



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:51 PM UTC

PDB ID : 6NYS / pdb_00006nys
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

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 Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

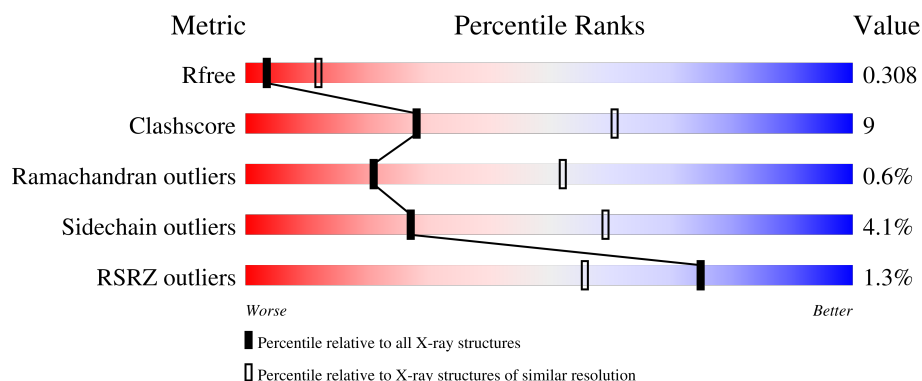
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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 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	681	 75% 22% •
1	B	681	 2% 75% 22% •

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 ⓘ

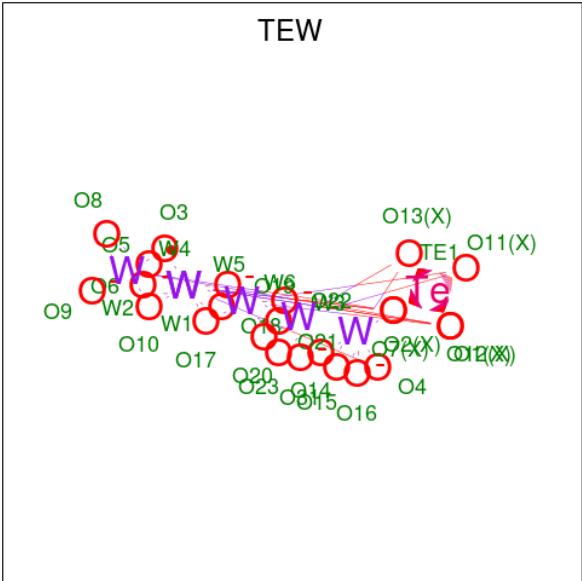
There are 2 unique types of molecules in this entry. The entry contains 11520 atoms, of which 0 are hydrogens and 0 are deuteriums.

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) (CCD ID: TEW) (formula: O₂₄TeW₆).



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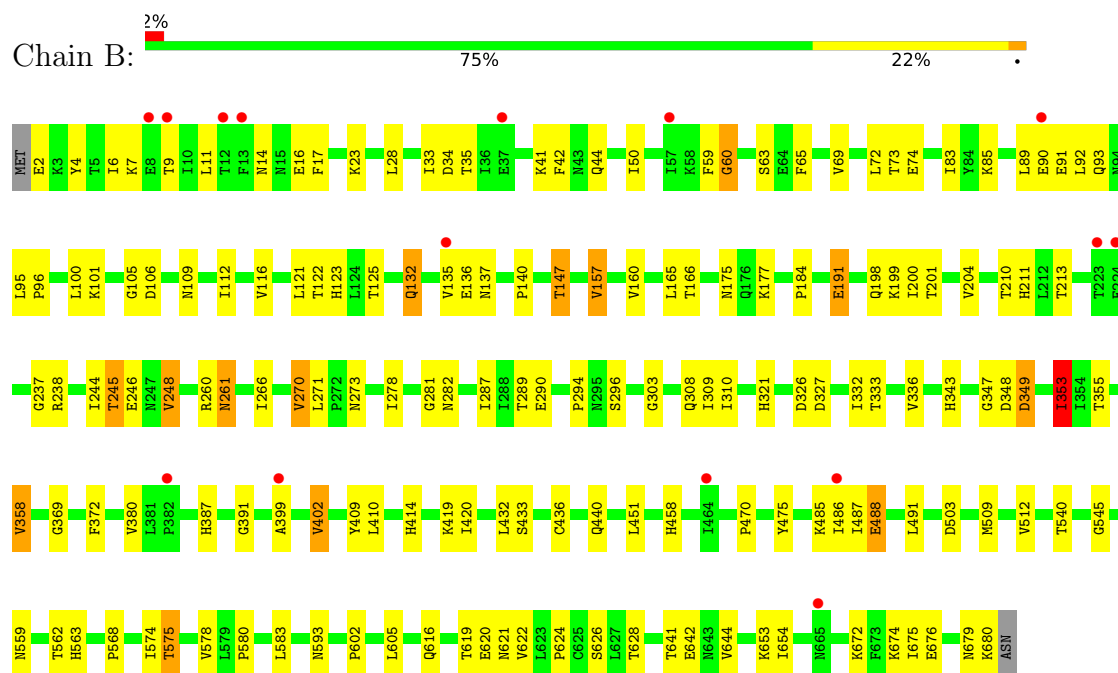
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total 31	O 24	Te 1	W 6	0	0
2	B	1	Total 31	O 24	Te 1	W 6	0	0
2	B	1	Total 31	O 24	Te 1	W 6	0	0
2	A	1	Total 31	O 24	Te 1	W 6	1	0
2	A	1	Total 31	O 24	Te 1	W 6	0	0
2	A	1	Total 31	O 24	Te 1	W 6	1	0
2	A	1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

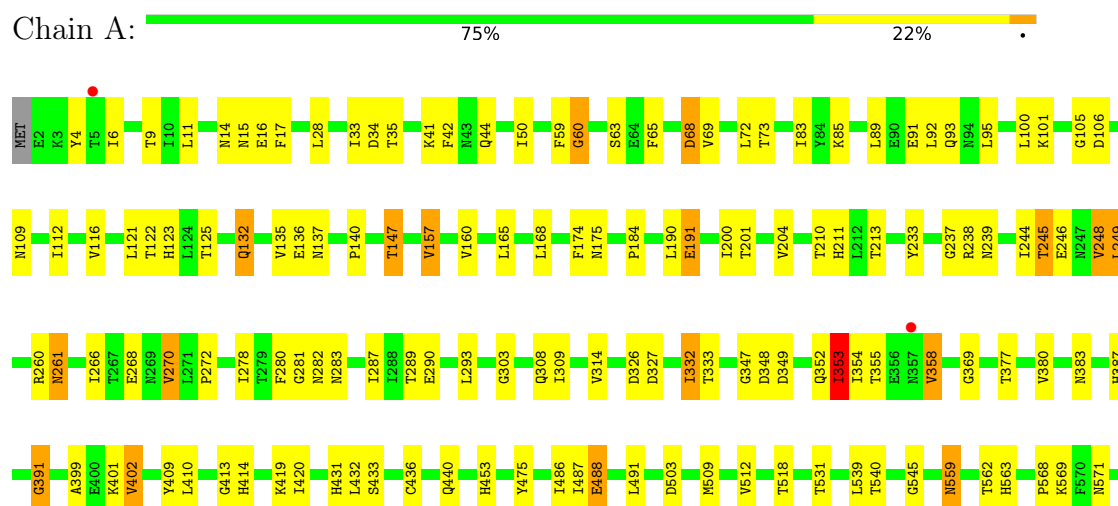
3 Residue-property plots

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, α , β , γ	65.29Å 171.76Å 92.03Å 90.00° 90.12° 90.00°	Depositor
Resolution (Å)	46.02 – 3.10 46.02 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.02-3.10) 99.5 (46.02-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	82.4	Xtriage
Anisotropy	1.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 121.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.439 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11520	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	1.15	9/5687 (0.2%)	1.52	36/7745 (0.5%)
1	B	1.15	8/5665 (0.1%)	1.52	21/7715 (0.3%)
All	All	1.15	17/11352 (0.1%)	1.52	57/15460 (0.4%)

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 (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	191	GLU	C-O	-7.56	1.15	1.24
1	B	358	VAL	C-O	7.21	1.31	1.23
1	B	355	THR	C-O	6.72	1.30	1.23
1	A	503	ASP	C-O	6.58	1.32	1.24
1	A	355	THR	C-O	6.33	1.30	1.23
1	B	50	ILE	N-CA	6.33	1.50	1.45
1	A	358	VAL	C-O	6.18	1.30	1.23
1	A	50	ILE	N-CA	6.15	1.50	1.45
1	B	503	ASP	C-O	6.13	1.31	1.24
1	B	327	ASP	C-O	6.11	1.31	1.24
1	A	377	THR	C-O	5.66	1.31	1.24
1	B	349	ASP	C-O	5.49	1.31	1.24
1	A	280	PHE	C-O	5.36	1.30	1.23
1	A	191	GLU	C-O	-5.29	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	327	ASP	C-O	5.24	1.30	1.24
1	A	272	PRO	C-O	-5.06	1.18	1.23
1	B	321	HIS	CE1-NE2	5.04	1.37	1.32

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	282	ASN	CA-CB-CG	-9.31	103.29	112.60
1	B	282	ASN	CA-CB-CG	-6.93	105.67	112.60
1	A	280	PHE	CA-C-N	6.79	127.84	120.44
1	A	280	PHE	C-N-CA	6.79	127.84	120.44
1	A	68	ASP	CA-CB-CG	6.19	118.79	112.60
1	B	348	ASP	CB-CA-C	6.14	121.29	110.85
1	B	261	ASN	CA-CB-CG	-6.14	106.46	112.60
1	A	545	GLY	CA-C-O	-6.10	116.18	122.28
1	B	132	GLN	CA-C-N	6.09	129.52	120.87
1	B	132	GLN	C-N-CA	6.09	129.52	120.87
1	A	261	ASN	CA-CB-CG	-5.94	106.66	112.60
1	A	606	THR	CA-CB-OG1	-5.87	100.79	109.60
1	A	383	ASN	CA-CB-CG	5.84	118.44	112.60
1	A	380	VAL	CA-C-N	5.80	128.44	120.67
1	A	380	VAL	C-N-CA	5.80	128.44	120.67
1	B	580	PRO	CA-C-N	5.73	128.23	120.38
1	B	580	PRO	C-N-CA	5.73	128.23	120.38
1	B	237	GLY	CA-C-O	-5.69	115.90	121.93
1	B	380	VAL	O-C-N	5.69	127.04	121.98
1	A	237	GLY	CA-C-O	-5.67	115.92	121.93
1	B	358	VAL	CA-C-N	5.61	128.19	120.67
1	B	358	VAL	C-N-CA	5.61	128.19	120.67
1	A	174	PHE	CA-C-O	-5.55	114.91	120.96
1	B	545	GLY	CA-C-O	-5.53	116.19	122.33
1	A	355	THR	CA-C-N	5.51	127.93	120.65
1	A	355	THR	C-N-CA	5.51	127.93	120.65
1	B	353	ILE	CA-C-O	-5.51	116.07	121.58
1	B	380	VAL	CA-C-N	5.45	127.97	120.67
1	B	380	VAL	C-N-CA	5.45	127.97	120.67
1	B	372	PHE	CA-C-O	-5.43	114.45	120.70
1	A	559	ASN	N-CA-C	-5.42	106.86	112.93
1	A	147	THR	CA-CB-OG1	-5.39	101.51	109.60
1	A	358	VAL	CA-C-N	5.35	127.84	120.67
1	A	358	VAL	C-N-CA	5.35	127.84	120.67
1	A	383	ASN	N-CA-C	-5.29	106.85	113.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	348	ASP	CB-CA-C	5.23	119.75	110.85
1	A	132	GLN	CA-C-N	5.22	128.28	120.87
1	A	132	GLN	C-N-CA	5.22	128.28	120.87
1	A	391	GLY	CA-C-N	5.18	127.49	120.65
1	A	391	GLY	C-N-CA	5.18	127.49	120.65
1	A	678	PHE	CA-C-O	-5.13	115.62	121.58
1	A	622	VAL	N-CA-C	-5.13	107.74	111.90
1	A	332	ILE	CA-C-N	5.13	131.15	122.12
1	A	332	ILE	C-N-CA	5.13	131.15	122.12
1	A	571	ASN	CA-C-O	-5.13	116.90	121.67
1	A	611	GLY	CA-C-O	-5.12	116.55	121.92
1	A	531	THR	CA-CB-OG1	-5.11	101.93	109.60
1	B	575	THR	CA-C-N	5.09	128.00	120.82
1	B	575	THR	C-N-CA	5.09	128.00	120.82
1	A	352	GLN	CA-C-N	5.09	127.42	120.35
1	A	352	GLN	C-N-CA	5.09	127.42	120.35
1	A	353	ILE	CA-C-O	-5.08	116.50	121.58
1	B	391	GLY	CA-C-N	5.07	127.04	120.44
1	B	391	GLY	C-N-CA	5.07	127.04	120.44
1	A	268	GLU	CB-CA-C	5.04	118.27	109.65
1	A	610	PHE	CB-CA-C	5.00	117.96	109.50
1	B	147	THR	CA-CB-OG1	-5.00	102.10	109.60

