



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 04:20 PM BST

PDB ID : 6ARF  
Title : Aspergillus fumigatus Cytosolic Thiolase: Apo enzyme in complex with potassium ions  
Authors : Marshall, A.C.; Bond, C.S.; Bruning, J.B.  
Deposited on : 2017-08-22  
Resolution : 1.70 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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13

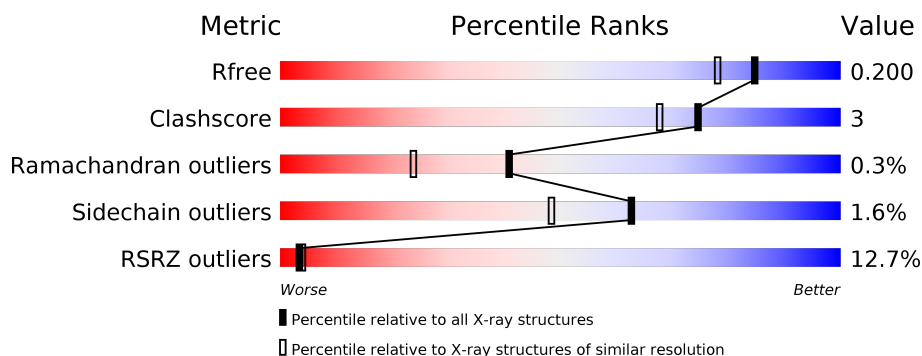
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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))
$R_{free}$	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 on 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	399	<div> <div>27%</div> <div> <div></div> <div>91%</div> <div>8%</div> <div></div> </div> </div>
1	B	399	<div> <div>17%</div> <div> <div></div> <div>89%</div> <div>11%</div> <div></div> </div> </div>
1	C	399	<div> <div>3%</div> <div> <div></div> <div>92%</div> <div>8%</div> <div></div> </div> </div>
1	D	399	<div> <div>4%</div> <div> <div></div> <div>92%</div> <div>7%</div> <div></div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13073 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	4	0
			2848	1797	491	549	11			
1	B	397	Total	C	N	O	S	0	2	0
			2852	1793	494	553	12			
1	C	396	Total	C	N	O	S	0	9	0
			2885	1821	495	558	11			
1	D	395	Total	C	N	O	S	0	7	0
			2872	1810	495	555	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 CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by author).

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

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by author).

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

- Molecule 4 is GLYCEROL (three-letter code: 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
4	D	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	172	Total O 172 172	0	0

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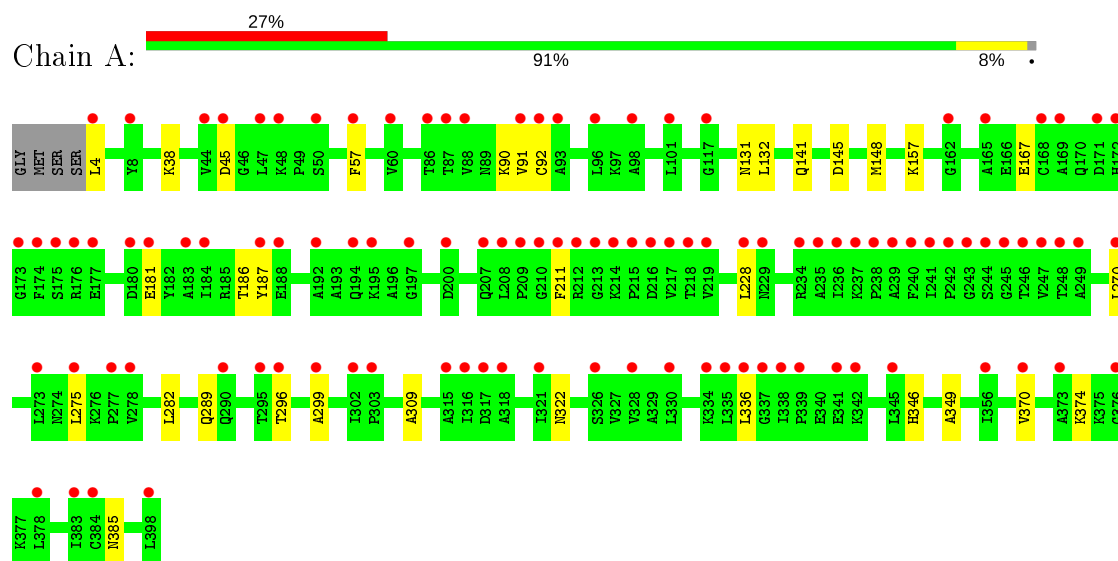
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	194	Total 194	O 194	0	0
5	C	578	Total 578	O 578	0	0
5	D	625	Total 625	O 625	0	0

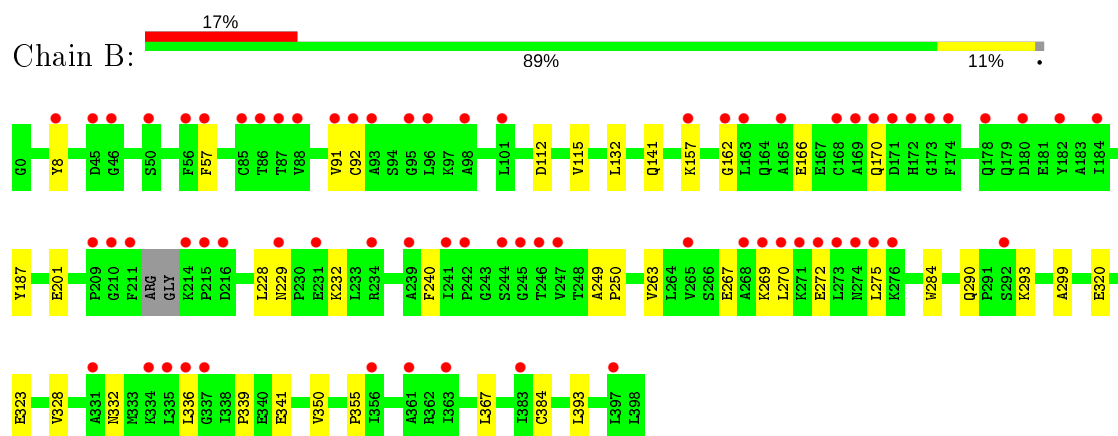
### 3 Residue-property plots [i](#)

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

- Molecule 1: Acetyl-CoA acetyltransferase

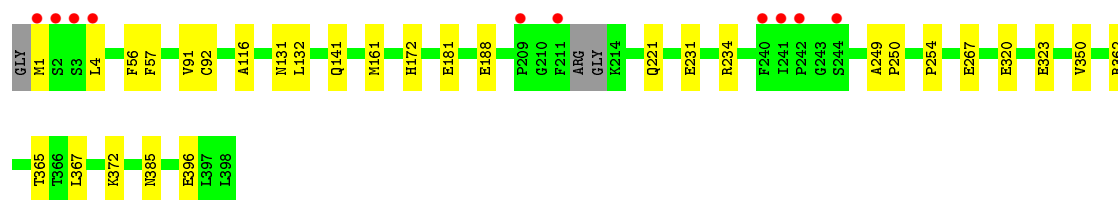


- Molecule 1: Acetyl-CoA acetyltransferase

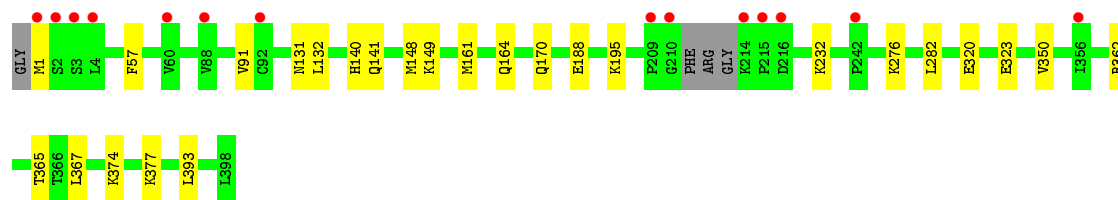
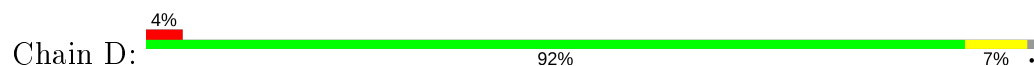


- Molecule 1: Acetyl-CoA acetyltransferase





• 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, $\alpha$ , $\beta$ , $\gamma$	71.44Å 105.41Å 110.42Å 90.00° 108.74° 90.00°	Depositor
Resolution (Å)	36.26 – 1.70 36.26 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (36.26-1.70) 99.9 (36.26-1.70)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 1.70Å)	Xtriage
Refinement program	PHENIX dev_2686	Depositor
R, $R_{free}$	0.165 , 0.200 0.166 , 0.200	Depositor DCC
$R_{free}$ test set	8518 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.7	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 57.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	13073	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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, K, CL

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	0.28	0/2905	0.48	0/3943
1	B	0.29	0/2901	0.49	0/3935
1	C	0.42	0/2952	0.57	0/4007
1	D	0.43	0/2927	0.57	0/3970
All	All	0.36	0/11685	0.53	0/15855

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	355	PRO	Peptide

### 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	2848	0	2904	22	0
1	B	2852	0	2904	20	0
1	C	2885	0	2958	18	0
1	D	2872	0	2933	17	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	1	0
2	D	1	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	4	0	0	0	0
4	C	12	0	16	0	0
4	D	18	0	24	1	0
5	A	172	0	0	7	0
5	B	194	0	0	1	0
5	C	578	0	0	8	2
5	D	625	0	0	9	1
All	All	13073	0	11739	74	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 3.

