



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2020 – 06:58 PM BST

PDB ID : 6NYS  
Title : The crystal structure of CroV588 a novel circular LRR protein structure  
Authors : Huyton, T.; Jaiswal, M.; Gorlich, D.  
Deposited on : 2019-02-12  
Resolution : 3.10 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

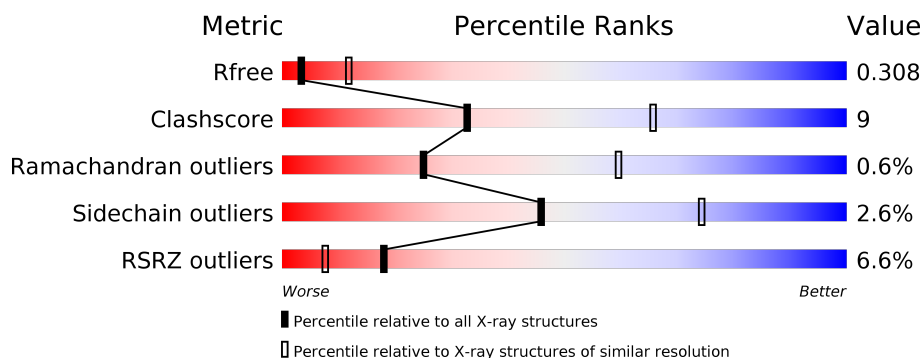
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 on 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	681	<div> <div>6%</div> <div> <div></div> <div>79%</div> <div>20%</div> </div> <div></div> </div>
1	B	681	<div> <div>8%</div> <div> <div></div> <div>79%</div> <div>20%</div> </div> <div></div> </div>

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	TEW	A	707	-	-	X	-

## 2 Entry composition i

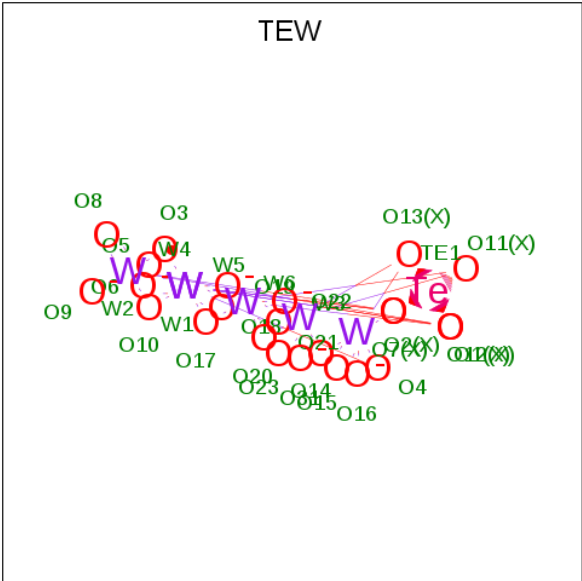
There are 2 unique types of molecules in this entry. The entry contains 11520 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 crov588.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	679	Total	C	N	O	S	0	1	0
			5533	3567	901	1058	7			
1	A	679	Total	C	N	O	S	0	3	0
			5553	3579	907	1060	7			

- Molecule 2 is 6-tungstotellurate(VI) (three-letter code: TEW) (formula: O<sub>24</sub>TeW<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	O	Te	W	1	0
			31	24	1	6		
2	B	1	Total	O	Te	W	1	0
			31	24	1	6		
2	B	1	Total	O	Te	W	0	0
			31	24	1	6		
2	B	1	Total	O	Te	W	1	0
			31	24	1	6		

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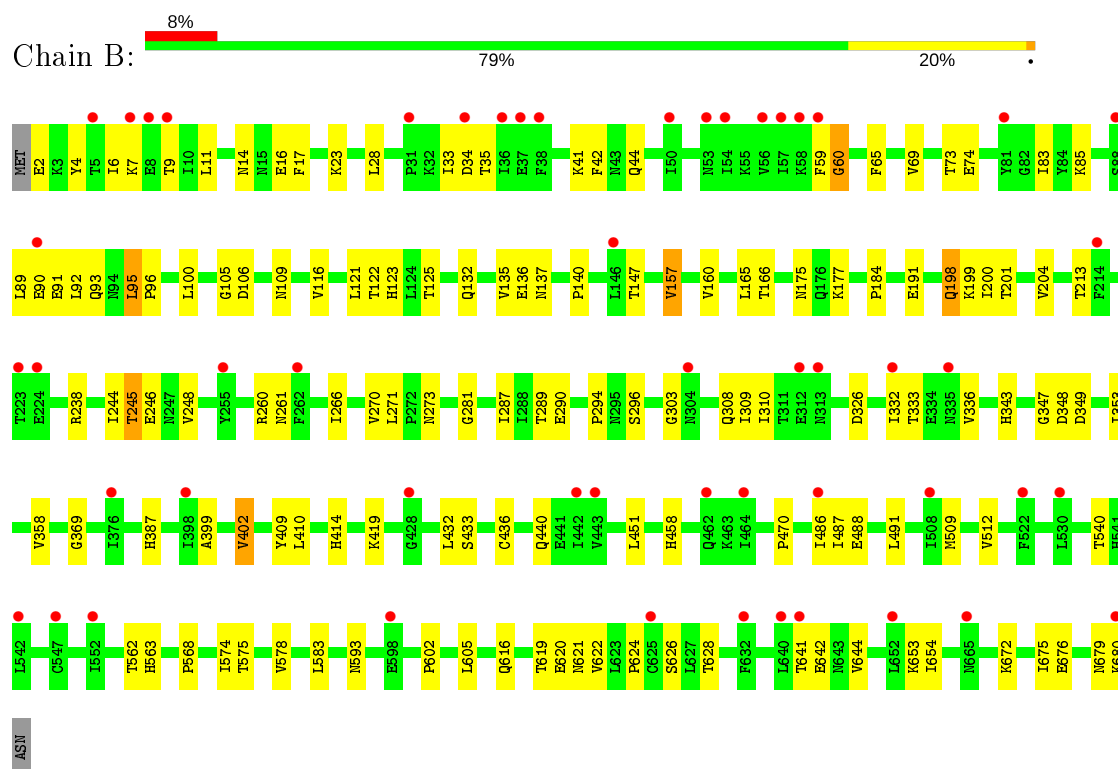
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total 31	O 24	Te 1	W 6	0	0
2	B	1	Total 31	O 24	Te 1	W 6	0	0
2	B	1	Total 31	O 24	Te 1	W 6	0	0
2	A	1	Total 31	O 24	Te 1	W 6	1	0
2	A	1	Total 31	O 24	Te 1	W 6	0	0
2	A	1	Total 31	O 24	Te 1	W 6	1	0
2	A	1	Total 31	O 24	Te 1	W 6	1	0
2	A	1	Total 31	O 24	Te 1	W 6	1	0
2	A	1	Total 31	O 24	Te 1	W 6	0	0
2	A	1	Total 31	O 24	Te 1	W 6	0	0

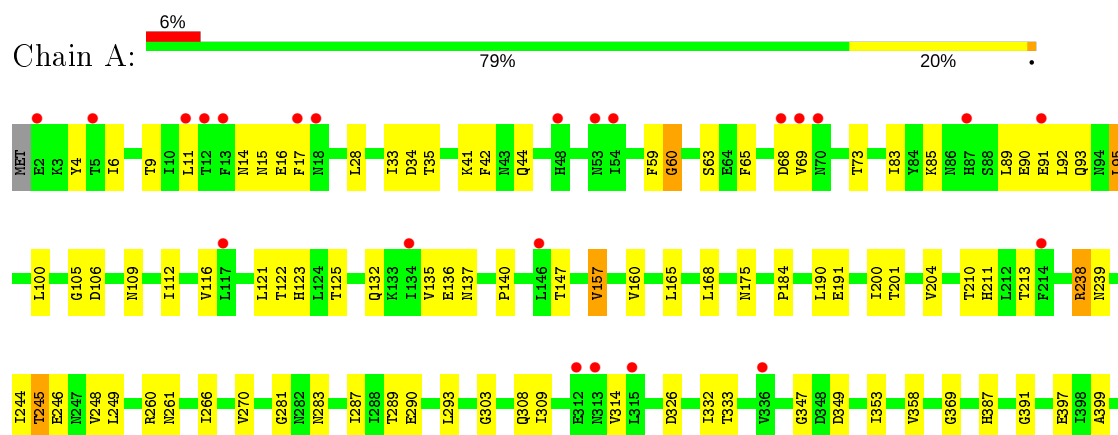
### 3 Residue-property plots [i](#)

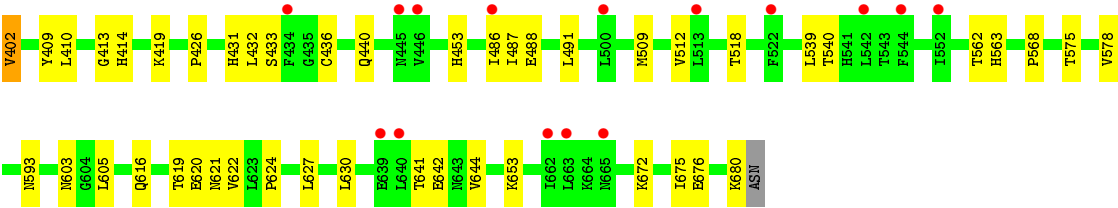
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: crov588



- Molecule 1: crov588





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.29Å 171.76Å 92.03Å 90.00° 90.12° 90.00°	Depositor
Resolution (Å)	46.02 – 3.10 48.61 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.02-3.10) 99.5 (48.61-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.261 , 0.296 0.258 , 0.308	Depositor DCC
$R_{free}$ test set	1851 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	82.4	Xtriage
Anisotropy	1.061	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 52.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.439 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11520	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% 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

### 5.1 Standard geometry

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

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	0.77	1/5687 (0.0%)	0.96	2/7745 (0.0%)
1	B	0.76	0/5665	0.95	1/7715 (0.0%)
All	All	0.76	1/11352 (0.0%)	0.96	3/15460 (0.0%)

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	4
1	B	0	4
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	397	GLU	CD-OE2	5.08	1.31	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	ARG	NE-CZ-NH2	-8.92	115.84	120.30
1	A	238	ARG	NE-CZ-NH1	8.75	124.68	120.30
1	B	348	ASP	CB-CA-C	5.45	121.29	110.40

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	135	VAL	Peptide
1	A	289	THR	Peptide
1	A	333	THR	Peptide
1	A	509	MET	Peptide
1	B	135	VAL	Peptide
1	B	289	THR	Peptide
1	B	333	THR	Peptide
1	B	509	MET	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5553	0	5432	95	0
1	B	5533	0	5420	93	0
2	A	217	0	0	11	0
2	B	217	0	0	20	0
All	All	11520	0	10852	195	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 9.

