Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2024 – 12:04 PM EDT

PDB ID	:	9BED
Title	:	Tungstate binding protein (Tungbindin) from Eubacterium limosum with eight molybdates bound
Authors	:	Zhou, D.; Rose, J.P.; Chen, L.; Wang, B.C.
Deposited on	:	2024-04-15
Resolution	:	2.02 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

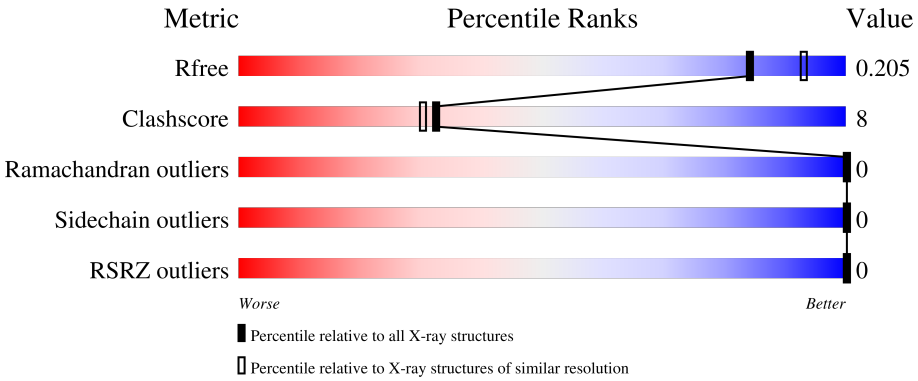
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.02 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}	164625	12358 (2.04-2.00)
Clashscore	180529	13897 (2.04-2.00)
Ramachandran outliers	177936	13770 (2.04-2.00)
Sidechain outliers	177891	13769 (2.04-2.00)
RSRZ outliers	164620	12358 (2.04-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	74	88% 12%
1	B	74	85% 8% 7%
1	C	74	91% • 7%
1	D	74	88% 5% 7%
1	E	74	92% • •

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Mol	Chain	Length	Quality of chain
1	F	74	

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
2	MOO	A	101	-	-	X	-
2	MOO	A	102	-	-	X	-
2	MOO	B	101	-	-	X	-
2	MOO	B	102	-	-	X	-
2	MOO	C	101	-	-	X	-
2	MOO	D	101	-	-	X	-
2	MOO	E	101	-	-	X	-
2	MOO	F	101	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6701 atoms, of which 3150 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 Molybdenum-pterin-binding protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	74	Total	C	H	N	O	S	0	0	0
			1092	334	556	93	106	3			
1	B	69	Total	C	H	N	O	S	0	0	0
			1014	305	523	85	98	3			
1	C	69	Total	C	H	N	O	S	0	0	0
			1014	305	523	85	98	3			
1	D	69	Total	C	H	N	O	S	0	0	0
			988	305	497	85	98	3			
1	E	71	Total	C	H	N	O	S	0	0	0
			1050	320	537	88	102	3			
1	F	70	Total	C	H	N	O	S	0	0	0
			1013	309	514	86	101	3			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	71	TRP	-	expression tag	UNP A0A0U3FVB3
A	72	SER	-	expression tag	UNP A0A0U3FVB3
A	73	HIS	-	expression tag	UNP A0A0U3FVB3
A	74	PRO	-	expression tag	UNP A0A0U3FVB3
B	71	TRP	-	expression tag	UNP A0A0U3FVB3
B	72	SER	-	expression tag	UNP A0A0U3FVB3
B	73	HIS	-	expression tag	UNP A0A0U3FVB3
B	74	PRO	-	expression tag	UNP A0A0U3FVB3
C	71	TRP	-	expression tag	UNP A0A0U3FVB3
C	72	SER	-	expression tag	UNP A0A0U3FVB3
C	73	HIS	-	expression tag	UNP A0A0U3FVB3
C	74	PRO	-	expression tag	UNP A0A0U3FVB3
D	71	TRP	-	expression tag	UNP A0A0U3FVB3
D	72	SER	-	expression tag	UNP A0A0U3FVB3
D	73	HIS	-	expression tag	UNP A0A0U3FVB3
D	74	PRO	-	expression tag	UNP A0A0U3FVB3
E	71	TRP	-	expression tag	UNP A0A0U3FVB3

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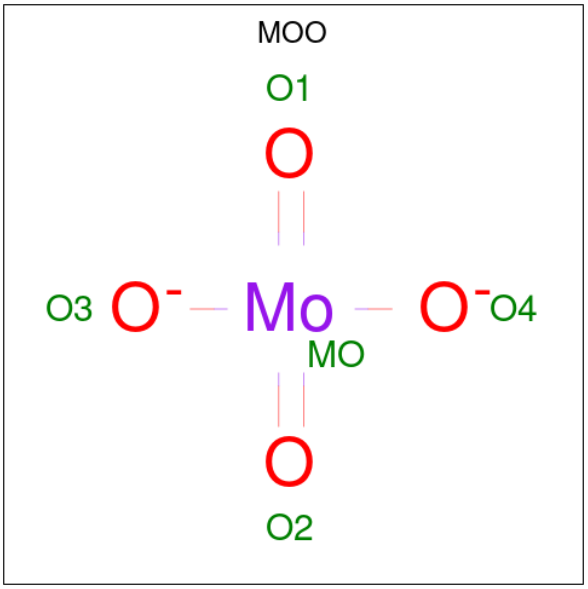
Chain	Residue	Modelled	Actual	Comment	Reference
E	72	SER	-	expression tag	UNP A0A0U3FVB3
E	73	HIS	-	expression tag	UNP A0A0U3FVB3
E	74	PRO	-	expression tag	UNP A0A0U3FVB3
F	71	TRP	-	expression tag	UNP A0A0U3FVB3
F	72	SER	-	expression tag	UNP A0A0U3FVB3
F	73	HIS	-	expression tag	UNP A0A0U3FVB3
F	74	PRO	-	expression tag	UNP A0A0U3FVB3

- Molecule 2 is MOLYBDATE ION (three-letter code: MOO) (formula: MoO_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Mo	O	0	0
			5	1	4		
2	A	1	Total	Mo	O	0	0
			5	1	4		
2	B	1	Total	Mo	O	0	0
			5	1	4		
2	B	1	Total	Mo	O	0	0
			5	1	4		
2	C	1	Total	Mo	O	0	0
			5	1	4		
2	D	1	Total	Mo	O	0	0
			5	1	4		
2	E	1	Total	Mo	O	0	0
			5	1	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total Mo O 5 1 4	0	0

- Molecule 3 is water.

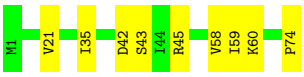
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	92	Total O 92 92	0	0
3	B	94	Total O 94 94	0	0
3	C	89	Total O 89 89	0	0
3	D	78	Total O 78 78	0	0
3	E	76	Total O 76 76	0	0
3	F	61	Total O 61 61	0	0

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: Molybdenum-pterin-binding protein

Chain A:

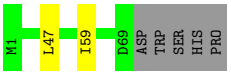


• Molecule 1: Molybdenum-pterin-binding protein

Chain B:

• Molecule 1: Molybdenum-pterin-binding protein

Chain C:

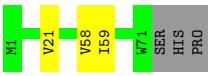


• Molecule 1: Molybdenum-pterin-binding protein

Chain D:

• Molecule 1: Molybdenum-pterin-binding protein

Chain E:



• Molecule 1: Molybdenum-pterin-binding protein

Chain F:


M1
N7
K17
I29
G30
G31
D42
R45
Q50
S53
V58
I59
M65
D70
TRP
SER
HIS
PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	74.71Å 74.71Å 156.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.36 – 2.02 37.36 – 2.02	Depositor EDS
% Data completeness (in resolution range)	97.7 (37.36-2.02) 97.7 (37.36-2.02)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.62 (at 2.01Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.151 , 0.205 0.151 , 0.205	Depositor DCC
R_{free} test set	27800 reflections (6.80%)	wwPDB-VP
Wilson B-factor (Å^2)	23.5	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 51.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6701	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MOO

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	0.44	0/540	0.70	0/728
1	B	0.49	0/491	0.71	0/659
1	C	0.46	0/491	0.71	0/659
1	D	0.51	0/491	0.74	0/659
1	E	0.49	0/515	0.78	0/693
1	F	0.48	0/499	0.72	0/670
All	All	0.48	0/3027	0.73	0/4068

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	536	556	556	9	0
1	B	491	523	523	8	0
1	C	491	523	523	3	0
1	D	491	497	523	6	0
1	E	513	537	537	4	0
1	F	499	514	527	10	0
2	A	10	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	10	0	0	6	0
2	C	5	0	0	4	0
2	D	5	0	0	3	0
2	E	5	0	0	2	0
2	F	5	0	0	3	0
3	A	92	0	0	1	3
3	B	94	0	0	1	3
3	C	89	0	0	0	1
3	D	78	0	0	0	0
3	E	76	0	0	0	0
3	F	61	0	0	3	0
All	All	3551	3150	3189	49	4

