



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 04:03 PM JST

PDB ID : 7VE3  
Title : Structure of the complex of sheep lactoperoxidase with hypoiodite at 2.70 Å resolution  
Authors : Singh, P.K.; Yamini, S.; Singh, R.P.; Singh, A.K.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.  
Deposited on : 2021-09-07  
Resolution : 2.70 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)

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<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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

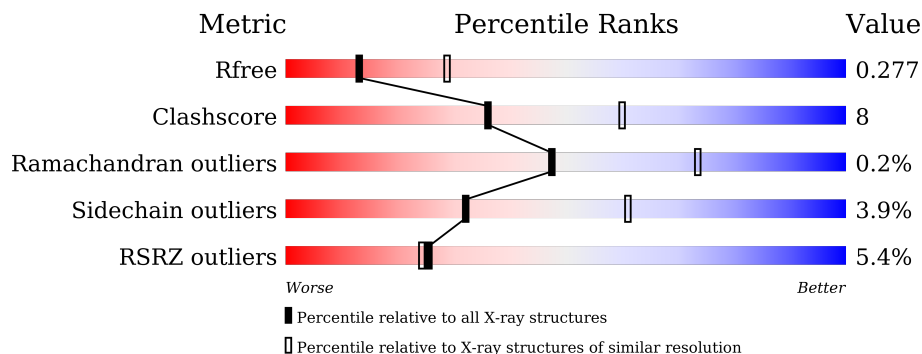
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 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.

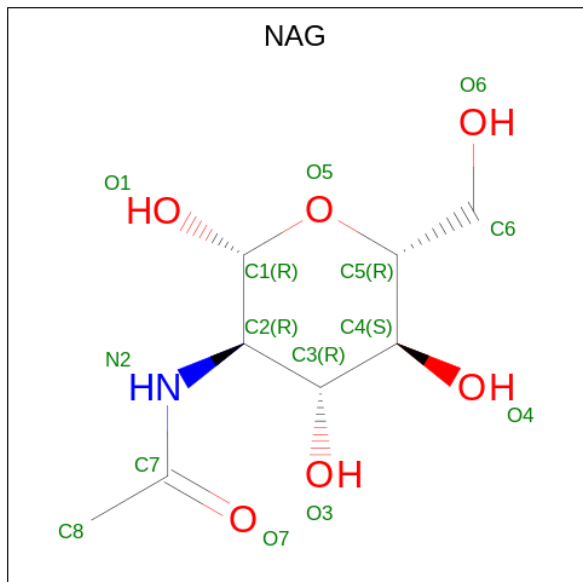
Mol	Chain	Length	Quality of chain
1	A	595	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	61D	A	612	-	-	X	-
7	61D	A	618	-	-	X	-
7	61D	A	621	-	-	X	-



- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is IODIDE ION (three-letter code: IOD) (formula: I).

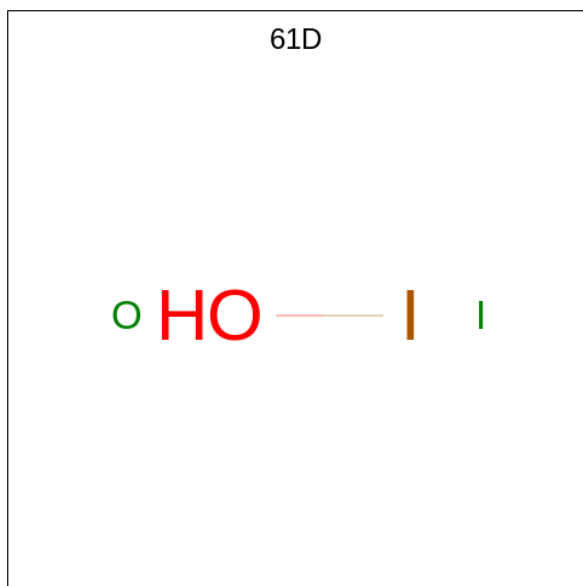
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total	I	0	0
			6	6		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



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

- Molecule 7 is hypoiodous acid (three-letter code: 61D) (formula: HIO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	I	O	0	0
			2	1	1		
7	A	1	Total	I	O	0	0
			2	1	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	I	O	0	0
			2	1	1		
7	A	1	Total	I	O	0	0
			2	1	1		
7	A	1	Total	I	O	0	0
			2	1	1		
7	A	1	Total	I	O	0	0
			2	1	1		
7	A	1	Total	I	O	0	0
			2	1	1		
7	A	1	Total	I	O	0	0
			2	1	1		
7	A	1	Total	I	O	0	0
			2	1	1		

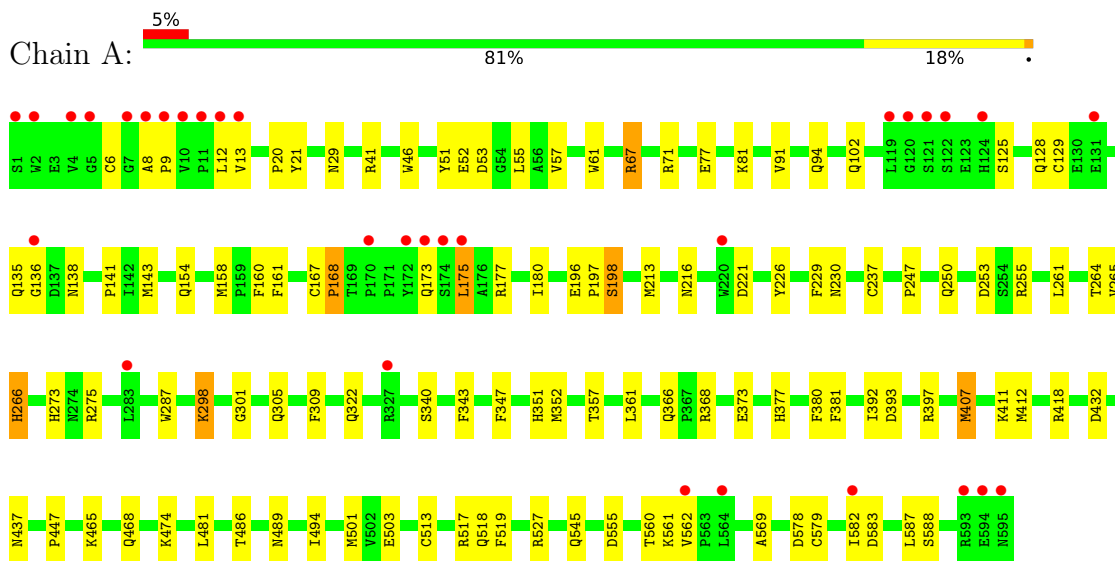
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	157	Total	O	0	0
			157	157		

### 3 Residue-property plots

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

- Molecule 1: Lactoperoxidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.94Å 80.18Å 76.12Å 90.00° 102.86° 90.00°	Depositor
Resolution (Å)	43.97 – 2.70 43.97 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.6 (43.97-2.70) 97.7 (43.97-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	11.72 (at 2.69Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.195 , 0.277 0.195 , 0.277	Depositor DCC
$R_{free}$ test set	860 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.0	Xtrriage
Anisotropy	0.031	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 44.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5031	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% 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: SO4, NAG, 61D, CA, HEM, IOD

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	0.32	0/4894	0.71	2/6637 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	GLN	CB-CA-C	-9.23	91.94	110.40
1	A	168	PRO	N-CA-C	5.74	127.03	112.10

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	4769	0	4687	72	0
2	A	43	0	30	3	0
3	A	1	0	0	0	0
4	A	28	0	26	0	0
5	A	6	0	0	1	0
6	A	5	0	0	0	0
7	A	22	0	0	9	0
8	A	157	0	0	9	0
All	All	5031	0	4743	77	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 8.

All (77) 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:A:198[A]:SER:OG	7:A:621:61D:I	2.22	1.27
1:A:6:CYS:O	1:A:167:CYS:SG	2.00	1.18
7:A:612:61D:O	7:A:613:61D:O	1.68	1.11
1:A:216:ASN:ND2	5:A:610:IOD:I	2.58	1.05
7:A:614:61D:I	8:A:849:HOH:O	2.68	0.81
1:A:351:HIS:HD1	1:A:437:ASN:HD21	1.29	0.79
1:A:52:GLU:HB3	1:A:57:VAL:HG23	1.66	0.79
1:A:51:TYR:CD2	1:A:55:LEU:O	2.37	0.78
1:A:230:ASN:HB2	1:A:250:GLN:OE1	1.91	0.71
1:A:418:ARG:O	1:A:432:ASP:HA	1.93	0.67
1:A:91:VAL:HG12	1:A:411:LYS:HD3	1.81	0.63
1:A:266:HIS:HE1	8:A:759:HOH:O	1.82	0.62
1:A:468:GLN:HG2	1:A:474:LYS:HA	1.83	0.61
2:A:601:HEM:HBB2	2:A:601:HEM:HMB2	1.82	0.60
1:A:264:THR:HG23	1:A:392:ILE:HB	1.86	0.58
1:A:322:GLN:HB2	8:A:798:HOH:O	2.04	0.58
1:A:125:SER:HA	1:A:128:GLN:HB2	1.86	0.57
1:A:197:PRO:HD2	7:A:621:61D:I	2.75	0.56
1:A:173:GLN:HG3	1:A:177:ARG:HA	1.88	0.56
1:A:61:TRP:HH2	1:A:136:GLY:O	1.89	0.56
1:A:418:ARG:O	1:A:432:ASP:CB	2.54	0.55
1:A:561:LYS:NZ	7:A:618:61D:I	3.10	0.55
1:A:393:ASP:HB2	8:A:760:HOH:O	2.05	0.55
1:A:351:HIS:HD1	1:A:437:ASN:ND2	2.04	0.55
1:A:562:VAL:CG2	1:A:582:ILE:CD1	2.86	0.54
1:A:418:ARG:O	1:A:432:ASP:CA	2.56	0.53
1:A:237:CYS:HA	1:A:381:PHE:O	2.09	0.53
1:A:230:ASN:CB	1:A:250:GLN:OE1	2.56	0.53
1:A:261:LEU:O	1:A:265:VAL:HG23	2.10	0.52
1:A:12:LEU:O	1:A:13:VAL:HG23	2.10	0.52
1:A:8:ALA:HB3	1:A:9:PRO:HD3	1.92	0.51
1:A:352:MET:HB3	1:A:412:MET:O	2.10	0.51
1:A:229:PHE:HB3	1:A:247:PRO:HG2	1.92	0.51
1:A:158:MET:HE1	1:A:432:ASP:H	1.76	0.51
1:A:196:GLU:HB3	7:A:621:61D:I	2.83	0.49
2:A:601:HEM:HMC2	2:A:601:HEM:HBC2	1.94	0.49
1:A:102:GLN:CG	1:A:265:VAL:HG21	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.48	0.49
1:A:29:ASN:O	1:A:527:ARG:NH1	2.46	0.48
1:A:501:MET:HE1	8:A:801:HOH:O	2.14	0.48
1:A:373:GLU:HB3	7:A:617:61D:I	2.83	0.48
1:A:397:ARG:NH1	7:A:618:61D:I	3.16	0.48
1:A:560:THR:HA	1:A:579:CYS:SG	2.54	0.48
1:A:46:TRP:CE2	1:A:340:SER:HB3	2.48	0.48
2:A:601:HEM:HBB2	2:A:601:HEM:CMB	2.43	0.48
1:A:578:ASP:OD1	1:A:579:CYS:N	2.48	0.47
1:A:275:ARG:CD	1:A:555:ASP:HB3	2.44	0.47
1:A:407:MET:HG3	8:A:795:HOH:O	2.13	0.47
1:A:447:PRO:HD3	8:A:707:HOH:O	2.15	0.47
1:A:53:ASP:CG	1:A:57:VAL:HG22	2.36	0.46
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.50	0.46
1:A:102:GLN:HG3	1:A:265:VAL:HG21	1.97	0.46
1:A:135:GLN:HG3	1:A:141:PRO:HD2	1.98	0.45
1:A:141:PRO:HG2	1:A:143:MET:CE	2.46	0.45
1:A:309:PHE:HZ	1:A:519:PHE:O	1.99	0.45
1:A:343:PHE:CG	1:A:518:GLN:HG2	2.51	0.45
1:A:255:ARG:HD2	7:A:612:61D:I	2.87	0.45
1:A:175:LEU:HD13	1:A:175:LEU:HA	1.80	0.45
1:A:287:TRP:HA	8:A:784:HOH:O	2.18	0.44
1:A:77:GLU:OE2	1:A:81:LYS:NZ	2.40	0.44
1:A:61:TRP:CH2	1:A:136:GLY:O	2.70	0.44
1:A:298:LYS:HB2	1:A:298:LYS:HE2	1.67	0.43
1:A:138:ASN:O	1:A:161:PHE:HA	2.18	0.43
1:A:343:PHE:CD1	1:A:518:GLN:HG2	2.54	0.43
1:A:253:ASP:HA	8:A:780:HOH:O	2.18	0.43
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.54	0.42
1:A:67:ARG:HB3	1:A:489:ASN:ND2	2.34	0.42
1:A:301:GLY:O	1:A:305:GLN:HG3	2.20	0.42
1:A:494:ILE:HD12	1:A:494:ILE:HA	1.81	0.42
1:A:513:CYS:O	1:A:517:ARG:HG3	2.20	0.42
1:A:20:PRO:HG2	1:A:21:TYR:CE2	2.54	0.42
1:A:361:LEU:HA	1:A:366:GLN:O	2.20	0.41
1:A:229:PHE:CG	1:A:247:PRO:HG2	2.55	0.41
1:A:309:PHE:CZ	1:A:519:PHE:O	2.73	0.41
1:A:94:GLN:O	1:A:569:ALA:CB	2.68	0.41
1:A:160:PHE:O	1:A:161:PHE:CD1	2.73	0.41
1:A:129:CYS:SG	1:A:161:PHE:HE1	2.43	0.41

