



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 02:59 AM UTC

PDB ID : 9RJV / pdb\_00009rjv  
Title : W-formate dehydrogenase from Nitratidesulfovibrio vulgaris (Desulfovibrio vulgaris) - aerobic soaked with 55 bar oxygen  
Authors : Vilela-Alves, G.; Manuel, R.R.; Carpentier, P.; Pereira, I.C.; Romao, M.J.; Mota, C.  
Deposited on : 2025-06-12  
Resolution : 1.83 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

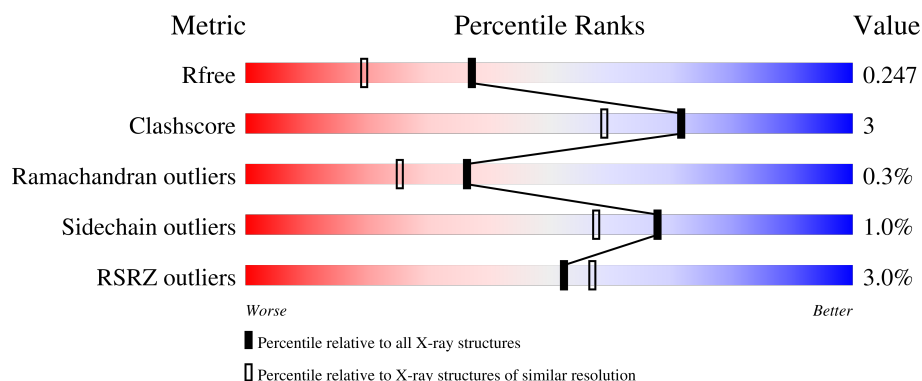
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 1.83 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	1013	
2	B	215	

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	GOL	A	1118	-	-	X	-
7	GOL	B	304	-	-	X	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 9830 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 Formate dehydrogenase, alpha subunit, selenocysteine-containing.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	967	Total	C	N	O	S	Se	0	0	0
			7570	4825	1320	1383	41	1			

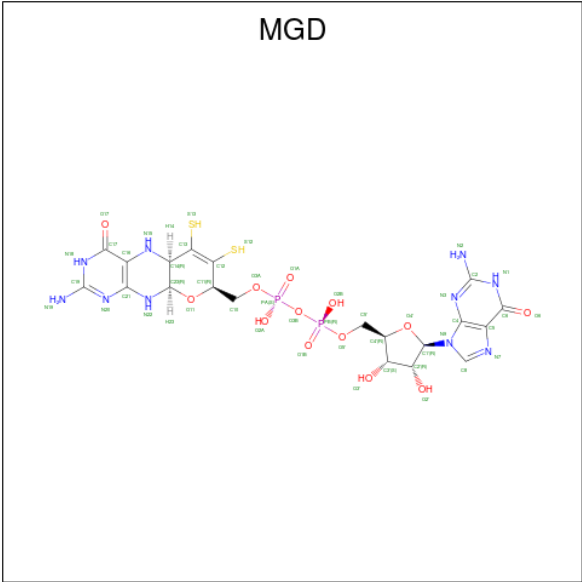
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1006	TRP	-	expression tag	UNP Q72EJ1
A	1007	SER	-	expression tag	UNP Q72EJ1
A	1008	HIS	-	expression tag	UNP Q72EJ1
A	1009	PRO	-	expression tag	UNP Q72EJ1
A	1010	GLN	-	expression tag	UNP Q72EJ1
A	1011	PHE	-	expression tag	UNP Q72EJ1
A	1012	GLU	-	expression tag	UNP Q72EJ1
A	1013	LYS	-	expression tag	UNP Q72EJ1

- Molecule 2 is a protein called Formate dehydrogenase, beta subunit, putative.

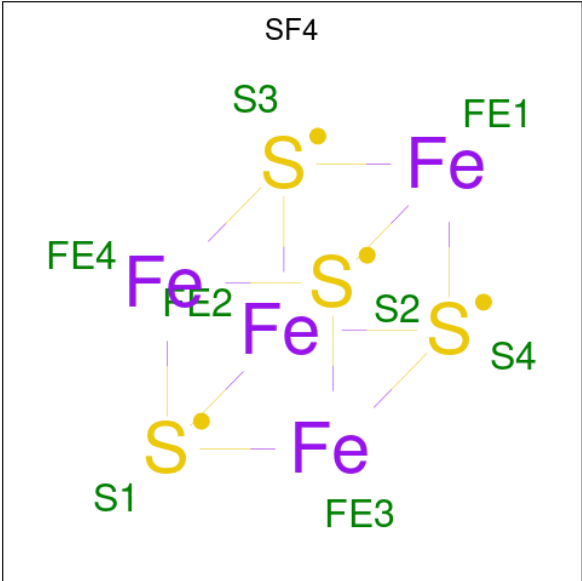
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	1	0
			1673	1046	293	318	16			

- Molecule 3 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (CCD ID: MGD) (formula: C<sub>20</sub>H<sub>26</sub>N<sub>10</sub>O<sub>13</sub>P<sub>2</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
3	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



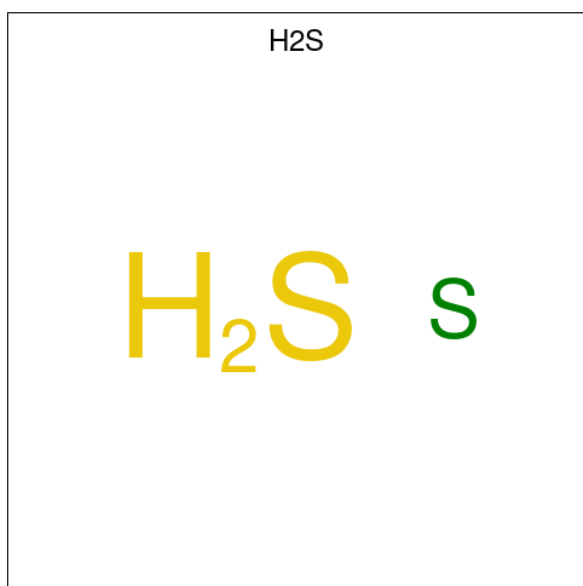
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is HYDROSULFURIC ACID (CCD ID: H2S) (formula: H<sub>2</sub>S) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is TUNGSTEN ION (CCD ID: W) (formula: W) (labeled as "Ligand of Interest" by depositor).

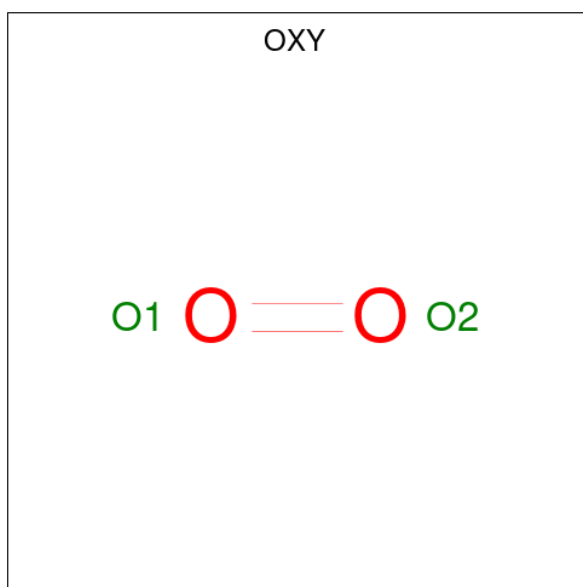
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	W	0	0
			1	1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 8 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O 2 2	0	0
8	A	1	Total O 2 2	0	0
8	A	1	Total O 2 2	0	0
8	A	1	Total O 2 2	0	0
8	A	1	Total O 2 2	0	0
8	A	1	Total O 2 2	0	0
8	A	1	Total O 2 2	0	0
8	A	1	Total O 2 2	0	0
8	A	1	Total O 2 2	0	0
8	A	1	Total O 2 2	0	0
8	B	1	Total O 2 2	0	0
8	B	1	Total O 2 2	0	0
8	B	1	Total O 2 2	0	0

- Molecule 9 is water.

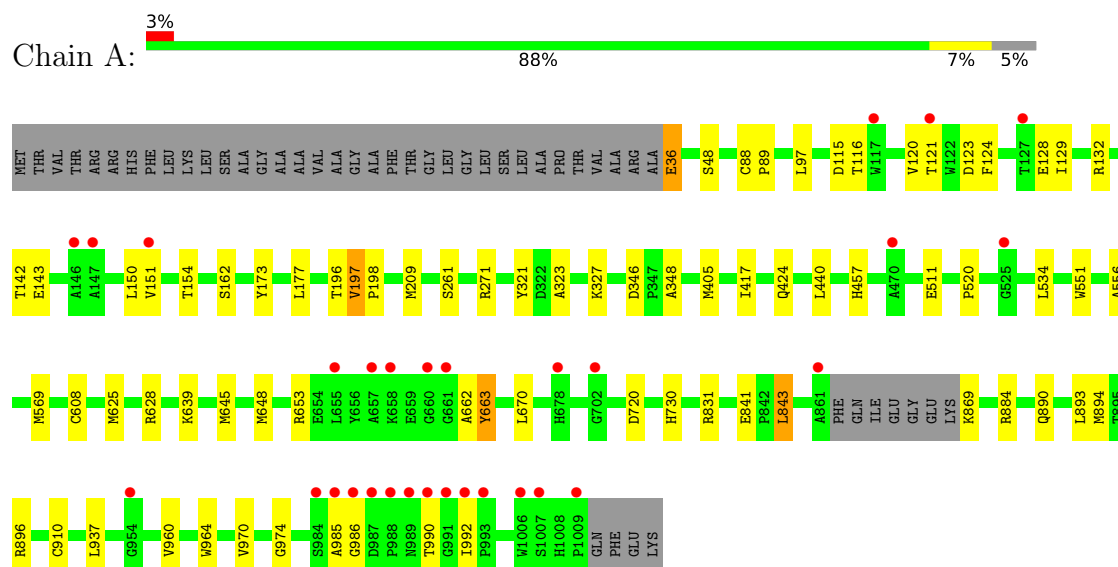


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	329	Total 329	O 329	0	0
9	B	74	Total 74	O 74	0	0

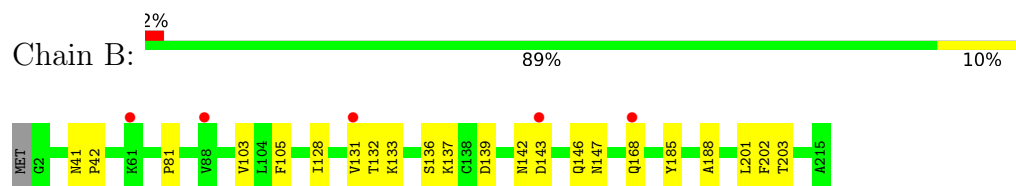
### 3 Residue-property plots [i](#)

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: Formate dehydrogenase, alpha subunit, selenocysteine-containing



- Molecule 2: Formate dehydrogenase, beta subunit, putative



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.84Å 128.38Å 148.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.65 – 1.83 43.65 – 1.83	Depositor EDS
% Data completeness (in resolution range)	99.7 (43.65-1.83) 99.1 (43.65-1.83)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.09 (at 1.83Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.195 , 0.241 0.203 , 0.247	Depositor DCC
$R_{free}$ test set	5550 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.5	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 28.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9830	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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: H2S, MGD, GOL, OXY, SF4, W, SEC

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	1.03	0/7774	1.31	2/10548 (0.0%)
2	B	1.04	0/1708	1.30	1/2314 (0.0%)
All	All	1.03	0/9482	1.31	3/12862 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	143	ASP	CA-CB-CG	9.17	121.77	112.60
1	A	97	LEU	CA-C-N	5.26	125.68	119.94
1	A	97	LEU	C-N-CA	5.26	125.68	119.94

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	7570	0	7395	48	0
2	B	1673	0	1640	15	0
3	A	94	0	44	1	0
4	A	8	0	0	0	0
4	B	24	0	0	1	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	1	0	0	0	0
7	A	24	0	32	4	0
7	B	6	0	8	4	0
8	A	20	0	0	1	0
8	B	6	0	0	0	0
9	A	329	0	0	3	0
9	B	74	0	0	1	0
All	All	9830	0	9119	62	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 3.

All (62) 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:B:137:LYS:O	7:B:304:GOL:H2	1.88	0.73
1:A:121:THR:HG23	9:A:1474:HOH:O	1.90	0.69
1:A:120:VAL:HG21	1:A:124:PHE:CD2	2.28	0.68
1:A:457:HIS:NE2	7:A:1118:GOL:H31	2.10	0.66
2:B:142:ASN:ND2	2:B:146[B]:GLN:OE1	2.31	0.64
1:A:121:THR:HG22	1:A:123:ASP:N	2.14	0.62
1:A:457:HIS:NE2	7:A:1118:GOL:C3	2.64	0.60
2:B:136:SER:HA	7:B:304:GOL:O2	2.06	0.56
1:A:120:VAL:CG2	1:A:124:PHE:CD2	2.89	0.55
1:A:937:LEU:C	1:A:937:LEU:HD12	2.33	0.54
1:A:209:MET:HE1	1:A:440:LEU:HD23	1.91	0.52
1:A:36:GLU:HA	2:B:147:ASN:OD1	2.08	0.52
1:A:128:GLU:O	1:A:132:ARG:HG2	2.10	0.52
1:A:121:THR:HG22	1:A:123:ASP:H	1.75	0.51
1:A:841:GLU:OE2	1:A:843:LEU:HB2	2.11	0.51
1:A:346:ASP:OD1	1:A:348:ALA:HB3	2.10	0.51
1:A:974:GLY:HA3	8:A:1109:OXY:O1	2.11	0.51
1:A:534:LEU:CD2	1:A:986:GLY:HA3	2.41	0.51
1:A:556:ALA:HB2	1:A:569:MET:HE1	1.93	0.51
1:A:88:CYS:HB2	1:A:89:PRO:HD2	1.93	0.50
1:A:893:LEU:C	1:A:893:LEU:HD23	2.36	0.50
2:B:41:ASN:HA	2:B:42:PRO:C	2.37	0.49
1:A:209:MET:CE	1:A:440:LEU:HD23	2.43	0.49
2:B:201:LEU:C	2:B:201:LEU:HD23	2.39	0.48
1:A:910:CYS:SG	1:A:960:VAL:HG13	2.53	0.47
1:A:653:ARG:NH2	1:A:670:LEU:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:890:GLN:HA	1:A:964:TRP:CH2	2.49	0.46
1:A:405:MET:HE1	1:A:884:ARG:HH12	1.81	0.46
1:A:173:TYR:CE2	1:A:177:LEU:HD11	2.51	0.46
2:B:128:ILE:HG22	9:B:460:HOH:O	2.16	0.45
1:A:48:SER:HA	1:A:628:ARG:HB2	1.98	0.45
1:A:162:SER:HB2	1:A:551:TRP:O	2.16	0.45
1:A:115:ASP:OD1	1:A:116:THR:HG23	2.16	0.44
1:A:196:THR:HB	1:A:417:ILE:HG13	2.00	0.44
2:B:185:TYR:CD1	2:B:203:THR:HB	2.53	0.44
2:B:139:ASP:HB3	7:B:304:GOL:H11	1.99	0.43
1:A:129:ILE:HG21	1:A:648:MET:HE2	2.00	0.43
1:A:937:LEU:HD12	1:A:937:LEU:O	2.17	0.43
1:A:151:VAL:O	1:A:520:PRO:HA	2.19	0.43
1:A:894:MET:SD	3:A:1102:MGD:H2'	2.59	0.43
1:A:720:ASP:OD1	1:A:720:ASP:C	2.61	0.43
2:B:105:PHE:HB2	7:B:304:GOL:C3	2.49	0.43
1:A:831:ARG:NH1	9:A:1211:HOH:O	2.52	0.42
2:B:103:VAL:O	2:B:137:LYS:NZ	2.50	0.42
1:A:990:THR:O	1:A:992:ILE:HD12	2.19	0.42
2:B:168:GLN:H	2:B:168:GLN:CD	2.27	0.42
1:A:197:VAL:CG2	7:A:1118:GOL:H2	2.49	0.42
1:A:321:TYR:CE2	1:A:323:ALA:HA	2.54	0.42
1:A:173:TYR:CZ	1:A:177:LEU:HD11	2.53	0.42
1:A:608:CYS:HA	1:A:639:LYS:O	2.20	0.42
1:A:424:GLN:HA	1:A:424:GLN:OE1	2.19	0.42
1:A:662:ALA:O	1:A:663:TYR:C	2.62	0.42
1:A:173:TYR:HB2	1:A:645:MET:HE1	2.02	0.41
2:B:132:THR:O	2:B:133:LYS:HB2	2.20	0.41
1:A:625:MET:HE3	1:A:730:HIS:CE1	2.55	0.41
2:B:188:ALA:HA	2:B:202:PHE:O	2.21	0.41
1:A:121:THR:CG2	9:A:1474:HOH:O	2.62	0.41
1:A:457:HIS:NE2	7:A:1118:GOL:H32	2.34	0.41
2:B:81:PRO:HD2	4:B:302:SF4:S3	2.61	0.40
1:A:143:GLU:O	1:A:150:LEU:HD12	2.22	0.40
1:A:896:ARG:HD2	1:A:970:VAL:O	2.22	0.40
1:A:197:VAL:N	1:A:198:PRO:CD	2.85	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	962/1013 (95%)	922 (96%)	38 (4%)	2 (0%)	43	34
2	B	213/215 (99%)	204 (96%)	8 (4%)	1 (0%)	24	12
All	All	1175/1228 (96%)	1126 (96%)	46 (4%)	3 (0%)	36	25