All (74) 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:C:172:HIS:NE2	5:C:501:HOH:O	2.08	0.86
5:A:640:HOH:O	1:D:148:MET:SD	2.35	0.83
1:D:188:GLU:OE1	5:D:501:HOH:O	2.11	0.69
1:B:299:ALA:HA	1:B:336:LEU:HD21	1.77	0.67
1:A:90:LYS:NZ	5:A:503:HOH:O	2.27	0.67
1:A:299:ALA:HA	1:A:336:LEU:HD21	1.76	0.67
1:C:131[B]:ASN:OD1	5:C:502:HOH:O	2.13	0.67
1:A:4:LEU:N	5:A:504:HOH:O	2.28	0.66
1:A:157:LYS:NZ	1:A:167:GLU:OE1	2.26	0.65
1:D:377[B]:LYS:NZ	5:D:508:HOH:O	2.30	0.65
1:A:132:LEU:HD21	1:C:141:GLN:HG3	1.83	0.60
1:B:323:GLU:HB3	1:B:350:VAL:HG23	1.85	0.59
1:C:1:MET:N	5:C:513:HOH:O	2.38	0.57
1:D:377[B]:LYS:NZ	5:D:510:HOH:O	2.38	0.56
1:A:349:ALA:N	5:A:508:HOH:O	2.36	0.55
1:A:322:ASN:ND2	5:A:502:HOH:O	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ASP:HB3	1:A:148:MET:CE	2.38	0.54
1:A:374:LYS:NZ	5:A:509:HOH:O	2.41	0.54
1:B:162:GLY:HA3	1:B:240:PHE:CZ	2.43	0.53
1:A:187:TYR:HB3	1:A:228:LEU:HD22	1.91	0.52
1:A:141:GLN:HG3	1:C:132:LEU:HD21	1.90	0.52
1:A:148:MET:HE3	1:D:140:HIS:CE1	2.44	0.52
1:D:131:ASN:N	1:D:131:ASN:OD1	2.42	0.52
1:D:232:LYS:NZ	5:D:511:HOH:O	2.42	0.52
1:B:328:VAL:O	1:B:332:ASN:ND2	2.41	0.51
1:C:320:GLU:HG3	1:C:367:LEU:HB2	1.91	0.51
1:C:1:MET:HA	1:C:4:LEU:HD12	1.92	0.51
1:D:320:GLU:HG3	1:D:367:LEU:HB2	1.93	0.51
1:B:270:LEU:HD12	1:B:275:LEU:HB2	1.93	0.51
1:C:181:GLU:OE2	1:C:234:ARG:NH2	2.44	0.50
1:A:145:ASP:HB3	1:A:148:MET:HE3	1.93	0.50
1:B:132:LEU:HD21	1:D:141:GLN:HG3	1.92	0.50
1:C:323:GLU:HB3	1:C:350:VAL:HG23	1.93	0.49
1:A:187:TYR:CD1	1:A:228:LEU:HB2	2.47	0.49
1:B:320:GLU:HG3	1:B:367:LEU:HB2	1.93	0.49
1:B:339:PRO:HB2	1:B:341:GLU:HG2	1.95	0.48
1:C:188:GLU:OE2	5:C:503:HOH:O	2.20	0.48
1:A:282:LEU:HB3	1:A:309:ALA:HB1	1.95	0.47
1:A:45:ASP:OD1	1:A:45:ASP:N	2.47	0.47
1:B:92:CYS:HB2	1:B:384:CYS:O	2.15	0.47
1:B:115:VAL:HG22	1:B:263:VAL:HG22	1.95	0.47
1:D:362:ARG:O	1:D:365[B]:THR:HG22	2.13	0.47
4:D:403:GOL:O3	5:D:503:HOH:O	2.20	0.46
1:D:170:GLN:OE1	5:D:502:HOH:O	2.20	0.46
1:C:372:LYS:HD3	5:C:842:HOH:O	2.16	0.46
1:B:284:TRP:HB3	1:B:393:LEU:HD12	1.97	0.46
1:C:249:ALA:HB3	1:C:250:PRO:HD3	1.97	0.46
1:C:396:GLU:OE2	5:C:504:HOH:O	2.21	0.45
1:B:290[B]:GLN:HB3	1:B:293:LYS:HG3	1.98	0.45
1:A:289:GLN:OE1	1:A:296:THR:HG23	2.17	0.45
1:B:157[B]:LYS:NZ	5:B:513:HOH:O	2.50	0.44
1:D:323:GLU:HB3	1:D:350:VAL:HG23	1.98	0.44
1:B:249:ALA:HB3	1:B:250:PRO:HD3	2.00	0.43
1:C:161:MET:HE1	5:C:833:HOH:O	2.18	0.43
1:B:141:GLN:HG3	1:D:132:LEU:HD21	2.00	0.42
1:B:229:ASN:ND2	1:B:232:LYS:HD2	2.34	0.42
1:B:187:TYR:HB3	1:B:228:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:MET:HA	1:D:164:GLN:OE1	2.18	0.42
2:C:401:CL:CL	5:D:789:HOH:O	2.58	0.42
1:D:1:MET:HG2	1:D:282:LEU:O	2.20	0.42
1:A:131:ASN:N	1:A:131:ASN:OD1	2.53	0.42
1:A:346:HIS:ND1	1:A:370:VAL:HG22	2.34	0.42
1:A:270:LEU:HD12	1:A:275:LEU:HB2	2.01	0.42
1:B:8:TYR:OH	1:B:267:GLU:OE1	2.30	0.42
1:D:149:LYS:NZ	5:D:522:HOH:O	2.52	0.41
1:B:166:GLU:O	1:B:170:GLN:HG3	2.20	0.41
1:A:92:CYS:HB2	1:A:385:ASN:HA	2.03	0.41
1:C:172:HIS:CD2	5:C:501:HOH:O	2.69	0.41
1:A:374:LYS:O	5:A:501:HOH:O	2.21	0.41
1:D:195:LYS:HE3	5:D:833:HOH:O	2.20	0.41
1:B:112:ASP:HB3	1:B:269:LYS:HG3	2.03	0.40
1:C:56:PHE:O	1:C:116:ALA:HA	2.21	0.40
1:C:362:ARG:O	1:C:365[B]:THR:HG22	2.21	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:956:HOH:O	5:D:856:HOH:O[1_455]	2.13	0.07
5:C:599:HOH:O	5:C:772:HOH:O[2_547]	2.15	0.05

## 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	397/399 (100%)	385 (97%)	11 (3%)	1 (0%)	41	24
1	B	395/399 (99%)	385 (98%)	9 (2%)	1 (0%)	41	24
1	C	401/399 (100%)	394 (98%)	6 (2%)	1 (0%)	47	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	398/399 (100%)	391 (98%)	6 (2%)	1 (0%)	41	24
All	All	1591/1596 (100%)	1555 (98%)	32 (2%)	4 (0%)	41	24

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	VAL
1	B	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	293/298 (98%)	288 (98%)	5 (2%)	60	46
1	B	294/298 (99%)	291 (99%)	3 (1%)	76	67
1	C	300/298 (101%)	293 (98%)	7 (2%)	50	33
1	D	297/298 (100%)	293 (99%)	4 (1%)	69	56
All	All	1184/1192 (99%)	1165 (98%)	19 (2%)	62	48

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LYS
1	A	57	PHE
1	A	181	GLU
1	A	186	THR
1	A	211	PHE
1	B	57	PHE
1	B	201	GLU
1	B	272	GLU
1	C	57	PHE
1	C	92	CYS

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Mol	Chain	Res	Type
1	C	221	GLN
1	C	231	GLU
1	C	254	PRO
1	C	267	GLU
1	C	385	ASN
1	D	57	PHE
1	D	276	LYS
1	D	374	LYS
1	D	393	LEU

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 17 are monoatomic - leaving 5 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	C	402	-	5,5,5	1.08	0	5,5,5	0.75	0
4	GOL	D	402	-	5,5,5	1.02	0	5,5,5	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	D	404	-	5,5,5	0.86	0	5,5,5	1.04	0
4	GOL	C	403	-	5,5,5	0.71	0	5,5,5	1.06	1 (20%)
4	GOL	D	403	-	5,5,5	0.71	0	5,5,5	1.09	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	C	402	-	-	0/4/4/4	-
4	GOL	D	402	-	-	0/4/4/4	-
4	GOL	D	404	-	-	0/4/4/4	-
4	GOL	C	403	-	-	4/4/4/4	-
4	GOL	D	403	-	-	1/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	403	GOL	C3-C2-C1	-2.09	103.59	111.70
4	C	403	GOL	C3-C2-C1	-2.06	103.71	111.70

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	403	GOL	C1-C2-C3-O3
4	C	403	GOL	O1-C1-C2-C3
4	C	403	GOL	O1-C1-C2-O2
4	C	403	GOL	O2-C2-C3-O3
4	D	403	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	403	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	395/399 (98%)	1.37	108 (27%) 0 0	28, 62, 95, 127	0
1	B	397/399 (99%)	0.80	69 (17%) 1 1	27, 51, 79, 110	0
1	C	396/399 (99%)	-0.09	10 (2%) 57 61	11, 22, 45, 88	0
1	D	395/399 (98%)	-0.14	14 (3%) 44 49	12, 20, 42, 101	0
All	All	1583/1596 (99%)	0.48	201 (12%) 3 4	11, 36, 83, 127	0