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	594/595 (100%)	577 (97%)	16 (3%)	1 (0%)	47 73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	168	PRO

### 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	519/518 (100%)	498 (96%)	21 (4%)	31 60

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ARG
1	A	67	ARG
1	A	71	ARG
1	A	175	LEU
1	A	180	ILE
1	A	198[A]	SER
1	A	198[B]	SER
1	A	266	HIS
1	A	298	LYS
1	A	347	PHE

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Mol	Chain	Res	Type
1	A	357	THR
1	A	368	ARG
1	A	407	MET
1	A	465	LYS
1	A	481	LEU
1	A	486	THR
1	A	503	GLU
1	A	545	GLN
1	A	583	ASP
1	A	587	LEU
1	A	588	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	GLN
1	A	468	GLN
1	A	571	ASN

### 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, 7 are monoatomic - leaving 15 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
7	61D	A	616	-	0,1,1	-	-	-		
7	61D	A	612	-	0,1,1	-	-	-		
7	61D	A	615	-	0,1,1	-	-	-		
4	NAG	A	604	1	14,14,15	0.75	0	17,19,21	1.62	3 (17%)
7	61D	A	620	-	0,1,1	-	-	-		
7	61D	A	614	-	0,1,1	-	-	-		
4	NAG	A	603	1	14,14,15	0.64	0	17,19,21	1.47	2 (11%)
6	SO4	A	611	-	4,4,4	0.32	0	6,6,6	0.22	0
7	61D	A	622	-	0,1,1	-	-	-		
7	61D	A	617	-	0,1,1	-	-	-		
7	61D	A	621	-	0,1,1	-	-	-		
7	61D	A	618	-	0,1,1	-	-	-		
7	61D	A	619	-	0,1,1	-	-	-		
7	61D	A	613	-	0,1,1	-	-	-		
2	HEM	A	601	1	41,50,50	1.44	7 (17%)	45,82,82	2.21	14 (31%)

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	NAG	A	604	1	-	0/6/23/26	0/1/1/1
4	NAG	A	603	1	-	4/6/23/26	0/1/1/1
2	HEM	A	601	1	-	4/12/54/54	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	C1B-NB	-3.95	1.33	1.40
2	A	601	HEM	CHB-C1B	2.98	1.42	1.35
2	A	601	HEM	C4D-ND	-2.89	1.35	1.40
2	A	601	HEM	C4B-NB	-2.34	1.34	1.38
2	A	601	HEM	C1D-ND	-2.31	1.34	1.38
2	A	601	HEM	FE-NB	2.26	2.08	1.96
2	A	601	HEM	FE-ND	-2.07	1.86	1.96

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	HEM	CHC-C4B-NB	5.76	130.69	124.43
2	A	601	HEM	CHD-C1D-ND	5.42	130.32	124.43
2	A	601	HEM	C1B-NB-C4B	4.69	109.92	105.07
2	A	601	HEM	CHA-C4D-ND	4.46	129.89	124.38
2	A	601	HEM	CBA-CAA-C2A	-3.80	106.13	112.62
4	A	603	NAG	C1-O5-C5	3.78	117.31	112.19
2	A	601	HEM	CHD-C1D-C2D	-3.66	119.26	124.98
4	A	604	NAG	C1-O5-C5	3.63	117.11	112.19
2	A	601	HEM	C4B-C3B-C2B	-3.51	104.33	107.11
2	A	601	HEM	CHB-C1B-NB	3.20	128.33	124.38
4	A	603	NAG	O5-C5-C6	2.94	111.82	107.20
4	A	604	NAG	O4-C4-C3	2.91	117.08	110.35
2	A	601	HEM	CHC-C4B-C3B	-2.69	120.45	124.57
2	A	601	HEM	CHA-C4D-C3D	-2.57	120.50	125.33
4	A	604	NAG	O3-C3-C2	-2.45	104.40	109.47
2	A	601	HEM	C4D-ND-C1D	2.39	107.54	105.07
2	A	601	HEM	C3B-C2B-C1B	2.35	108.23	106.49
2	A	601	HEM	CBD-CAD-C3D	-2.26	106.36	112.63
2	A	601	HEM	O2D-CGD-CBD	2.01	120.48	114.03

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	603	NAG	O5-C5-C6-O6
4	A	603	NAG	C4-C5-C6-O6
4	A	603	NAG	C8-C7-N2-C2
4	A	603	NAG	O7-C7-N2-C2
2	A	601	HEM	CAD-CBD-CGD-O1D
2	A	601	HEM	CAD-CBD-CGD-O2D
2	A	601	HEM	CAA-CBA-CGA-O1A
2	A	601	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	612	61D	2	0
7	A	614	61D	1	0
7	A	617	61D	1	0

