)	293 (99%)	2 (1%)	76	66
1	C	299/298 (100%)	293 (98%)	6 (2%)	48	29
1	D	293/298 (98%)	288 (98%)	5 (2%)	53	36
All	All	1182/1192 (99%)	1164 (98%)	18 (2%)	57	41

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	PHE
1	A	186	THR
1	A	198	LEU
1	A	336	LEU
1	A	372	LYS
1	B	57	PHE
1	B	91	VAL
1	C	1	MET
1	C	57	PHE
1	C	91	VAL
1	C	92	CYS
1	C	231[A]	GLU
1	C	231[B]	GLU
1	D	57	PHE
1	D	91	VAL
1	D	92	CYS
1	D	217	VAL
1	D	276	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	289	GLN
1	A	322	ASN
1	B	67	GLN
1	B	164	GLN
1	B	170	GLN
1	B	221	GLN
1	B	322	ASN
1	C	104	GLN
1	C	158	GLN
1	C	221	GLN
1	D	290	GLN
1	D	322	ASN
1	D	332	ASN

5.3.3 RNA ⓘ

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 20 ligands modelled in this entry, 17 are monoatomic - leaving 3 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	D	406	-	5,5,5	1.06	0	5,5,5	1.04	0
4	GOL	C	406	-	5,5,5	0.96	0	5,5,5	1.61	2 (40%)
4	GOL	C	405	-	5,5,5	0.83	0	5,5,5	1.17	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	D	406	-	-	2/4/4/4	-
4	GOL	C	406	-	-	2/4/4/4	-
4	GOL	C	405	-	-	0/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	406	GOL	C3-C2-C1	-2.82	101.45	111.80
4	C	405	GOL	C3-C2-C1	-2.09	104.14	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	406	GOL	O2-C2-C3	2.00	117.48	109.18

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	406	GOL	C1-C2-C3-O3
4	C	406	GOL	O1-C1-C2-C3
4	D	406	GOL	O2-C2-C3-O3
4	C	406	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	406	GOL	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, 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	395/399 (98%)	0.93	45 (11%)	10 11	15, 47, 73, 130	6 (1%)
1	B	396/399 (99%)	0.53	18 (4%)	38 44	20, 39, 67, 98	2 (0%)
1	C	396/399 (99%)	-0.38	7 (1%)	67 75	6, 17, 38, 94	8 (2%)
1	D	395/399 (98%)	-0.43	8 (2%)	65 73	7, 16, 34, 99	4 (1%)
All	All	1582/1596 (99%)	0.16	78 (4%)	35 41	6, 27, 66, 130	20 (1%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	211	PHE	4.7
1	B	210	GLY	4.4
1	B	215	PRO	3.9
1	B	214	LYS	3.8
1	C	211	PHE	3.6
1	B	0	GLY	3.6
1	C	2	SER	3.6
1	A	373	ALA	3.6
1	B	243	GLY	3.5
1	D	1	MET	3.4
1	D	2	SER	3.3
1	C	4	LEU	3.3
1	C	1	MET	3.2
1	B	209	PRO	3.1
1	B	273	LEU	3.1
1	A	174	PHE	3.1
1	B	242	PRO	3.0
1	D	210	GLY	3.0
1	D	215	PRO	3.0
1	A	299	ALA	2.9
1	A	240	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	209	PRO	2.9
1	A	278	VAL	2.9
1	D	3	SER	2.8
1	A	271[A]	LYS	2.8
1	D	4	LEU	2.7
1	A	212	ARG	2.7
1	B	245	GLY	2.7
1	A	184	ILE	2.7
1	B	335	LEU	2.7
1	A	236	ILE	2.7
1	A	169	ALA	2.7
1	A	294	PHE	2.6
1	C	157	LYS	2.6
1	B	241	ILE	2.6
1	A	345	LEU	2.6
1	B	239	ALA	2.6
1	A	209	PRO	2.6
1	A	296	THR	2.6
1	A	397	LEU	2.6
1	A	228	LEU	2.5
1	A	8	TYR	2.5
1	A	330	LEU	2.5
1	A	336	LEU	2.5
1	A	314	ASP	2.4
1	A	311	VAL	2.4
1	A	327	VAL	2.4
1	A	168	CYS	2.4
1	A	4	LEU	2.4
1	A	170	GLN	2.3
1	A	246	THR	2.3
1	A	350	VAL	2.3
1	A	239	ALA	2.3
1	A	233	LEU	2.3
1	A	398	LEU	2.3
1	B	372	LYS	2.3
1	D	214	LYS	2.3
1	A	213	GLY	2.2
1	A	328	VAL	2.2
1	A	370	VAL	2.2
1	A	45	ASP	2.2
1	B	240	PHE	2.2
1	C	3	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	173	GLY	2.2
1	A	270	LEU	2.1
1	A	241	ILE	2.1
1	A	165	ALA	2.1
1	B	247	VAL	2.1
1	B	168	CYS	2.1
1	A	160	LEU	2.1
1	B	336	LEU	2.1
1	A	331	ALA	2.0
1	A	198	LEU	2.0
1	A	207	GLN	2.0
1	A	312	GLY	2.0
1	C	241	ILE	2.0
1	A	196	ALA	2.0
1	A	216	ASP	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(Å ²)	Q<0.9
4	GOL	C	406	6/6	0.80	0.17	20,20,20,20	0
4	GOL	C	405	6/6	0.87	0.12	20,20,20,20	0
4	GOL	D	406	6/6	0.92	0.11	24,33,45,51	0
3	CL	A	404	1/1	0.96	0.07	30,30,30,30	1
2	RB	D	404	1/1	0.96	0.09	48,48,48,48	1
2	RB	A	402	1/1	0.97	0.06	66,66,66,66	1
3	CL	B	404	1/1	0.97	0.06	30,30,30,30	1
3	CL	C	404	1/1	0.97	0.08	25,25,25,25	0

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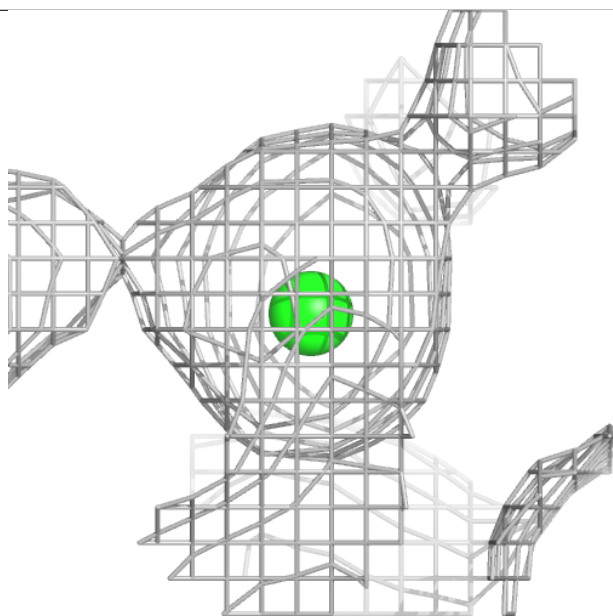
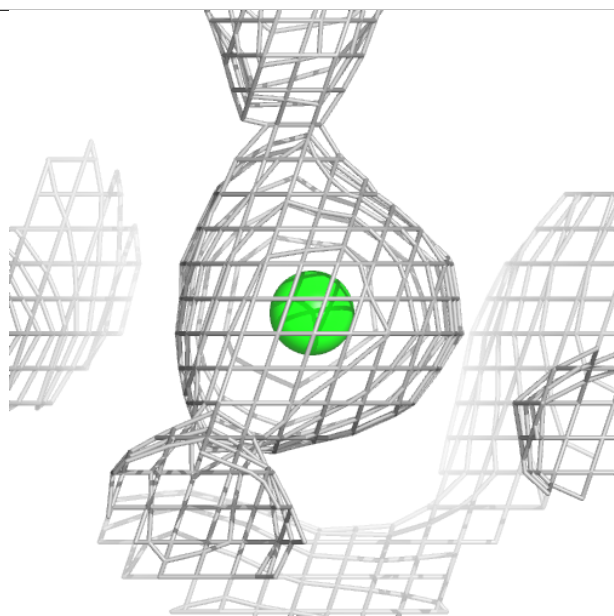
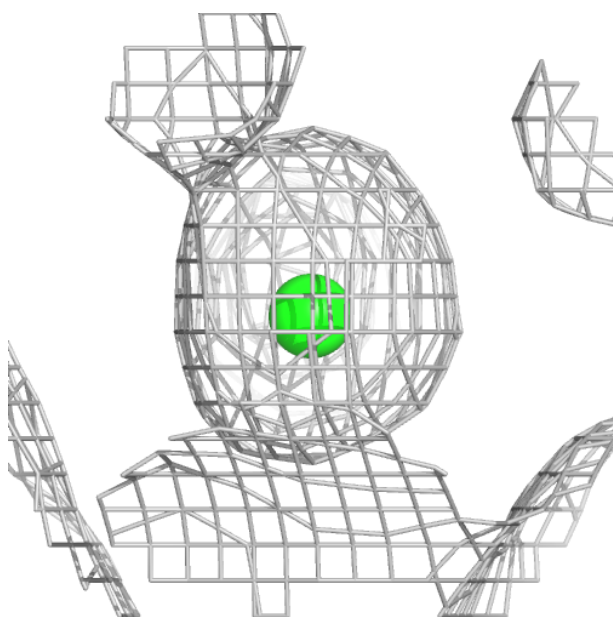
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	D	405	1/1	0.98	0.05	21,21,21,21	0
2	RB	B	403	1/1	0.98	0.06	88,88,88,88	0
2	RB	A	401	1/1	0.99	0.03	40,40,40,40	1
2	RB	A	403	1/1	0.99	0.05	65,65,65,65	1
2	RB	B	402	1/1	0.99	0.04	51,51,51,51	0
2	RB	C	401	1/1	1.00	0.02	18,18,18,18	0
2	RB	C	402	1/1	1.00	0.02	19,19,19,19	1
2	RB	C	403	1/1	1.00	0.02	20,20,20,20	1
2	RB	D	401	1/1	1.00	0.01	16,16,16,16	0
2	RB	D	402	1/1	1.00	0.02	19,19,19,19	1
2	RB	D	403	1/1	1.00	0.02	23,23,23,23	1
2	RB	B	401	1/1	1.00	0.03	40,40,40,40	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.