All (201) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	211	PHE	11.8
1	B	211	PHE	9.0
1	A	215	PRO	8.8
1	A	184	ILE	8.3
1	A	213	GLY	8.1
1	A	235	ALA	7.7
1	A	236	ILE	7.6
1	A	245	GLY	7.2
1	A	209	PRO	6.8
1	B	273	LEU	6.7
1	D	215	PRO	6.7
1	D	209	PRO	6.5
1	A	242	PRO	6.4
1	B	209	PRO	6.1
1	B	268	ALA	5.9
1	B	214	LYS	5.8
1	B	335	LEU	5.7
1	B	215	PRO	5.6
1	A	210	GLY	5.6
1	B	88	VAL	5.6
1	B	336	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	168	CYS	5.4
1	A	212	ARG	5.3
1	A	241	ILE	5.3
1	A	373	ALA	5.2
1	A	243	GLY	5.1
1	A	169	ALA	5.1
1	C	211	PHE	5.1
1	A	356	ILE	5.0
1	A	216	ASP	4.9
1	B	168	CYS	4.9
1	A	334	LYS	4.8
1	A	208	LEU	4.8
1	D	2	SER	4.8
1	B	275	LEU	4.6
1	D	210	GLY	4.6
1	A	370	VAL	4.5
1	B	239	ALA	4.5
1	A	336	LEU	4.4
1	A	45	ASP	4.4
1	A	383	ILE	4.3
1	B	246	THR	4.3
1	A	214	LYS	4.2
1	B	174	PHE	4.2
1	D	216	ASP	4.2
1	B	210	GLY	4.2
1	B	241	ILE	4.1
1	A	296	THR	4.1
1	B	242	PRO	4.1
1	A	240	PHE	4.1
1	A	303	PRO	4.1
1	A	180	ASP	4.1
1	B	231	GLU	4.0
1	A	174	PHE	4.0
1	A	172	HIS	4.0
1	D	214	LYS	3.9
1	B	244	SER	3.9
1	B	46	GLY	3.9
1	C	2	SER	3.9
1	A	44	VAL	3.8
1	A	92	CYS	3.8
1	B	171	ASP	3.7
1	A	244	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	93	ALA	3.7
1	B	383	ILE	3.7
1	A	91	VAL	3.7
1	A	200	ASP	3.6
1	A	229	ASN	3.6
1	A	217	VAL	3.6
1	B	93	ALA	3.6
1	D	88[A]	VAL	3.6
1	A	337	GLY	3.5
1	A	302	ILE	3.5
1	A	341	GLU	3.4
1	A	317	ASP	3.4
1	B	45	ASP	3.3
1	A	218	THR	3.3
1	D	1	MET	3.3
1	B	363	ILE	3.3
1	B	173	GLY	3.3
1	A	101	LEU	3.3
1	A	175	SER	3.3
1	B	270	LEU	3.3
1	A	197	GLY	3.2
1	C	241	ILE	3.2
1	D	4	LEU	3.2
1	A	335	LEU	3.2
1	B	8	TYR	3.2
1	A	338	ILE	3.1
1	A	345	LEU	3.1
1	A	342	LYS	3.1
1	A	228	LEU	3.1
1	A	339	PRO	3.1
1	C	3	SER	3.0
1	B	87	THR	3.0
1	A	173	GLY	3.0
1	B	337	GLY	3.0
1	A	165	ALA	3.0
1	A	234	ARG	2.9
1	A	181	GLU	2.9
1	D	242	PRO	2.9
1	B	271	LYS	2.9
1	B	229	ASN	2.9
1	A	249	ALA	2.9
1	A	318	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	8	TYR	2.8
1	A	248	THR	2.8
1	A	177	GLU	2.8
1	A	330	LEU	2.8
1	B	96	LEU	2.8
1	B	163	LEU	2.8
1	A	88	VAL	2.8
1	B	356	ILE	2.7
1	A	278	VAL	2.7
1	C	4	LEU	2.7
1	B	245	GLY	2.7
1	B	165	ALA	2.7
1	A	48	LYS	2.7
1	C	244	SER	2.7
1	B	331	ALA	2.7
1	B	247	VAL	2.7
1	B	169	ALA	2.6
1	A	187	TYR	2.6
1	B	157[A]	LYS	2.6
1	B	56	PHE	2.6
1	B	272	GLU	2.6
1	A	321	ILE	2.6
1	B	397	LEU	2.6
1	A	238	PRO	2.6
1	B	216	ASP	2.6
1	B	95	GLY	2.6
1	A	273	LEU	2.6
1	B	170	GLN	2.6
1	C	209	PRO	2.6
1	B	234	ARG	2.5
1	A	195	LYS	2.5
1	B	57	PHE	2.5
1	C	242	PRO	2.5
1	A	117	GLY	2.5
1	B	184	ILE	2.5
1	B	101	LEU	2.5
1	B	276	LYS	2.5
1	A	87	THR	2.5
1	A	275	LEU	2.5
1	A	183	ALA	2.5
1	A	50	SER	2.5
1	A	96	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	178	GLN	2.4
1	A	299	ALA	2.4
1	A	219	VAL	2.4
1	A	316	ILE	2.4
1	B	274	ASN	2.4
1	A	398	LEU	2.4
1	D	3	SER	2.4
1	A	239	ALA	2.4
1	A	194	GLN	2.4
1	A	270	LEU	2.3
1	B	92	CYS	2.3
1	A	290[A]	GLN	2.3
1	B	172	HIS	2.3
1	A	176	ARG	2.3
1	A	192	ALA	2.3
1	C	240	PHE	2.3
1	D	92	CYS	2.3
1	C	1	MET	2.3
1	A	98	ALA	2.2
1	A	378	LEU	2.2
1	A	57	PHE	2.2
1	B	50	SER	2.2
1	B	292	SER	2.2
1	A	86	THR	2.2
1	A	207	GLN	2.2
1	B	269	LYS	2.2
1	A	47	LEU	2.2
1	A	326[A]	SER	2.2
1	A	376	GLY	2.2
1	A	60	VAL	2.2
1	A	188	GLU	2.2
1	B	334	LYS	2.2
1	A	295	THR	2.1
1	B	86	THR	2.1
1	B	361	ALA	2.1
1	A	162	GLY	2.1
1	B	91	VAL	2.1
1	D	60	VAL	2.1
1	A	237	LYS	2.1
1	D	356	ILE	2.1
1	B	180	ASP	2.1
1	A	246	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	247	VAL	2.1
1	A	315	ALA	2.0
1	A	171	ASP	2.0
1	A	328	VAL	2.0
1	A	384	CYS	2.0
1	B	85	CYS	2.0
1	A	277	PRO	2.0
1	B	162	GLY	2.0
1	B	98	ALA	2.0
1	B	182	TYR	2.0
1	B	265	VAL	2.0
1	A	4	LEU	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 monosaccharides 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, 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
3	K	A	404	1/1	0.67	0.07	68,68,68,68	0
4	GOL	D	404	6/6	0.81	0.15	50,57,61,64	0
3	K	B	403	1/1	0.84	0.06	57,57,57,57	0
3	K	B	404	1/1	0.88	0.15	77,77,77,77	0
3	K	A	403	1/1	0.90	0.22	69,69,69,69	0
4	GOL	D	403	6/6	0.91	0.21	33,43,50,54	0
4	GOL	C	403	6/6	0.91	0.16	33,53,57,61	0
4	GOL	C	402	6/6	0.92	0.12	25,33,46,48	0
2	CL	B	401	1/1	0.93	0.14	48,48,48,48	1
4	GOL	D	402	6/6	0.94	0.07	22,30,39,42	0
3	K	B	402	1/1	0.95	0.05	42,42,42,42	0

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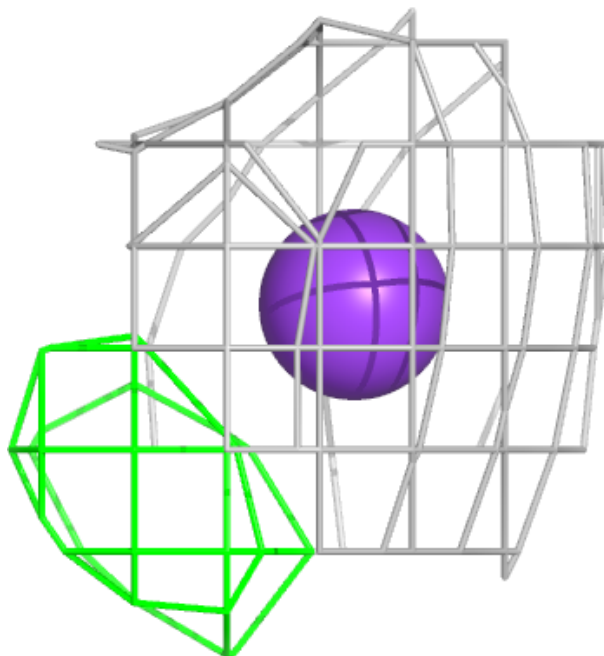
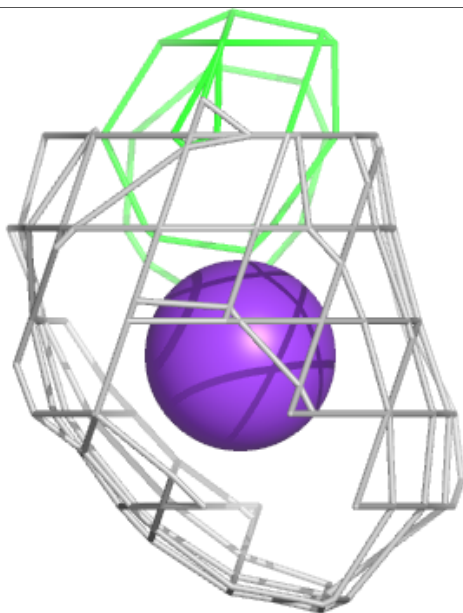
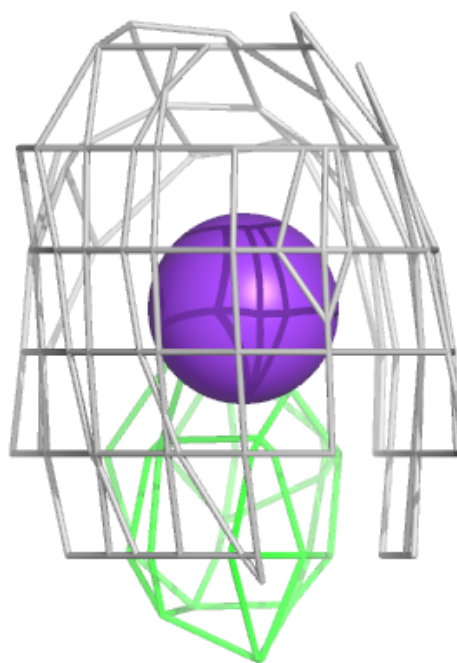
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	K	D	408	1/1	0.95	0.06	36,36,36,36	1
2	CL	A	401	1/1	0.96	0.22	58,58,58,58	1
3	K	A	402	1/1	0.97	0.05	39,39,39,39	1
2	CL	D	401	1/1	0.97	0.16	22,22,22,22	1
3	K	D	406	1/1	0.99	0.06	20,20,20,20	0
3	K	C	406	1/1	0.99	0.04	23,23,23,23	0
3	K	C	404	1/1	0.99	0.06	20,20,20,20	0
2	CL	C	401	1/1	0.99	0.12	23,23,23,23	1
3	K	D	407	1/1	0.99	0.07	21,21,21,21	1
3	K	C	405	1/1	0.99	0.06	20,20,20,20	0
3	K	D	405	1/1	1.00	0.06	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 K A 404:**

