



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 17, 2025 – 01:09 pm BST

PDB ID : 9FPP / pdb_00009fpp
Title : FGD2 (Rv0132c) from Mycobacterium tuberculosis with cofactor F420 crystallised with Anderson-Evans polyoxotungstate
Authors : Aderemi, A.; Snee, M.; Levy, C.; Leys, D.
Deposited on : 2024-06-13
Resolution : 2.35 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4-5-2 with Phenix2.0rc1
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

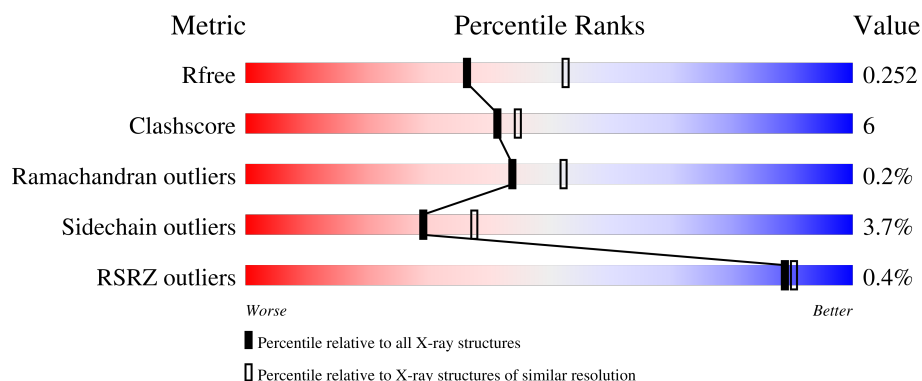
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.35 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	1460 (2.36-2.36)
Clashscore	180529	1571 (2.36-2.36)
Ramachandran outliers	177936	1559 (2.36-2.36)
Sidechain outliers	177891	1559 (2.36-2.36)
RSRZ outliers	164620	1460 (2.36-2.36)

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 $\leq 5\%$. 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	332	 83% 11% . .
1	B	332	 81% 13% . .
1	E	332	 82% 12% . .
1	F	332	 81% 12% . .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10957 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.

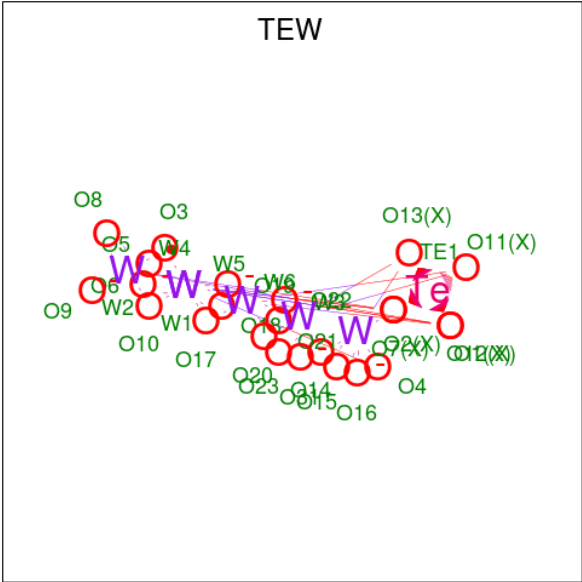
- Molecule 1 is a protein called F420-dependent hydroxymycolic acid dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	2	0
			2463	1566	440	454	3			
1	B	319	Total	C	N	O	S	0	2	0
			2456	1562	436	455	3			
1	E	319	Total	C	N	O	S	0	1	0
			2452	1559	436	454	3			
1	F	318	Total	C	N	O	S	0	2	0
			2458	1562	441	452	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	GLY	-	expression tag	UNP P96809
A	30	SER	-	expression tag	UNP P96809
B	29	GLY	-	expression tag	UNP P96809
B	30	SER	-	expression tag	UNP P96809
E	29	GLY	-	expression tag	UNP P96809
E	30	SER	-	expression tag	UNP P96809
F	29	GLY	-	expression tag	UNP P96809
F	30	SER	-	expression tag	UNP P96809

- Molecule 2 is 6-tungstotellurate(VI) (CCD ID: TEW) (formula: O₂₄TeW₆).



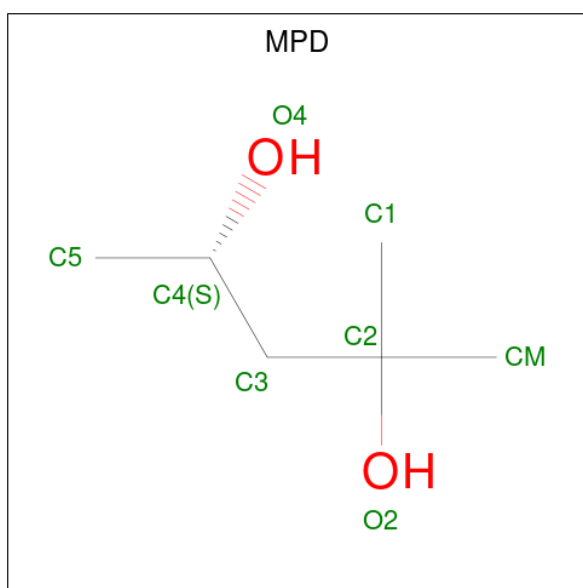
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	O	Te	W	0	1
			62	48	2	12		
2	A	1	Total	O	Te	W	0	0
			31	24	1	6		
2	A	1	Total	O	Te	W	0	0
			31	24	1	6		
2	B	1	Total	O	Te	W	0	0
			31	24	1	6		
2	E	1	Total	O	Te	W	0	0
			27	20	1	6		
2	E	1	Total	O	Te	W	0	1
			62	48	2	12		
2	E	1	Total	O	Te	W	0	0
			31	24	1	6		

- Molecule 3 is IMIDAZOLE (CCD ID: IMD) (formula: C₃H₅N₂).



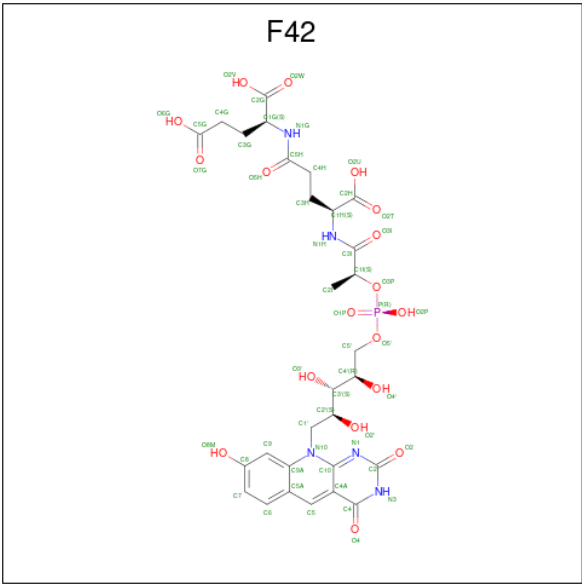
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			5	3	2		
3	E	1	Total	C	N	0	0
			5	3	2		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			8	6	2		
4	F	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is COENZYME F420 (CCD ID: F42) (formula: C₂₉H₃₆N₅O₁₈P) (labeled as "Ligand of Interest" by depositor).

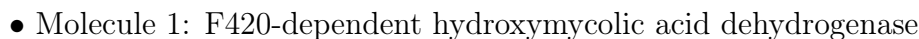


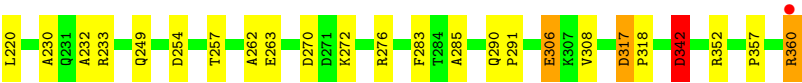
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			53	29	5	18	1		
5	F	1	Total	C	N	O	P	0	0
			53	29	5	18	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	182	Total	O	0	0
			182	182		
6	B	163	Total	O	0	0
			163	163		
6	E	178	Total	O	0	0
			178	178		
6	F	198	Total	O	0	0
			198	198		

- Molecule 1: F420-dependent hydroxymycolic acid dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.31Å 89.31Å 155.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.82 – 2.35 77.82 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (77.82-2.35) 100.0 (77.82-2.35)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.210 , 0.251 0.211 , 0.252	Depositor DCC
R_{free} test set	2615 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10957	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 59.91 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6460e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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: IMD, MPD, TEW, F42

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	0.61	0/2534	1.18	5/3459 (0.1%)
1	B	0.60	0/2527	1.17	6/3451 (0.2%)
1	E	0.62	0/2520	1.19	10/3442 (0.3%)
1	F	0.60	1/2528 (0.0%)	1.22	13/3448 (0.4%)
All	All	0.61	1/10109 (0.0%)	1.19	34/13800 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	E	0	1
1	F	0	3
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	276	ARG	NE-CZ	5.03	1.38	1.33

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	342	ASP	CA-CB-CG	9.30	121.90	112.60
1	B	147	GLU	CB-CA-C	-7.93	92.81	109.38
1	F	276	ARG	CA-CB-CG	7.57	129.24	114.10
1	A	147	GLU	CB-CA-C	-7.48	93.74	109.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	147	GLU	CB-CA-C	-7.38	93.95	109.38

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	192	ARG	Sidechain
1	A	57	ARG	Sidechain
1	B	162	ARG	Sidechain
1	B	298	ARG	Sidechain
1	E	192	ARG	Sidechain

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	2463	0	2392	26	0
1	B	2456	0	2377	29	0
1	E	2452	0	2370	25	0
1	F	2458	0	2388	35	0
2	A	124	0	0	13	0
2	B	31	0	0	1	0
2	E	120	0	0	6	0
3	A	5	0	5	2	0
3	E	5	0	5	2	0
4	B	8	0	14	0	0
4	F	8	0	14	0	0
5	B	53	0	31	0	0
5	F	53	0	31	1	0
6	A	182	0	0	8	0
6	B	163	0	0	5	0
6	E	178	0	0	9	0
6	F	198	0	0	13	0
All	All	10957	0	9627	125	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 6.