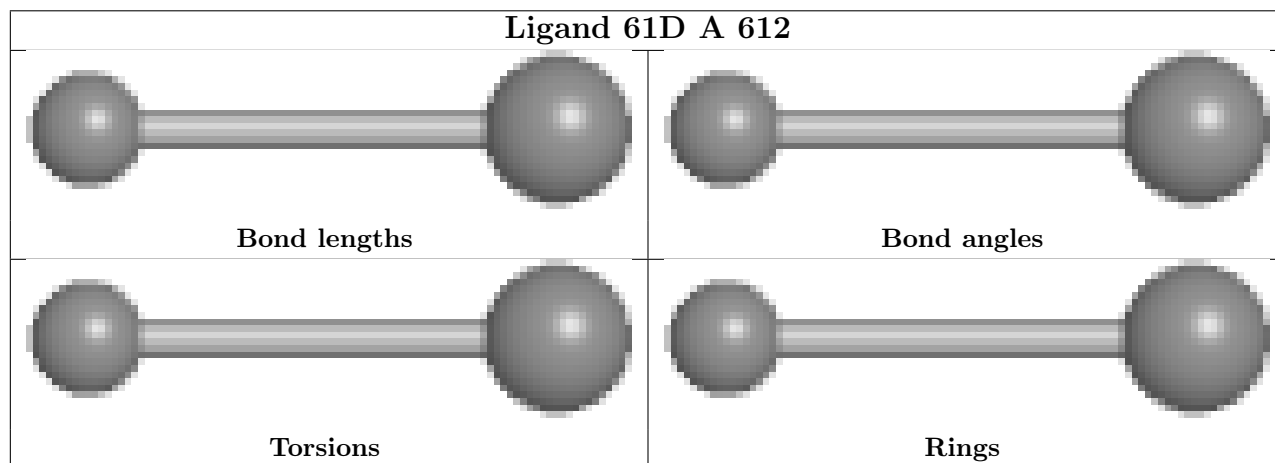
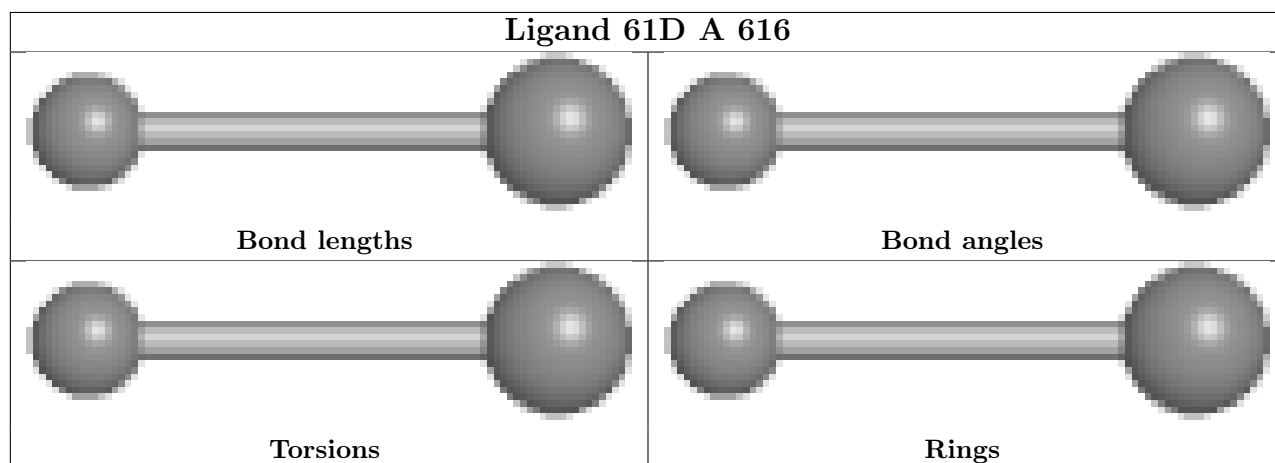
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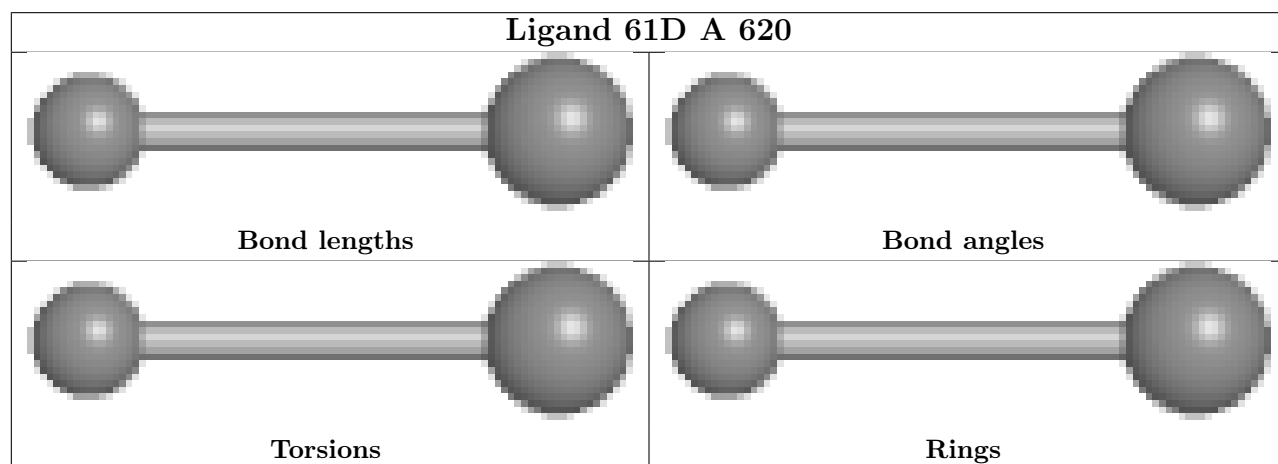
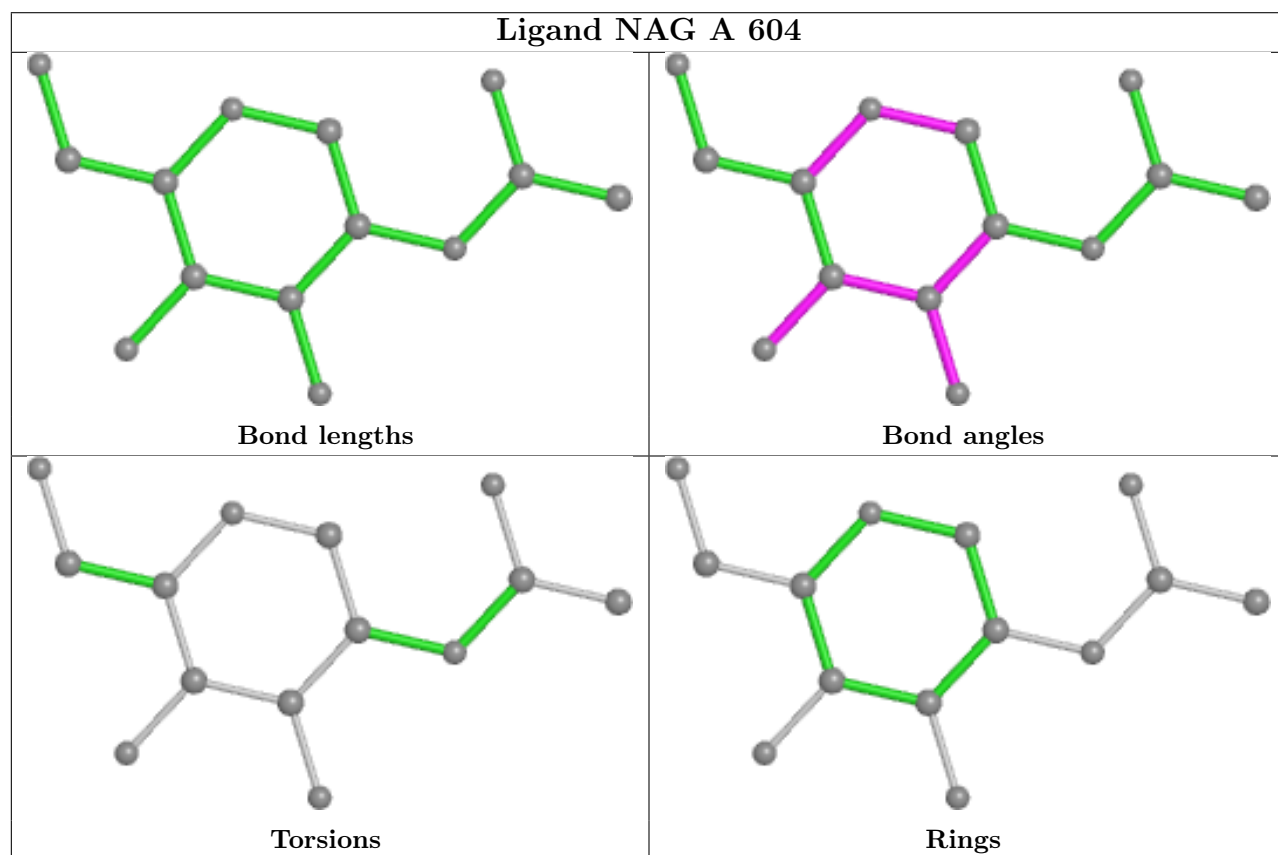
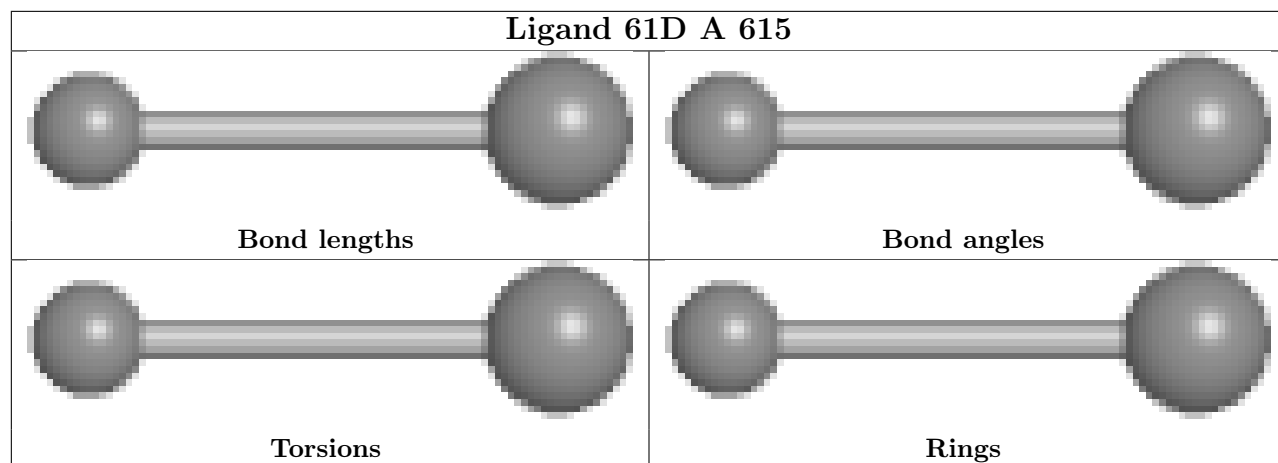