All (195) 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:B:166:THR:HG21	2:B:706:TEW:O8	1.40	1.17
1:A:260:ARG:HD3	1:A:261:ASN:OD1	1.49	1.09
1:B:238:ARG:NH2	2:B:707:TEW:O17	1.99	0.96
1:A:431[B]:HIS:NE2	1:A:453[B]:HIS:CE1	2.41	0.88
1:B:166:THR:CG2	2:B:706:TEW:O8	2.22	0.84
2:B:707:TEW:O15	2:B:707:TEW:O5	1.95	0.84
1:A:260:ARG:NH2	2:A:707:TEW:O31	2.08	0.84
1:A:260:ARG:NH1	2:A:707:TEW:O23	2.14	0.81
1:A:575:THR:O	1:A:578:VAL:HG12	1.80	0.80
1:A:431[B]:HIS:CE1	1:A:453[B]:HIS:CE1	2.70	0.79
1:B:575:THR:O	1:B:578:VAL:HG12	1.82	0.78
1:B:679:ASN:ND2	2:B:704:TEW:O22	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431[B]:HIS:CD2	1:A:453[B]:HIS:CG	2.76	0.73
2:B:707:TEW:O18	2:B:707:TEW:O21	2.08	0.72
1:B:245:THR:OG1	1:B:246:GLU:N	2.21	0.71
1:A:245:THR:OG1	1:A:246:GLU:N	2.24	0.70
1:B:69:VAL:O	1:B:91:GLU:HG3	1.93	0.68
1:A:14:ASN:ND2	2:A:706:TEW:O16	2.27	0.68
1:A:69:VAL:O	1:A:91:GLU:HG3	1.94	0.67
1:B:4:TYR:HB2	1:B:11:LEU:HD11	1.75	0.67
1:A:347:GLY:O	1:A:369:GLY:HA3	1.95	0.66
1:A:353:ILE:HD12	1:A:353:ILE:H	1.60	0.66
1:B:353:ILE:HD12	1:B:353:ILE:H	1.59	0.65
1:B:347:GLY:O	1:B:369:GLY:HA3	1.96	0.65
1:A:261:ASN:ND2	2:A:707:TEW:O23	2.31	0.64
1:A:4:TYR:HB2	1:A:11:LEU:HD11	1.80	0.62
1:B:83:ILE:HD12	1:B:106:ASP:OD2	1.99	0.62
1:B:6:ILE:CG1	1:B:11:LEU:HD13	2.30	0.62
1:A:353:ILE:N	1:A:353:ILE:HD12	2.15	0.62
2:B:701:TEW:O1	2:B:701:TEW:O12	2.18	0.62
1:A:260:ARG:CD	1:A:261:ASN:OD1	2.37	0.62
1:B:353:ILE:N	1:B:353:ILE:HD12	2.16	0.61
2:B:707:TEW:O16	2:B:707:TEW:O31	2.19	0.61
1:A:83:ILE:HD12	1:A:106:ASP:OD2	2.01	0.61
1:A:6:ILE:CG1	1:A:11:LEU:HD13	2.32	0.60
1:A:92:LEU:HA	1:A:95:LEU:HD12	1.83	0.60
1:A:266:ILE:HG23	1:A:270:VAL:CG2	2.31	0.60
1:A:431[B]:HIS:NE2	1:A:453[B]:HIS:NE2	2.50	0.59
1:B:266:ILE:HG23	1:B:270:VAL:CG2	2.32	0.59
1:B:14:ASN:ND2	2:B:704:TEW:O16	2.36	0.59
1:B:414:HIS:HD2	2:B:705:TEW:O6	1.87	0.58
1:A:85:LYS:HD2	1:A:85:LYS:N	2.19	0.57
1:B:165:LEU:HB3	1:B:184:PRO:HG2	1.86	0.56
1:A:353:ILE:CD1	1:A:353:ILE:H	2.19	0.56
1:A:593:ASN:OD1	1:A:616:GLN:NE2	2.33	0.56
1:B:92:LEU:HA	1:B:95:LEU:HD12	1.87	0.56
1:A:122:THR:HG23	1:A:123:HIS:ND1	2.22	0.55
1:B:353:ILE:H	1:B:353:ILE:CD1	2.20	0.55
1:B:16:GLU:OE1	2:B:704:TEW:O14	2.25	0.55
1:B:177:LYS:HG3	1:B:198:GLN:HG2	1.89	0.55
1:B:679:ASN:ND2	2:B:704:TEW:O21	2.40	0.55
1:B:85:LYS:N	1:B:85:LYS:HD2	2.21	0.55
1:A:16:GLU:HA	1:A:41:LYS:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:GLU:HG3	1:B:213:THR:HB	1.89	0.54
1:B:122:THR:HG23	1:B:123:HIS:ND1	2.23	0.54
1:B:6:ILE:HG13	1:B:11:LEU:HD13	1.88	0.54
1:A:562:THR:HG23	1:A:563:HIS:ND1	2.23	0.54
1:A:260:ARG:NH1	1:A:283:ASN:HD21	2.06	0.54
1:A:281:GLY:O	1:A:303:GLY:HA3	2.08	0.53
1:A:157:VAL:O	1:A:160:VAL:HG12	2.09	0.53
1:B:157:VAL:O	1:B:160:VAL:HG12	2.09	0.53
1:B:562:THR:HG23	1:B:563:HIS:ND1	2.24	0.53
1:B:593:ASN:OD1	1:B:616:GLN:NE2	2.35	0.52
1:B:16:GLU:HA	1:B:41:LYS:HB2	1.89	0.52
1:B:281:GLY:O	1:B:303:GLY:HA3	2.10	0.52
1:B:166:THR:CB	2:B:706:TEW:O8	2.58	0.52
1:A:89:LEU:N	1:A:89:LEU:HD12	2.25	0.52
1:A:238:ARG:NH1	2:A:707:TEW:O22	2.36	0.51
1:A:6:ILE:HG13	1:A:11:LEU:HD13	1.91	0.51
1:A:165:LEU:HB3	1:A:184:PRO:HG2	1.92	0.51
1:A:605:LEU:HD23	1:A:624:PRO:HG2	1.92	0.51
1:A:238:ARG:NE	1:A:239:ASN:OD1	2.41	0.51
1:A:332:ILE:HG22	1:A:358:VAL:CG1	2.41	0.50
1:B:332:ILE:HG22	1:B:358:VAL:CG1	2.41	0.50
1:B:266:ILE:HG23	1:B:270:VAL:HG21	1.94	0.50
1:B:387:HIS:CD2	1:B:409:TYR:CD1	3.00	0.50
1:A:620:GLU:HA	1:A:644:VAL:HG23	1.94	0.50
1:A:16:GLU:OE1	2:A:706:TEW:O14	2.29	0.49
1:A:121:LEU:HB3	1:A:140:PRO:HG2	1.94	0.49
1:A:85:LYS:HB2	1:A:105:GLY:HA3	1.94	0.49
1:A:431[B]:HIS:CD2	1:A:453[B]:HIS:ND1	2.80	0.49
1:B:89:LEU:HD12	1:B:89:LEU:N	2.27	0.49
1:B:2:GLU:HG3	2:B:702:TEW:O9	2.12	0.49
1:B:487:ILE:HG22	1:B:488:GLU:H	1.78	0.49
1:B:486:ILE:HG22	1:B:512:VAL:HG13	1.93	0.49
1:B:125:THR:HG23	1:B:147:THR:HB	1.95	0.49
1:B:419:LYS:NZ	1:B:440:GLN:OE1	2.46	0.48
1:B:410:LEU:HD23	1:B:432:LEU:HD13	1.95	0.48
1:A:619:THR:O	1:A:622:VAL:HG22	2.14	0.48
1:B:273:ASN:O	1:B:296:SER:OG	2.23	0.48
1:A:414:HIS:CD2	1:A:436:CYS:HB3	2.48	0.48
2:B:707:TEW:O19	2:B:707:TEW:O9	2.32	0.48
1:A:653:LYS:HA	1:A:676:GLU:O	2.14	0.48
1:B:260:ARG:HD3	1:B:261:ASN:OD1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:GLN:HG2	1:B:116:VAL:HG13	1.96	0.48
1:B:59:PHE:O	1:B:60:GLY:O	2.32	0.48
1:A:201:THR:O	1:A:204:VAL:HG22	2.13	0.48
1:B:574:ILE:HG23	1:B:578:VAL:HG11	1.96	0.48
1:B:620:GLU:HA	1:B:644:VAL:HG23	1.95	0.48
1:B:414:HIS:CD2	2:B:705:TEW:O6	2.67	0.48
1:B:34:ASP:OD1	1:B:35:THR:HG23	2.14	0.48
1:A:419:LYS:NZ	1:A:440:GLN:OE1	2.45	0.47
1:A:266:ILE:HG23	1:A:270:VAL:HG21	1.97	0.47
1:B:653:LYS:HA	1:B:676:GLU:O	2.14	0.47
2:B:707:TEW:O1	2:B:707:TEW:O3	2.33	0.47
1:B:458:HIS:CE1	1:A:603:ASN:HB3	2.50	0.47
1:A:59:PHE:O	1:A:60:GLY:O	2.33	0.47
1:B:121:LEU:HB3	1:B:140:PRO:HG2	1.96	0.47
1:A:287:ILE:HD13	1:A:308:GLN:HB3	1.97	0.47
1:B:605:LEU:HD23	1:B:624:PRO:HG2	1.96	0.47
1:A:200:ILE:HG23	1:A:204:VAL:HG21	1.95	0.47
1:B:287:ILE:HD13	1:B:308:GLN:HB3	1.97	0.47
1:B:619:THR:O	1:B:622:VAL:HG22	2.15	0.47
1:A:34:ASP:OD1	1:A:35:THR:HG23	2.16	0.46
1:A:93:GLN:HG2	1:A:116:VAL:HG13	1.97	0.46
1:A:621:ASN:HD22	1:A:621:ASN:N	2.13	0.46
1:B:414:HIS:CD2	1:B:436:CYS:HB3	2.50	0.46
1:B:583:LEU:HB3	1:B:602:PRO:HG2	1.96	0.46
1:A:486:ILE:HG22	1:A:512:VAL:HG13	1.97	0.46
1:A:487:ILE:HG22	1:A:488:GLU:H	1.80	0.46
1:A:414:HIS:CD2	1:A:436:CYS:CB	2.99	0.46
1:B:487:ILE:CG2	1:B:488:GLU:H	2.29	0.46
1:A:191:GLU:HG3	1:A:213:THR:HB	1.97	0.45
1:A:387:HIS:CD2	1:A:409:TYR:CD1	3.04	0.45
1:A:431[B]:HIS:CD2	1:A:453[B]:HIS:CD2	3.04	0.45
1:B:201:THR:O	1:B:204:VAL:HG22	2.16	0.45
1:B:540:THR:HB	1:B:562:THR:HG22	1.98	0.45
1:B:574:ILE:HG23	1:B:578:VAL:CG1	2.46	0.45
1:A:540:THR:HB	1:A:562:THR:HG22	1.98	0.45
1:A:42:PHE:CE1	1:A:44:GLN:HB2	2.52	0.45
1:B:200:ILE:HG23	1:B:204:VAL:HG21	1.98	0.45
1:B:85:LYS:HB2	1:B:105:GLY:HA3	1.99	0.45
2:A:705:TEW:O2	2:A:705:TEW:O7	2.35	0.45
1:B:6:ILE:HG12	1:B:11:LEU:HD13	1.99	0.44
1:A:210:THR:OG1	1:A:211:HIS:ND1	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:ILE:HG21	1:A:491:LEU:HD11	2.00	0.44
1:A:410:LEU:HD23	1:A:432:LEU:HD13	2.00	0.44
1:A:244:ILE:HG23	1:A:248:VAL:HG21	2.00	0.44
1:B:310:ILE:HG22	1:B:336:VAL:HG13	2.00	0.44
1:B:343:HIS:HE1	2:B:703:TEW:O8	2.00	0.44
1:B:109:ASN:OD1	1:B:132:GLN:HG2	2.17	0.43
1:A:200:ILE:CG2	1:A:204:VAL:HG21	2.47	0.43
1:A:260:ARG:NH1	2:A:707:TEW:O31	2.51	0.43
1:A:6:ILE:HG12	1:A:11:LEU:HD13	2.00	0.43
1:A:260:ARG:CZ	2:A:707:TEW:O31	2.65	0.43
1:B:414:HIS:CD2	1:B:436:CYS:CB	3.02	0.43
1:A:9:THR:O	1:A:33:ILE:HG23	2.18	0.43
1:B:626:SER:O	1:B:628:THR:HG23	2.18	0.43
1:A:431[B]:HIS:NE2	1:A:453[B]:HIS:CD2	2.87	0.43
1:A:109:ASN:OD1	1:A:132:GLN:HG2	2.18	0.43
1:A:518:THR:HA	1:A:539:LEU:HA	2.00	0.43
1:A:92:LEU:HA	1:A:95:LEU:CD1	2.47	0.43
1:B:399:ALA:O	1:B:402:VAL:CG2	2.67	0.43
1:B:621:ASN:N	1:B:621:ASN:HD22	2.17	0.43
1:B:9:THR:O	1:B:33:ILE:HG23	2.18	0.43
1:A:641:THR:O	1:A:644:VAL:HG12	2.19	0.43
1:B:74:GLU:HA	1:B:96:PRO:HB2	2.00	0.42
1:A:125:THR:HG23	1:A:147:THR:HB	2.00	0.42
1:B:653:LYS:O	1:B:654:ILE:HD13	2.19	0.42
1:A:487:ILE:HG22	1:A:488:GLU:N	2.35	0.42
1:B:486:ILE:HG21	1:B:491:LEU:HD11	2.01	0.42
1:A:136:GLU:HG2	1:A:137:ASN:OD1	2.20	0.42
1:B:679:ASN:CG	2:B:704:TEW:O21	2.58	0.42
1:A:326:ASP:O	1:A:349:ASP:HB2	2.20	0.42
1:B:271:LEU:HB3	1:B:294:PRO:HD3	2.02	0.42
1:A:332:ILE:HG22	1:A:358:VAL:HG13	2.01	0.42
1:A:399:ALA:O	1:A:402:VAL:CG2	2.68	0.42
1:A:487:ILE:CG2	1:A:488:GLU:H	2.33	0.42
1:A:15:ASN:HB2	2:A:706:TEW:O15	2.19	0.42
1:A:391:GLY:O	1:A:413:GLY:HA3	2.20	0.41
1:B:641:THR:O	1:B:644:VAL:HG12	2.20	0.41
1:B:42:PHE:CE1	1:B:44:GLN:HB2	2.55	0.41
1:A:238:ARG:NH1	2:A:707:TEW:O20	2.53	0.41
1:A:168:LEU:HD23	1:A:190:LEU:HD13	2.01	0.41
1:A:244:ILE:HG21	1:A:249:LEU:HD11	2.02	0.41
1:B:244:ILE:HG23	1:B:248:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:ARG:HG2	1:B:261:ASN:OD1	2.20	0.41
2:B:701:TEW:O1	2:B:701:TEW:O7	2.38	0.41
1:B:136:GLU:HG2	1:B:137:ASN:OD1	2.21	0.41
1:A:293:LEU:HD12	1:A:314:VAL:O	2.20	0.41
1:B:157:VAL:O	1:B:160:VAL:CG1	2.69	0.41
1:A:65:PHE:HB3	1:A:85:LYS:HE3	2.02	0.41
1:B:238:ARG:O	1:B:261:ASN:HB2	2.20	0.41
1:B:326:ASP:O	1:B:349:ASP:HB2	2.20	0.41
1:A:627:LEU:HD21	1:A:630:LEU:HB2	2.03	0.41
1:B:11:LEU:CD2	1:B:28:LEU:HD23	2.51	0.41
1:B:23:LYS:HE3	1:B:23:LYS:HB2	1.97	0.41
1:B:451:LEU:HB3	1:B:470:PRO:HG3	2.03	0.41
1:A:85:LYS:CD	1:A:85:LYS:N	2.84	0.40
1:B:486:ILE:HG22	1:B:512:VAL:CG1	2.52	0.40
1:B:7:LYS:HA	1:B:7:LYS:HE2	2.02	0.40
1:B:487:ILE:HG22	1:B:488:GLU:N	2.35	0.40
1:A:11:LEU:CD2	1:A:28:LEU:CD2	2.99	0.40
1:A:63:SER:CB	1:A:85:LYS:HZ1	2.34	0.40
1:B:65:PHE:HB3	1:B:85:LYS:HE3	2.03	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	680/681 (100%)	601 (88%)	75 (11%)	4 (1%)	25	59
1	B	678/681 (100%)	597 (88%)	77 (11%)	4 (1%)	25	59
All	All	1358/1362 (100%)	1198 (88%)	152 (11%)	8 (1%)	25	59

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	60	GLY
1	A	60	GLY
1	B	73	THR
1	A	175	ASN
1	B	17	PHE
1	B	175	ASN
1	A	17	PHE
1	A	73	THR

### 5.3.2 Protein sidechains ⓘ

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	646/645 (100%)	629 (97%)	17 (3%)	46	74
1	B	644/645 (100%)	628 (98%)	16 (2%)	47	75
All	All	1290/1290 (100%)	1257 (97%)	33 (3%)	46	74

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	90	GLU
1	B	95	LEU
1	B	100	LEU
1	B	157	VAL
1	B	198	GLN
1	B	199	LYS
1	B	245	THR
1	B	290	GLU
1	B	309	ILE
1	B	402	VAL
1	B	433	SER
1	B	568	PRO
1	B	642	GLU
1	B	672	LYS
1	B	675	ILE
1	B	680	LYS

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Mol	Chain	Res	Type
1	A	68	ASP
1	A	90	GLU
1	A	95	LEU
1	A	100	LEU
1	A	112	ILE
1	A	157	VAL
1	A	245	THR
1	A	290	GLU
1	A	309	ILE
1	A	402	VAL
1	A	426	PRO
1	A	433	SER
1	A	568	PRO
1	A	642	GLU
1	A	672	LYS
1	A	675	ILE
1	A	680	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	94	ASN
1	B	467	ASN
1	B	621	ASN
1	B	665	ASN
1	A	94	ASN
1	A	283	ASN
1	A	467	ASN
1	A	621	ASN
1	A	665	ASN

### 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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

14 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	TEW	B	704	1	29,42,42	0.97	1 (3%)	12,129,129	32.63	11 (91%)
2	TEW	A	704	-	29,42,42	0.96	2 (6%)	12,129,129	13.26	11 (91%)
2	TEW	B	701	-	29,42,42	1.05	2 (6%)	12,129,129	12.18	12 (100%)
2	TEW	A	703	-	29,42,42	0.95	1 (3%)	12,129,129	9.62	11 (91%)
2	TEW	B	705	-	29,42,42	0.88	1 (3%)	12,129,129	1.52	2 (16%)
2	TEW	A	707	1	29,42,42	0.94	1 (3%)	12,129,129	1.34	1 (8%)
2	TEW	A	702	-	29,42,42	0.92	0	12,129,129	1.44	2 (16%)
2	TEW	B	702	-	29,42,42	0.93	1 (3%)	12,129,129	10.53	10 (83%)
2	TEW	A	706	1	29,42,42	0.92	1 (3%)	12,129,129	2.24	4 (33%)
2	TEW	B	706	-	29,42,42	1.00	2 (6%)	12,129,129	1.79	4 (33%)
2	TEW	B	703	-	29,42,42	0.94	0	12,129,129	1.29	2 (16%)
2	TEW	A	701	-	29,42,42	2.19	3 (10%)	12,129,129	2.96	7 (58%)
2	TEW	B	707	1	29,42,42	1.74	10 (34%)	12,129,129	5.04	9 (75%)
2	TEW	A	705	-	29,42,42	1.04	2 (6%)	12,129,129	10.62	11 (91%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	TEW	W6-O13	-8.72	1.89	2.34
2	A	701	TEW	W6-O11	-6.08	2.02	2.34
2	B	707	TEW	W3-O2	-3.48	2.16	2.34
2	B	707	TEW	W4-O12	-3.36	2.17	2.34
2	B	707	TEW	W6-O13	-3.22	2.17	2.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	707	TEW	W2-O7	-3.17	2.18	2.34
2	B	707	TEW	W1-O6	2.66	1.77	1.72
2	B	707	TEW	W5-O12	-2.53	2.21	2.34
2	B	707	TEW	W5-O11	-2.40	2.22	2.34
2	B	707	TEW	W4-O7	-2.39	2.22	2.34
2	B	706	TEW	W6-O13	-2.26	2.22	2.34
2	A	704	TEW	W6-O13	-2.22	2.23	2.34
2	B	706	TEW	W2-O7	-2.22	2.23	2.34
2	A	705	TEW	W2-O7	-2.19	2.23	2.34
2	B	701	TEW	W6-O13	-2.19	2.23	2.34
2	A	701	TEW	W5-O11	-2.17	2.23	2.34
2	B	707	TEW	W3-O13	-2.16	2.23	2.34
2	B	704	TEW	W2-O7	-2.12	2.23	2.34
2	A	707	TEW	W6-O13	-2.12	2.23	2.34
2	A	706	TEW	W2-O7	-2.12	2.23	2.34
2	A	704	TEW	W2-O7	-2.08	2.23	2.34
2	B	707	TEW	W1-O5	-2.06	1.70	2.10
2	A	705	TEW	W6-O13	-2.06	2.23	2.34
2	A	703	TEW	W6-O13	-2.03	2.24	2.34
2	B	701	TEW	W5-O11	-2.02	2.24	2.34
2	B	702	TEW	W6-O13	-2.01	2.24	2.34
2	B	705	TEW	W3-O2	-2.01	2.24	2.34