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 (49) 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:101:MOO:O2	2:B:101:MOO:MO	1.64	0.67
2:B:102:MOO:O4	2:B:102:MOO:MO	1.66	0.67
2:F:101:MOO:O1	2:F:101:MOO:MO	1.66	0.66
2:A:101:MOO:O1	2:A:101:MOO:MO	1.66	0.65
2:A:102:MOO:O1	2:A:102:MOO:MO	1.68	0.63
2:E:101:MOO:MO	2:E:101:MOO:O3	1.69	0.63
2:A:101:MOO:MO	2:A:101:MOO:O2	1.70	0.63
2:B:102:MOO:MO	2:B:102:MOO:O3	1.70	0.62
2:F:101:MOO:MO	2:F:101:MOO:O3	1.71	0.62
2:C:101:MOO:O4	2:C:101:MOO:MO	1.70	0.62
2:D:101:MOO:O3	2:D:101:MOO:MO	1.70	0.62
1:C:59:ILE:HD13	1:E:59:ILE:HD13	1.82	0.62
2:D:101:MOO:MO	2:D:101:MOO:O4	1.69	0.62
1:D:59:ILE:HD13	1:F:59:ILE:HD13	1.81	0.61
2:D:101:MOO:MO	2:D:101:MOO:O1	1.71	0.61
2:C:101:MOO:MO	2:C:101:MOO:O1	1.72	0.61
2:E:101:MOO:MO	2:E:101:MOO:O2	1.70	0.61
2:A:102:MOO:MO	2:A:102:MOO:O3	1.72	0.60
2:B:101:MOO:MO	2:B:101:MOO:O4	1.72	0.60
2:C:101:MOO:MO	2:C:101:MOO:O3	1.72	0.60
2:A:101:MOO:MO	2:A:101:MOO:O3	1.71	0.60
2:B:101:MOO:MO	2:B:101:MOO:O1	1.71	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:101:MOO:MO	2:F:101:MOO:O4	1.73	0.59
2:C:101:MOO:MO	2:C:101:MOO:O2	1.73	0.59
2:B:102:MOO:MO	2:B:102:MOO:O1	1.72	0.59
1:A:35:ILE:HD11	1:B:9:LEU:HD11	1.88	0.55
1:A:42:ASP:OD1	1:A:45:ARG:NH2	2.42	0.53
1:A:35:ILE:CD1	1:B:9:LEU:HD11	2.39	0.53
1:B:2:LYS:HD3	1:C:47:LEU:HD23	1.91	0.52
1:D:17:LYS:HE3	1:E:21:VAL:HG12	1.94	0.49
1:A:59:ILE:HD13	1:B:59:ILE:HD13	1.95	0.49
1:B:2:LYS:HD3	1:C:47:LEU:CD2	2.43	0.49
1:F:29:ILE:O	3:F:201:HOH:O	2.20	0.48
1:A:21:VAL:HG12	1:F:17:LYS:HG2	1.95	0.48
3:A:268:HOH:O	1:D:6:ARG:HD2	2.15	0.47
1:F:42:ASP:OD1	1:F:45:ARG:NH2	2.46	0.47
1:B:58:VAL:C	1:B:59:ILE:HG13	2.33	0.47
1:A:60:LYS:HD2	1:F:65:MET:HG3	1.96	0.47
1:F:31:GLY:HA3	3:F:206:HOH:O	2.16	0.45
1:A:74:PRO:HB3	1:B:48:GLY:HA3	1.99	0.45
1:F:58:VAL:C	1:F:59:ILE:HG13	2.36	0.44
1:E:58:VAL:C	1:E:59:ILE:HG13	2.37	0.44
1:B:45:ARG:NH1	3:B:201:HOH:O	2.30	0.43
1:F:31:GLY:CA	3:F:206:HOH:O	2.66	0.42
1:A:43:SER:OG	1:D:6:ARG:NE	2.52	0.42
1:F:50:GLN:HG2	1:F:53:SER:OG	2.19	0.42
1:D:17:LYS:CE	1:E:21:VAL:HG12	2.49	0.41
1:D:35:ILE:HA	1:F:7:ASN:OD1	2.20	0.41
1:A:58:VAL:C	1:A:59:ILE:HG13	2.40	0.41

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:271:HOH:O	3:B:268:HOH:O[5_545]	1.92	0.28
3:A:234:HOH:O	3:B:268:HOH:O[5_545]	1.97	0.23
3:C:282:HOH:O	3:C:282:HOH:O[7_556]	2.05	0.15
3:A:262:HOH:O	3:B:270:HOH:O[5_545]	2.10	0.10

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	72/74 (97%)	71 (99%)	1 (1%)	0	100	100
1	B	67/74 (90%)	66 (98%)	1 (2%)	0	100	100
1	C	67/74 (90%)	67 (100%)	0	0	100	100
1	D	67/74 (90%)	67 (100%)	0	0	100	100
1	E	69/74 (93%)	67 (97%)	2 (3%)	0	100	100
1	F	68/74 (92%)	67 (98%)	1 (2%)	0	100	100
All	All	410/444 (92%)	405 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	59/59 (100%)	59 (100%)	0	100	100
1	B	54/59 (92%)	54 (100%)	0	100	100
1	C	54/59 (92%)	54 (100%)	0	100	100
1	D	54/59 (92%)	54 (100%)	0	100	100
1	E	56/59 (95%)	56 (100%)	0	100	100
1	F	55/59 (93%)	55 (100%)	0	100	100
All	All	332/354 (94%)	332 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	E	50	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	MOO	B	102	-	2,4,4	0.33	0	-		
2	MOO	F	101	-	2,4,4	1.74	1 (50%)	-		
2	MOO	B	101	-	2,4,4	2.10	1 (50%)	-		
2	MOO	A	101	-	2,4,4	1.77	1 (50%)	-		
2	MOO	C	101	-	2,4,4	0.34	0	-		
2	MOO	D	101	-	2,4,4	0.42	0	-		
2	MOO	A	102	-	2,4,4	1.26	0	-		
2	MOO	E	101	-	2,4,4	0.74	0	-		

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	101	MOO	O2-MO	-2.87	1.64	1.73
2	F	101	MOO	O1-MO	-2.43	1.66	1.73
2	A	101	MOO	O1-MO	-2.31	1.66	1.73

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

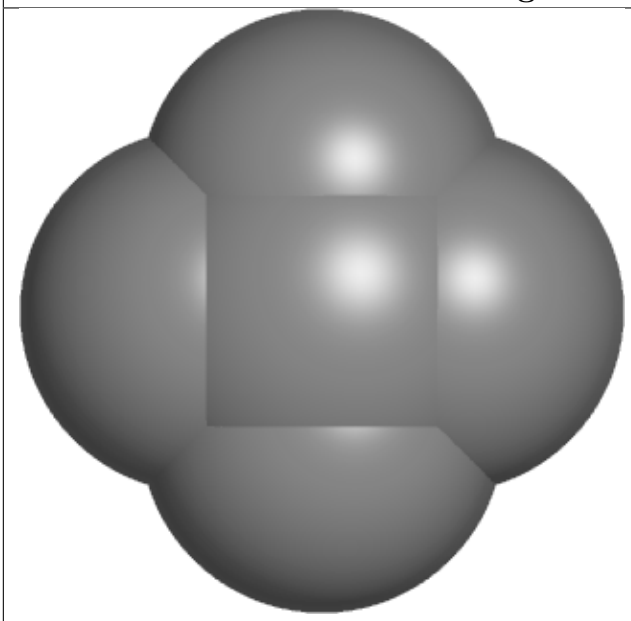
There are no ring outliers.

8 monomers are involved in 23 short contacts:

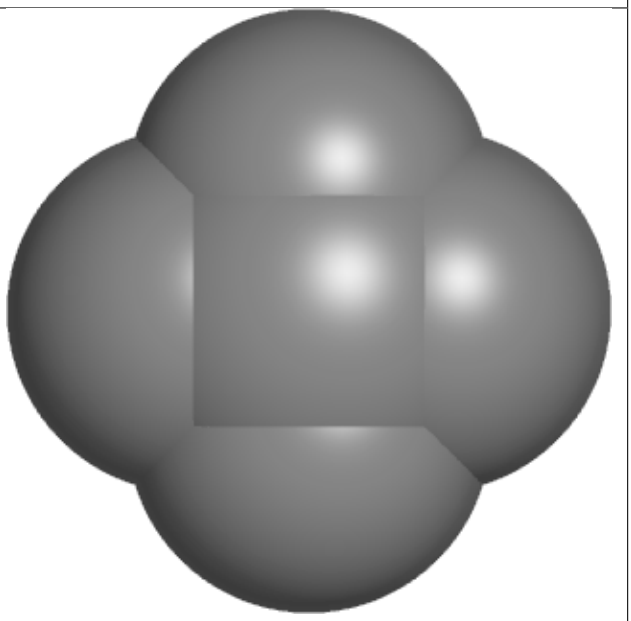
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	102	MOO	3	0
2	F	101	MOO	3	0
2	B	101	MOO	3	0
2	A	101	MOO	3	0
2	C	101	MOO	4	0
2	D	101	MOO	3	0
2	A	102	MOO	2	0
2	E	101	MOO	2	0

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 then 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.

