



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 22, 2026 – 07:29 pm BST

PDB ID : 9SQ3 / pdb_00009sq3
Title : Crystal structure of the Molybdenum-containing nitrogenase from Methanocaldococcus infernus refined to 1.21 Å resolution - crystalline form B.
Authors : Maslac, N.; Torer, M.R.; Bolte, P.; Wagner, T.
Deposited on : 2025-09-19
Resolution : 1.21 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

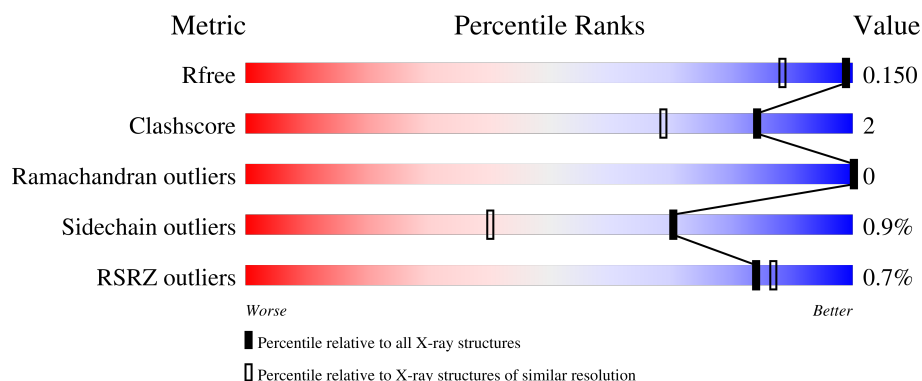
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.21 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	2002 (1.24-1.20)
Clashscore	190562	2061 (1.24-1.20)
Ramachandran outliers	187476	2009 (1.24-1.20)
Sidechain outliers	187428	2008 (1.24-1.20)
RSRZ outliers	180081	2000 (1.24-1.20)

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	477	% 94% 5% .
1	C	477	94% 5% .
2	B	462	% 92% 7%
2	D	462	% 92% 7% .

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.

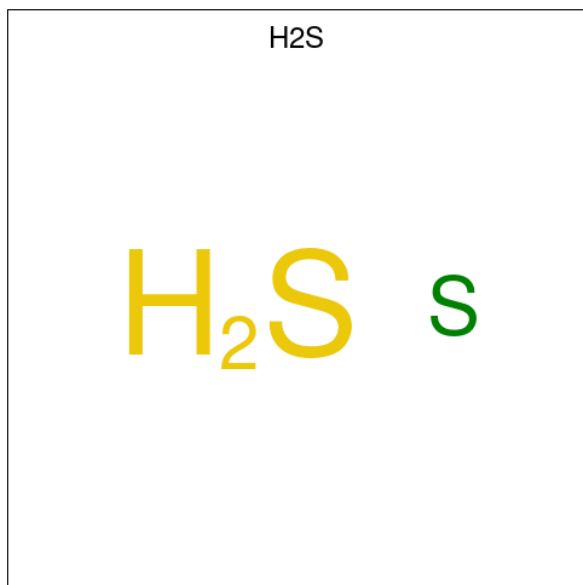
- Molecule 2 is a protein called Nitrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	461	Total 7683	C 2457	H 3857	N 641	O 708	S 20	0	41	0
2	D	461	Total 7645	C 2445	H 3844	N 636	O 700	S 20	0	37	0

-
- Chemical structure of HCA (3-Hydroxybutyrate) showing atom labels:
- Carbons: C1, C2, C3(R), C4, C5, C6, C7
 - Oxygens: O1, O2, O3, O4, O5, O6, O7
- The structure illustrates the 3D arrangement of atoms, with C3(R) indicating a chiral center. The hydroxyl group (OH) is attached to C3(R) with a dashed bond, indicating its orientation in space.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			20	7	6	7		
3	C	1	Total	C	H	O	0	0
			20	7	6	7		

- Molecule 4 is HYDROSULFURIC ACID (CCD ID: H2S) (formula: H₂S) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