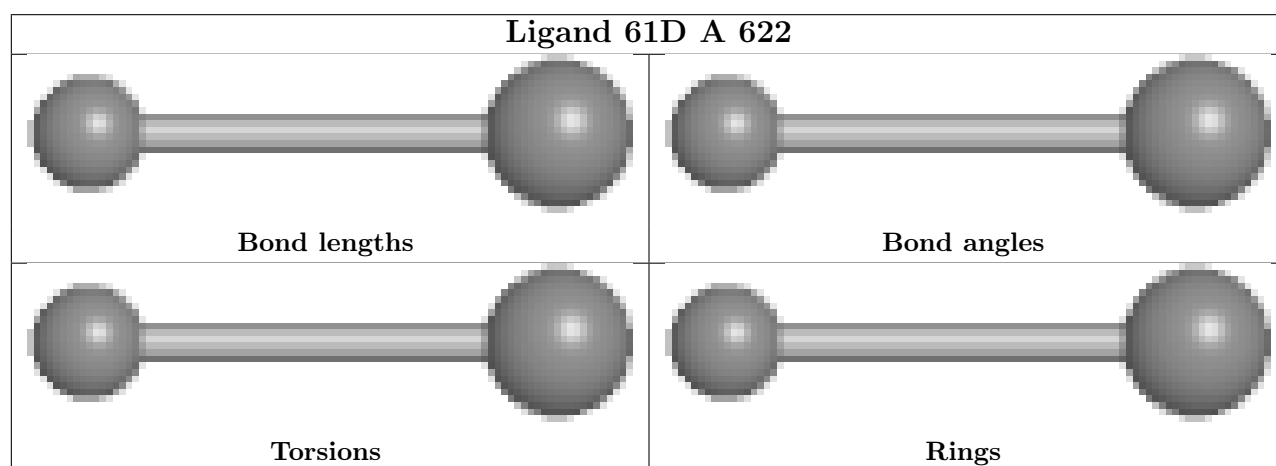
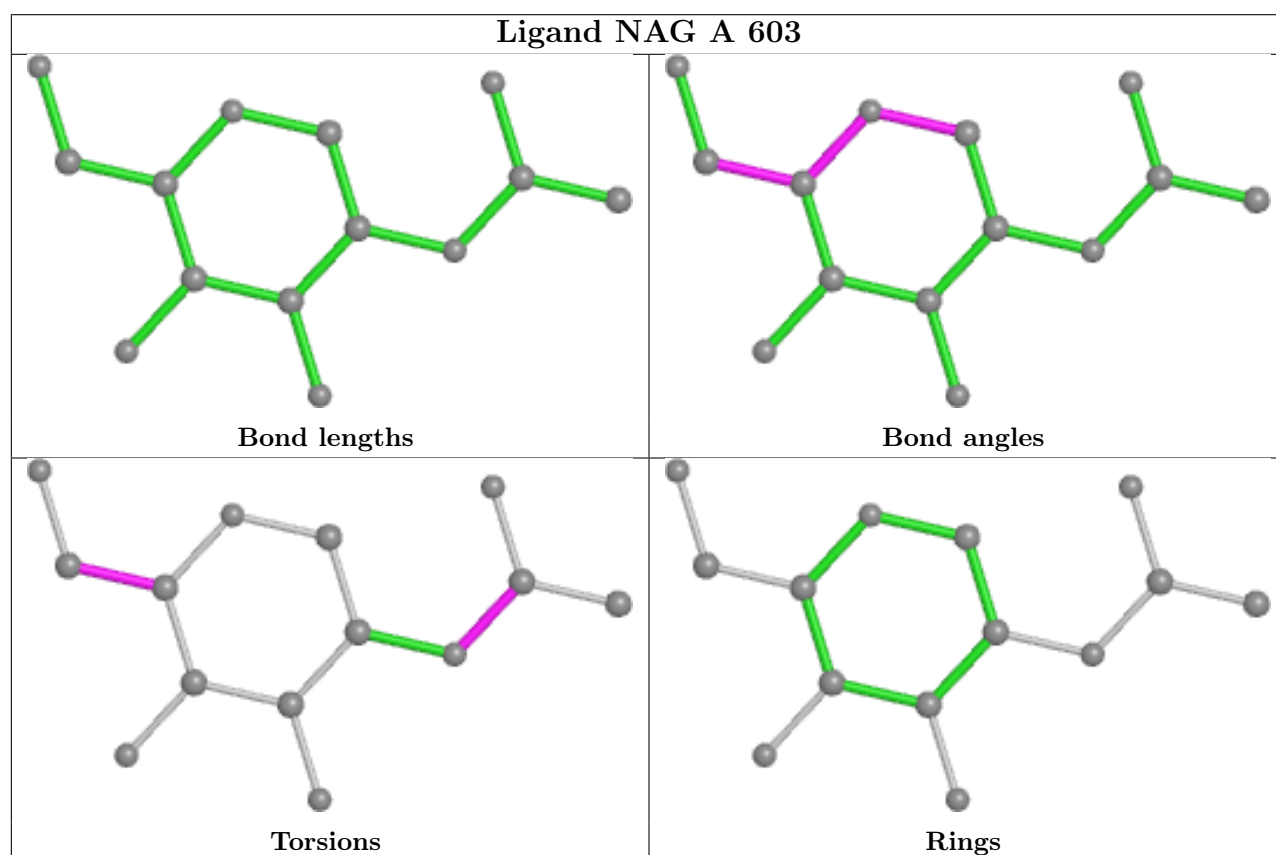
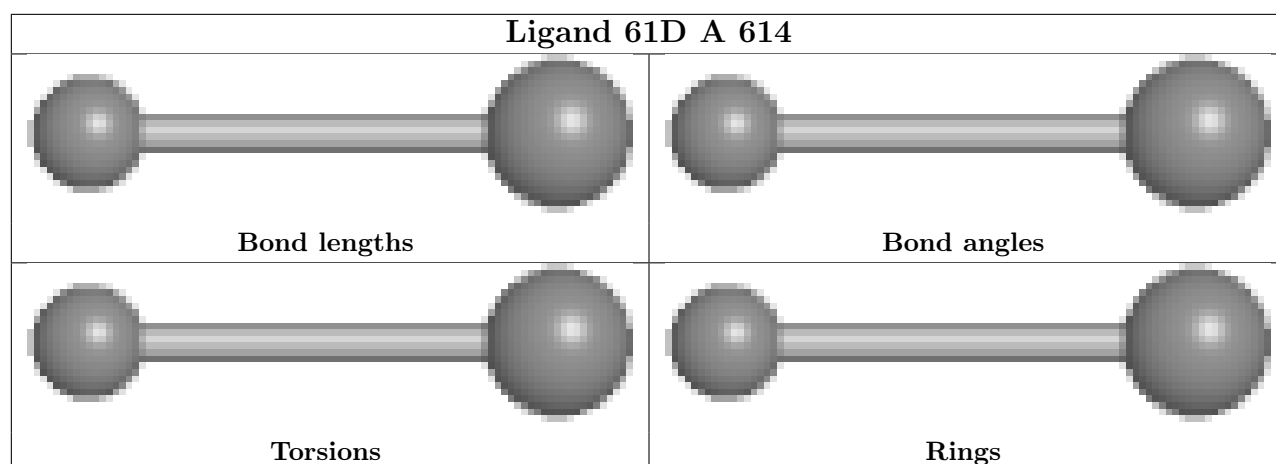
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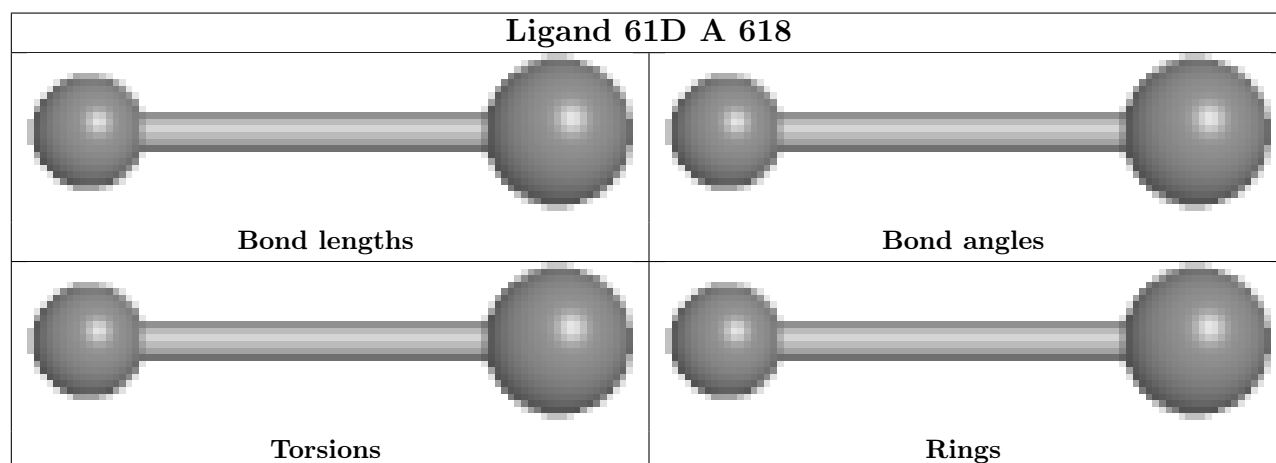
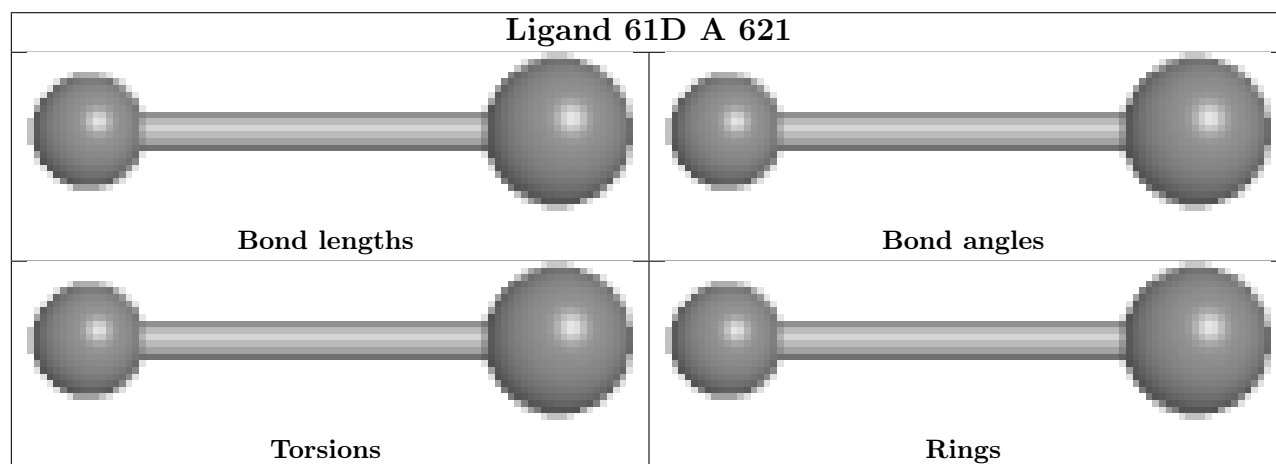
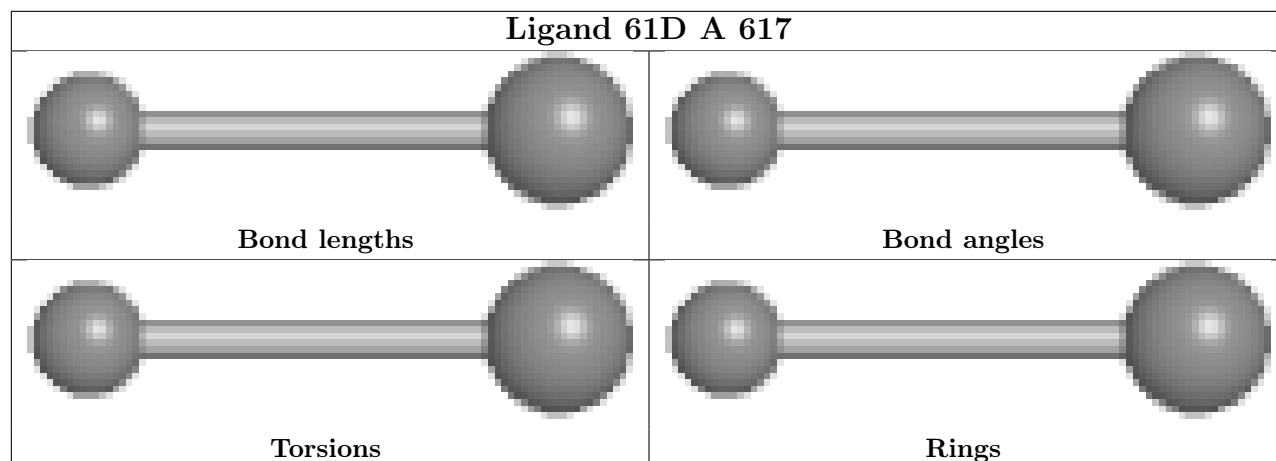
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	621	61D	3	0
7	A	618	61D	2	0
7	A	613	61D	1	0
2	A	601	HEM	3	0

