



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:21 AM UTC

PDB ID : 7FF8 / pdb\_00007ff8  
Title : Pseudomonas aeruginosa Virulence Factor Regulator with cAMP ligand and Cl(triethylphosphine)gold(I)  
Authors : Chew, B.L.A.; Luo, D.  
Deposited on : 2021-07-22  
Resolution : 2.80 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)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

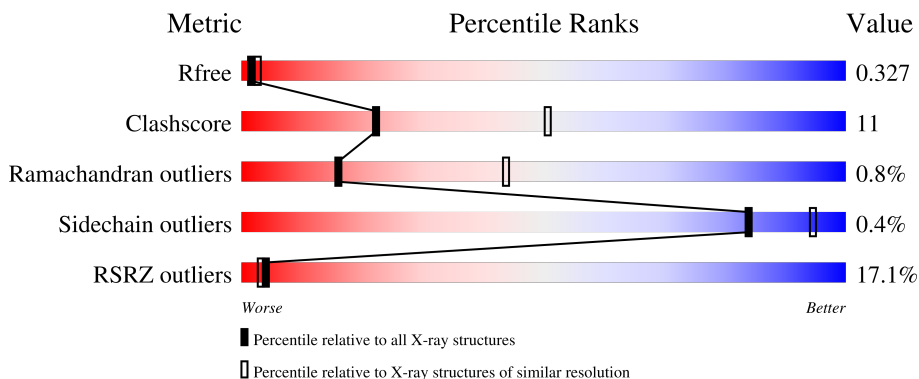
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	210	
1	B	210	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 2924 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.

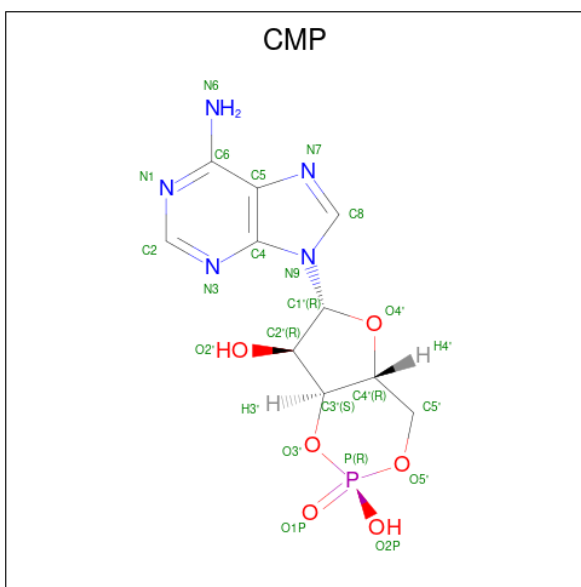
- Molecule 1 is a protein called cAMP-activated global transcriptional regulator Vfr.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	197	Total 1462	C 924	N 254	O 274	S 10	0	0	0
1	B	188	Total 1375	C 869	N 243	O 255	S 8	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	85	GLU	GLN	conflict	UNP P55222
B	85	GLU	GLN	conflict	UNP P55222

- Molecule 2 is ADENOSINE-3',5'-CYCLIC-MONOPHOSPHATE (CCD ID: CMP) (formula: C<sub>10</sub>H<sub>12</sub>N<sub>5</sub>O<sub>6</sub>P) (labeled as "Ligand of Interest" by depositor).



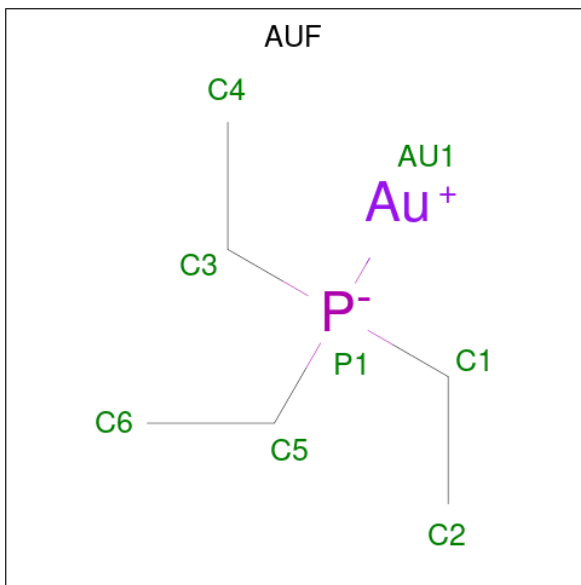
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 22	C 10	N 5	O 6	P 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	B	1	22	10	5	6	1	0	0

- Molecule 3 is triethylphosphanuidylgold(1+) (CCD ID: AUF) (formula: C<sub>6</sub>H<sub>15</sub>AuP) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Au	C	P		
3	A	1	8	1	6	1	0	0
3	B	1	8	1	6	1	0	0

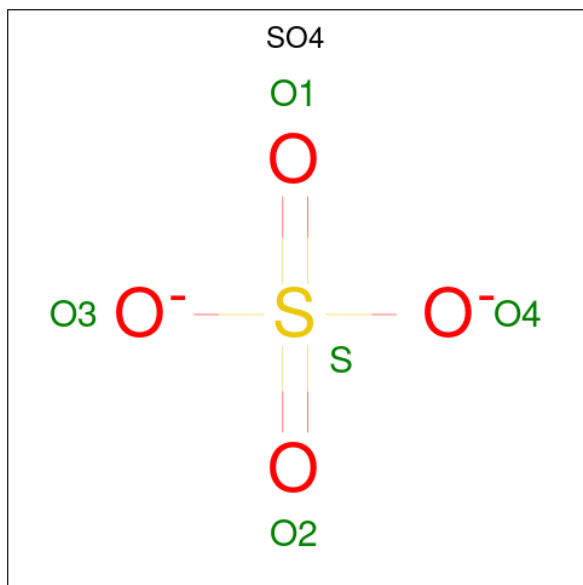
- Molecule 4 is GOLD ION (CCD ID: AU) (formula: Au) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Au		
4	A	2	2	2	0	0
4	B	3	3	3	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0
5	B	1	Total Cl 1 1	0	0

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.26Å 49.93Å 62.38Å 90.00° 100.14° 90.00°	Depositor
Resolution (Å)	34.52 – 2.80 34.52 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.52-2.80) 92.7 (34.52-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.08 (at 2.81Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.269 , 0.327 0.271 , 0.327	Depositor DCC
$R_{free}$ test set	560 reflections (5.24%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.3	Xtrriage
Anisotropy	0.418	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 64.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	2924	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.35% 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: CMP, SO4, AUF, AU, 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	0.58	5/1479 (0.3%)	0.79	6/1997 (0.3%)
1	B	0.43	1/1391 (0.1%)	0.67	2/1879 (0.1%)
All	All	0.51	6/2870 (0.2%)	0.74	8/3876 (0.2%)

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	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	158	GLN	C-N	-9.78	1.24	1.34
1	A	162	MET	SD-CE	9.39	2.03	1.79
1	A	190	ARG	CB-CG	-8.46	1.27	1.52
1	A	202	HIS	CG-CD2	7.97	1.44	1.35
1	A	162	MET	CB-CG	5.68	1.69	1.52
1	A	190	ARG	CZ-NH2	-5.37	1.26	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	MET	CA-CB-CG	11.64	137.39	114.10
1	A	190	ARG	CG-CD-NE	-10.92	87.98	112.00
1	A	190	ARG	NE-CZ-NH2	-8.90	111.19	119.20
1	B	101	GLU	CA-CB-CG	6.70	127.50	114.10
1	B	200	LEU	CA-CB-CG	6.28	138.29	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	ARG	NE-CZ-NH1	6.25	127.75	121.50
1	A	162	MET	CB-CG-SD	5.12	128.07	112.70
1	A	190	ARG	N-CA-CB	-5.01	102.81	110.07