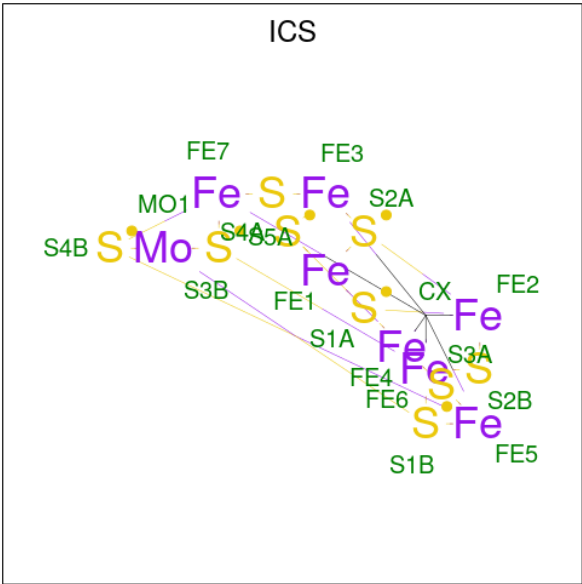
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	A	1	Total	C	H	O	0	1
			14	3	8	3		
5	B	1	Total	C	H	O	0	0
			14	3	8	3		
5	B	1	Total	C	H	O	0	0
			14	3	8	3		
5	C	1	Total	C	H	O	0	0
			14	3	8	3		
5	C	1	Total	C	H	O	0	0
			14	3	8	3		
5	D	1	Total	C	H	O	0	0
			14	3	8	3		
5	D	1	Total	C	H	O	0	0
			14	3	8	3		
5	D	1	Total	C	H	O	0	0
			14	3	8	3		

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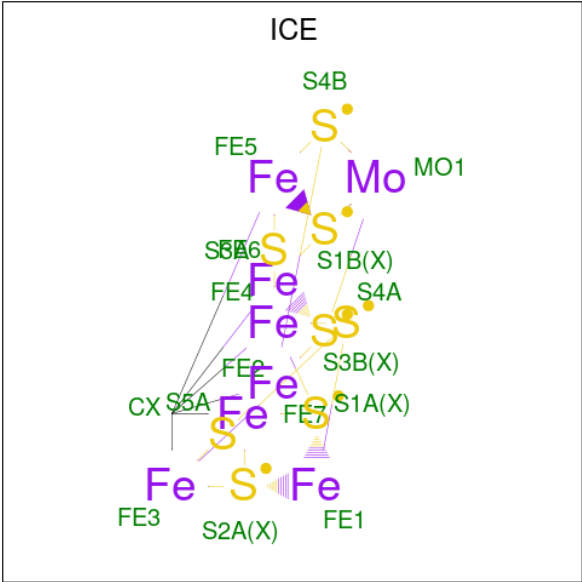
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	H	O	0	0
			14	3	8	3		
5	D	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 6 is iron-sulfur-molybdenum cluster with interstitial carbon (CCD ID: ICS) (formula: CFe₇MoS₉) (labeled as "Ligand of Interest" by depositor).



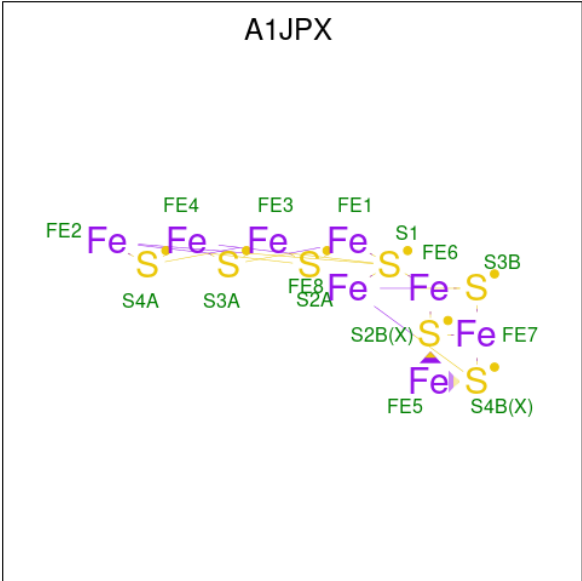
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Fe	Mo	S	0	1
			18	1	7	1	9		
6	C	1	Total	C	Fe	Mo	S	0	1
			18	1	7	1	9		

- Molecule 7 is iron-sulfur-molybdenum cluster with interstitial carbon (CCD ID: ICE) (formula: CFe₇MoS₈).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total 17	C 1	Fe 7	Mo 1	S 8	0	1
7	C	1	Total 17	C 1	Fe 7	Mo 1	S 8	0	1