The worst 5 of 125 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:F:232:ALA:HB2	6:F:501:HOH:O	1.54	1.06
1:E:276:ARG:NH1	2:E:401:TEW:O9	1.95	1.00
1:B:60:ALA:HB2	6:B:531:HOH:O	1.71	0.89
2:A:401[B]:TEW:O22	1:B:298:ARG:NH2	2.07	0.88
1:B:276:ARG:NH1	1:B:342:ASP:OD2	2.08	0.84

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	319/332 (96%)	310 (97%)	7 (2%)	2 (1%)	22	24
1	B	319/332 (96%)	308 (97%)	10 (3%)	1 (0%)	37	43
1	E	318/332 (96%)	309 (97%)	9 (3%)	0	100	100
1	F	317/332 (96%)	308 (97%)	9 (3%)	0	100	100
All	All	1273/1328 (96%)	1235 (97%)	35 (3%)	3 (0%)	44	52

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	89	SER
1	A	89	SER
1	A	115	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	245/254 (96%)	236 (96%)	9 (4%)	29	38
1	B	244/254 (96%)	236 (97%)	8 (3%)	33	42
1	E	243/254 (96%)	232 (96%)	11 (4%)	23	29
1	F	244/254 (96%)	235 (96%)	9 (4%)	29	38
All	All	976/1016 (96%)	939 (96%)	37 (4%)	29	37

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	74	TRP
1	F	317	ASP
1	F	102	SER
1	F	193	THR
1	B	193	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	85	ASN
1	F	311	ASN
1	B	354	ASN
1	E	63	GLN
1	E	67	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

15 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$
4	MPD	F	401	-	7,7,7	0.22	0	9,10,10	0.50	0
2	TEW	A	402	6	29,42,42	0.89	1 (3%)	12,129,129	3.04	6 (50%)
2	TEW	A	403	-	29,42,42	0.84	0	12,129,129	2.32	4 (33%)
2	TEW	E	403	-	29,42,42	0.88	1 (3%)	12,129,129	3.10	5 (41%)
3	IMD	A	404	-	3,5,5	0.25	0	4,5,5	0.56	0
4	MPD	B	401	-	7,7,7	0.23	0	9,10,10	0.43	0
2	TEW	A	401[B]	-	29,42,42	0.92	1 (3%)	12,129,129	3.73	5 (41%)
2	TEW	E	401	1	18,38,42	0.65	0	12,111,129	3.22	7 (58%)
2	TEW	E	402[B]	6	29,42,42	0.87	1 (3%)	12,129,129	4.86	7 (58%)
5	F42	B	402	-	51,55,55	1.33	5 (9%)	64,79,79	2.24	5 (7%)
2	TEW	A	401[A]	6	29,42,42	0.95	2 (6%)	12,129,129	3.23	8 (66%)
2	TEW	E	402[A]	-	29,42,42	0.89	1 (3%)	12,129,129	3.77	7 (58%)
5	F42	F	402	-	51,55,55	1.20	4 (7%)	64,79,79	2.19	7 (10%)
2	TEW	B	403	-	29,42,42	0.82	0	12,129,129	2.34	5 (41%)
3	IMD	E	404	-	3,5,5	0.25	0	4,5,5	0.58	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
4	MPD	F	401	-	-	2/5/5/5	-
3	IMD	A	404	-	-	-	0/1/1/1
4	MPD	B	401	-	-	3/5/5/5	-
5	F42	B	402	-	-	5/53/53/53	0/3/3/3
5	F42	F	402	-	-	10/53/53/53	0/3/3/3
3	IMD	E	404	-	-	-	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	402	F42	C10-N1	4.73	1.39	1.33
5	F	402	F42	C10-N1	4.04	1.38	1.33
5	B	402	F42	C9-C8	3.94	1.44	1.37
5	B	402	F42	C4-N3	3.81	1.39	1.33
5	F	402	F42	O8M-C8	-3.75	1.28	1.37

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	402	F42	C4A-C4-N3	-11.37	116.47	124.40
5	F	402	F42	C4A-C4-N3	-11.04	116.70	124.40
5	B	402	F42	C2-N3-C4	11.03	124.46	115.14
2	E	402[B]	TEW	O11-TE1-O7	10.87	104.44	94.65
5	F	402	F42	C2-N3-C4	10.60	124.09	115.14

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

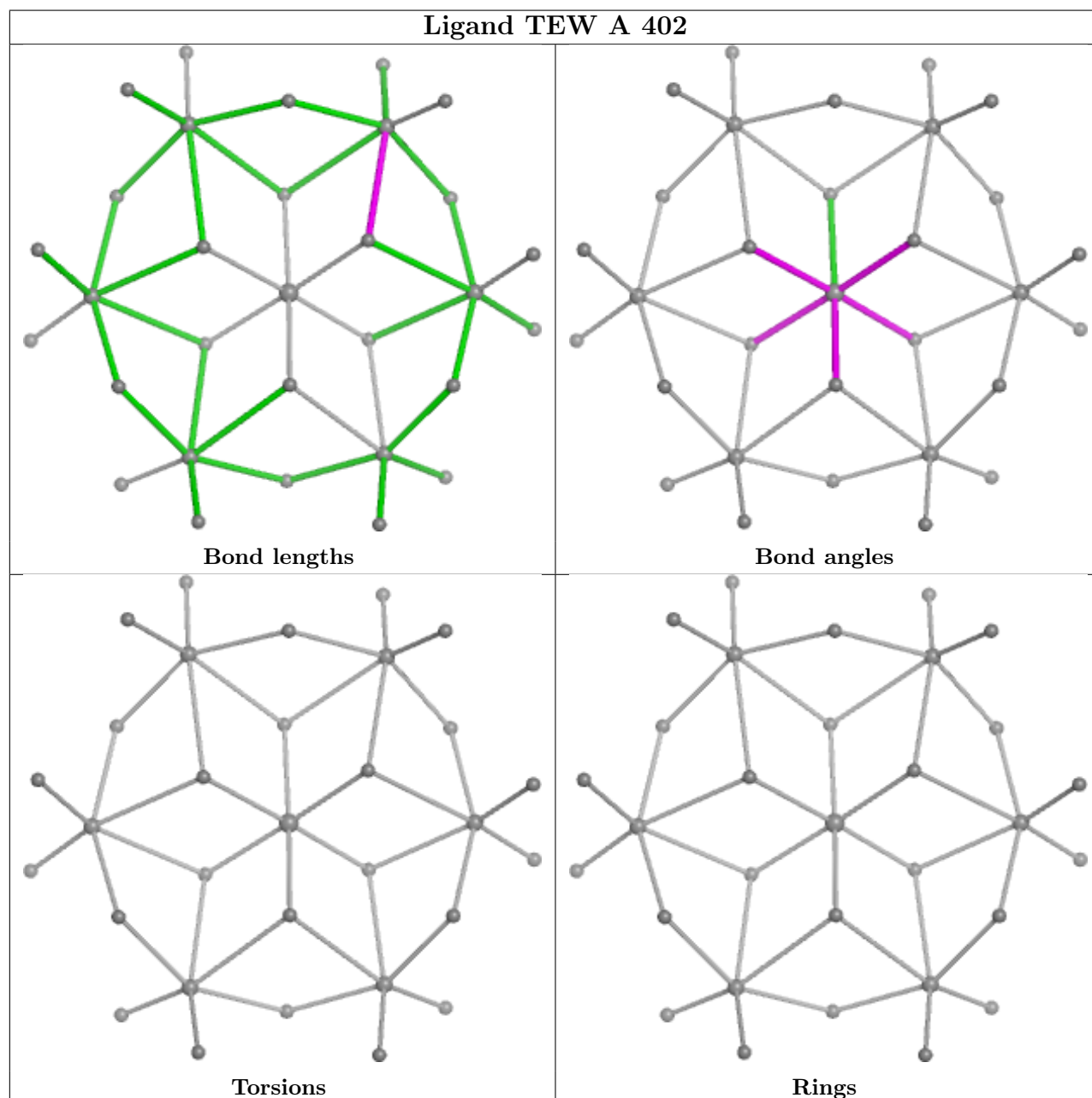
Mol	Chain	Res	Type	Atoms
4	B	401	MPD	CM-C2-C3-C4
5	F	402	F42	C5'-O5'-P-O1P
5	F	402	F42	N1G-C1G-C3G-C4G
5	F	402	F42	C5'-O5'-P-O3P
5	B	402	F42	C1G-C3G-C4G-C5G

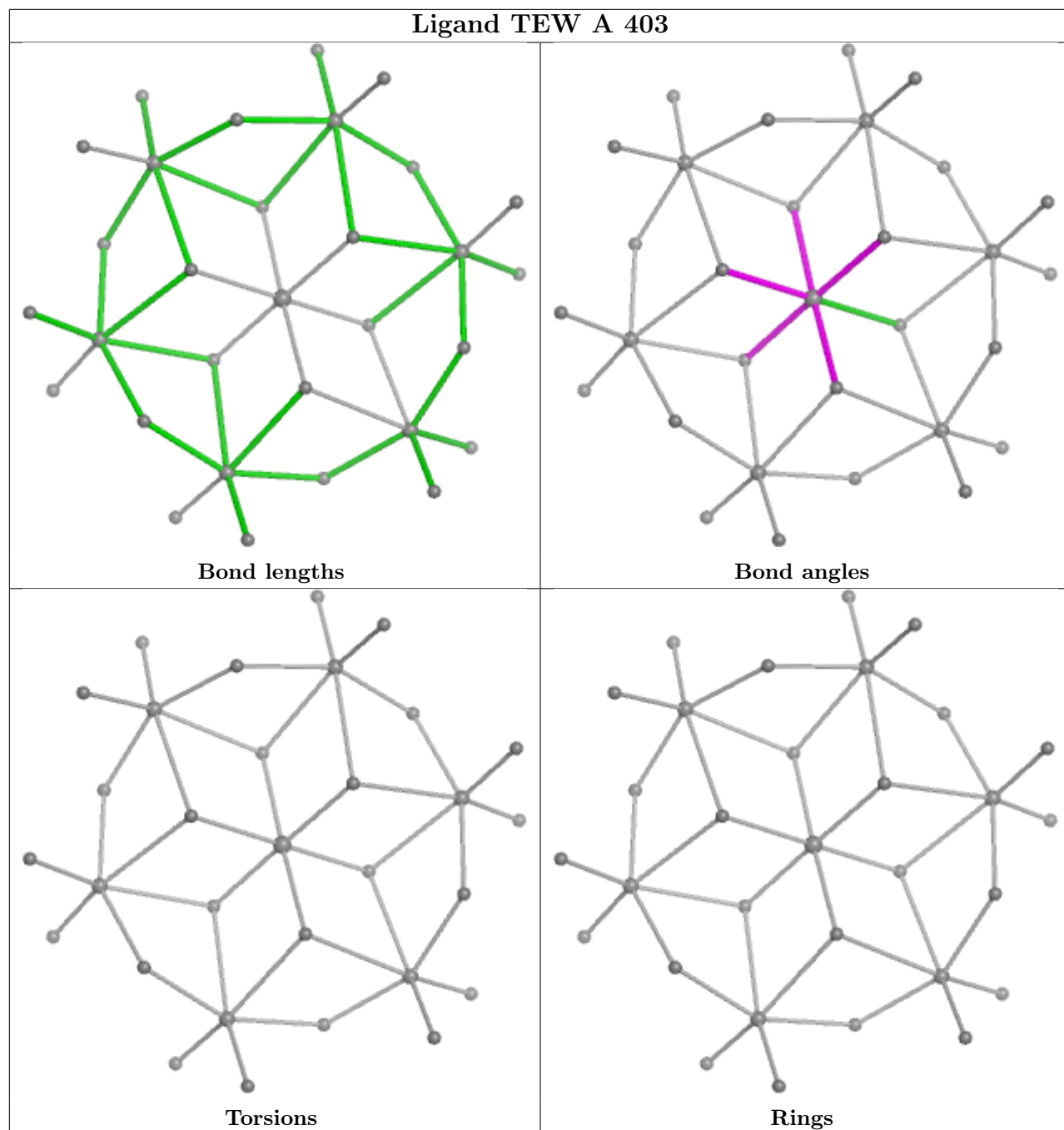
There are no ring outliers.