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	131	VAL
1	A	985	ALA
1	A	663	TYR

### 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	786/819 (96%)	776 (99%)	10 (1%)	61	47
2	B	186/186 (100%)	186 (100%)	0	100	100
All	All	972/1005 (97%)	962 (99%)	10 (1%)	68	58

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	GLU
1	A	142	THR
1	A	154	THR

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Mol	Chain	Res	Type
1	A	197	VAL
1	A	261	SER
1	A	271	ARG
1	A	327	LYS
1	A	511	GLU
1	A	843	LEU
1	A	869	LYS

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	383	GLN
1	A	595	ASN
1	A	855	GLN

### 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 [i](#)

Of 26 ligands modelled in this entry, 1 is modelled with single atom and 1 is monoatomic - leaving 24 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	GOL	A	1108	-	5,5,5	0.22	0	5,5,5	0.56	0
7	GOL	A	1118	-	5,5,5	0.12	0	5,5,5	0.37	0
3	MGD	A	1102	6	47,52,52	0.81	3 (6%)	58,81,81	0.97	3 (5%)
7	GOL	A	1107	-	5,5,5	0.16	0	5,5,5	0.46	0
8	OXY	A	1114	-	1,1,1	0.03	0	-		
8	OXY	A	1109	-	1,1,1	0.22	0	-		
8	OXY	A	1115	-	1,1,1	0.02	0	-		
8	OXY	A	1112	-	1,1,1	0.06	0	-		
8	OXY	A	1117	-	1,1,1	0.13	0	-		
8	OXY	B	306	-	1,1,1	0.11	0	-		
4	SF4	B	303	2	0,12,12	-	-	-		
8	OXY	A	1119	-	1,1,1	0.04	0	-		
4	SF4	B	301	2	0,12,12	-	-	-		
4	SF4	B	302	2	0,12,12	-	-	-		
8	OXY	A	1110	-	1,1,1	0.04	0	-		
8	OXY	B	307	-	1,1,1	0.14	0	-		
8	OXY	A	1111	-	1,1,1	0.09	0	-		
7	GOL	A	1106	-	5,5,5	0.10	0	5,5,5	0.34	0
4	SF4	A	1103	1	0,12,12	-	-	-		
3	MGD	A	1101	6	47,52,52	0.86	2 (4%)	58,81,81	1.15	7 (12%)
7	GOL	B	304	-	5,5,5	0.27	0	5,5,5	1.07	0
8	OXY	A	1116	-	1,1,1	0.06	0	-		
8	OXY	A	1113	-	1,1,1	0.09	0	-		
8	OXY	B	305	-	1,1,1	0.10	0	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	A	1108	-	-	4/4/4/4	-
7	GOL	A	1118	-	-	0/4/4/4	-
3	MGD	A	1102	6	-	3/22/66/66	0/6/6/6
3	MGD	A	1101	6	-	1/22/66/66	0/6/6/6
7	GOL	B	304	-	-	0/4/4/4	-
4	SF4	B	301	2	-	-	0/6/5/5
4	SF4	B	302	2	-	-	0/6/5/5
7	GOL	A	1107	-	-	0/4/4/4	-
4	SF4	B	303	2	-	-	0/6/5/5
7	GOL	A	1106	-	-	2/4/4/4	-
4	SF4	A	1103	1	-	-	0/6/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	MGD	C23-C14	3.42	1.56	1.53
3	A	1102	MGD	C23-C14	3.00	1.56	1.53
3	A	1102	MGD	PA-O3B	2.83	1.62	1.59
3	A	1101	MGD	PB-O3B	2.81	1.62	1.59
3	A	1102	MGD	PB-O3B	2.06	1.61	1.59

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	MGD	O11-C23-C14	3.34	111.19	108.96
3	A	1101	MGD	C23-C14-N15	3.28	111.09	107.87
3	A	1101	MGD	C19-N20-C21	3.23	119.06	113.36
3	A	1102	MGD	C19-N20-C21	2.99	118.64	113.36
3	A	1102	MGD	O4'-C1'-C2'	-2.67	100.90	106.62
3	A	1101	MGD	O11-C23-N22	2.55	110.92	108.61
3	A	1102	MGD	C17-C16-N15	2.25	122.41	116.27
3	A	1101	MGD	O2A-PA-O3B	2.22	113.28	107.27
3	A	1101	MGD	C17-C16-N15	2.13	122.07	116.27
3	A	1101	MGD	C4'-O4'-C1'	-2.09	104.85	109.47

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1102	MGD	C4'-C5'-O5'-PB
3	A	1102	MGD	O4'-C4'-C5'-O5'
7	A	1106	GOL	C1-C2-C3-O3
7	A	1108	GOL	C1-C2-C3-O3
7	A	1106	GOL	O2-C2-C3-O3
7	A	1108	GOL	O2-C2-C3-O3
3	A	1102	MGD	C3'-C4'-C5'-O5'
3	A	1101	MGD	PA-O3B-PB-O5'
7	A	1108	GOL	O1-C1-C2-C3
7	A	1108	GOL	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 11 short contacts:

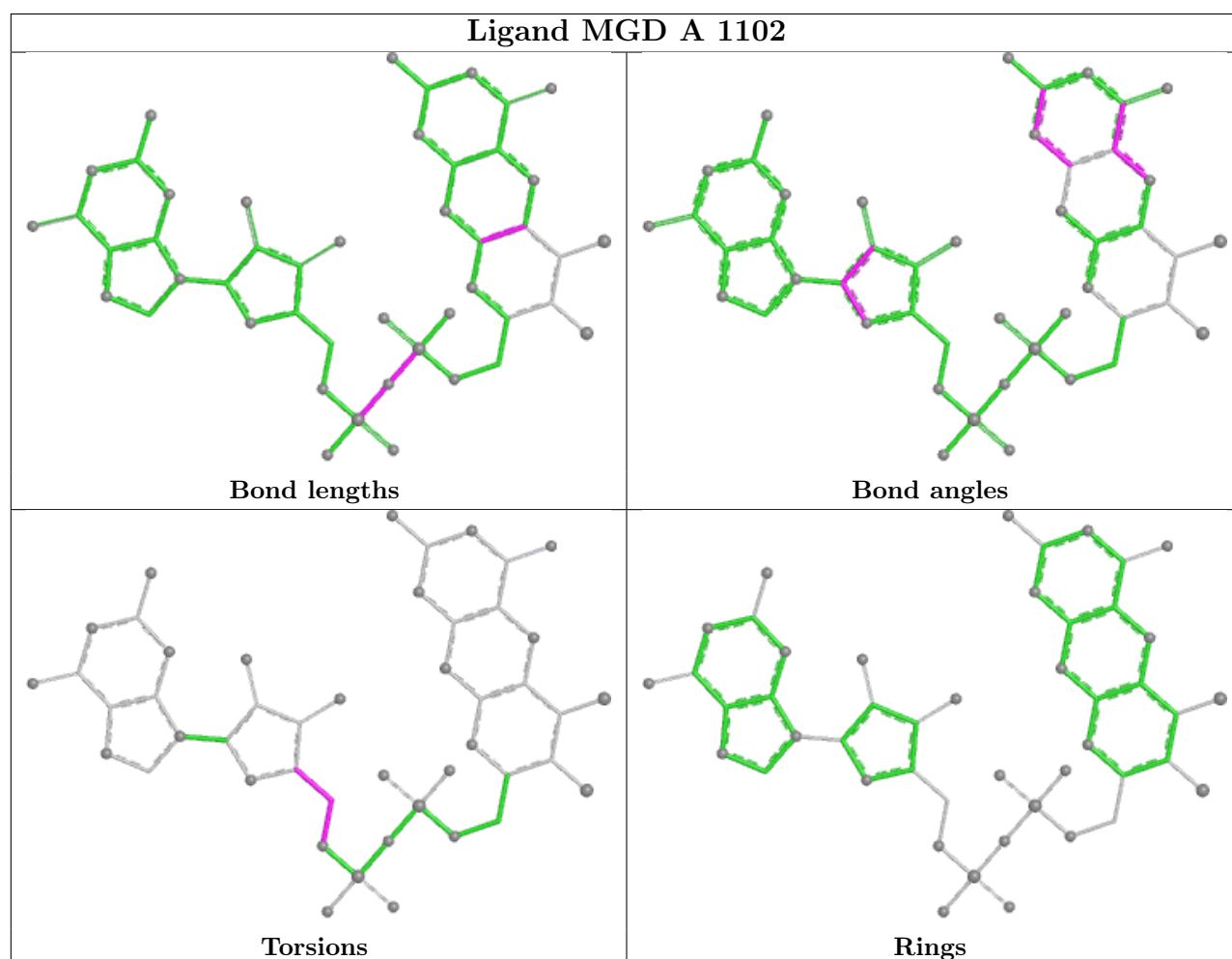
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1118	GOL	4	0