- Molecule 8 is FE(8)-S(7) CLUSTER, P1+ state conformer B (CCD ID: A1JPX) (formula: Fe₈S₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	Fe	S	0	1
			15	8	7		

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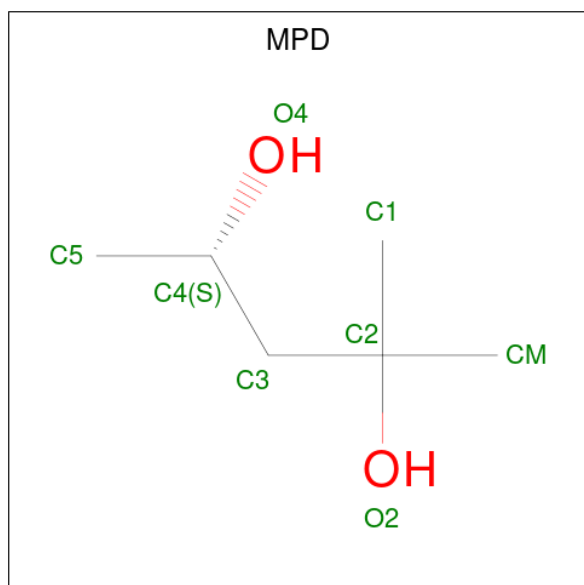
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	Fe	S	0	1
			15	8	7		

- Molecule 9 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X) (labeled as "Ligand of Interest" by depositor).

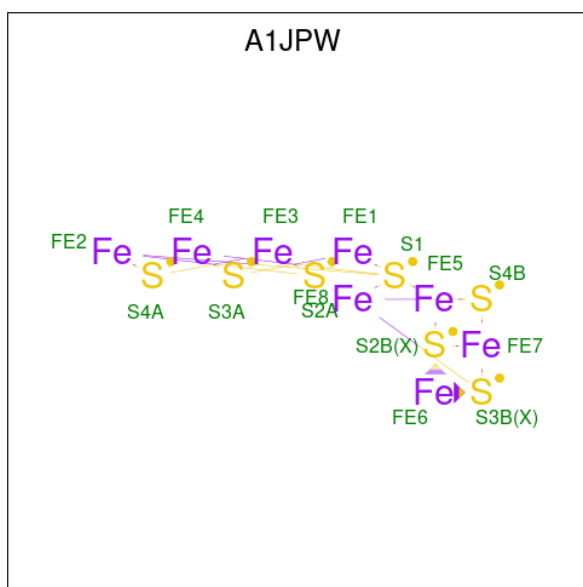
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	X	0	1
			1	1		
9	C	1	Total	X	0	1
			1	1		

- Molecule 10 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	H	O	0	0
			22	6	14	2		
10	D	1	Total	C	H	O	0	0
			22	6	14	2		
10	D	1	Total	C	H	O	0	0
			22	6	14	2		

- Molecule 11 is FE(8)-S(7) CLUSTER, P1+ state conformer A (CCD ID: A1JPW) (formula: Fe₈S₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	Fe	S	0	1
			15	8	7		
11	D	1	Total	Fe	S	0	1
			15	8	7		

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	B	2	Total	Mg	0	0
			2	2		

- Molecule 13 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	3	Total	Cl	0	0
			3	3		
13	D	3	Total	Cl	0	0
			3	3		

- Molecule 14 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	D	1	Total	Na	0	0
			1	1		

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	444	Total 444	O 444	0	15
15	B	513	Total 513	O 513	0	51
15	C	508	Total 508	O 508	0	17
15	D	556	Total 556	O 556	0	65

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	68.50Å 80.24Å 105.74Å 74.49° 82.25° 65.02°	Depositor
Resolution (Å)	33.62 – 1.21 33.62 – 1.21	Depositor EDS
% Data completeness (in resolution range)	62.0 (33.62-1.21) 62.1 (33.62-1.21)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 1.21Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.121 , 0.146 0.129 , 0.150	Depositor DCC
R_{free} test set	18808 reflections (3.14%)	wwPDB-VP
Wilson B-factor (Å ²)	11.9	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	33411	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, GOL, ICS, UNX, CL, ICE, HCA, A1JPW, H2S, MPD, A1JPX, MG