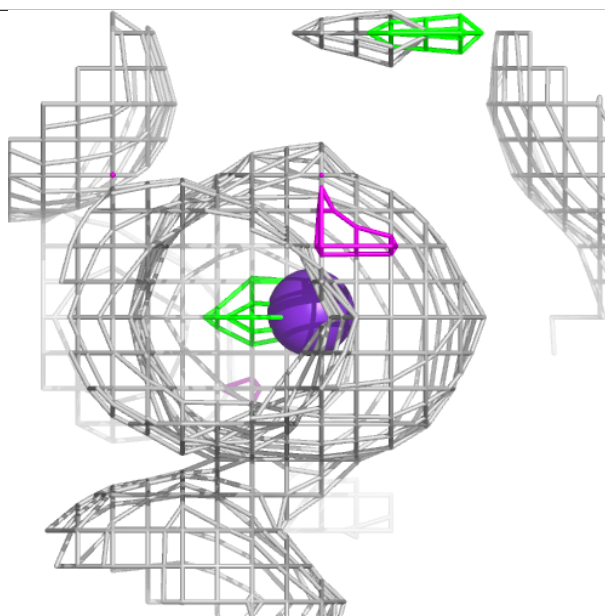
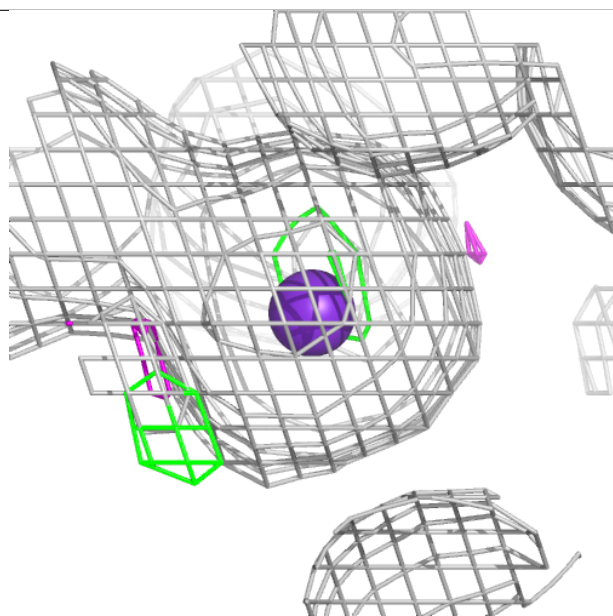
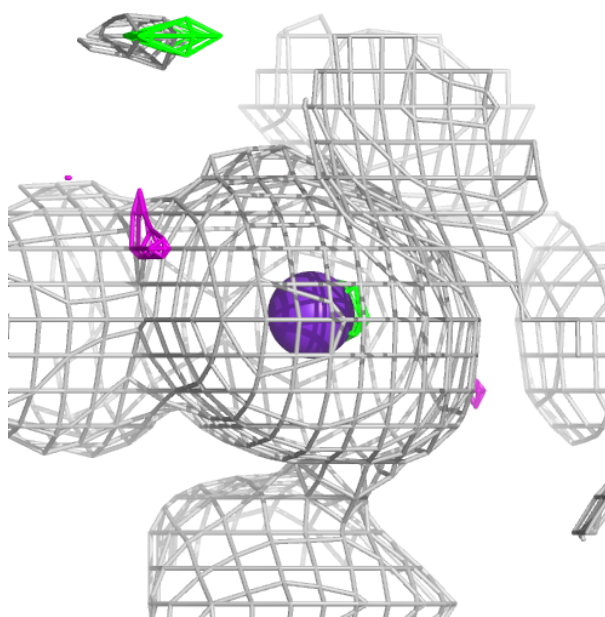
Electron density around CL A 404:

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



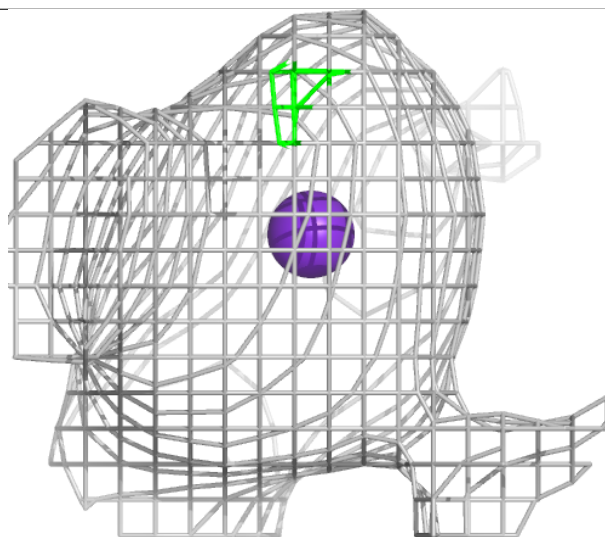
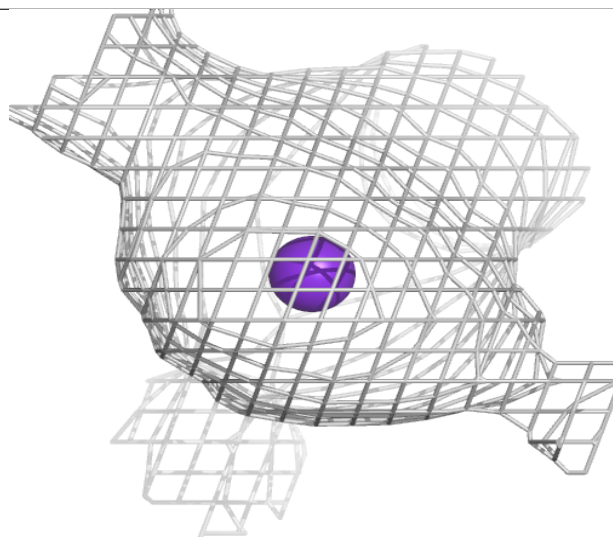
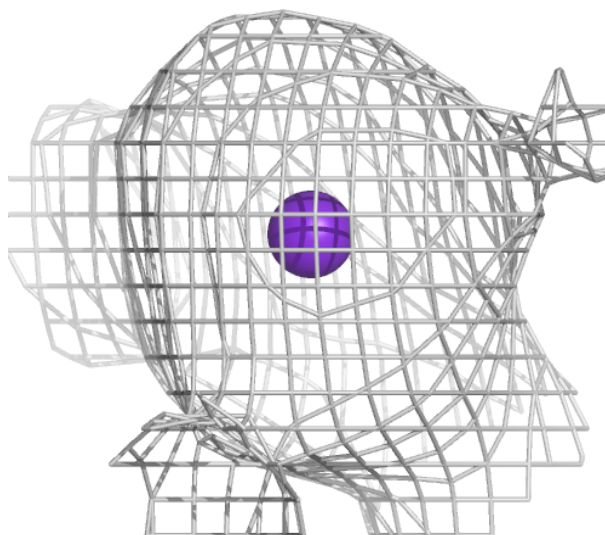
Electron density around RB D 404:

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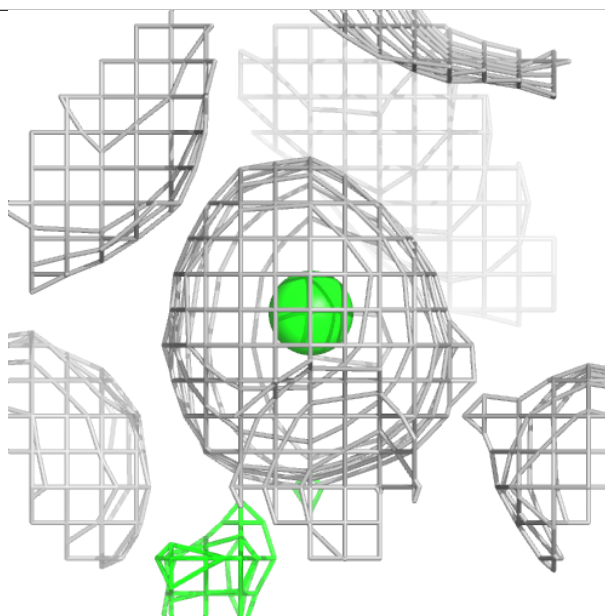
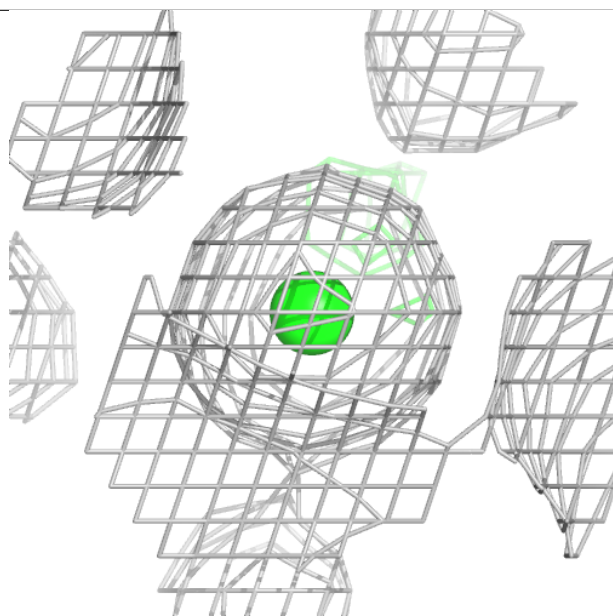
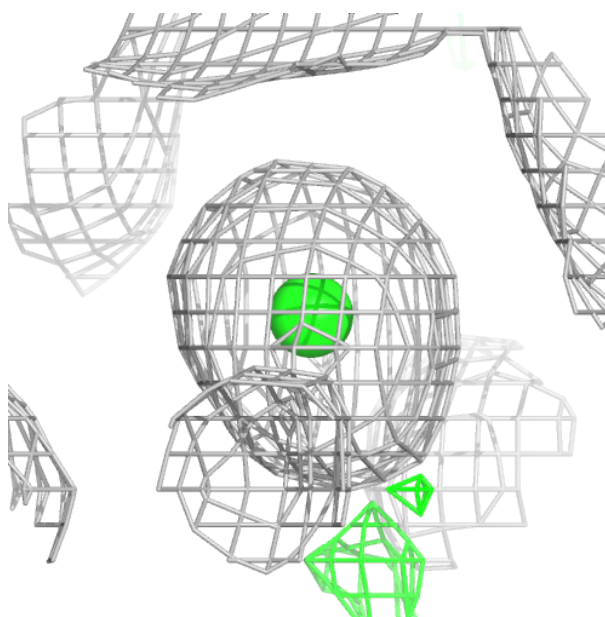
Electron density around RB A 402:

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and green (positive)



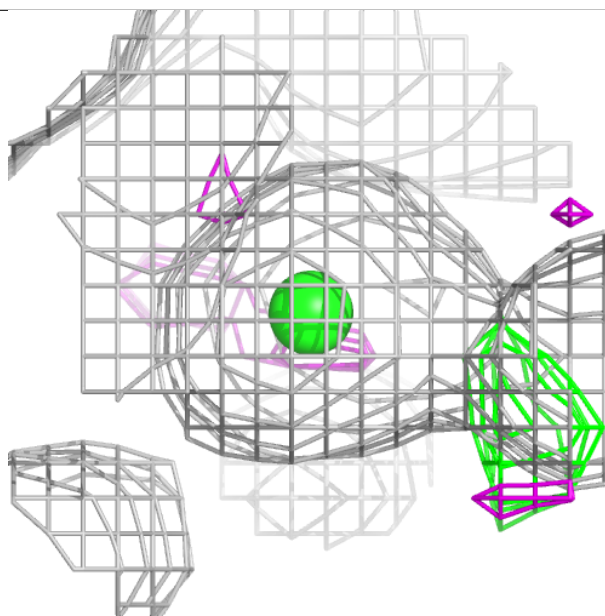
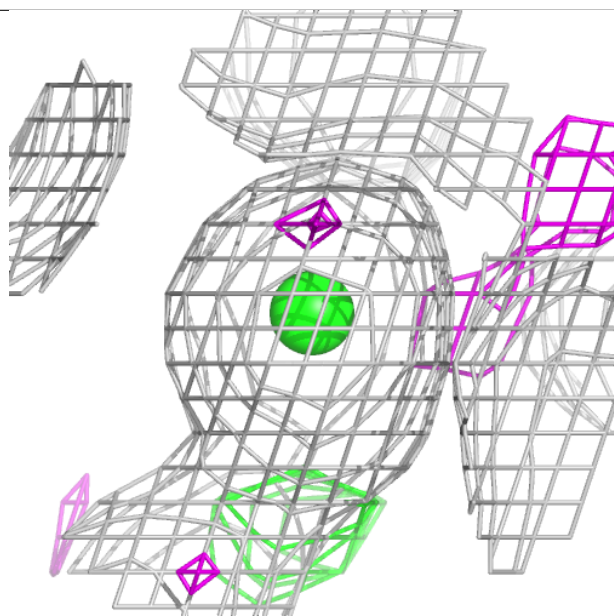
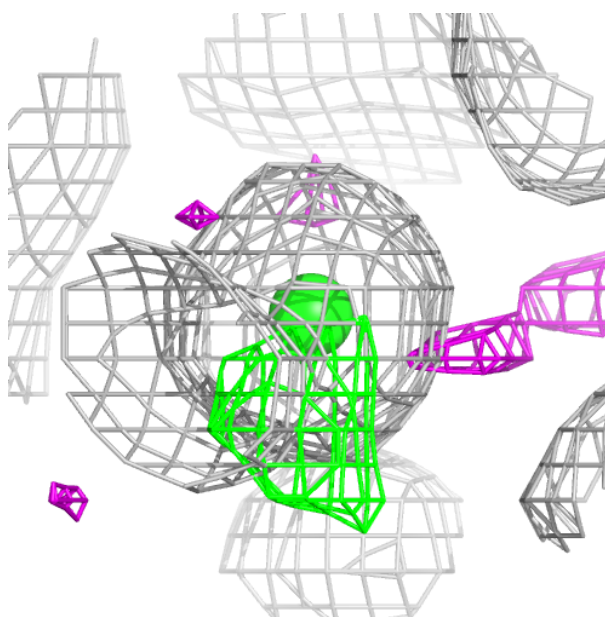
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and green (positive)