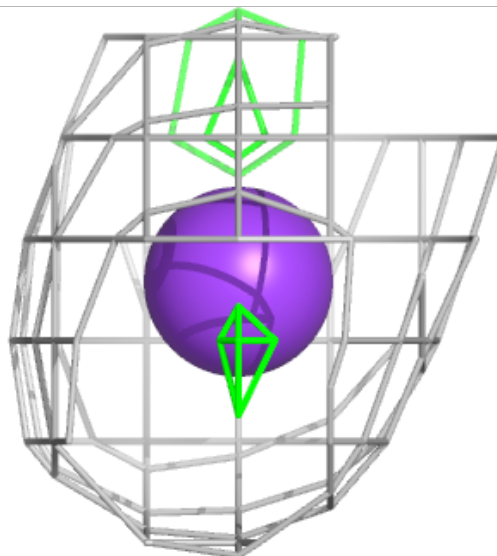
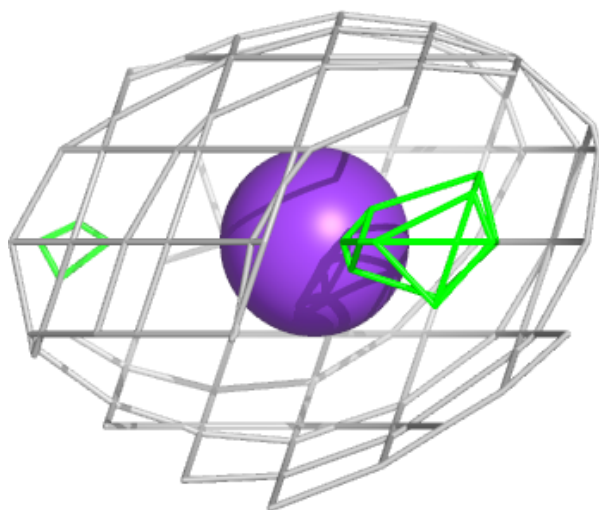
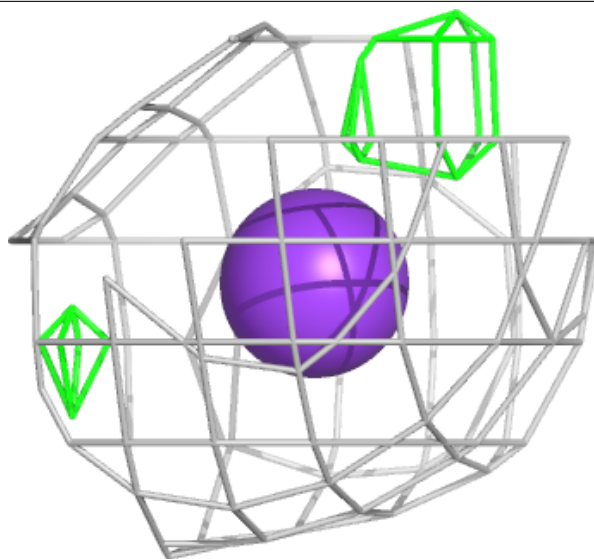
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





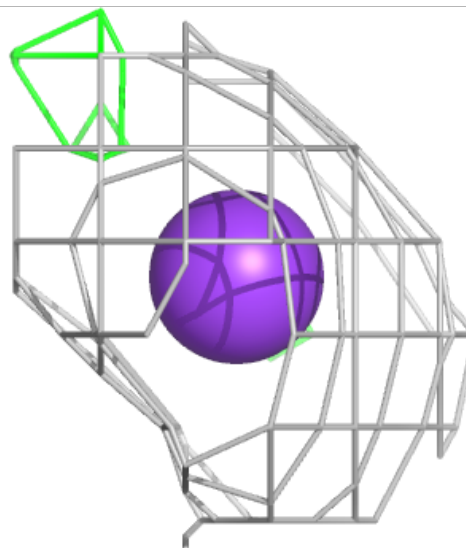
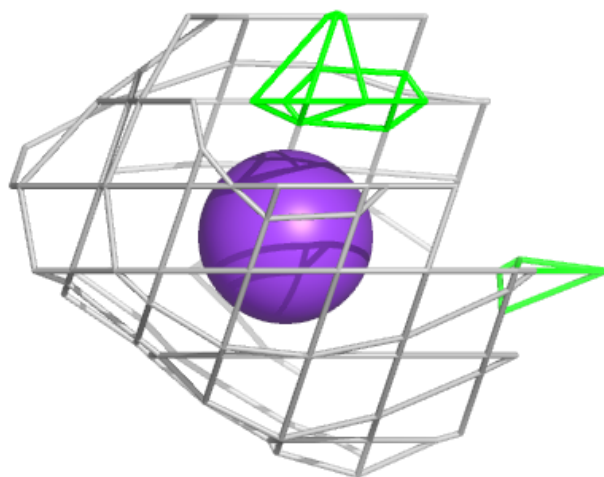
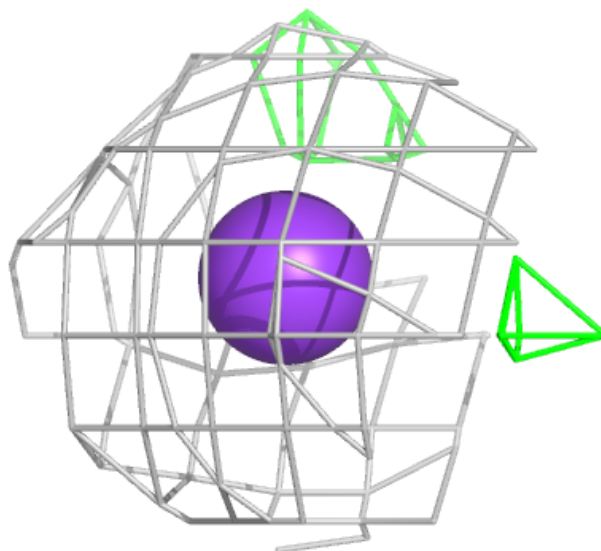
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and green (positive)



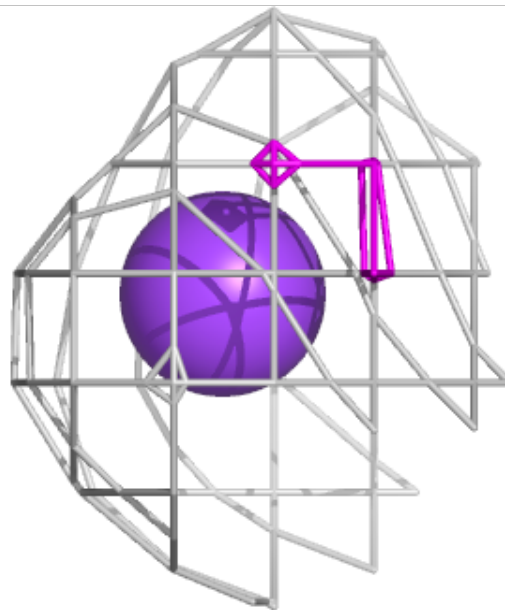
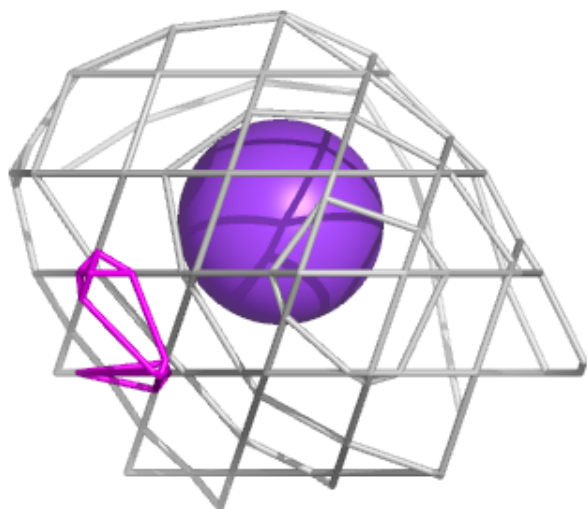
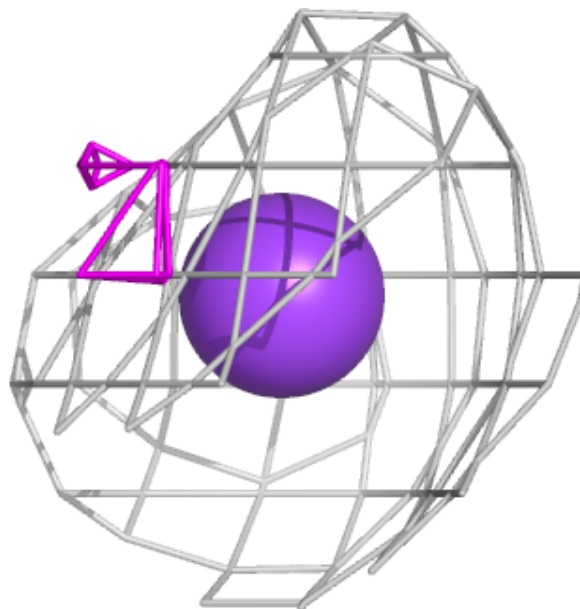
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and green (positive)