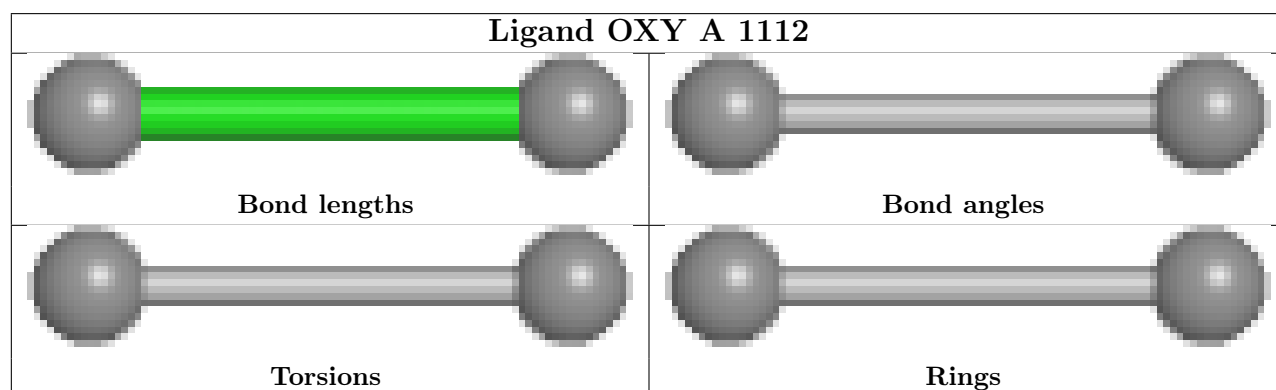
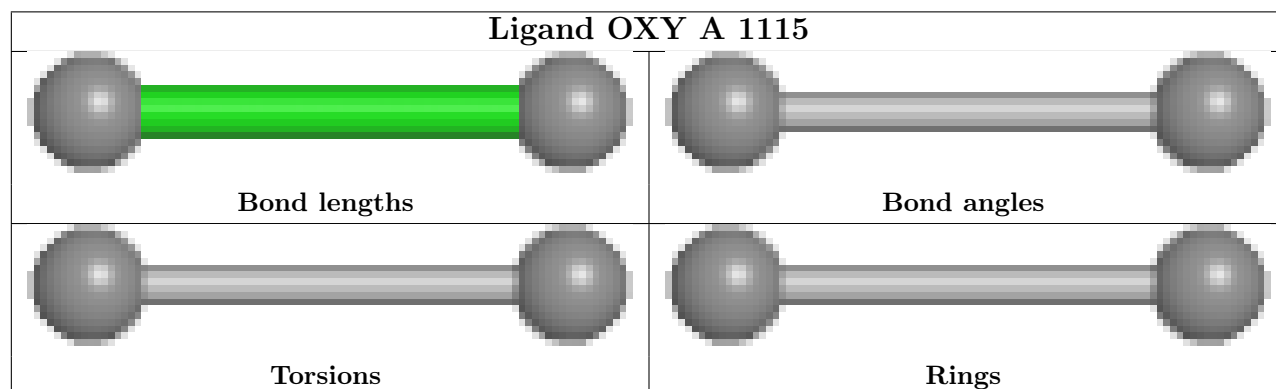
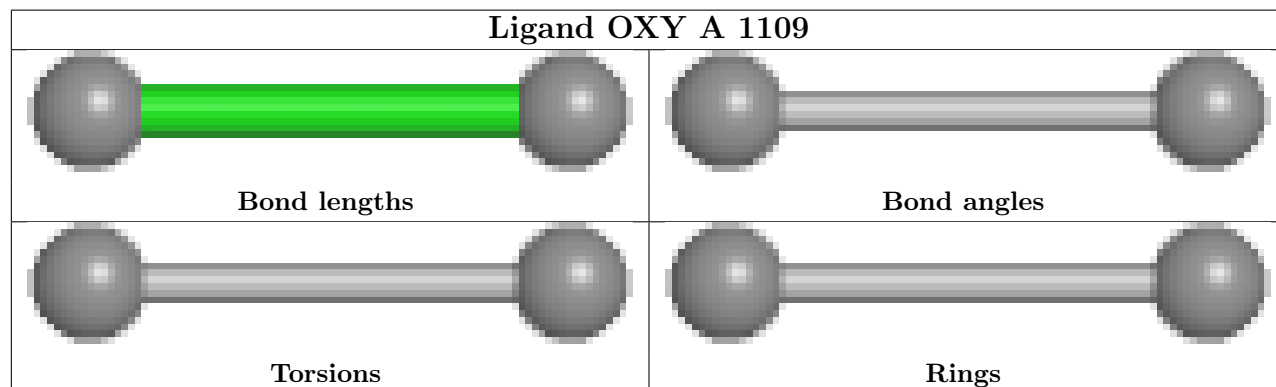
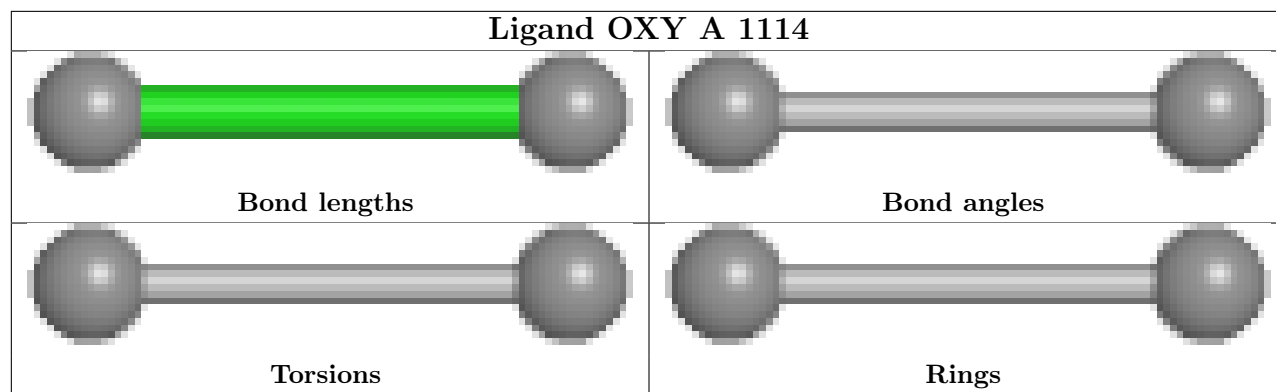
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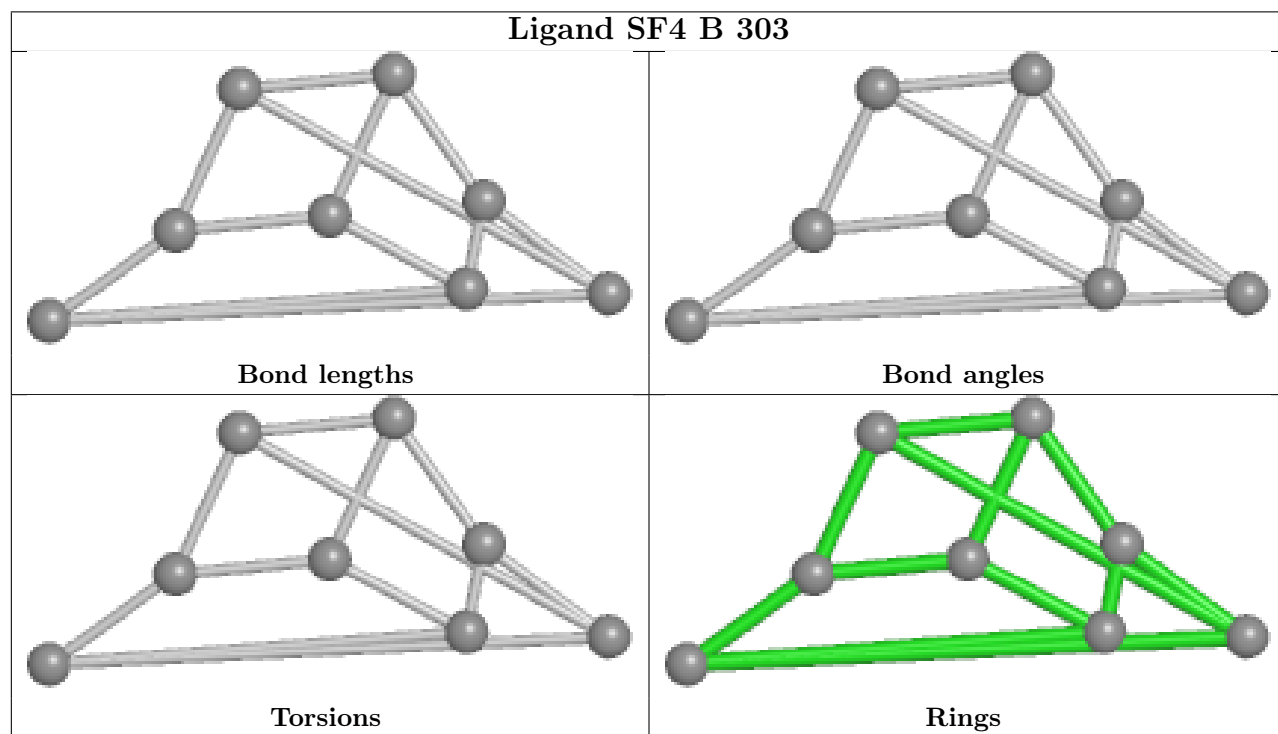
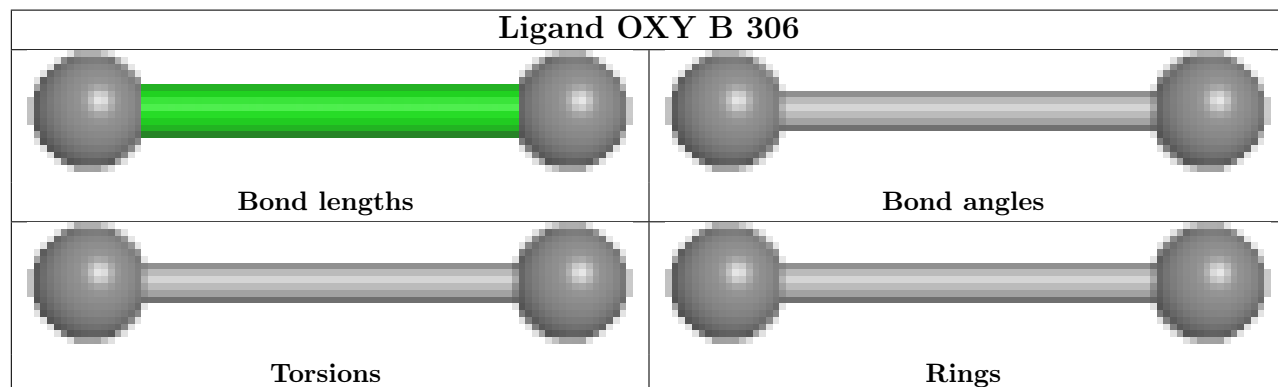
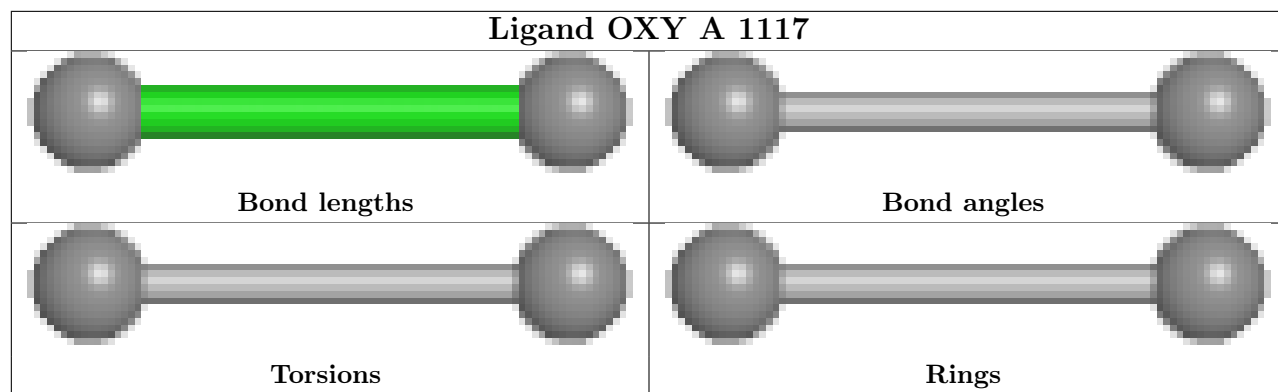
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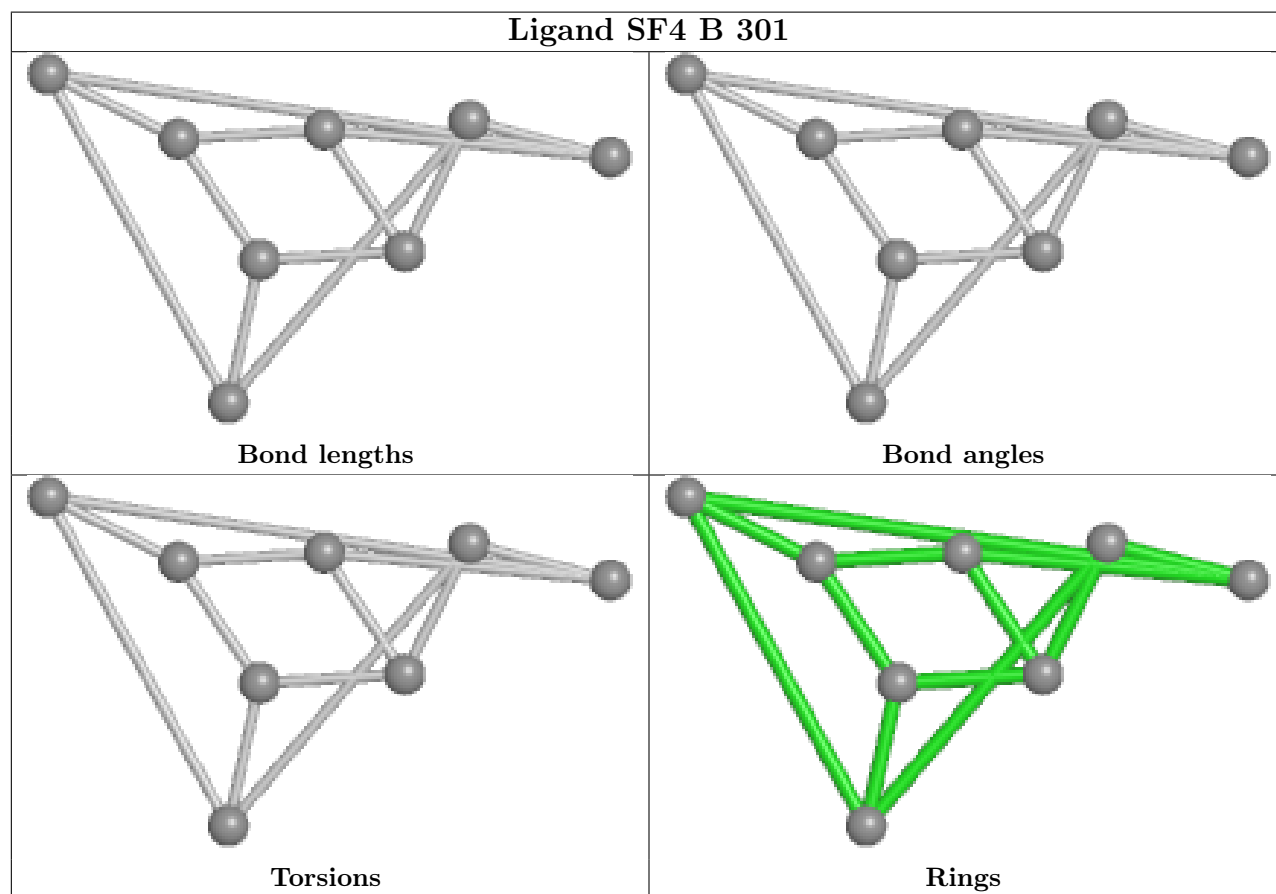
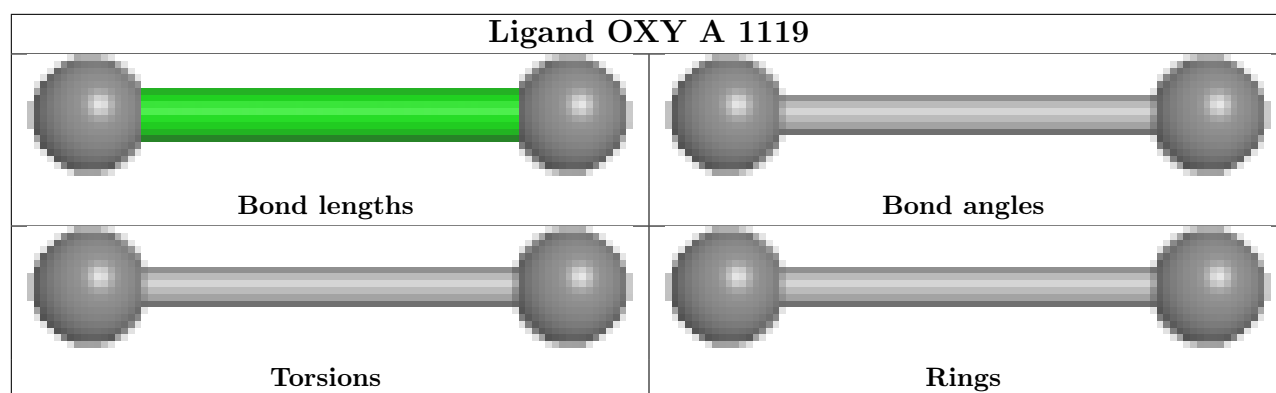
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1102	MGD	1	0
8	A	1109	OXY	1	0
4	B	302	SF4	1	0
7	B	304	GOL	4	0