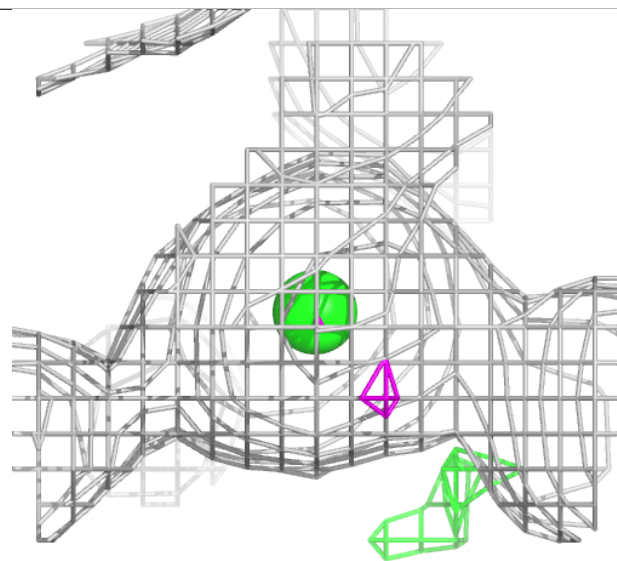
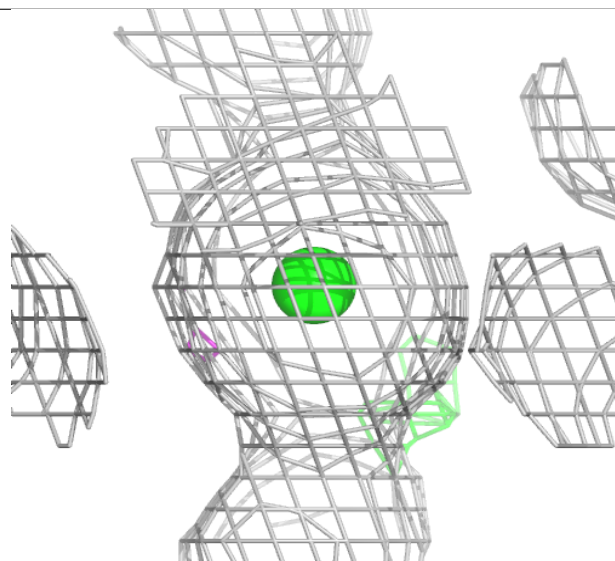
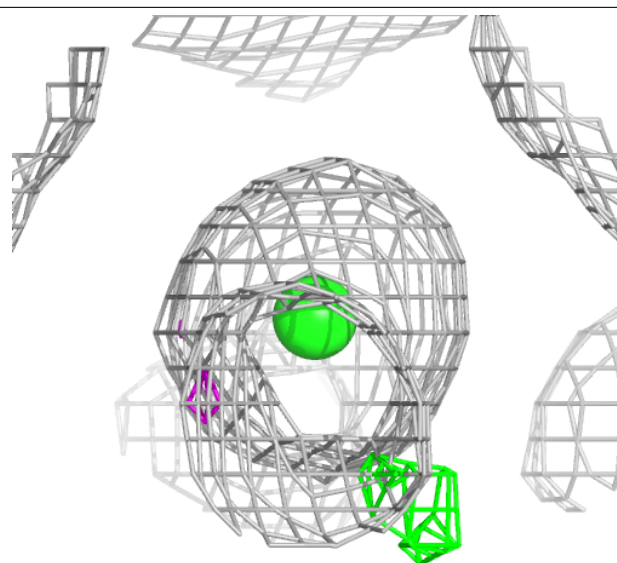
Electron density around CL C 404:

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and green (positive)



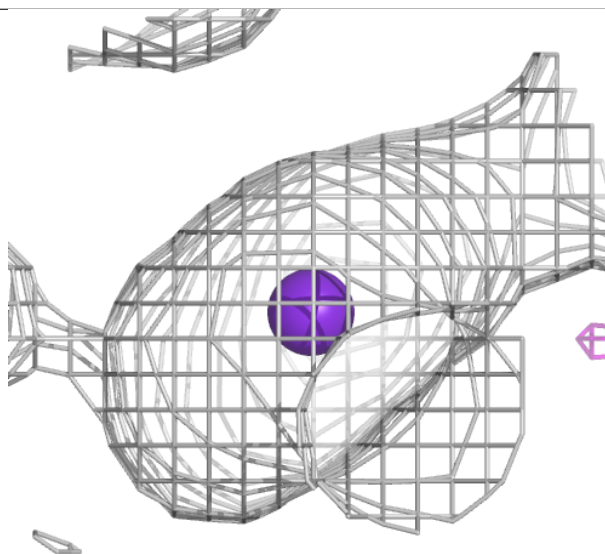
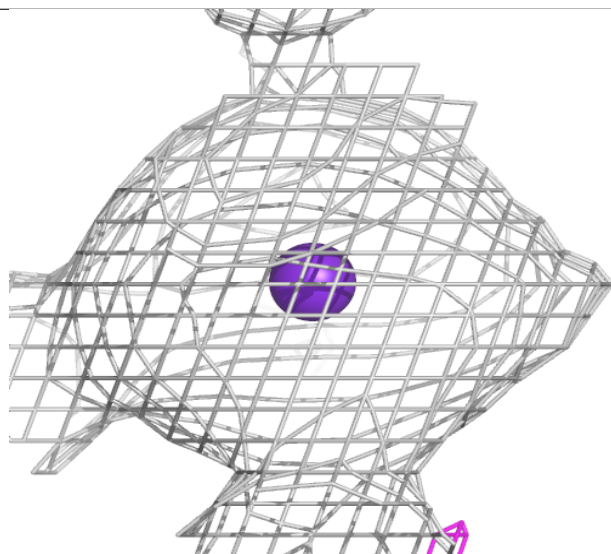
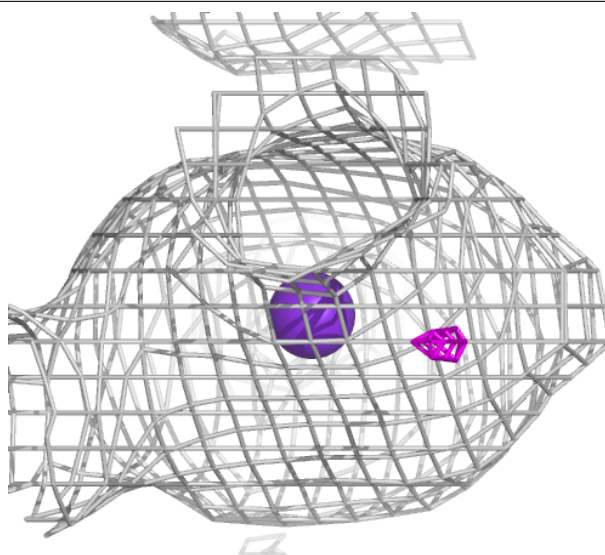
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and green (positive)