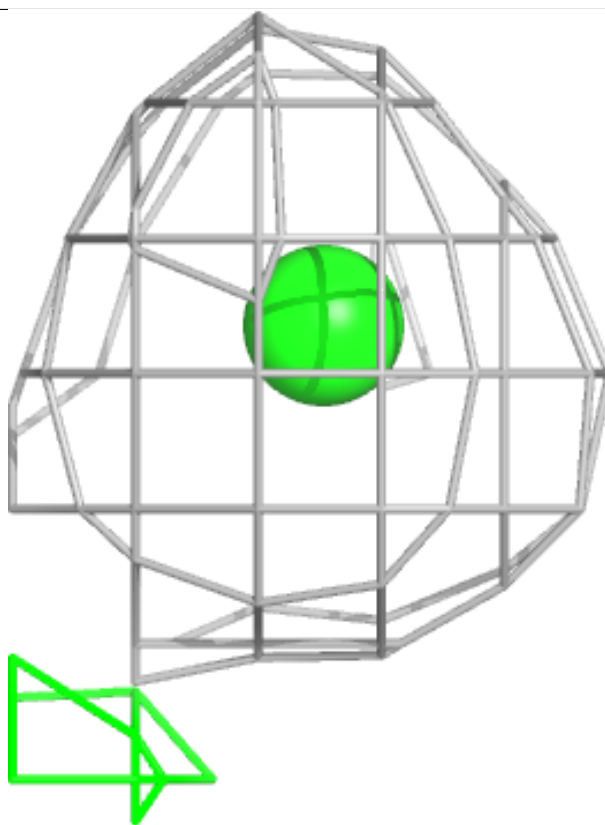
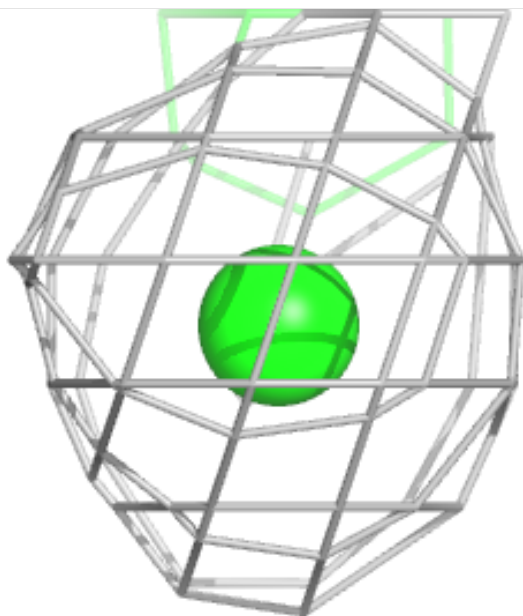
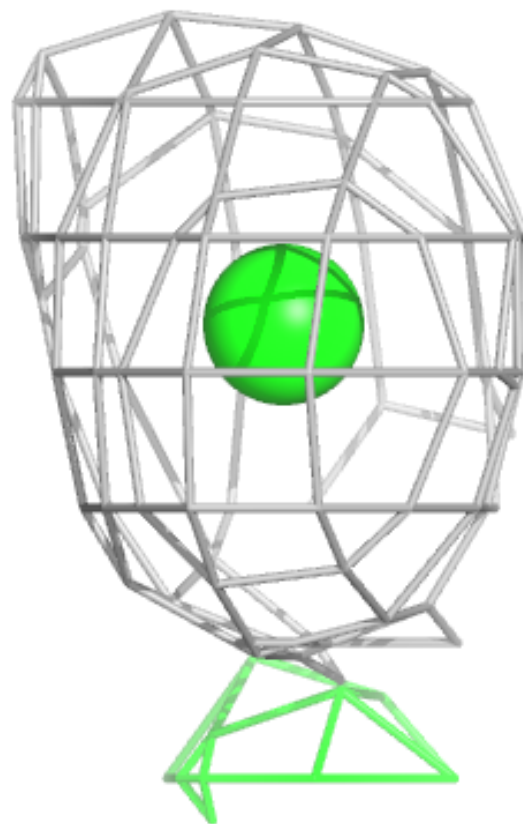
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and green (positive)



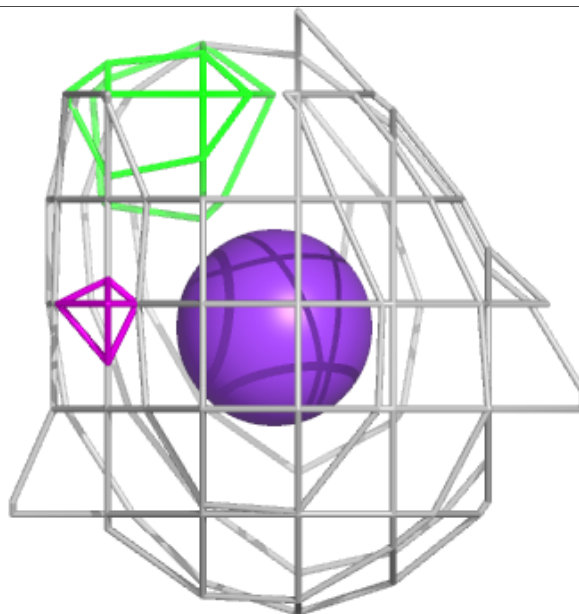
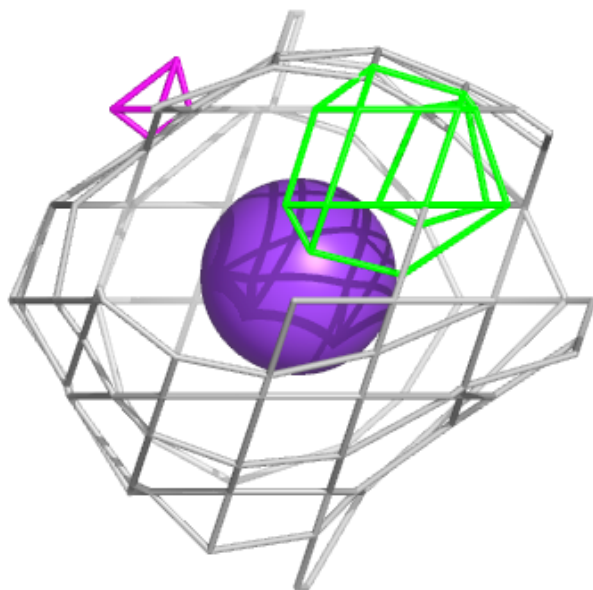
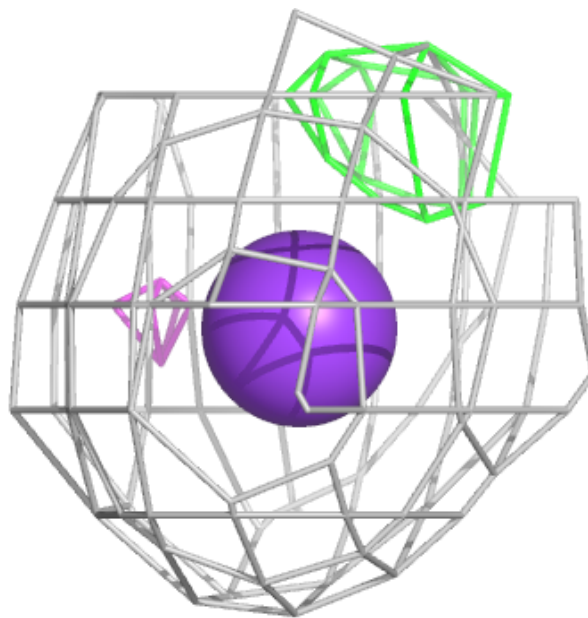
**Electron density around CL B 401:**

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



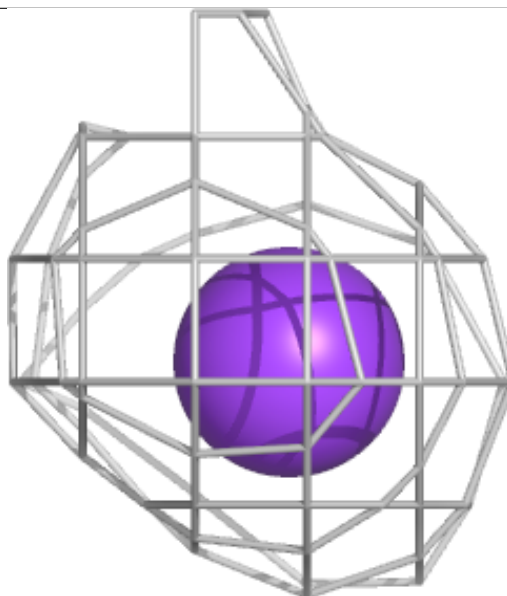
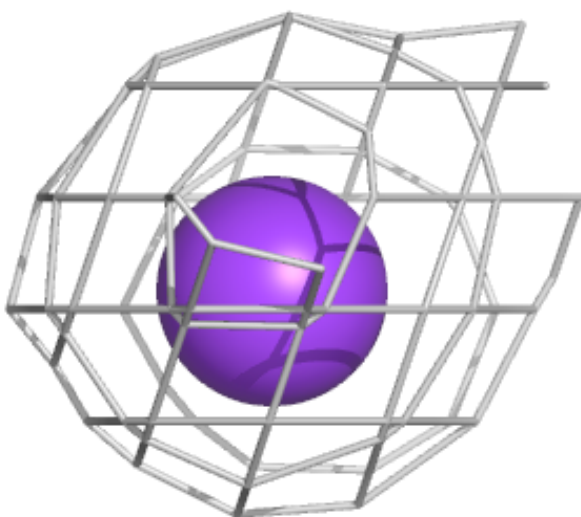
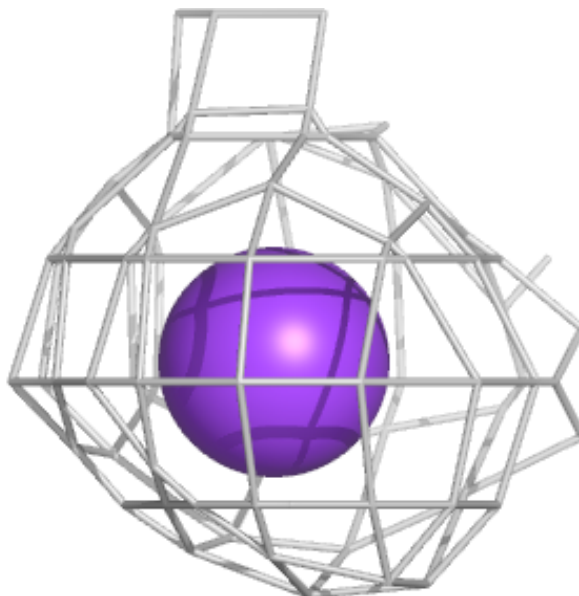
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and green (positive)