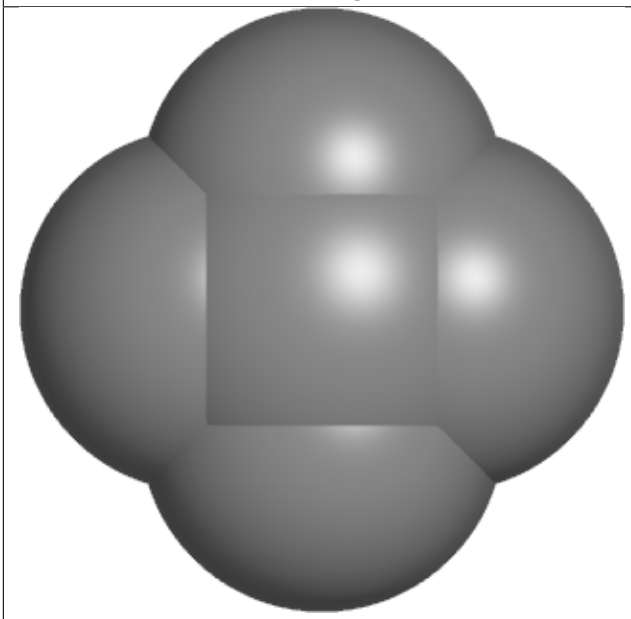
Ligand MOO B 102



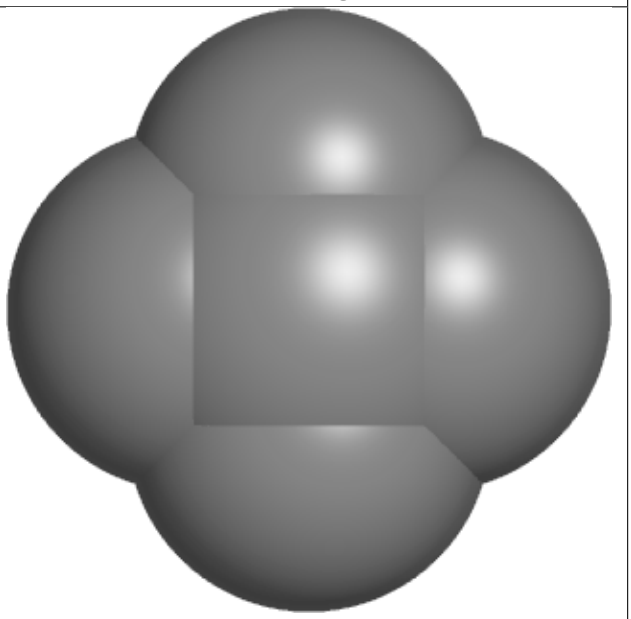
Bond lengths



Bond angles

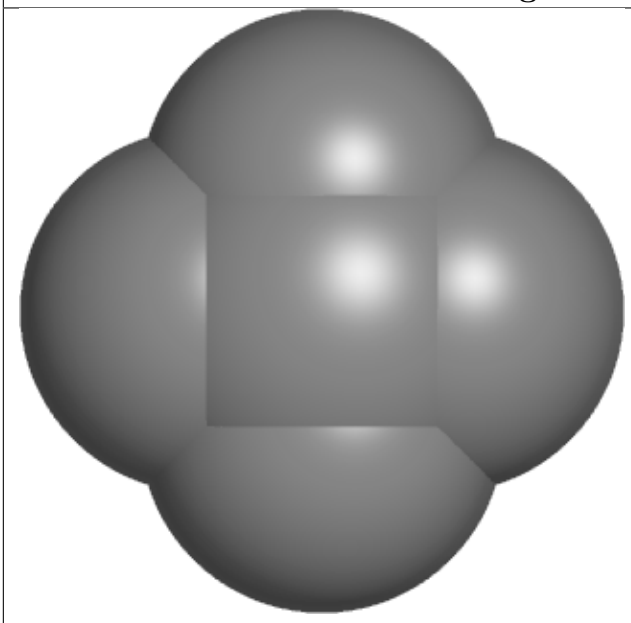


Torsions

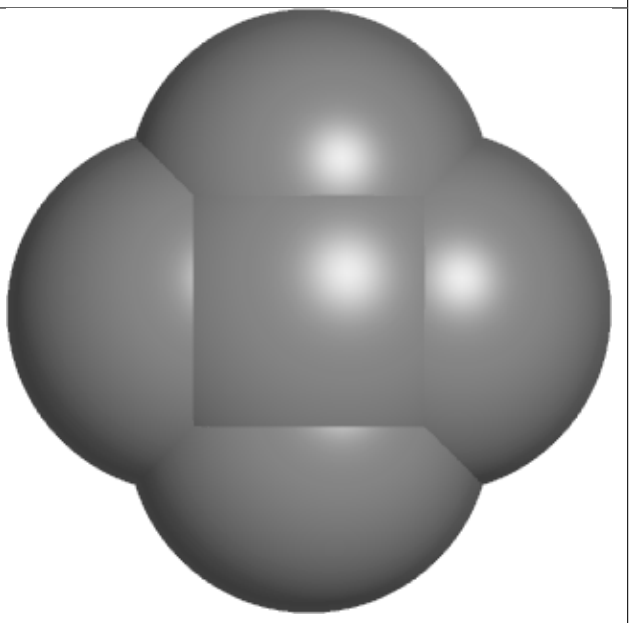


Rings

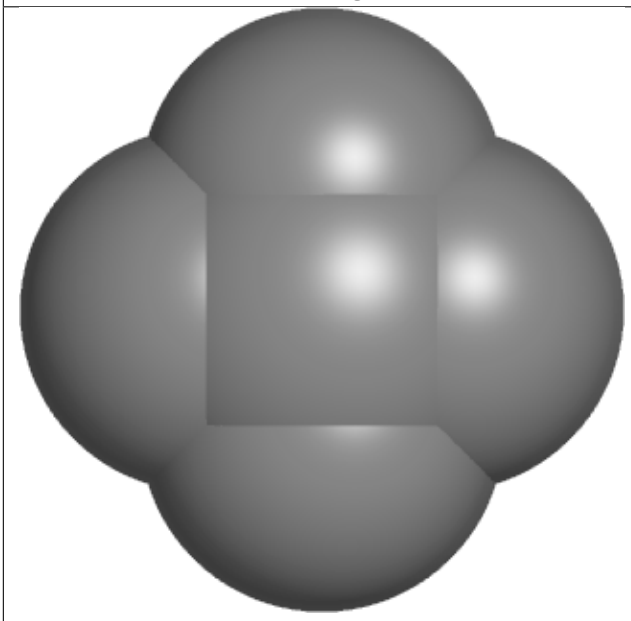
Ligand MOO F 101



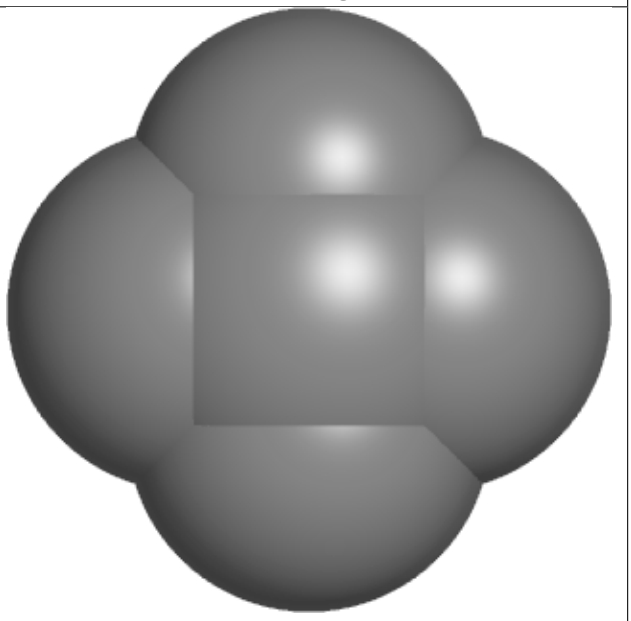
Bond lengths



Bond angles

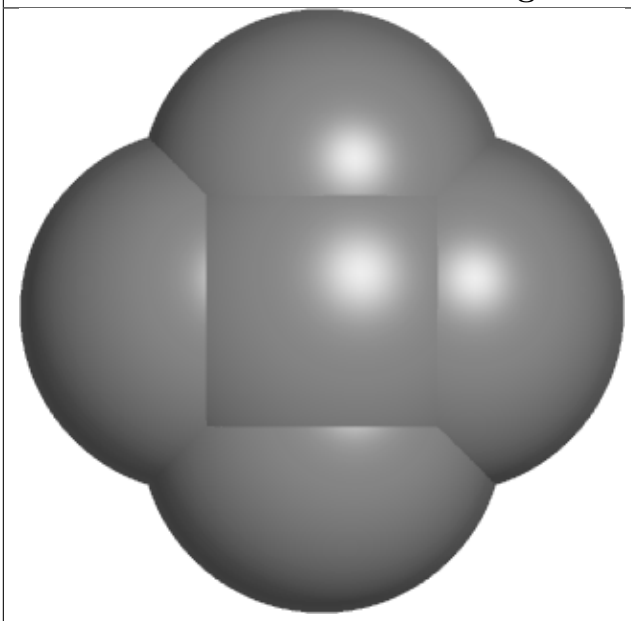


Torsions

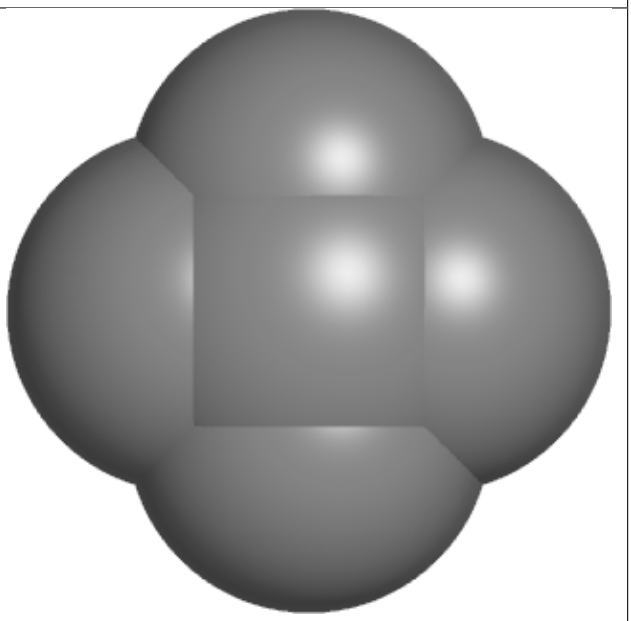