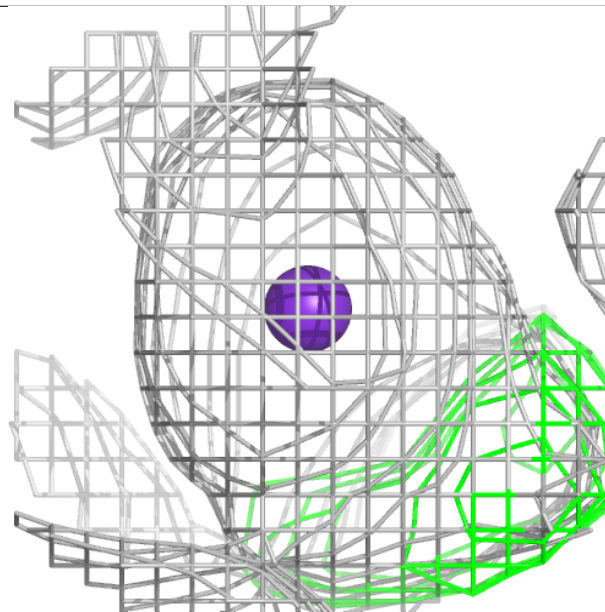
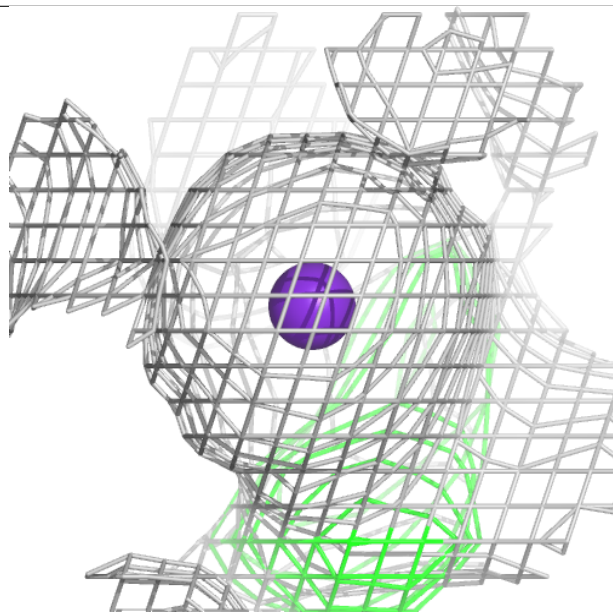
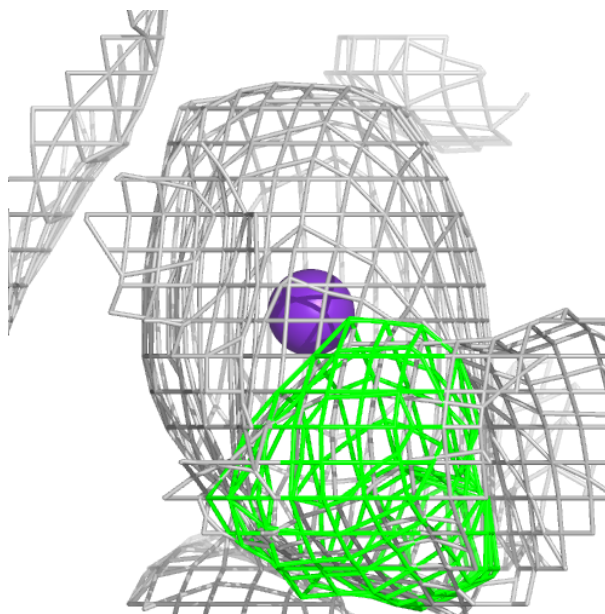
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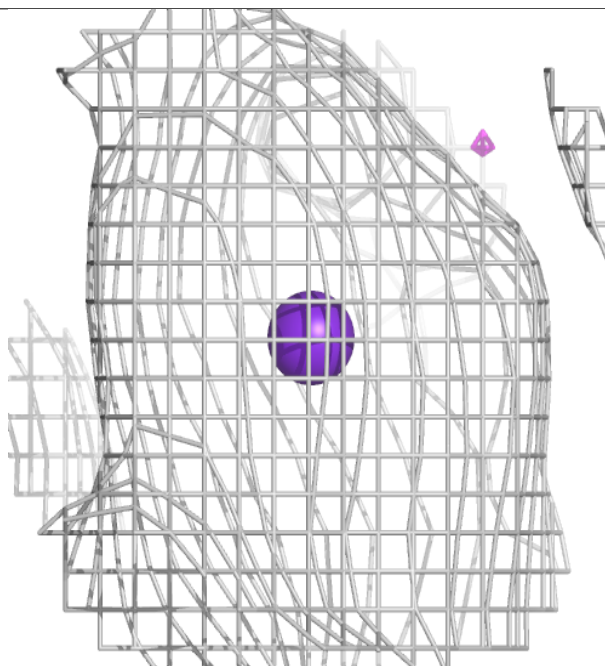
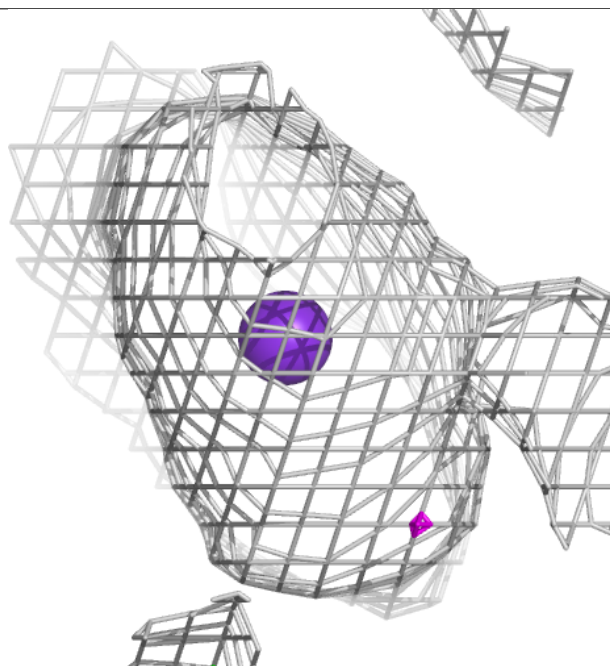
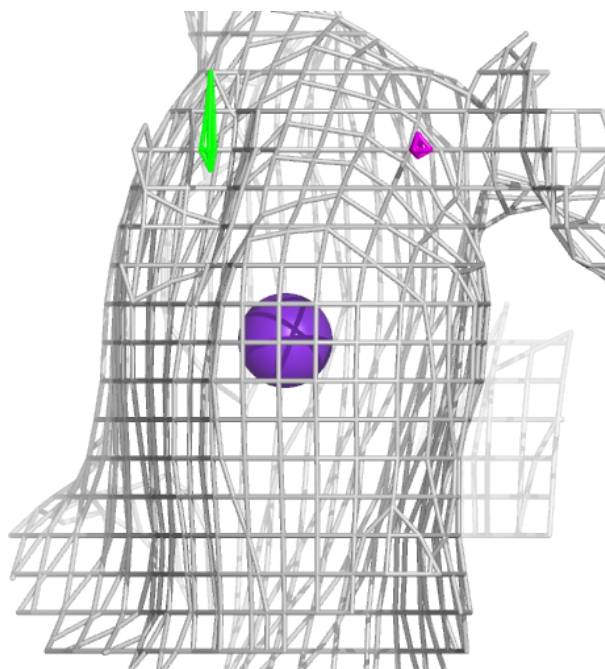
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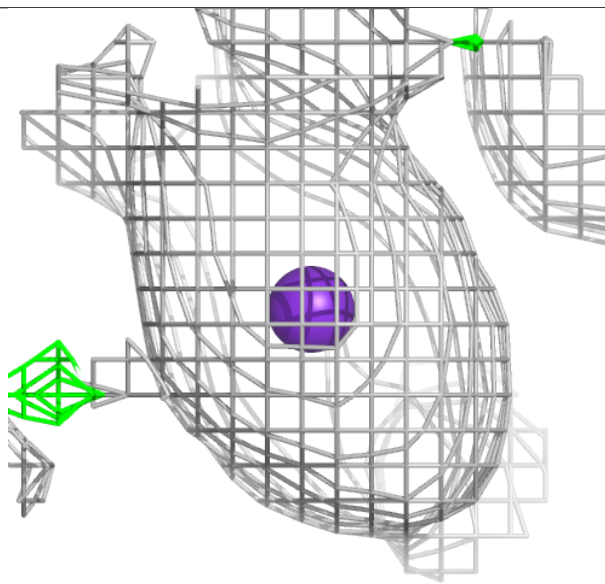
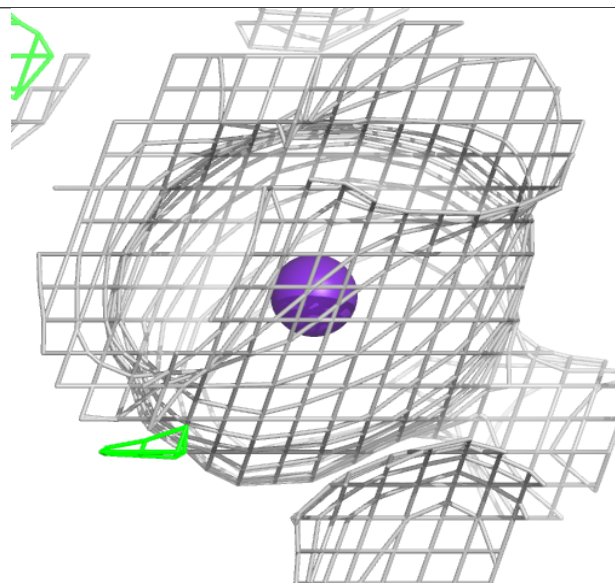
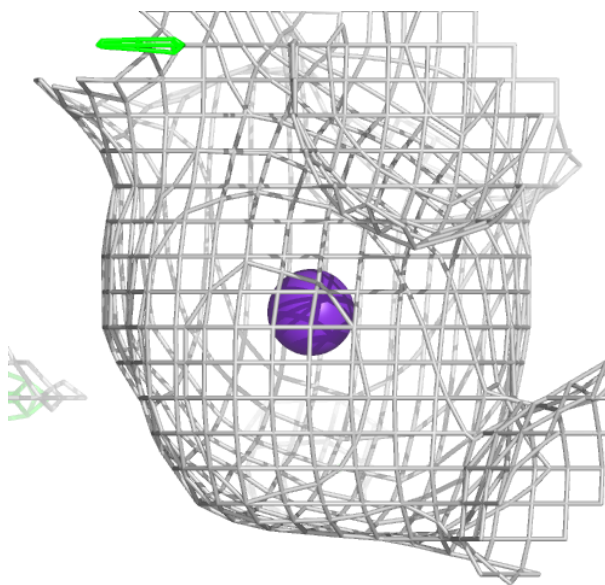
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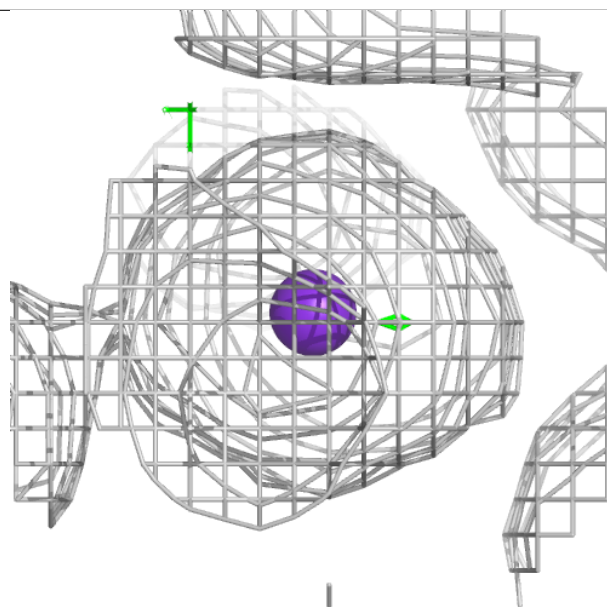
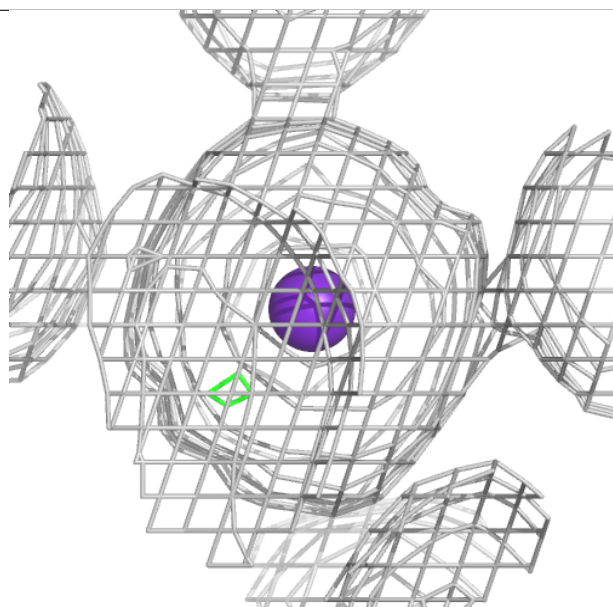
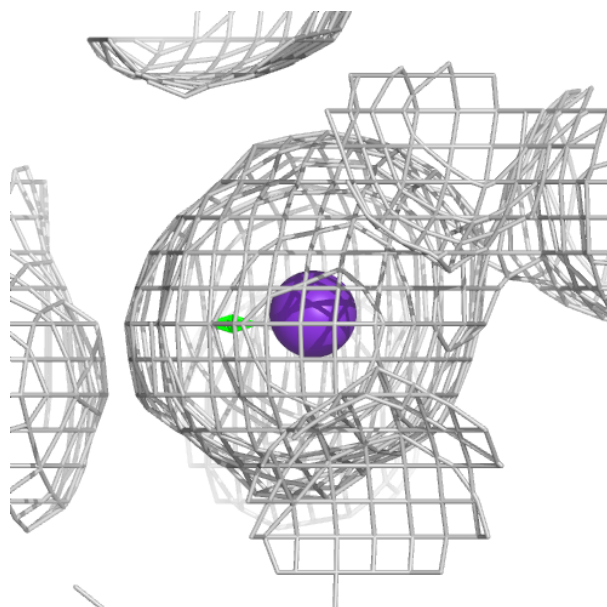
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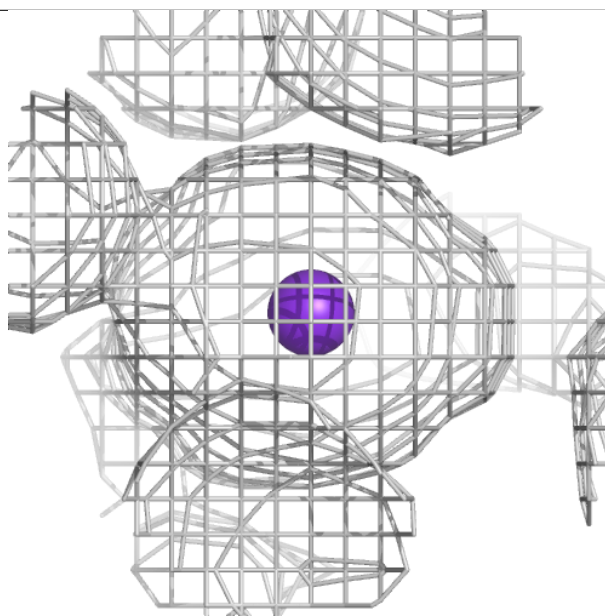
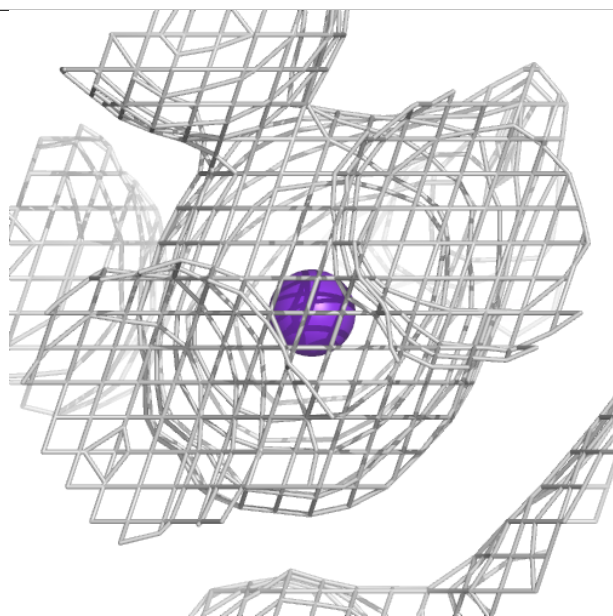
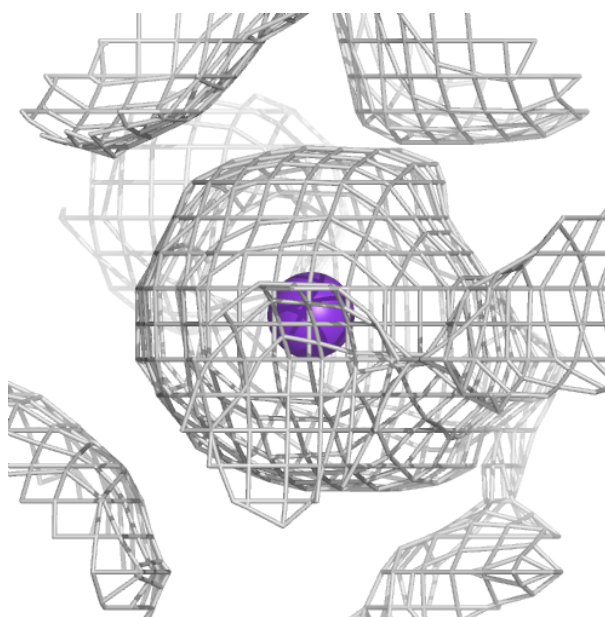
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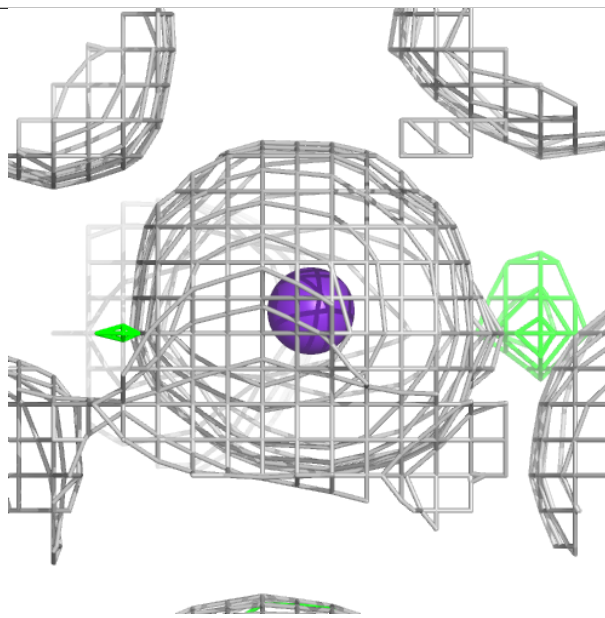
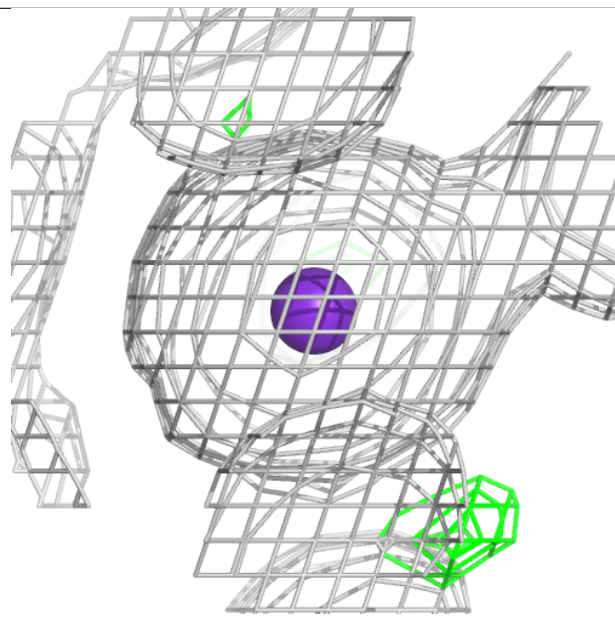
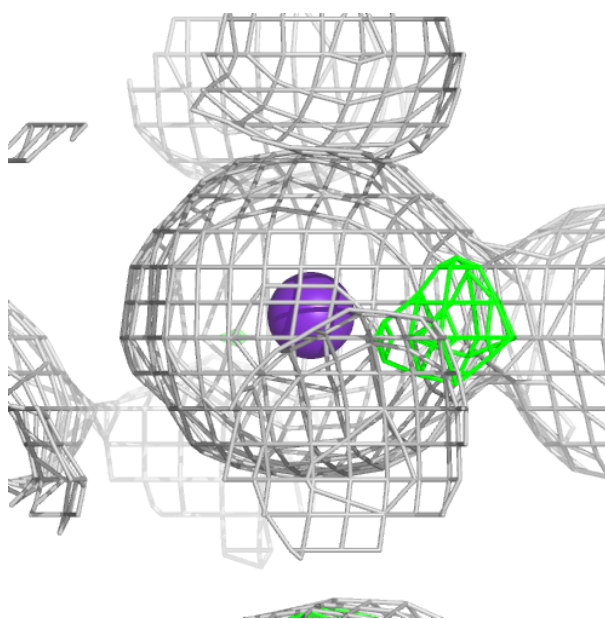
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and green (positive)