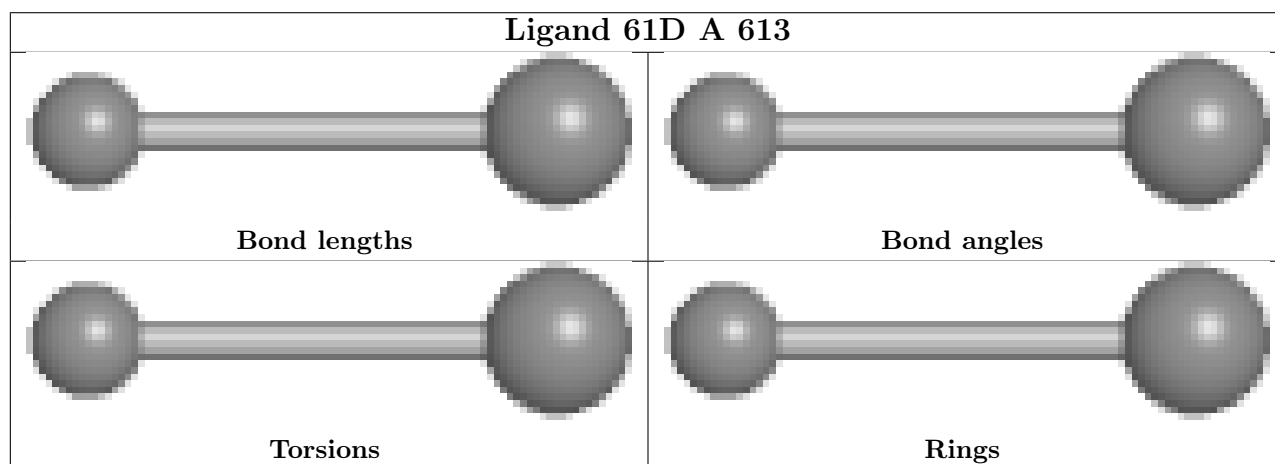
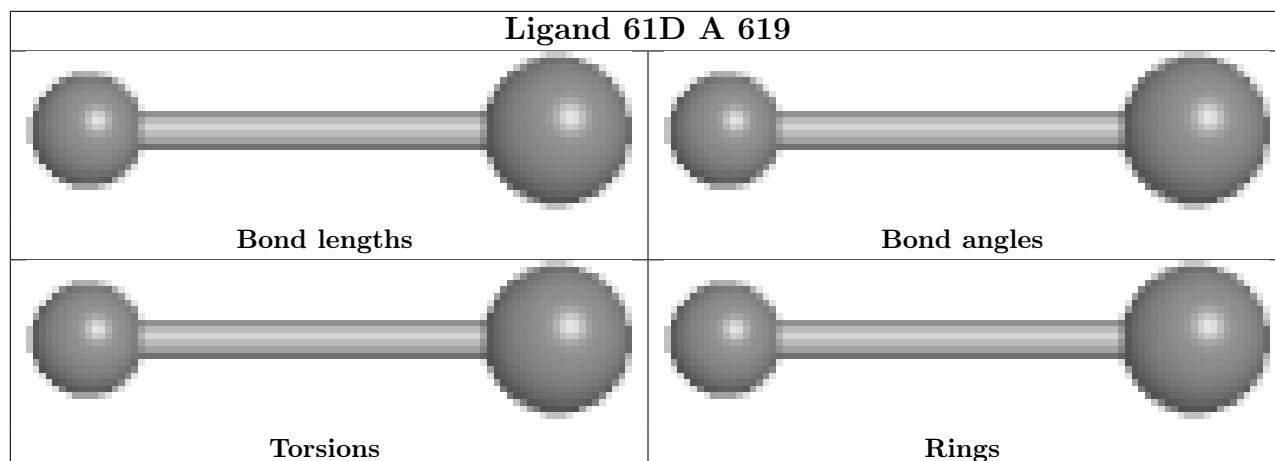
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

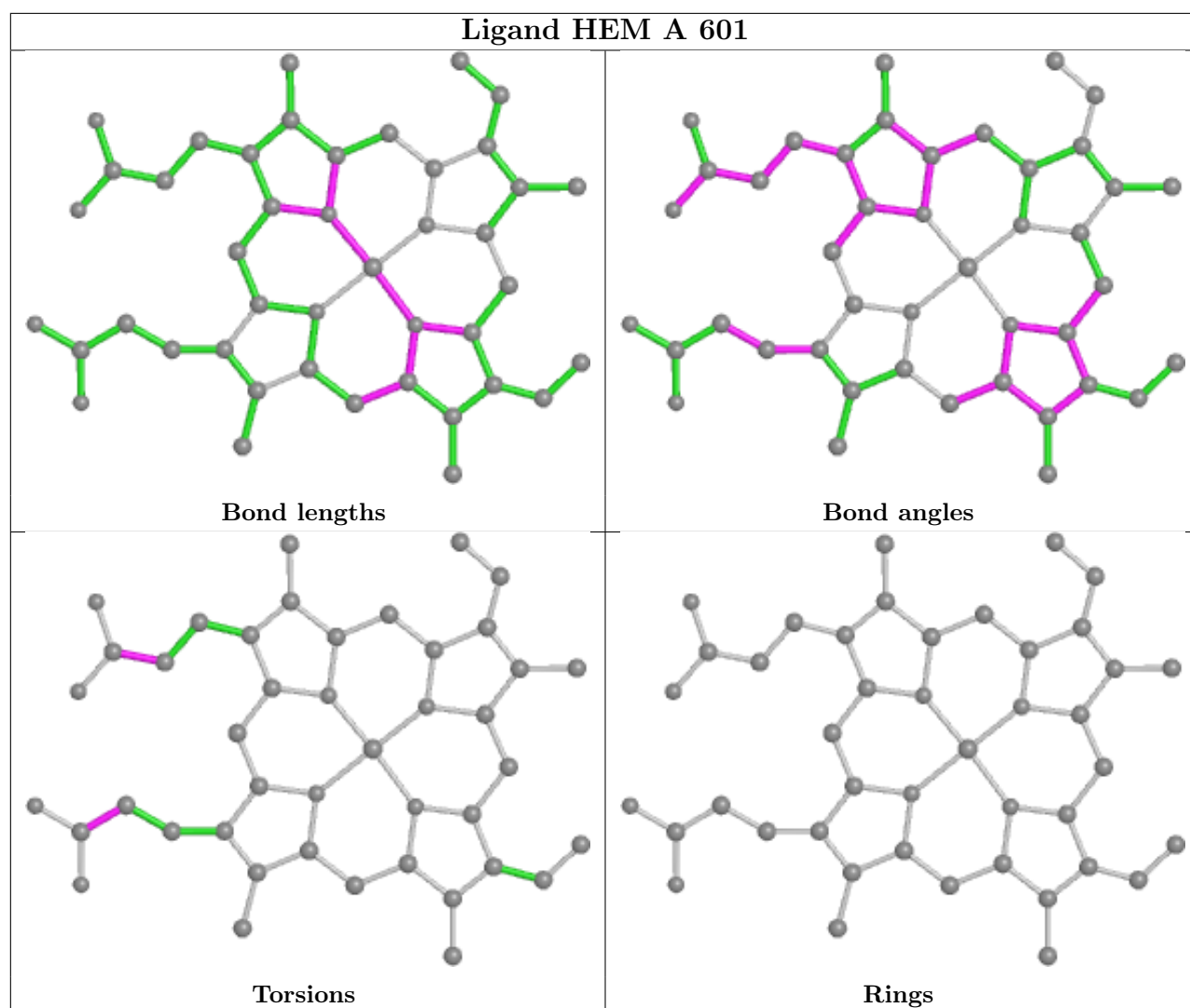












## 5.7 Other polymers [i](#)

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	595/595 (100%)	0.03	32 (5%) <span style="border: 1px solid red; padding: 2px;">25</span> <span style="border: 1px solid red; padding: 2px;">24</span>	38, 60, 128, 233	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	SER	15.3
1	A	174	SER	14.7
1	A	8	ALA	14.4
1	A	121	SER	13.9
1	A	595	ASN	11.1
1	A	173	GLN	11.1
1	A	2	TRP	7.7
1	A	4	VAL	7.3
1	A	12	LEU	7.3
1	A	13	VAL	6.9
1	A	594	GLU	5.8
1	A	5	GLY	5.7
1	A	7	GLY	5.7
1	A	175	LEU	4.3
1	A	122	SER	4.1
1	A	9	PRO	3.9
1	A	10	VAL	3.5
1	A	120	GLY	3.2
1	A	327	ARG	3.2
1	A	582	ILE	3.2
1	A	119	LEU	2.7
1	A	11	PRO	2.7
1	A	172	TYR	2.7
1	A	170	PRO	2.6
1	A	124	HIS	2.4
1	A	131	GLU	2.4
1	A	593	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	220	TRP	2.3
1	A	136	GLY	2.2
1	A	562	VAL	2.2
1	A	564	LEU	2.0
1	A	283	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
4	NAG	A	603	14/15	0.86	0.21	83,93,99,106	0
7	61D	A	620	2/2	0.91	0.11	74,74,74,98	2
5	IOD	A	607	1/1	0.93	0.07	89,89,89,89	1
4	NAG	A	604	14/15	0.93	0.14	58,66,74,75	0
6	SO4	A	611	5/5	0.94	0.15	48,52,65,71	0
5	IOD	A	605	1/1	0.95	0.08	76,76,76,76	1
7	61D	A	617	2/2	0.97	0.05	85,85,85,104	2
7	61D	A	619	2/2	0.97	0.09	57,57,57,70	2
7	61D	A	614	2/2	0.97	0.09	89,89,89,101	2
7	61D	A	613	2/2	0.98	0.22	57,57,57,76	2
5	IOD	A	609	1/1	0.98	0.04	85,85,85,85	1
5	IOD	A	610	1/1	0.98	0.06	68,68,68,68	1
2	HEM	A	601	43/43	0.98	0.19	34,40,43,52	0
7	61D	A	612	2/2	0.98	0.18	55,55,55,67	2
7	61D	A	618	2/2	0.99	0.10	66,66,66,81	2
5	IOD	A	608	1/1	0.99	0.08	74,74,74,74	1
3	CA	A	602	1/1	0.99	0.16	49,49,49,49	0
7	61D	A	621	2/2	0.99	0.08	52,52,52,62	2