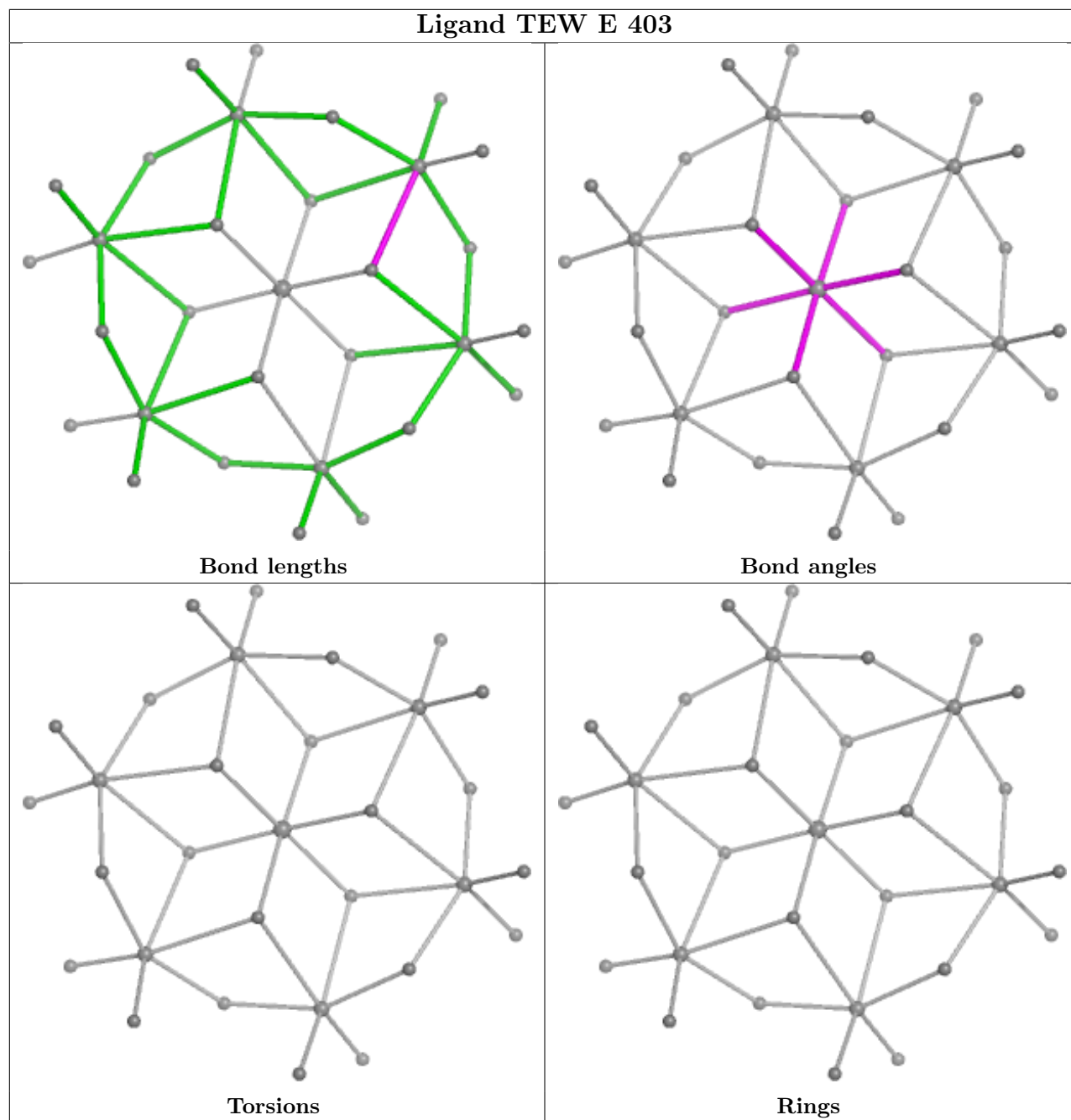
11 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	402	TEW	1	0
2	A	403	TEW	6	0
2	E	403	TEW	2	0
3	A	404	IMD	2	0
2	A	401[B]	TEW	4	0
2	E	401	TEW	1	0
2	E	402[B]	TEW	3	0
2	A	401[A]	TEW	2	0
5	F	402	F42	1	0
2	B	403	TEW	1	0
3	E	404	IMD	2	0

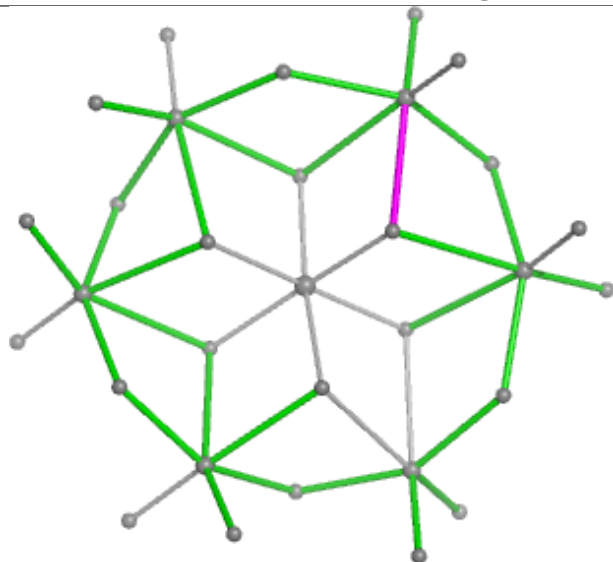
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



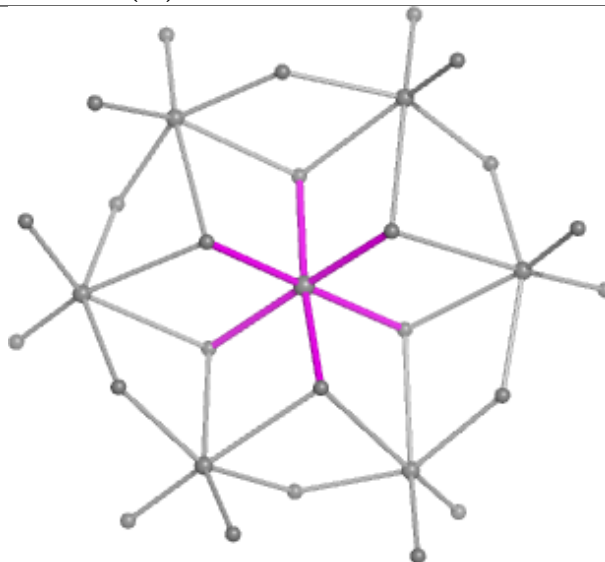




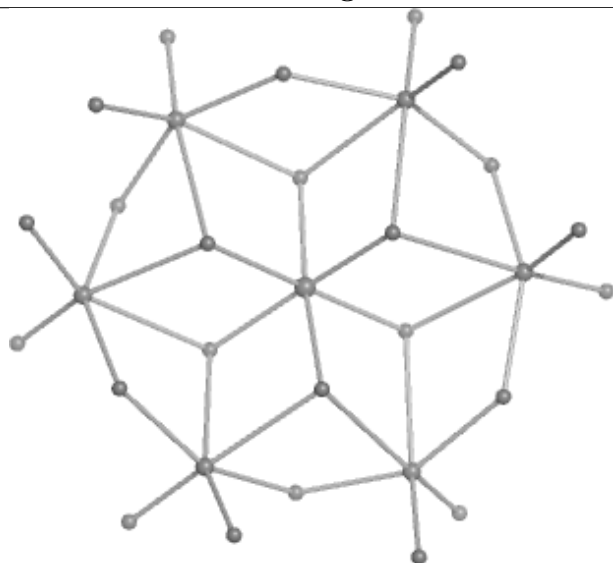
Ligand TEW A 401 (B)