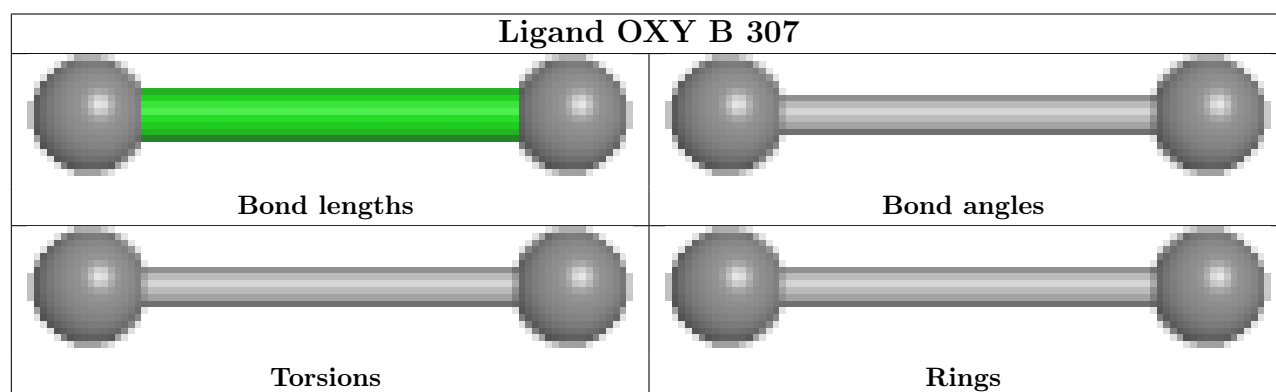
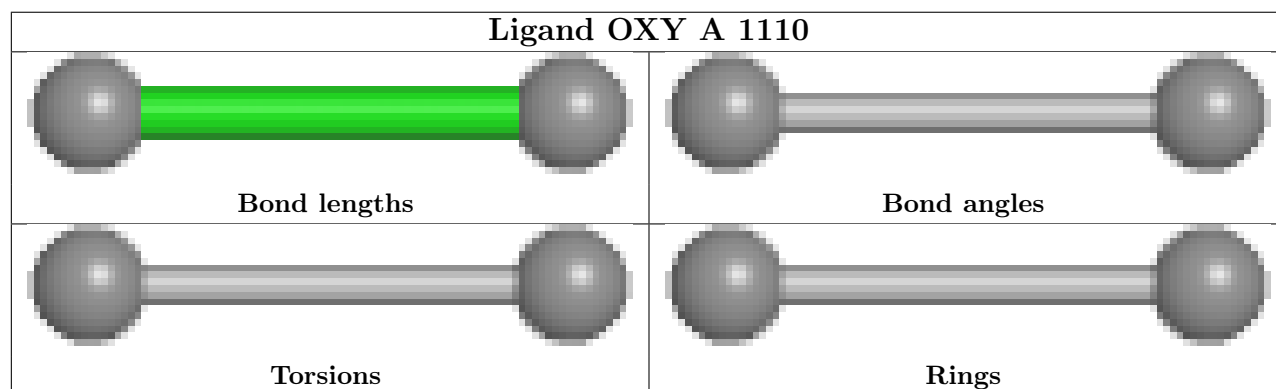
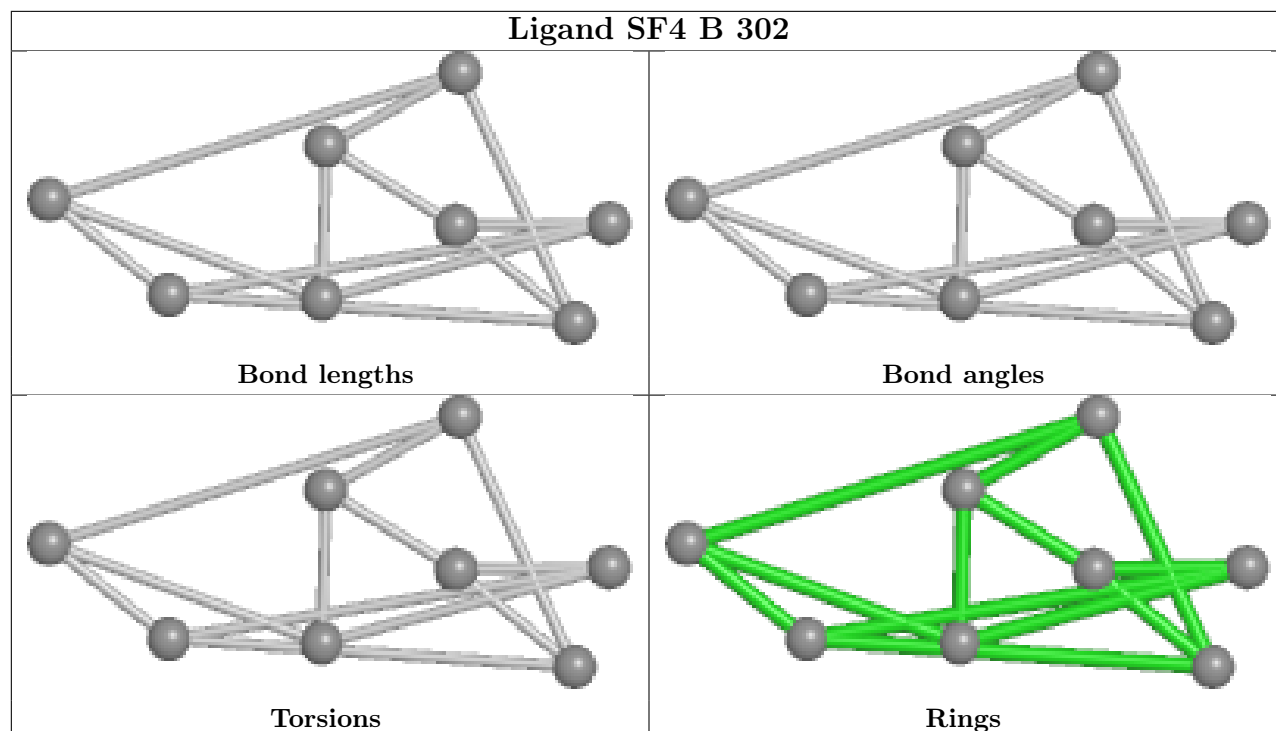
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

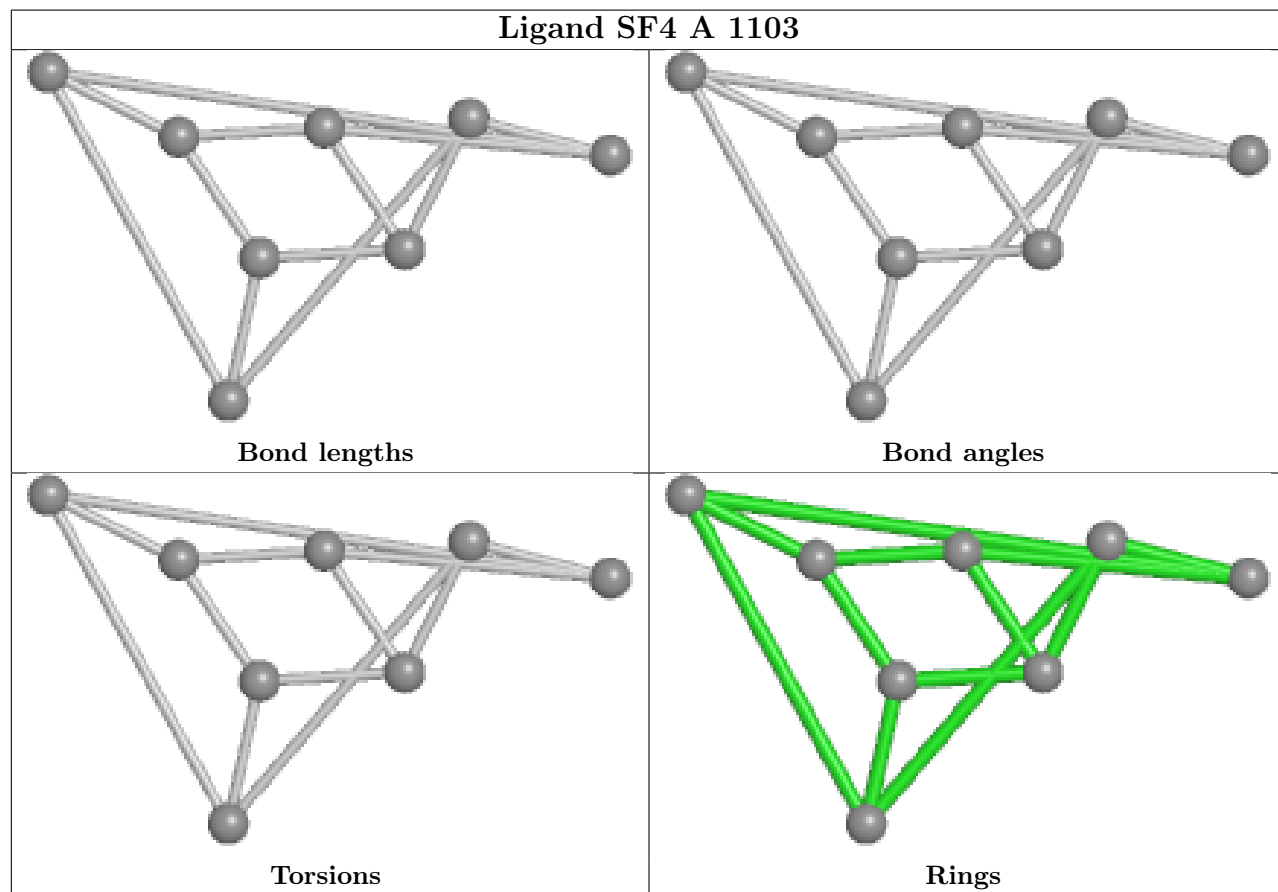
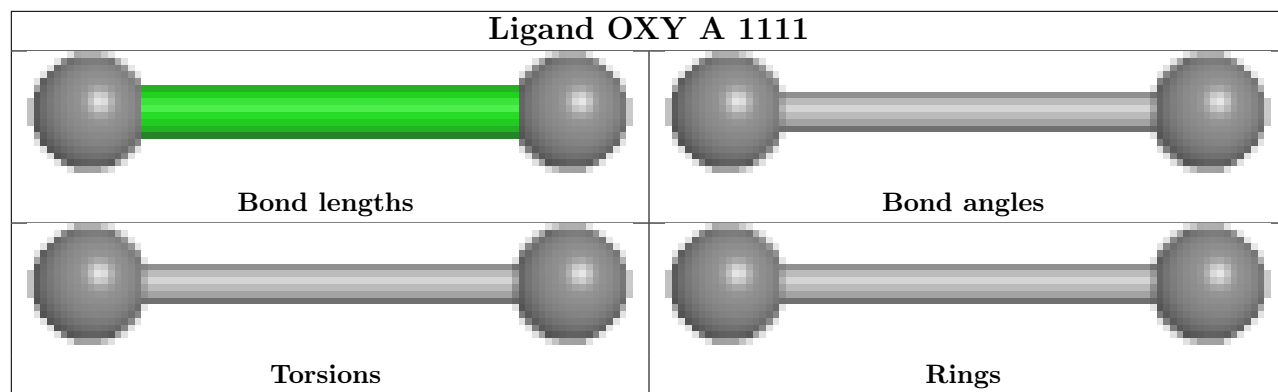




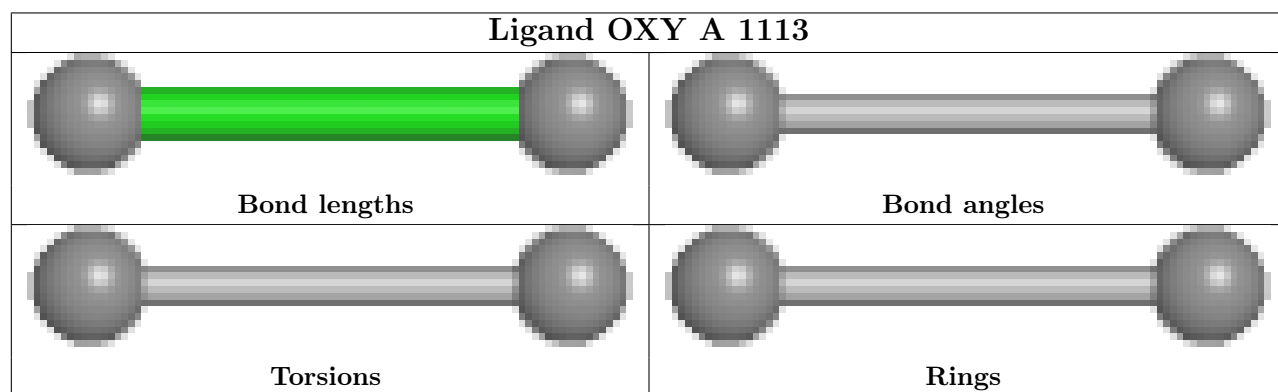
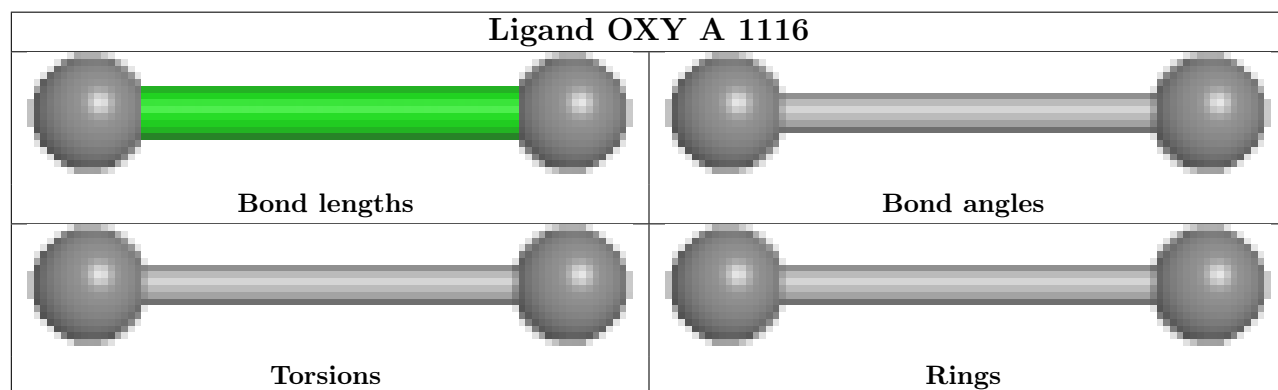
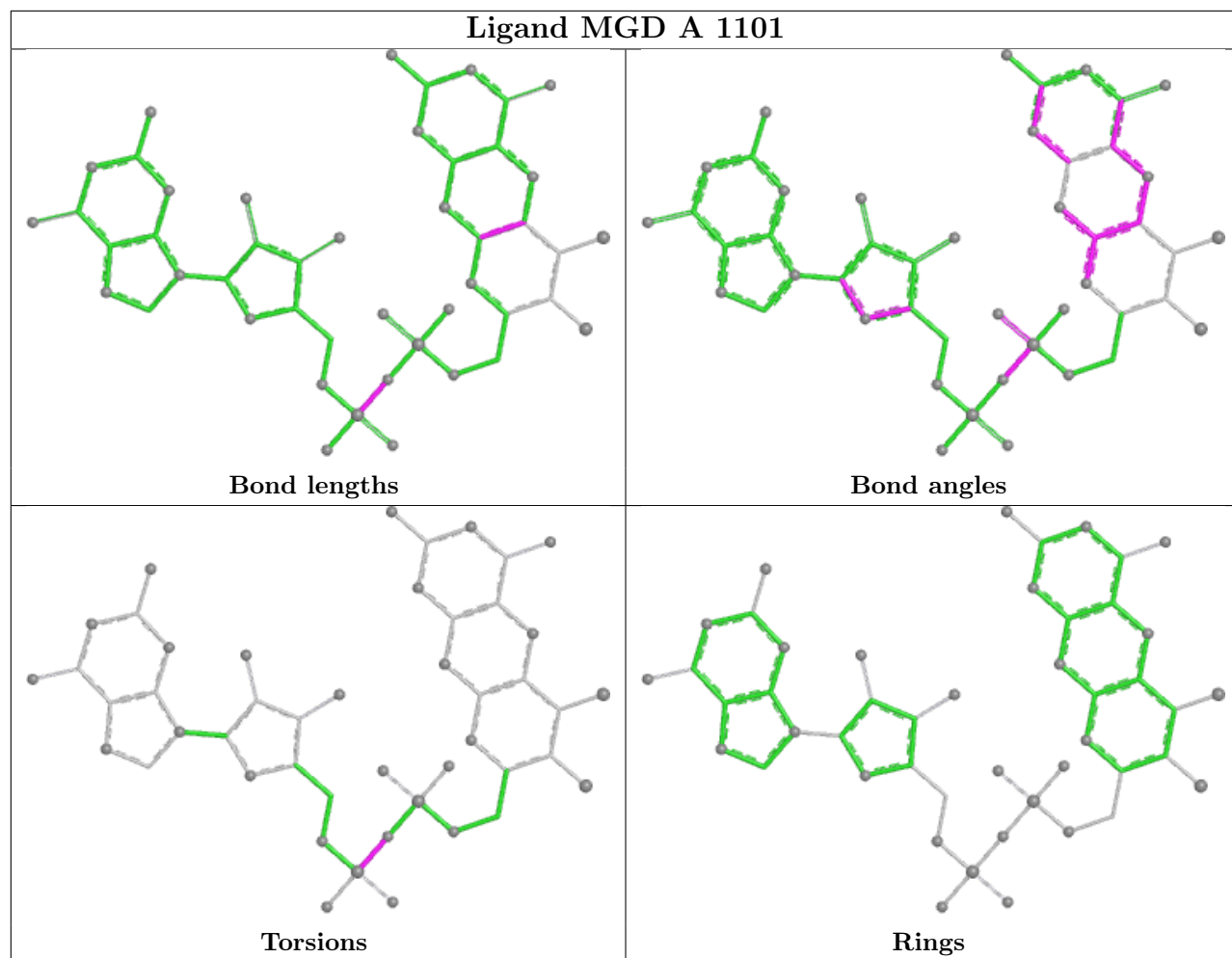