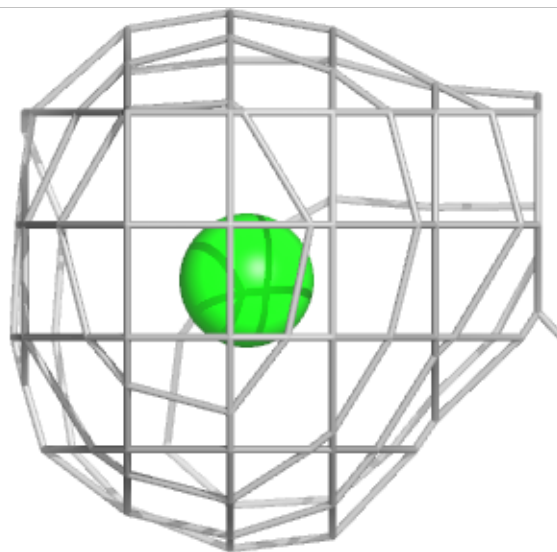
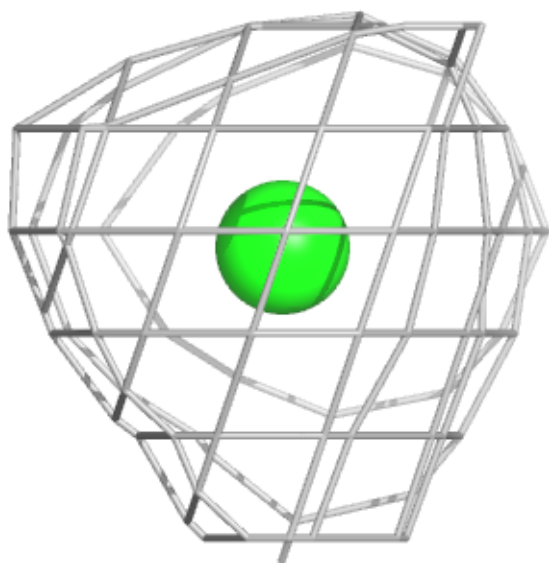
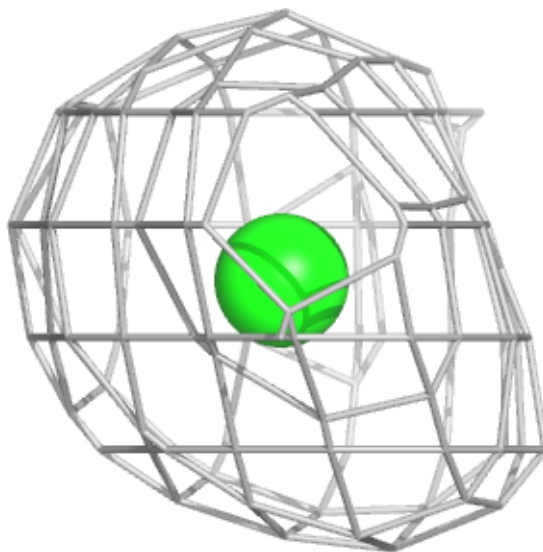
**Electron density around K D 408:**

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



**Electron density around CL A 401:**

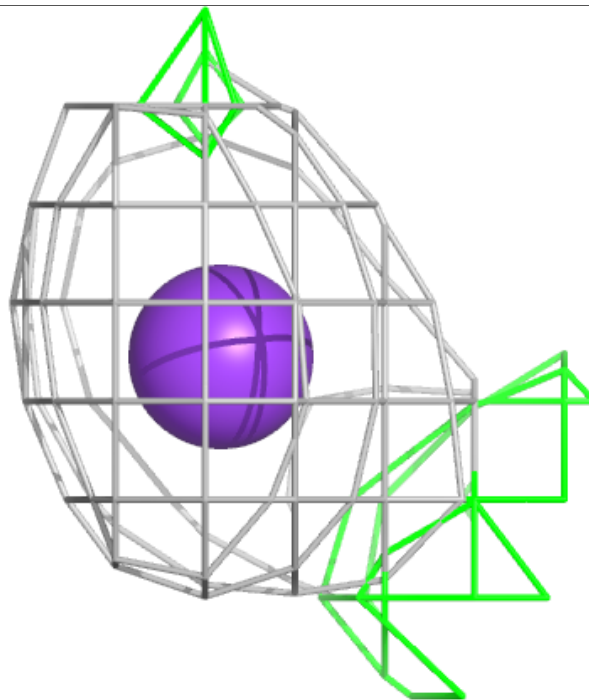
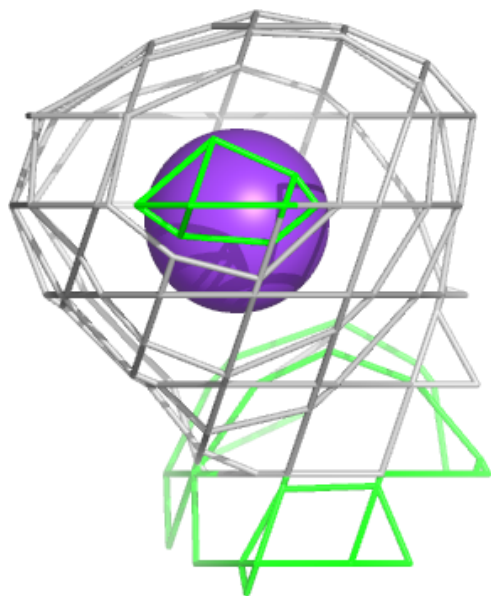
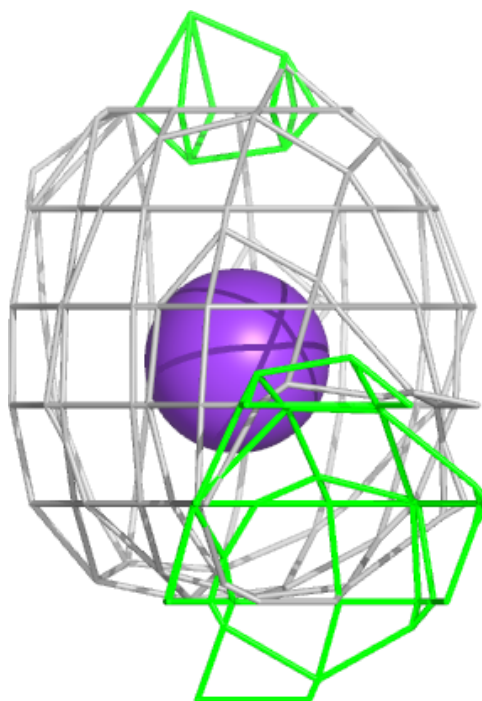
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and green (positive)





**Electron density around K A 402:**

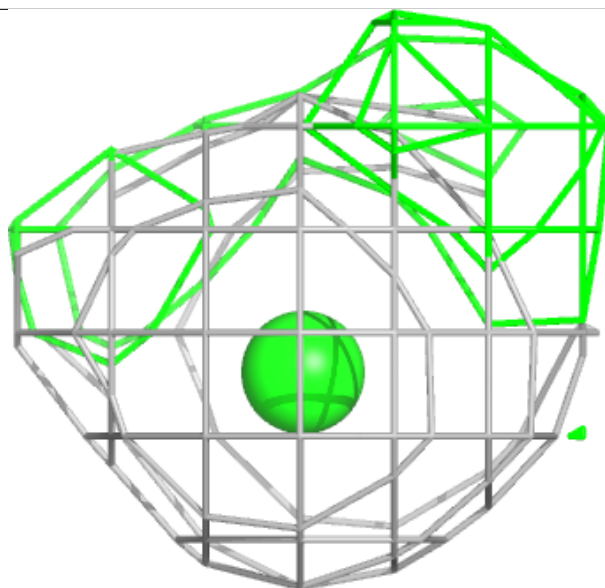
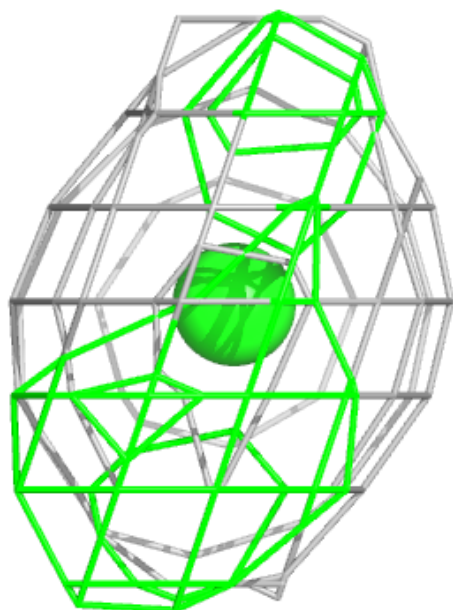
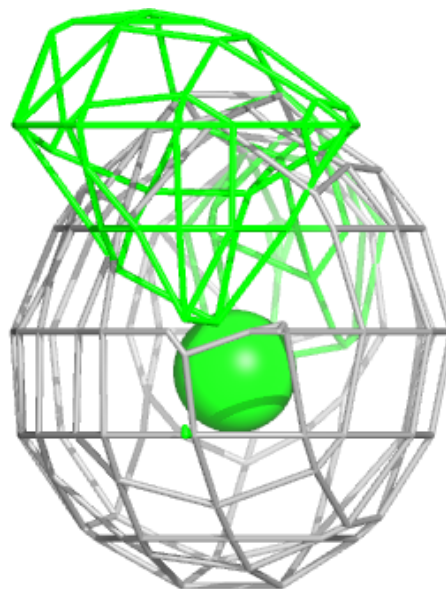
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