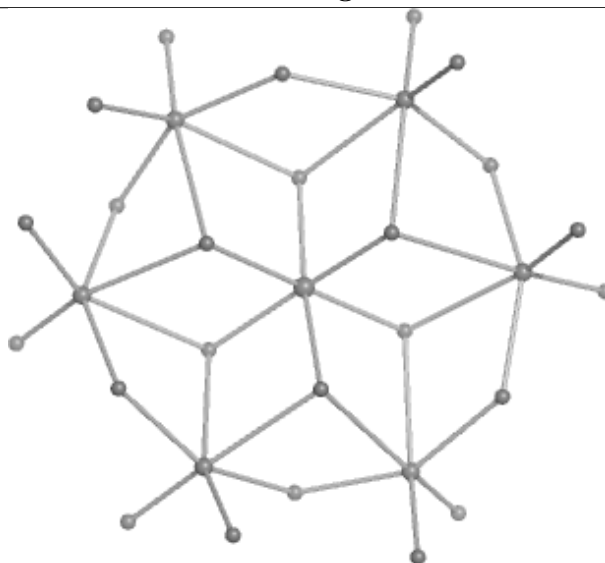
Bond lengths



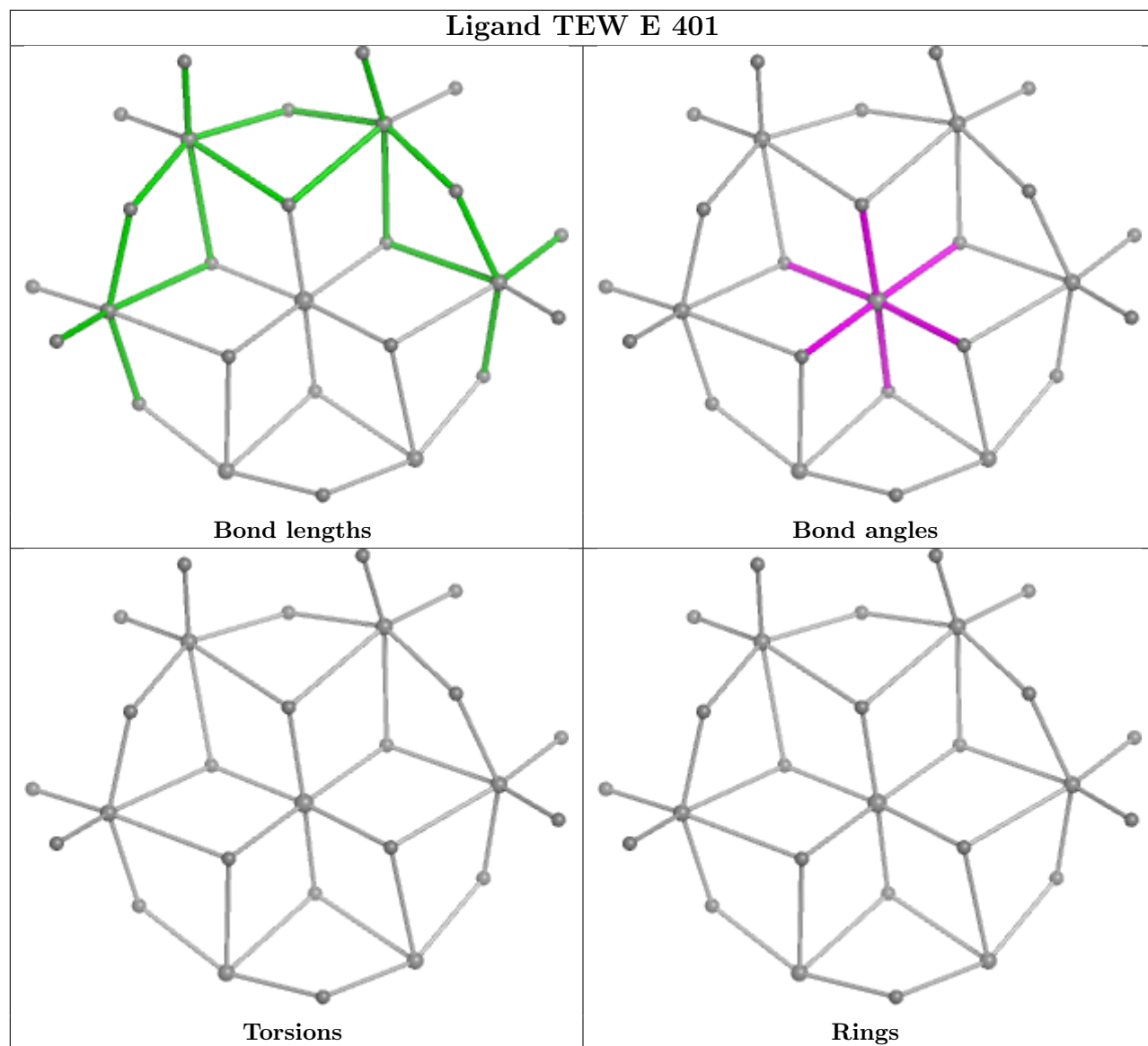
Bond angles



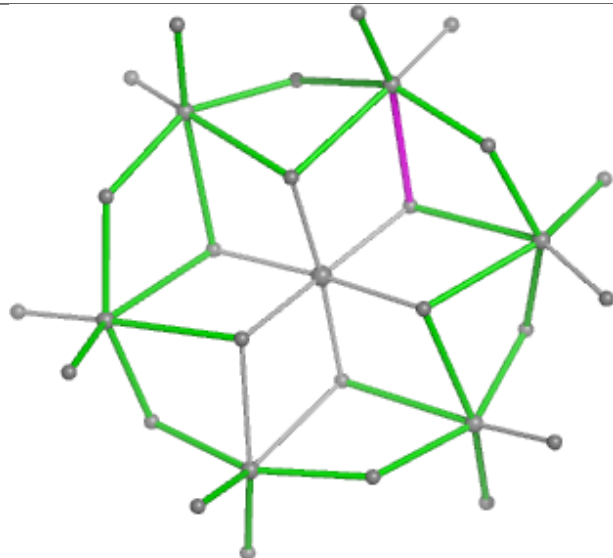
Torsions



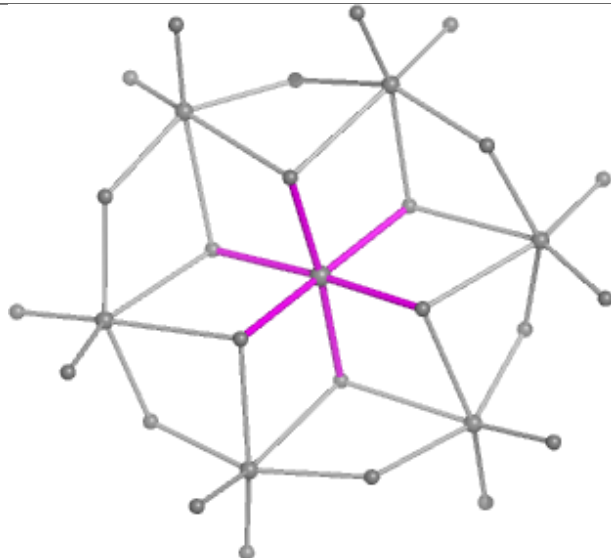
Rings



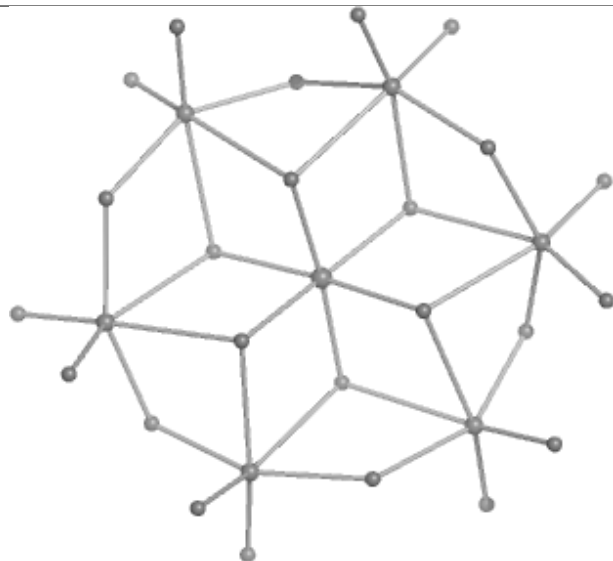
Ligand TEW E 402 (B)



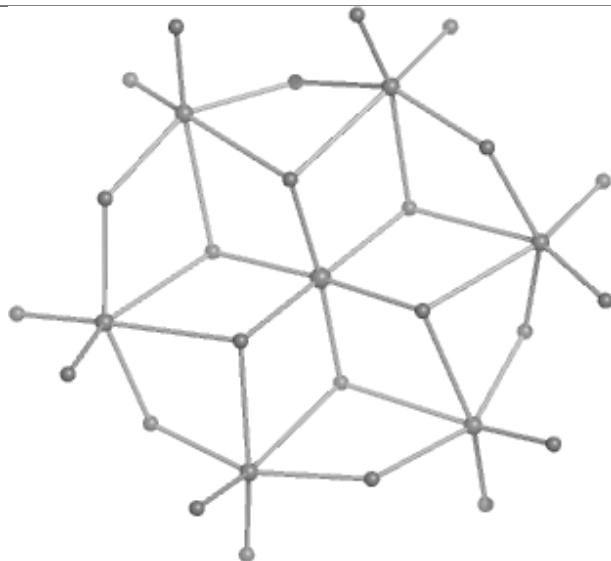
Bond lengths



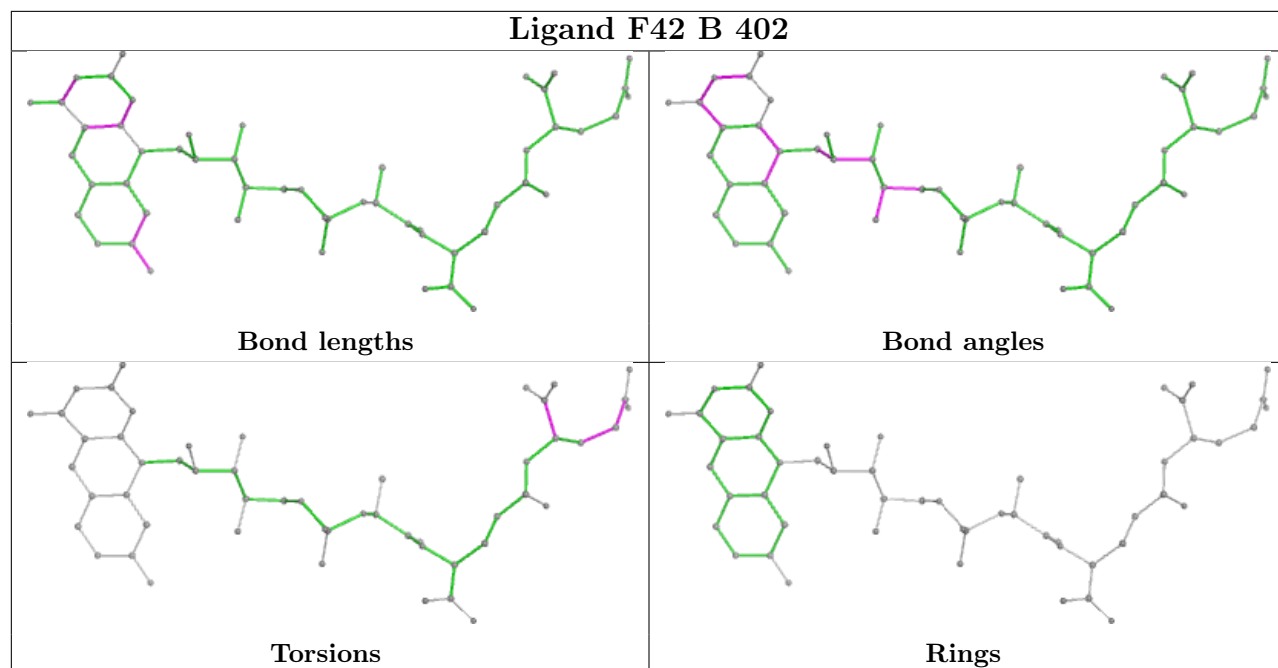
Bond angles



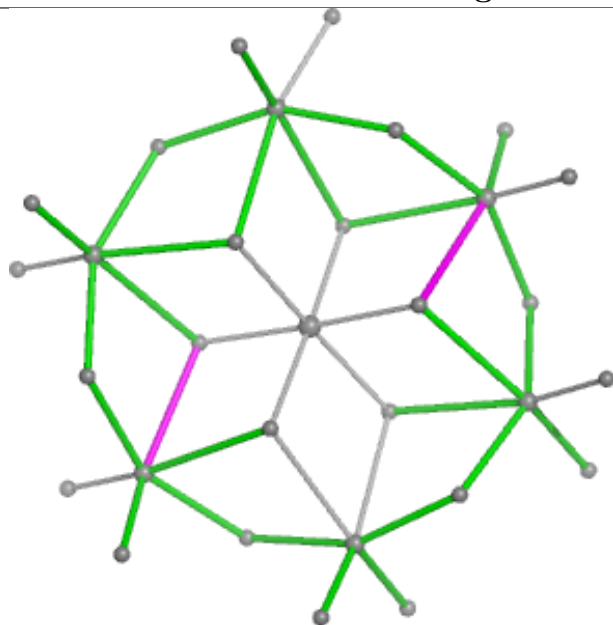
Torsions



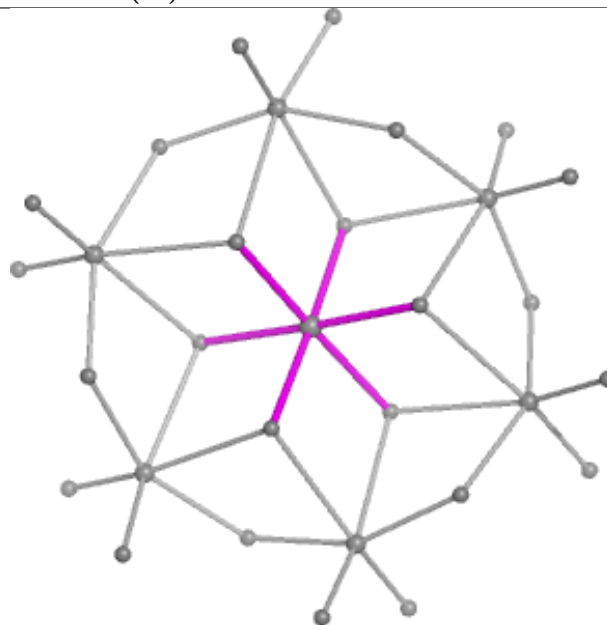
Rings



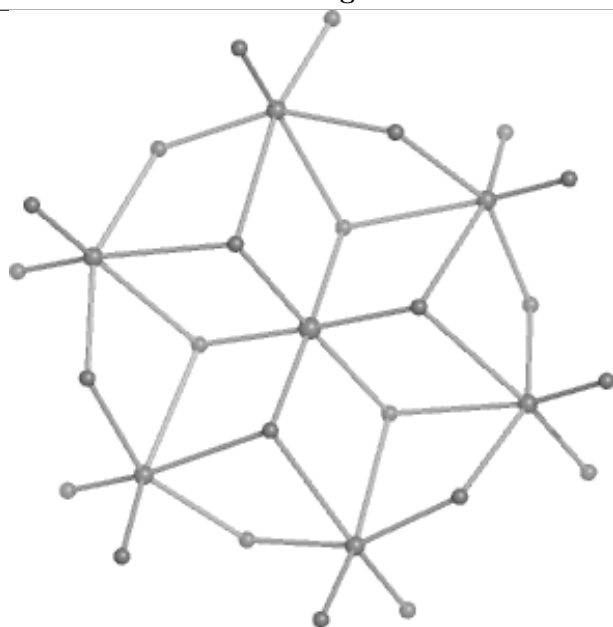
Ligand TEW A 401 (A)