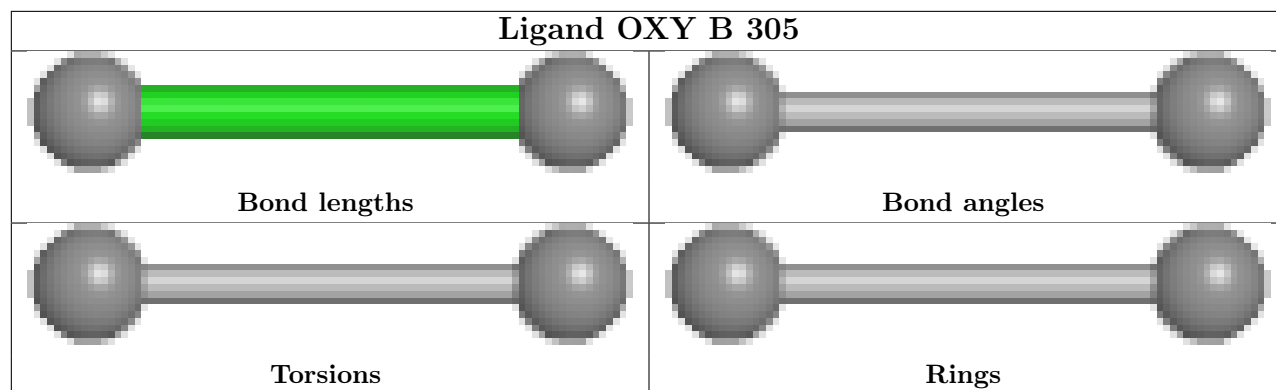












## 5.7 Other polymers [i](#)

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	966/1013 (95%)	0.22	30 (3%) 51 56	17, 29, 50, 77	0
2	B	214/215 (99%)	0.23	5 (2%) 61 67	17, 31, 46, 58	1 (0%)
All	All	1180/1228 (96%)	0.22	35 (2%) 52 57	17, 29, 50, 77	1 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1006	TRP	5.1
1	A	985	ALA	4.6
1	A	146	ALA	4.0
1	A	988	PRO	3.6
1	A	992	ILE	3.4
1	A	986	GLY	3.3
1	A	1009	PRO	3.0
1	A	661	GLY	2.9
1	A	655	LEU	2.8
1	A	147	ALA	2.7
1	A	657	ALA	2.6
1	A	954	GLY	2.6
1	A	991	GLY	2.5
2	B	131	VAL	2.5
1	A	470	ALA	2.5
2	B	168	GLN	2.5
1	A	525	GLY	2.4
1	A	989	ASN	2.4
1	A	658	LYS	2.4
1	A	660	GLY	2.4
1	A	151	VAL	2.3
2	B	88	VAL	2.3
1	A	121	THR	2.3
1	A	984	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1007	SER	2.2
1	A	678	HIS	2.2
1	A	127	THR	2.2
1	A	987	ASP	2.2
1	A	993	PRO	2.2
1	A	702	GLY	2.1
1	A	990	THR	2.1
1	A	861	ALA	2.1
2	B	143	ASP	2.1
1	A	117	TRP	2.0
2	B	61	LYS	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( $\text{\AA}^2$ )	Q<0.9
8	OXY	A	1114	2/2	0.74	0.15	43,43,43,52	0
8	OXY	A	1116	2/2	0.75	0.19	42,42,42,42	0
8	OXY	A	1110	2/2	0.82	0.15	46,46,46,50	0
8	OXY	B	305	2/2	0.82	0.12	49,49,49,55	0
8	OXY	B	307	2/2	0.82	0.14	59,59,59,61	0
8	OXY	A	1115	2/2	0.83	0.21	47,47,47,50	0
8	OXY	A	1113	2/2	0.83	0.11	50,50,50,54	0
8	OXY	A	1111	2/2	0.84	0.12	43,43,43,51	0
8	OXY	A	1119	2/2	0.85	0.11	37,37,37,44	0
8	OXY	A	1117	2/2	0.86	0.21	51,51,51,56	0
8	OXY	A	1112	2/2	0.86	0.13	40,40,40,45	0
7	GOL	A	1118	6/6	0.87	0.12	32,41,42,46	0

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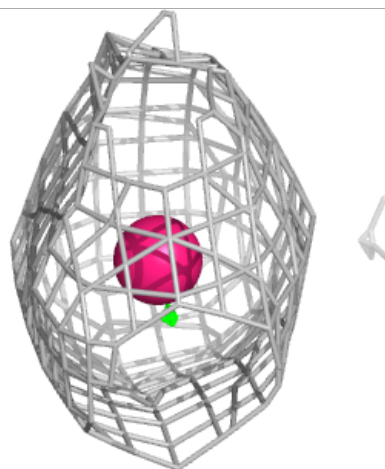
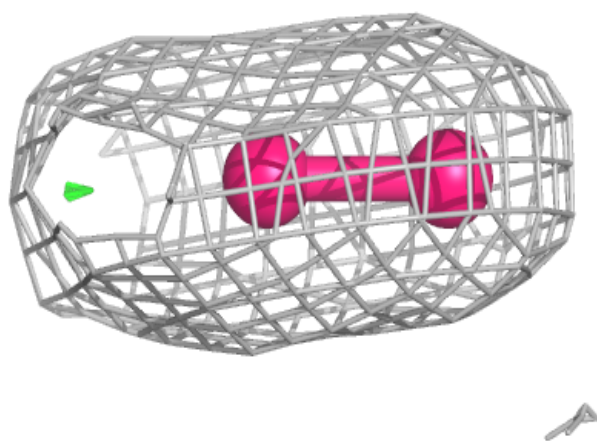
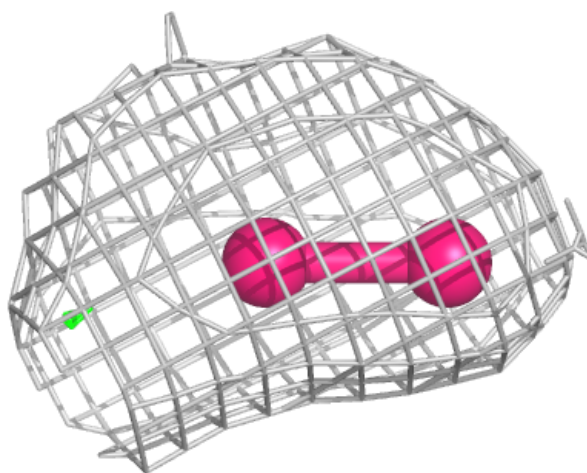
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	GOL	A	1108	6/6	0.90	0.10	30,32,35,37	0
7	GOL	B	304	6/6	0.91	0.15	18,33,36,36	0
7	GOL	A	1106	6/6	0.93	0.10	33,36,39,39	0
8	OXY	B	306	2/2	0.94	0.13	39,39,39,40	0
8	OXY	A	1109	2/2	0.94	0.14	42,42,42,43	0
7	GOL	A	1107	6/6	0.96	0.06	22,26,27,27	0
3	MGD	A	1102	47/47	0.97	0.05	20,22,25,27	0
5	H2S	A	1104	1/1	0.97	0.10	26,26,26,26	0
3	MGD	A	1101	47/47	0.98	0.05	15,19,22,24	0
4	SF4	B	303	8/8	0.99	0.04	24,25,26,27	0
4	SF4	B	302	8/8	0.99	0.04	28,31,33,33	0
4	SF4	B	301	8/8	1.00	0.02	20,20,21,22	0
4	SF4	A	1103	8/8	1.00	0.02	18,18,19,19	0
6	W	A	1105	1/1	1.00	0.02	23,23,23,23	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.

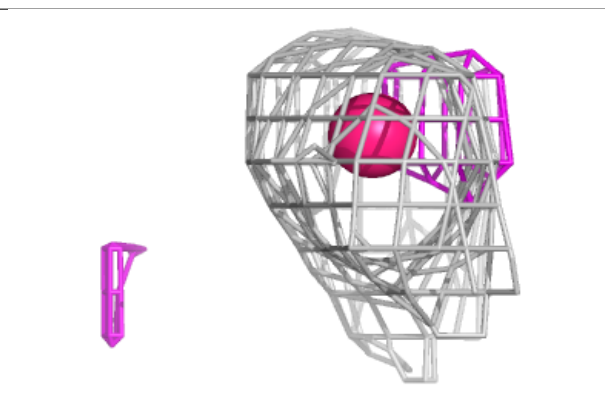
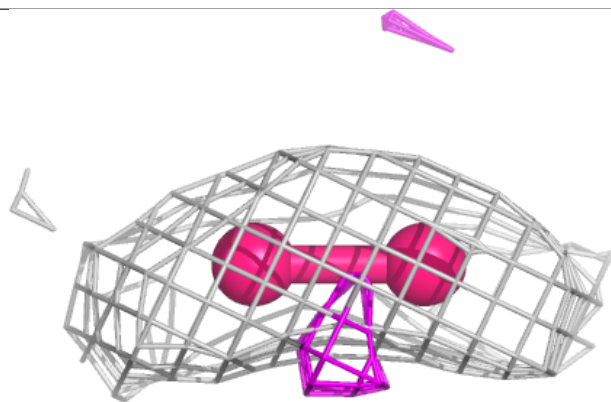
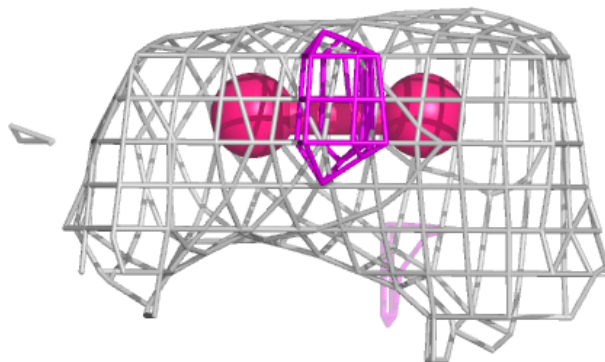
**Electron density around OXY A 1114:**

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

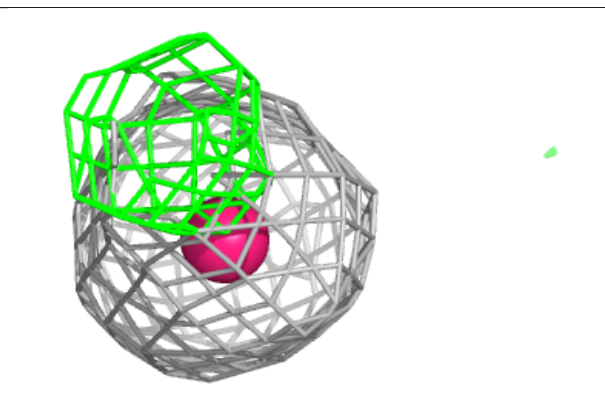
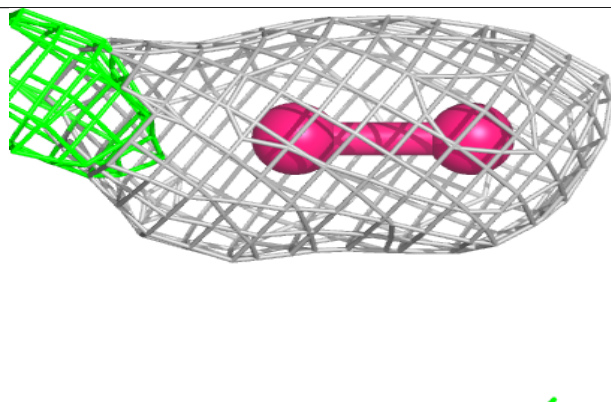
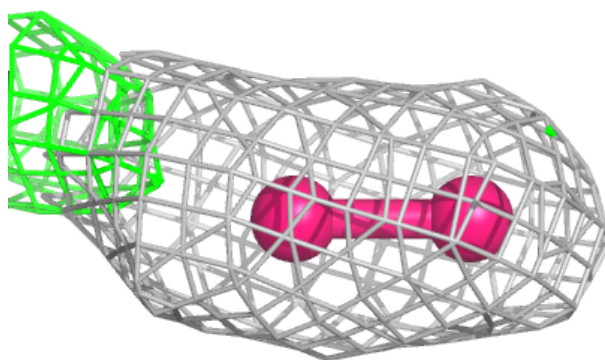


**Electron density around OXY A 1116:**

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and green (positive)

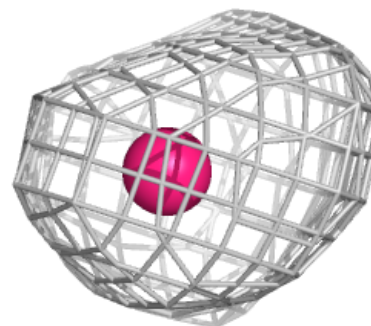
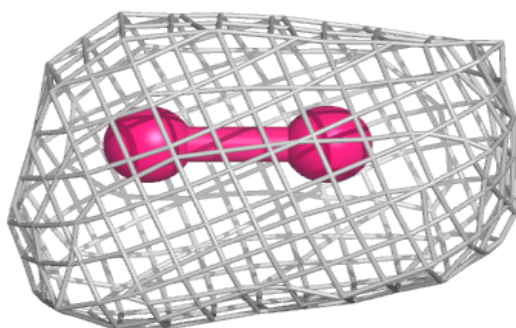
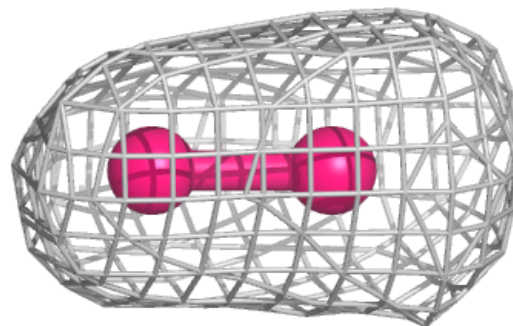
**Electron density around OXY A 1110:**