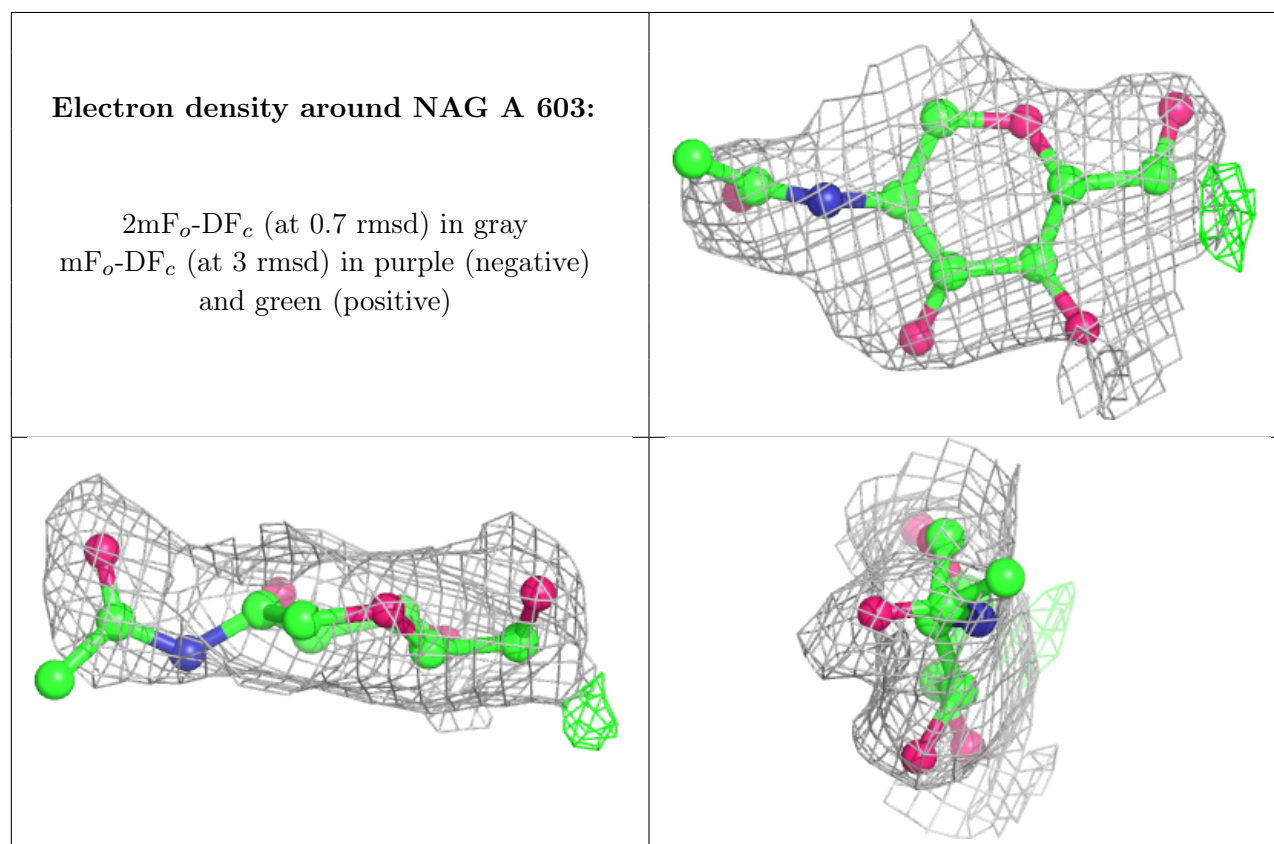
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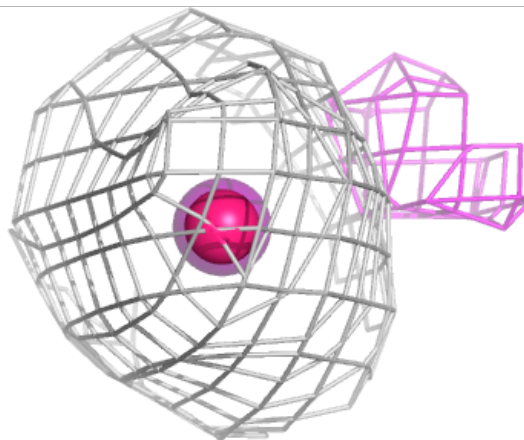
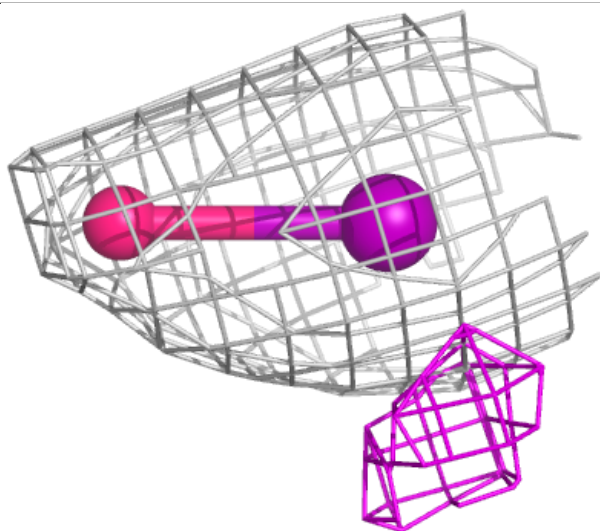
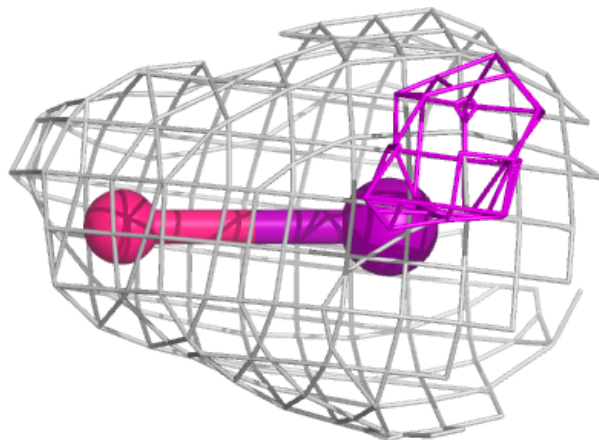
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	61D	A	616	2/2	1.00	0.11	39,39,39,54	2
5	IOD	A	606	1/1	1.00	0.07	61,61,61,61	1
7	61D	A	615	2/2	1.00	0.07	60,60,60,68	2
7	61D	A	622	2/2	1.00	0.11	46,46,46,54	2

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.



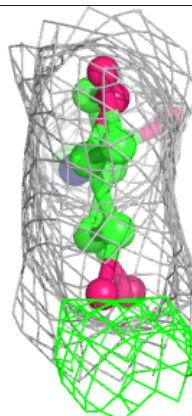
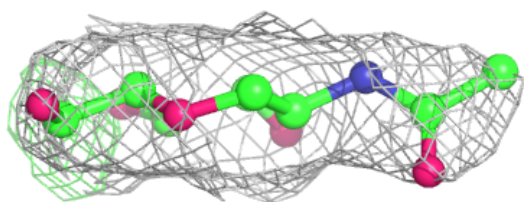
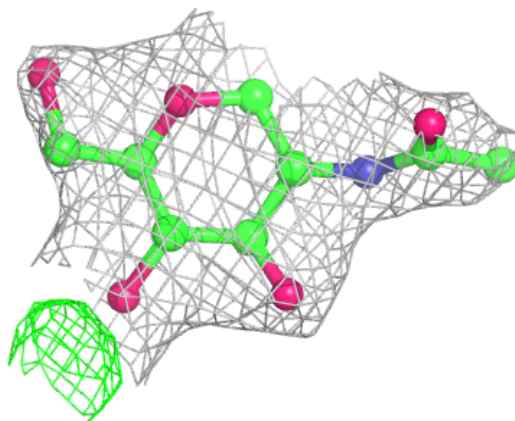
**Electron density around 61D A 620:**

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

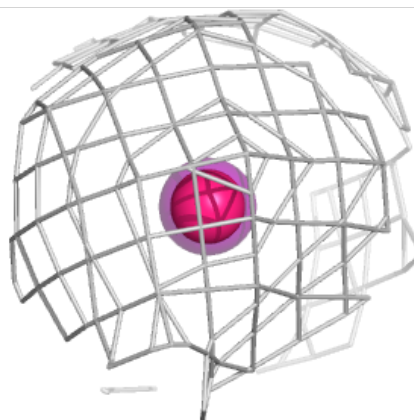
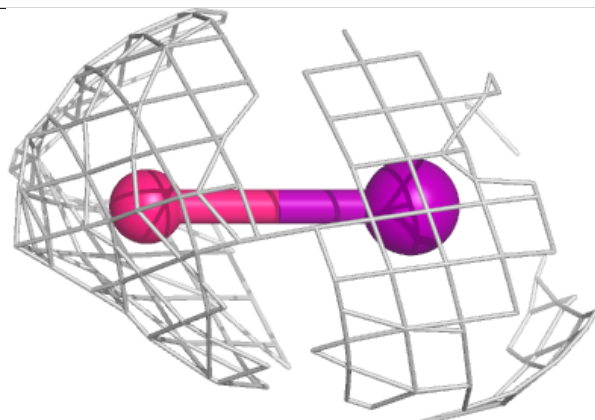
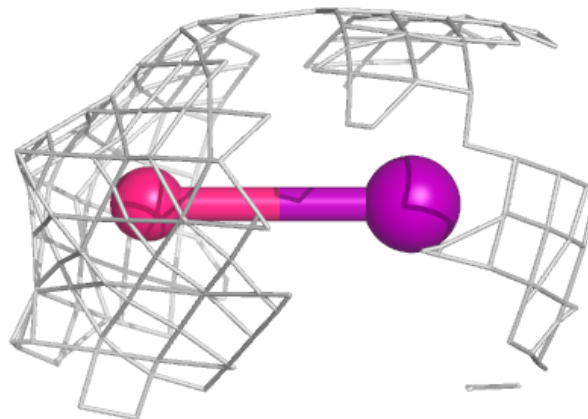


**Electron density around NAG A 604:**

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

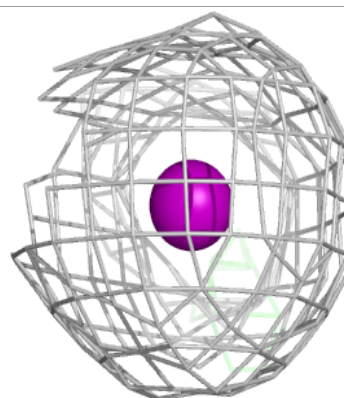
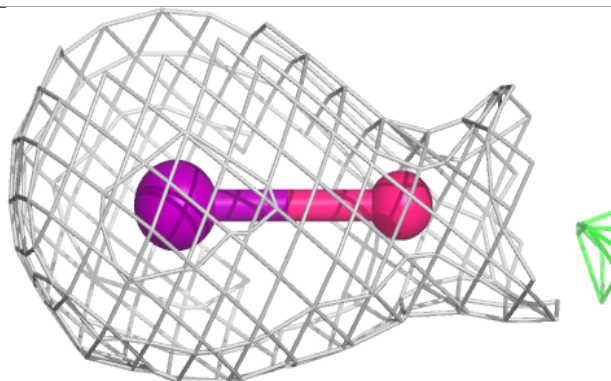
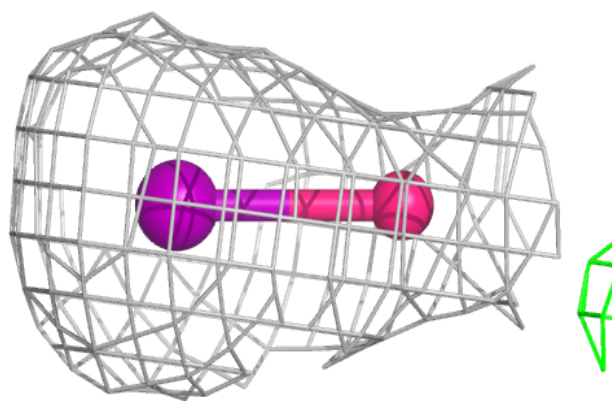
**Electron density around 61D A 617:**

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and green (positive)