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	101	GLU	Sidechain,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	1462	0	1414	32	0
1	B	1375	0	1313	29	0
2	A	22	0	11	1	0
2	B	22	0	11	2	0
3	A	8	0	0	0	0
3	B	8	0	0	1	0
4	A	2	0	0	0	0
4	B	3	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	10	0	0	0	0
6	B	10	0	0	0	0
All	All	2924	0	2749	58	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (58) 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)
2:A:301:CMP:H2	2:A:301:CMP:C2	0.97	1.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:302:CMP:H2	2:B:302:CMP:C2	0.97	1.48
1:A:162:MET:SD	1:A:162:MET:CE	2.03	1.46
1:A:190:ARG:HG3	1:A:190:ARG:NH1	1.91	0.82
1:B:21:HIS:HA	1:B:101:GLU:HG3	1.62	0.79
1:B:156:CYS:SG	3:B:303:AUF:C1	2.70	0.79
1:B:150:ARG:HG2	1:B:154:ASP:OD1	1.82	0.79
1:A:190:ARG:O	1:A:194:SER:N	2.14	0.77
1:A:71:PHE:O	1:A:128:ARG:NH1	2.18	0.77
1:B:74:GLU:HG3	1:B:121:LEU:HD21	1.73	0.71
1:A:148:VAL:HB	1:A:191:VAL:HG11	1.74	0.69
1:B:71:PHE:O	1:B:128:ARG:NH1	2.24	0.66
1:B:150:ARG:O	1:B:154:ASP:N	2.26	0.66
1:B:60:GLU:OE1	1:B:92:ARG:NH1	2.27	0.65
1:A:55:ASP:N	1:A:55:ASP:OD1	2.24	0.63
1:A:54:GLU:O	1:B:134:ARG:NH2	2.34	0.60
1:A:61:MET:HE1	1:B:136:VAL:HG12	1.87	0.56
1:A:191:VAL:O	1:A:195:LEU:HG	2.05	0.56
1:A:150:ARG:HG3	1:A:154:ASP:OD1	2.06	0.56
1:A:114:ASP:OD2	1:A:116:GLU:N	2.28	0.54
1:A:139:LEU:HD23	1:A:147:ARG:HD2	1.89	0.54
1:B:139:LEU:HD22	1:B:147:ARG:HD3	1.89	0.54
1:B:95:VAL:HG12	1:B:96:GLU:H	1.72	0.53
1:B:54:GLU:HB2	1:B:90:TRP:CZ3	2.43	0.53
1:A:143:ASP:O	1:A:147:ARG:HG3	2.10	0.52
1:B:41:LEU:O	1:B:102:ILE:N	2.39	0.52
1:A:138:ASP:O	1:A:142:LEU:HB2	2.10	0.52
1:B:194:SER:O	1:B:198:GLN:HG3	2.10	0.52
1:A:136:VAL:HG22	1:B:136:VAL:HG22	1.92	0.51
1:A:119:TYR:CE1	1:B:118:LEU:HD21	2.45	0.51
1:B:36:ASP:O	1:B:87:ARG:HG2	2.13	0.49
1:A:192:LEU:HB3	1:A:203:VAL:HG21	1.94	0.48
1:B:132:THR:O	1:B:136:VAL:HG23	2.14	0.47
1:A:190:ARG:HG3	1:A:190:ARG:HH11	1.78	0.47
1:B:140:ALA:O	1:B:141:PHE:HB2	2.14	0.47
1:A:54:GLU:HA	1:A:59:ARG:O	2.15	0.47
1:A:101:GLU:HG3	1:A:102:ILE:N	2.30	0.46
1:B:69:GLY:O	1:B:124:GLN:NE2	2.48	0.46
1:B:74:GLU:OE1	2:B:302:CMP:O2'	2.32	0.46
1:A:168:MET:HE3	1:A:168:MET:HB3	1.81	0.45
1:A:190:ARG:NH1	1:A:190:ARG:CG	2.69	0.45
1:A:53:ILE:O	1:A:61:MET:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:HIS:O	1:B:21:HIS:N	2.50	0.45
1:A:129:LEU:HD23	1:B:75:LEU:HD11	1.99	0.45
1:B:188:VAL:O	1:B:192:LEU:HG	2.17	0.44
1:A:106:LYS:O	1:A:110:LEU:HG	2.19	0.42
1:B:162:MET:N	1:B:169:GLN:O	2.50	0.42
1:A:114:ASP:CG	1:A:116:GLU:HG2	2.45	0.42
1:A:72:PHE:CE1	1:A:91:VAL:HG11	2.55	0.41
1:A:74:GLU:N	1:A:74:GLU:OE2	2.50	0.41
1:A:67:ASN:O	1:A:70:ASP:HB2	2.19	0.41
1:A:114:ASP:OD2	1:A:116:GLU:HG2	2.20	0.41
1:A:114:ASP:OD2	1:A:115:SER:N	2.54	0.41
1:A:159:PRO:O	1:A:160:ASP:HB2	2.20	0.41
1:B:117:ILE:HD12	1:B:117:ILE:HA	1.96	0.41
1:B:151:THR:HA	1:B:154:ASP:HB2	2.02	0.41
1:B:201:VAL:HA	1:B:209:VAL:O	2.20	0.41
1:B:38:CYS:SG	1:B:87:ARG:NH1	2.84	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	193/210 (92%)	180 (93%)	13 (7%)	0	100	100
1	B	182/210 (87%)	173 (95%)	6 (3%)	3 (2%)	7	27
All	All	375/420 (89%)	353 (94%)	19 (5%)	3 (1%)	16	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	21	HIS
1	B	39	GLU

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Mol	Chain	Res	Type
1	B	20	CYS

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	145/181 (80%)	144 (99%)	1 (1%)	76	91
1	B	132/181 (73%)	132 (100%)	0	100	100
All	All	277/362 (76%)	276 (100%)	1 (0%)	84	94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	190	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 15 ligands modelled in this entry, 7 are monoatomic - leaving 8 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
6	SO4	B	307	-	4,4,4	0.23	0	6,6,6	0.07	0
2	CMP	A	301	-	25,25,25	1.75	8 (32%)	37,39,39	1.97	10 (27%)
3	AUF	A	302	-	6,7,7	0.74	0	6,9,9	1.34	1 (16%)
6	SO4	A	306	-	4,4,4	0.24	0	6,6,6	0.08	0
3	AUF	B	303	-	6,7,7	0.97	0	6,9,9	1.32	1 (16%)
6	SO4	A	307	-	4,4,4	0.24	0	6,6,6	0.08	0
6	SO4	B	308	-	4,4,4	0.25	0	6,6,6	0.08	0
2	CMP	B	302	-	25,25,25	1.75	8 (32%)	37,39,39	1.97	10 (27%)

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
3	AUF	A	302	-	-	2/6/9/9	-
2	CMP	B	302	-	-	0/4/31/31	0/4/4/4
3	AUF	B	303	-	-	4/6/9/9	-
2	CMP	A	301	-	-	0/4/31/31	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	CMP	C5-C4	4.71	1.47	1.39
2	B	302	CMP	C5-C4	4.70	1.47	1.39
2	B	302	CMP	P-O3'	3.00	1.62	1.57
2	A	301	CMP	P-O5'	2.99	1.61	1.57
2	B	302	CMP	P-O5'	2.99	1.61	1.57
2	A	301	CMP	P-O3'	2.98	1.62	1.57
2	A	301	CMP	C5-C6	2.72	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	302	CMP	C5-C6	2.71	1.48	1.41
2	B	302	CMP	C8-N7	2.35	1.36	1.31
2	A	301	CMP	C8-N7	2.31	1.36	1.31
2	A	301	CMP	C5-N7	-2.26	1.35	1.39
2	B	302	CMP	C5-N7	-2.25	1.35	1.39
2	A	301	CMP	O5'-C5'	-2.16	1.43	1.46
2	B	302	CMP	O5'-C5'	-2.14	1.43	1.46
2	A	301	CMP	O3'-C3'	-2.11	1.41	1.44
2	B	302	CMP	O3'-C3'	-2.08	1.41	1.44

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	302	CMP	C5-C4-N3	-5.84	118.67	126.72
2	A	301	CMP	C5-C4-N3	-5.80	118.73	126.72
2	B	302	CMP	N3-C4-N9	4.60	134.99	127.17
2	A	301	CMP	N3-C4-N9	4.59	134.98	127.17
2	B	302	CMP	C2-N3-C4	3.73	120.93	111.83
2	A	301	CMP	C2-N3-C4	3.68	120.82	111.83
2	A	301	CMP	C4-C5-N7	-3.43	106.67	110.58
2	B	302	CMP	C4-C5-N7	-3.42	106.68	110.58
2	B	302	CMP	N3-C2-N1	-3.29	123.61	128.58
2	B	302	CMP	O2P-P-O1P	3.26	118.57	108.56
2	A	301	CMP	O2P-P-O1P	3.26	118.57	108.56
2	A	301	CMP	N3-C2-N1	-3.24	123.68	128.58
2	A	301	CMP	C4-N9-C8	2.59	108.45	105.74
2	A	301	CMP	C5-N7-C8	2.52	107.42	103.45
2	B	302	CMP	C4-N9-C8	2.52	108.38	105.74
2	B	302	CMP	C5-N7-C8	2.49	107.37	103.45
3	B	303	AUF	C1-P1-C3	2.41	125.26	103.72
2	B	302	CMP	O3'-C3'-C2'	2.13	117.69	115.61
2	A	301	CMP	O3'-C3'-C2'	2.08	117.64	115.61
2	B	302	CMP	C6-C5-N7	2.07	136.08	132.09
2	A	301	CMP	C6-C5-N7	2.05	136.05	132.09
3	A	302	AUF	C1-P1-C3	2.00	121.59	103.72

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	303	AUF	C6-C5-P1-C3
3	A	302	AUF	C2-C1-P1-C3