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	97	0
1	B	5533	0	5420	96	0
2	A	217	0	0	11	0
2	B	217	0	0	20	0
All	All	11520	0	10852	200	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 (200) 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:O5	2:B:707:TEW:O15	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
1:A:431[B]:HIS:CD2	1:A:453[B]:HIS:CG	2.76	0.73
2:B:707:TEW:O21	2:B:707:TEW:O18	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:B:4:TYR:HB2	1:B:11:LEU:HD11	1.75	0.67
1:A:69:VAL:O	1:A:91:GLU:HG3	1.94	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:H	1:B:353:ILE:HD12	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:B:83:ILE:HD12	1:B:106:ASP:OD2	1.99	0.62
1:A:4:TYR:HB2	1:A:11:LEU:HD11	1.80	0.62
1:B:6:ILE:CG1	1:B:11:LEU:HD13	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ILE:HD12	1:A:353:ILE:N	2.15	0.62
2:B:701:TEW:O12	2:B:701:TEW:O1	2.18	0.62
1:A:260:ARG:CD	1:A:261:ASN:OD1	2.37	0.62
1:B:353:ILE:HD12	1:B:353:ILE:N	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:B:266:ILE:HG23	1:B:270:VAL:CG2	2.32	0.59
1:A:431[B]:HIS:NE2	1:A:453[B]:HIS:NE2	2.50	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:N	1:A:85:LYS:HD2	2.19	0.57
1:B:165:LEU:HB3	1:B:184:PRO:HG2	1.86	0.56
1:B:92:LEU:HA	1:B:95:LEU:HD12	1.87	0.56
1:A:353:ILE:H	1:A:353:ILE:CD1	2.19	0.56
1:A:593:ASN:OD1	1:A:616:GLN:NE2	2.33	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:85:LYS:N	1:B:85:LYS:HD2	2.21	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:191:GLU:HG3	1:B:213:THR:HB	1.89	0.54
1:A:16:GLU:HA	1:A:41:LYS:HB2	1.88	0.54
1:B:6:ILE:HG13	1:B:11:LEU:HD13	1.88	0.54
1:B:122:THR:HG23	1:B:123:HIS:ND1	2.23	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:B:157:VAL:O	1:B:160:VAL:HG12	2.09	0.53
1:A:157:VAL:O	1:A: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:273:ASN:O	1:B:296:SER:OG	2.23	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:HD12	1:A:89:LEU:N	2.25	0.52
1:B:210:THR:OG1	1:B:211:HIS:ND1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:210:THR:OG1	1:A:211:HIS:ND1	2.40	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:B:332:ILE:HG22	1:B:358:VAL:CG1	2.41	0.50
1:A:332:ILE:HG22	1:A: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
2:B:707:TEW:O9	2:B:707:TEW:O19	2.32	0.48
1:A:414:HIS:CD2	1:A:436:CYS:HB3	2.48	0.48
1:B:260:ARG:HD3	1:B:261:ASN:OD1	2.13	0.48
1:A:653:LYS:HA	1:A:676:GLU:O	2.14	0.48
1:B:59:PHE:O	1:B:60:GLY:O	2.32	0.48
1:B:93:GLN:HG2	1:B:116:VAL:HG13	1.96	0.48
1:B:414:HIS:CD2	2:B:705:TEW:O6	2.67	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:A:201:THR:O	1:A:204:VAL:HG22	2.13	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:O3	2:B:707:TEW:O1	2.33	0.47
1:B:121:LEU:HB3	1:B:140:PRO:HG2	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:679:ASN:CG	2:B:704:TEW:O21	2.58	0.47
1:A:200:ILE:HG23	1:A:204:VAL:HG21	1.95	0.47
1:A:34:ASP:OD1	1:A:35:THR:HG23	2.16	0.46
1:B:414:HIS:CD2	1:B:436:CYS:HB3	2.50	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: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:B:63:SER:CB	1:B:85:LYS:HZ1	2.29	0.46
1:B:487:ILE:CG2	1:B:488:GLU:H	2.29	0.46
1:A:414:HIS:CD2	1:A:436:CYS:CB	2.99	0.46
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: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: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:B:200:ILE:HG23	1:B:204:VAL:HG21	1.98	0.45
1:A:42:PHE:CE1	1:A:44:GLN:HB2	2.52	0.45
1:B:85:LYS:HB2	1:B:105:GLY:HA3	1.99	0.45
1:B:475:TYR:C	1:B:475:TYR:CD1	2.94	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: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:B:414:HIS:CD2	1:B:436:CYS:CB	3.02	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:626:SER:O	1:B:628:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:THR:O	1:A:33:ILE: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:B:9:THR:O	1:B:33:ILE:HG23	2.18	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:A:92:LEU:HA	1:A:95:LEU:CD1	2.47	0.43
1:A:518:THR:HA	1:A:539:LEU:HA	2.00	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:475:TYR:C	1:A:475:TYR:CD1	2.96	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:233:TYR:C	1:A:233:TYR:CD1	2.98	0.42
1:A:136:GLU:HG2	1:A:137:ASN:OD1	2.20	0.42
1:B:271:LEU:HB3	1:B:294:PRO:HD3	2.02	0.42
1:A:326:ASP:O	1:A:349:ASP:HB2	2.20	0.42
1:A:15:ASN:HB2	2:A:706:TEW:O15	2.19	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:B:641:THR:O	1:B:644:VAL:HG12	2.20	0.41
1:A:391:GLY:O	1:A:413:GLY:HA3	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:B:244:ILE:HG23	1:B:248:VAL:HG21	2.02	0.41
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:A:63:SER:CB	1:A:85:LYS:HZ1	2.33	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:136:GLU:HG2	1:B:137:ASN:OD1	2.21	0.41
1:B:157:VAL:O	1:B:160:VAL:CG1	2.69	0.41
1:A:293:LEU:HD12	1:A:314:VAL:O	2.20	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:65:PHE:HB3	1:A:85:LYS:HE3	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:7:LYS:HA	1:B:7:LYS:HE2	2.02	0.40
1:B:486:ILE:HG22	1:B:512:VAL:CG1	2.52	0.40
1:A:85:LYS:N	1:A:85:LYS:CD	2.84	0.40
1:B:487:ILE:HG22	1:B:488:GLU:N	2.35	0.40
1:B:65:PHE:HB3	1:B:85:LYS:HE3	2.03	0.40
1:A:11:LEU:CD2	1:A:28:LEU:CD2	2.99	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%)	21	52	
1	B	678/681 (100%)	597 (88%)	77 (11%)	4 (1%)	21	52	
All	All	1358/1362 (100%)	1198 (88%)	152 (11%)	8 (1%)	21	52	

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%)	619 (96%)	27 (4%)	26	58
1	B	644/645 (100%)	618 (96%)	26 (4%)	28	60
All	All	1290/1290 (100%)	1237 (96%)	53 (4%)	27	59

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	72	LEU
1	B	90	GLU
1	B	100	LEU
1	B	101	LYS
1	B	112	ILE
1	B	157	VAL
1	B	199	LYS
1	B	245	THR
1	B	248	VAL
1	B	270	VAL
1	B	278	ILE
1	B	290	GLU
1	B	309	ILE
1	B	353	ILE
1	B	402	VAL
1	B	420	ILE
1	B	433	SER
1	B	485	LYS
1	B	488	GLU
1	B	559	ASN
1	B	568	PRO
1	B	642	GLU
1	B	672	LYS
1	B	674	LYS
1	B	675	ILE
1	B	680	LYS
1	A	68	ASP

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Mol	Chain	Res	Type
1	A	72	LEU
1	A	100	LEU
1	A	101	LYS
1	A	112	ILE
1	A	157	VAL
1	A	245	THR
1	A	248	VAL
1	A	249	LEU
1	A	270	VAL
1	A	278	ILE
1	A	290	GLU
1	A	309	ILE
1	A	353	ILE
1	A	354	ILE
1	A	401	LYS
1	A	402	VAL
1	A	420	ILE
1	A	433	SER
1	A	488	GLU
1	A	559	ASN
1	A	568	PRO
1	A	569	LYS
1	A	642	GLU
1	A	672	LYS
1	A	675	ILE
1	A	680	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	44	GLN
1	B	94	ASN
1	B	110	GLN
1	B	159	ASN
1	B	195	ASN
1	B	198	GLN
1	B	313	ASN
1	B	317	ASN
1	B	467	ASN
1	B	572	GLN
1	B	621	ASN
1	B	665	ASN

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Mol	Chain	Res	Type
1	A	44	GLN
1	A	94	ASN
1	A	110	GLN
1	A	195	ASN
1	A	198	GLN
1	A	269	ASN
1	A	283	ASN
1	A	458	HIS
1	A	467	ASN
1	A	550	GLN
1	A	572	GLN
1	A	621	ASN
1	A	665	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	A	705	-	24,42,42	1.13	0	12,129,129	10.62	11 (91%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TEW	B	704	1	24,42,42	1.11	0	12,129,129	32.63	11 (91%)
2	TEW	A	701	-	24,42,42	1.84	3 (12%)	12,129,129	2.96	7 (58%)
2	TEW	A	703	-	24,42,42	1.09	0	12,129,129	9.62	11 (91%)
2	TEW	A	707	1	24,42,42	1.08	1 (4%)	12,129,129	1.34	1 (8%)
2	TEW	A	706	1	24,42,42	1.09	0	12,129,129	2.24	4 (33%)
2	TEW	B	707	1	24,42,42	1.68	6 (25%)	12,129,129	5.04	9 (75%)
2	TEW	B	706	-	24,42,42	1.05	0	12,129,129	1.79	4 (33%)
2	TEW	B	702	-	24,42,42	1.08	0	12,129,129	10.53	10 (83%)
2	TEW	A	704	-	24,42,42	1.07	0	12,129,129	13.26	11 (91%)
2	TEW	B	701	-	24,42,42	1.15	0	12,129,129	12.18	12 (100%)
2	TEW	B	705	-	24,42,42	1.09	0	12,129,129	1.52	2 (16%)
2	TEW	B	703	-	24,42,42	1.09	1 (4%)	12,129,129	1.29	2 (16%)
2	TEW	A	702	-	24,42,42	1.08	0	12,129,129	1.44	2 (16%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	TEW	W6-O23	-6.61	1.59	1.72
2	B	707	TEW	W6-O23	4.08	1.80	1.72
2	B	707	TEW	W2-O8	3.64	1.79	1.72
2	A	701	TEW	W6-O31	-3.16	1.49	2.09
2	B	707	TEW	W1-O6	2.62	1.77	1.72
2	B	707	TEW	W6-O31	-2.10	1.69	2.09
2	A	701	TEW	W6-O14	-2.09	1.78	1.97
2	B	707	TEW	W1-O5	-2.06	1.70	2.09
2	B	707	TEW	W2-O9	-2.05	1.70	2.09
2	B	703	TEW	W5-O22	-2.01	1.71	2.09
2	A	707	TEW	W6-O31	-2.00	1.71	2.09

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	O1-TE1-O12	-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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	TEW	O1-TE1-O12	-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
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	O1-TE1-O2	-15.73	66.63	85.21
2	A	704	TEW	O11-TE1-O7	15.49	108.59	94.65
2	B	701	TEW	O1-TE1-O2	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	O1-TE1-O12	12.41	105.82	94.65
2	A	703	TEW	O1-TE1-O12	-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	O1-TE1-O2	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	O1-TE1-O2	-7.83	75.96	85.21
2	B	702	TEW	O12-TE1-O11	-7.61	76.22	85.21
2	B	707	TEW	O1-TE1-O12	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	O1-TE1-O2	4.72	90.78	85.21
2	B	701	TEW	O13-TE1-O1	-4.56	90.55	94.65
2	B	707	TEW	O13-TE1-O2	4.51	90.53	85.21
2	A	701	TEW	O1-TE1-O12	-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	O1-TE1-O12	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	O1-TE1-O12	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	O1-TE1-O12	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	O1-TE1-O2	-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	O1-TE1-O12	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	O1-TE1-O2	-2.44	82.33	85.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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.

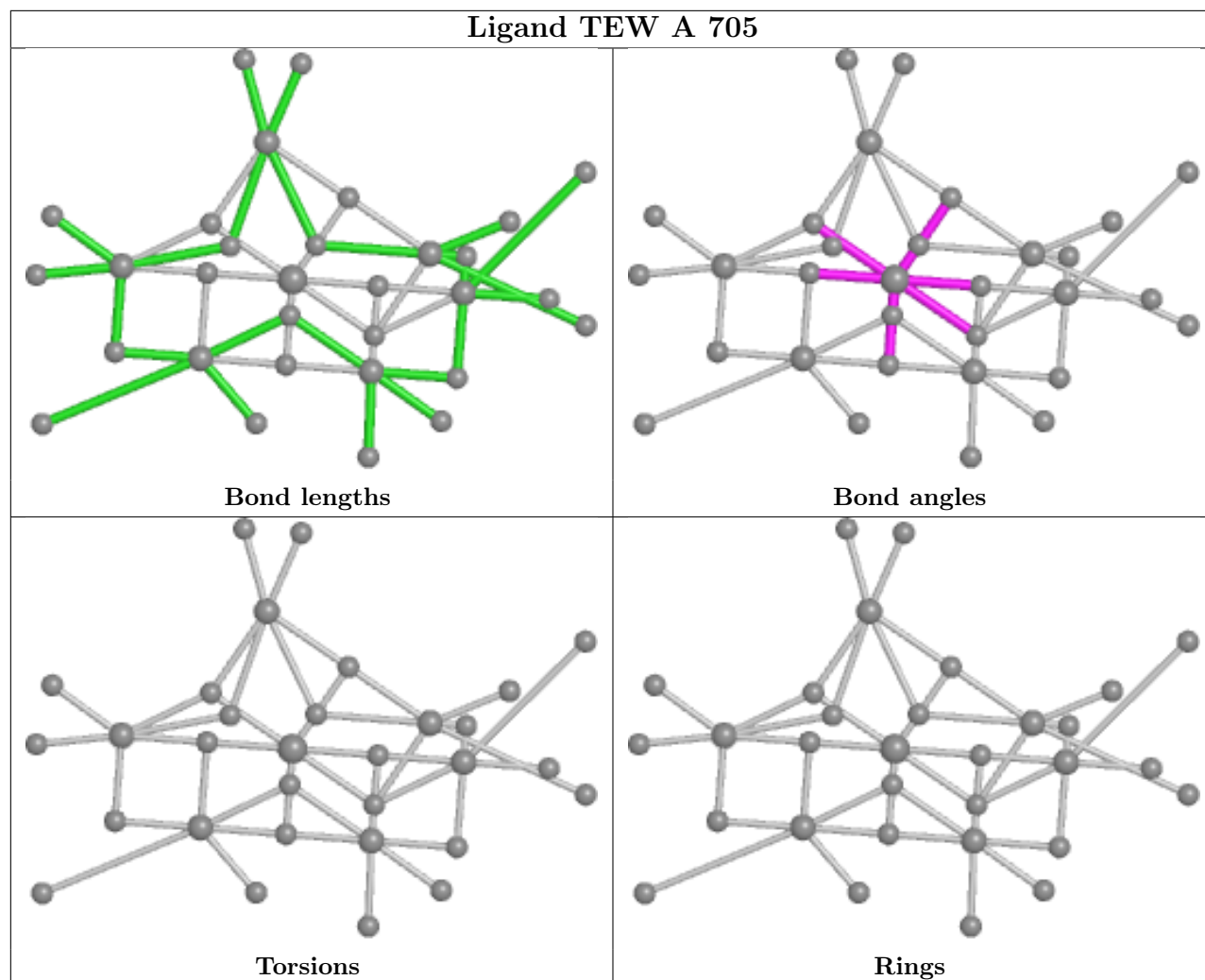
There are no torsion outliers.