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	704	TEW	O13-TE1-O12	-56.99	43.35	94.65
2	B	704	TEW	O12-TE1-O1	-46.23	53.04	94.65
2	B	704	TEW	O13-TE1-O1	-43.53	55.47	94.65
2	B	704	TEW	O7-TE1-O2	39.51	130.22	94.65
2	B	704	TEW	O12-TE1-O7	-29.73	50.09	85.21
2	B	704	TEW	O12-TE1-O11	-29.46	50.42	85.21
2	B	704	TEW	O13-TE1-O11	-29.01	50.94	85.21
2	B	701	TEW	O12-TE1-O1	-28.65	68.86	94.65
2	B	704	TEW	O13-TE1-O2	-26.40	54.03	85.21
2	A	704	TEW	O13-TE1-O1	-24.35	72.73	94.65
2	A	705	TEW	O13-TE1-O12	-21.51	75.29	94.65
2	B	702	TEW	O13-TE1-O1	20.52	113.12	94.65
2	B	701	TEW	O11-TE1-O2	20.40	113.02	94.65
2	A	705	TEW	O12-TE1-O7	19.60	108.36	85.21
2	B	702	TEW	O11-TE1-O7	-18.91	77.63	94.65
2	A	704	TEW	O12-TE1-O7	18.91	107.54	85.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	703	TEW	O13-TE1-O12	-18.31	78.17	94.65
2	B	704	TEW	O7-TE1-O1	-17.98	63.97	85.21
2	A	704	TEW	O13-TE1-O2	-16.42	65.82	85.21
2	A	704	TEW	O7-TE1-O1	15.94	104.04	85.21
2	B	704	TEW	O2-TE1-O1	-15.73	66.63	85.21
2	A	704	TEW	O11-TE1-O7	15.49	108.59	94.65
2	B	701	TEW	O2-TE1-O1	14.94	102.86	85.21
2	A	703	TEW	O13-TE1-O2	14.49	102.32	85.21
2	B	702	TEW	O11-TE1-O2	-13.28	82.70	94.65
2	A	705	TEW	O13-TE1-O1	-13.27	82.71	94.65
2	B	702	TEW	O12-TE1-O1	12.41	105.82	94.65
2	A	703	TEW	O12-TE1-O1	-12.18	83.69	94.65
2	A	705	TEW	O7-TE1-O1	11.30	98.55	85.21
2	A	704	TEW	O13-TE1-O11	-10.71	72.56	85.21
2	B	707	TEW	O7-TE1-O2	-10.31	85.38	94.65
2	A	704	TEW	O11-TE1-O2	-9.44	86.16	94.65
2	B	701	TEW	O13-TE1-O12	-9.27	86.31	94.65
2	A	703	TEW	O11-TE1-O2	9.25	102.98	94.65
2	B	701	TEW	O13-TE1-O2	9.10	95.96	85.21
2	A	704	TEW	O13-TE1-O12	-9.08	86.48	94.65
2	A	705	TEW	O11-TE1-O7	8.95	102.71	94.65
2	B	702	TEW	O12-TE1-O7	-8.93	74.66	85.21
2	A	703	TEW	O7-TE1-O2	8.71	102.50	94.65
2	B	704	TEW	O11-TE1-O7	-8.54	86.96	94.65
2	A	703	TEW	O2-TE1-O1	8.49	95.24	85.21
2	B	701	TEW	O12-TE1-O11	-8.30	75.41	85.21
2	A	705	TEW	O13-TE1-O11	-8.03	75.72	85.21
2	A	704	TEW	O2-TE1-O1	-7.83	75.96	85.21
2	B	702	TEW	O12-TE1-O11	-7.61	76.22	85.21
2	B	707	TEW	O12-TE1-O1	7.60	101.50	94.65
2	A	703	TEW	O12-TE1-O7	-6.94	77.01	85.21
2	B	707	TEW	O11-TE1-O7	-6.84	88.50	94.65
2	A	703	TEW	O7-TE1-O1	-6.50	77.53	85.21
2	A	701	TEW	O13-TE1-O12	6.33	100.36	94.65
2	A	704	TEW	O7-TE1-O2	6.13	100.17	94.65
2	A	703	TEW	O13-TE1-O1	6.11	100.16	94.65
2	A	703	TEW	O12-TE1-O11	-6.07	78.04	85.21
2	B	707	TEW	O12-TE1-O7	5.80	92.06	85.21
2	A	706	TEW	O13-TE1-O12	-5.02	90.14	94.65
2	B	702	TEW	O7-TE1-O2	-4.96	90.19	94.65
2	B	702	TEW	O2-TE1-O1	4.72	90.78	85.21
2	B	701	TEW	O13-TE1-O1	-4.56	90.55	94.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	707	TEW	O13-TE1-O2	4.51	90.53	85.21
2	A	701	TEW	O12-TE1-O1	-4.44	90.66	94.65
2	B	702	TEW	O13-TE1-O2	4.39	90.40	85.21
2	A	703	TEW	O11-TE1-O7	-4.27	90.81	94.65
2	B	701	TEW	O12-TE1-O7	-4.26	80.18	85.21
2	A	705	TEW	O12-TE1-O11	-4.13	80.33	85.21
2	B	702	TEW	O13-TE1-O12	4.08	98.33	94.65
2	A	706	TEW	O7-TE1-O2	3.84	98.11	94.65
2	B	701	TEW	O7-TE1-O2	3.68	97.97	94.65
2	A	705	TEW	O12-TE1-O1	3.62	97.91	94.65
2	B	706	TEW	O13-TE1-O1	-3.46	91.54	94.65
2	B	701	TEW	O11-TE1-O7	-3.45	91.55	94.65
2	A	705	TEW	O7-TE1-O2	-3.44	91.56	94.65
2	A	704	TEW	O12-TE1-O1	3.41	97.73	94.65
2	A	701	TEW	O13-TE1-O11	-3.36	81.23	85.21
2	B	701	TEW	O13-TE1-O11	-3.31	81.30	85.21
2	A	707	TEW	O11-TE1-O2	3.27	97.59	94.65
2	A	701	TEW	O13-TE1-O1	3.21	97.54	94.65
2	A	702	TEW	O12-TE1-O1	3.17	97.51	94.65
2	B	707	TEW	O13-TE1-O12	-3.12	91.84	94.65
2	B	707	TEW	O11-TE1-O2	-3.08	91.88	94.65
2	A	705	TEW	O11-TE1-O2	-3.05	91.91	94.65
2	B	705	TEW	O13-TE1-O2	3.02	88.78	85.21
2	B	707	TEW	O2-TE1-O1	-3.00	81.67	85.21
2	B	707	TEW	O13-TE1-O11	2.80	88.52	85.21
2	A	701	TEW	O12-TE1-O7	-2.76	81.95	85.21
2	B	703	TEW	O13-TE1-O1	2.75	97.13	94.65
2	B	706	TEW	O12-TE1-O1	2.72	97.11	94.65
2	B	703	TEW	O13-TE1-O12	-2.66	92.26	94.65
2	A	702	TEW	O7-TE1-O2	2.63	97.03	94.65
2	A	706	TEW	O11-TE1-O2	-2.60	92.31	94.65
2	B	701	TEW	O7-TE1-O1	2.49	88.14	85.21
2	A	705	TEW	O2-TE1-O1	-2.44	82.33	85.21
2	A	701	TEW	O11-TE1-O7	2.40	96.81	94.65
2	B	705	TEW	O7-TE1-O2	-2.34	92.55	94.65
2	A	701	TEW	O11-TE1-O2	2.32	96.74	94.65
2	B	706	TEW	O13-TE1-O11	2.32	87.95	85.21
2	B	706	TEW	O7-TE1-O1	2.08	87.66	85.21
2	A	706	TEW	O13-TE1-O1	2.00	96.46	94.65

There are no chirality outliers.

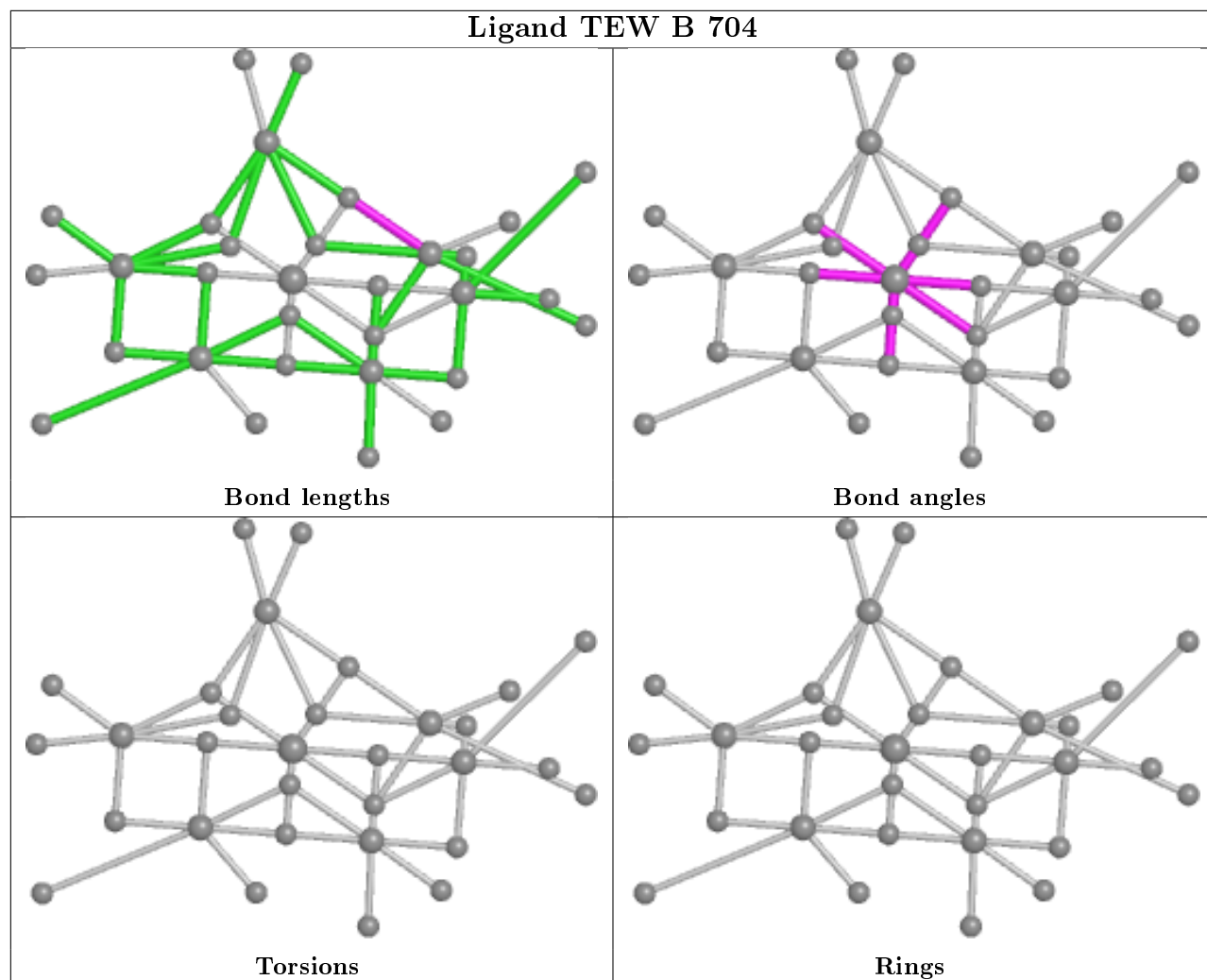
There are no torsion outliers.

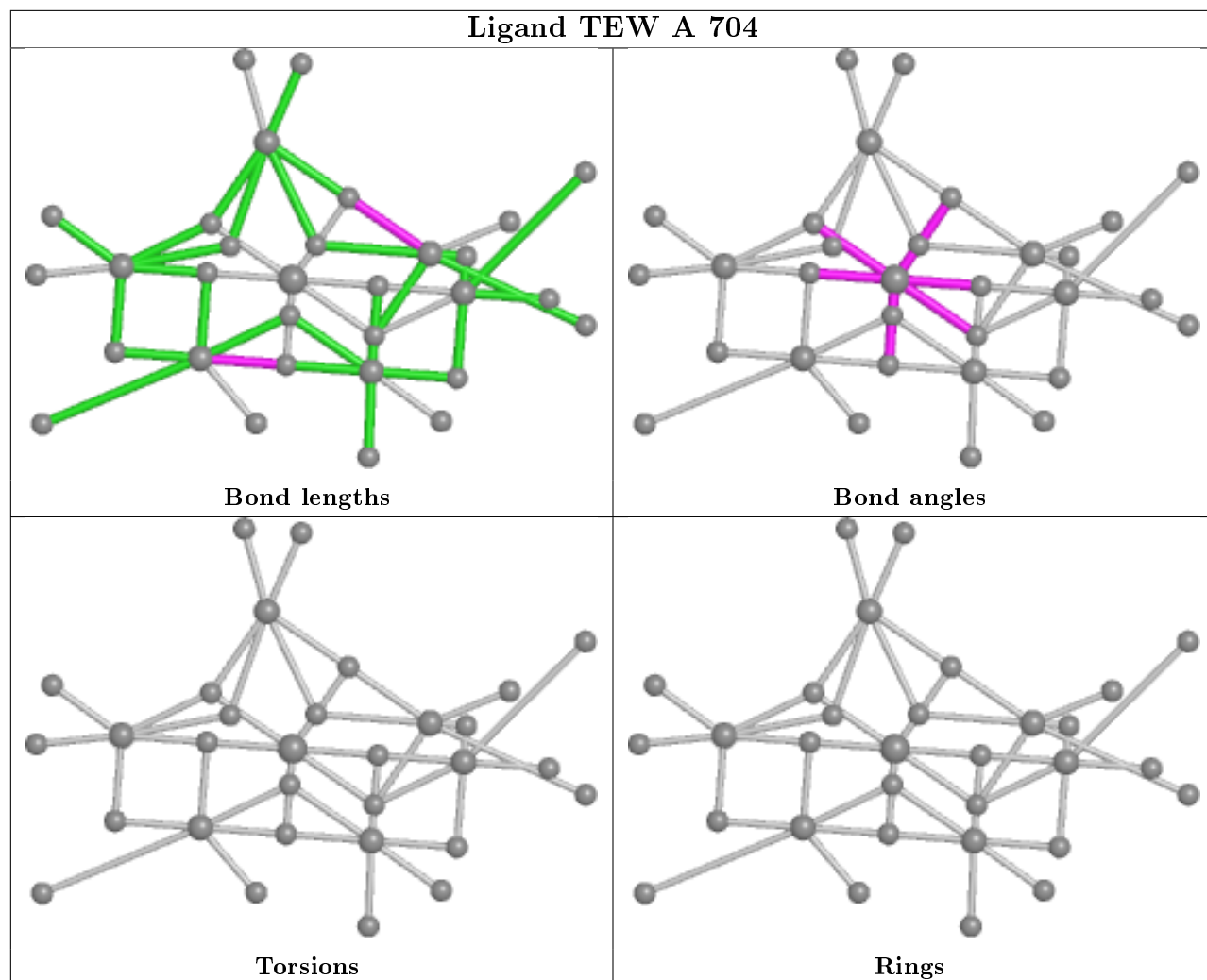
There are no ring outliers.