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	0.78	0/4056	0.94	1/5467 (0.0%)
1	C	0.86	2/4100 (0.0%)	1.02	3/5527 (0.1%)
2	B	0.85	1/4063 (0.0%)	1.03	3/5493 (0.1%)
2	D	0.88	2/4029 (0.0%)	1.02	5/5447 (0.1%)
All	All	0.85	5/16248 (0.0%)	1.00	12/21934 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	3
2	B	0	2
2	D	0	6
All	All	0	13

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	207[A]	SER	C-O	8.72	1.33	1.23
2	D	207[B]	SER	C-O	8.72	1.33	1.23
2	B	69	HIS	C-N	-8.62	1.22	1.34
1	C	171[A]	GLN	C-O	7.23	1.33	1.24
1	C	171[B]	GLN	C-O	7.23	1.33	1.24

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	433	ILE	N-CA-C	-8.55	104.80	113.10
2	B	433	ILE	N-CA-C	-8.38	104.97	113.10
1	C	419	PHE	CA-CB-CG	-7.26	106.54	113.80
2	D	207[A]	SER	CA-C-O	6.62	128.28	120.20
2	D	207[B]	SER	CA-C-O	6.62	128.28	120.20

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	184[A]	ARG	Sidechain
1	A	80[A]	ARG	Sidechain
2	B	418[B]	MET	Mainchain
2	B	441[A]	ARG	Sidechain
1	C	80[A]	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3887	3893	3819	16	0
1	C	3908	3901	3802	17	0
2	B	3826	3857	3703	23	0
2	D	3801	3844	3706	22	0
3	A	14	6	6	2	0
3	C	14	6	6	3	0
4	A	1	0	0	1	0
4	C	1	0	0	1	0
5	A	36	48	48	0	0
5	B	12	16	16	0	0
5	C	12	16	16	0	0
5	D	36	48	48	0	0
6	A	18	0	0	2	0
6	C	18	0	0	1	0
7	A	17	0	0	1	0
7	C	17	0	0	2	0
8	A	15	0	0	1	0
8	C	15	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	1	0	0	0	0
9	C	1	0	0	0	0
10	B	8	14	14	2	0
10	D	16	28	28	3	0
11	B	15	0	0	1	0
11	D	15	0	0	1	0
12	B	2	0	0	0	0
13	B	3	0	0	0	0
13	D	3	0	0	0	0
14	D	1	0	0	0	0
15	A	444	0	0	0	0
15	B	513	0	0	1	0
15	C	508	0	0	0	0
15	D	556	0	0	0	0
All	All	17734	15677	15212	72	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 2.

The worst 5 of 72 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)
8:C:507[B]:A1JPX:S2A	2:D:42[B]:SER:HB3	2.25	0.76
8:A:511[B]:A1JPX:S2A	2:B:42[B]:SER:HB3	2.36	0.66
2:D:417:ARG:HB3	2:D:422[B]:ILE:HD13	1.85	0.58
10:B:501:MPD:H51	2:D:437[B]:MET:HG3	1.86	0.58
2:D:432:PRO:HD3	10:D:502:MPD:HM3	1.88	0.56

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	487/477 (102%)	467 (96%)	20 (4%)	0	100	100
1	C	492/477 (103%)	476 (97%)	16 (3%)	0	100	100
2	B	500/462 (108%)	491 (98%)	9 (2%)	0	100	100
2	D	496/462 (107%)	486 (98%)	10 (2%)	0	100	100
All	All	1975/1878 (105%)	1920 (97%)	55 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	421/410 (103%)	416 (99%)	5 (1%)	63	28
1	C	426/410 (104%)	421 (99%)	5 (1%)	63	28
2	B	425/391 (109%)	421 (99%)	4 (1%)	70	40
2	D	422/391 (108%)	419 (99%)	3 (1%)	76	47
All	All	1694/1602 (106%)	1677 (99%)	17 (1%)	70	36

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	134	LEU
2	D	462	GLN
2	B	177[B]	ILE
2	B	462	GLN
1	C	80[A]	ARG