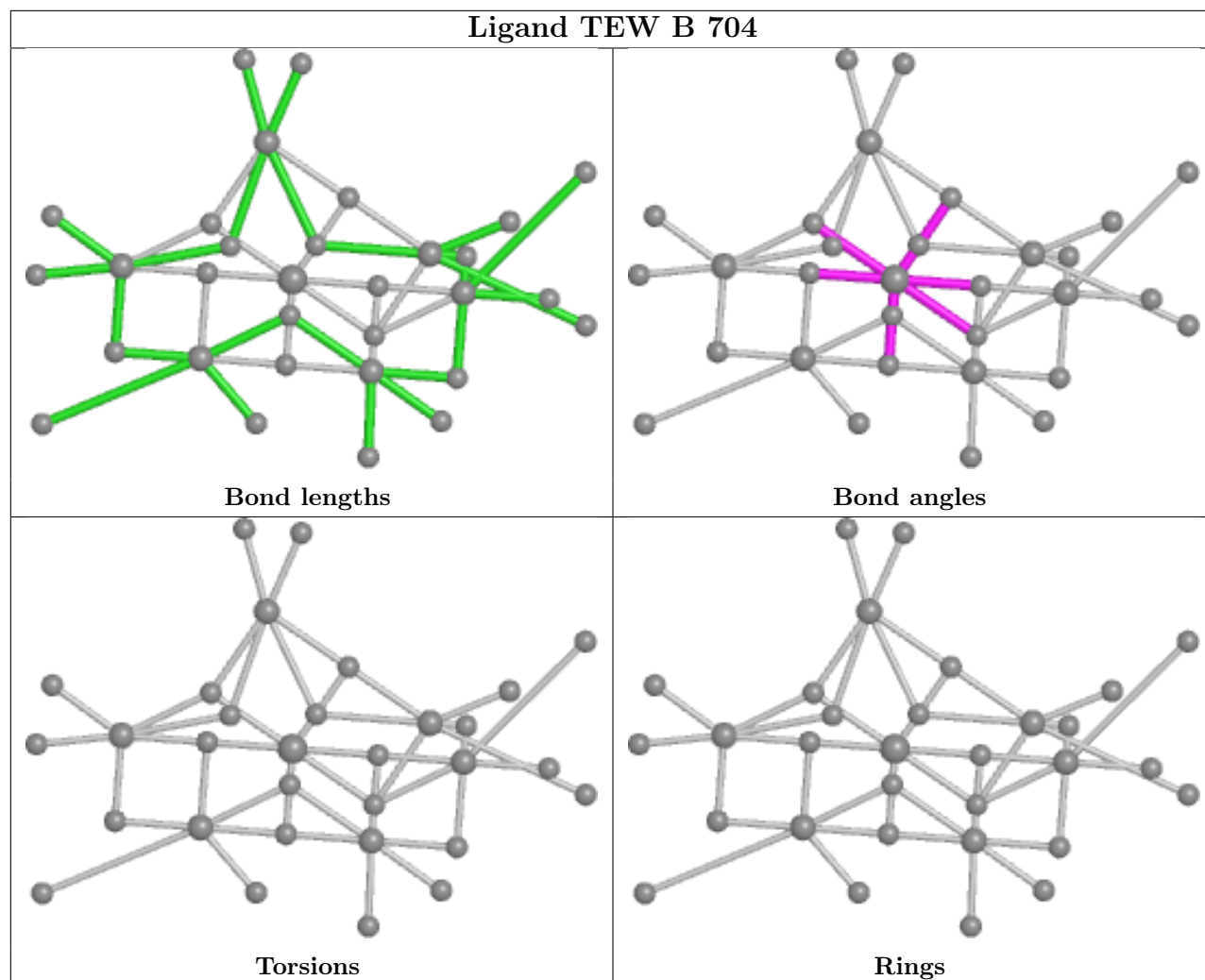
There are no ring outliers.

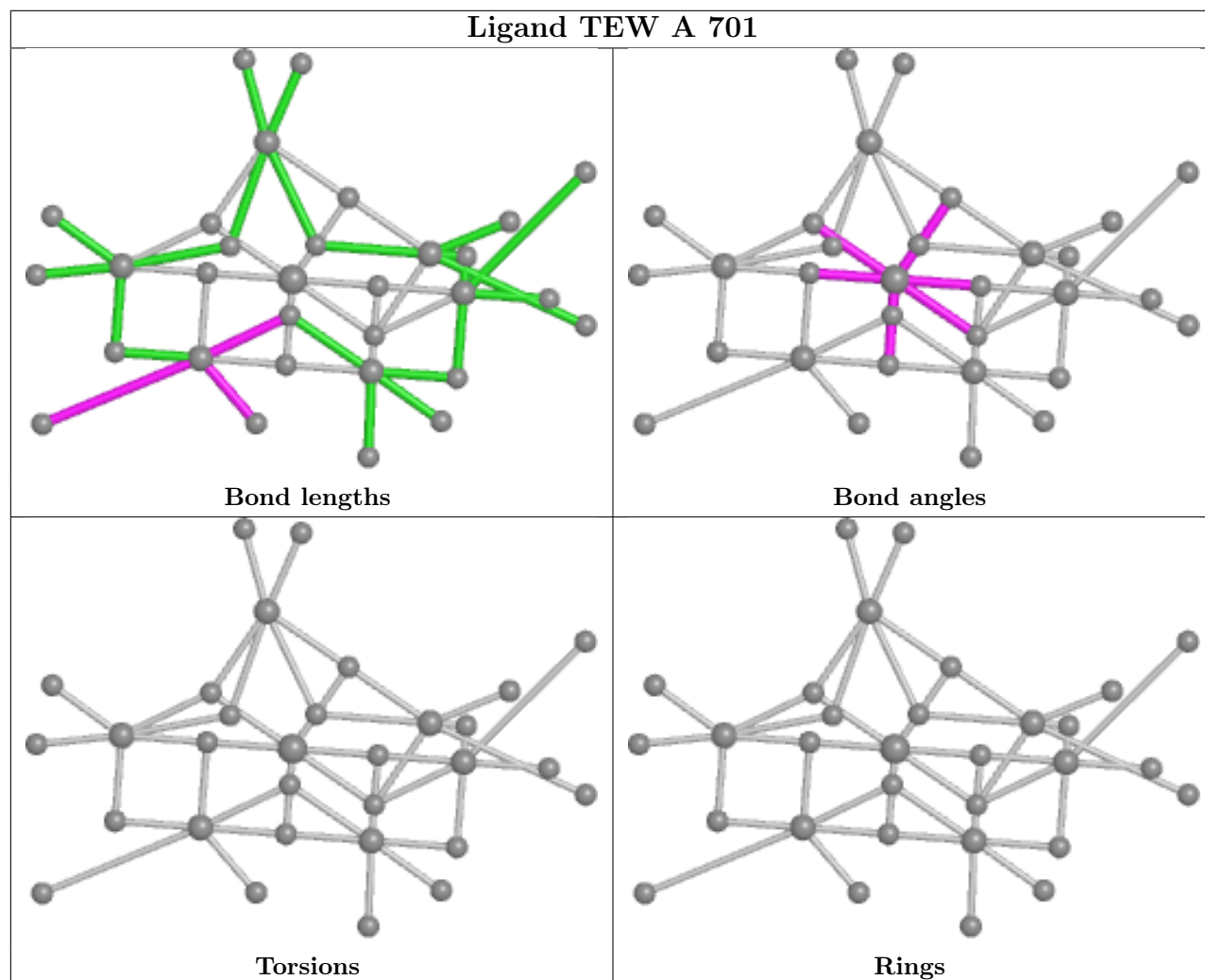
10 monomers are involved in 31 short contacts:

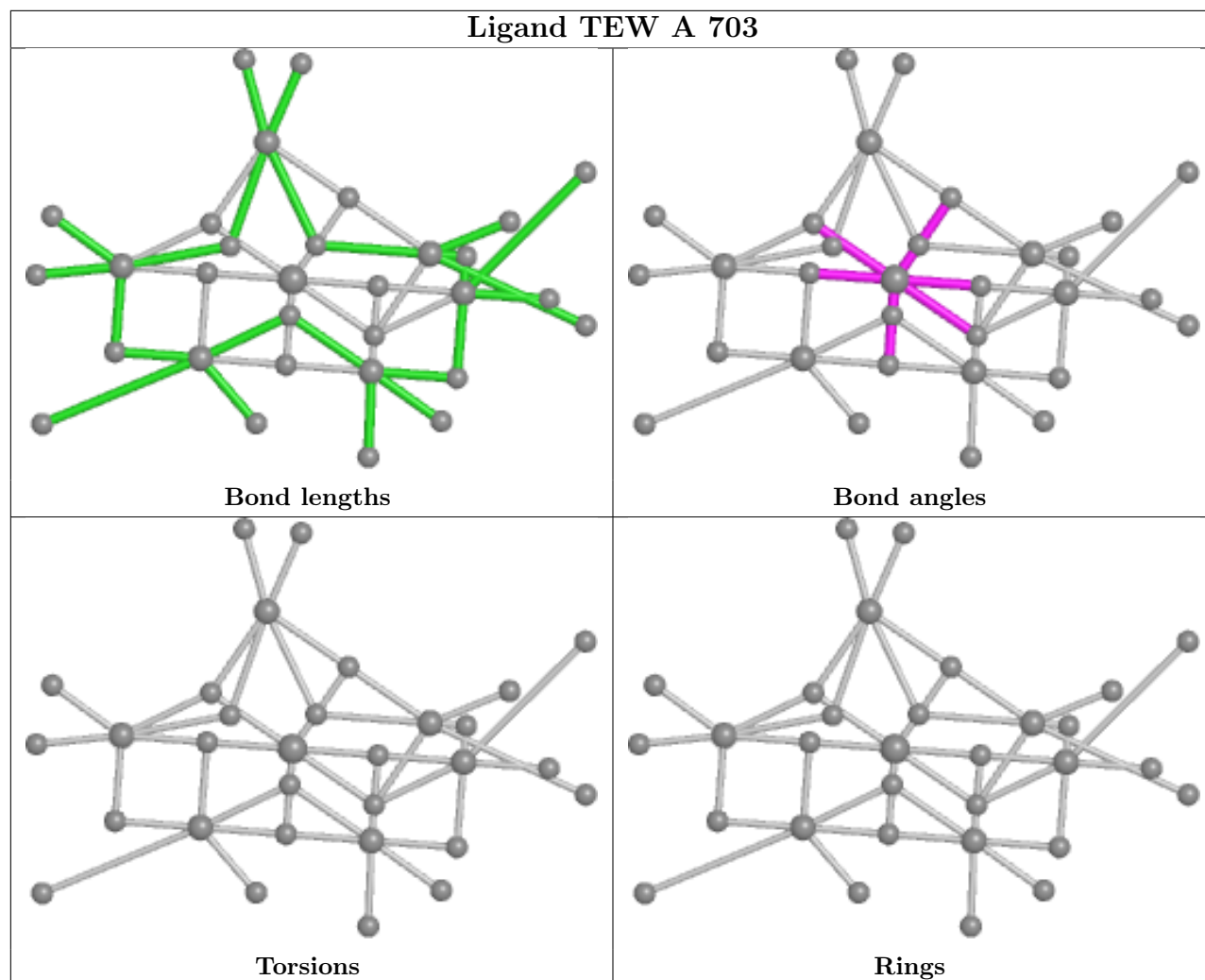
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	705	TEW	1	0
2	B	704	TEW	5	0
2	A	707	TEW	7	0
2	A	706	TEW	3	0
2	B	707	TEW	6	0
2	B	706	TEW	3	0
2	B	702	TEW	1	0
2	B	701	TEW	2	0
2	B	705	TEW	2	0
2	B	703	TEW	1	0

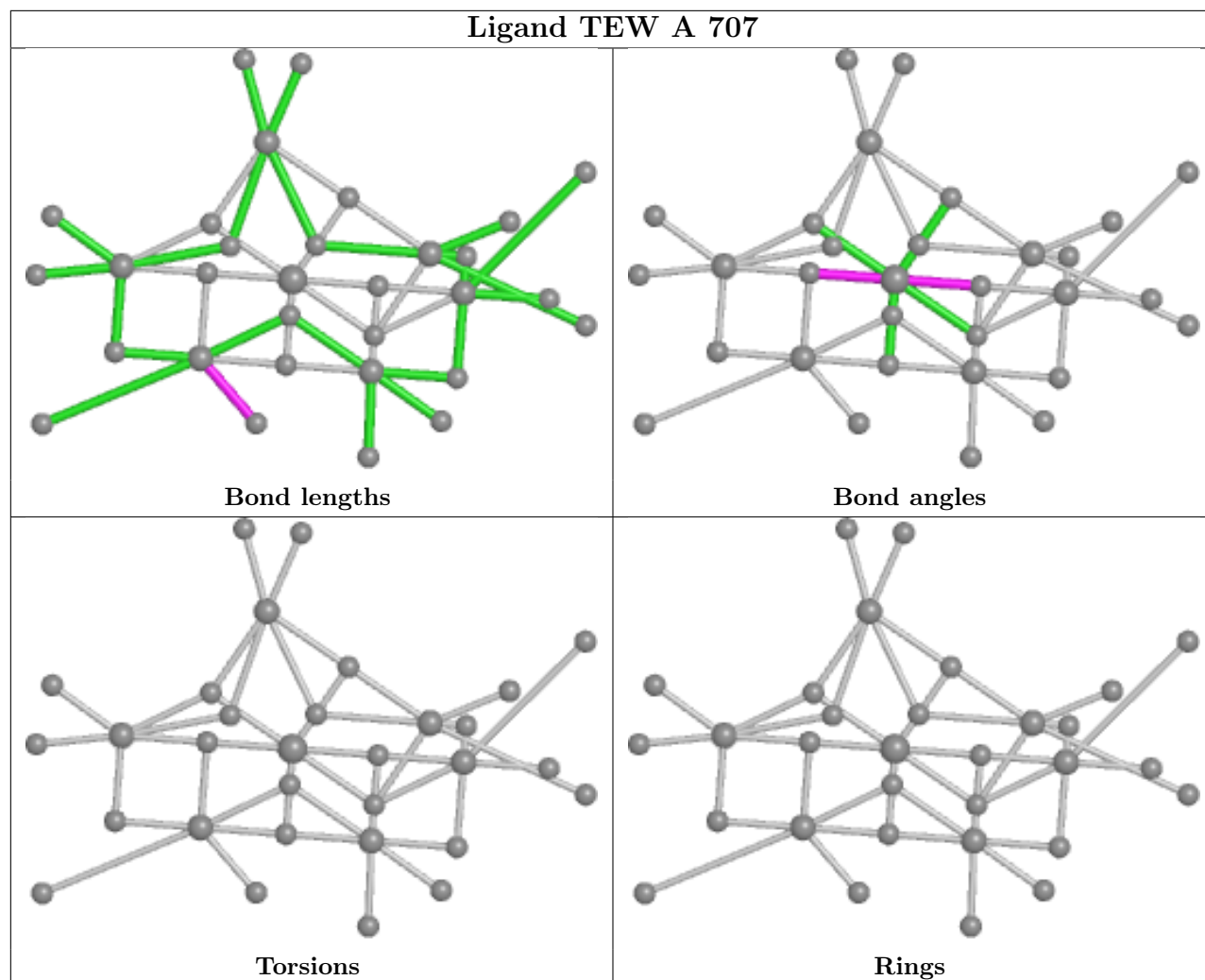
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