10 monomers are involved in 31 short contacts:

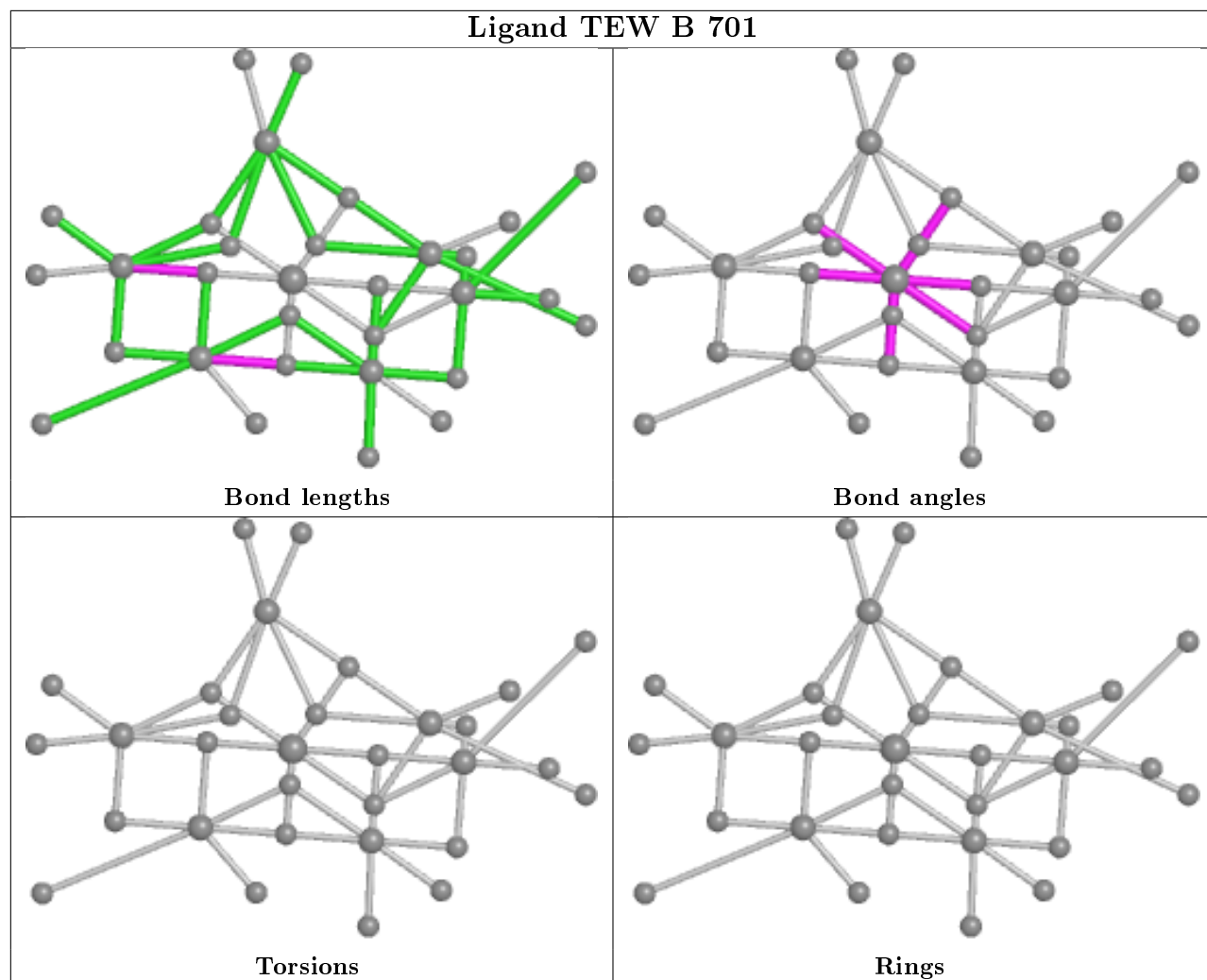
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	704	TEW	5	0
2	B	701	TEW	2	0
2	B	705	TEW	2	0
2	A	707	TEW	7	0
2	B	702	TEW	1	0
2	A	706	TEW	3	0
2	B	706	TEW	3	0
2	B	703	TEW	1	0
2	B	707	TEW	6	0
2	A	705	TEW	1	0

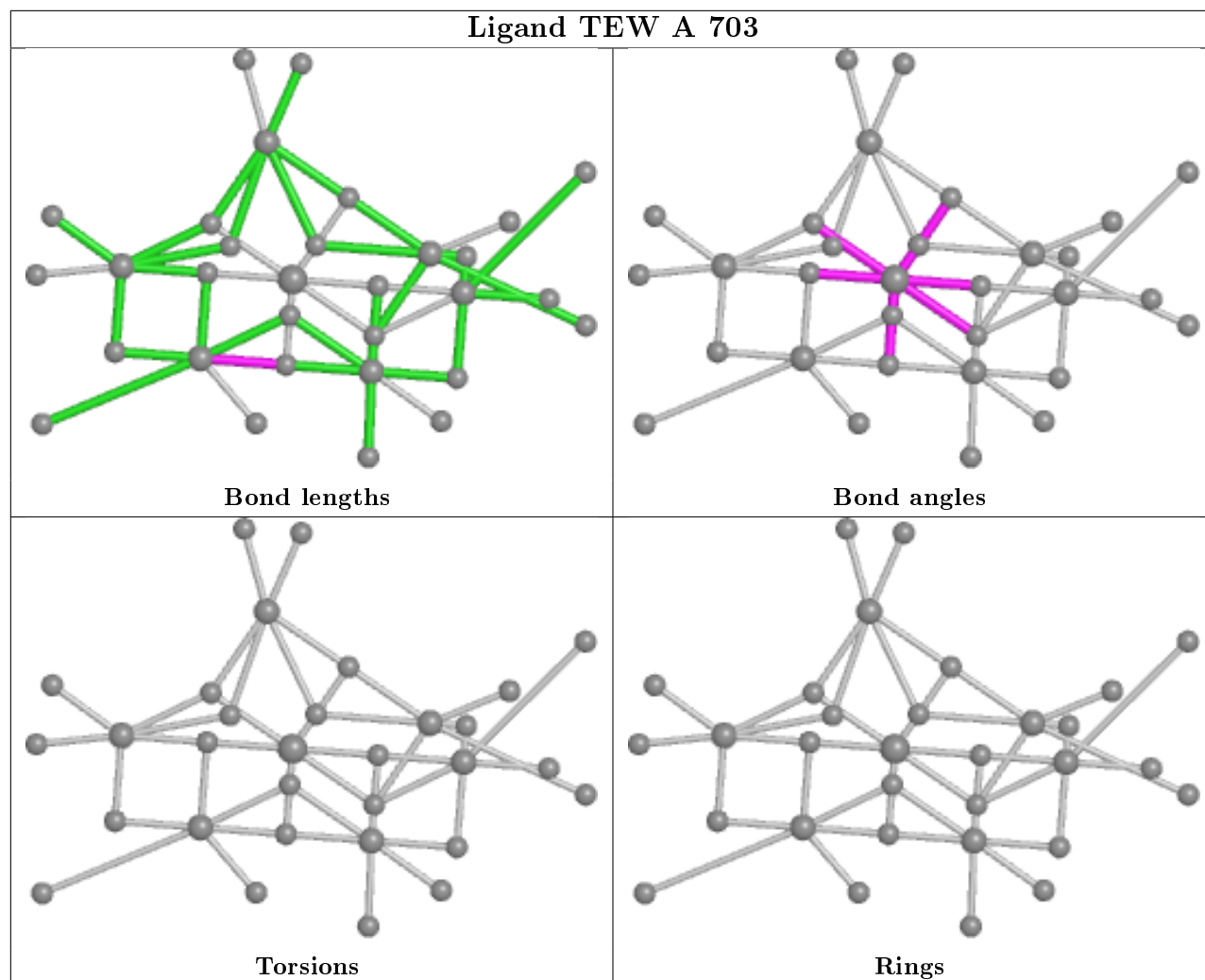
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