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and green (positive)



**Electron density around OXY B 305:**

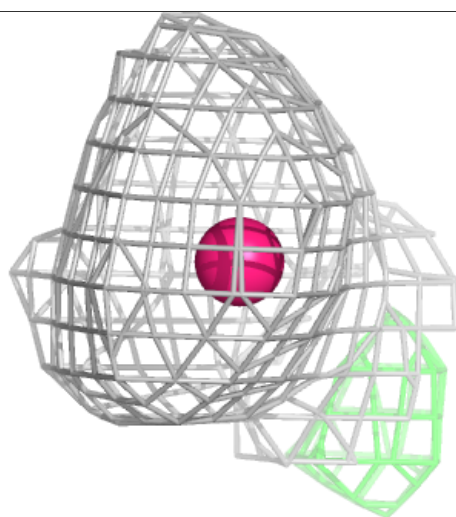
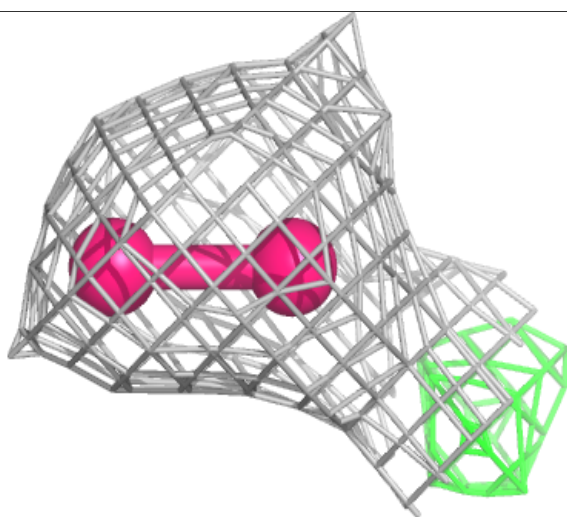
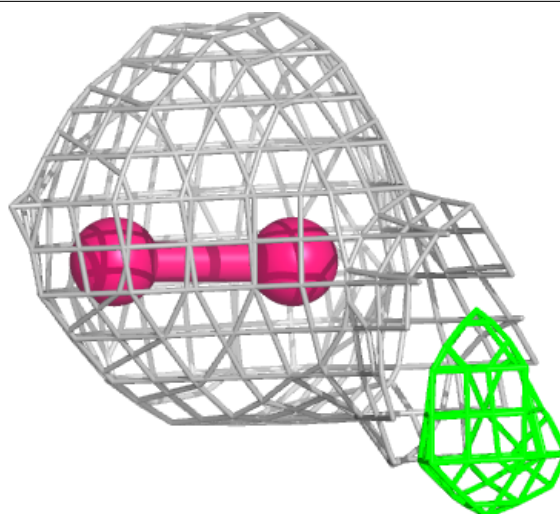
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and green (positive)





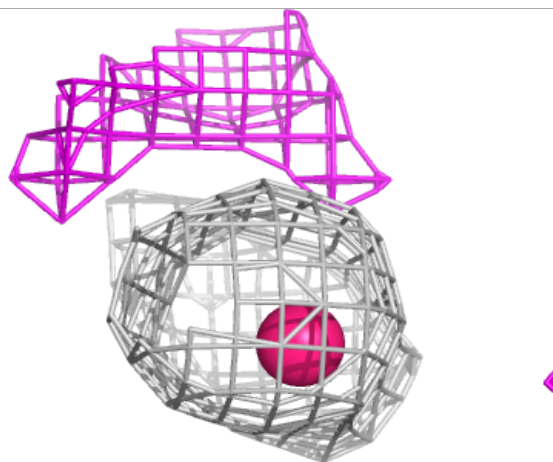
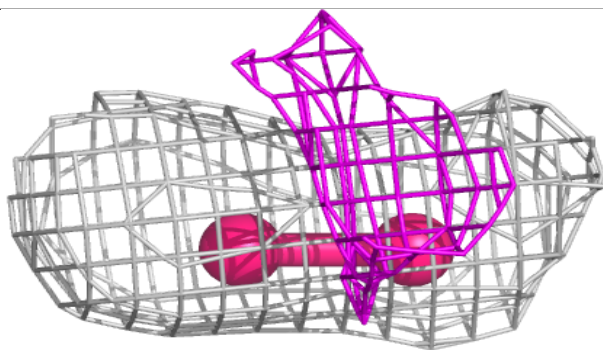
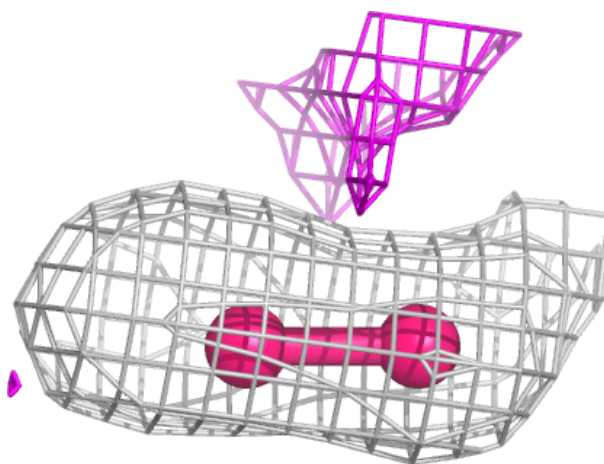
**Electron density around OXY B 307:**

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and green (positive)



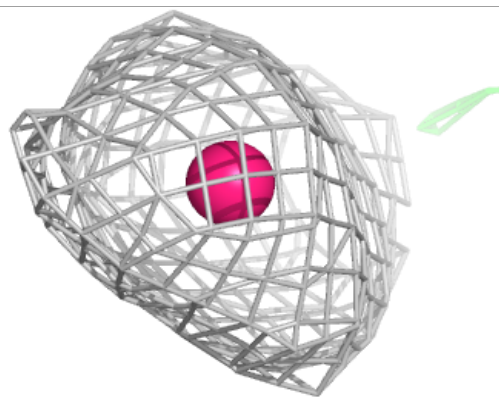
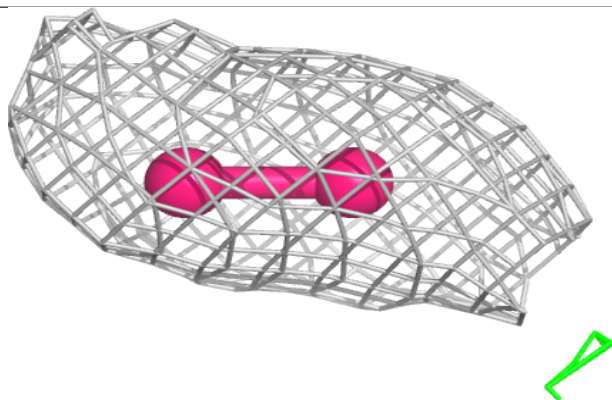
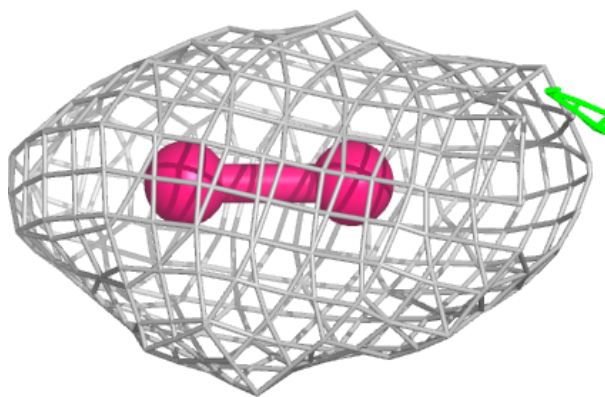
**Electron density around OXY A 1115:**

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and green (positive)



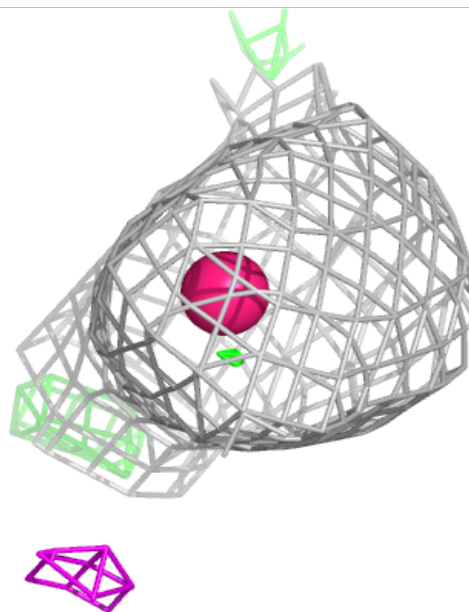
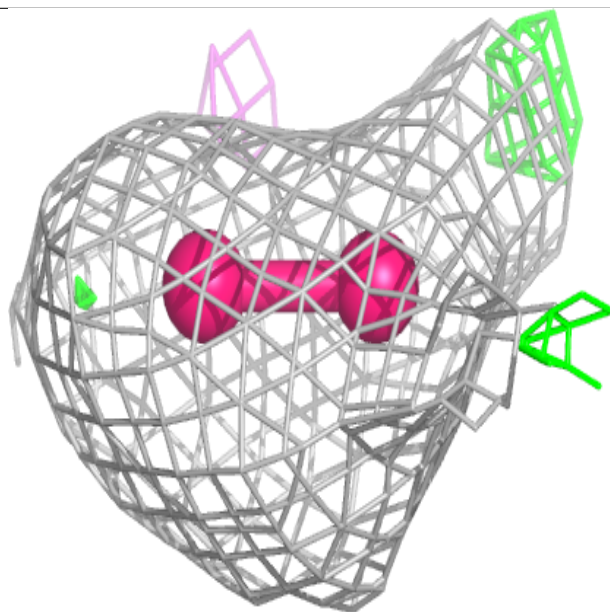
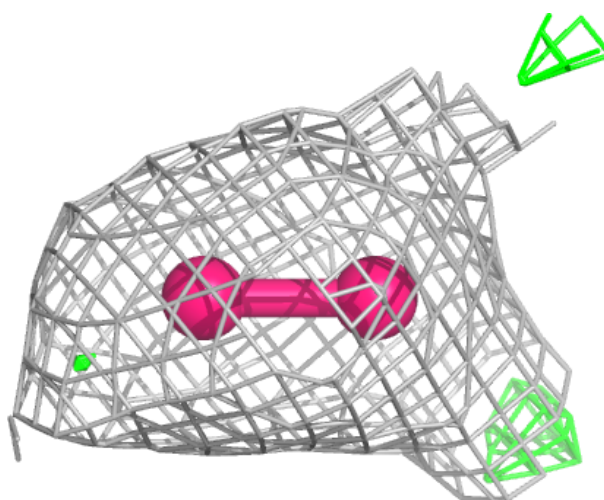
**Electron density around OXY A 1113:**

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



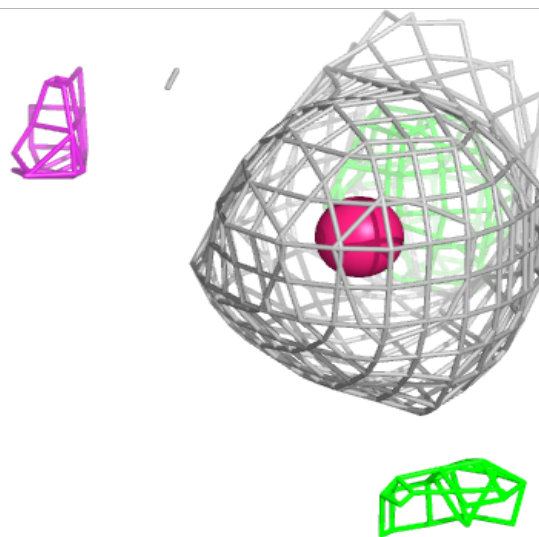
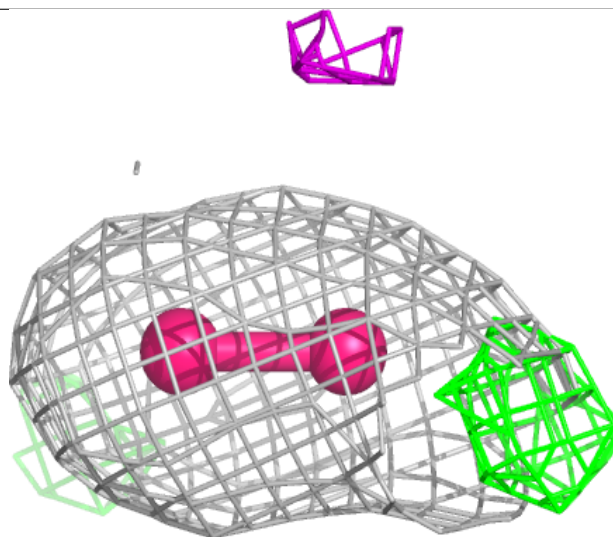
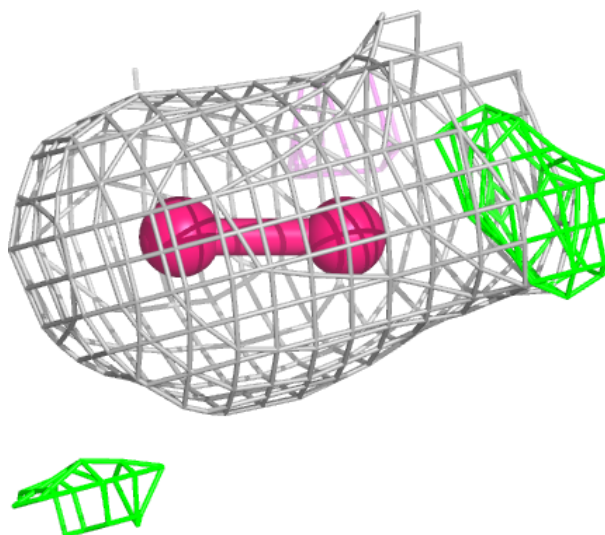
**Electron density around OXY A 1111:**