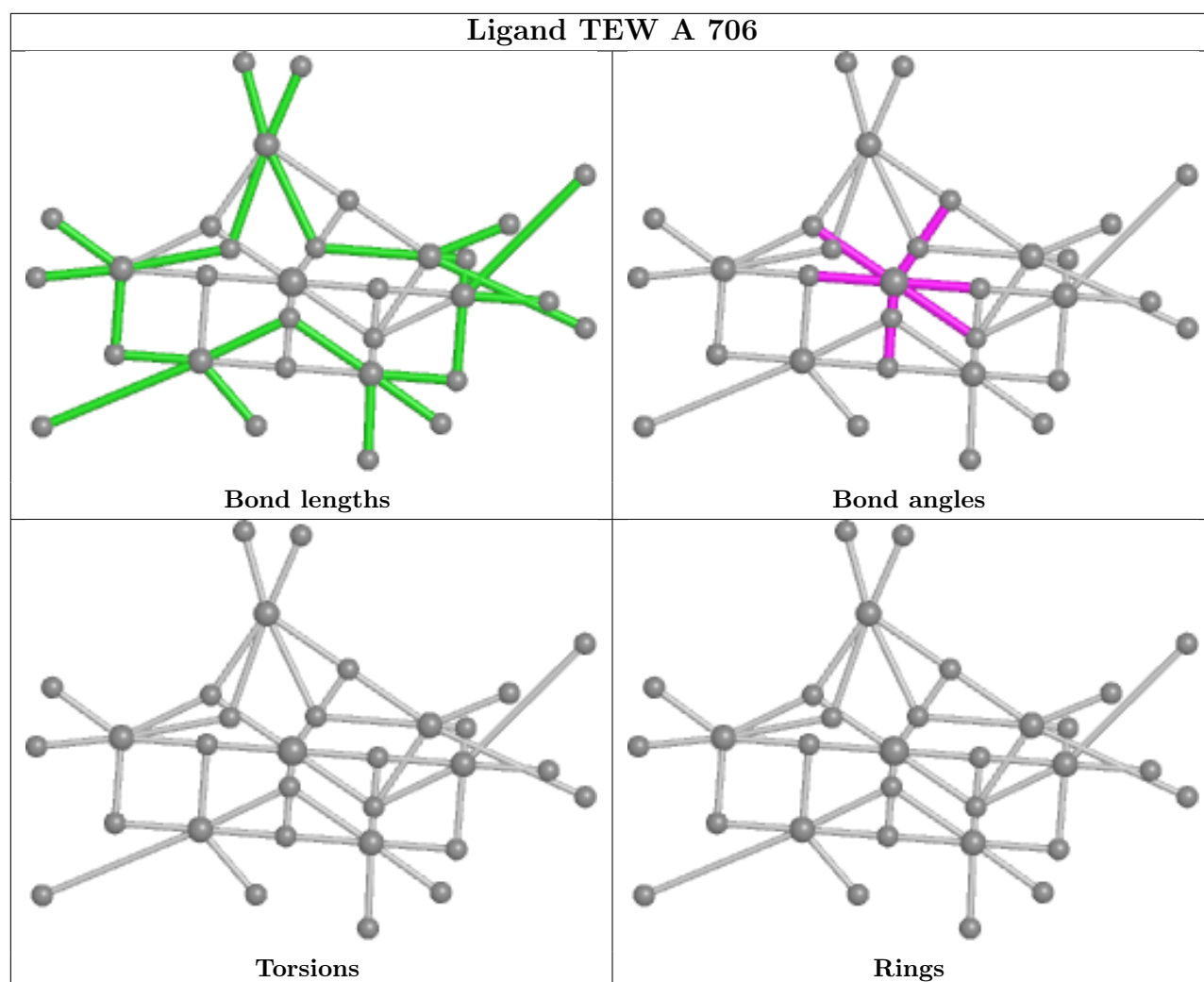


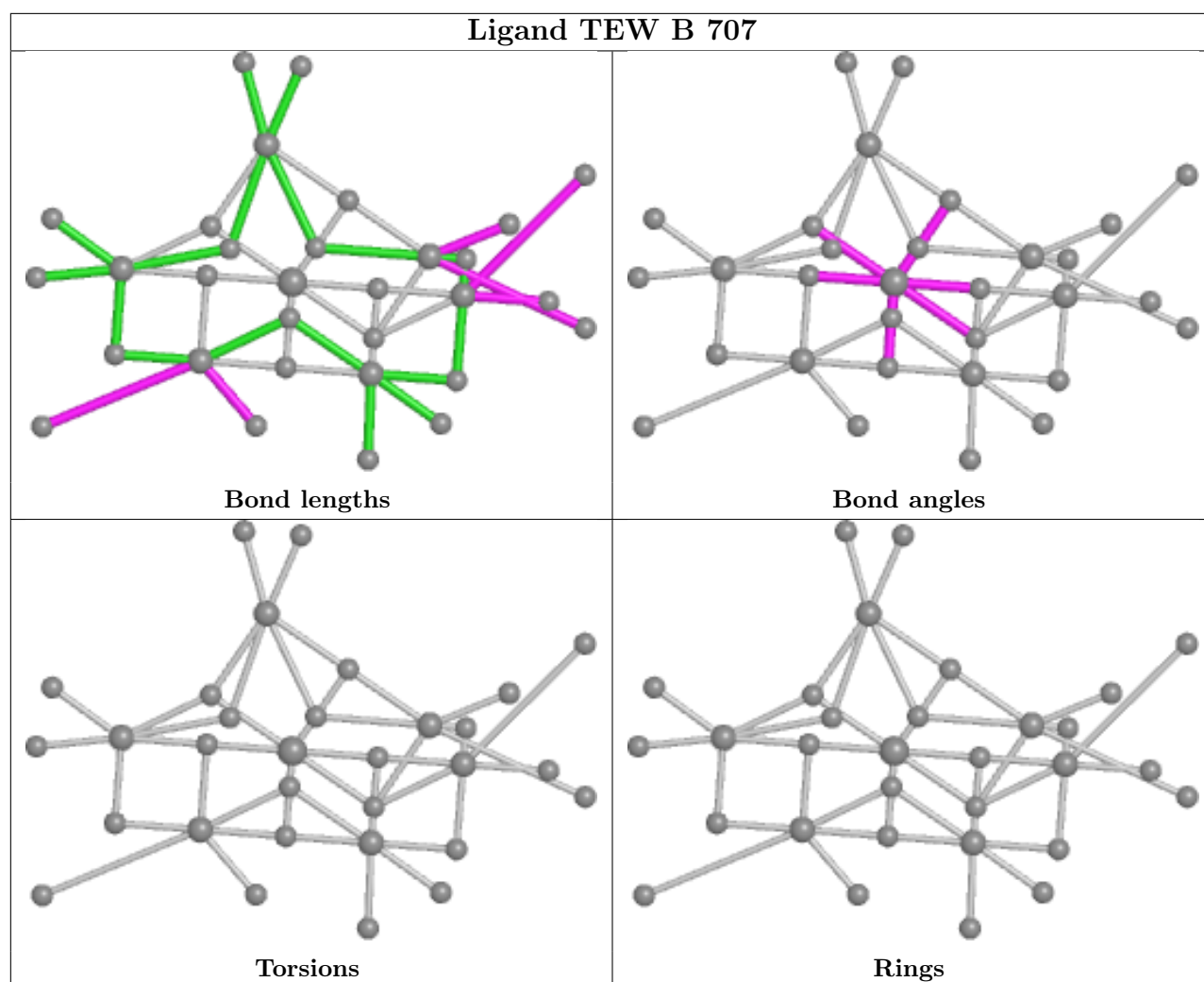


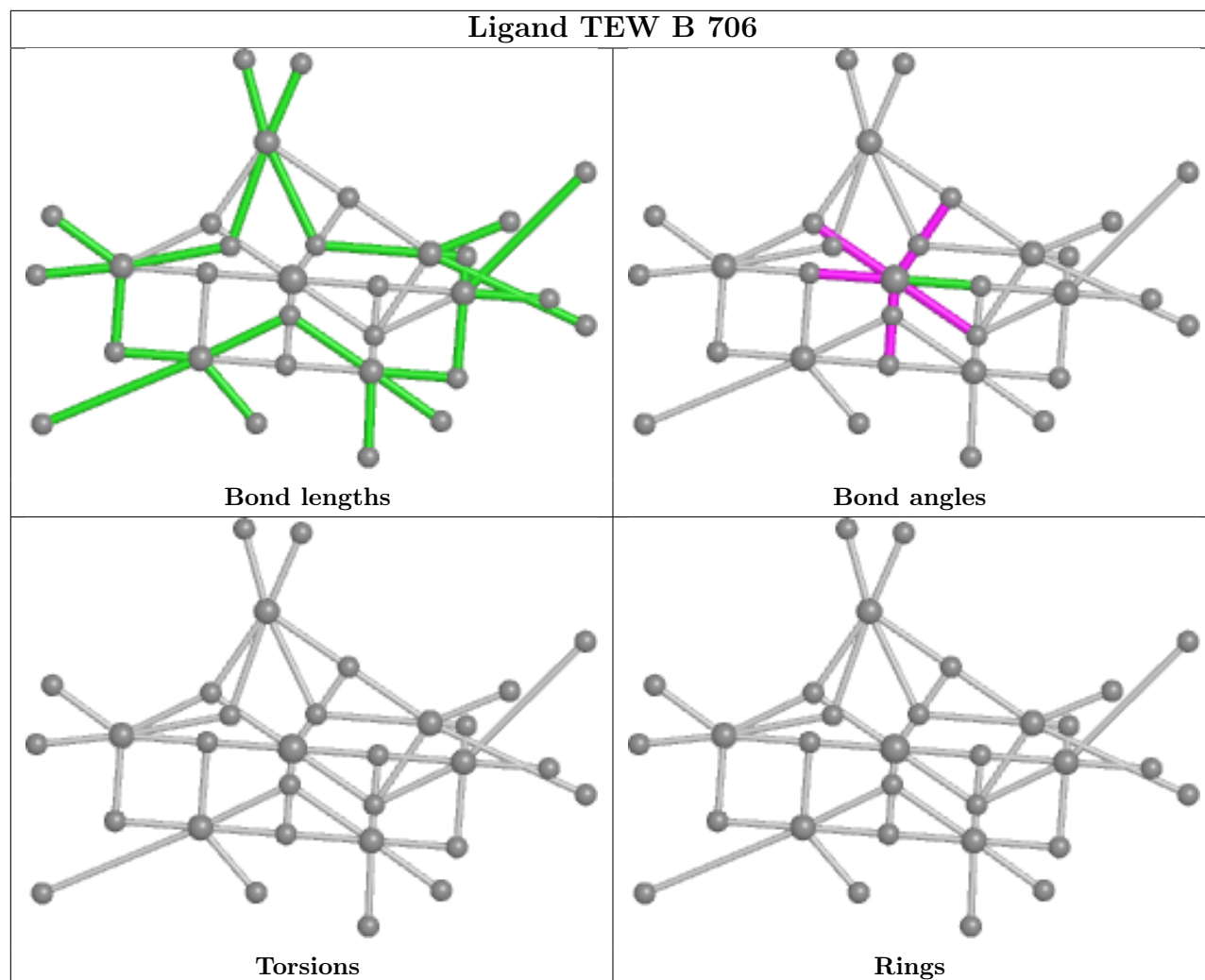


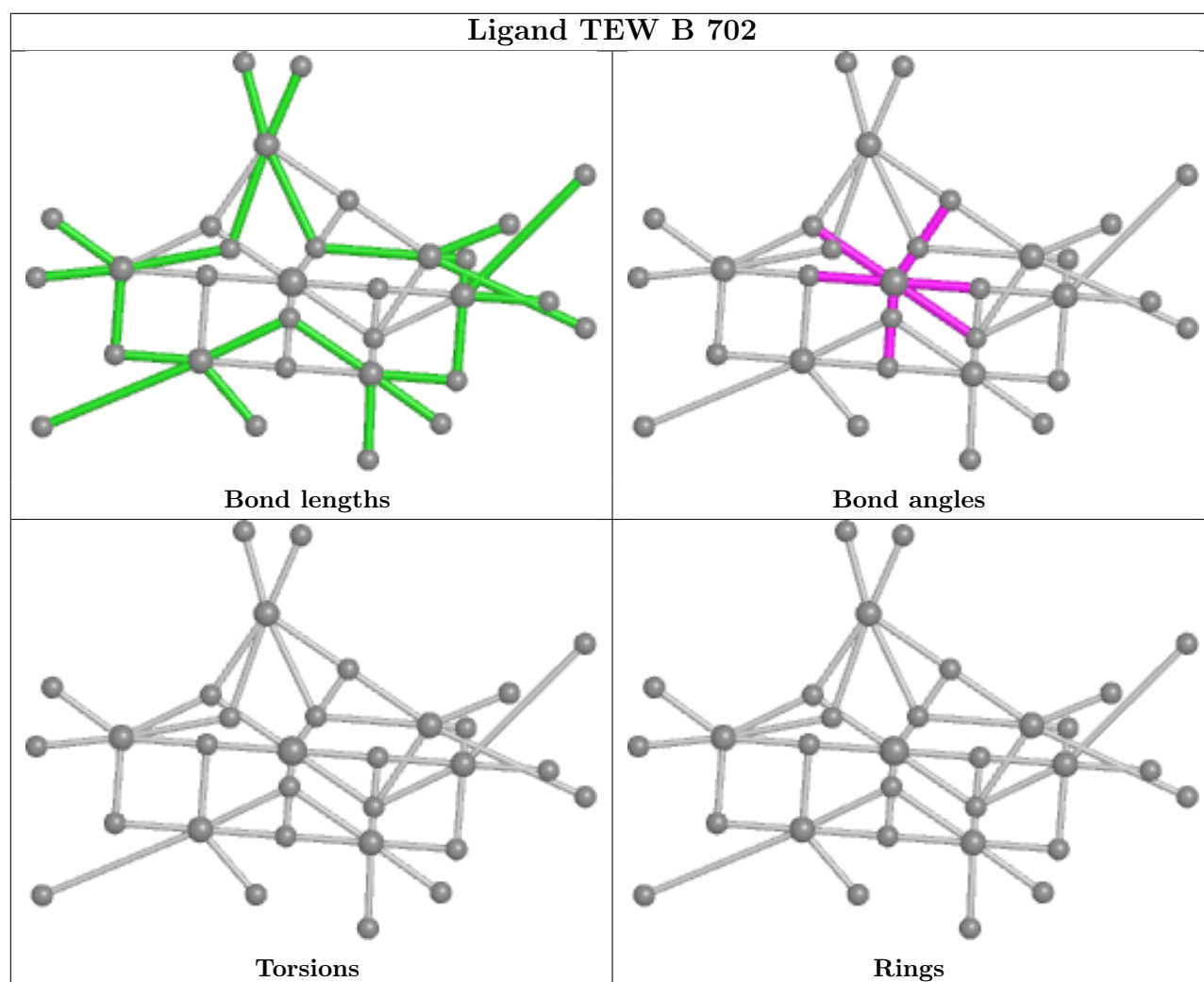


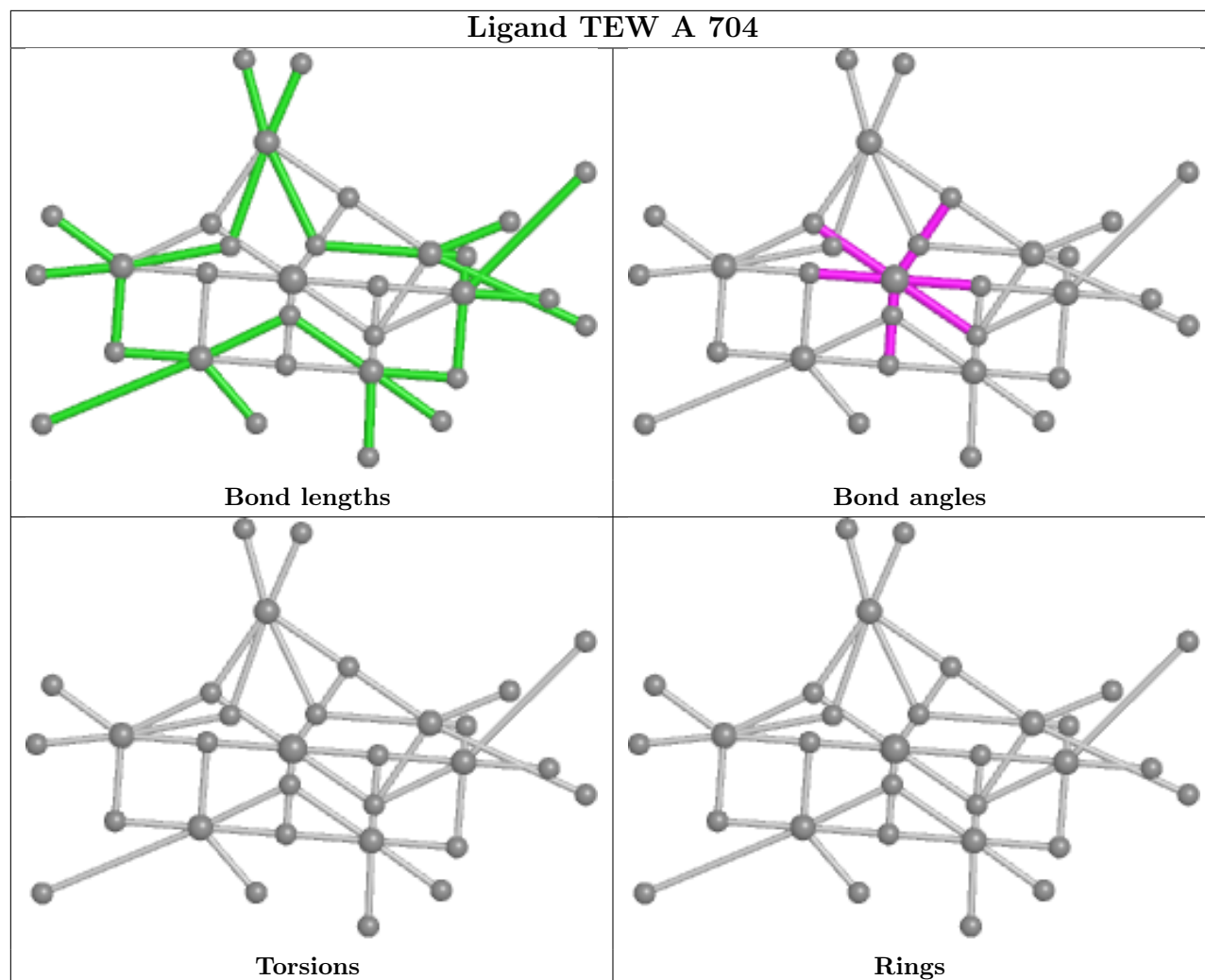


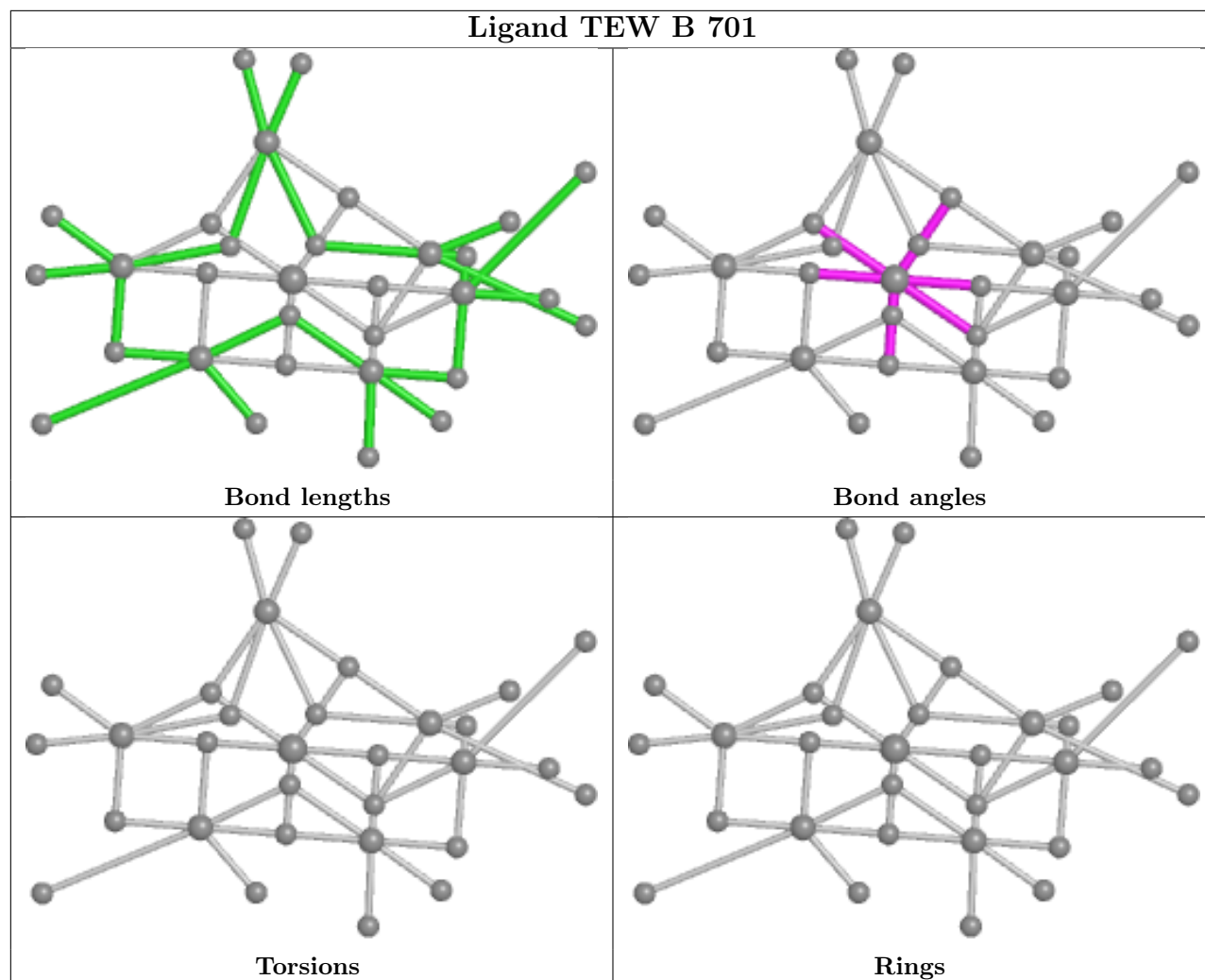


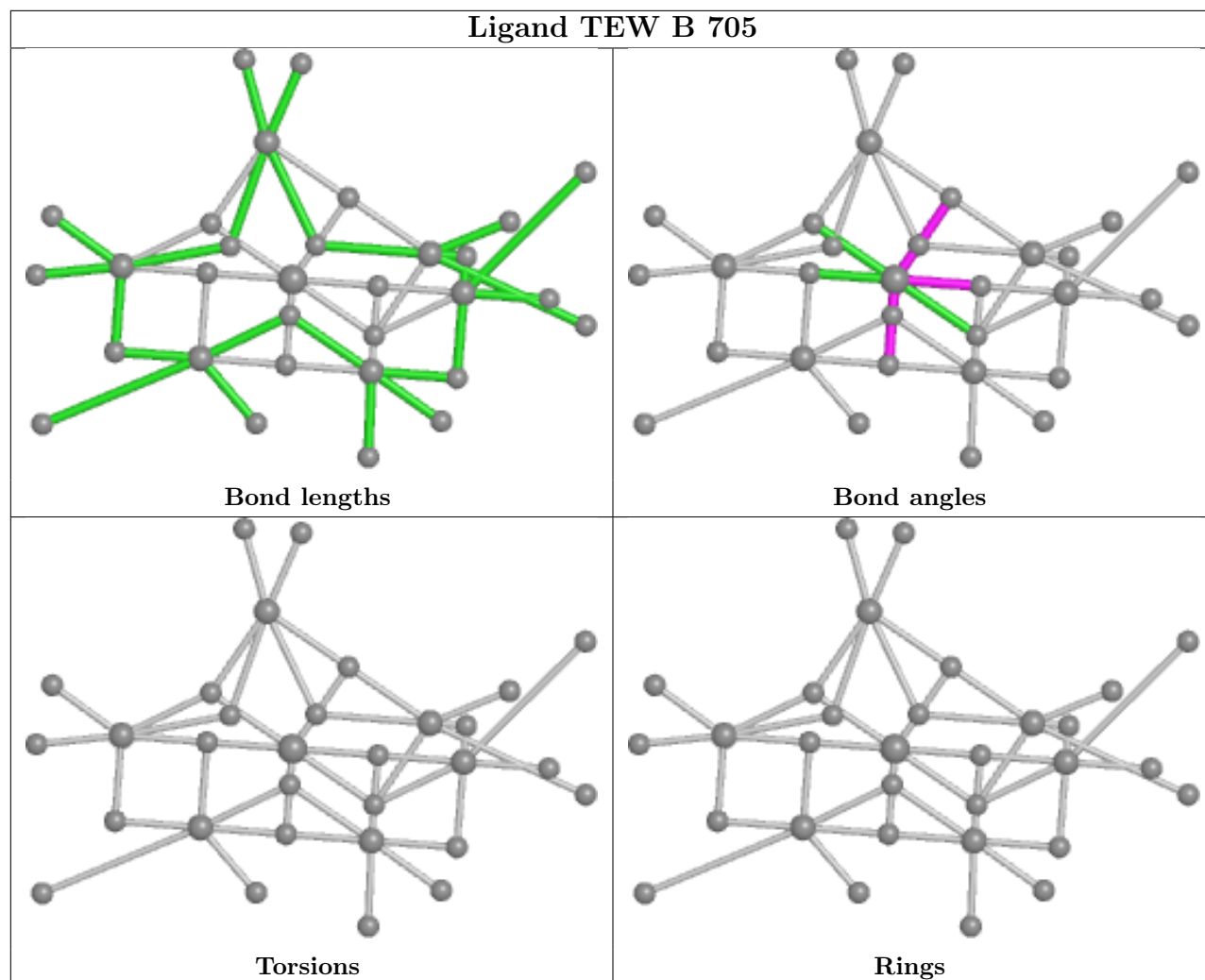


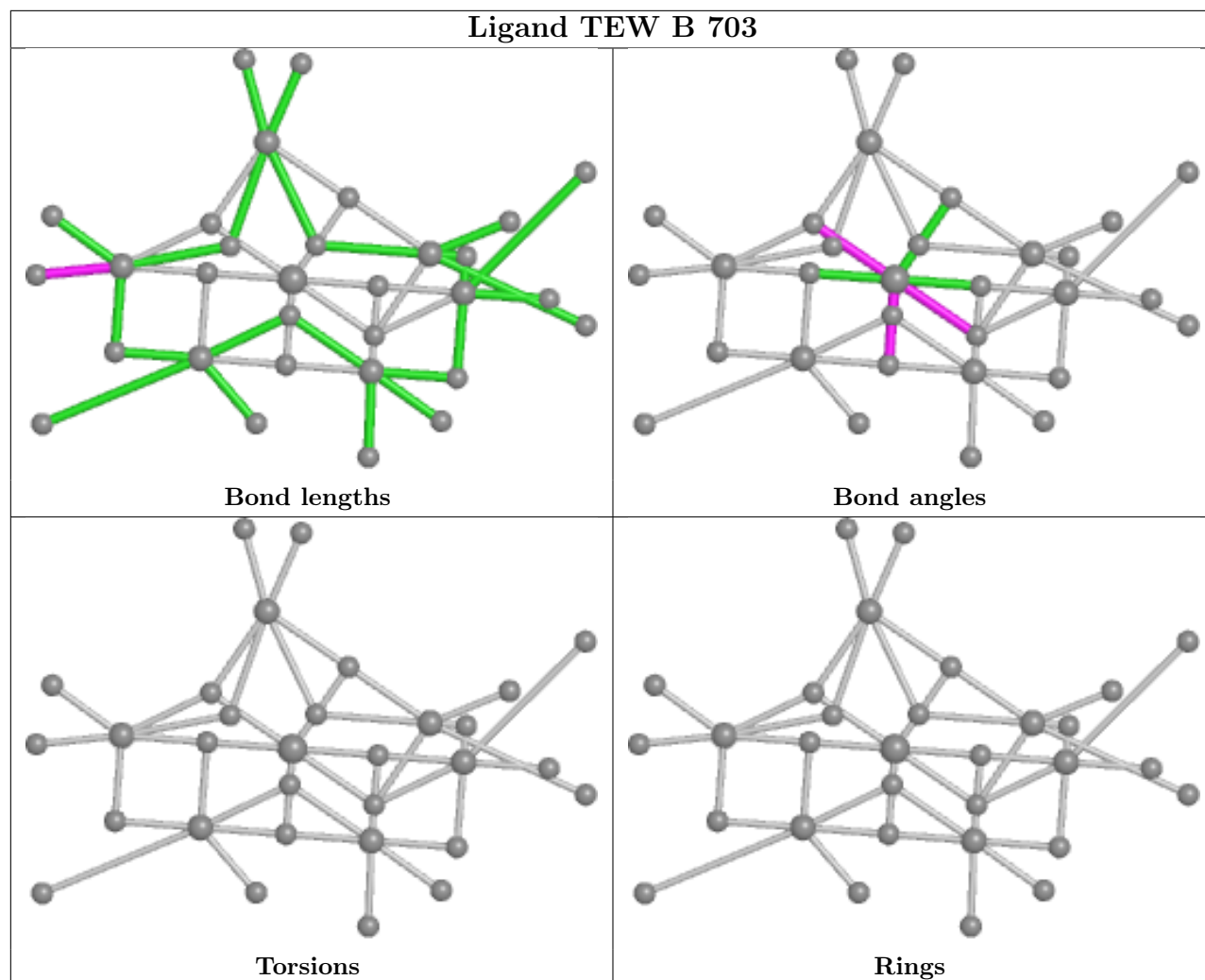


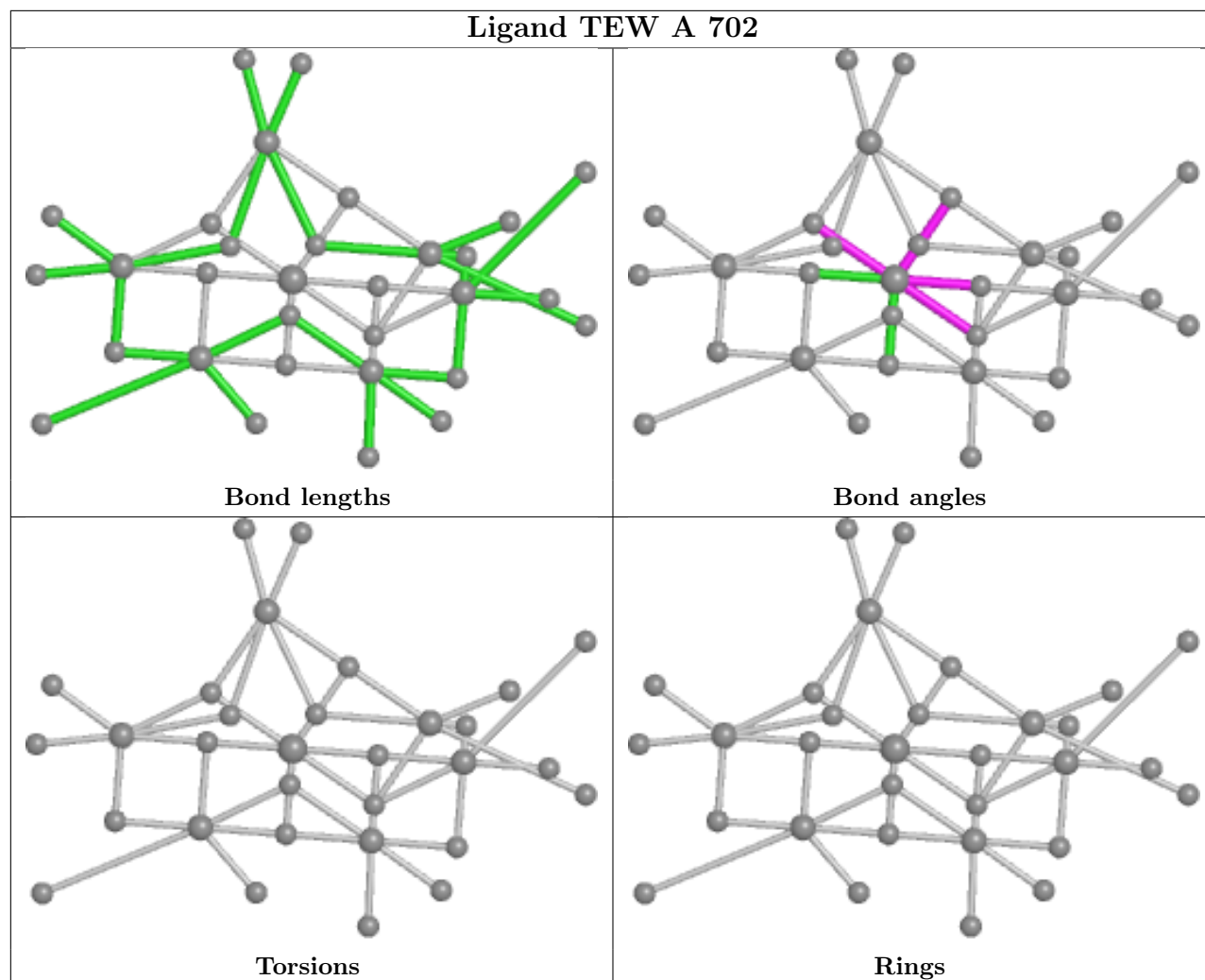












5.7 Other polymers [i](#)

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 [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	679/681 (99%)	0.11	3 (0%) 88 76	40, 109, 160, 189	3 (0%)
1	B	679/681 (99%)	0.13	15 (2%) 62 41	43, 106, 158, 203	1 (0%)
All	All	1358/1362 (99%)	0.12	18 (1%) 75 56	40, 108, 159, 203	4 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	THR	3.8
1	B	486	ILE	3.1
1	A	357	ASN	3.1
1	B	90	GLU	2.8
1	B	224	GLU	2.7