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

Mol	Chain	Res	Type
1	C	289	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 42 ligands modelled in this entry, 2 are modelled with single atom, 2 are unknown and 9 are monoatomic - leaving 29 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	GOL	B	504	-	5,5,5	0.08	0	5,5,5	0.26	0
5	GOL	D	507	-	5,5,5	0.09	0	5,5,5	0.34	0
8	A1JPX	C	507[B]	2,1	0,23,23	-	-	-		
5	GOL	C	504	-	5,5,5	0.09	0	5,5,5	0.32	0
5	GOL	A	508[A]	-	5,5,5	0.08	0	5,5,5	0.31	0
5	GOL	A	503	-	5,5,5	0.09	0	5,5,5	0.30	0
5	GOL	D	506	-	5,5,5	0.08	0	5,5,5	0.31	0
5	GOL	D	505	-	5,5,5	0.09	0	5,5,5	0.35	0
7	ICE	C	506[B]	3,1	12,28,28	2.65	8 (66%)	-		
5	GOL	A	505	-	5,5,5	0.09	0	5,5,5	0.33	0
6	ICS	A	509[A]	3,1	18,30,30	2.64	11 (61%)	-		
5	GOL	D	509	-	5,5,5	0.09	0	5,5,5	0.31	0
7	ICE	A	510[B]	3,1	12,28,28	2.57	8 (66%)	-		
8	A1JPX	A	511[B]	2,1	0,23,23	-	-	-		
11	A1JPW	B	502[A]	2,1	0,23,23	-	-	-		
3	HCA	C	501	6,7	13,13,13	1.13	1 (7%)	14,18,18	1.72	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	MPD	D	501	-	7,7,7	0.17	0	9,10,10	0.31	0
11	A1JPW	D	503[A]	2,1	0,23,23	-	-	-		
5	GOL	C	503	-	5,5,5	0.09	0	5,5,5	0.35	0
5	GOL	A	504	-	5,5,5	0.09	0	5,5,5	0.36	0
10	MPD	D	502	-	7,7,7	0.12	0	9,10,10	0.30	0
5	GOL	D	508	-	5,5,5	0.06	0	5,5,5	0.40	0
3	HCA	A	501	6,7	13,13,13	1.10	0	14,18,18	1.72	2 (14%)
6	ICS	C	505[A]	3,1	18,30,30	2.60	11 (61%)	-		
5	GOL	A	507	-	5,5,5	0.08	0	5,5,5	0.31	0
5	GOL	A	506	-	5,5,5	0.09	0	5,5,5	0.33	0
5	GOL	D	504	-	5,5,5	0.10	0	5,5,5	0.34	0
10	MPD	B	501	-	7,7,7	0.13	0	9,10,10	0.32	0
5	GOL	B	503	-	5,5,5	0.08	0	5,5,5	0.36	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	504	-	-	2/4/4/4	-
5	GOL	D	507	-	-	2/4/4/4	-
8	A1JPX	C	507[B]	2,1	-	-	0/10/9/9
5	GOL	C	504	-	-	4/4/4/4	-
5	GOL	A	508[A]	-	-	2/4/4/4	-
5	GOL	A	503	-	-	2/4/4/4	-
5	GOL	D	506	-	-	2/4/4/4	-
5	GOL	D	505	-	-	3/4/4/4	-
5	GOL	A	505	-	-	2/4/4/4	-
5	GOL	D	509	-	-	0/4/4/4	-
8	A1JPX	A	511[B]	2,1	-	-	0/10/9/9
11	A1JPW	B	502[A]	2,1	-	-	0/10/9/9
3	HCA	C	501	6,7	-	4/17/17/17	-
10	MPD	D	501	-	-	0/5/5/5	-
11	A1JPW	D	503[A]	2,1	-	-	0/10/9/9
5	GOL	C	503	-	-	0/4/4/4	-
5	GOL	A	504	-	-	0/4/4/4	-
10	MPD	D	502	-	-	1/5/5/5	-
5	GOL	D	508	-	-	0/4/4/4	-
3	HCA	A	501	6,7	-	4/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	507	-	-	2/4/4/4	-
5	GOL	A	506	-	-	3/4/4/4	-
5	GOL	D	504	-	-	0/4/4/4	-
10	MPD	B	501	-	-	0/5/5/5	-
5	GOL	B	503	-	-	4/4/4/4	-

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	509[A]	ICS	S4B-FE7	-4.04	2.22	2.32
6	A	509[A]	ICS	S1B-FE6	-4.02	2.22	2.32
7	A	510[B]	ICE	S4B-FE7	-3.96	2.22	2.32
6	C	505[A]	ICS	S4B-FE7	-3.91	2.22	2.32
7	C	506[B]	ICE	S4B-FE7	-3.91	2.22	2.32