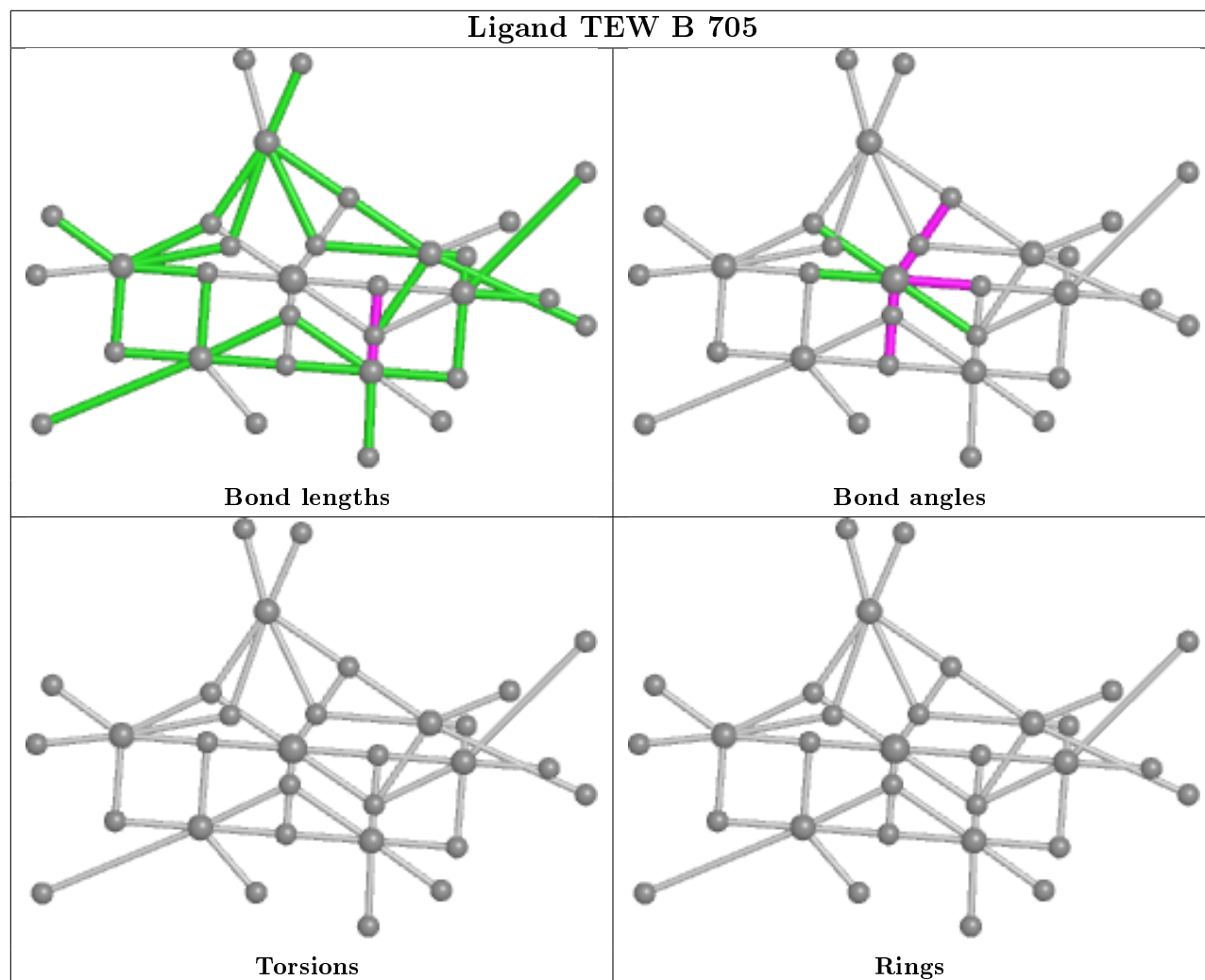


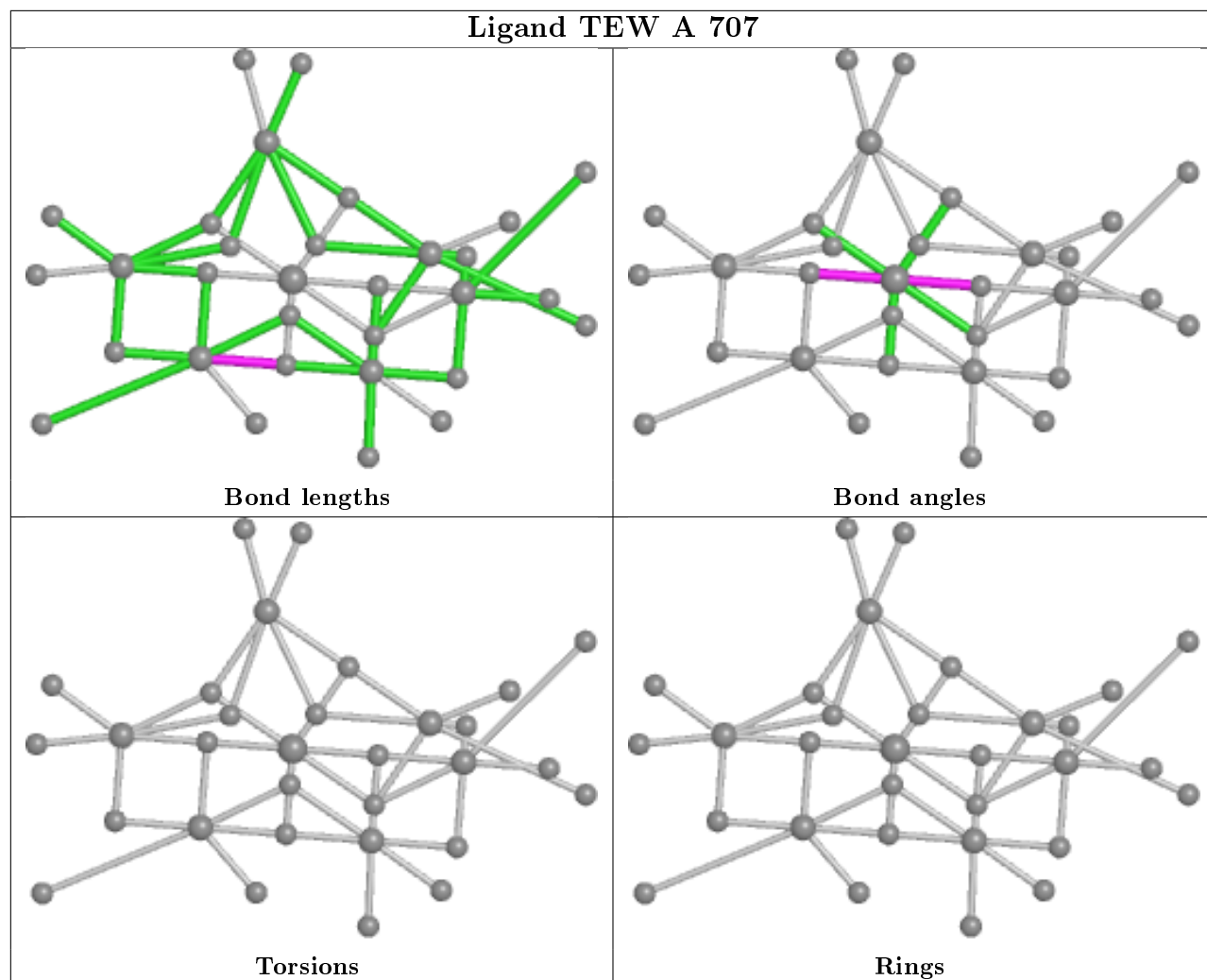


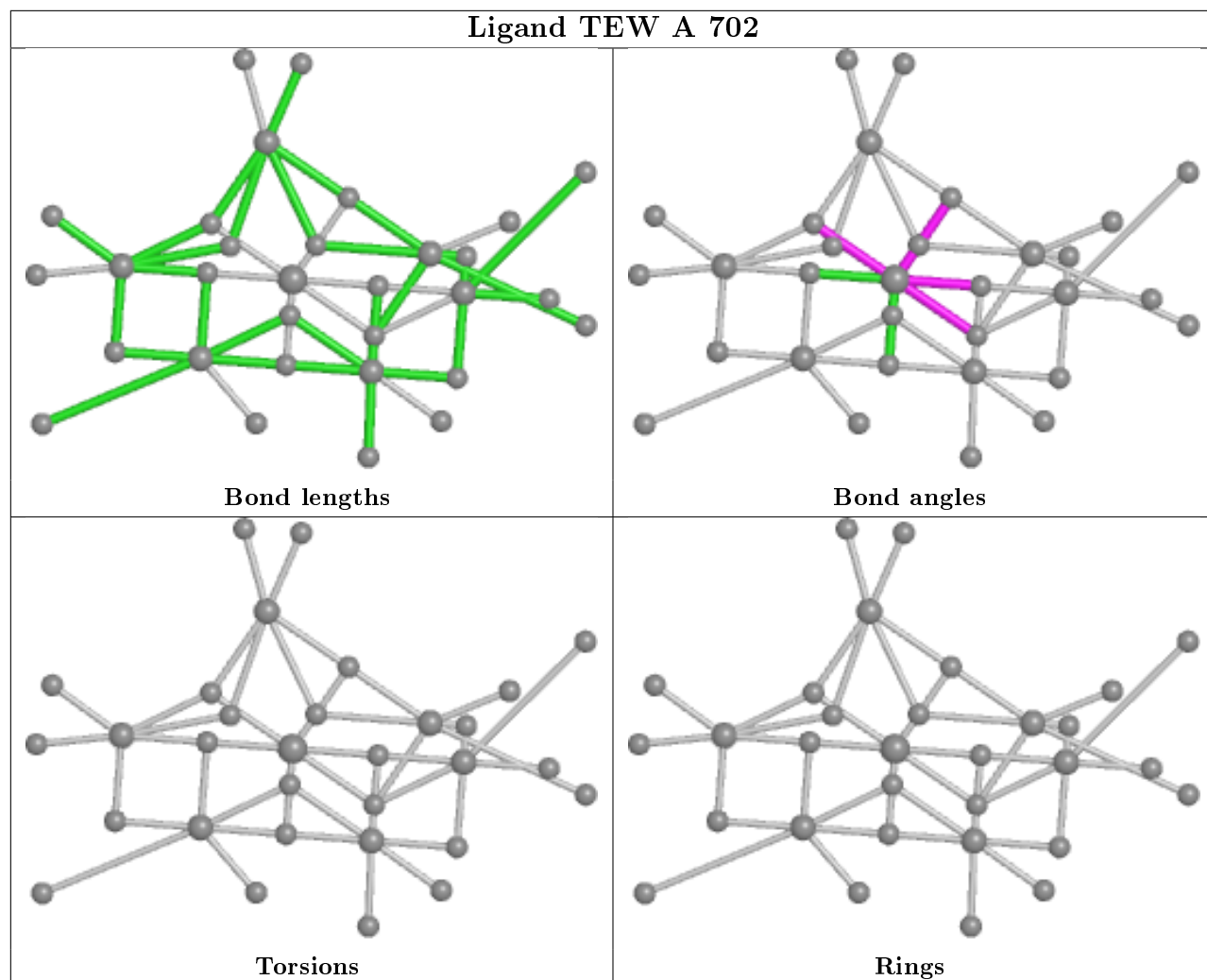


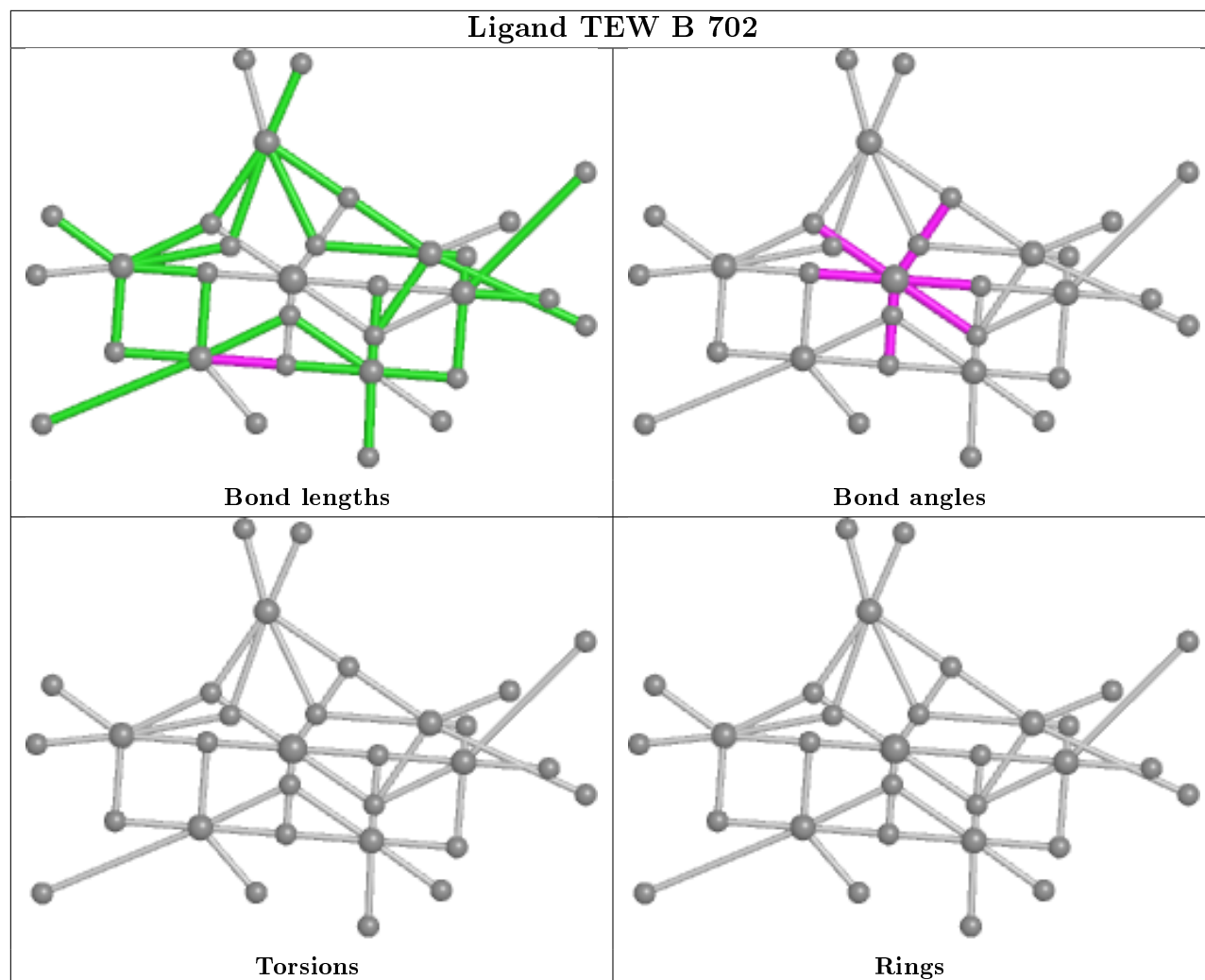


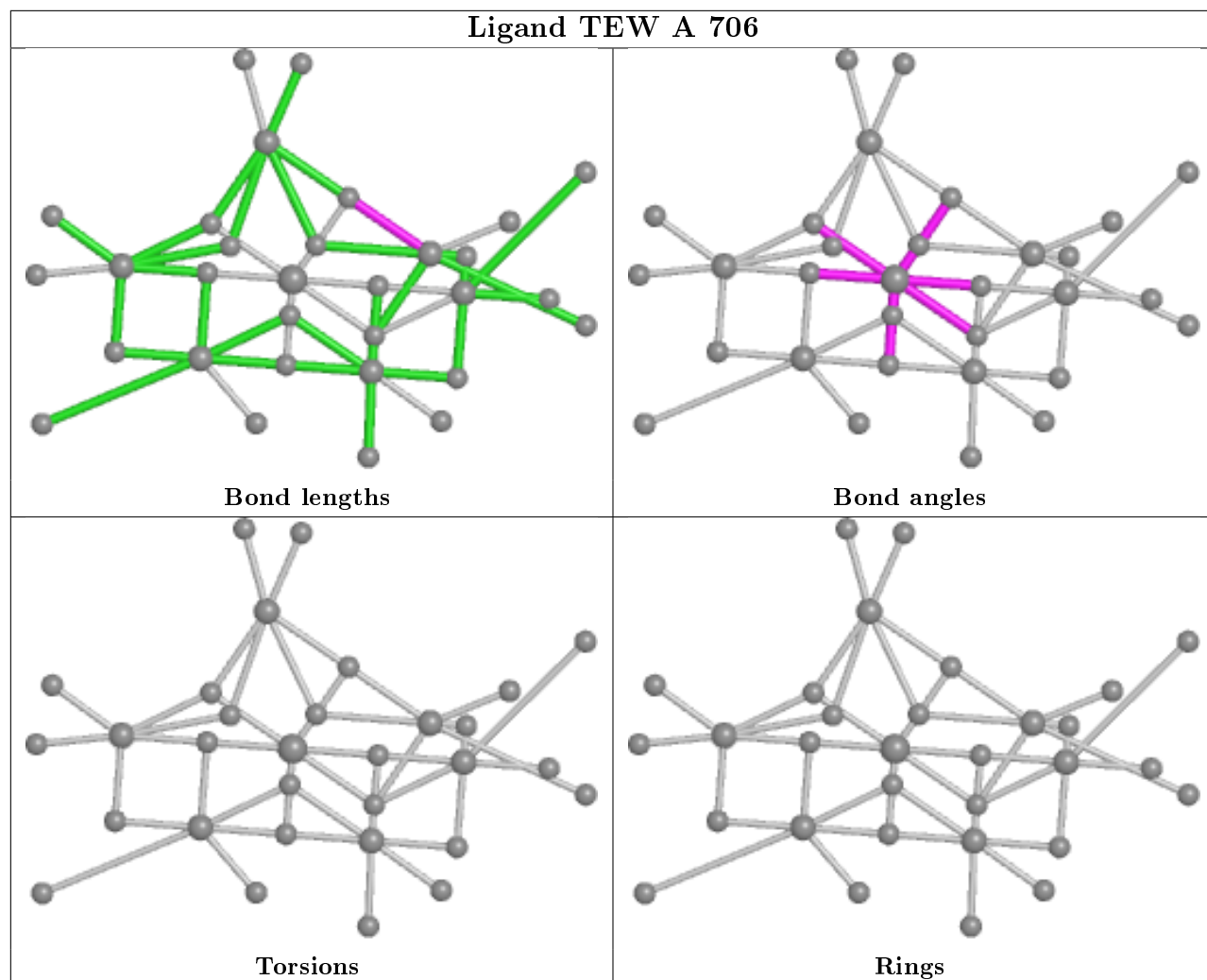


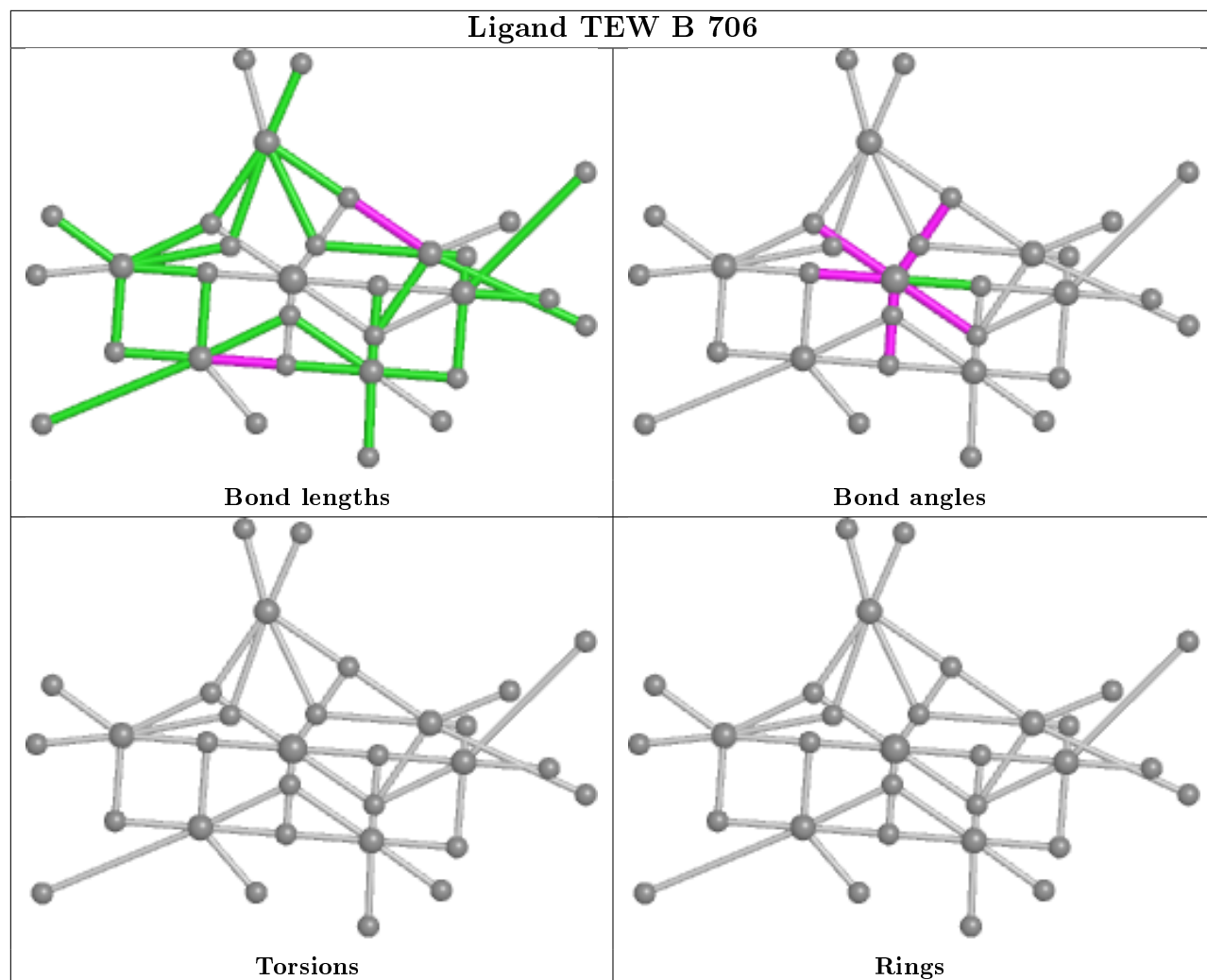




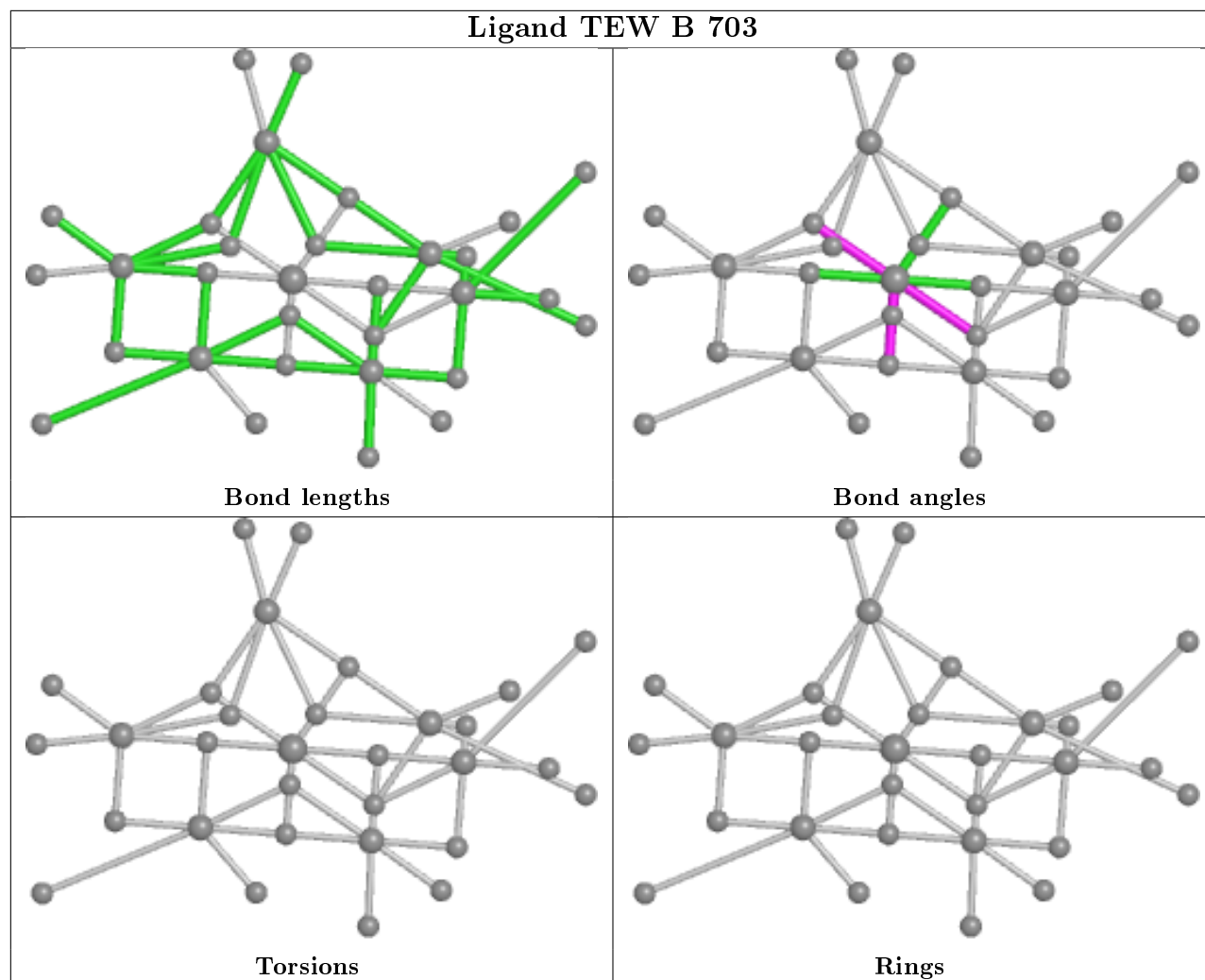


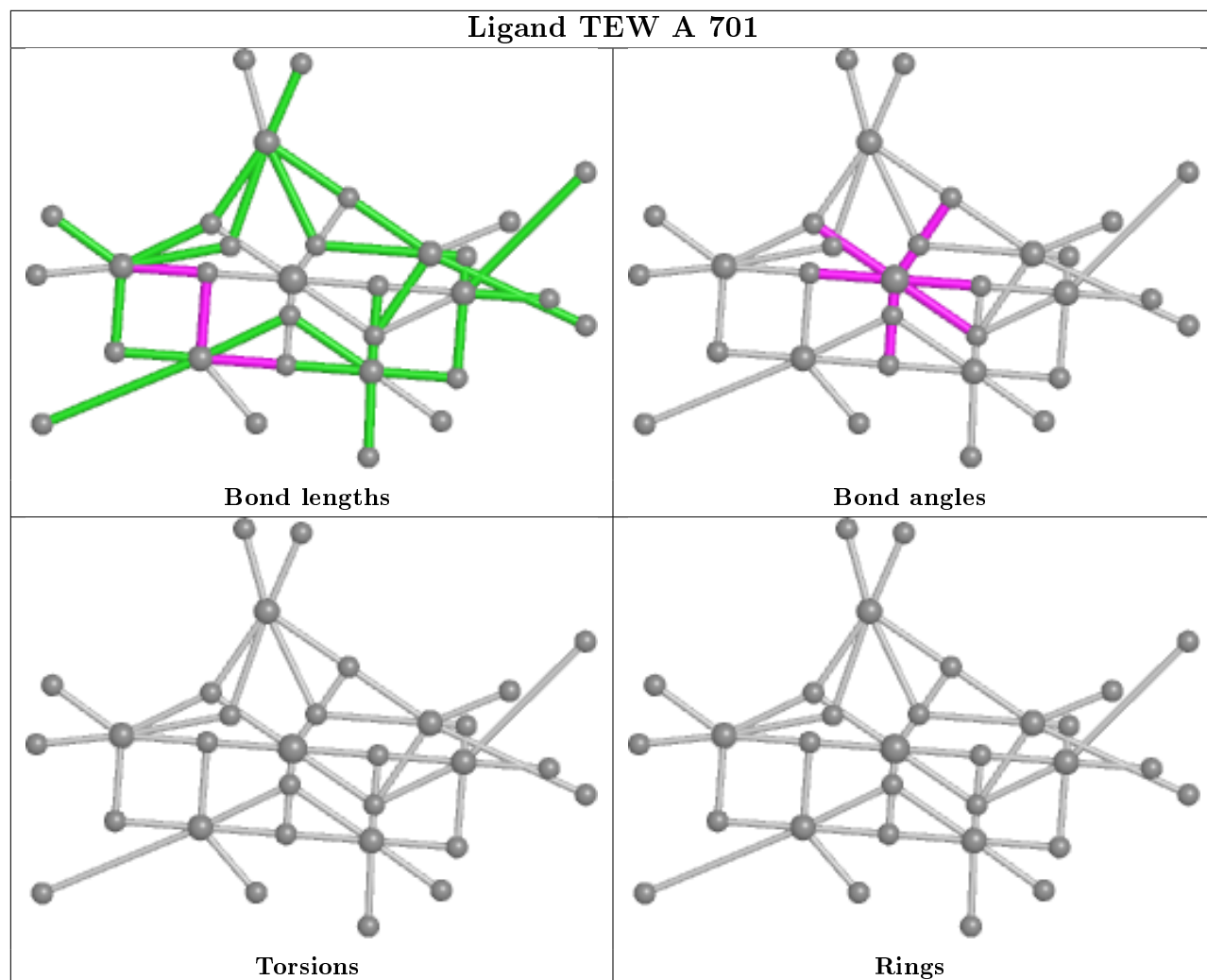


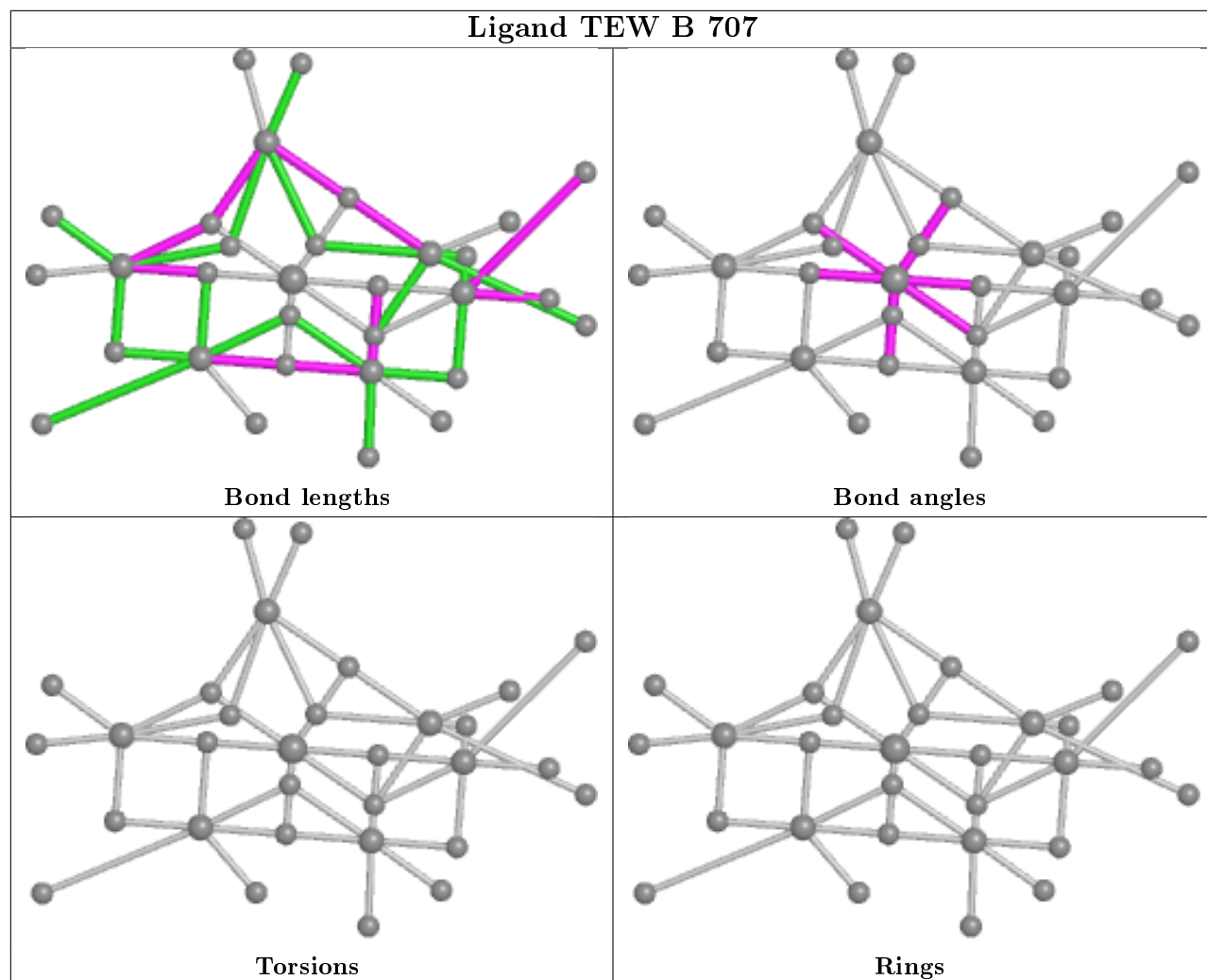


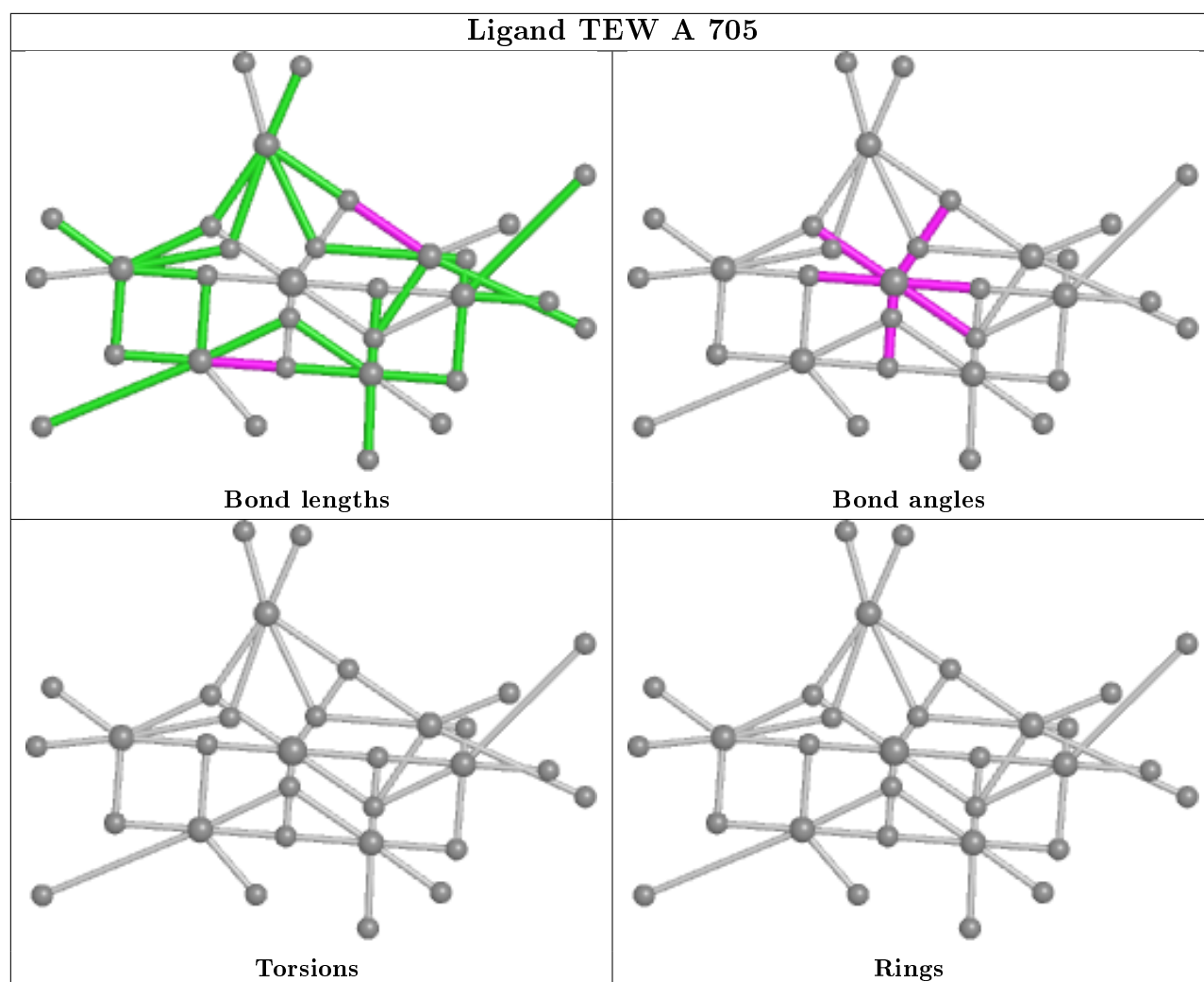












## 5.7 Other polymers [i](#)

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	679/681 (99%)	0.24	38 (5%)	24 11	76, 109, 160, 189	0
1	B	679/681 (99%)	0.33	52 (7%)	13 5	76, 106, 158, 203	0
All	All	1358/1362 (99%)	0.29	90 (6%)	18 7	76, 108, 159, 203	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	486	ILE	6.4
1	A	68	ASP	6.3
1	B	464	ILE	5.4
1	A	18	ASN	5.4
1	A	69	VAL	5.3
1	B	57	ILE	4.9
1	B	508	ILE	4.9
1	B	552	ILE	4.7
1	A	662	ILE	4.7
1	A	13	PHE	4.5
1	B	224	GLU	4.5
1	B	547	CYS	4.5
1	B	59	PHE	4.3
1	B	8	GLU	4.0
1	A	542	LEU	4.0
1	B	332	ILE	3.8
1	A	544	PHE	3.7
1	A	5	THR	3.6
1	B	313	ASN	3.6
1	A	522	PHE	3.5
1	A	500	LEU	3.5
1	B	88	SER	3.4
1	A	486	ILE	3.3
1	B	90	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	17	PHE	3.2
1	A	12	THR	3.2
1	B	54	ILE	3.1
1	A	313	ASN	3.1
1	B	38	PHE	3.1
1	A	214	PHE	2.9
1	A	87	HIS	2.9
1	B	641	THR	2.9
1	A	54	ILE	2.9
1	A	312	GLU	2.9
1	B	680	LYS	2.8
1	B	9	THR	2.8
1	B	522	PHE	2.8
1	A	91	GLU	2.7
1	B	81	TYR	2.7
1	A	639	GLU	2.7
1	B	665	ASN	2.7
1	B	50	ILE	2.7
1	B	442	ILE	2.7
1	B	5	THR	2.6
1	A	446	VAL	2.6
1	B	36	ILE	2.6
1	B	223	THR	2.6
1	B	255[A]	TYR	2.6
1	B	640	LEU	2.6
1	B	398	ILE	2.5
1	B	542	LEU	2.5