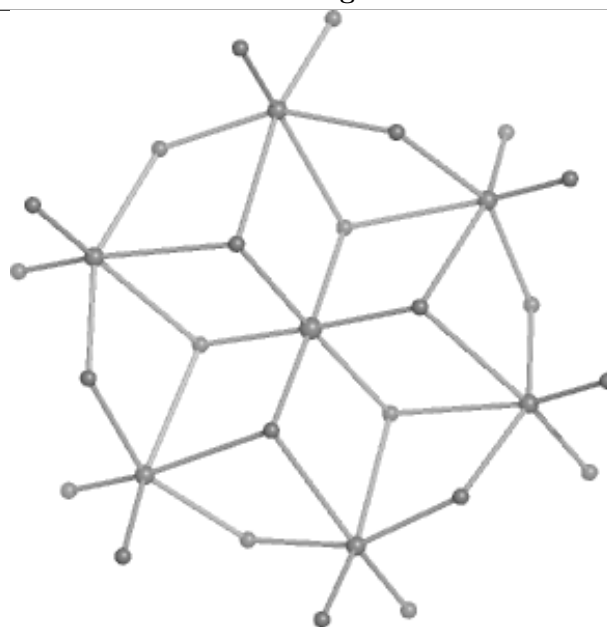
Bond lengths



Bond angles

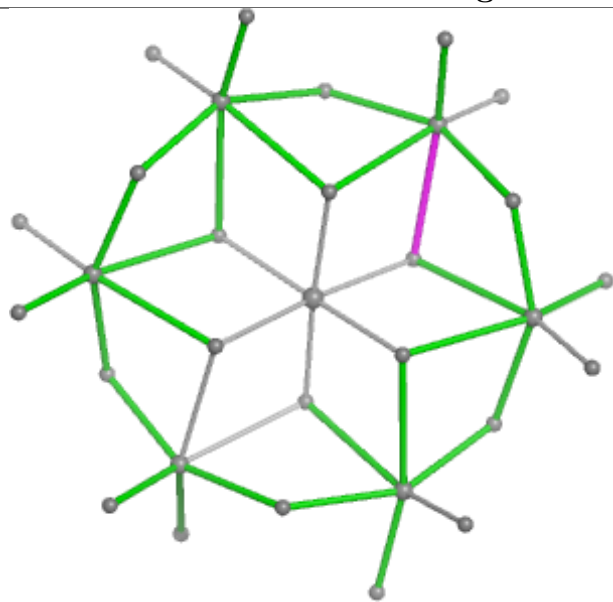


Torsions

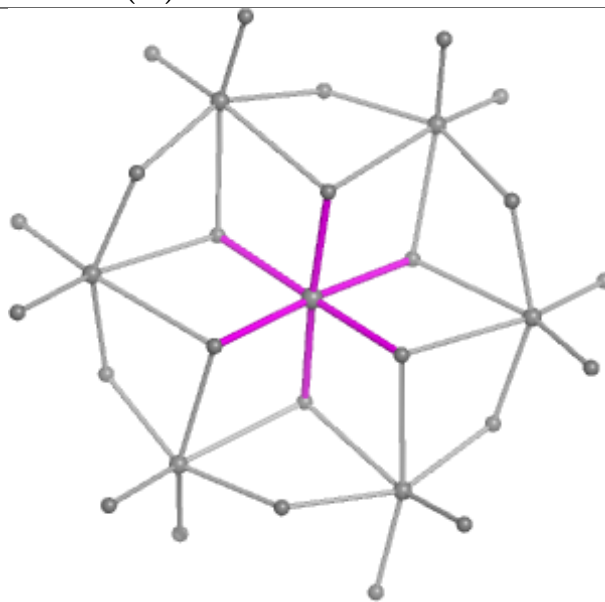


Rings

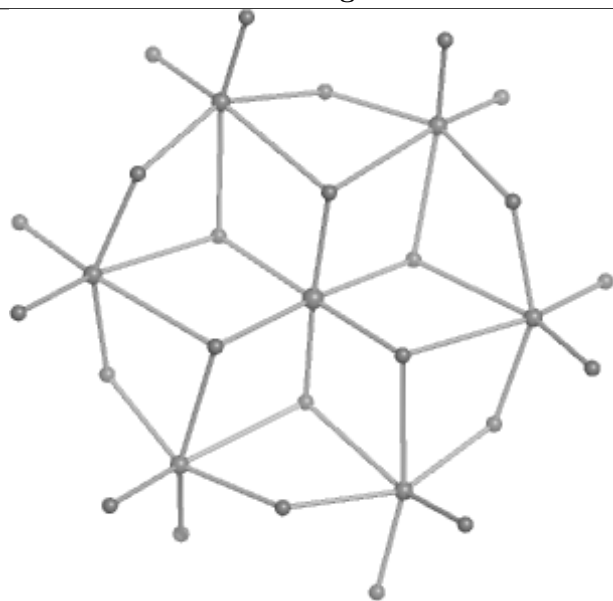
Ligand TEW E 402 (A)