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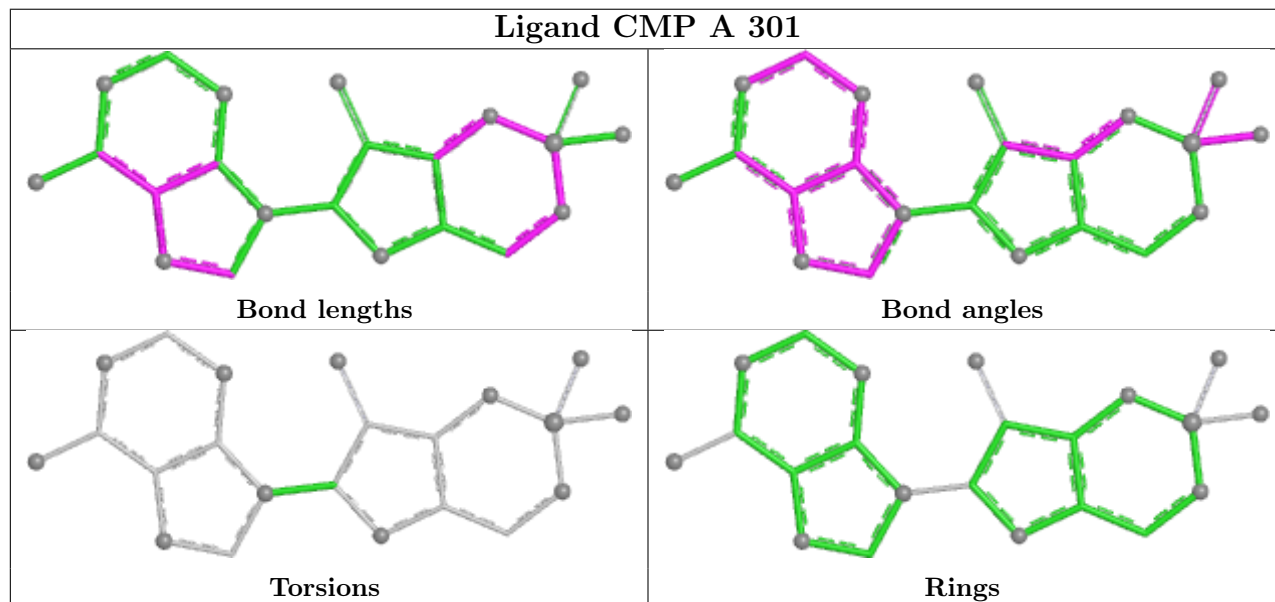
Mol	Chain	Res	Type	Atoms
3	B	303	AUF	C6-C5-P1-C1
3	A	302	AUF	C2-C1-P1-C5
3	B	303	AUF	C2-C1-P1-C3
3	B	303	AUF	C4-C3-P1-C5

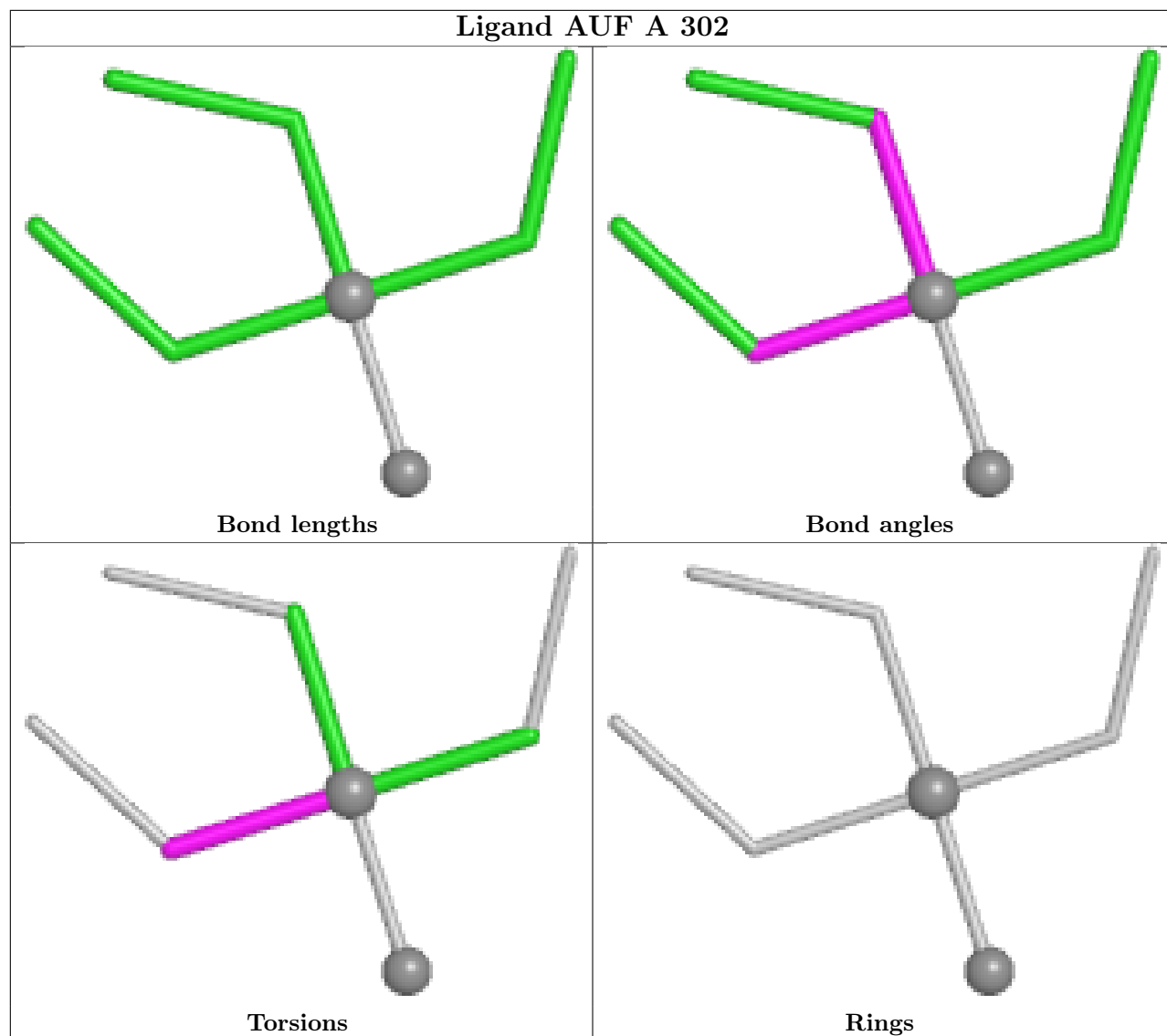
There are no ring outliers.