Rings

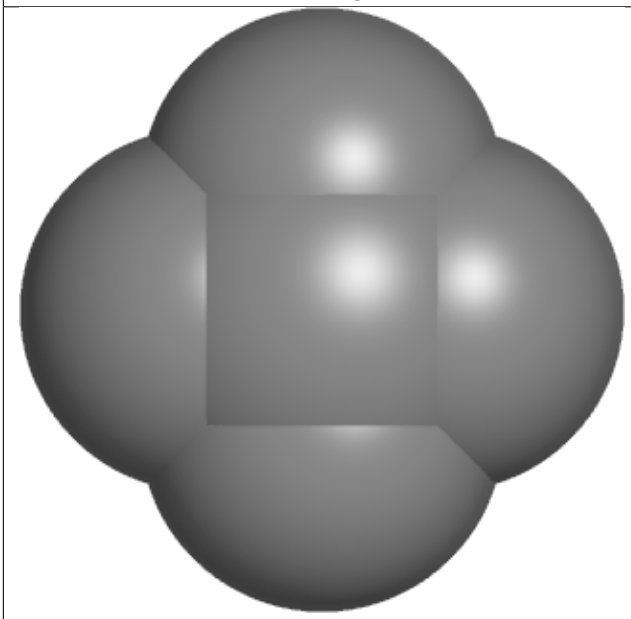
Ligand MOO B 101



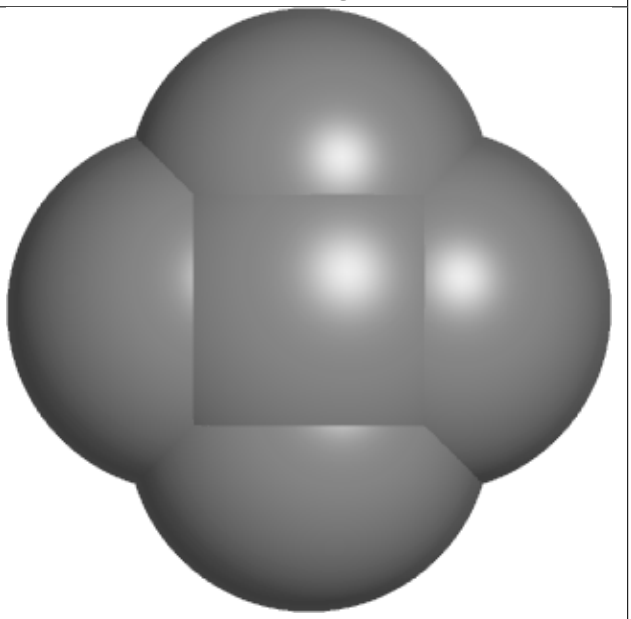
Bond lengths



Bond angles

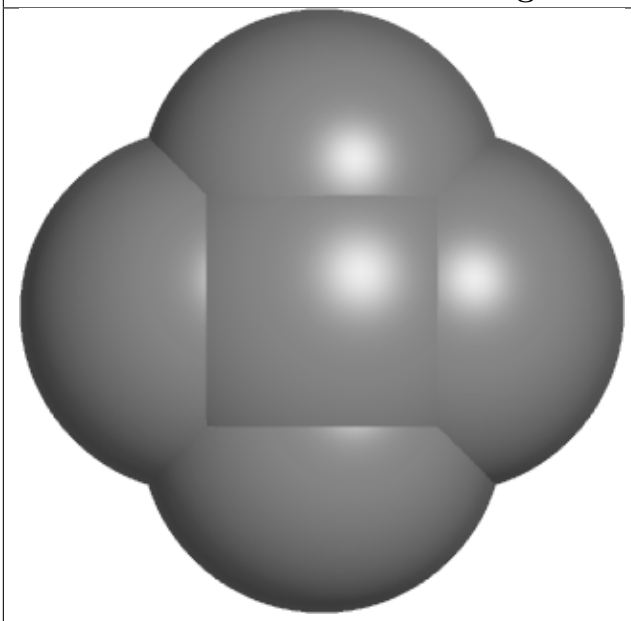


Torsions

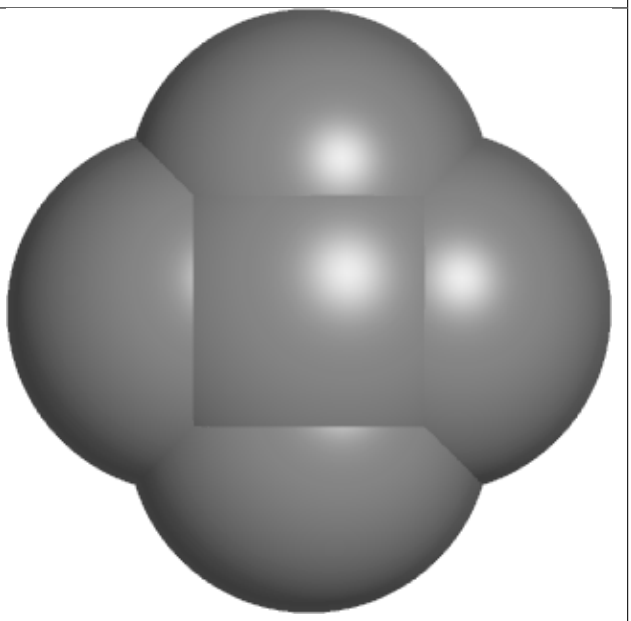


Rings

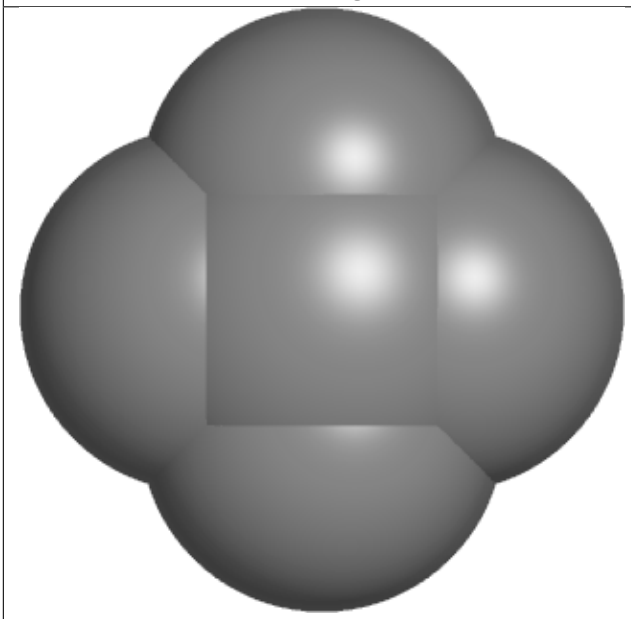
Ligand MOO A 101



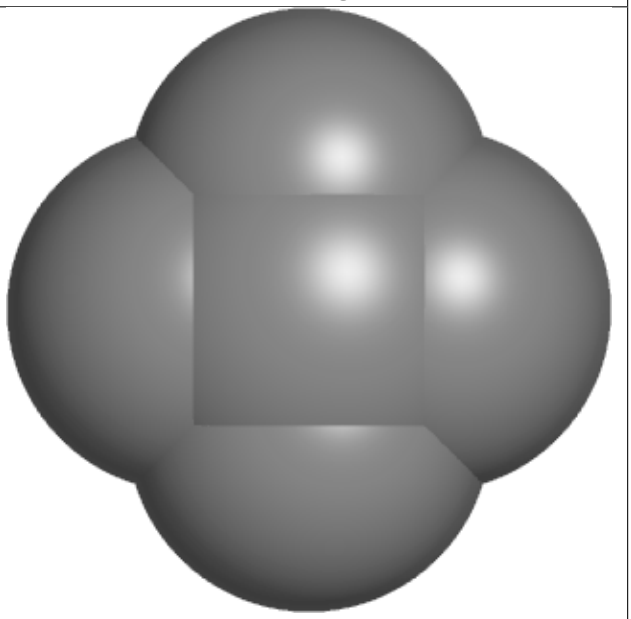
Bond lengths



Bond angles

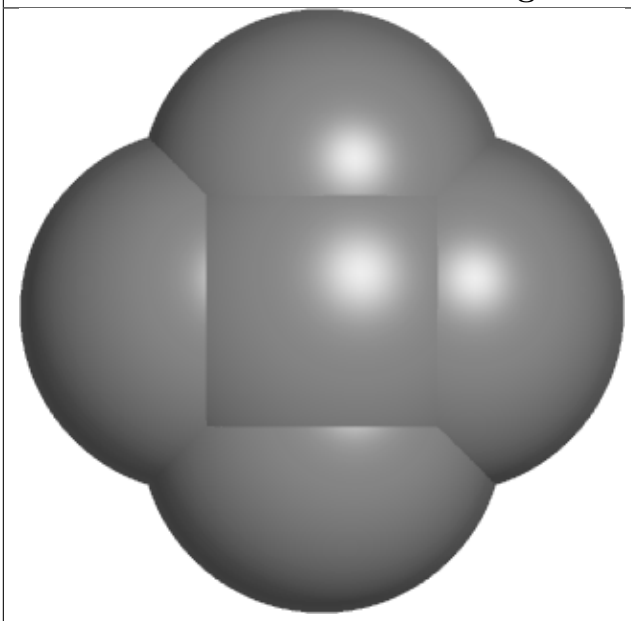


Torsions