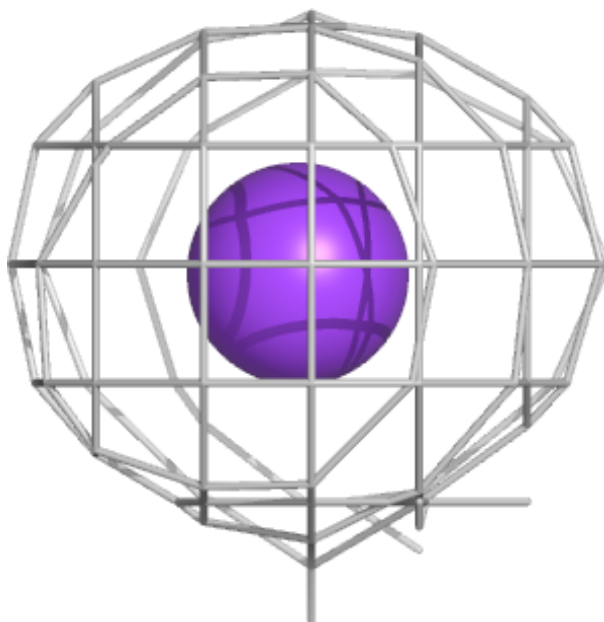
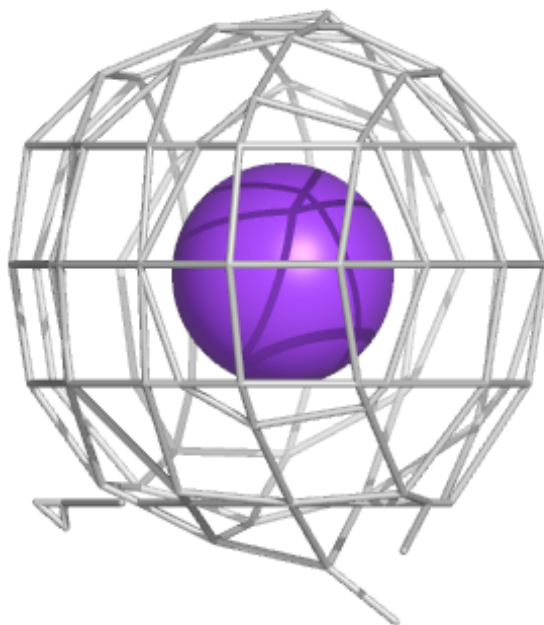
**Electron density around CL D 401:**

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



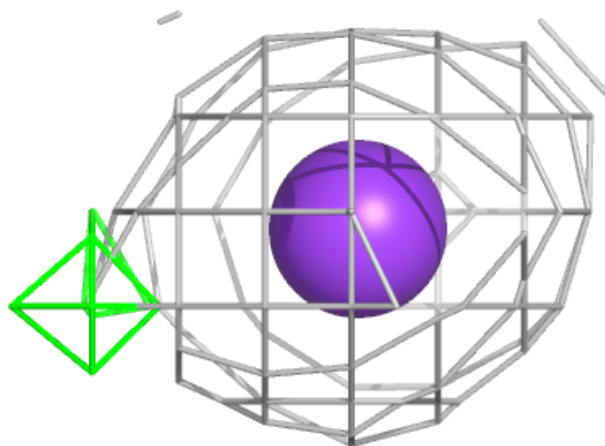
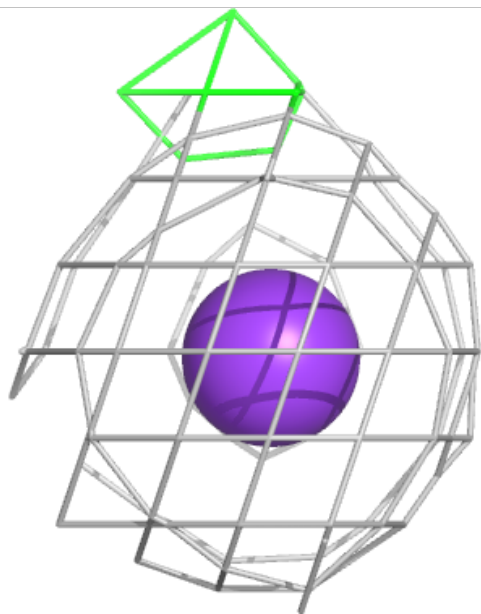
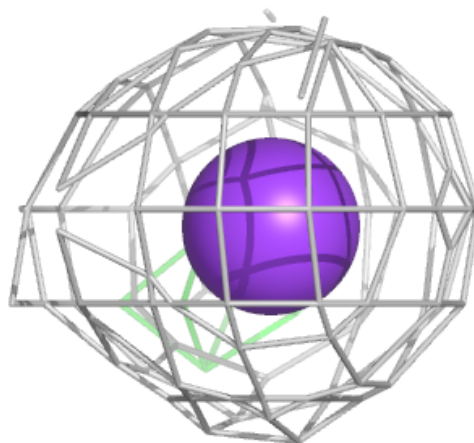
**Electron density around K D 406:**

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



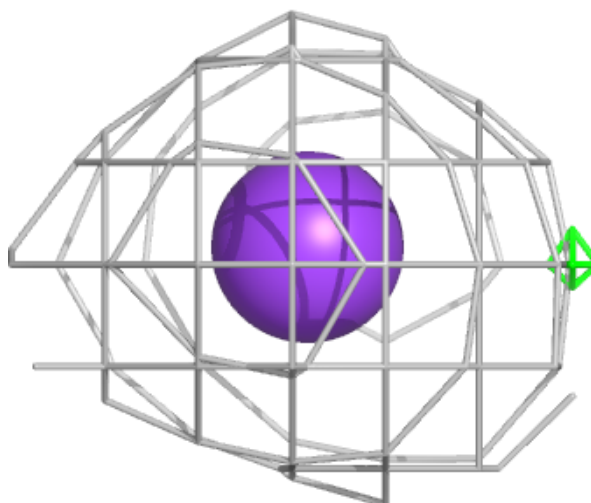
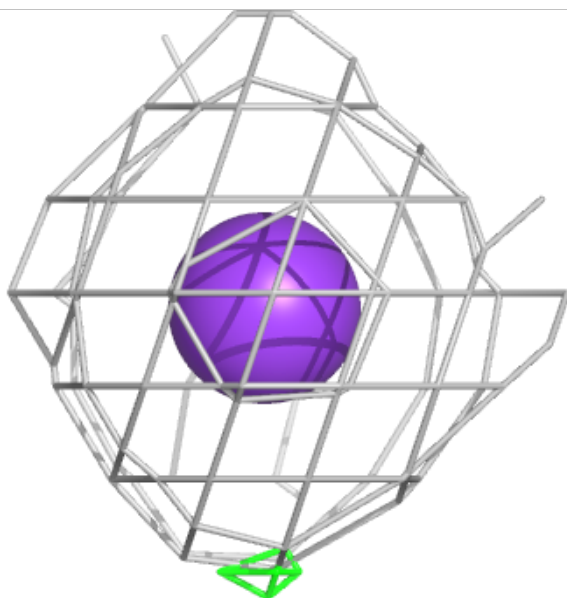
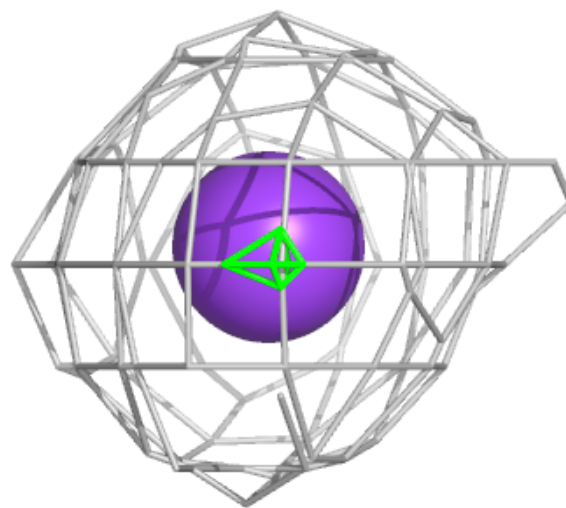
**Electron density around K C 406:**