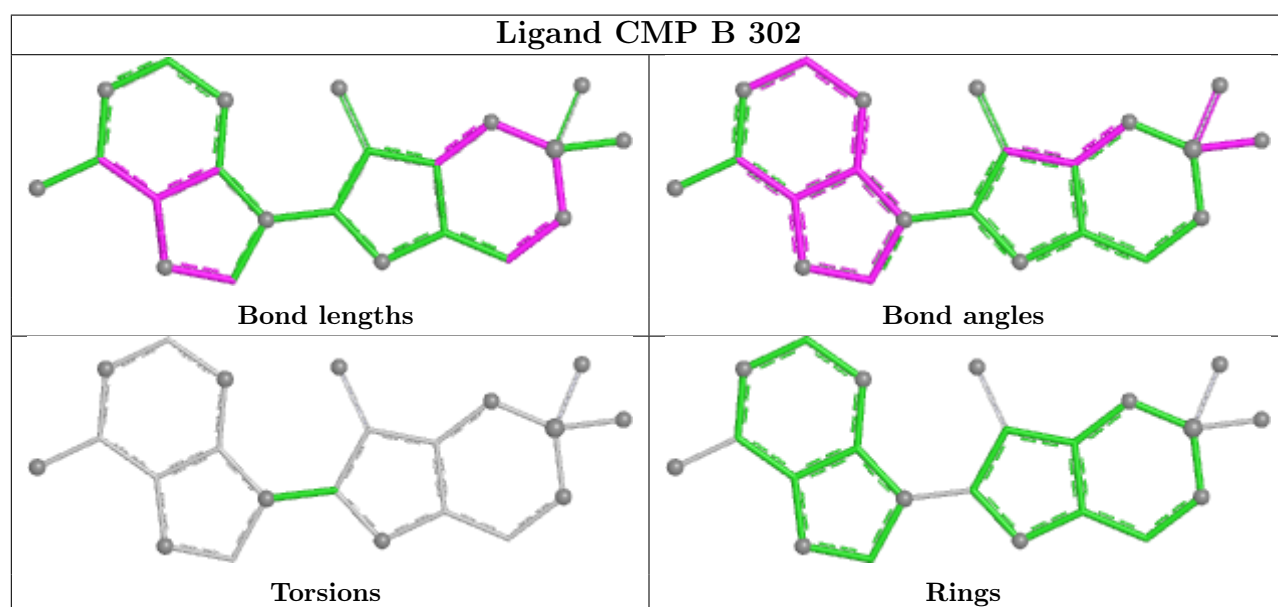
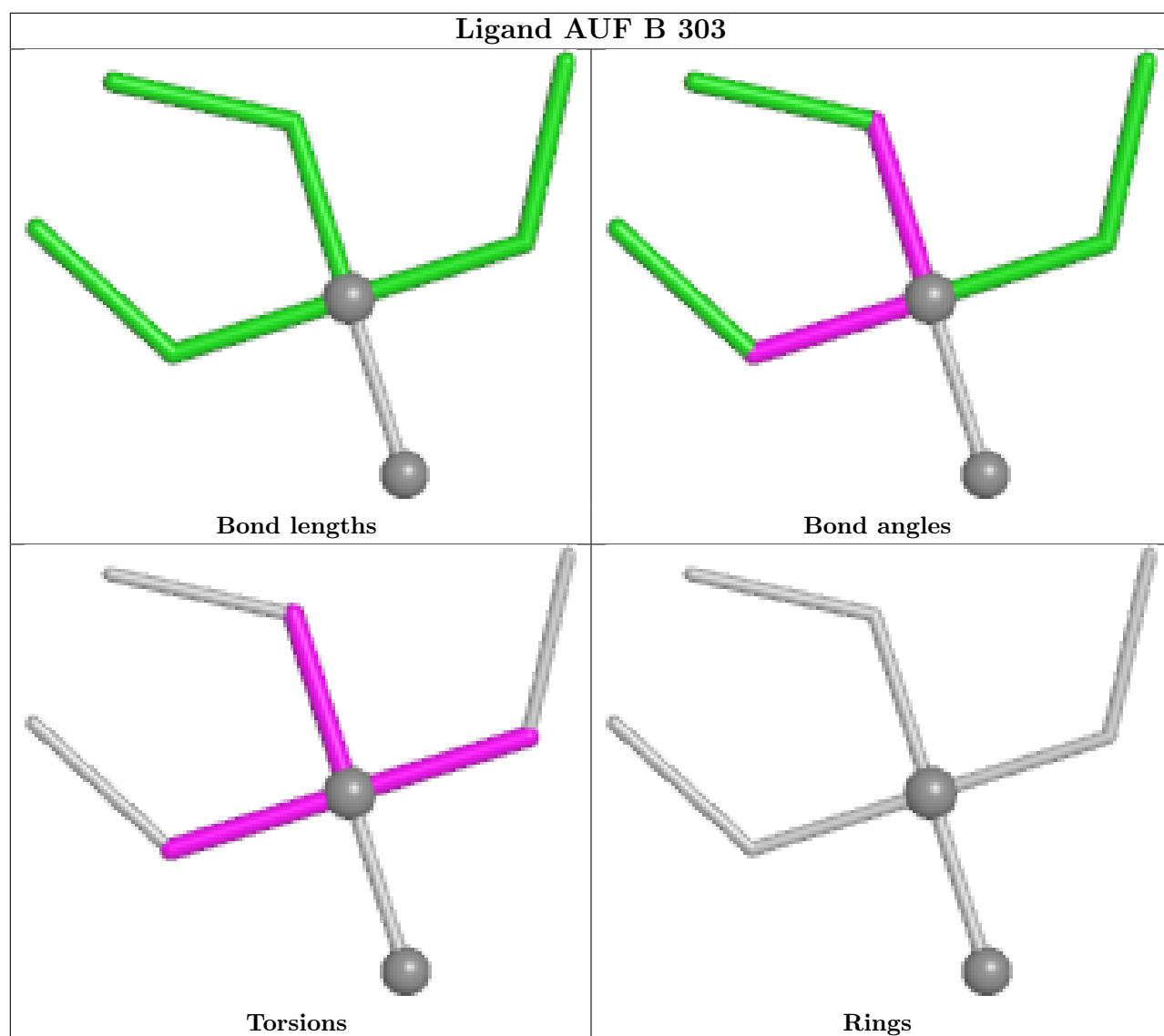
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	CMP	1	0
3	B	303	AUF	1	0
2	B	302	CMP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 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	197/210 (93%)	1.02	38 (19%) <b>3</b> <b>2</b>	19, 37, 64, 75	0
1	B	188/210 (89%)	1.06	28 (14%) <b>5</b> <b>4</b>	21, 41, 65, 76	0
All	All	385/420 (91%)	1.04	66 (17%) <b>4</b> <b>3</b>	19, 39, 64, 76	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	101	GLU	6.5
1	A	184	SER	6.0
1	B	21	HIS	5.8
1	A	162	MET	5.2
1	B	212	GLY	4.3
1	A	157	GLN	4.2
1	A	153	LEU	3.9
1	A	187	MET	3.8
1	A	9	LYS	3.7
1	B	115	SER	3.6
1	B	157	GLN	3.6
1	B	207	THR	3.6
1	B	112	GLN	3.4
1	A	190	ARG	3.4
1	A	202	HIS	3.4
1	B	19	HIS	3.4
1	A	59	ARG	3.4
1	A	57	ASP	3.3
1	B	38	CYS	3.1
1	A	186	GLU	3.0
1	A	201	VAL	3.0
1	B	154	ASP	2.9
1	A	127	ASP	2.8
1	B	47	GLY	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	54	GLU	2.8
1	B	77	LEU	2.8
1	B	200	LEU	2.7
1	B	117	ILE	2.7
1	A	58	GLY	2.7
1	B	205	GLY	2.7
1	B	22	ARG	2.6
1	A	101	GLU	2.6
1	A	191	VAL	2.6
1	A	169	GLN	2.6
1	A	160	ASP	2.6
1	A	56	ASP	2.5
1	A	38	CYS	2.5
1	B	58	GLY	2.5
1	B	156	CYS	2.5
1	A	10	LEU	2.5
1	A	207	THR	2.5
1	A	20	CYS	2.4
1	B	18	ALA	2.4
1	A	192	LEU	2.3
1	A	195	LEU	2.3
1	B	142	LEU	2.3
1	A	204	LYS	2.3
1	B	141	PHE	2.3
1	B	100	ALA	2.3
1	A	209	VAL	2.3
1	B	20	CYS	2.2
1	B	199	GLY	2.2
1	B	150	ARG	2.2
1	B	143	ASP	2.2
1	A	17	LEU	2.2
1	A	113	GLN	2.2
1	A	145	THR	2.2
1	A	79	GLU	2.2
1	A	21	HIS	2.1
1	A	166	ASP	2.1
1	A	199	GLY	2.1
1	A	161	ALA	2.1
1	A	117	ILE	2.0
1	A	54	GLU	2.0
1	A	200	LEU	2.0
1	B	79	GLU	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](#)

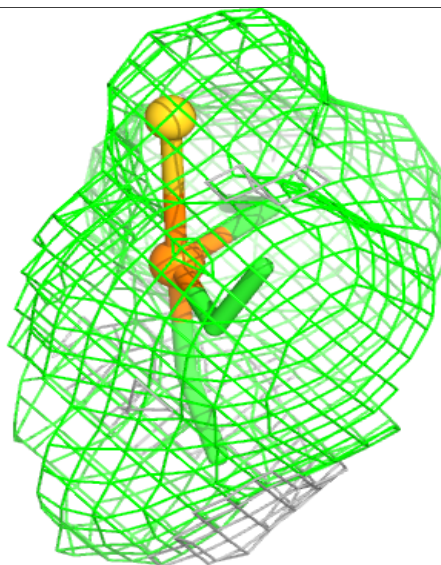
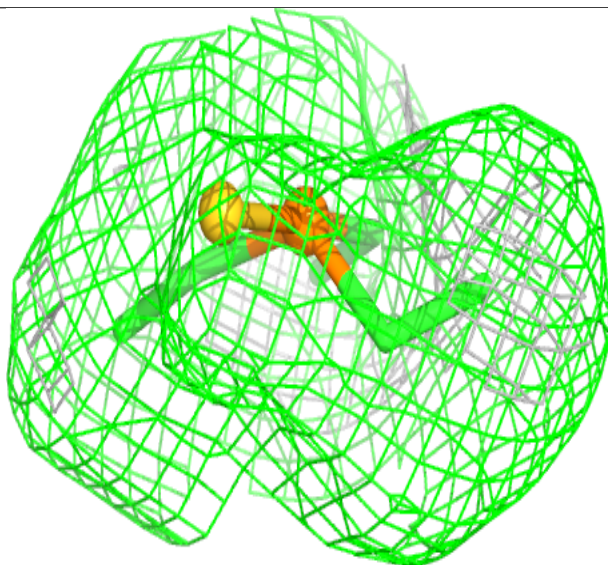
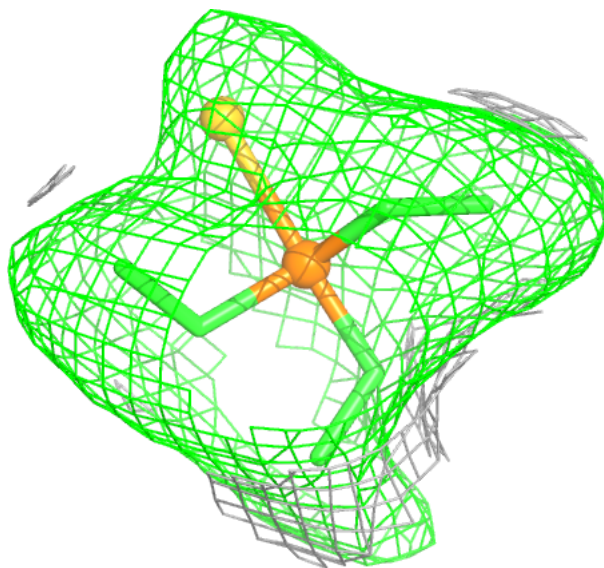
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	AUF	B	303	8/8	0.82	0.34	15,40,64,95	0
5	CL	A	305	1/1	0.86	0.15	70,70,70,70	0
6	SO4	A	307	5/5	0.86	0.10	46,53,59,65	0
3	AUF	A	302	8/8	0.87	0.24	33,45,64,106	0
6	SO4	A	306	5/5	0.88	0.15	36,39,46,47	0
4	AU	A	303	1/1	0.88	0.12	109,109,109,109	0
6	SO4	B	307	5/5	0.90	0.09	32,44,48,51	0
4	AU	B	304	1/1	0.92	0.10	135,135,135,135	0
2	CMP	A	301	22/22	0.93	0.09	12,23,30,34	0
6	SO4	B	308	5/5	0.94	0.07	35,36,43,46	0
2	CMP	B	302	22/22	0.95	0.07	15,24,33,35	0
4	AU	B	306	1/1	0.96	0.06	85,85,85,85	0
4	AU	A	304	1/1	0.97	0.07	65,65,65,65	0
5	CL	B	301	1/1	0.97	0.10	70,70,70,70	0
4	AU	B	305	1/1	0.99	0.08	71,71,71,71	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.