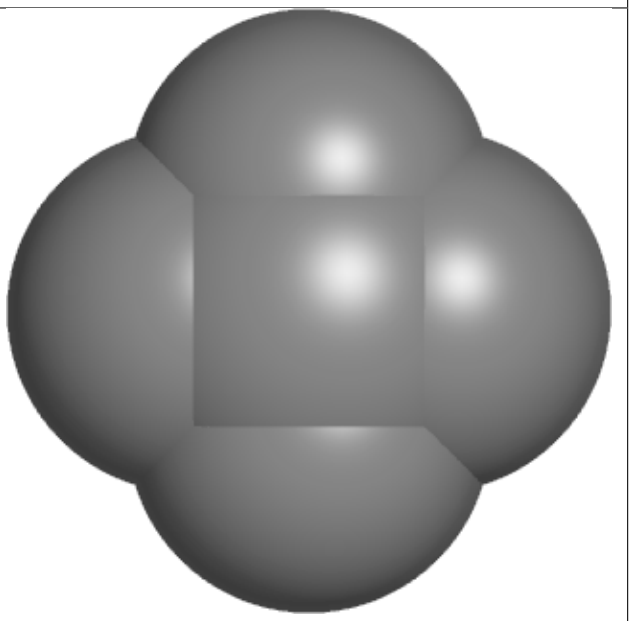


Rings

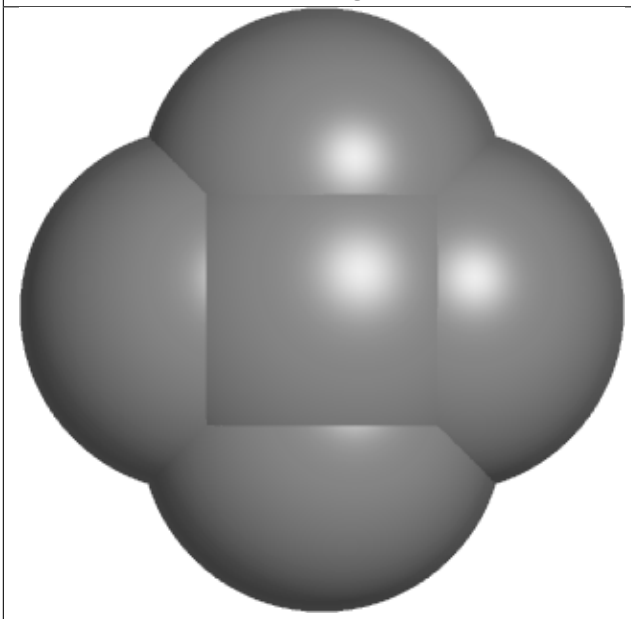
Ligand MOO C 101



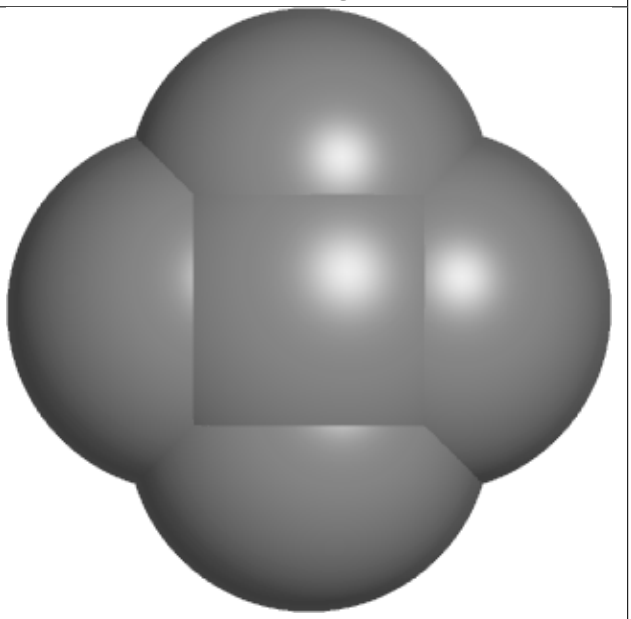
Bond lengths



Bond angles

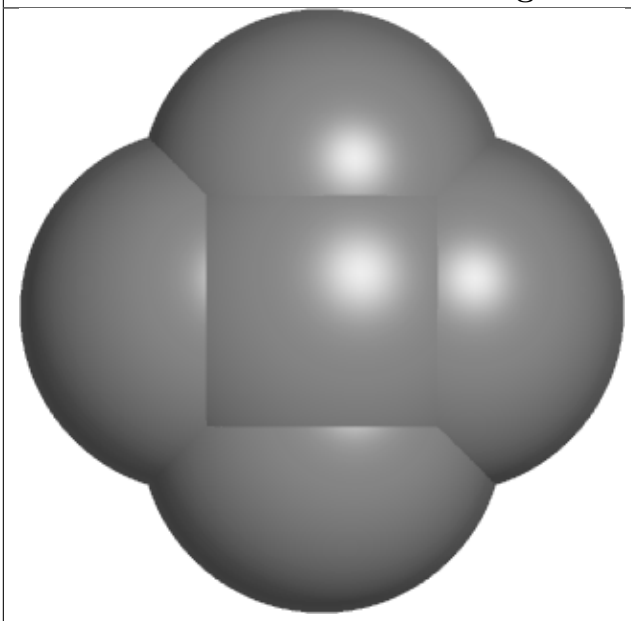


Torsions



Rings

Ligand MOO D 101



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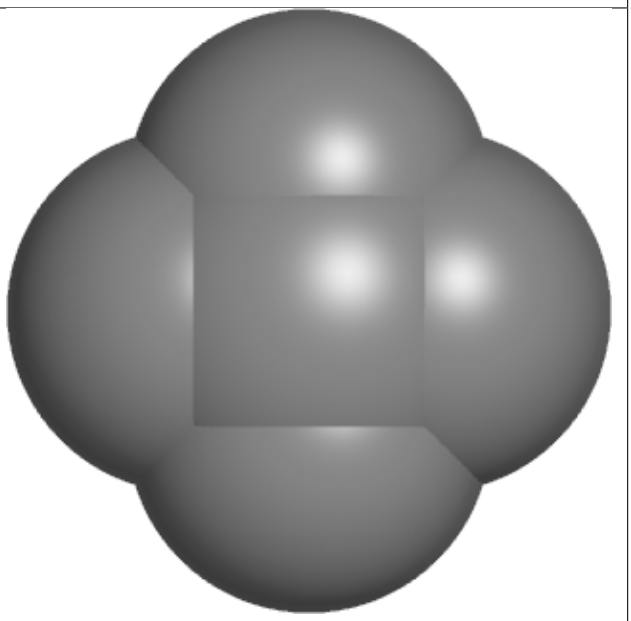
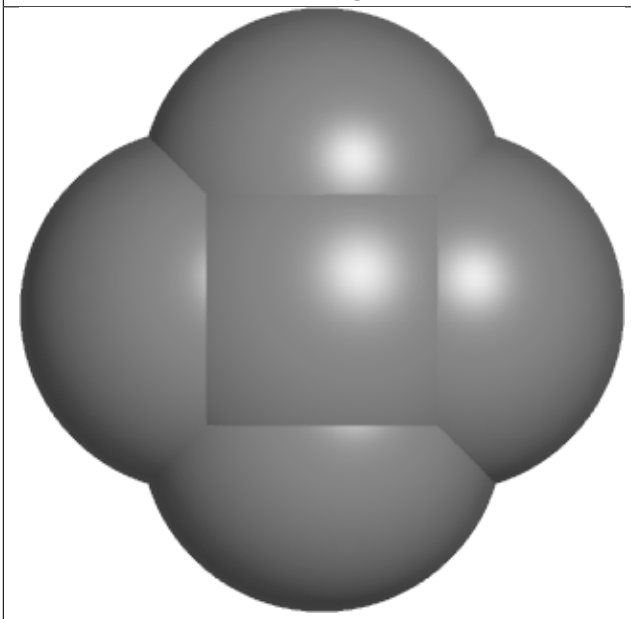
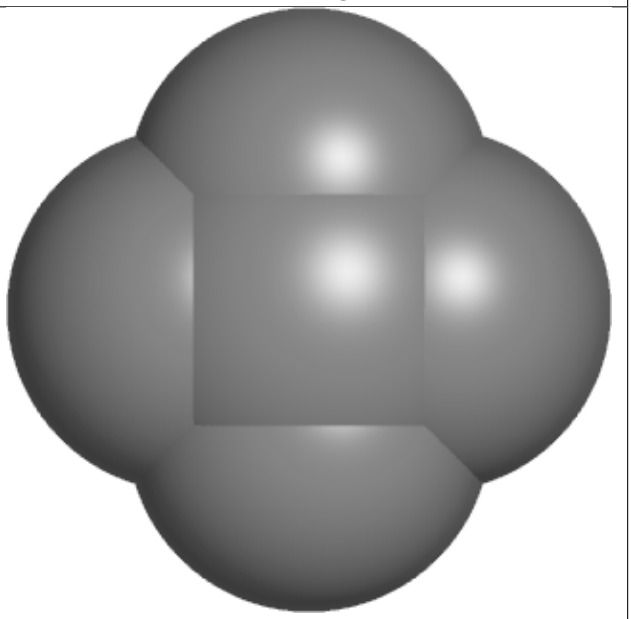