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



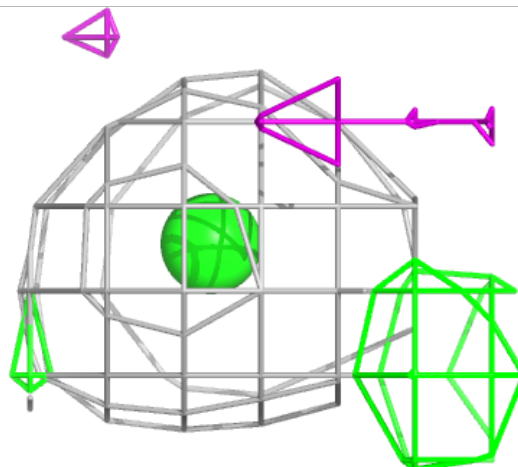
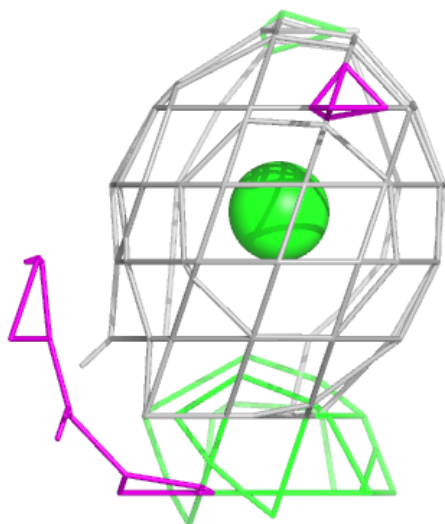
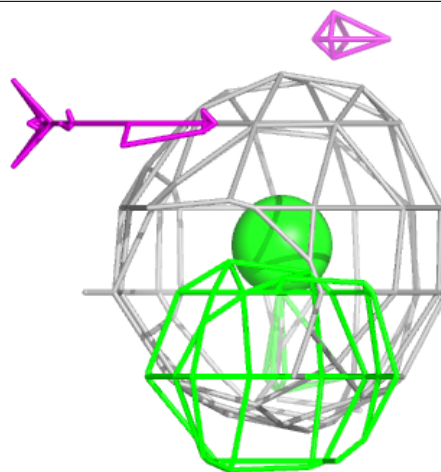
**Electron density around K C 404:**

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



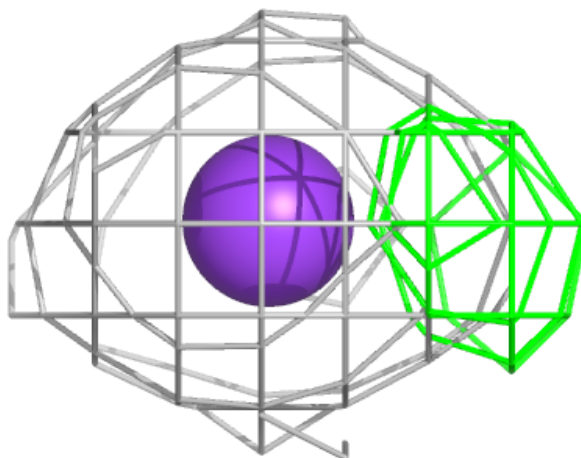
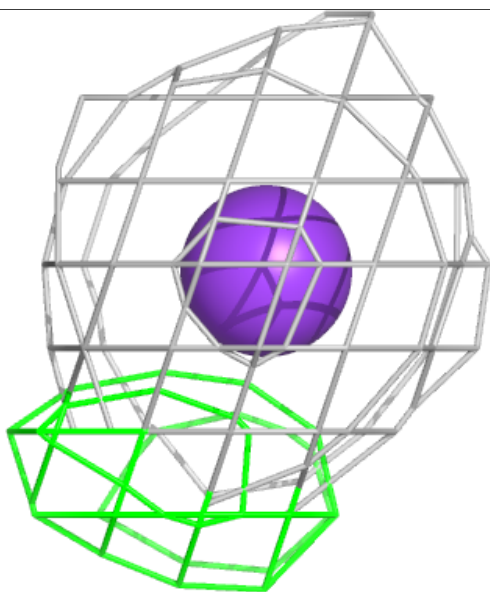
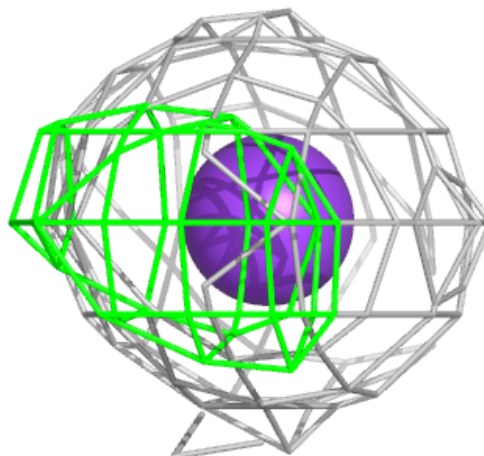
**Electron density around CL C 401:**

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



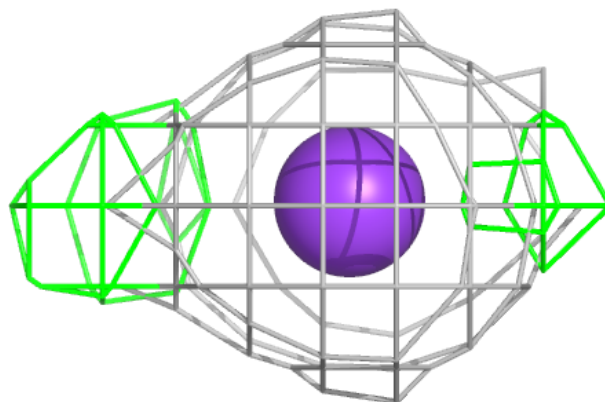
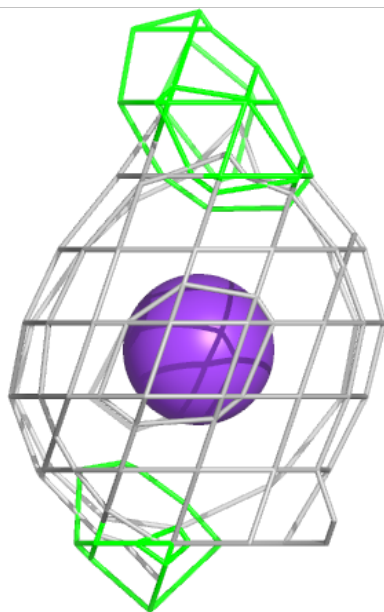
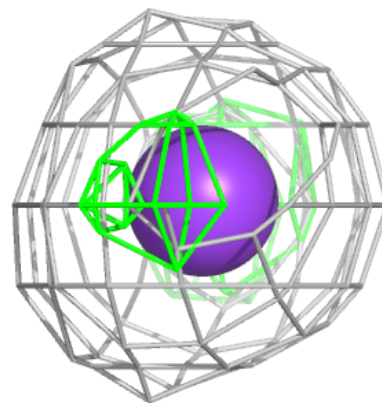
**Electron density around K D 407:**

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

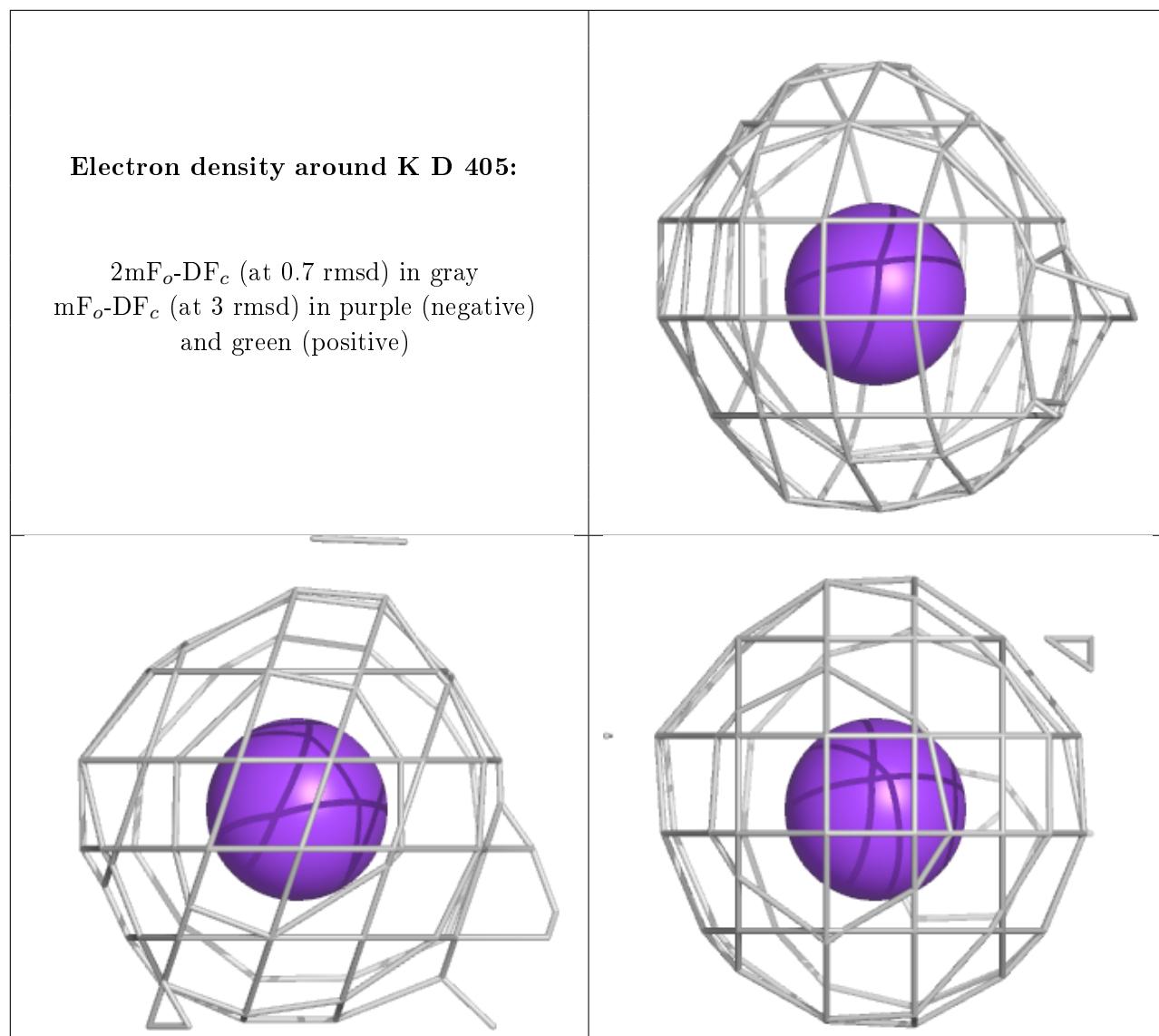


**Electron density around K C 405:**

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







## 6.5 Other polymers [i](#)

There are no such residues in this entry.