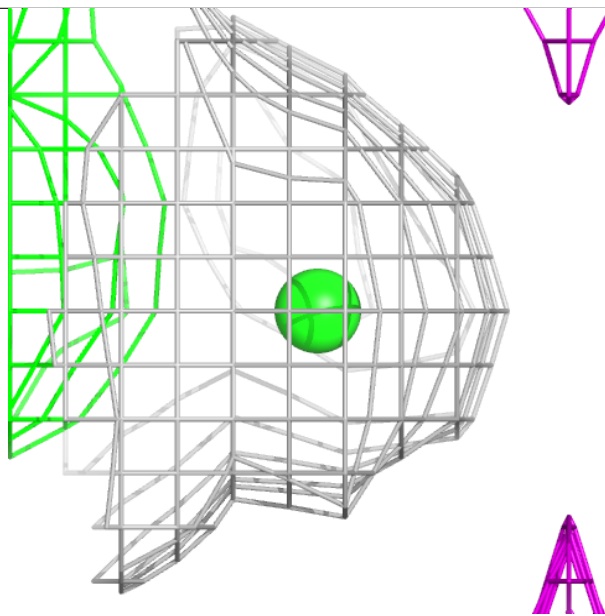
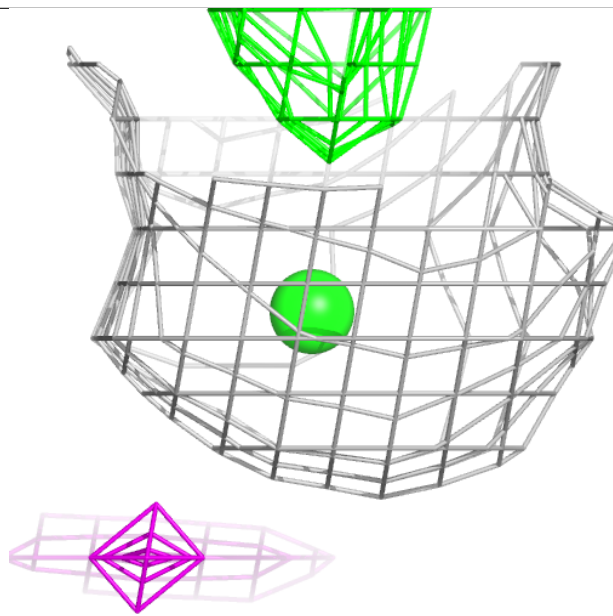
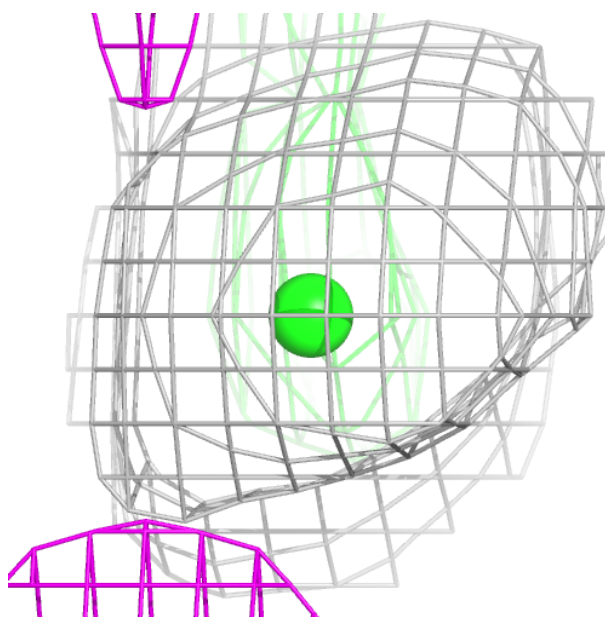
**Electron density around AUF B 303:**

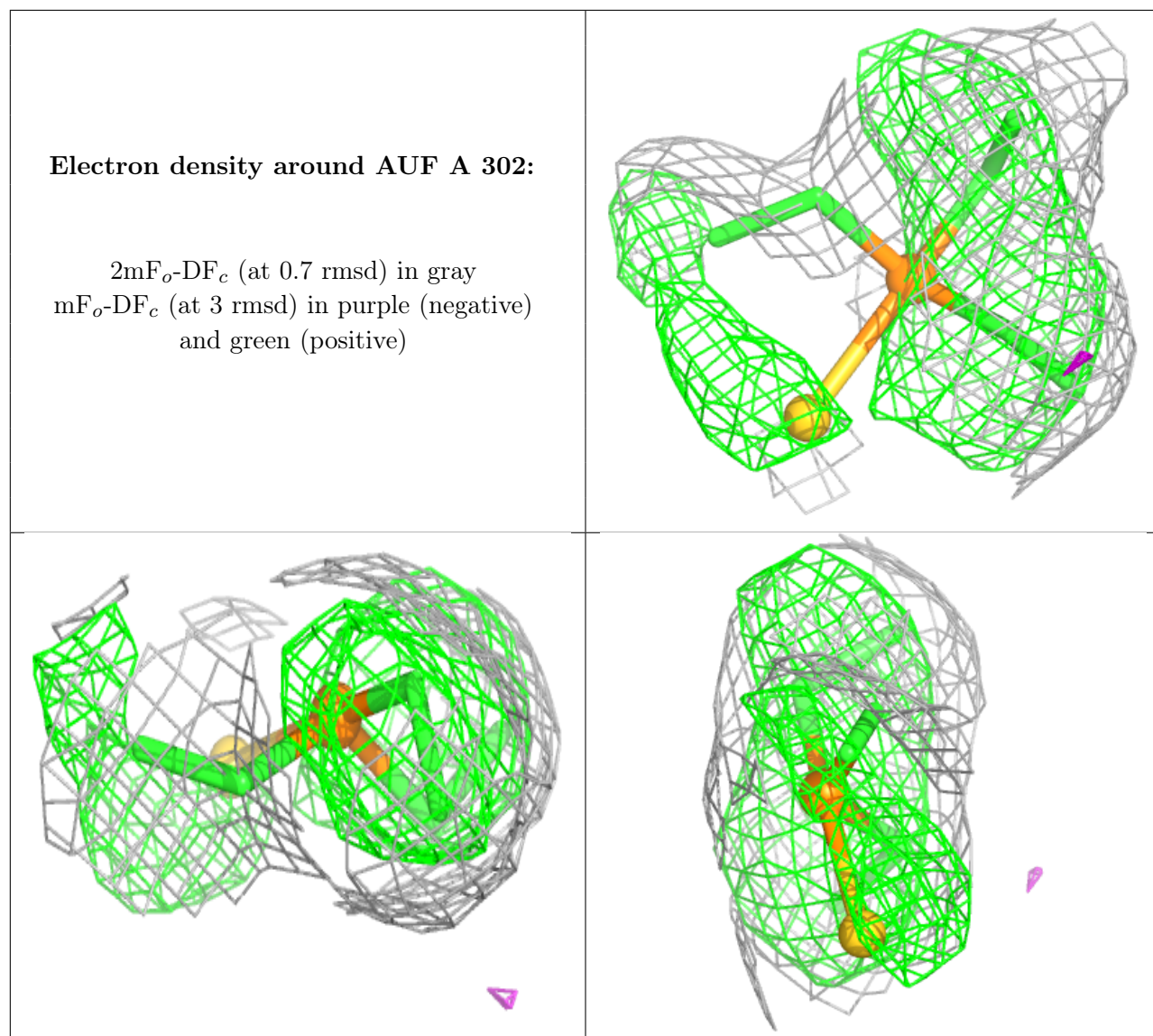
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CL A 305:**