1	B	312	GLU	2.5
1	A	445	ASN	2.5
1	A	663	LEU	2.5
1	A	11	LEU	2.5
1	B	34	ASP	2.5
1	B	376	ILE	2.5
1	B	652	LEU	2.4
1	A	134	ILE	2.4
1	A	434	PHE	2.4
1	A	552	ILE	2.4
1	B	56	VAL	2.3
1	B	428	GLY	2.3
1	B	598	GLU	2.3
1	A	70	ASN	2.3
1	A	2	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	304	ASN	2.2
1	B	58	LYS	2.2
1	B	214	PHE	2.2
1	B	262	PHE	2.2
1	A	665	ASN	2.2
1	A	513	LEU	2.2
1	B	443	VAL	2.2
1	B	335	ASN	2.2
1	A	336	VAL	2.2
1	A	146	LEU	2.1
1	B	530	LEU	2.1
1	B	37	GLU	2.1
1	A	315	LEU	2.1
1	B	462	GLN	2.1
1	A	53	ASN	2.1
1	A	117	LEU	2.1
1	B	625	CYS	2.1
1	A	48	HIS	2.1
1	B	31	PRO	2.1
1	B	7	LYS	2.0
1	B	146	LEU	2.0
1	B	632	PHE	2.0
1	B	53	ASN	2.0
1	A	640	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

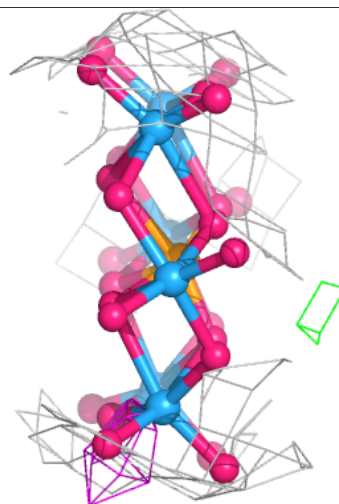
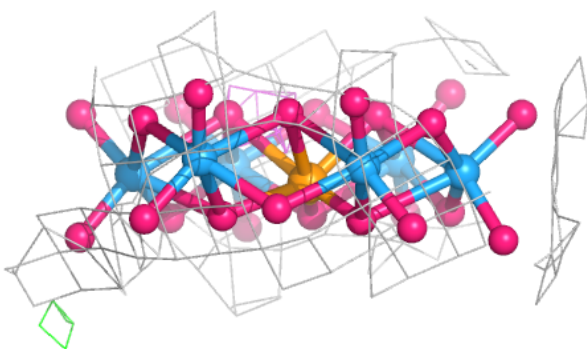
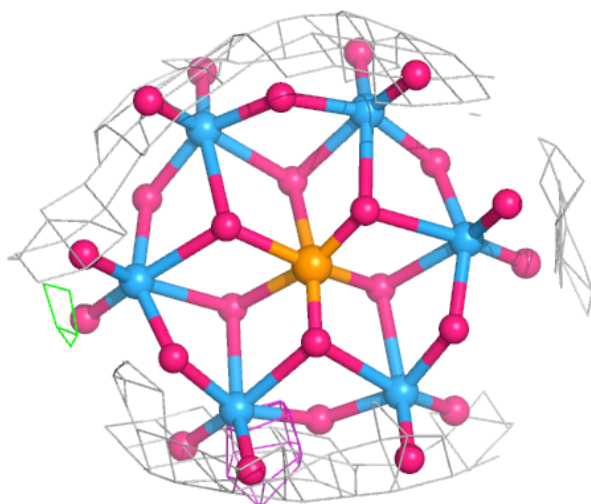
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	TEW	B	702	31/31	0.73	0.16	127,215,258,285	7
2	TEW	A	702	31/31	0.76	0.14	199,244,264,278	7
2	TEW	A	704	31/31	0.82	0.18	127,200,232,244	7
2	TEW	A	703	31/31	0.88	0.11	127,242,278,310	6
2	TEW	A	706	31/31	0.91	0.09	173,203,226,251	4
2	TEW	B	706	31/31	0.91	0.14	258,302,325,328	4
2	TEW	B	704	31/31	0.92	0.08	127,217,238,262	4
2	TEW	B	703	31/31	0.92	0.09	179,216,257,281	6
2	TEW	B	701	31/31	0.93	0.09	127,206,222,238	1
2	TEW	A	701	31/31	0.94	0.10	76,168,189,202	5
2	TEW	A	705	31/31	0.94	0.10	127,173,202,213	1
2	TEW	A	707	31/31	0.95	0.11	162,193,210,226	7
2	TEW	B	705	31/31	0.96	0.09	157,171,193,205	1
2	TEW	B	707	31/31	0.98	0.24	53,74,92,105	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.