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



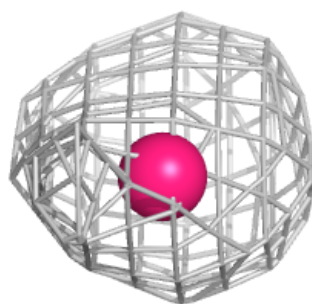
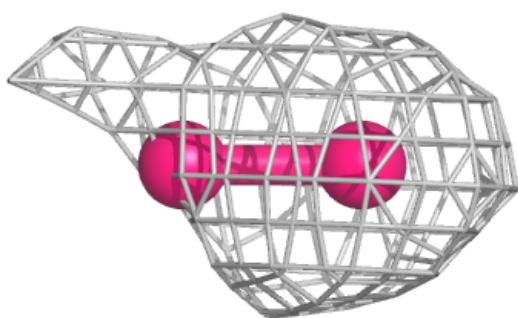
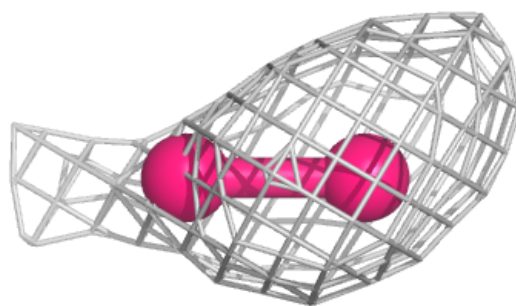
**Electron density around OXY A 1119:**

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



**Electron density around OXY A 1117:**

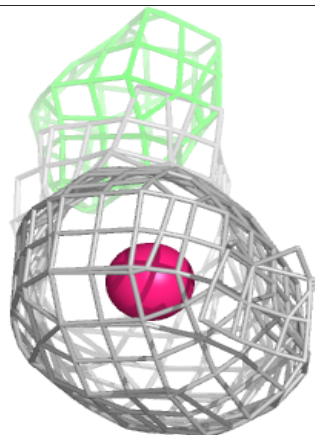
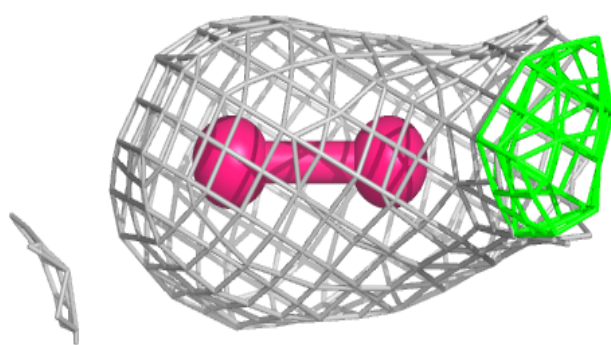
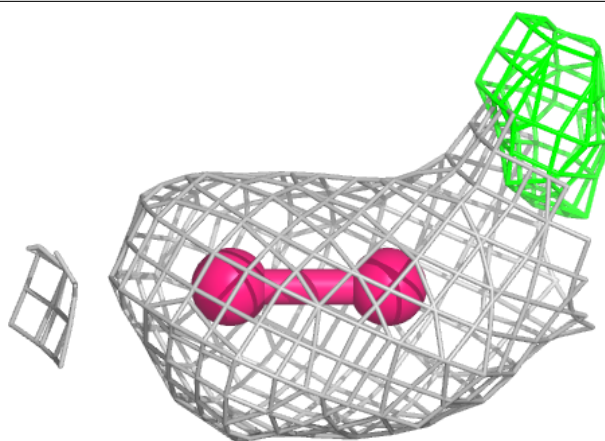
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





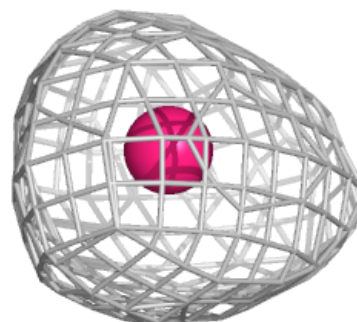
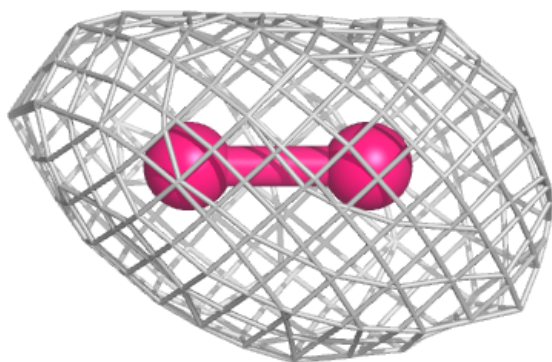
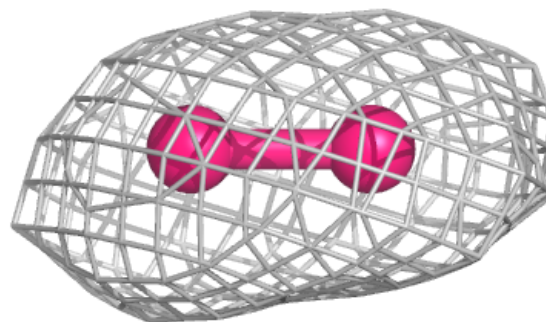
**Electron density around OXY A 1112:**

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

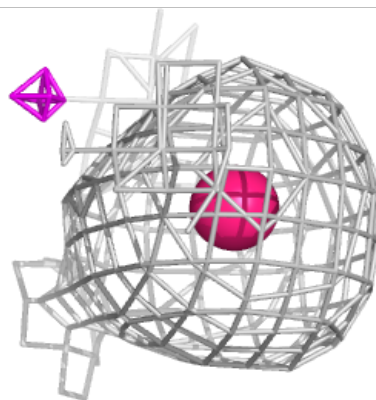
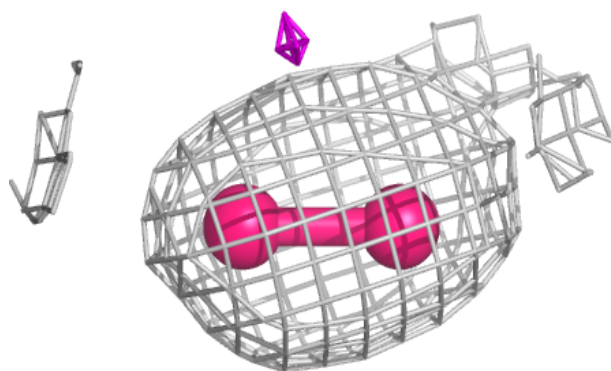
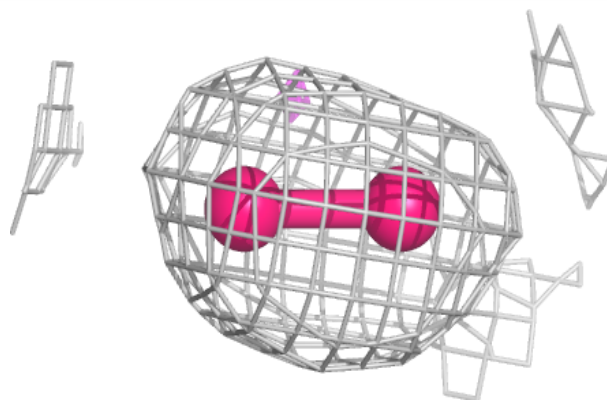


**Electron density around OXY B 306:**

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

**Electron density around OXY A 1109:**

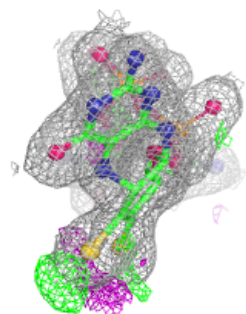
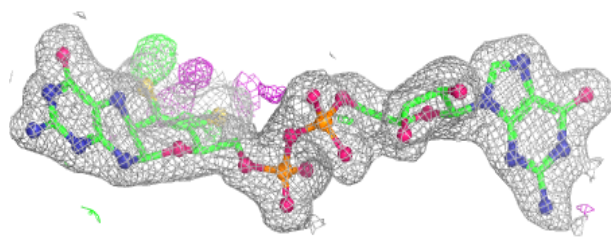
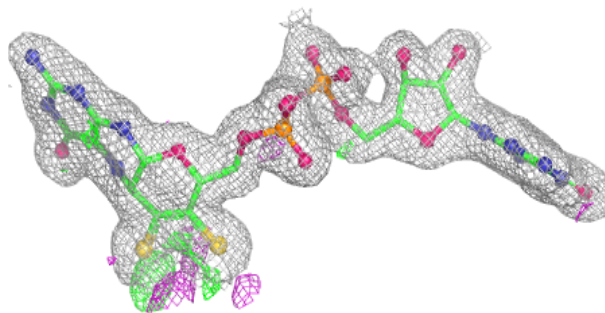
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





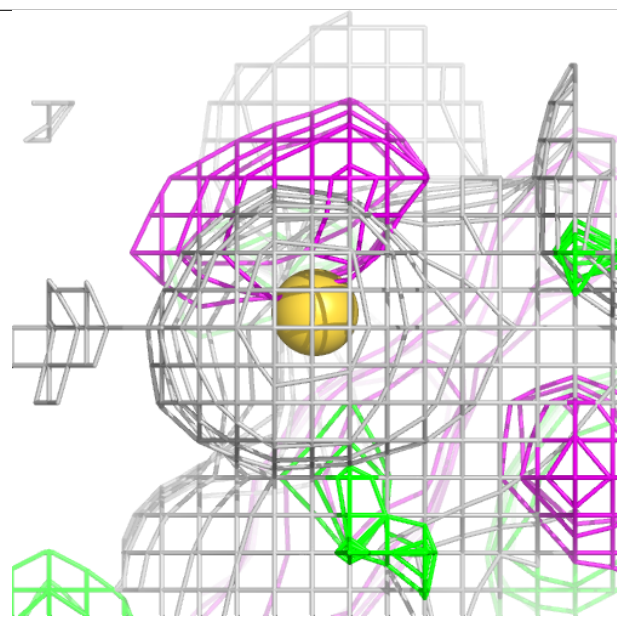
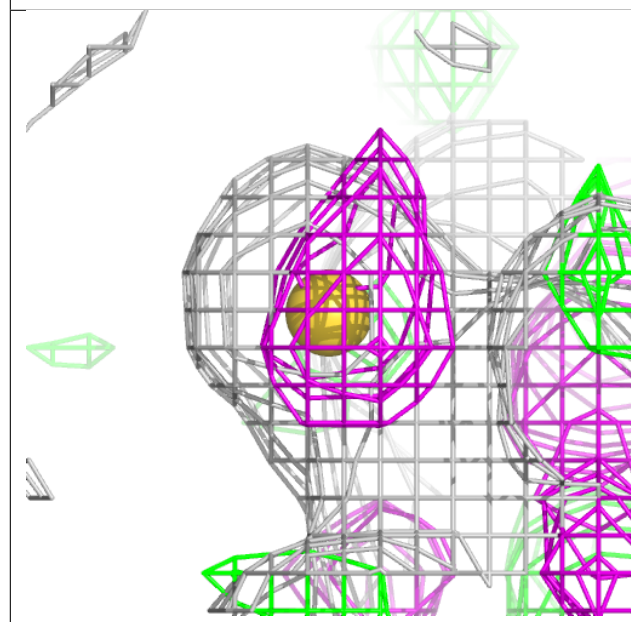
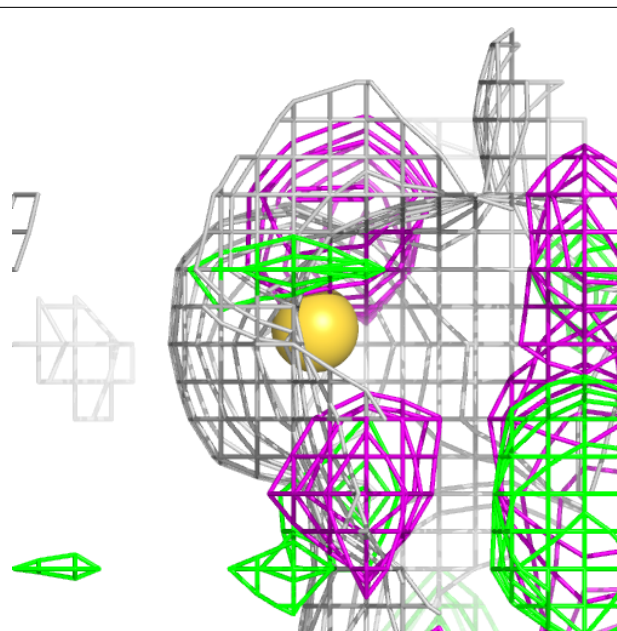
**Electron density around MGD A 1102:**

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



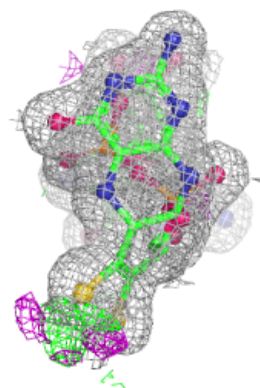
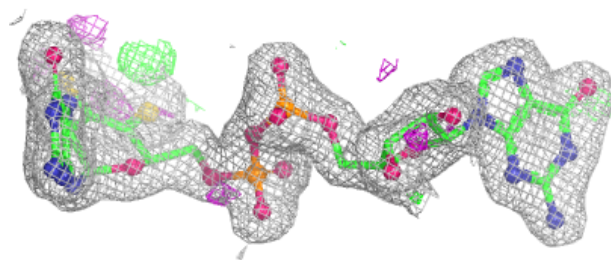
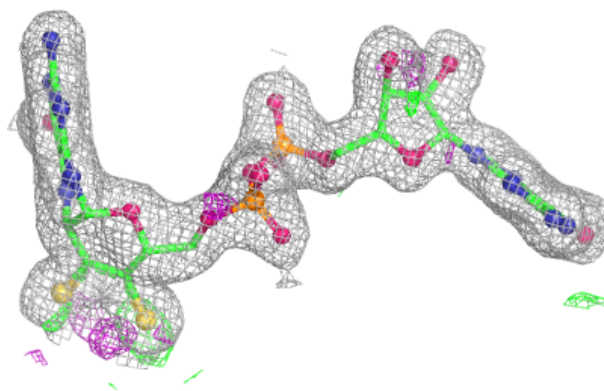
**Electron density around H2S A 1104:**

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



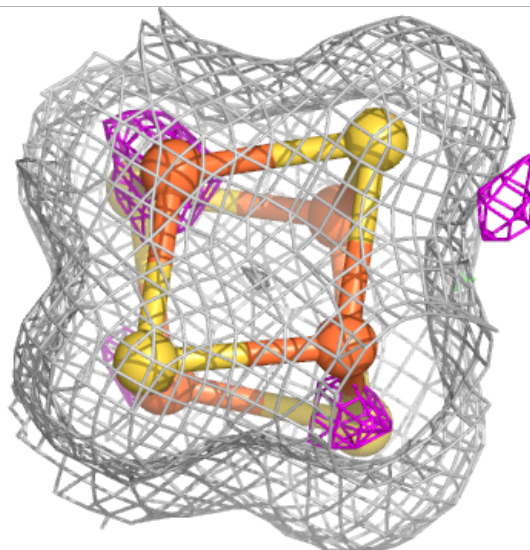
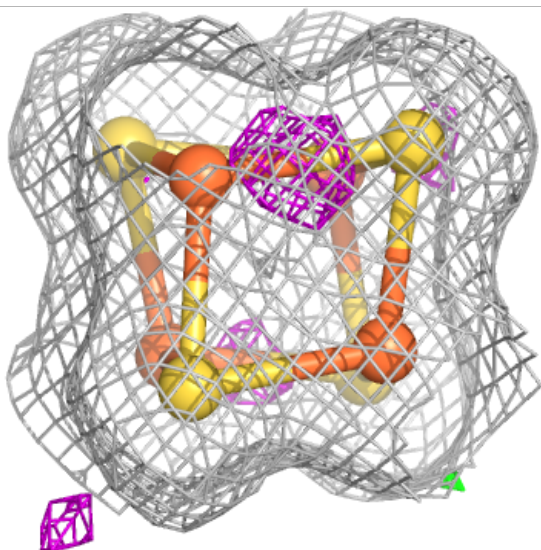
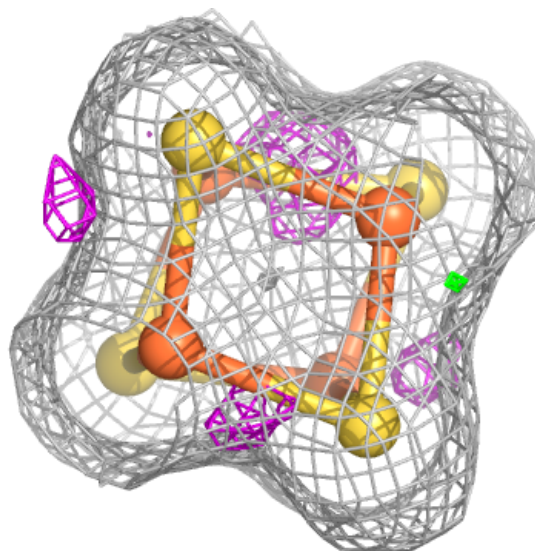
**Electron density around MGD A 1101:**