Bond angles

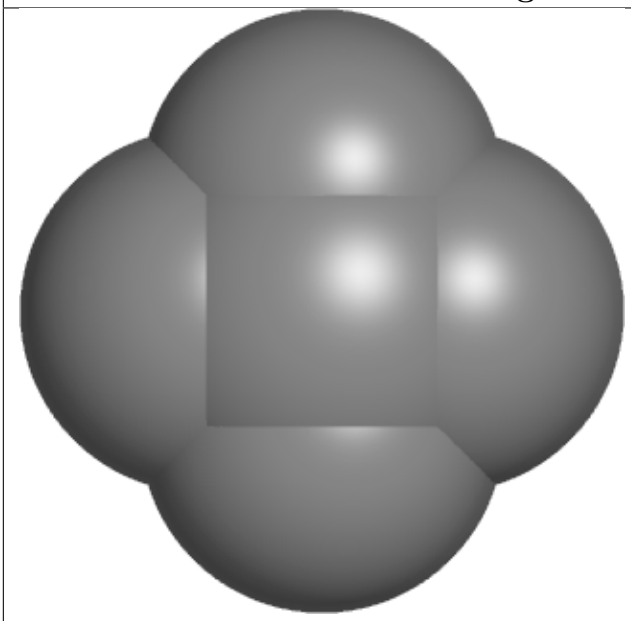


Torsions

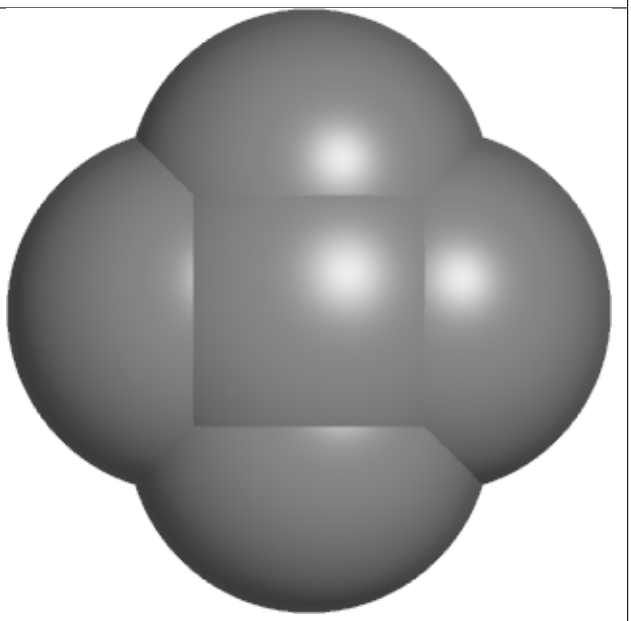


Rings

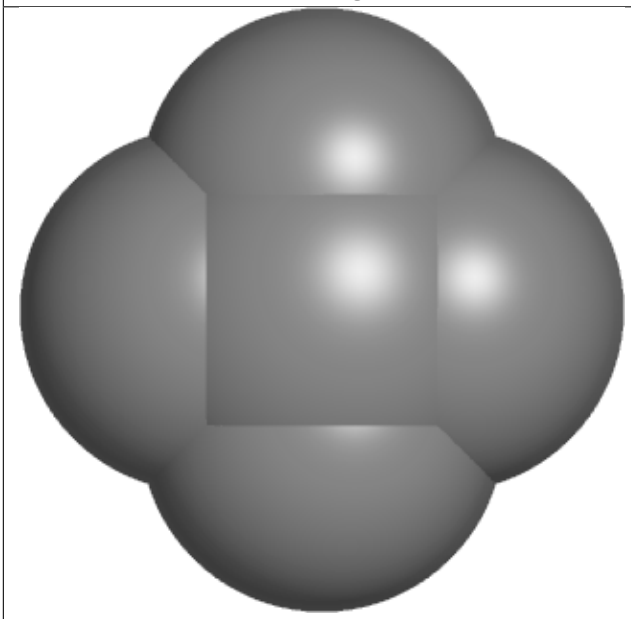
Ligand MOO A 102



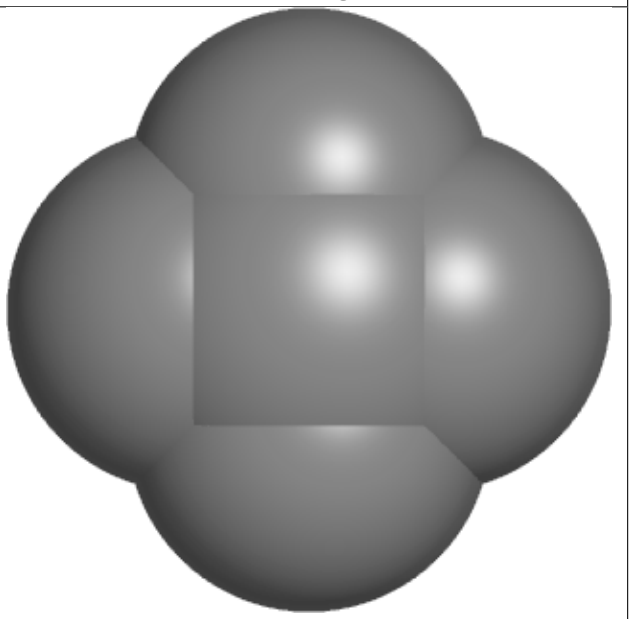
Bond lengths



Bond angles

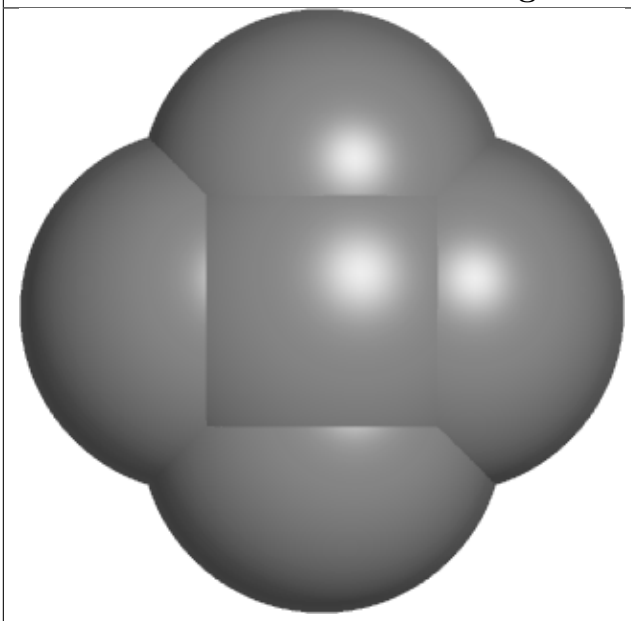


Torsions

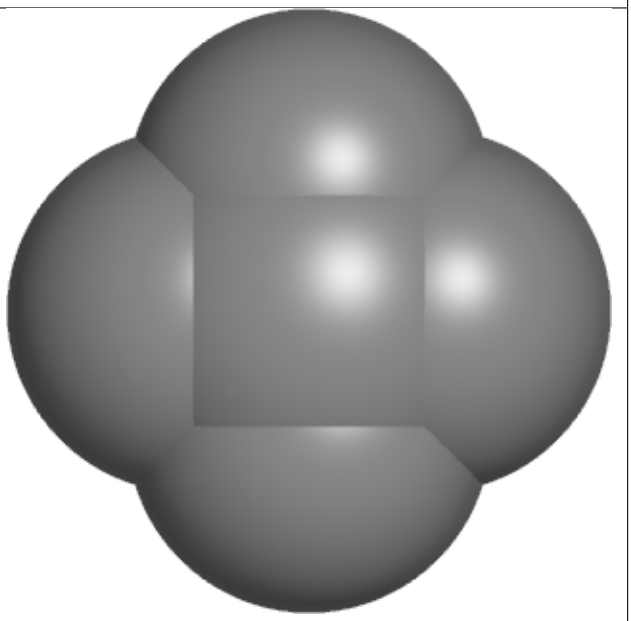


Rings

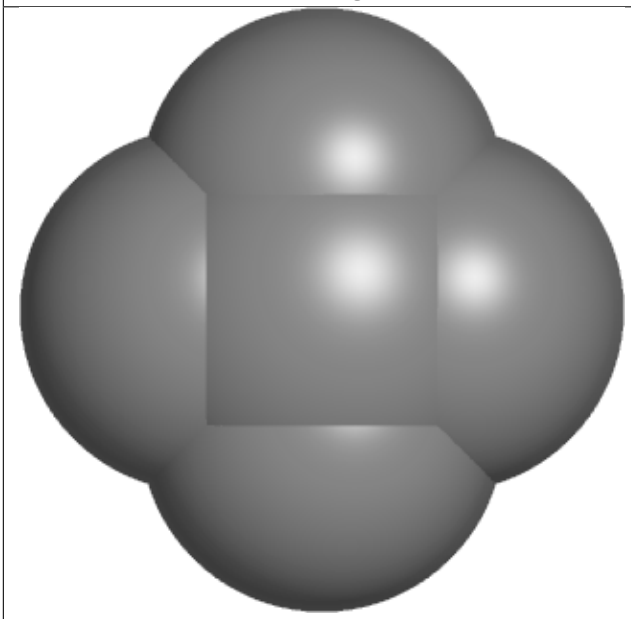
Ligand MOO E 101



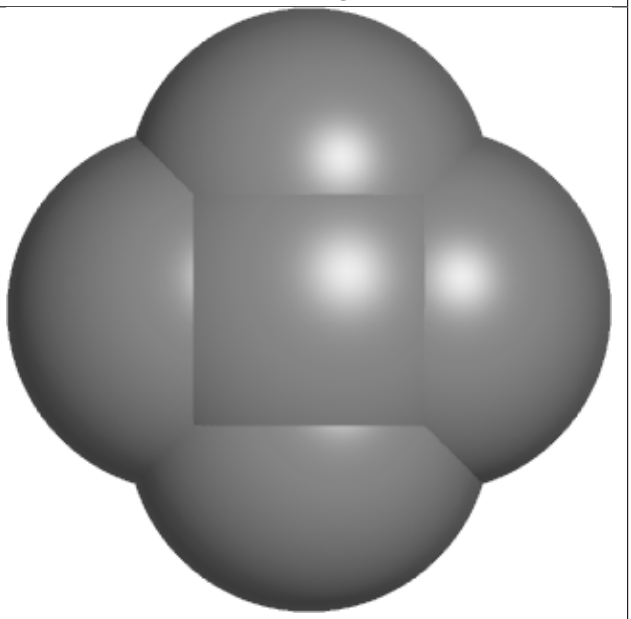
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	74/74 (100%)	-0.79	0	100	100	17, 25, 36, 46	0
1	B	69/74 (93%)	-0.83	0	100	100	17, 23, 32, 37	0
1	C	69/74 (93%)	-0.70	0	100	100	19, 26, 37, 40	0
1	D	69/74 (93%)	-0.55	0	100	100	18, 27, 37, 45	0
1	E	71/74 (95%)	-0.69	0	100	100	19, 28, 42, 46	0
1	F	70/74 (94%)	-0.42	0	100	100	19, 31, 46, 54	0
All	All	422/444 (95%)	-0.66	0	100	100	17, 26, 40, 54	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MOO	A	101	5/5	1.00	0.03	11,16,18,23	0

Continued on next page...

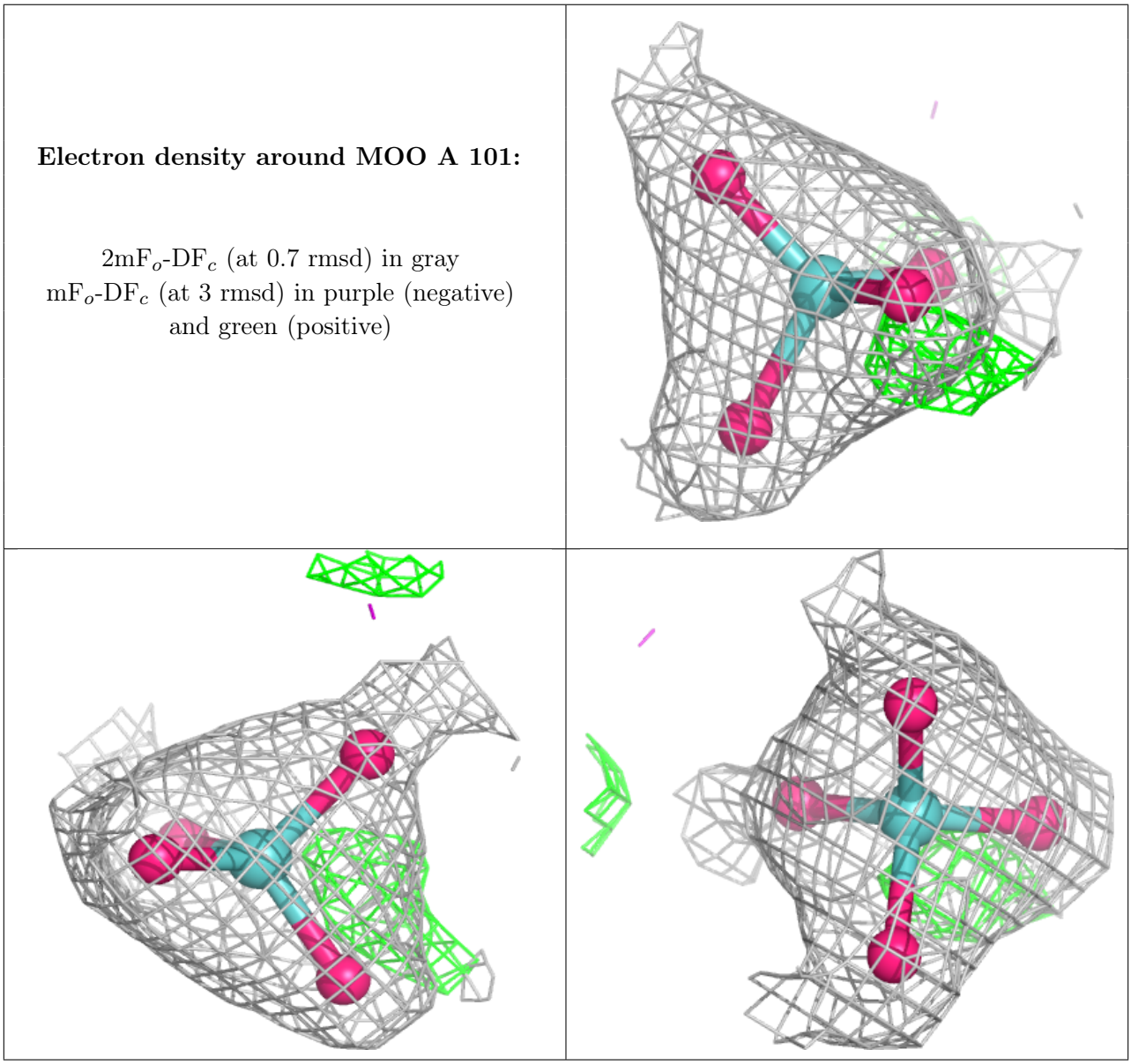
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MOO	A	102	5/5	1.00	0.03	16,17,19,19	0
2	MOO	B	101	5/5	1.00	0.03	14,15,17,19	0
2	MOO	B	102	5/5	1.00	0.03	14,17,19,21	0
2	MOO	C	101	5/5	1.00	0.03	16,18,20,20	0
2	MOO	D	101	5/5	1.00	0.02	15,16,18,19	0
2	MOO	E	101	5/5	1.00	0.03	14,20,21,21	0
2	MOO	F	101	5/5	1.00	0.04	13,15,19,20	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.

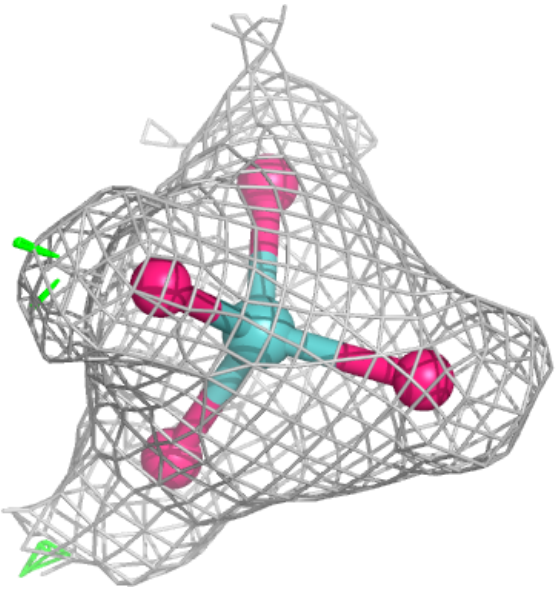
Electron density around MOO A 101:

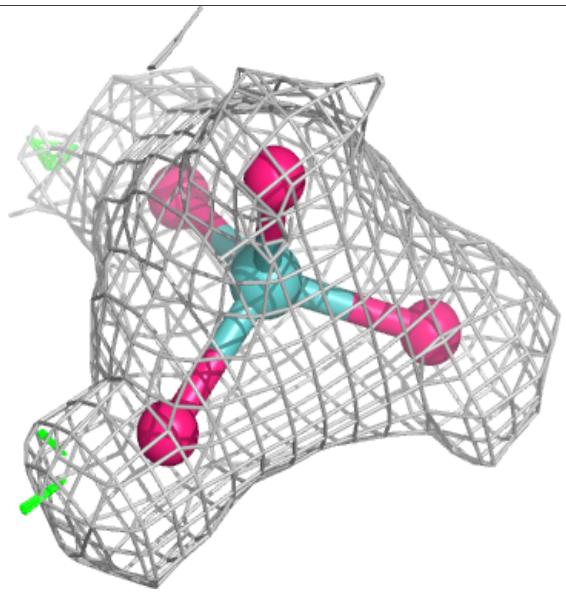
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