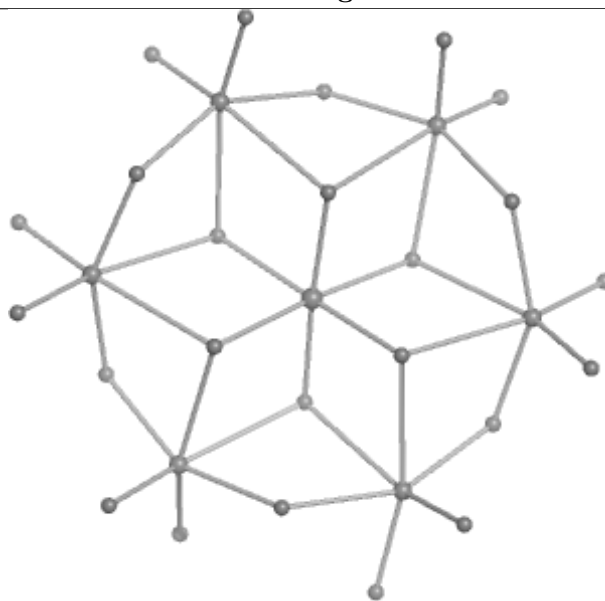
Bond lengths



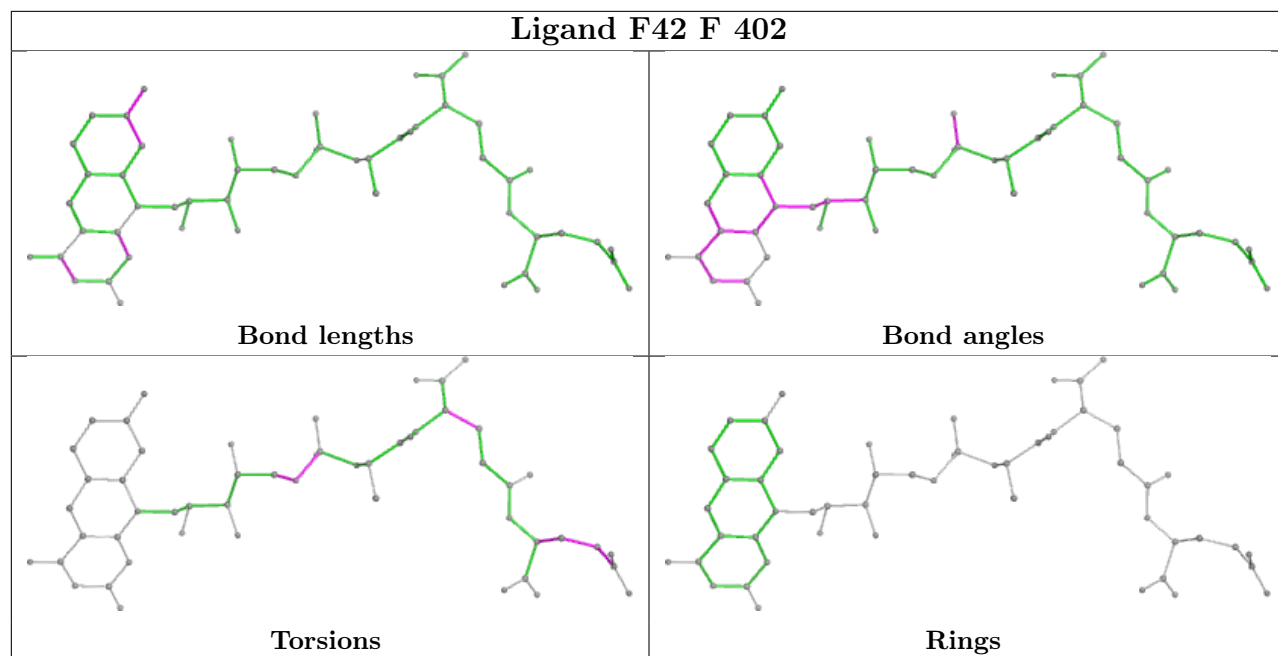
Bond angles

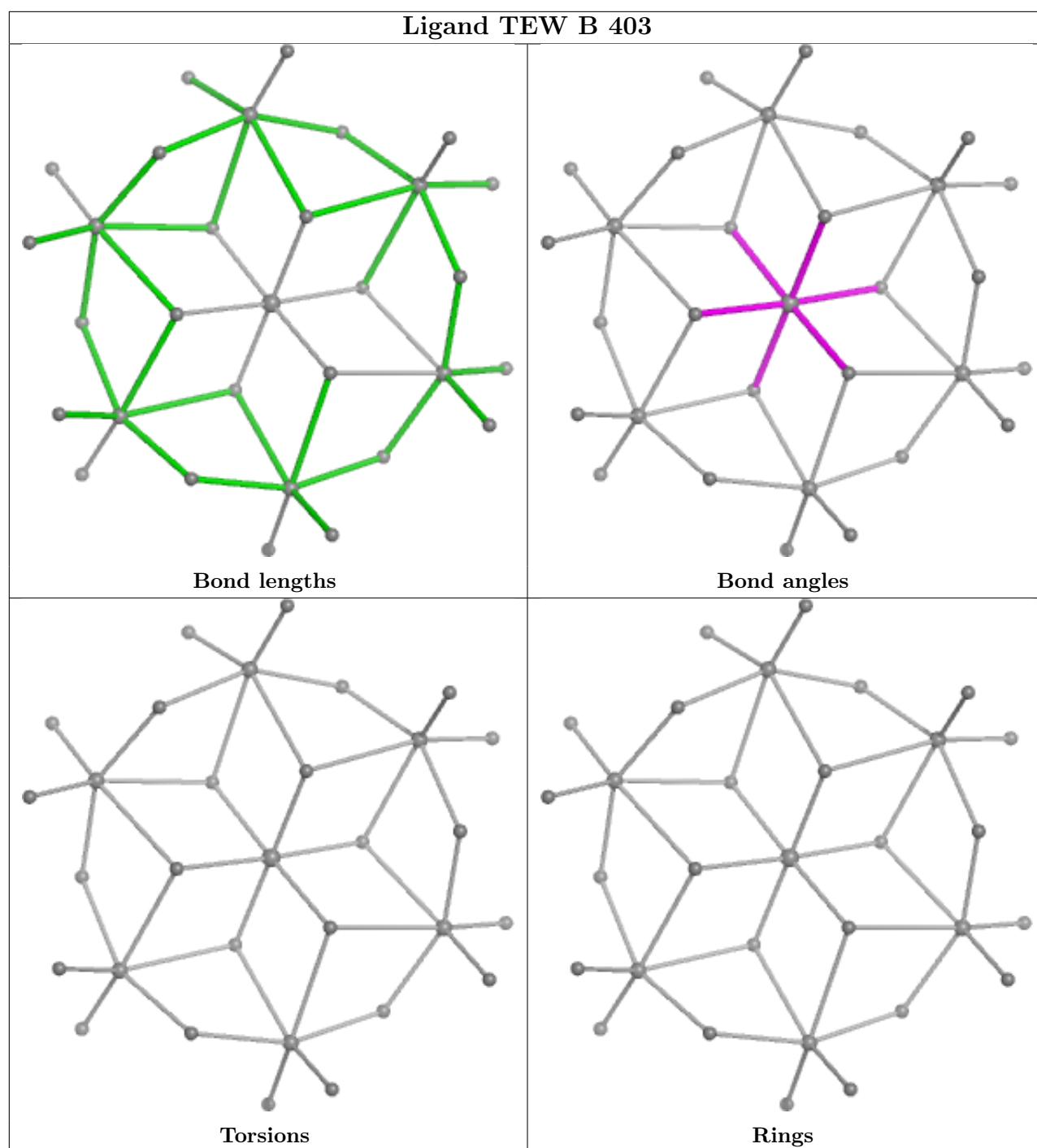


Torsions



Rings





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	319/332 (96%)	-0.10	0	100 100	8, 18, 35, 60	2 (0%)
1	B	319/332 (96%)	0.01	2 (0%)	85 88	9, 20, 43, 60	2 (0%)
1	E	319/332 (96%)	-0.02	2 (0%)	85 88	9, 18, 36, 50	1 (0%)
1	F	318/332 (95%)	0.10	1 (0%)	90 91	8, 20, 40, 63	2 (0%)
All	All	1275/1328 (96%)	-0.00	5 (0%)	89 90	8, 19, 38, 63	7 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	60	ALA	3.9
1	F	360[A]	ARG	3.7
1	B	203	ALA	2.8
1	E	306	GLU	2.2
1	E	298	ARG	2.2

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,

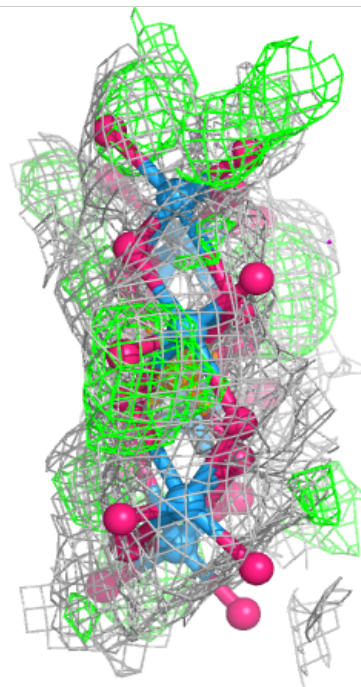
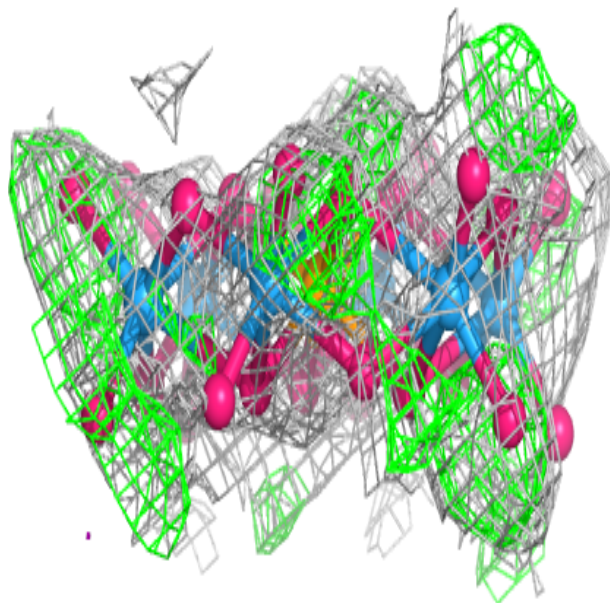
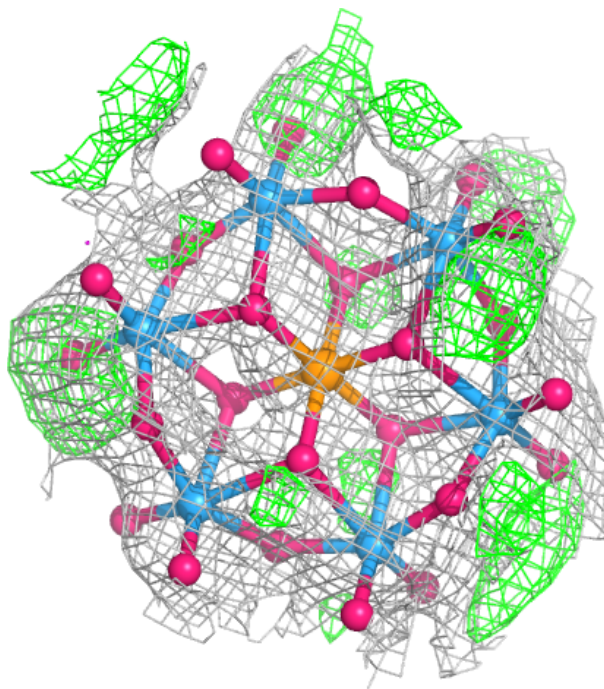
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	TEW	A	403	31/31	0.69	0.26	49,62,69,71	31
2	TEW	E	403	31/31	0.79	0.22	58,70,74,78	31
4	MPD	B	401	8/8	0.81	0.16	28,31,34,36	0
3	IMD	E	404	5/5	0.83	0.12	47,48,48,50	0
3	IMD	A	404	5/5	0.84	0.12	46,47,48,49	0
4	MPD	F	401	8/8	0.88	0.12	29,33,36,38	0
2	TEW	E	401	27/31	0.89	0.13	35,39,42,43	27
5	F42	B	402	53/53	0.90	0.11	19,25,63,71	0
5	F42	F	402	53/53	0.90	0.10	17,25,58,65	0
2	TEW	A	401[B]	31/31	0.98	0.08	30,32,37,43	31
2	TEW	E	402[A]	31/31	0.98	0.08	23,31,44,46	31
2	TEW	E	402[B]	31/31	0.98	0.08	25,32,35,41	31
2	TEW	A	402	31/31	0.98	0.07	26,38,50,57	7
2	TEW	A	401[A]	31/31	0.98	0.08	19,29,43,47	31
2	TEW	B	403	31/31	0.99	0.07	29,41,51,56	31

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.

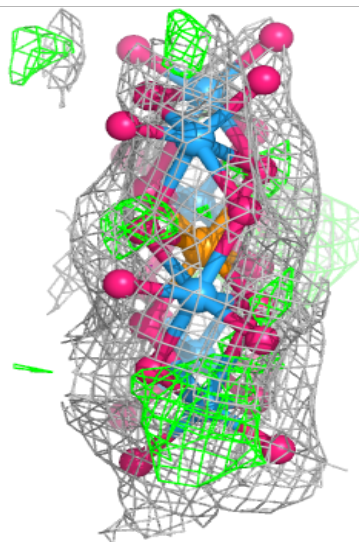
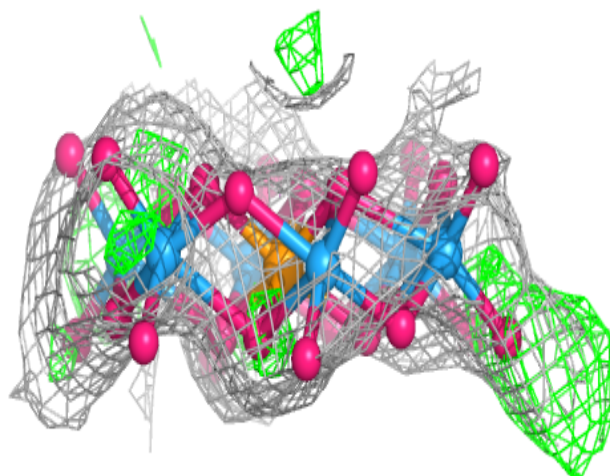
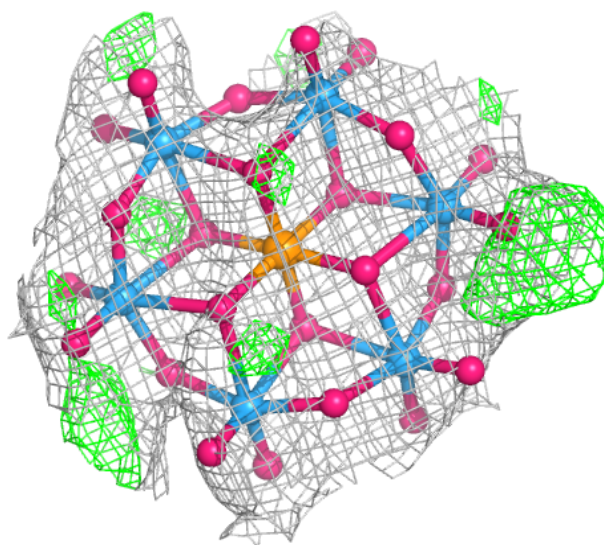
Electron density around TEW A 403:

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



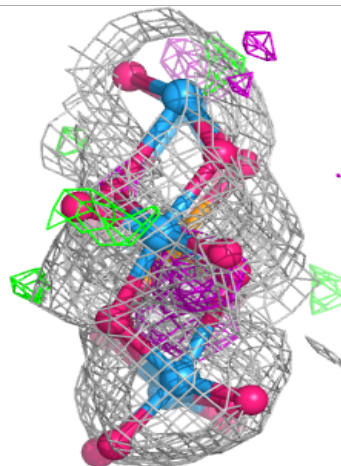
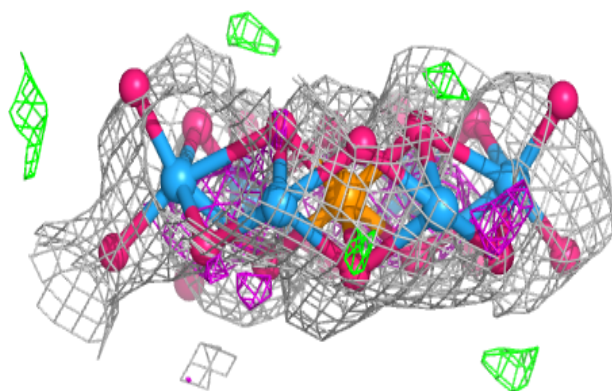
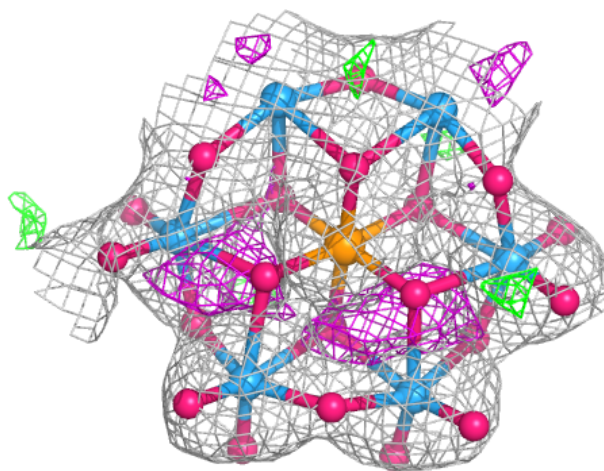
Electron density around TEW E 403:

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



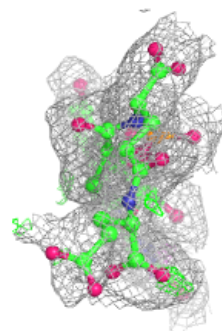
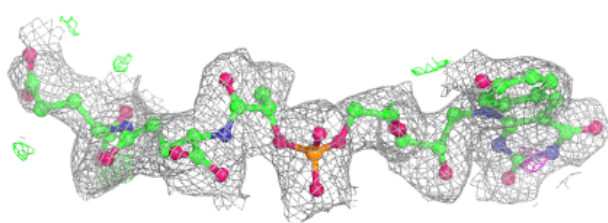
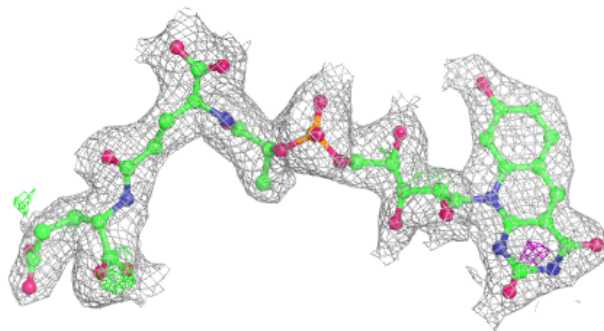
Electron density around TEW E 401:

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

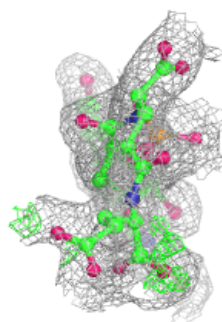
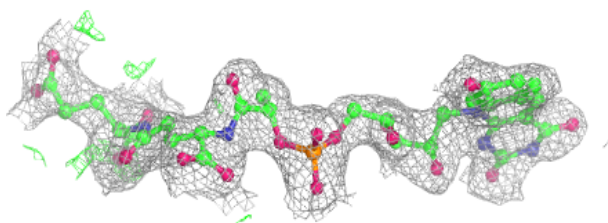
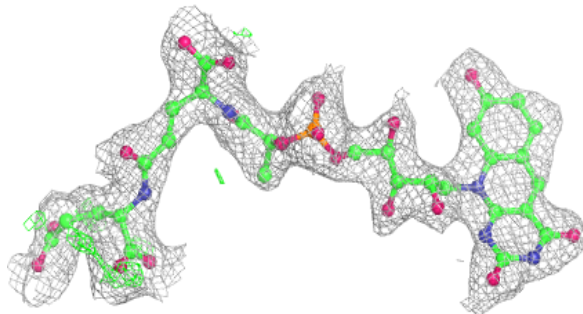


Electron density around F42 B 402:

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

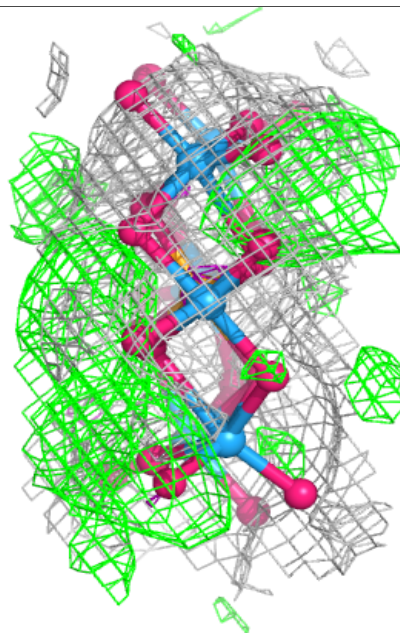
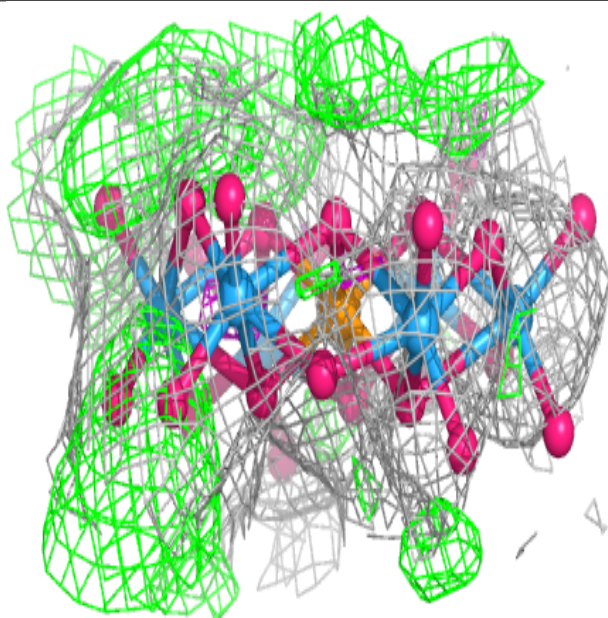
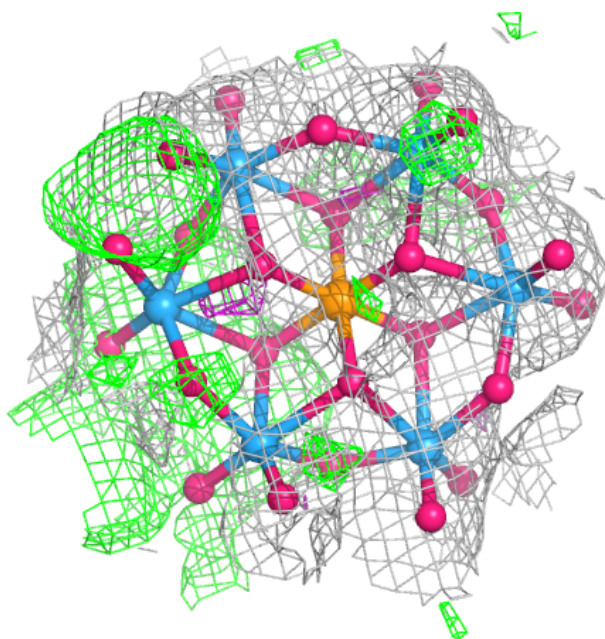
**Electron density around F42 F 402:**

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



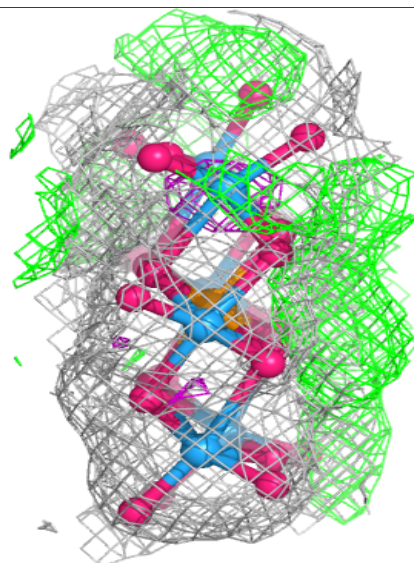
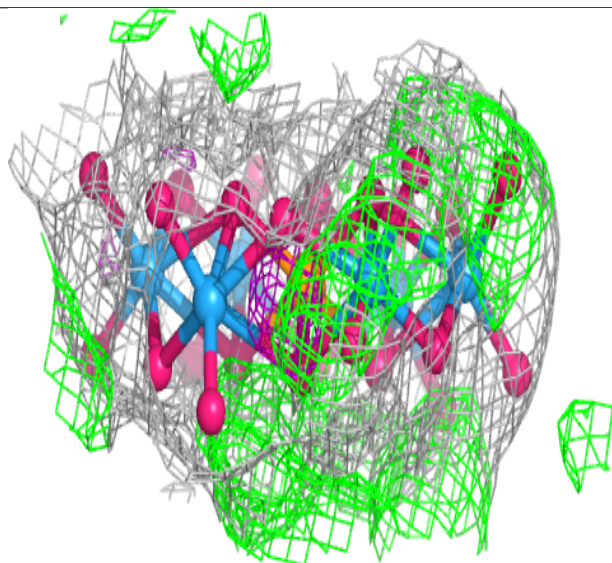
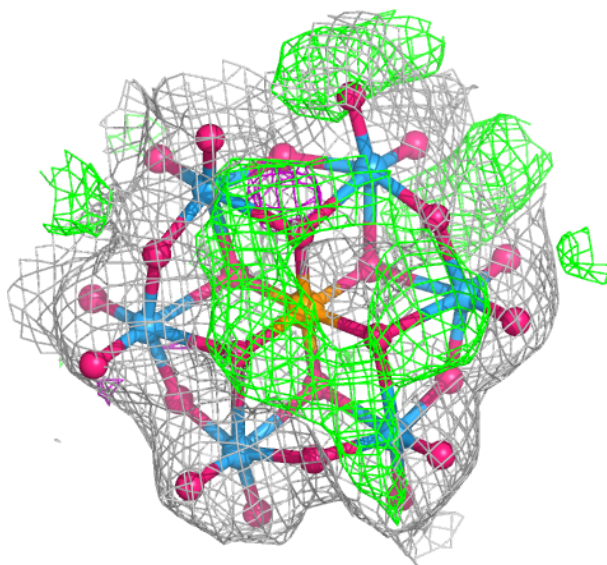
Electron density around TEW A 401 (B):