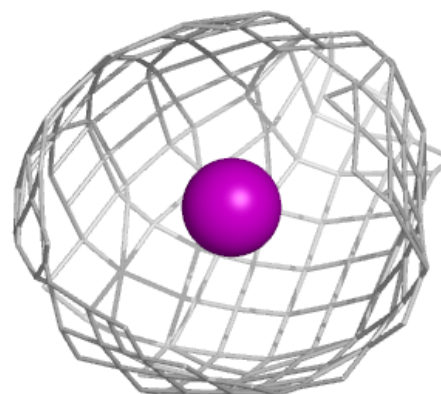
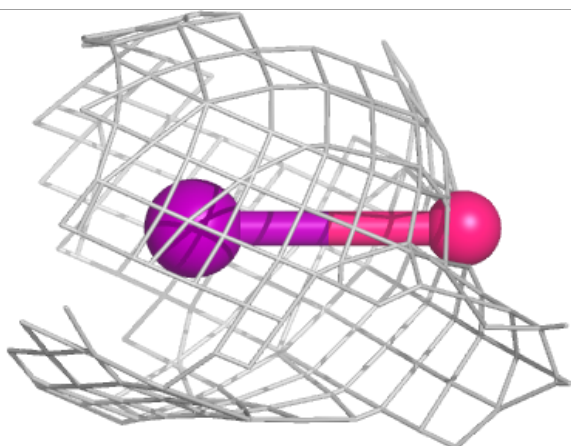
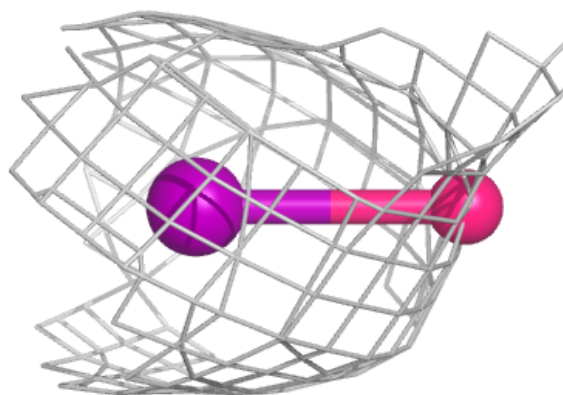


**Electron density around 61D A 619:**

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

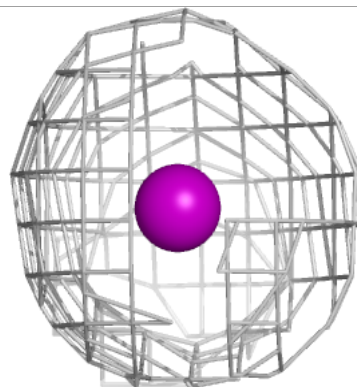
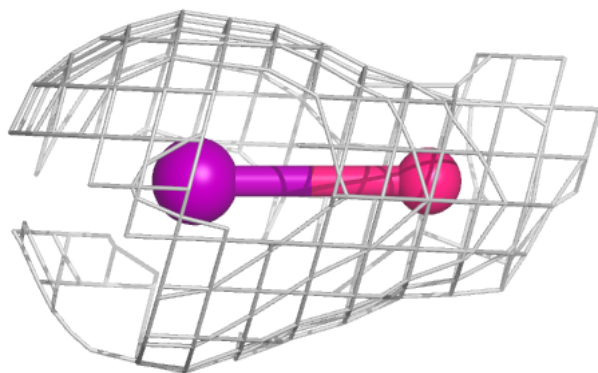
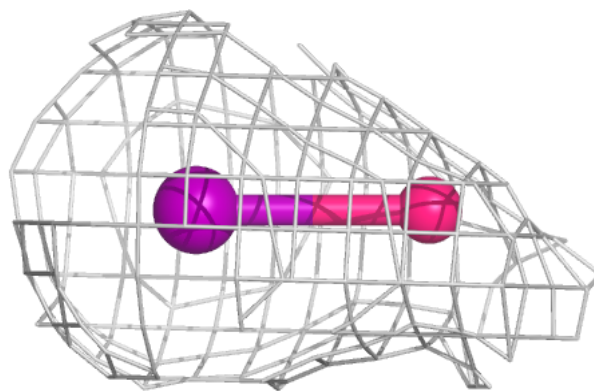
**Electron density around 61D A 614:**

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and green (positive)



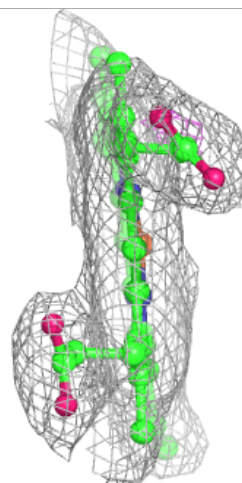
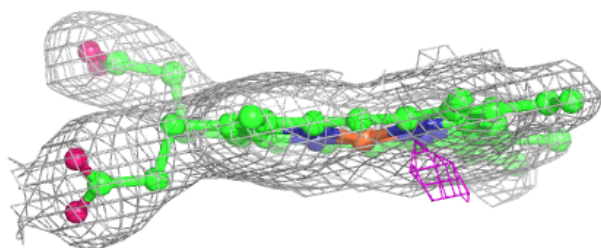
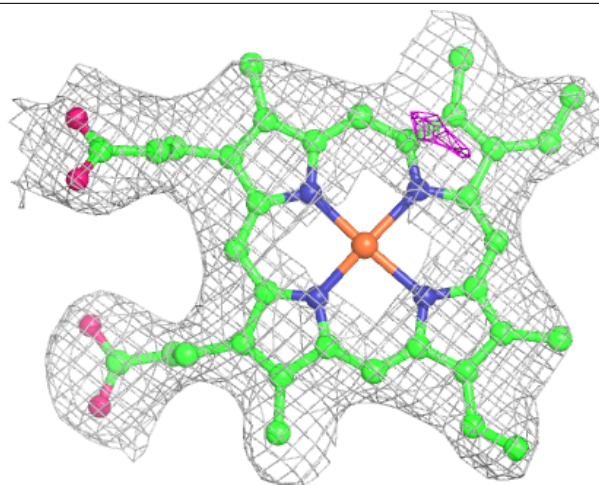
**Electron density around 61D A 613:**

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



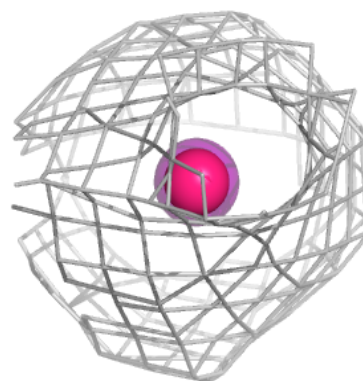
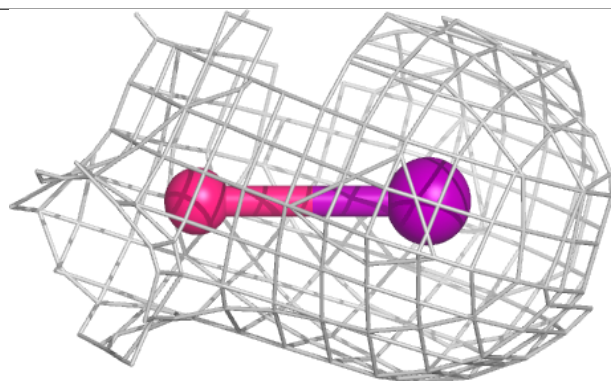
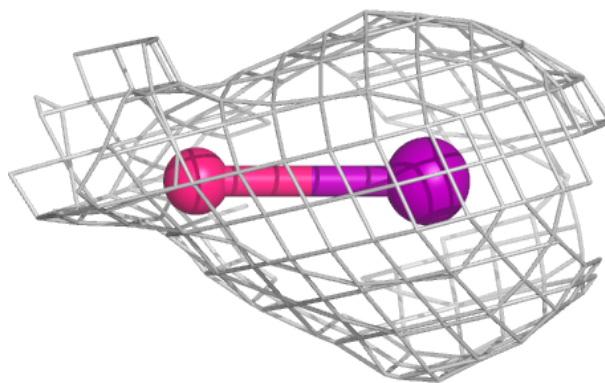
**Electron density around HEM A 601:**

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and green (positive)

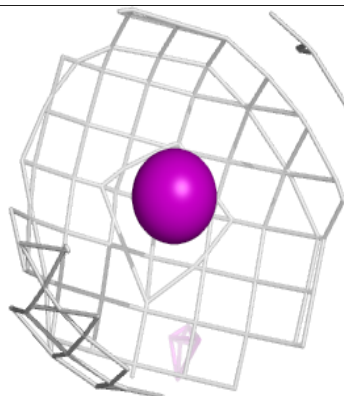
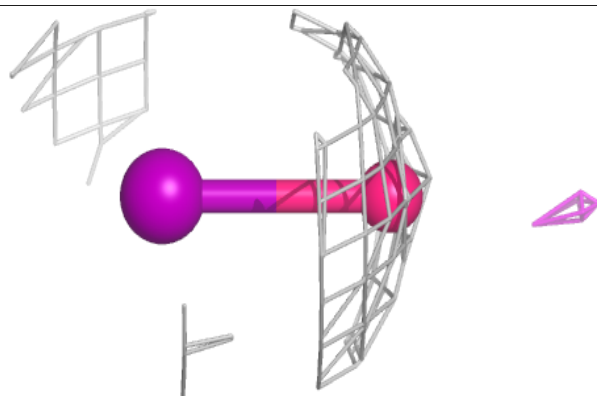
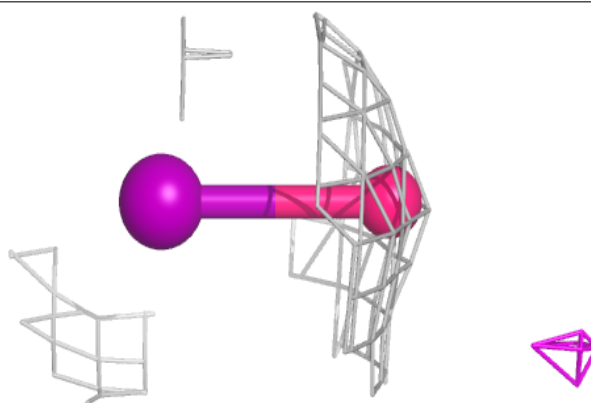