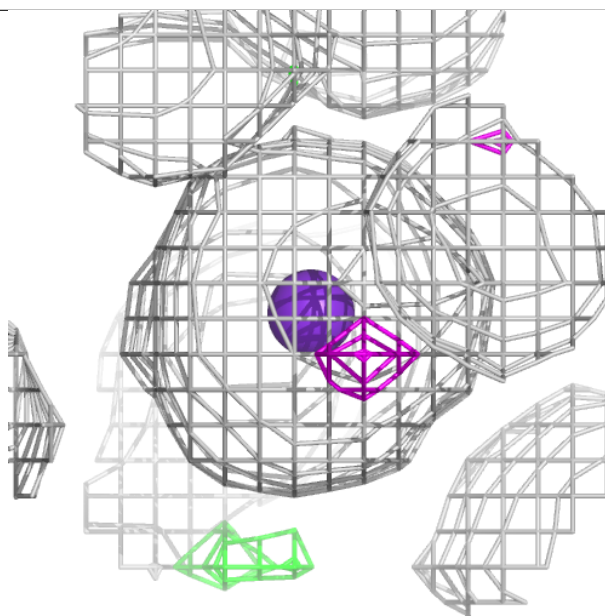
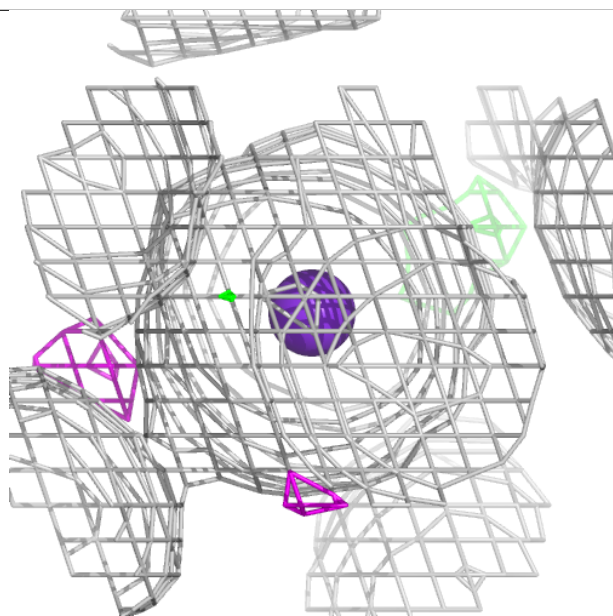
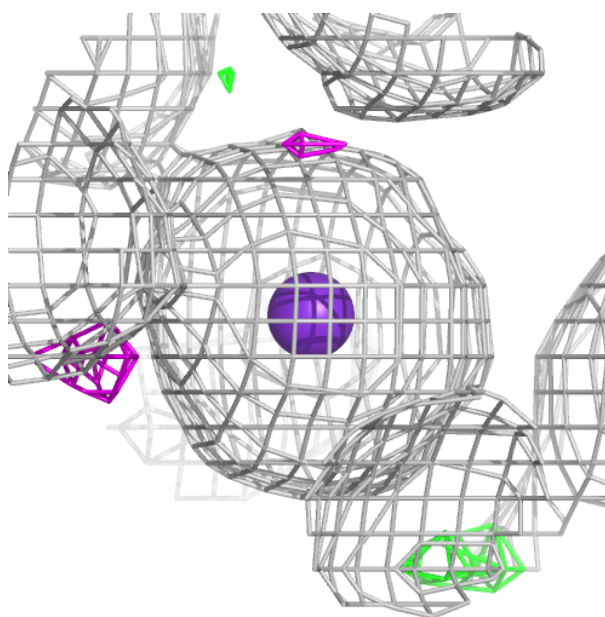
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and green (positive)