1	B	665	ASN	2.6
1	B	12	THR	2.5
1	B	9	THR	2.4
1	B	223	THR	2.3
1	B	382	PRO	2.3
1	B	37	GLU	2.3
1	B	464	ILE	2.2
1	A	649	LEU	2.2
1	B	13	PHE	2.1
1	B	135	VAL	2.1
1	B	57	ILE	2.1
1	B	399	ALA	2.1
1	B	8	GLU	2.1

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](#)

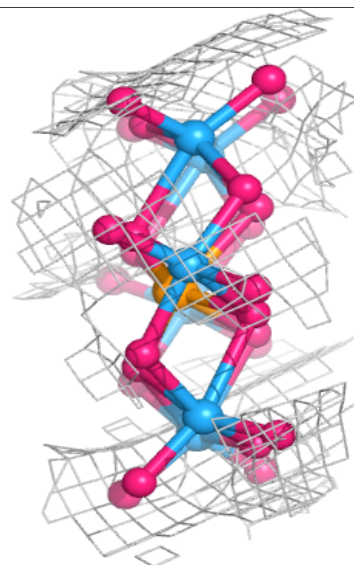
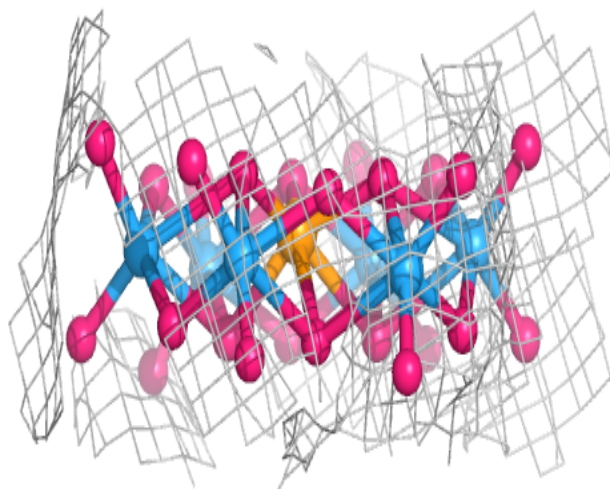
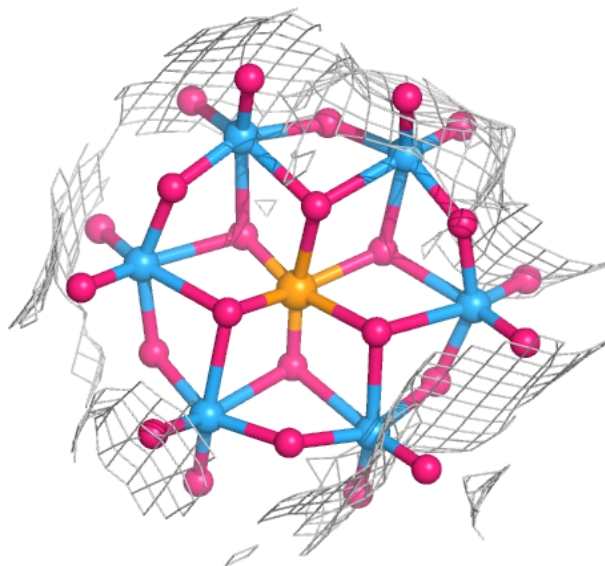
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	B	702	31/31	0.93	0.08	127,215,258,285	7
2	TEW	B	703	31/31	0.96	0.07	179,216,257,281	6
2	TEW	A	702	31/31	0.96	0.06	199,244,264,278	7
2	TEW	A	704	31/31	0.96	0.07	127,200,232,244	7
2	TEW	A	703	31/31	0.97	0.06	127,242,278,310	6
2	TEW	B	706	31/31	0.97	0.06	258,302,325,328	4
2	TEW	A	707	31/31	0.97	0.06	162,193,210,226	7
2	TEW	A	706	31/31	0.98	0.06	173,203,226,251	4
2	TEW	B	705	31/31	0.99	0.04	157,171,193,205	1