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



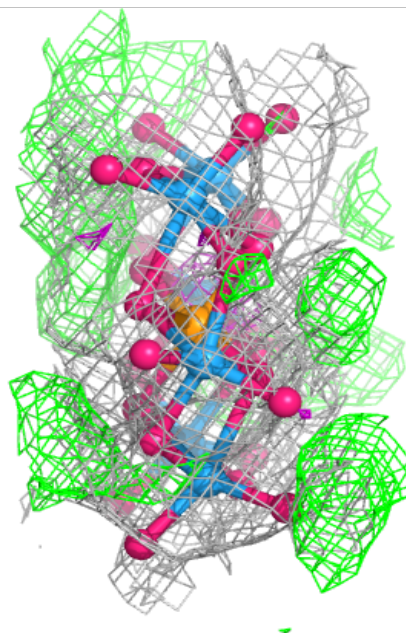
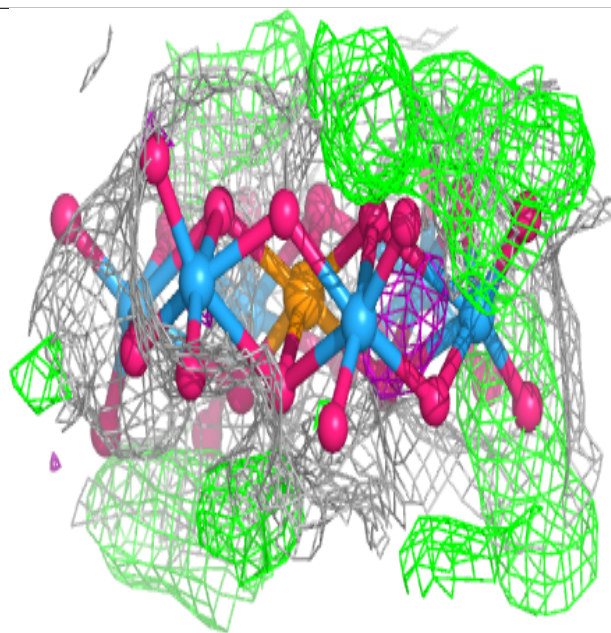
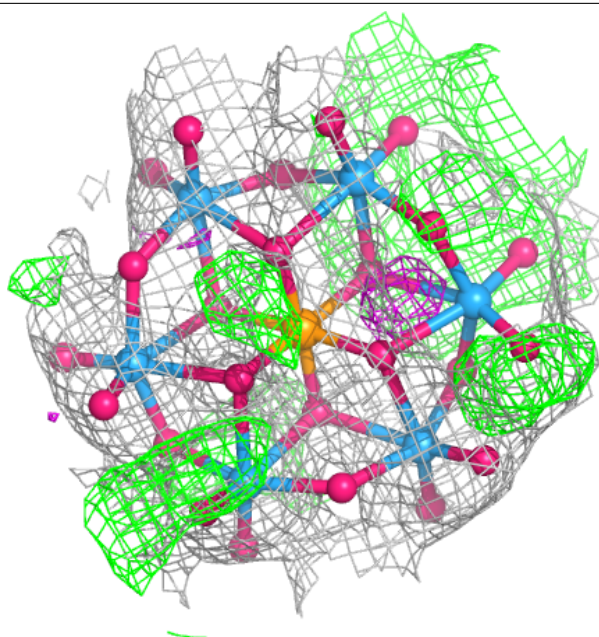
Electron density around TEW E 402 (A):

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



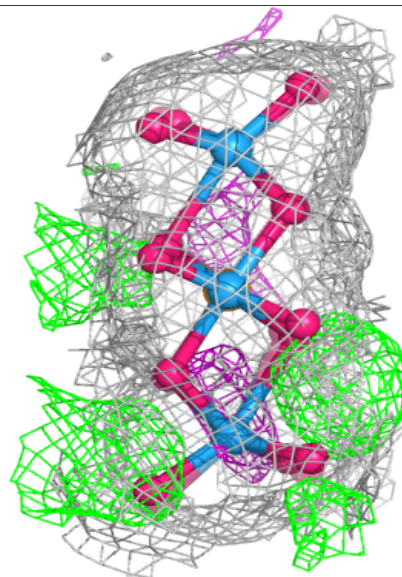
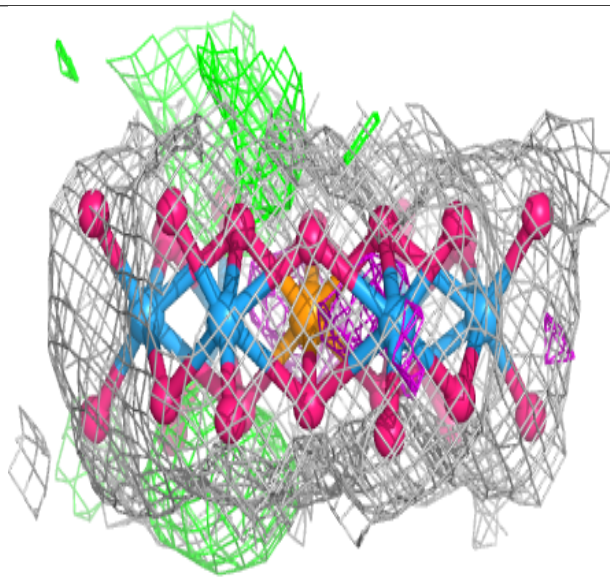
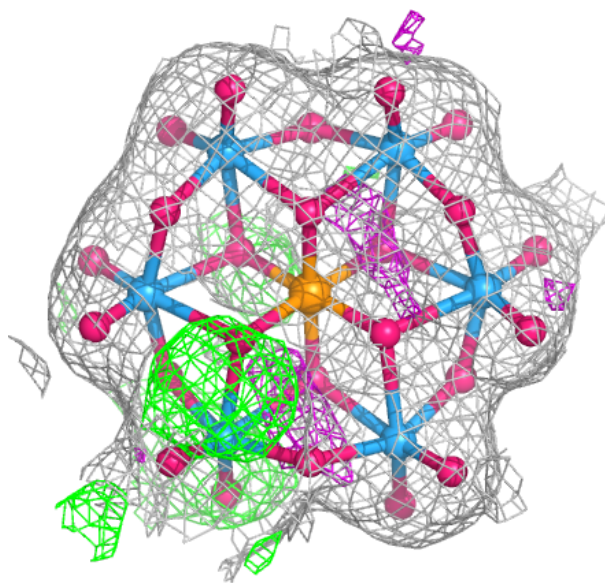
Electron density around TEW E 402 (B):

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



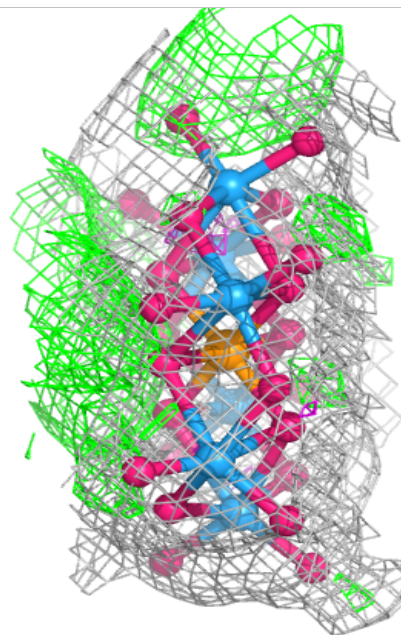
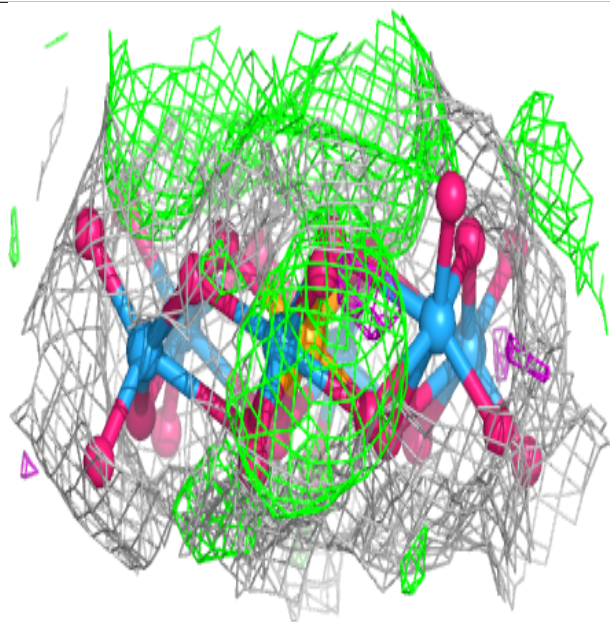
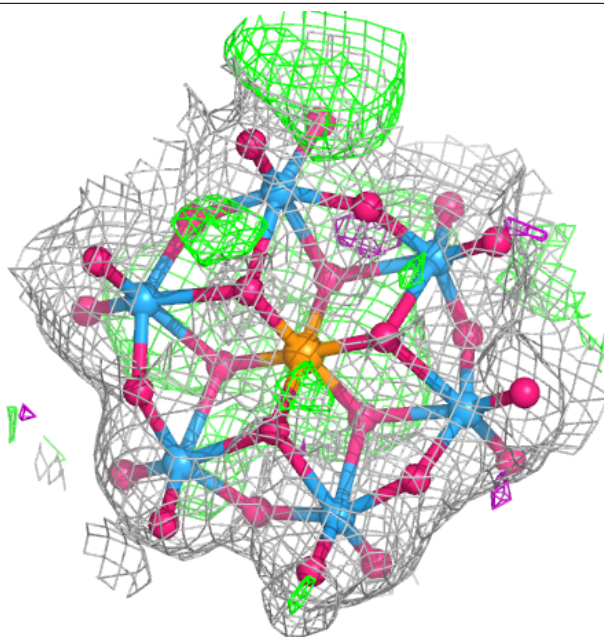
Electron density around TEW A 402:

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



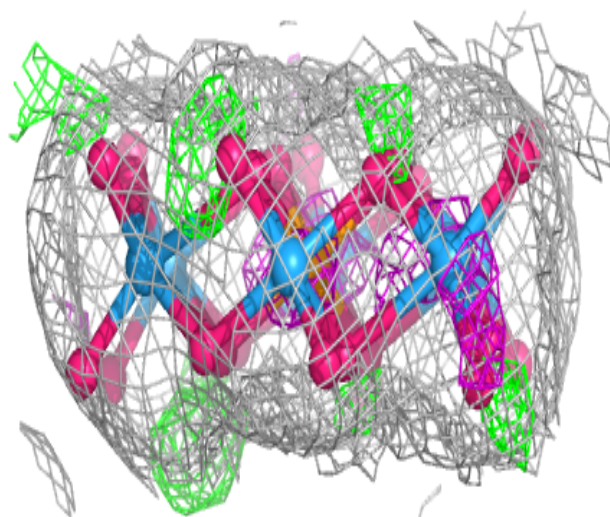
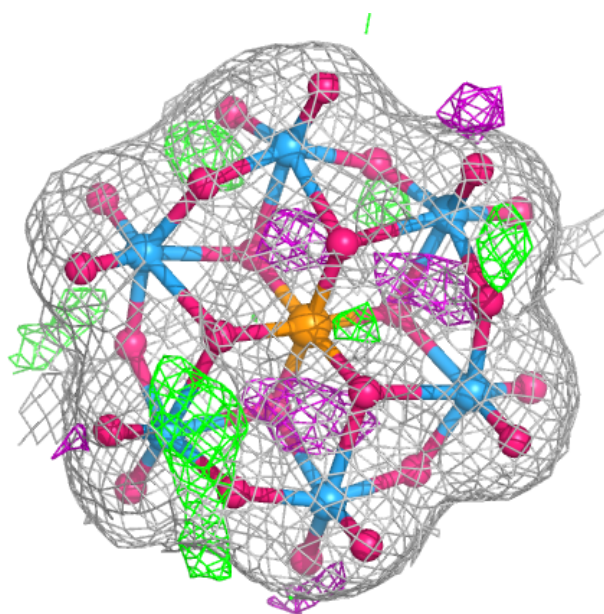
Electron density around TEW A 401 (A):

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



Electron density around TEW B 403:

$2mF_o - DF_c$ (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.