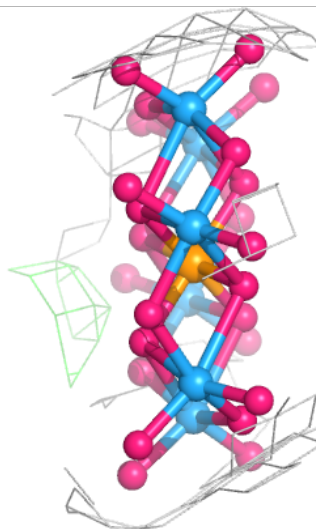
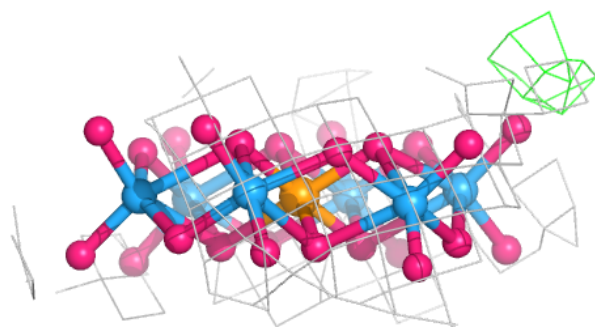
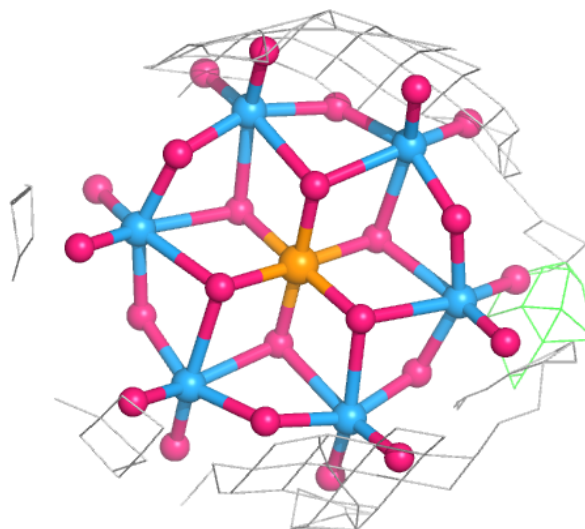
**Electron density around TEW B 702:**

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



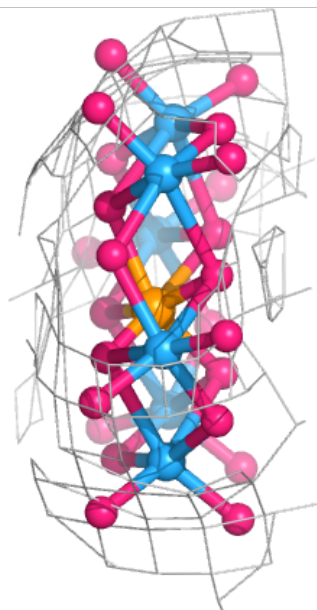
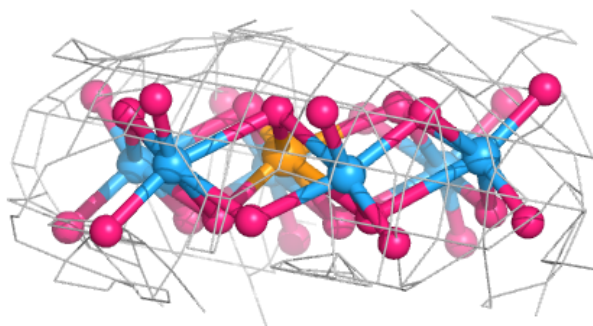
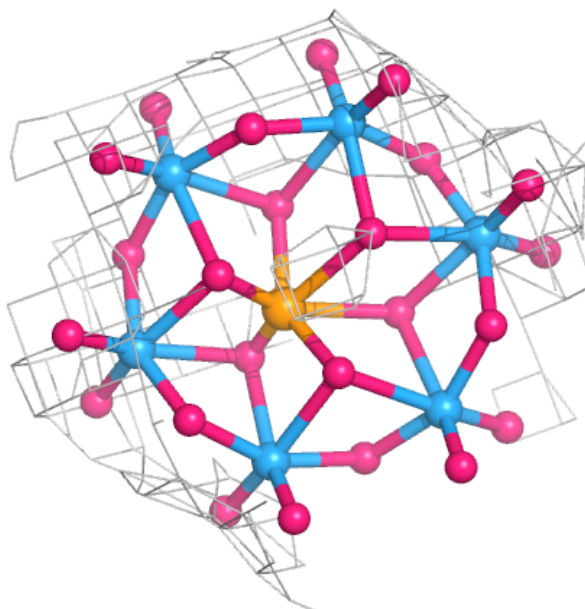
**Electron density around TEW A 702:**

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



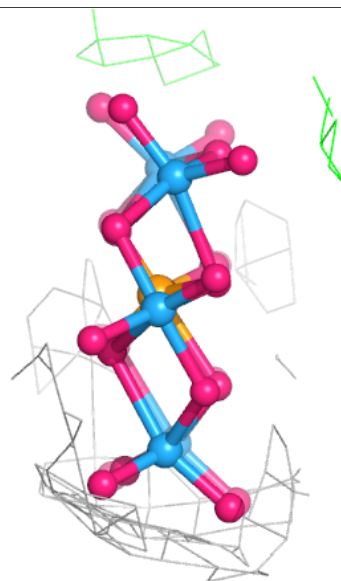
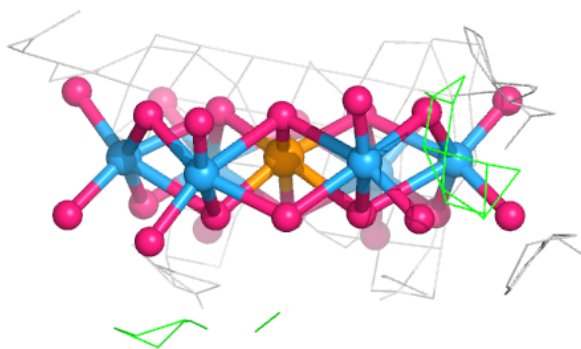
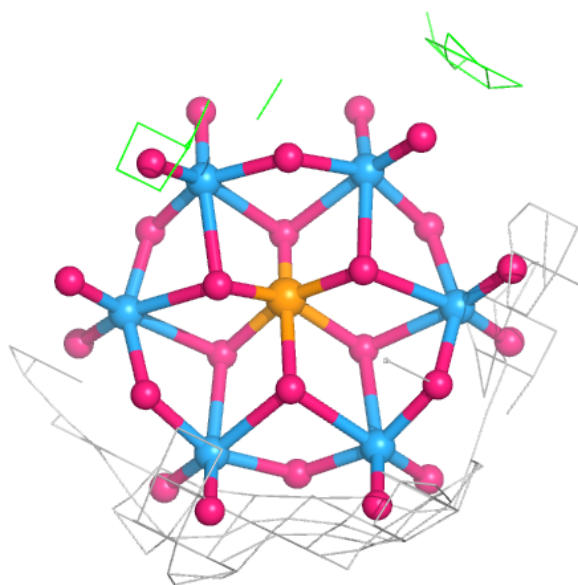
**Electron density around TEW A 704:**

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



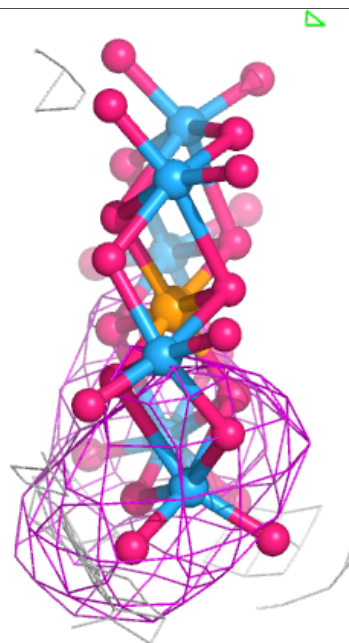
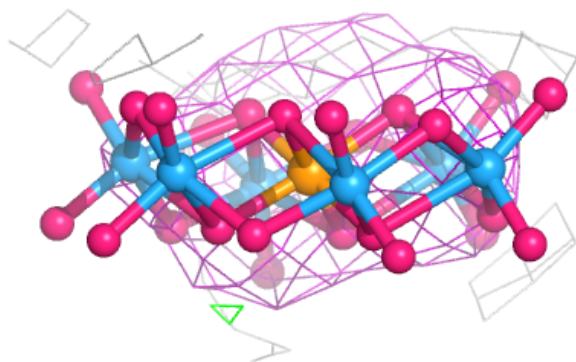
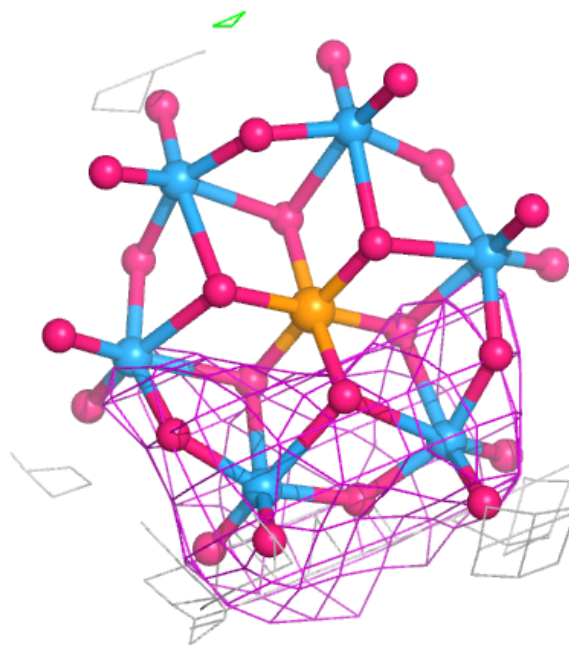
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



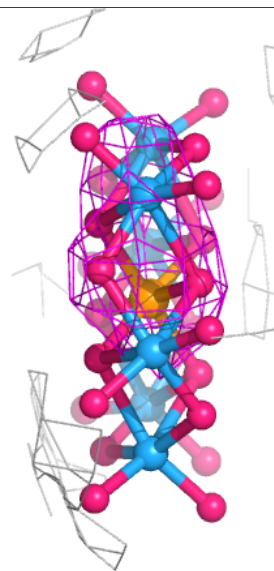
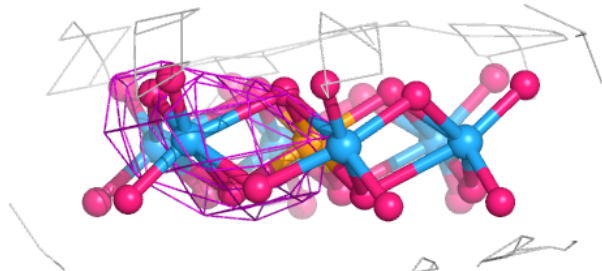
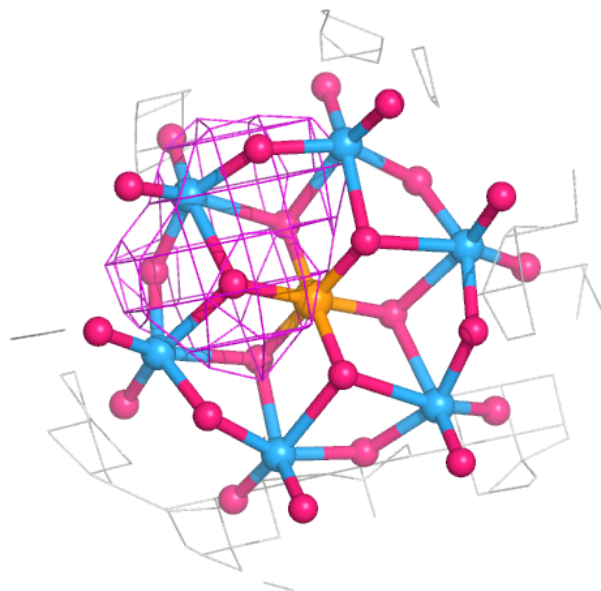
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and green (positive)



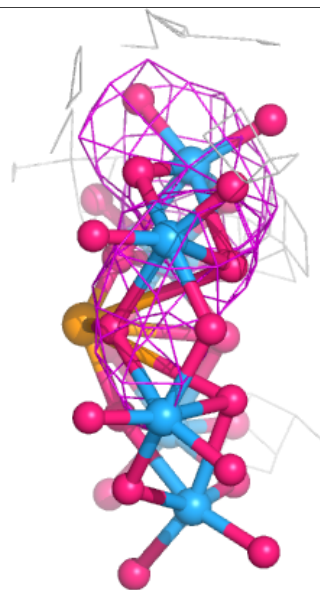
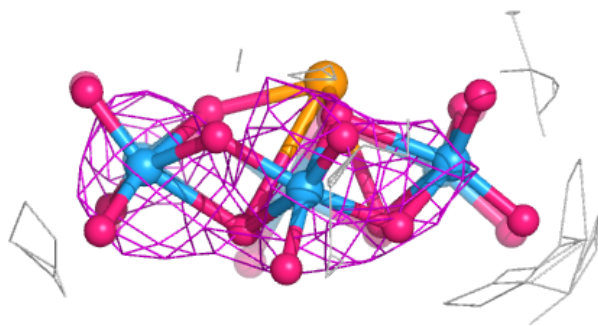
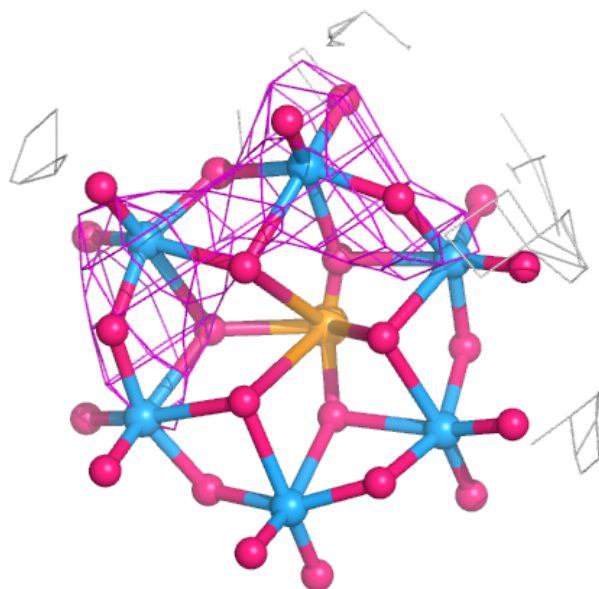
**Electron density around TEW B 706:**

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and green (positive)