2	TEW	B	701	31/31	0.99	0.04	127,206,222,238	1
2	TEW	A	705	31/31	0.99	0.04	127,173,202,213	1
2	TEW	A	701	31/31	0.99	0.05	76,168,189,202	5
2	TEW	B	704	31/31	0.99	0.04	127,217,238,262	4
2	TEW	B	707	31/31	1.00	0.03	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.

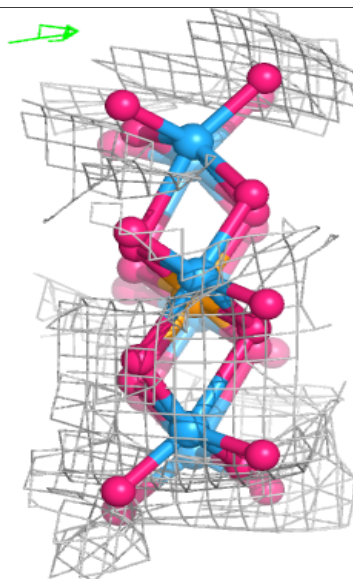
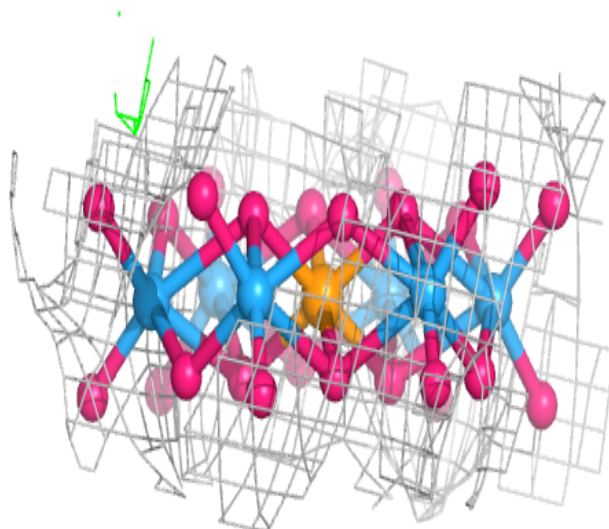
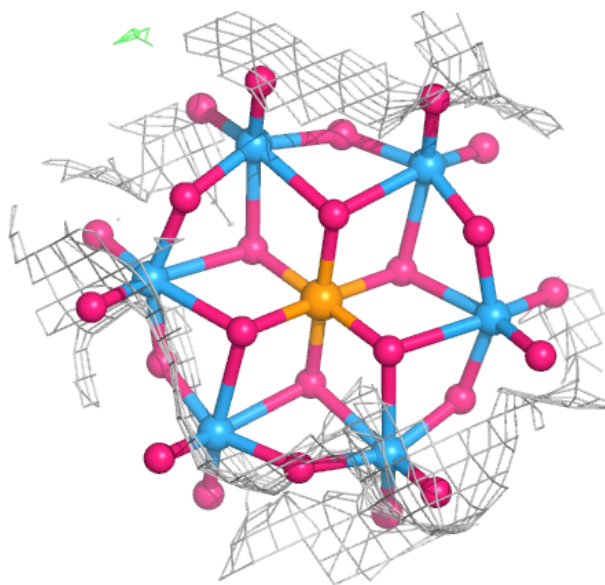
Electron density around TEW B 702:

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



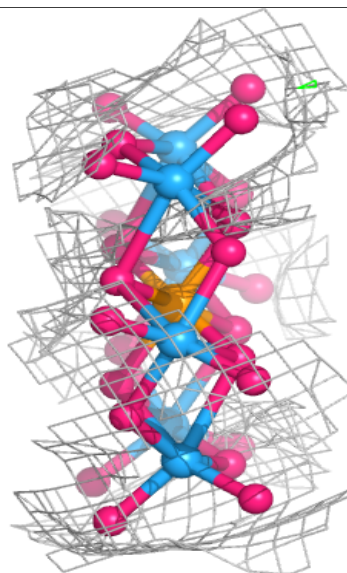
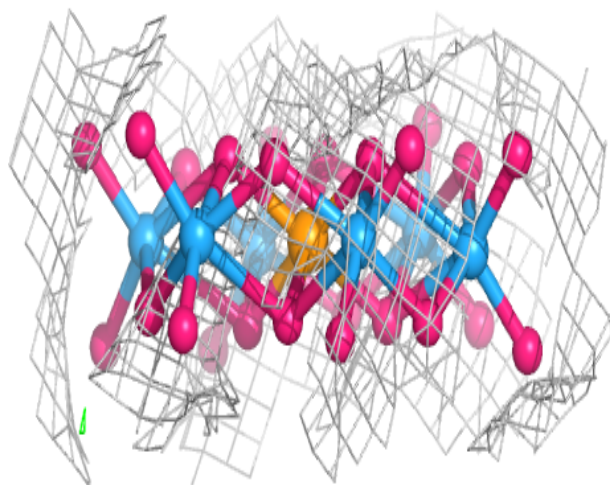
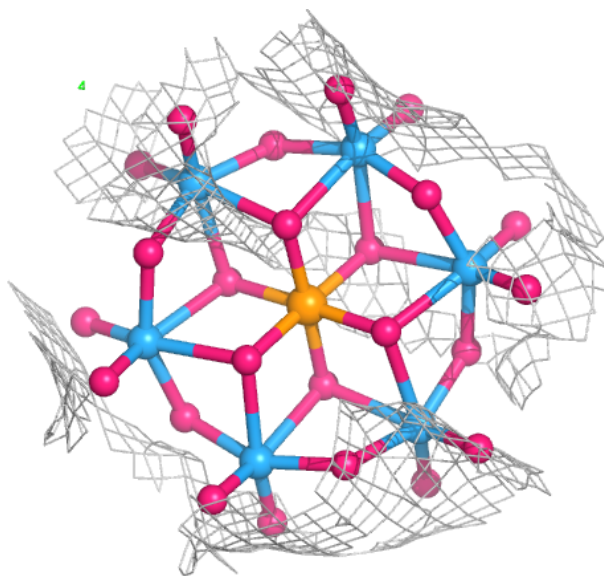
Electron density around TEW B 703:

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



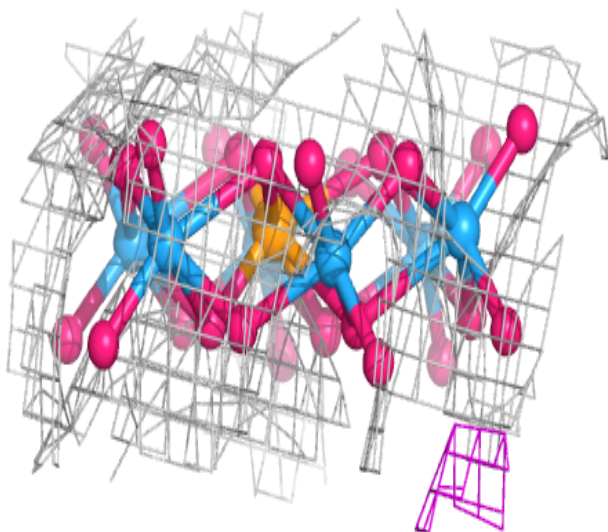
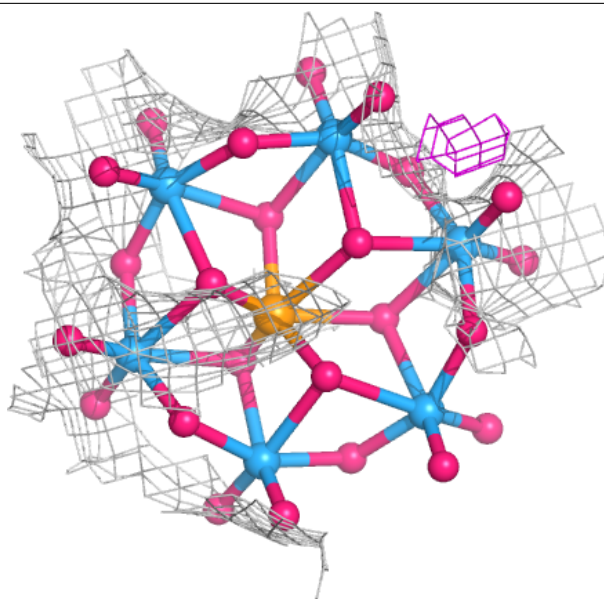
Electron density around TEW A 702:

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



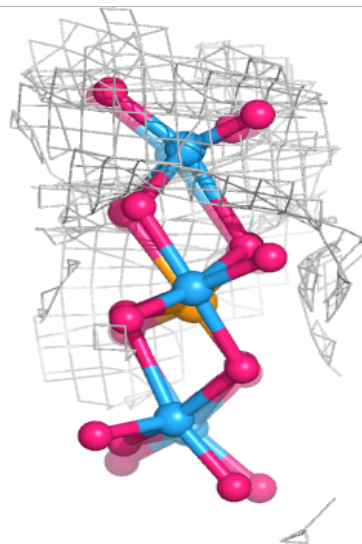
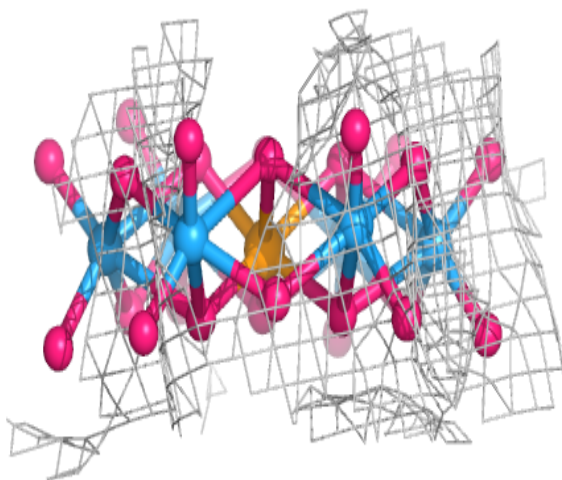
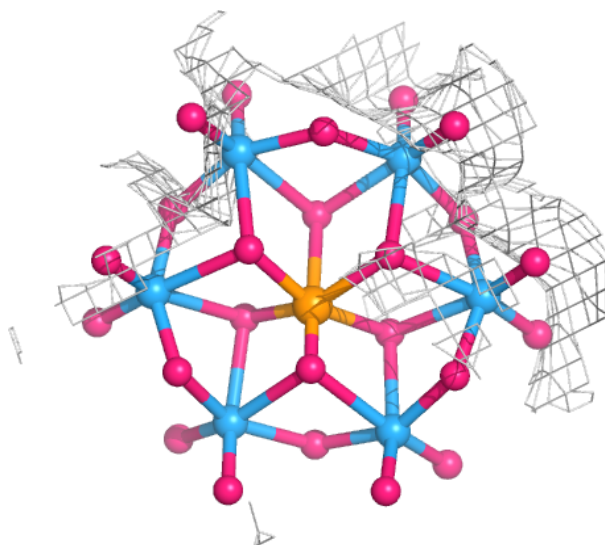
Electron density around TEW A 704:

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



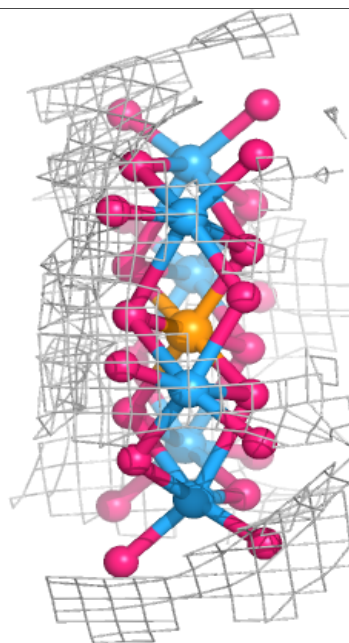
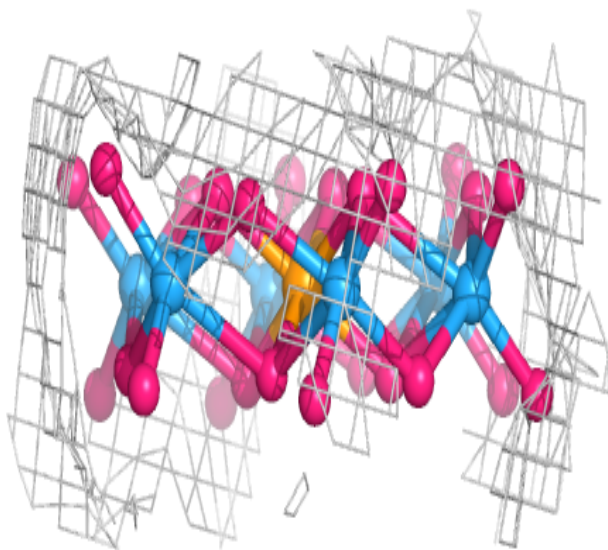
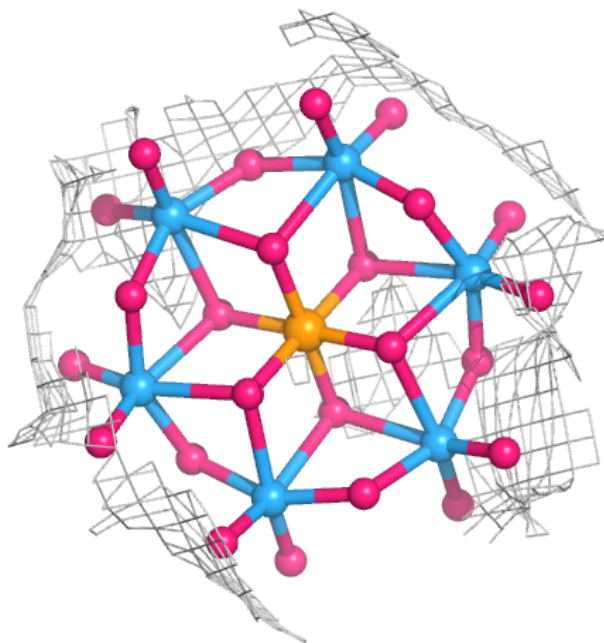
Electron density around TEW A 703:

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



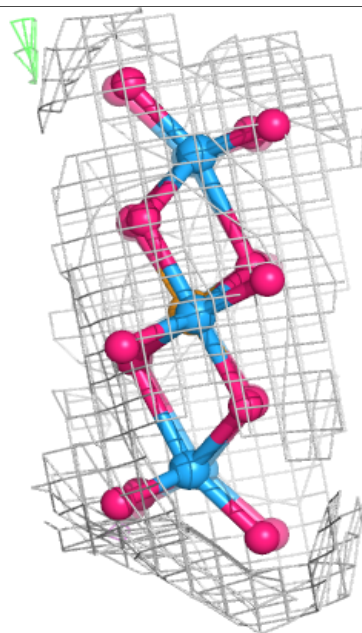
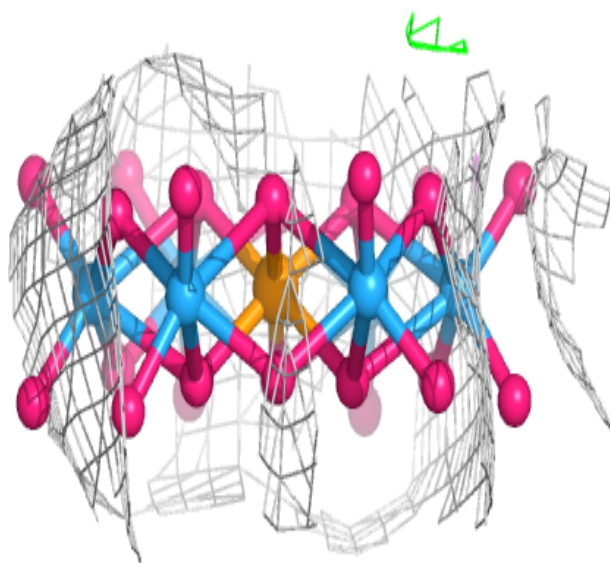
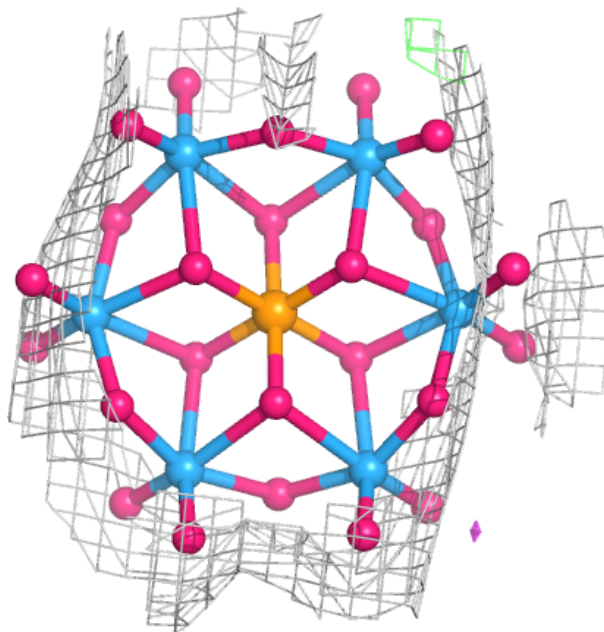
Electron density around TEW B 706:

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



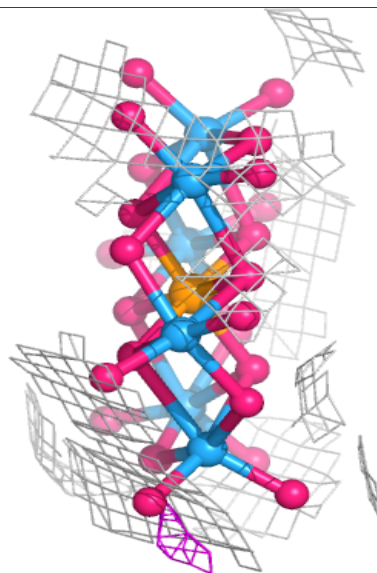
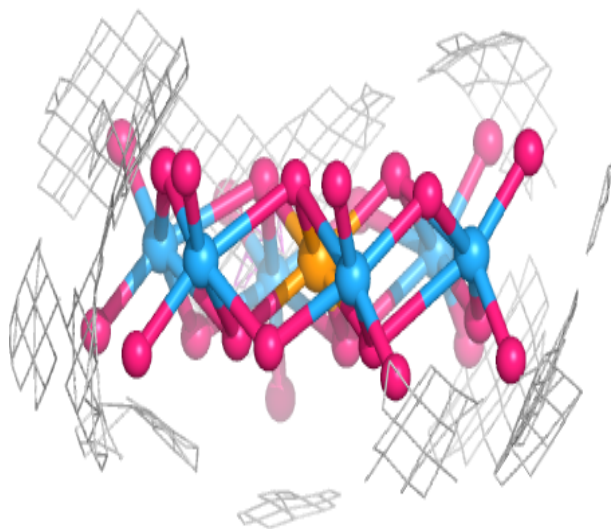
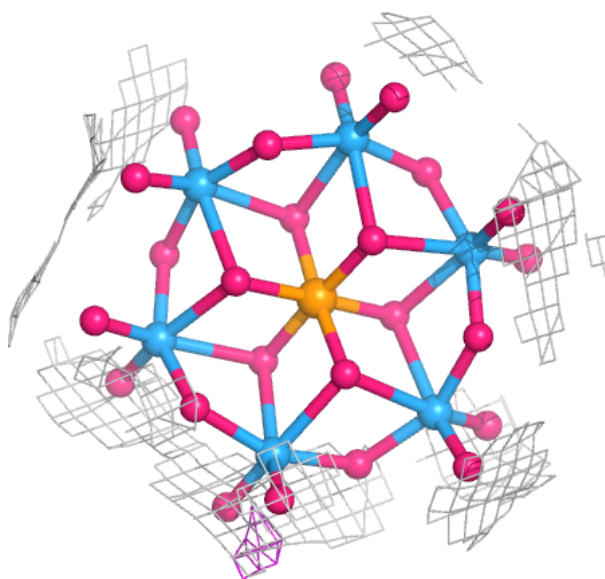
Electron density around TEW A 707:

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



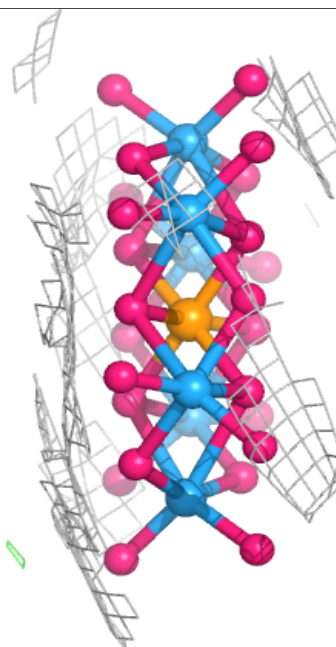
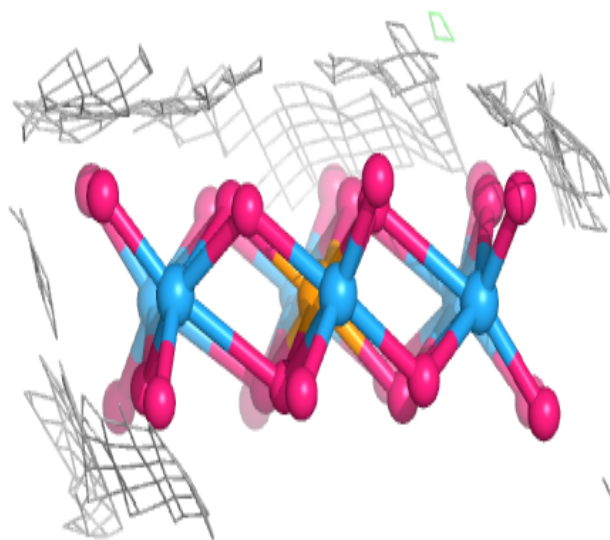
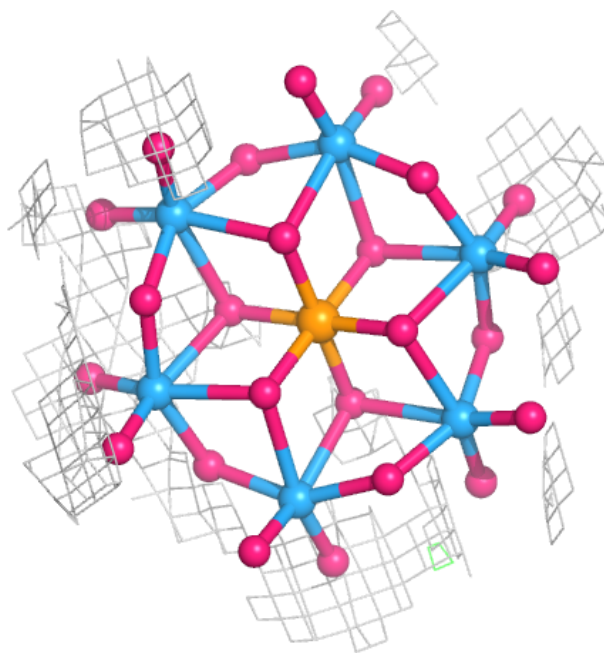
Electron density around TEW A 706:

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and green (positive)



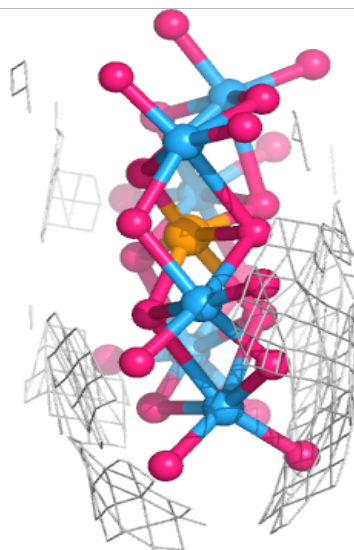
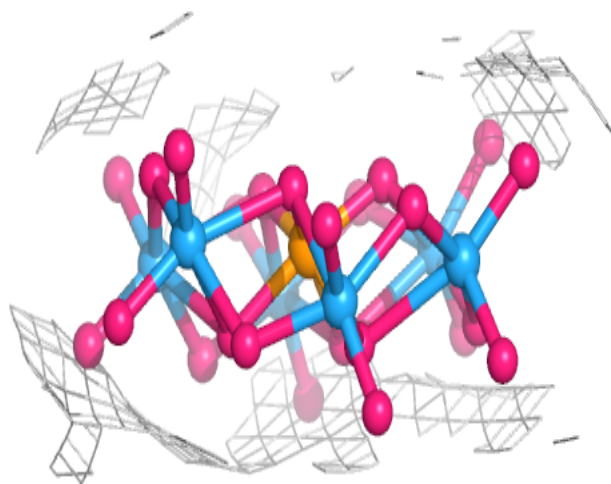
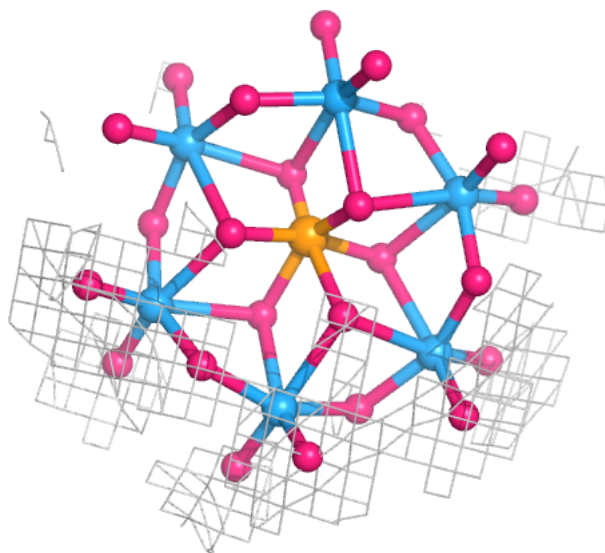
Electron density around TEW B 705:

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and green (positive)



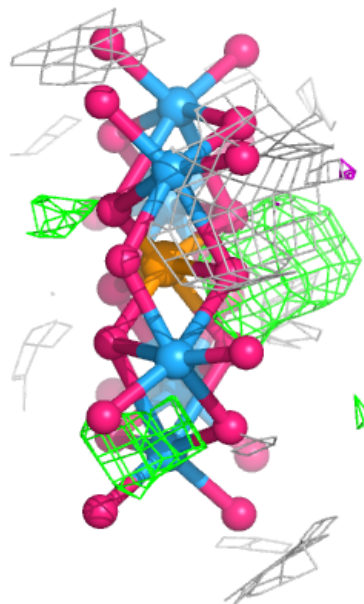
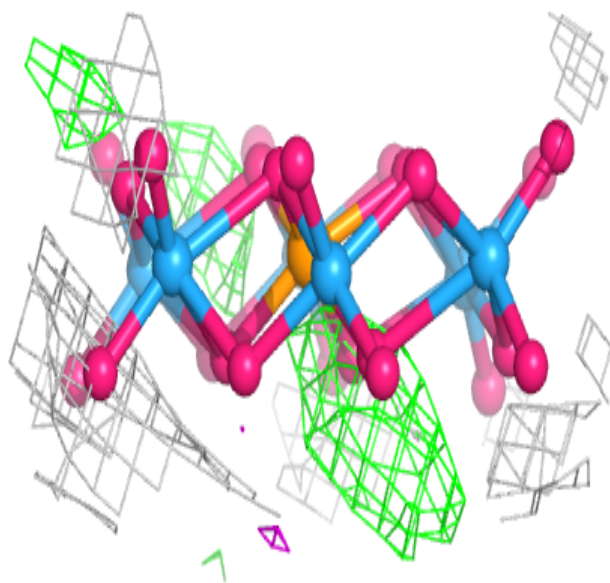
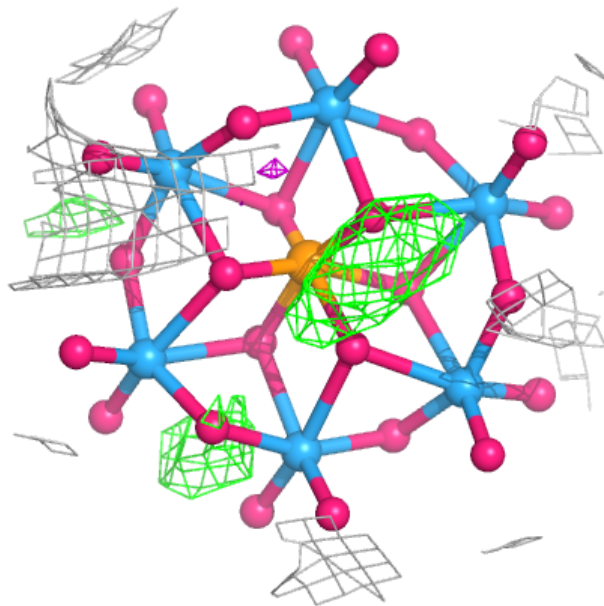
Electron density around TEW B 701:

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



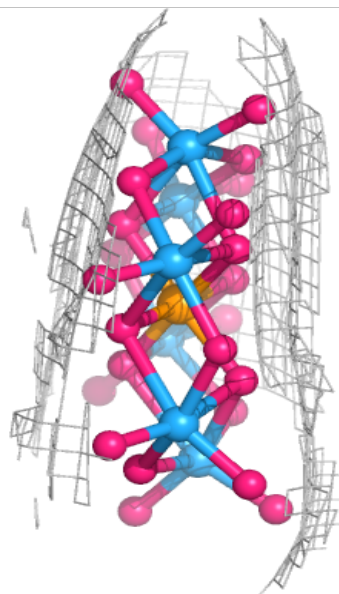
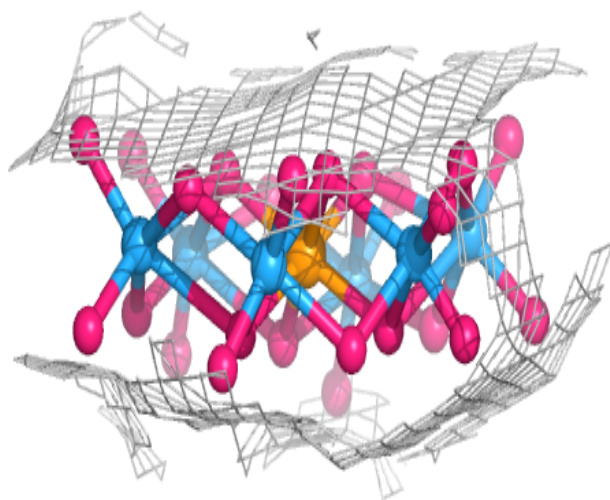
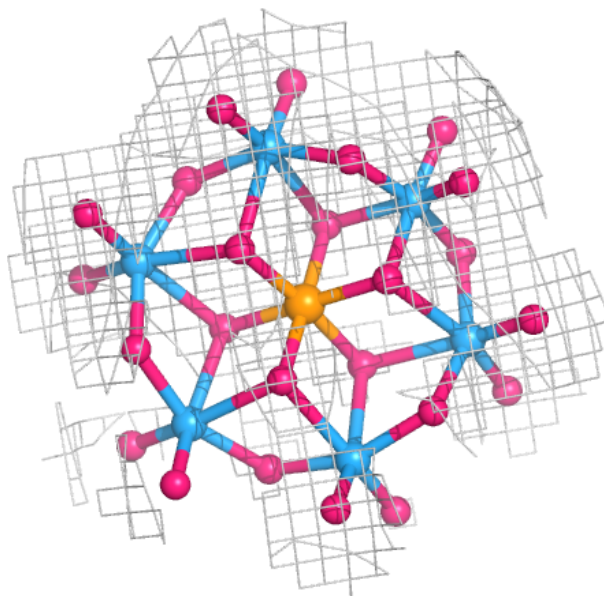
Electron density around TEW A 705:

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



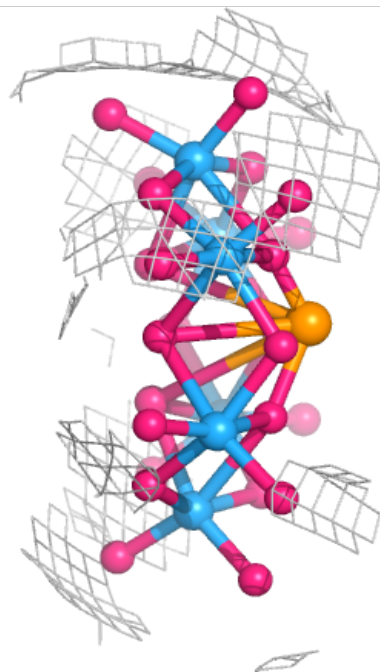
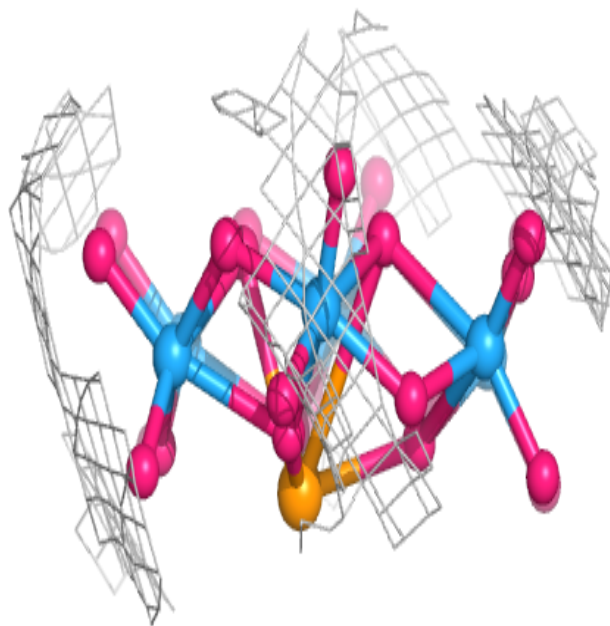
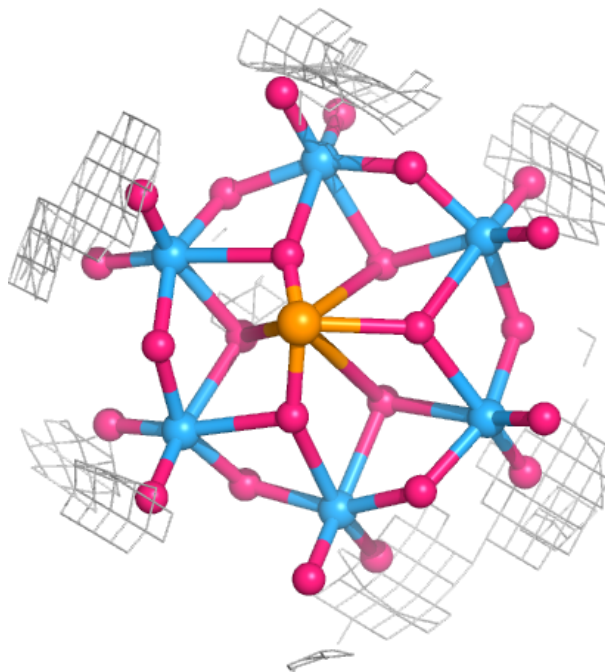
Electron density around TEW A 701:

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



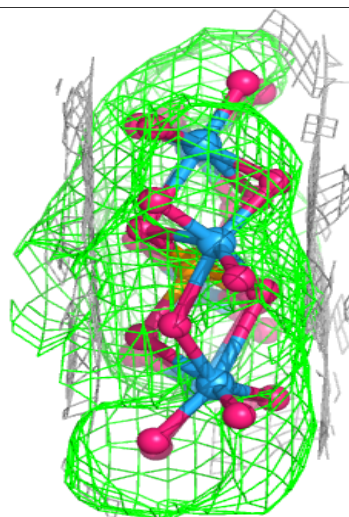
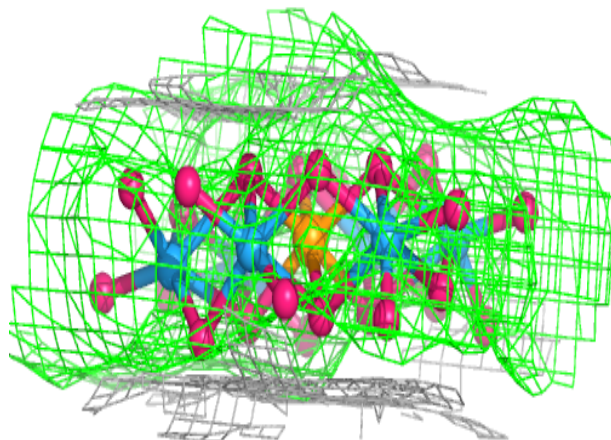
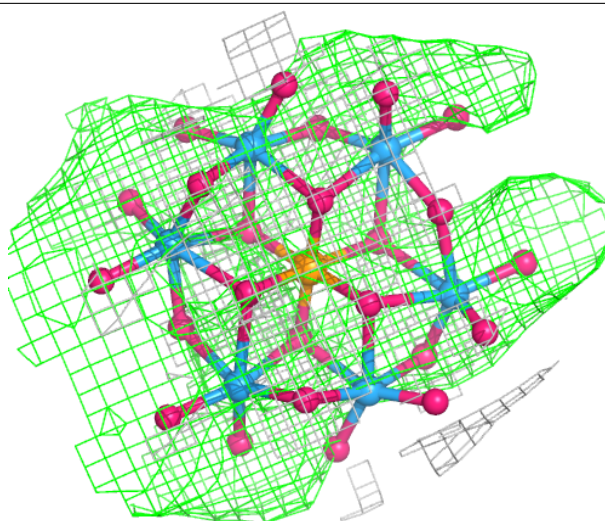
Electron density around TEW B 704:

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



Electron density around TEW B 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 [i](#)

There are no such residues in this entry.