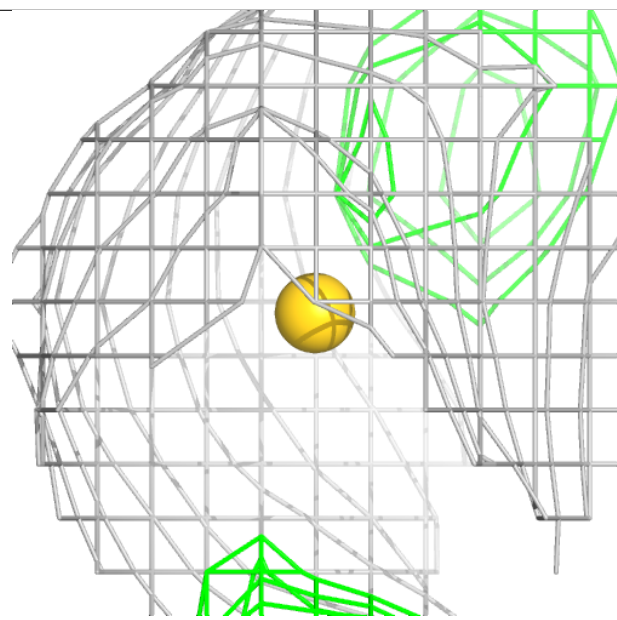
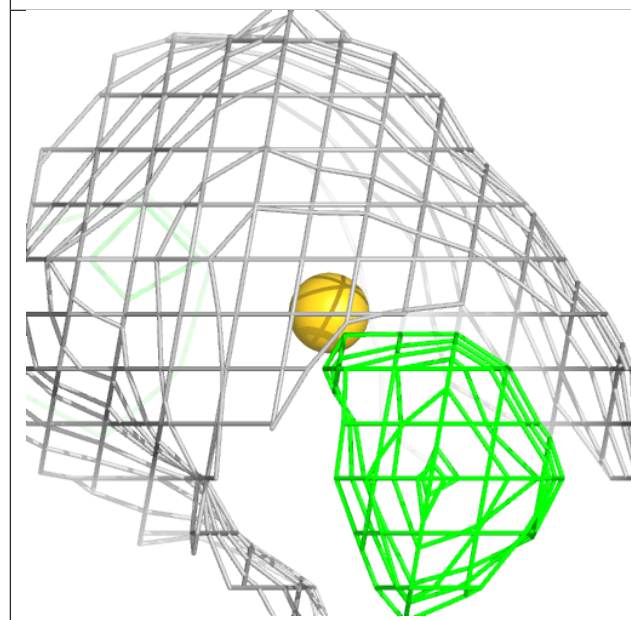
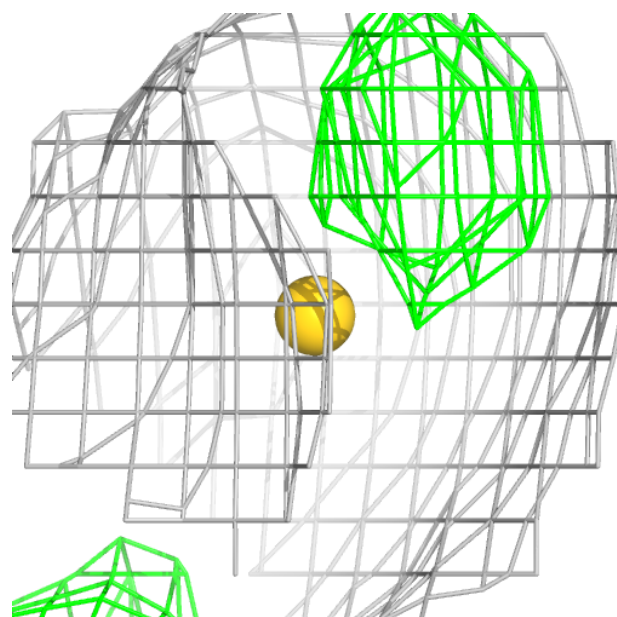
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





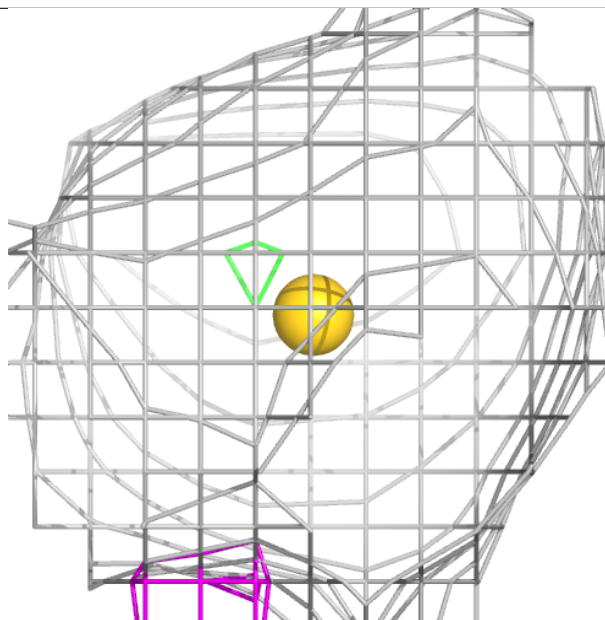
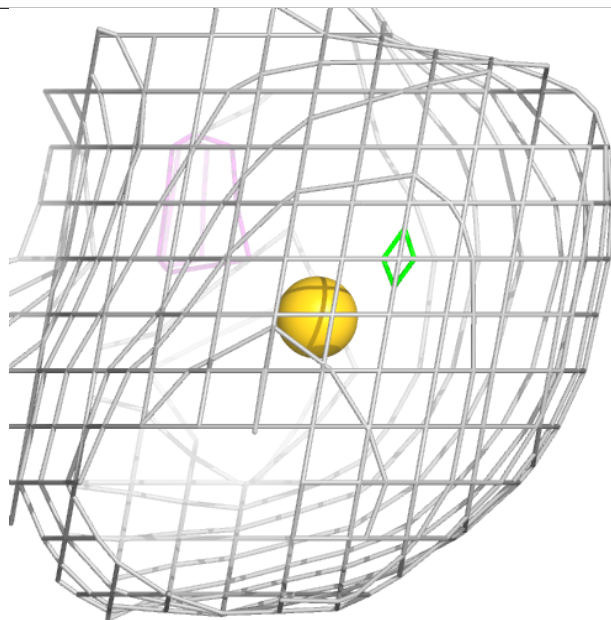
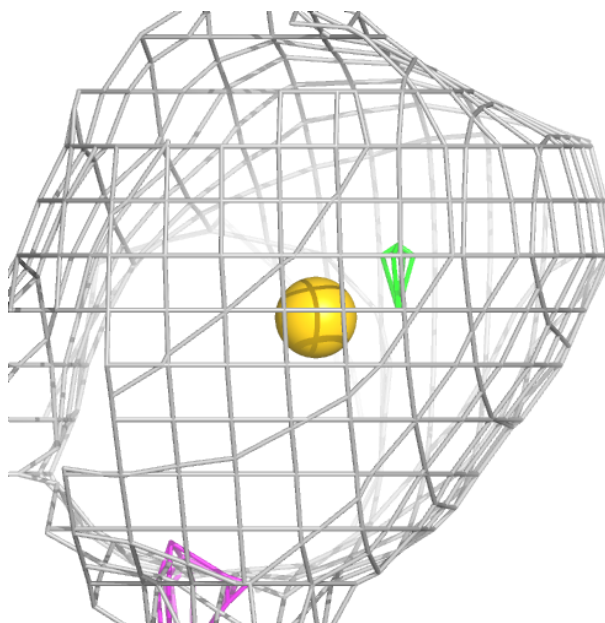
**Electron density around AU A 303:**

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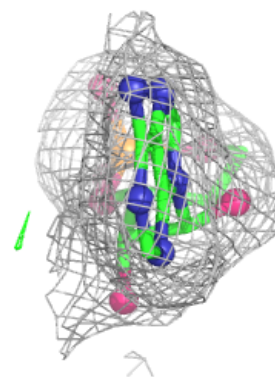
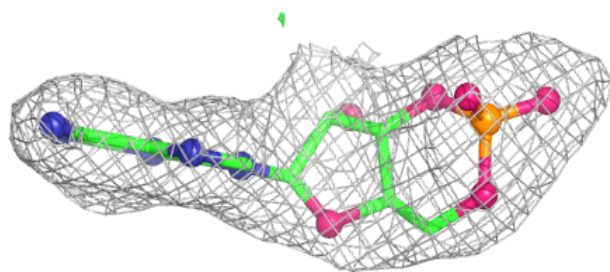
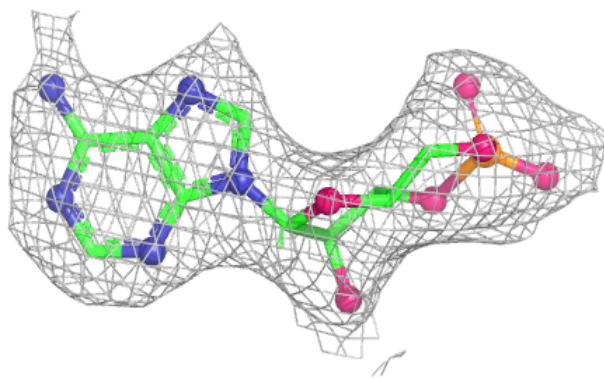
**Electron density around AU B 304:**