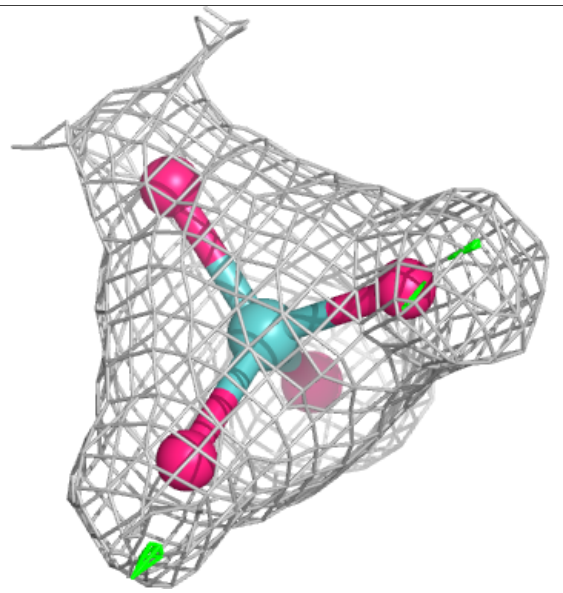


Electron density around MOO A 102:

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

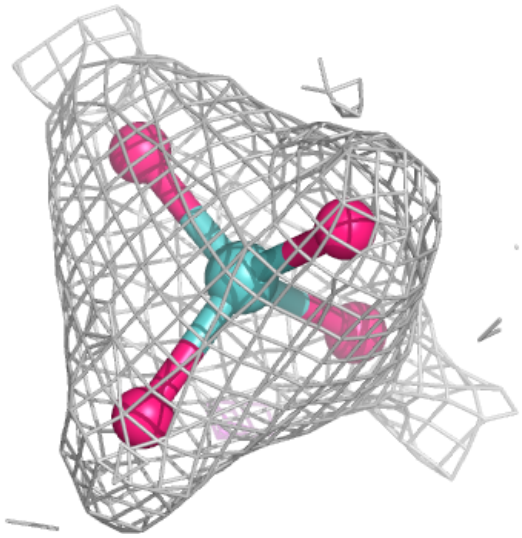


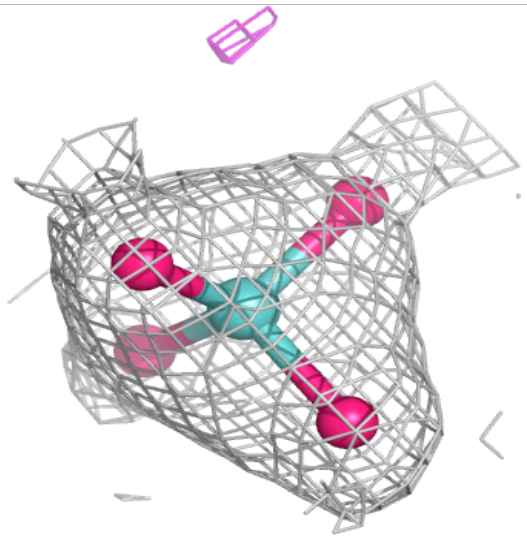


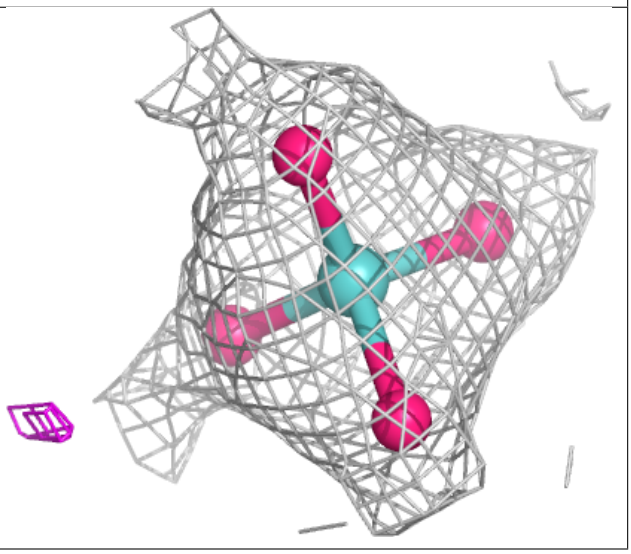


Electron density around MOO B 101:

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

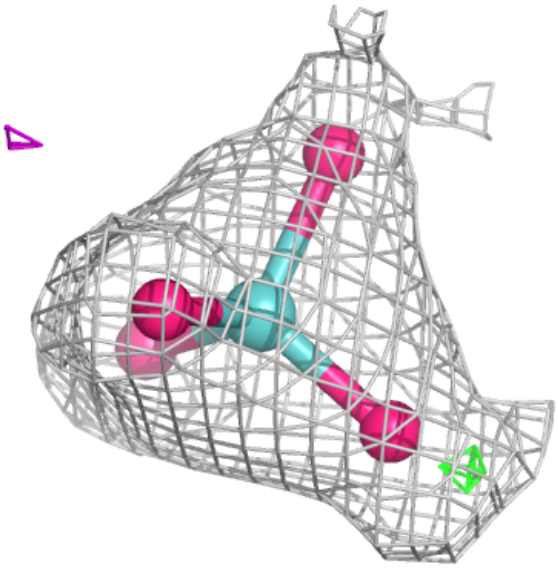


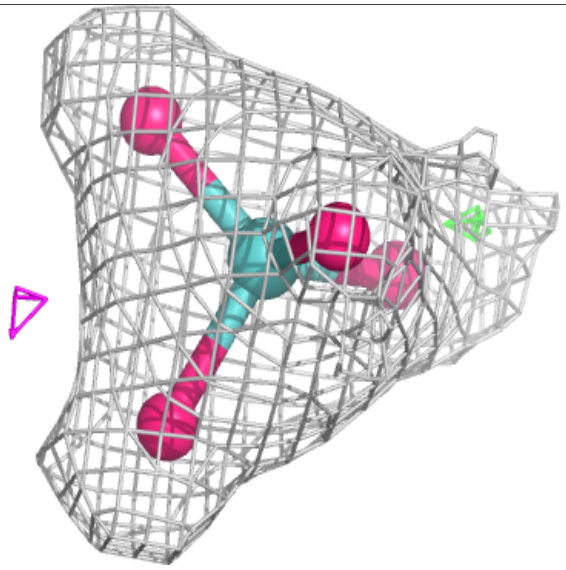


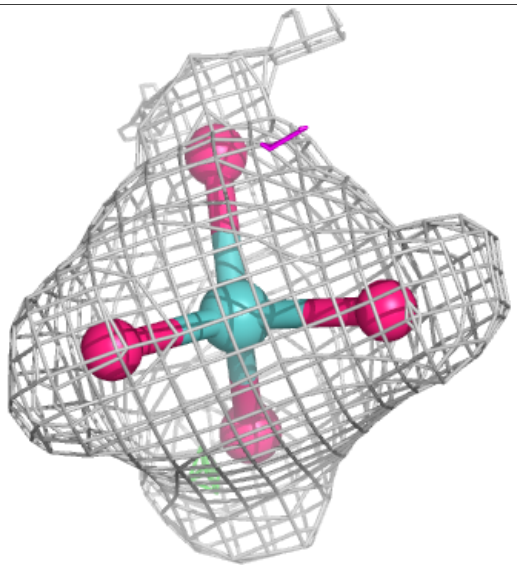


Electron density around MOO B 102:

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

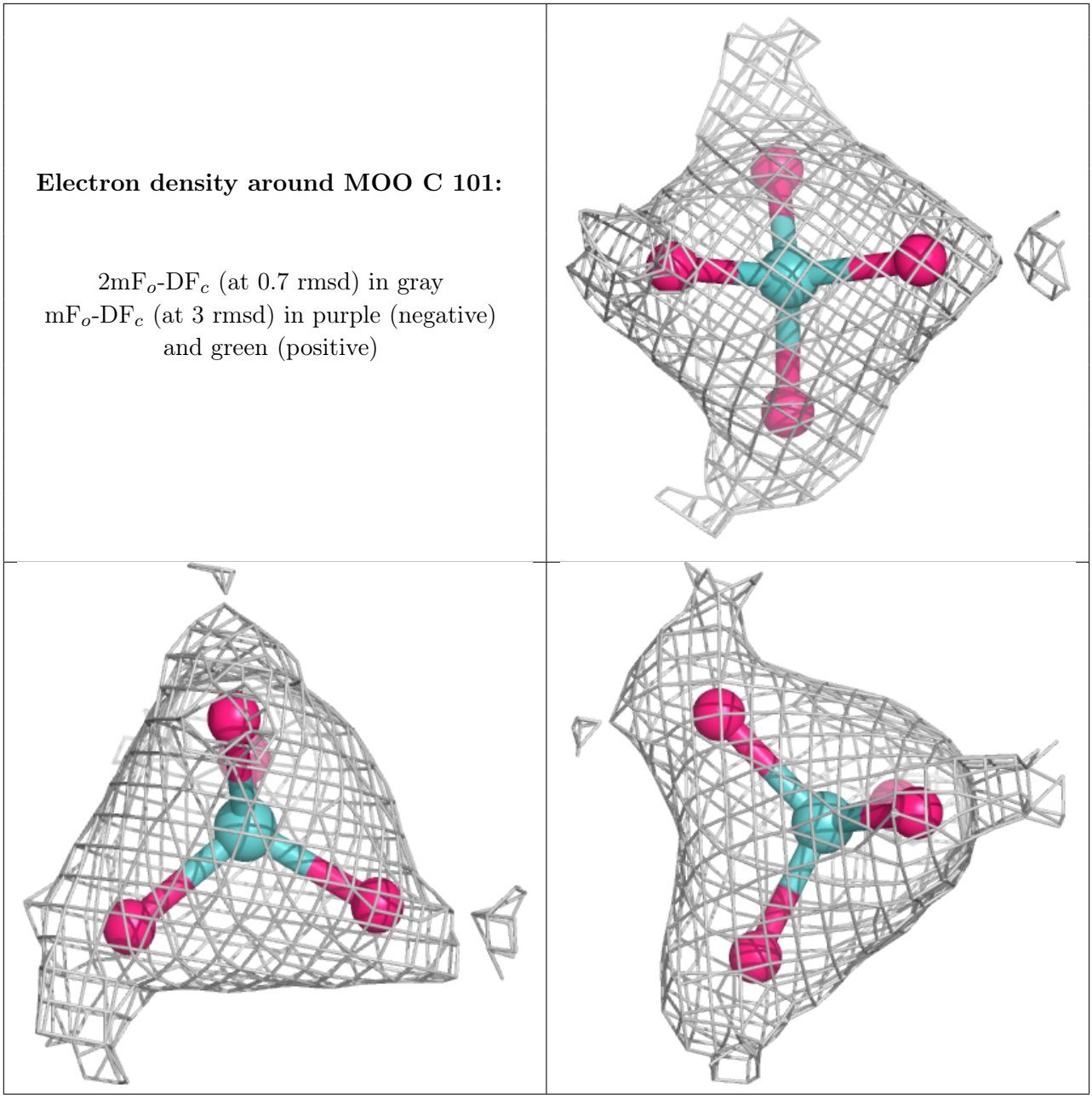






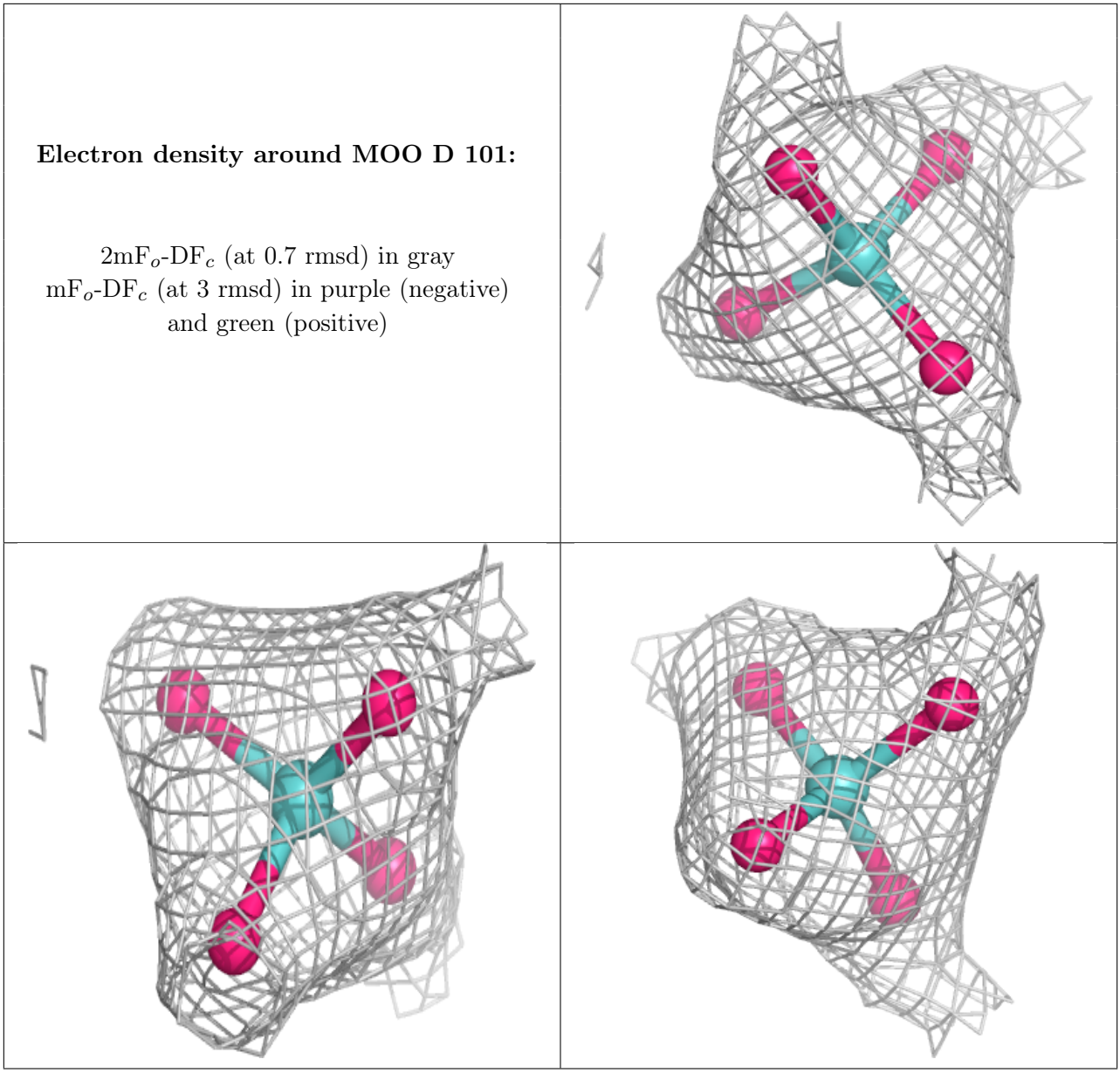
Electron density around MOO C 101:

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



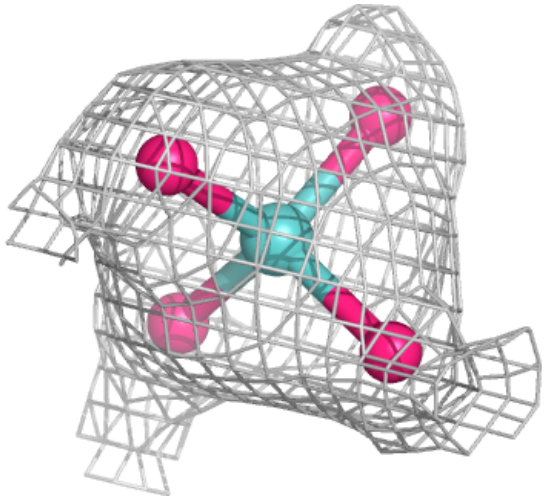
Electron density around MOO D 101:

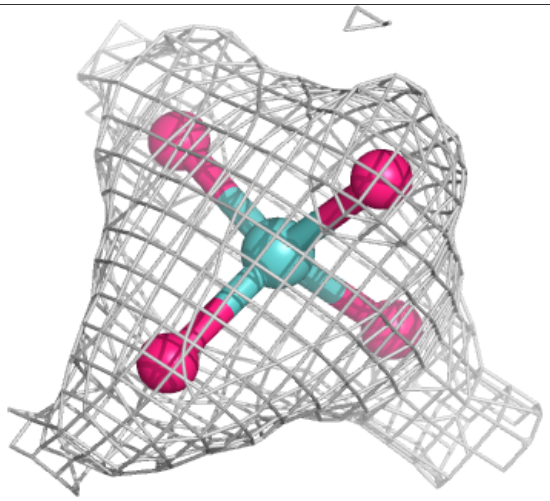
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

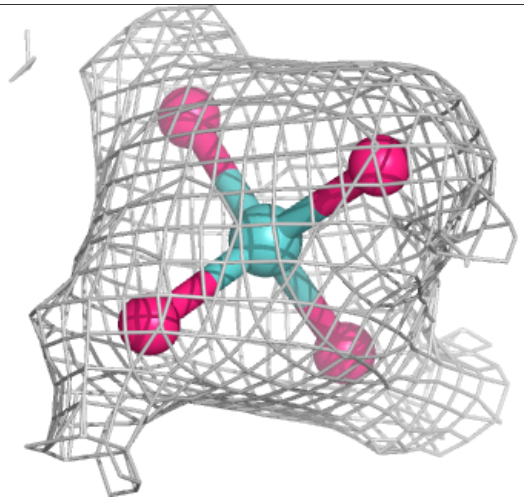


Electron density around MOO E 101:

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

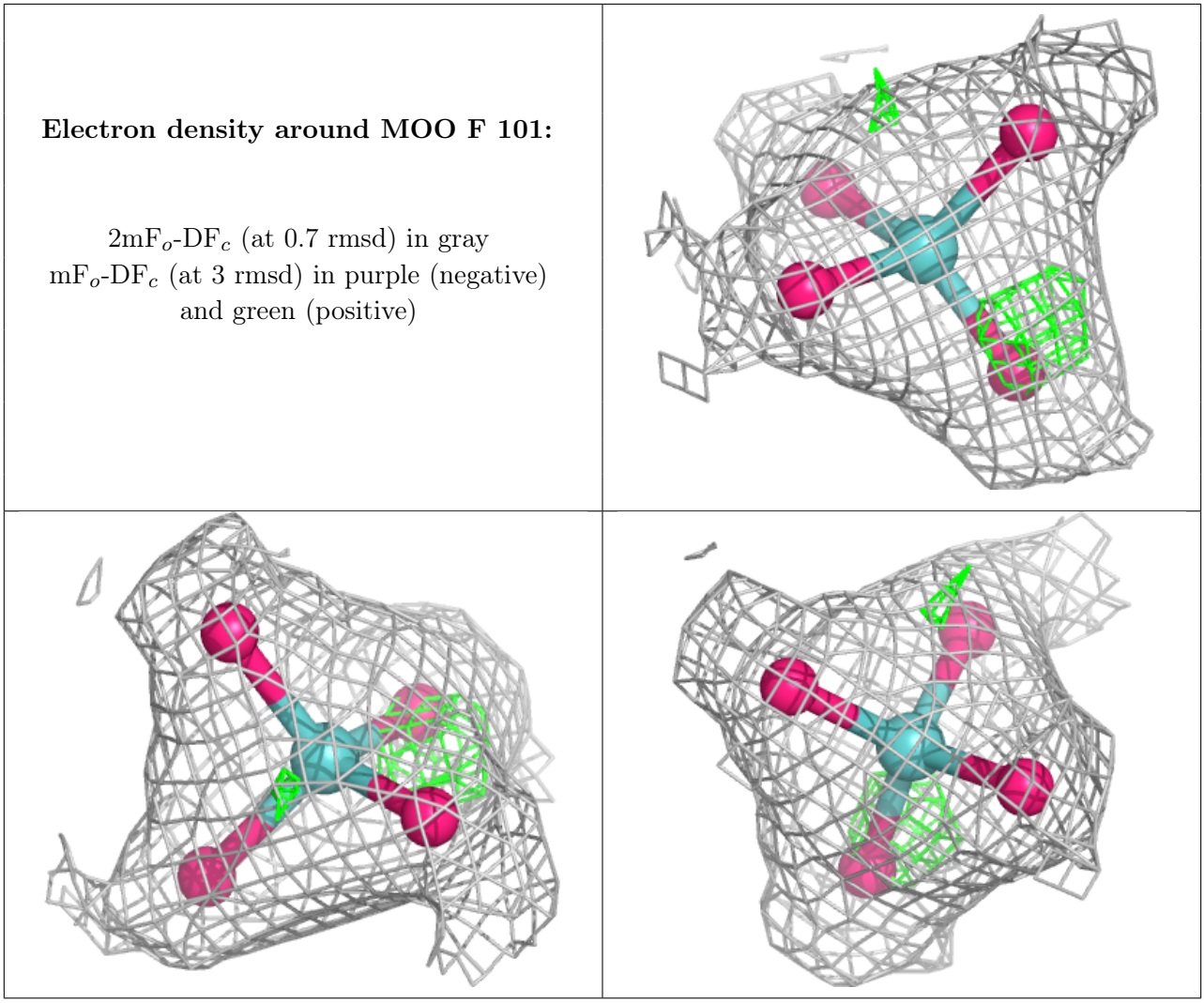






Electron density around MOO F 101:

$2mF_o$-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.