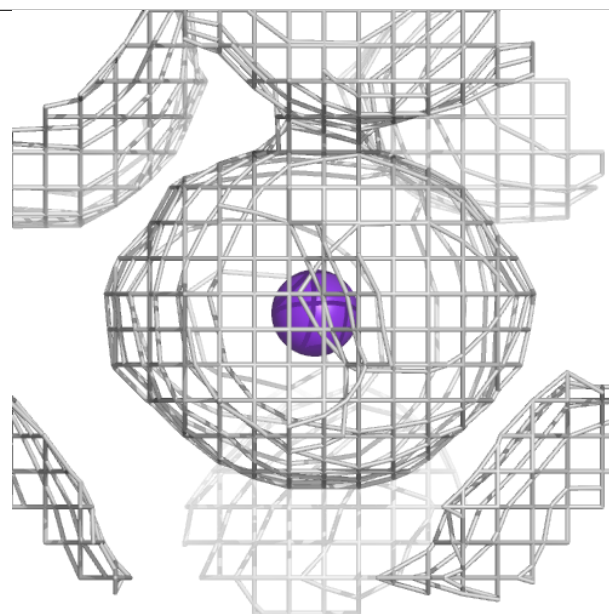
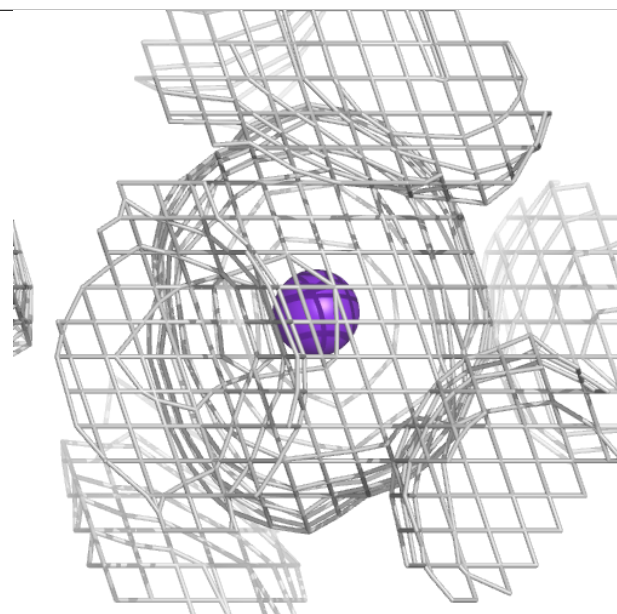
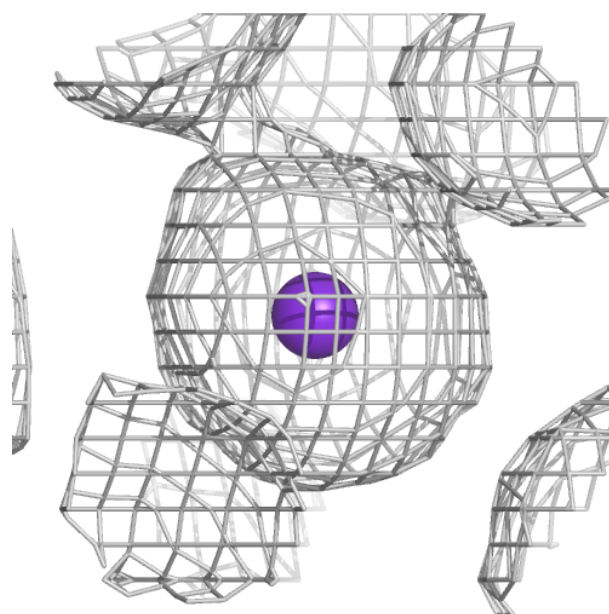
Electron density around RB D 401:

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



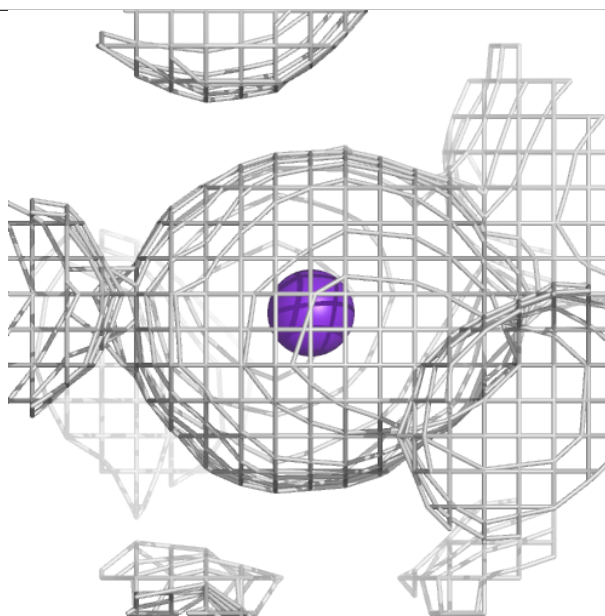
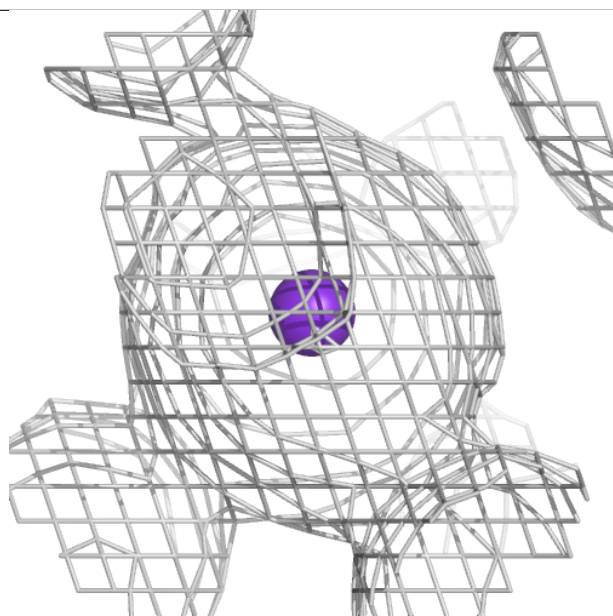
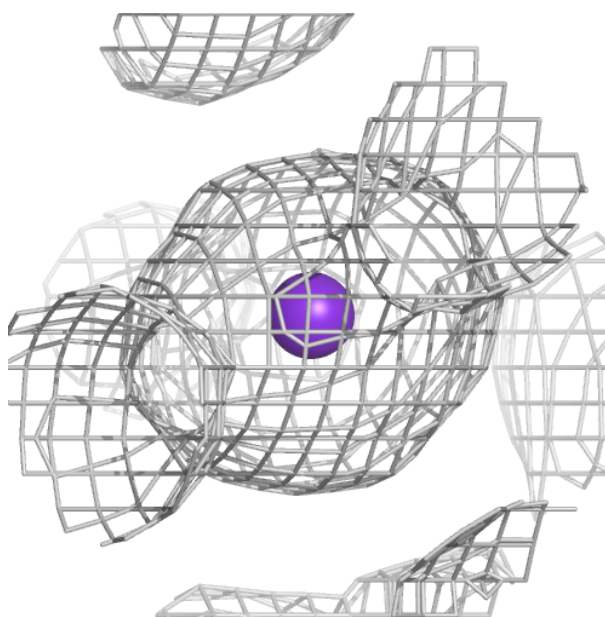
Electron density around RB D 402:

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



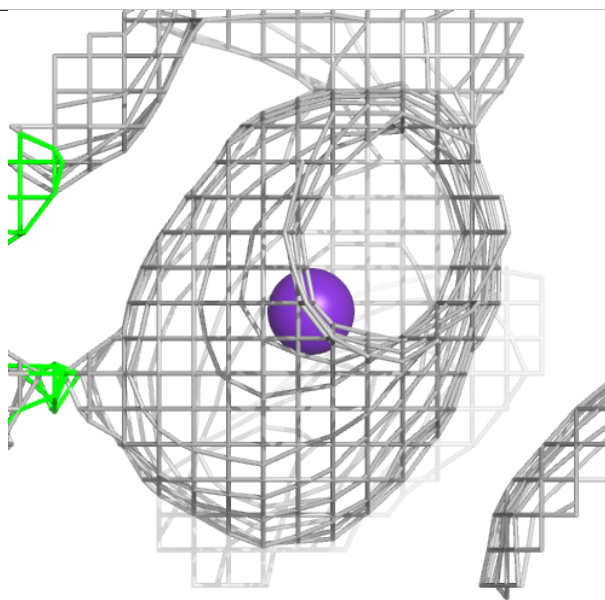
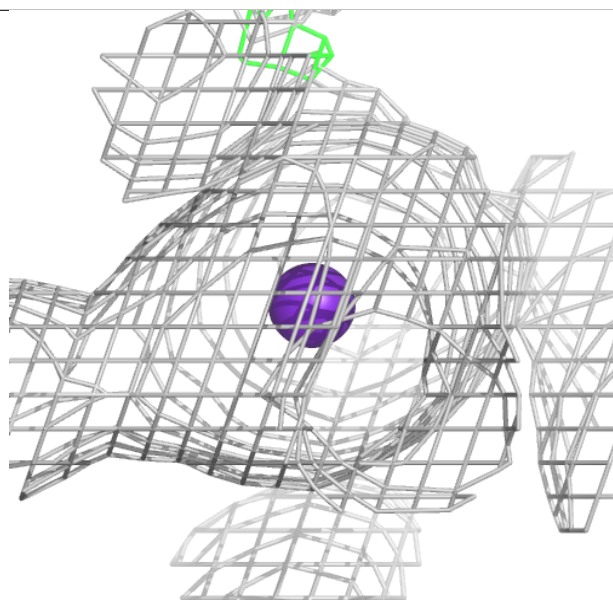
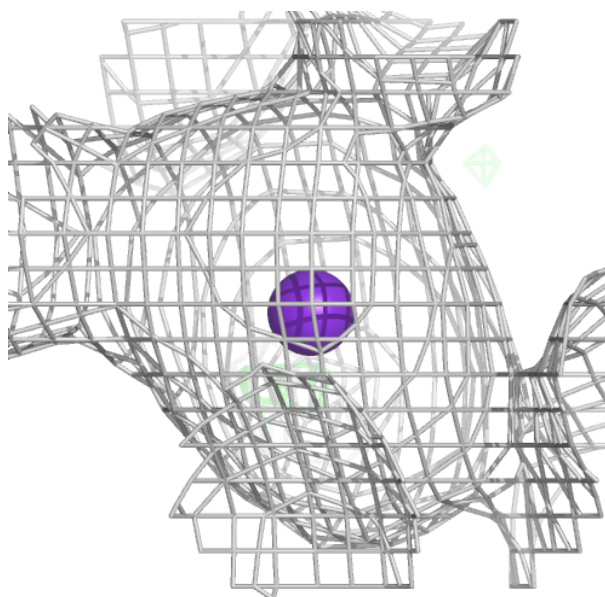
Electron density around RB D 403:

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



Electron density around RB B 401:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.