**Electron density around TEW B 704:**

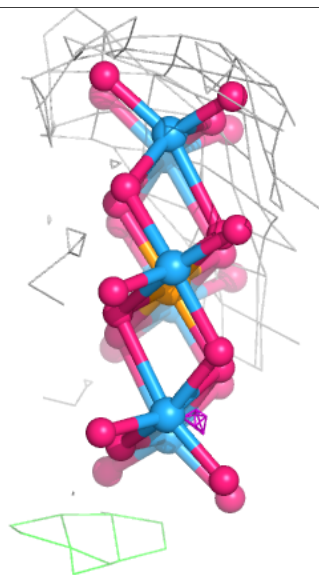
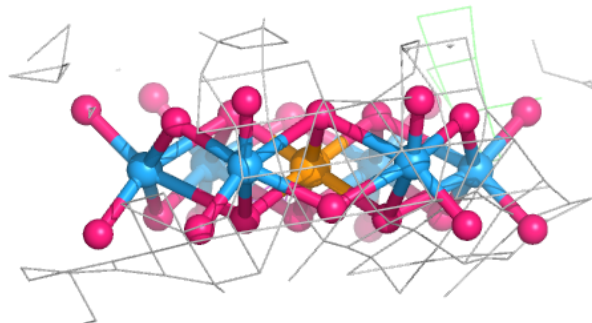
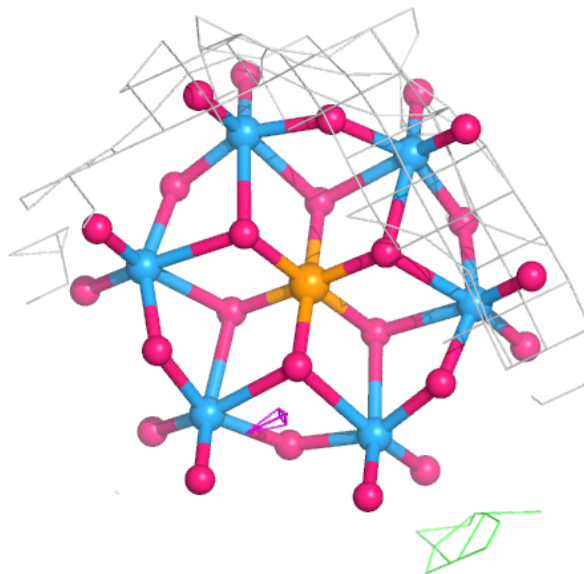
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around TEW B 703:**

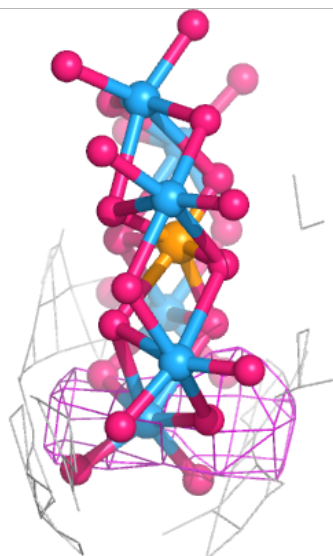
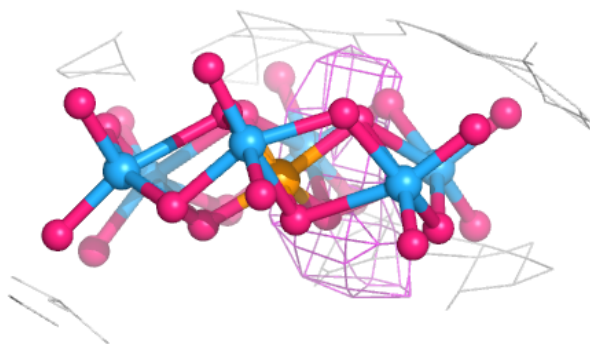
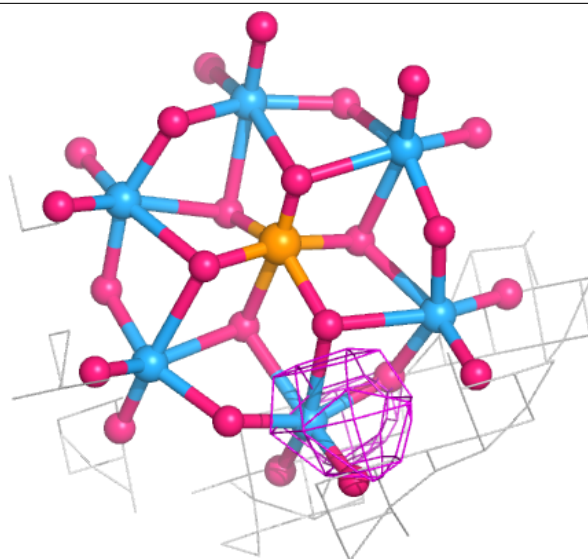
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





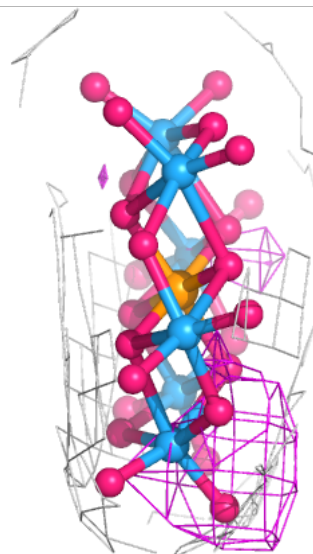
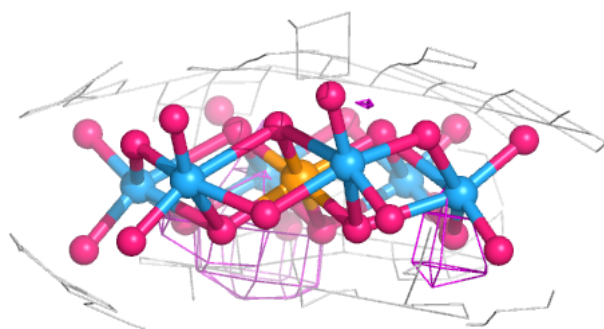
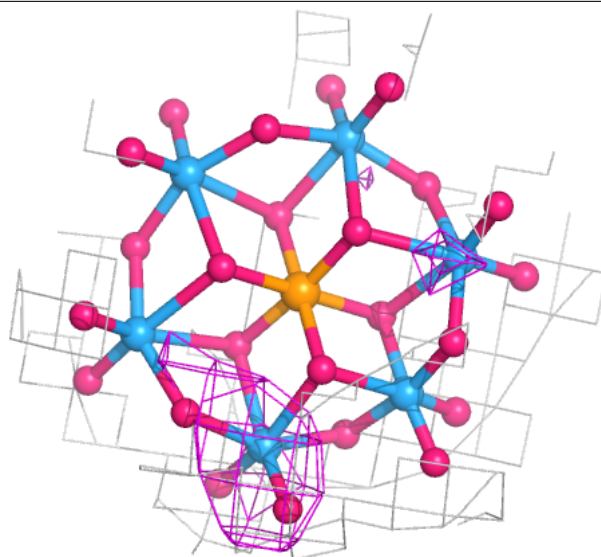
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and green (positive)



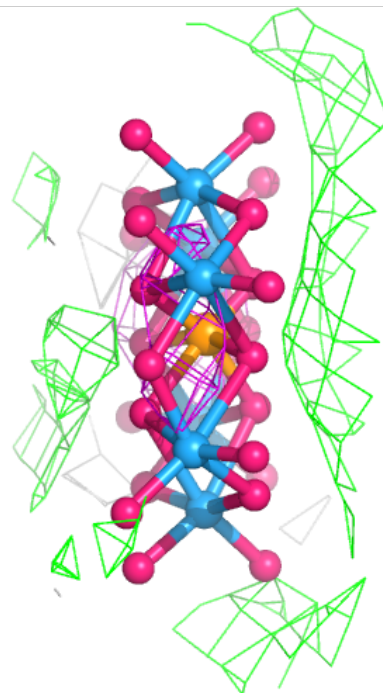
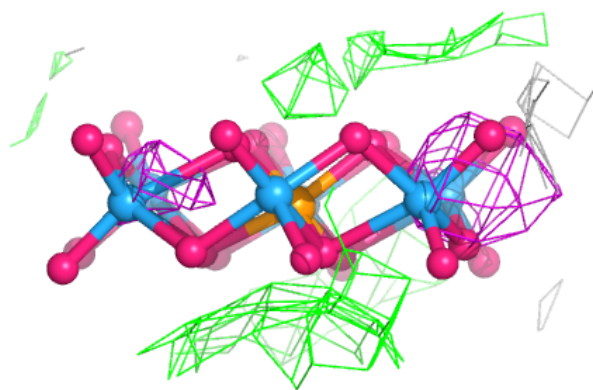
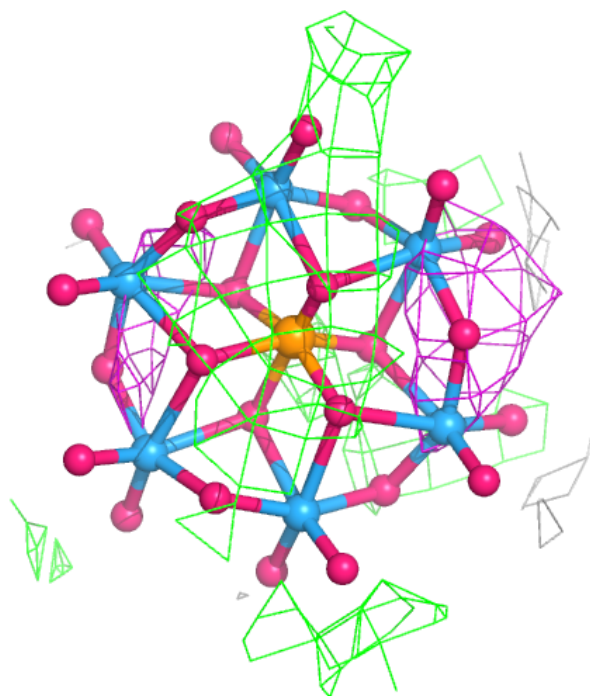
**Electron density around TEW A 701:**

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



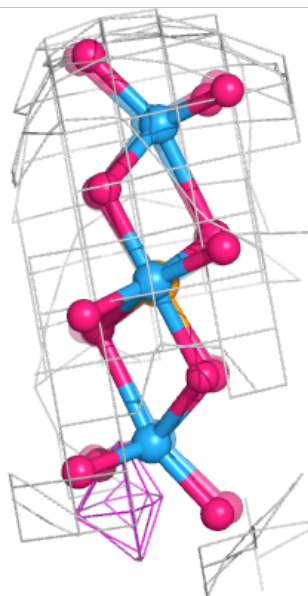
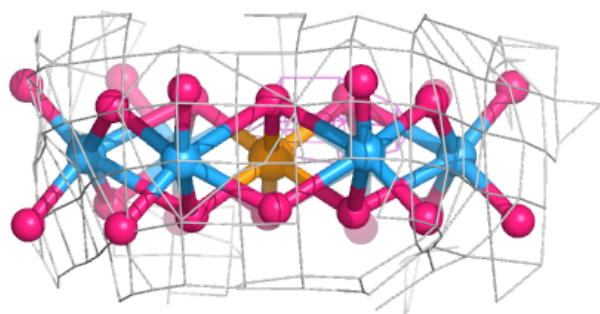
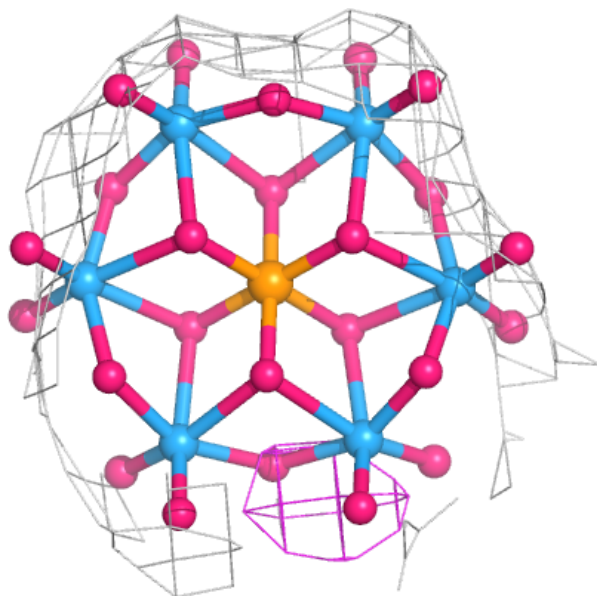
**Electron density around TEW A 705:**

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



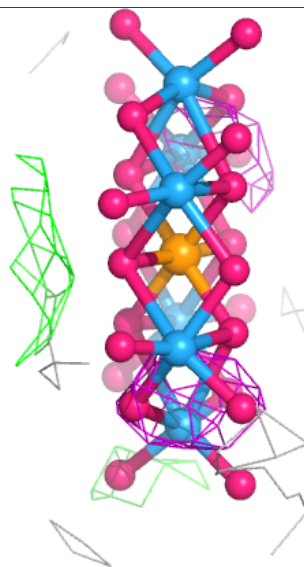
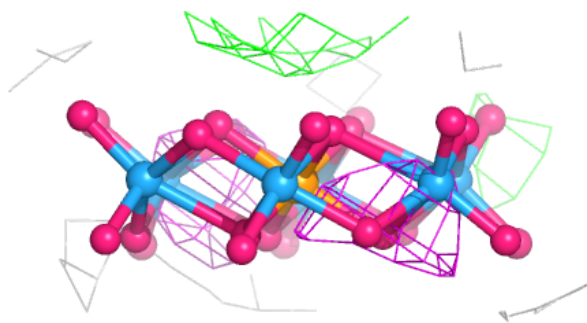
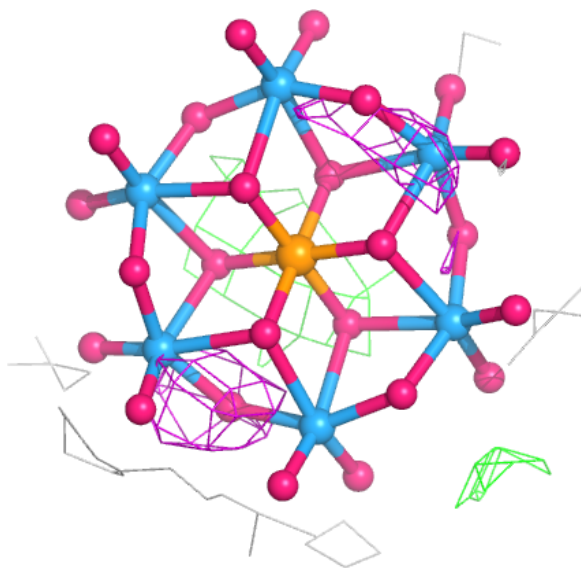
**Electron density around TEW A 707:**

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and green (positive)



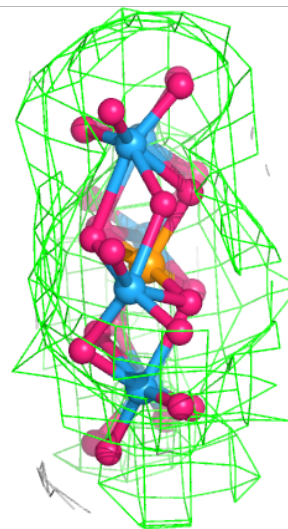
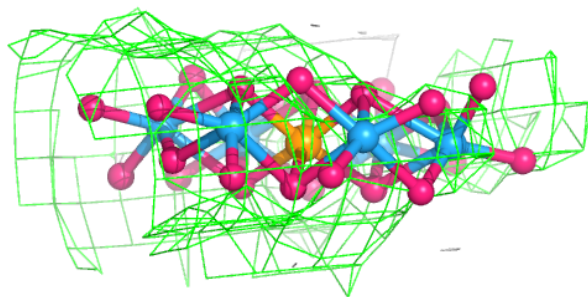
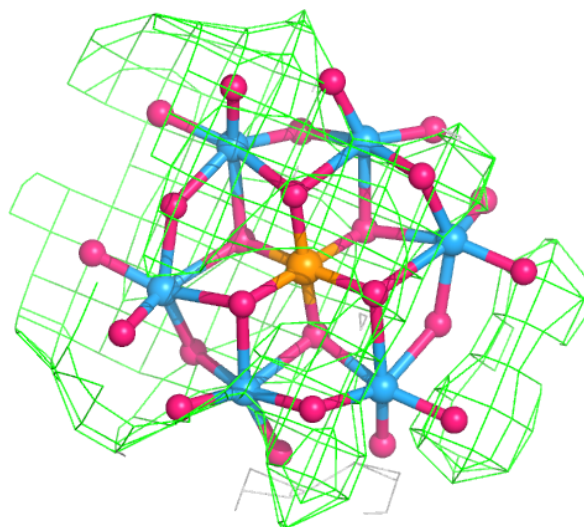
**Electron density around TEW B 705:**

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



**Electron density around TEW B 707:**

$2mF_o-DF_c$  (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.