**Electron density around 61D A 612:**

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

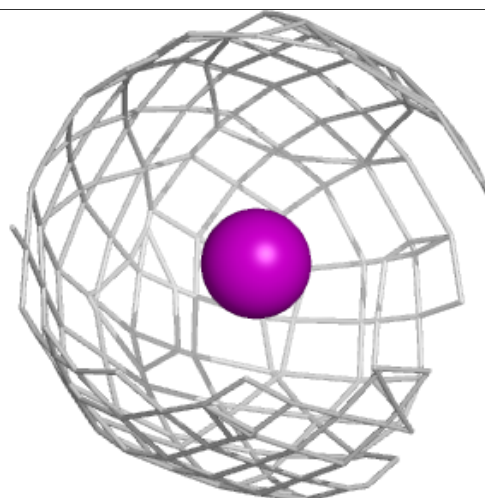
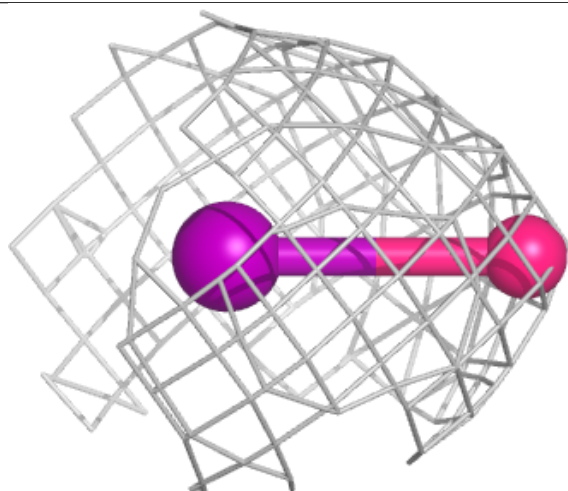
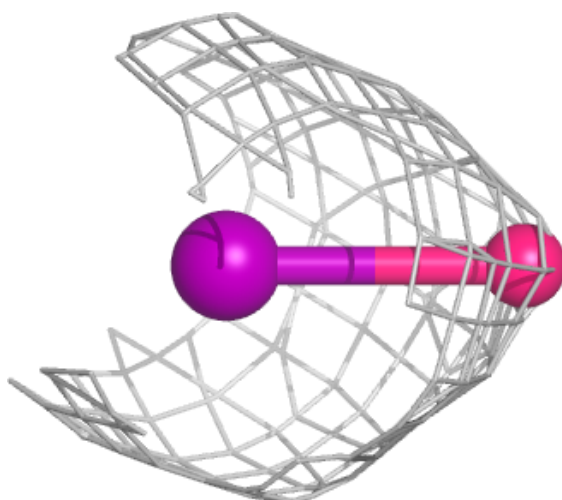
**Electron density around 61D A 618:**

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



**Electron density around 61D A 621:**

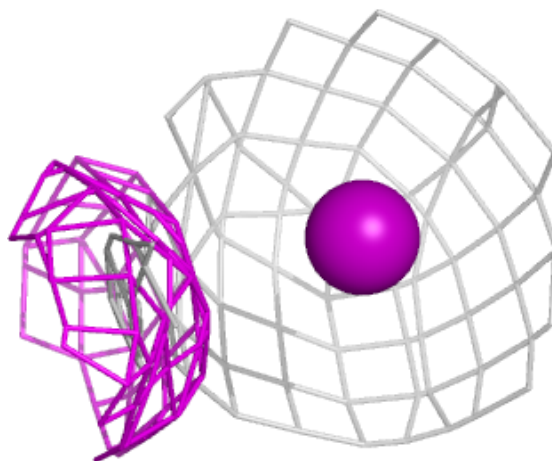
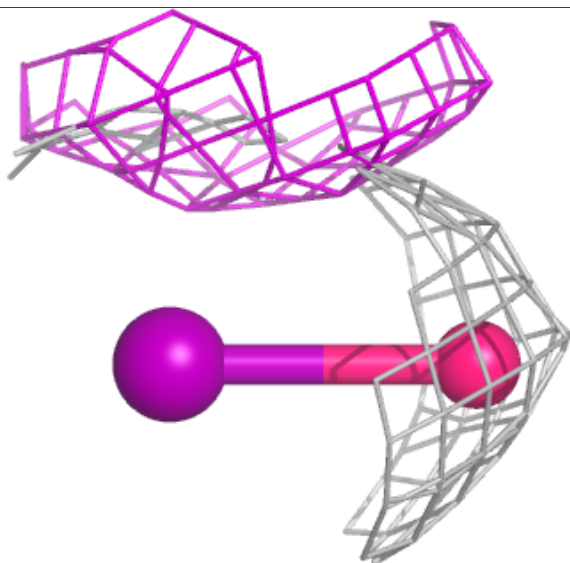
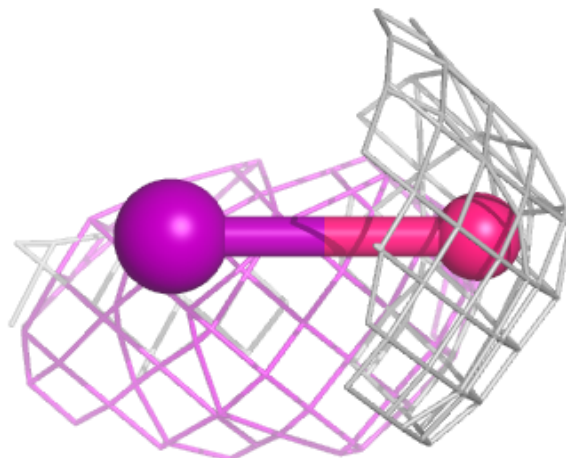
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





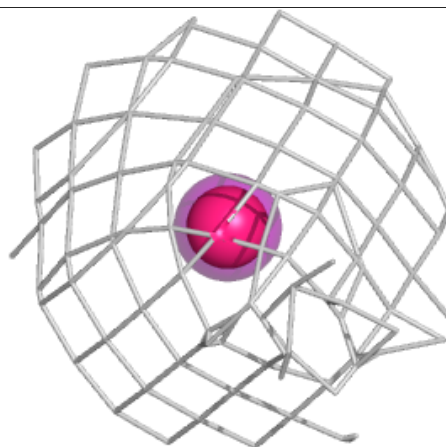
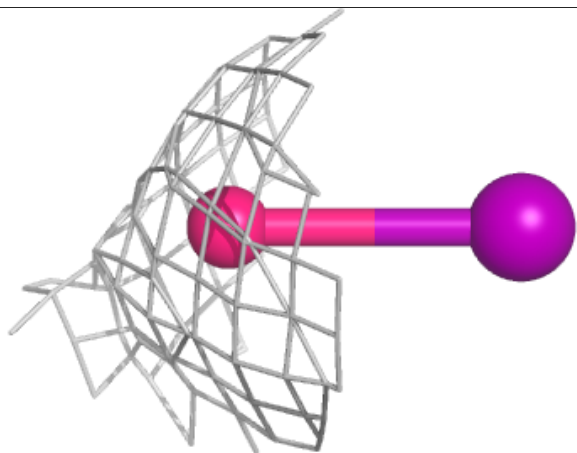
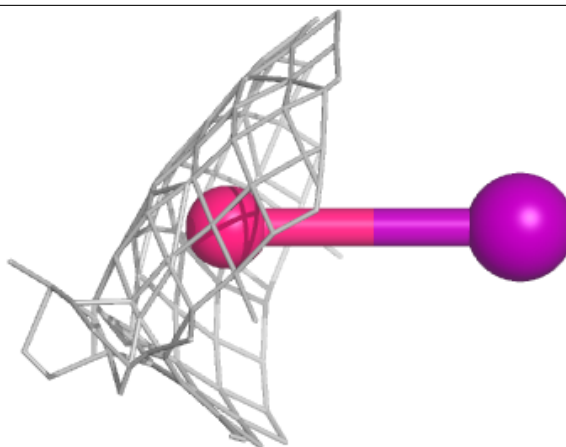
**Electron density around 61D A 616:**

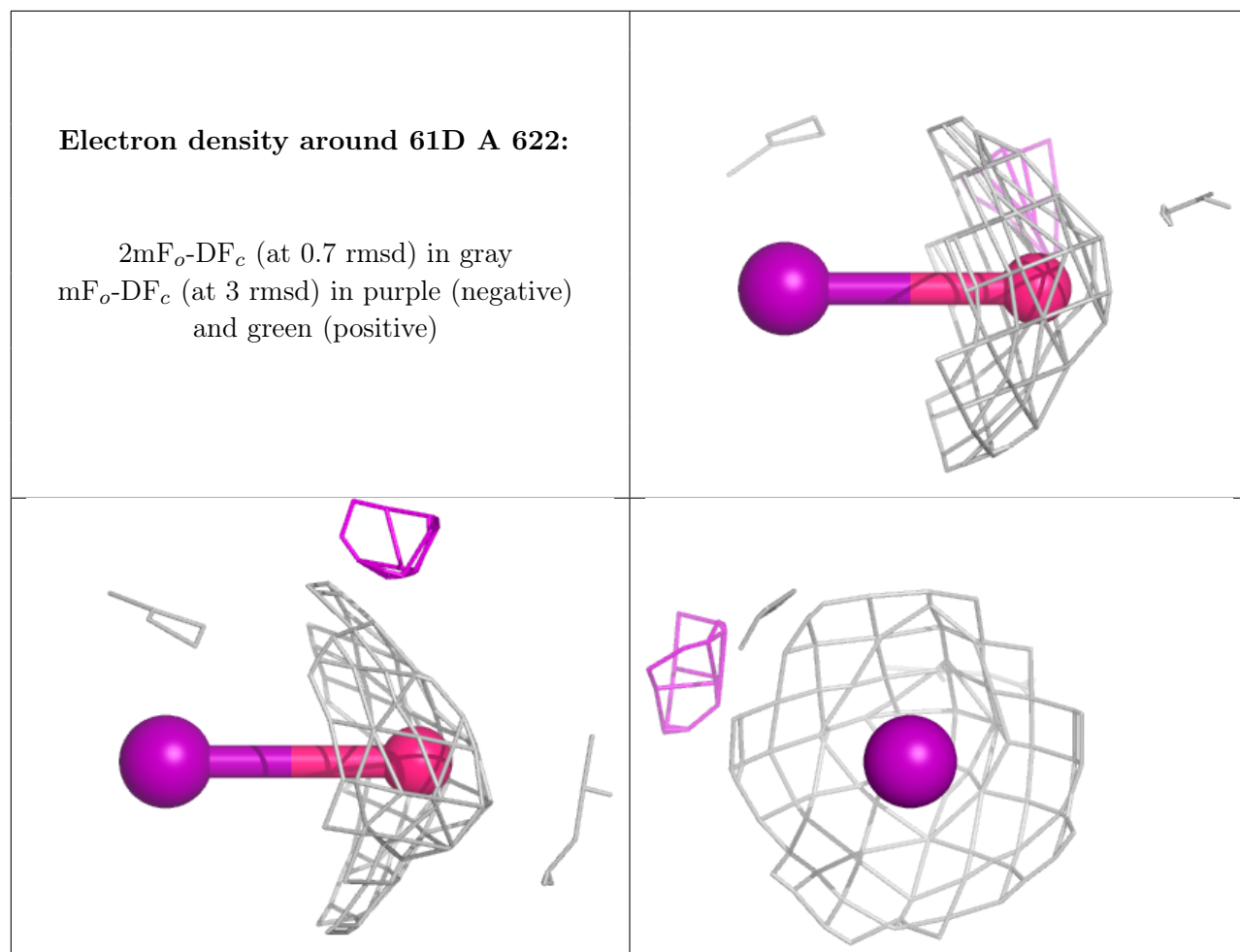
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 61D A 615:**

$2mF_o-DF_c$  (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.