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and green (positive)

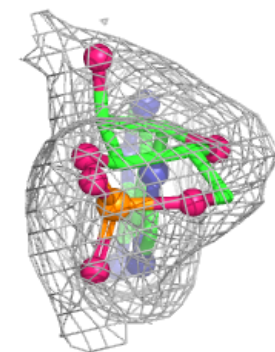
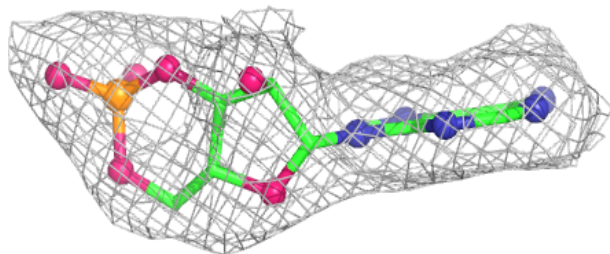
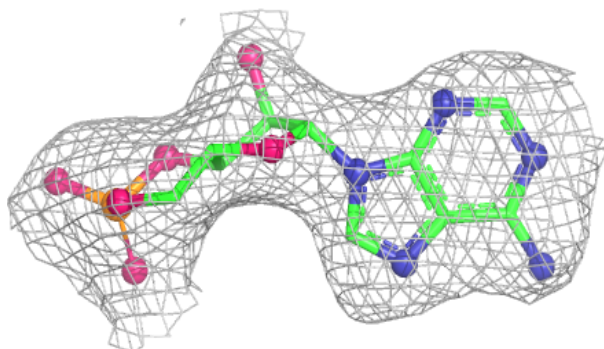


**Electron density around CMP A 301:**

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and green (positive)

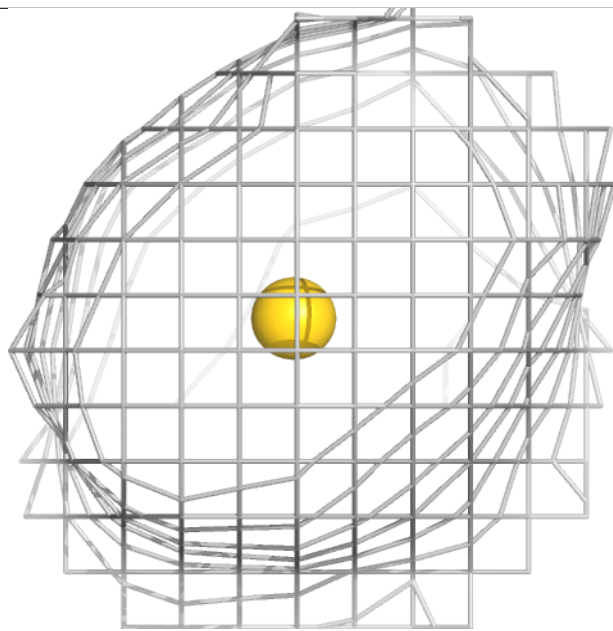
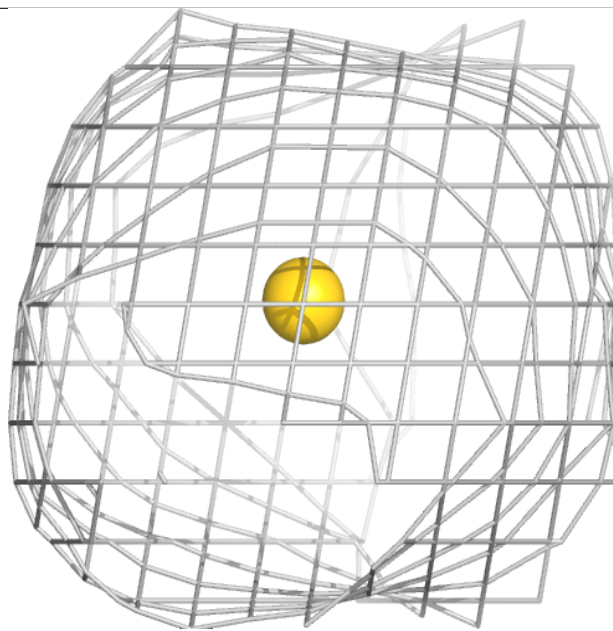
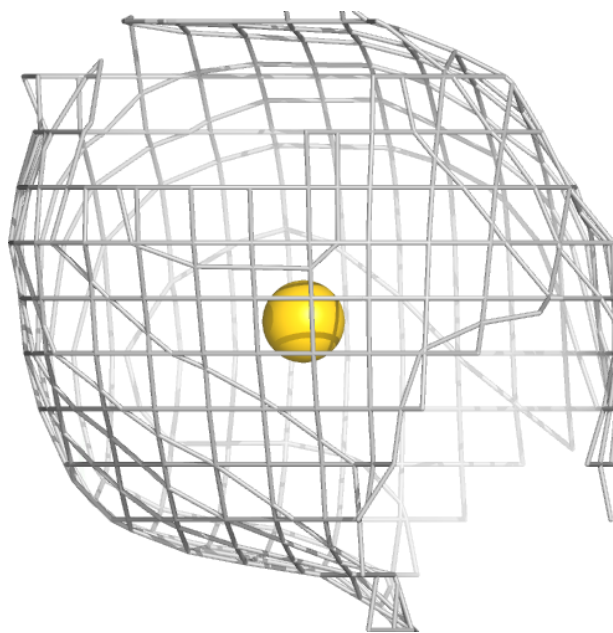
**Electron density around CMP B 302:**

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and green (positive)



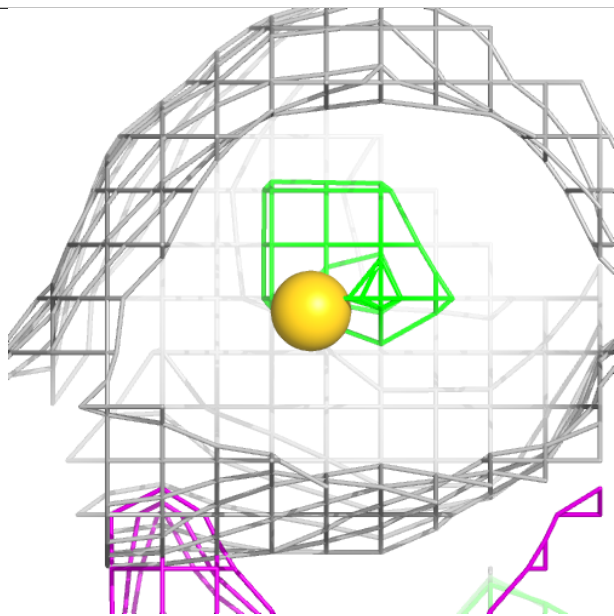
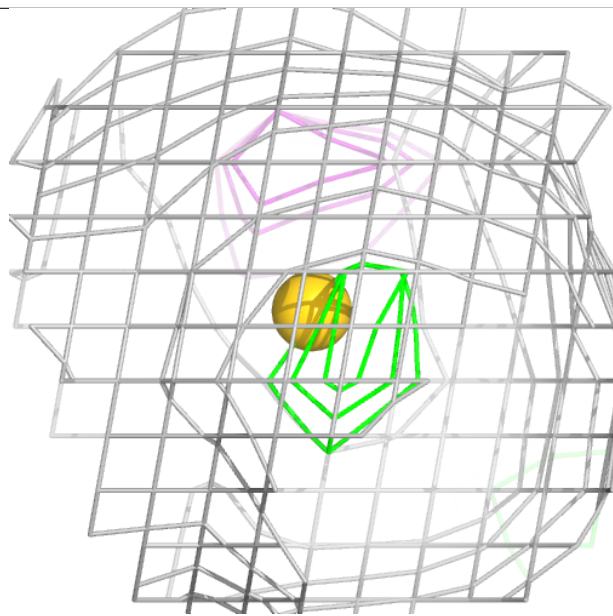
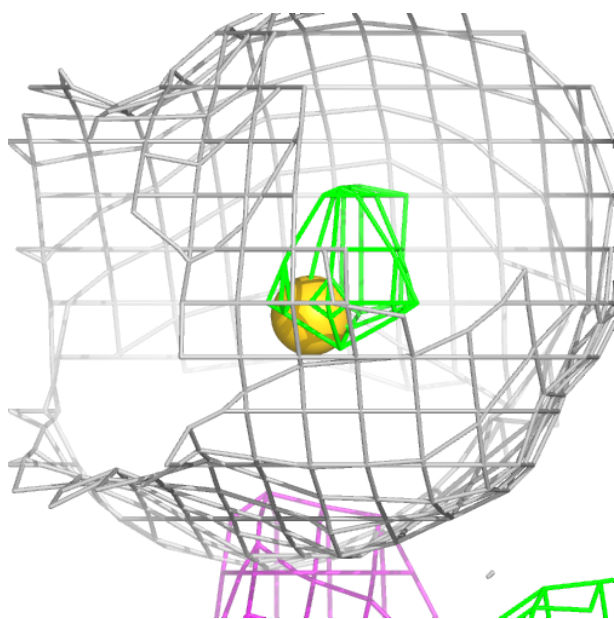
**Electron density around AU B 306:**