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



**Electron density around SF4 B 303:**

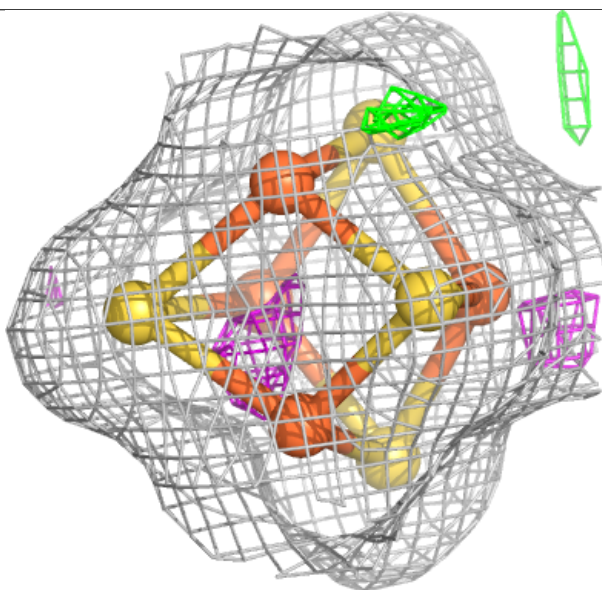
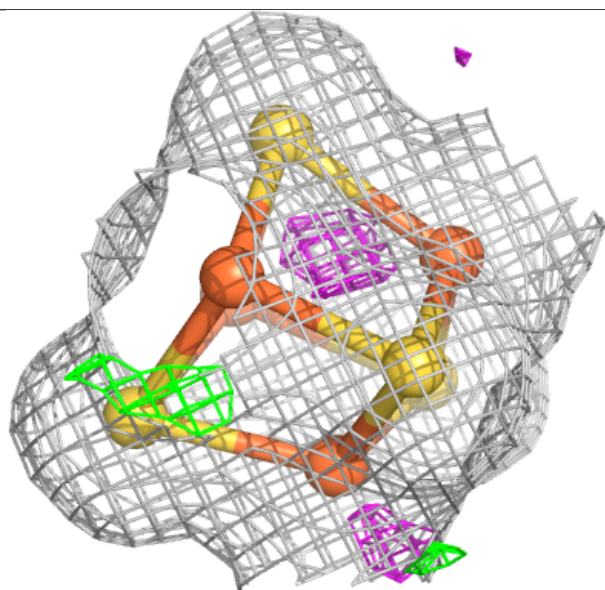
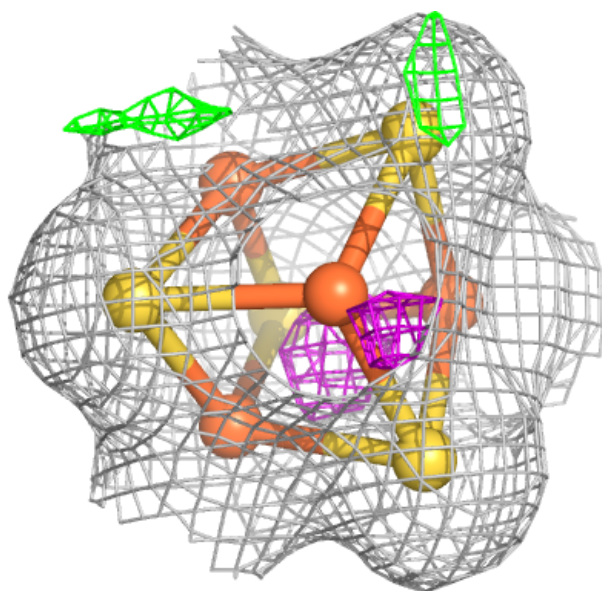
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





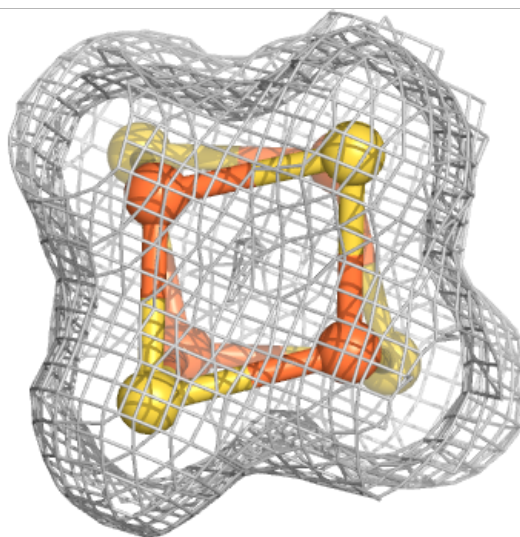
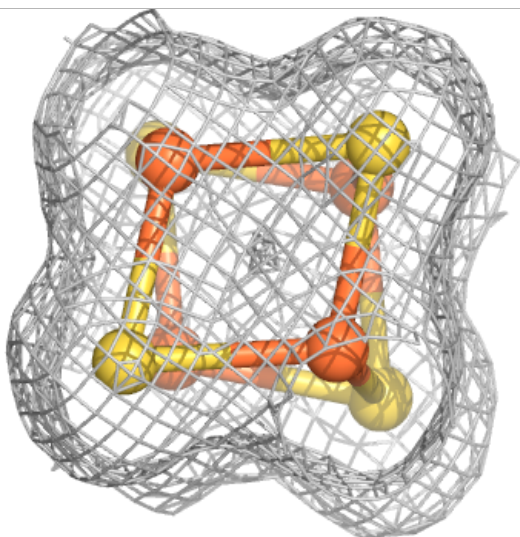
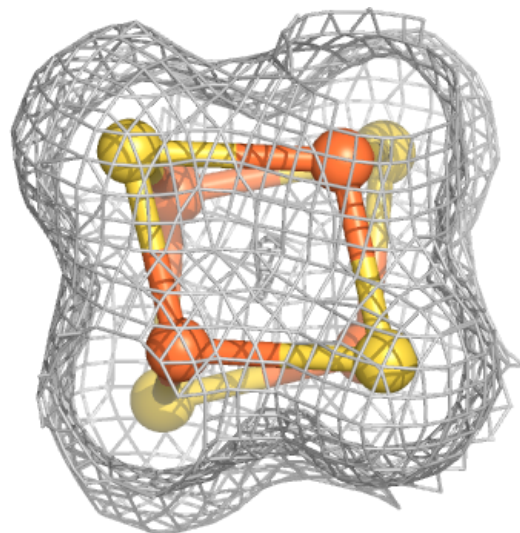
**Electron density around SF4 B 302:**

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



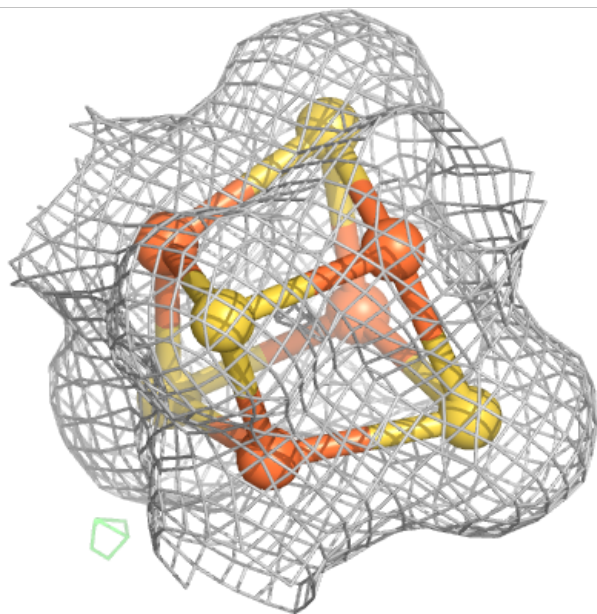
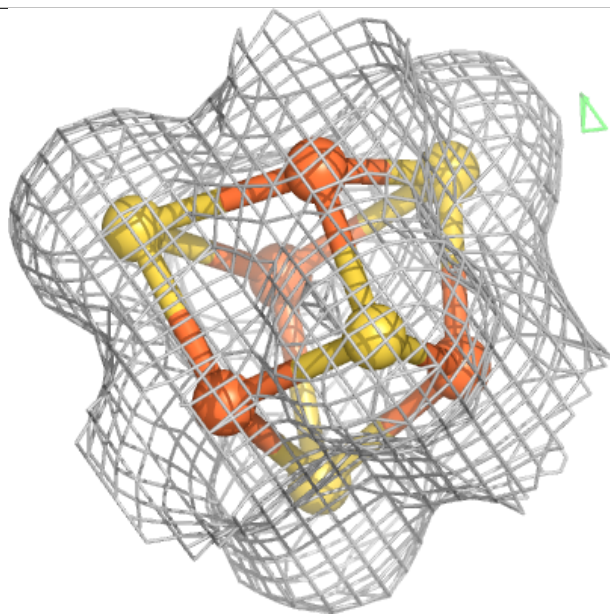
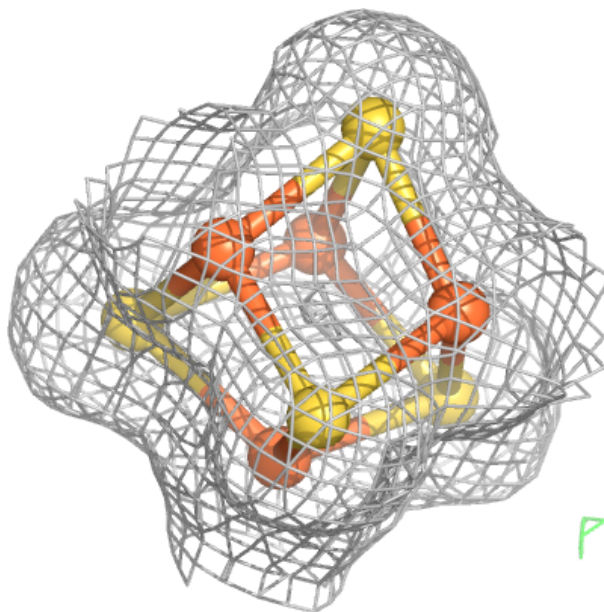
**Electron density around SF4 B 301:**

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



**Electron density around SF4 A 1103:**

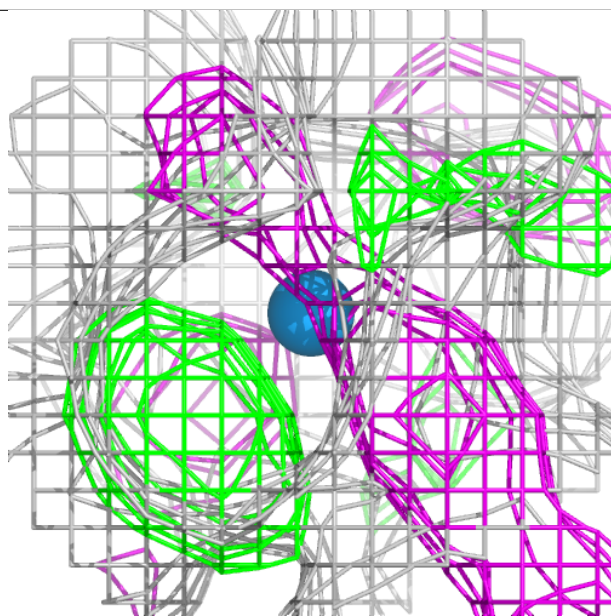
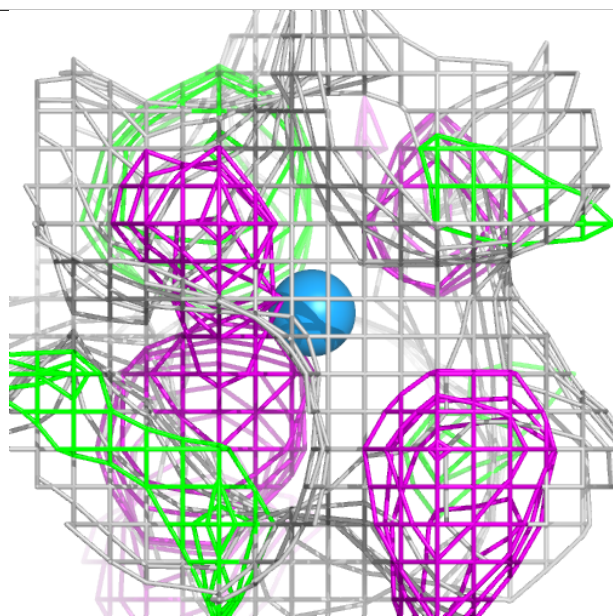
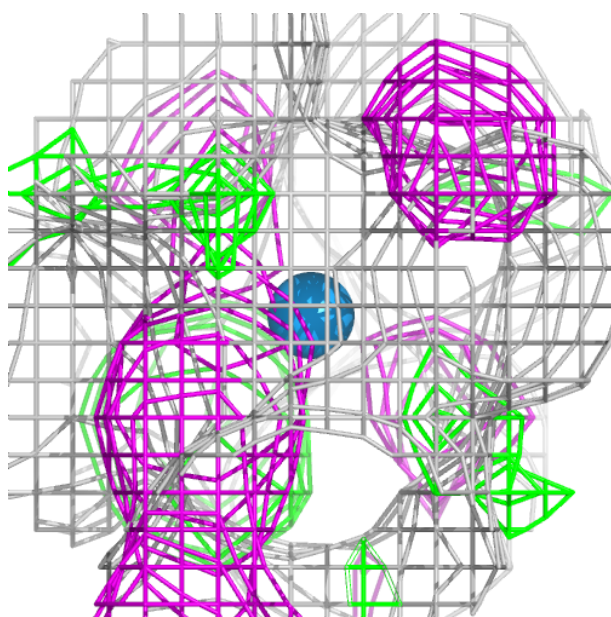
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around W A 1105:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.