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



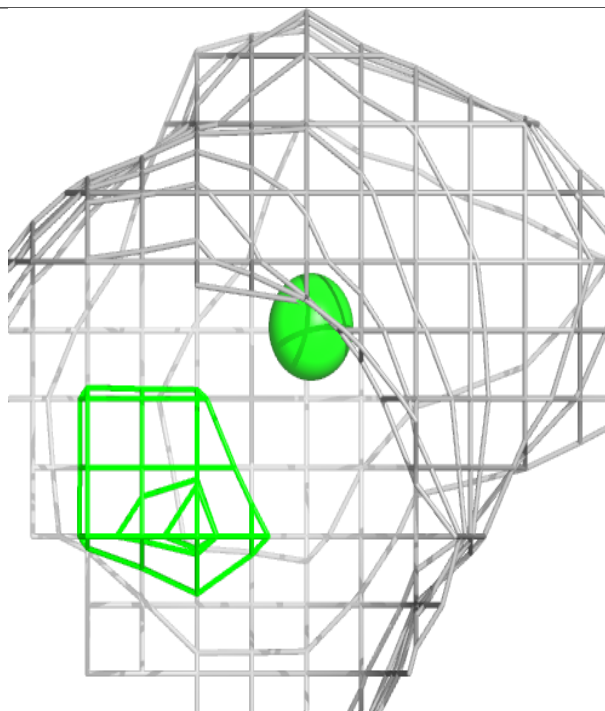
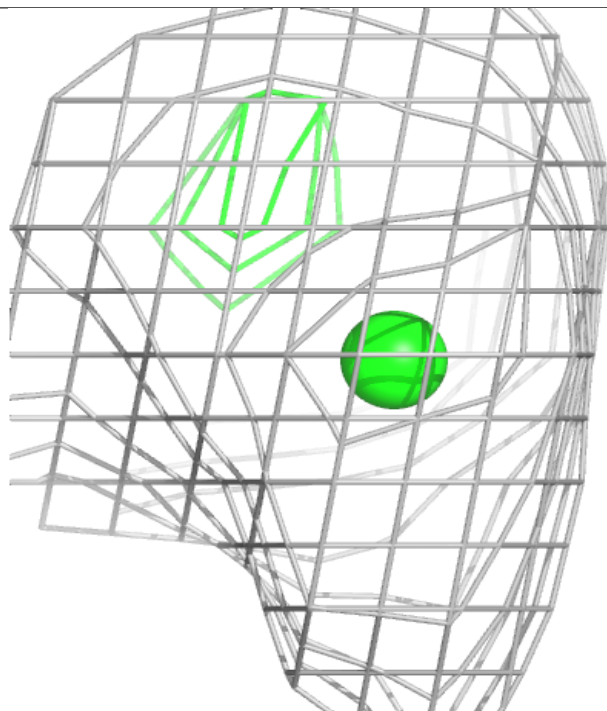
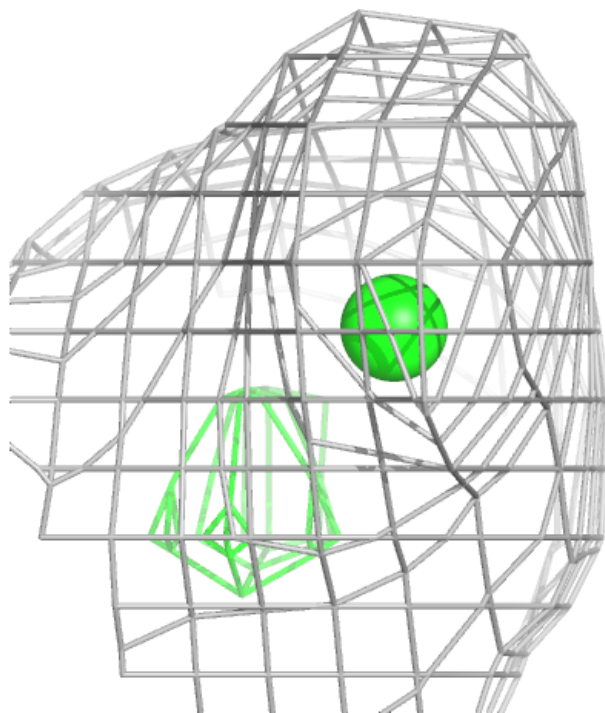
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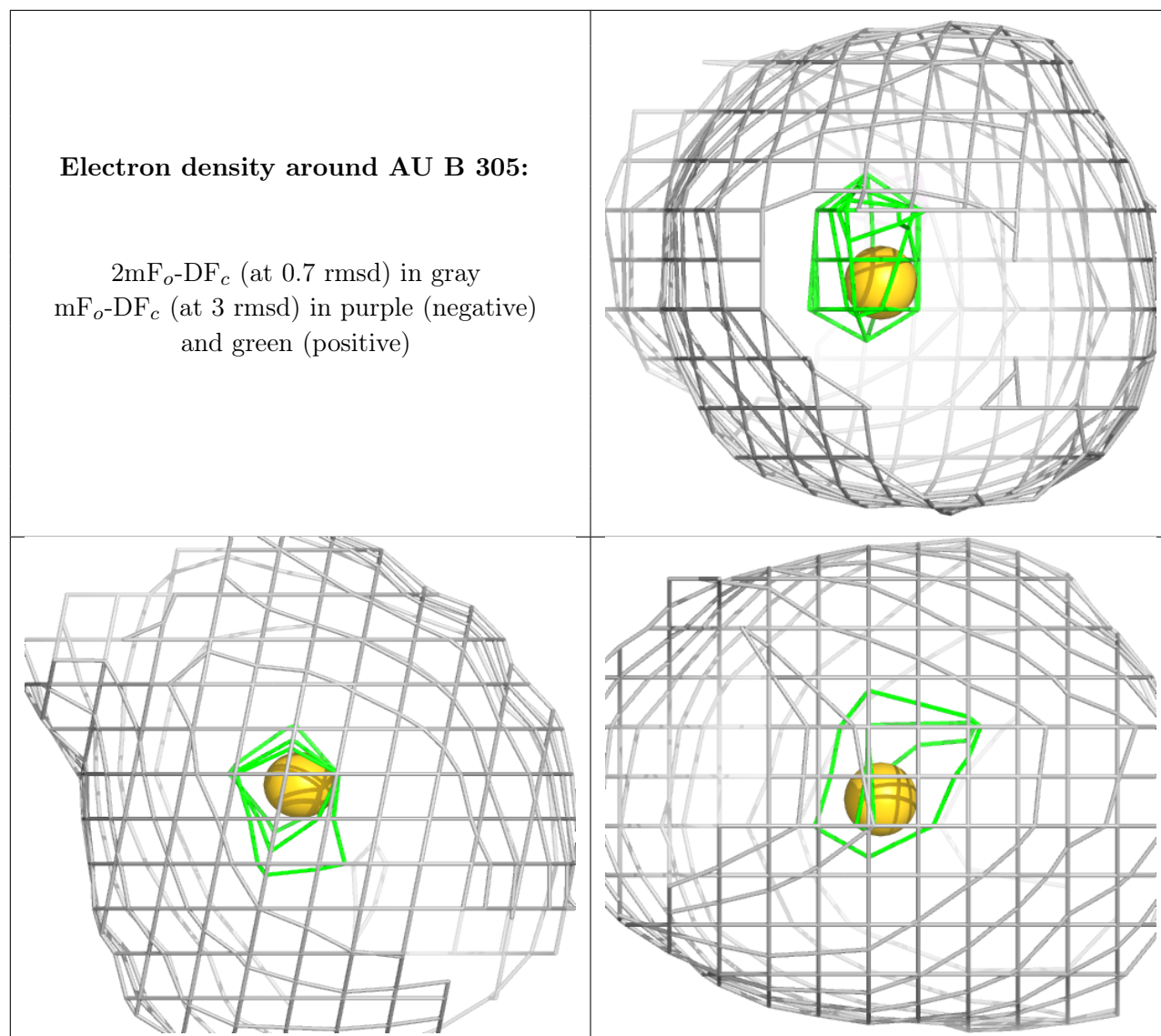
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CL B 301:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.