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	HCA	O5-C7-C3	-4.58	115.77	122.25
3	C	501	HCA	O5-C7-C3	-4.39	116.04	122.25
3	A	501	HCA	O6-C7-C3	2.95	118.17	113.05
3	C	501	HCA	O6-C7-C3	2.84	117.98	113.05
3	C	501	HCA	C4-C5-C6	2.23	117.80	112.75

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	505	GOL	O1-C1-C2-C3
5	A	506	GOL	C1-C2-C3-O3
5	A	508[A]	GOL	C1-C2-C3-O3
5	B	503	GOL	O1-C1-C2-C3
5	B	503	GOL	C1-C2-C3-O3

There are no ring outliers.

12 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	507[B]	A1JPX	1	0
7	C	506[B]	ICE	2	0

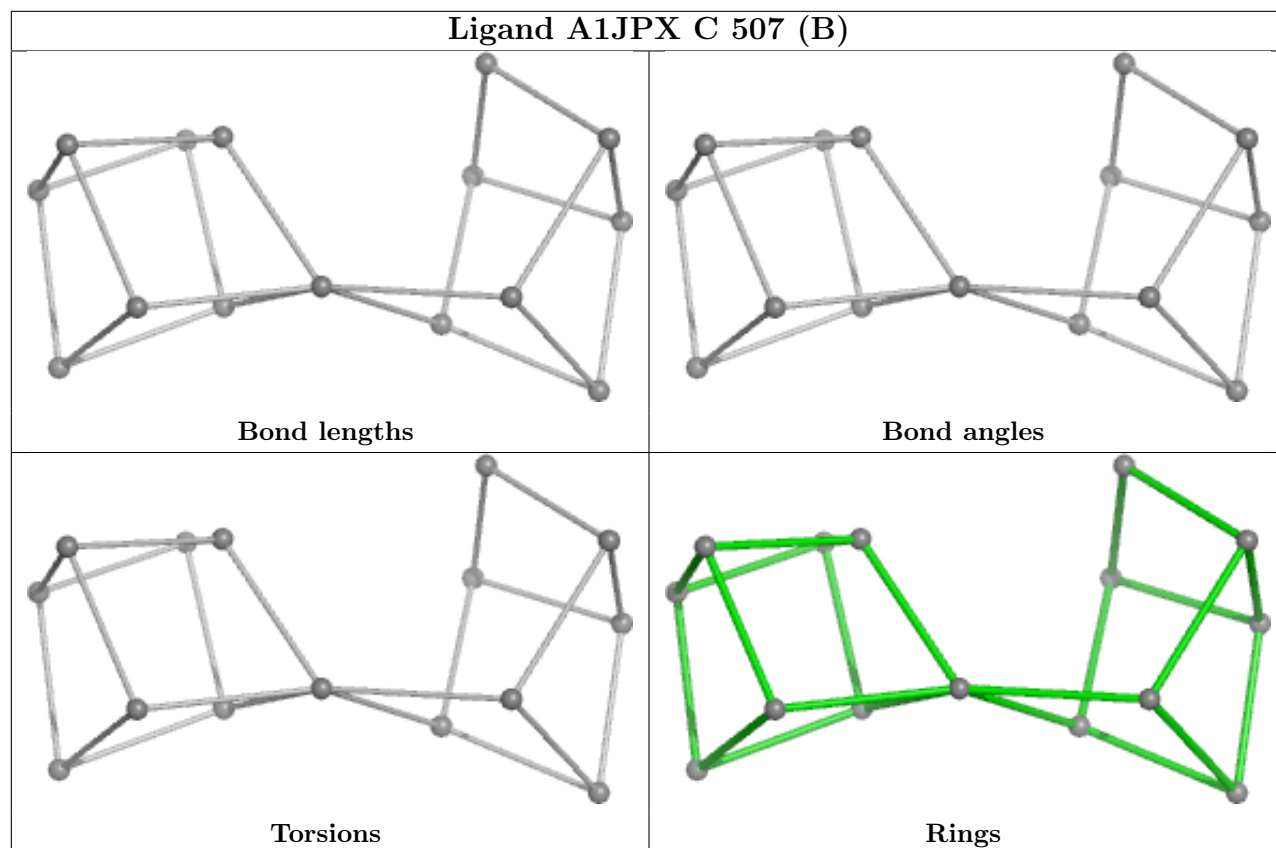
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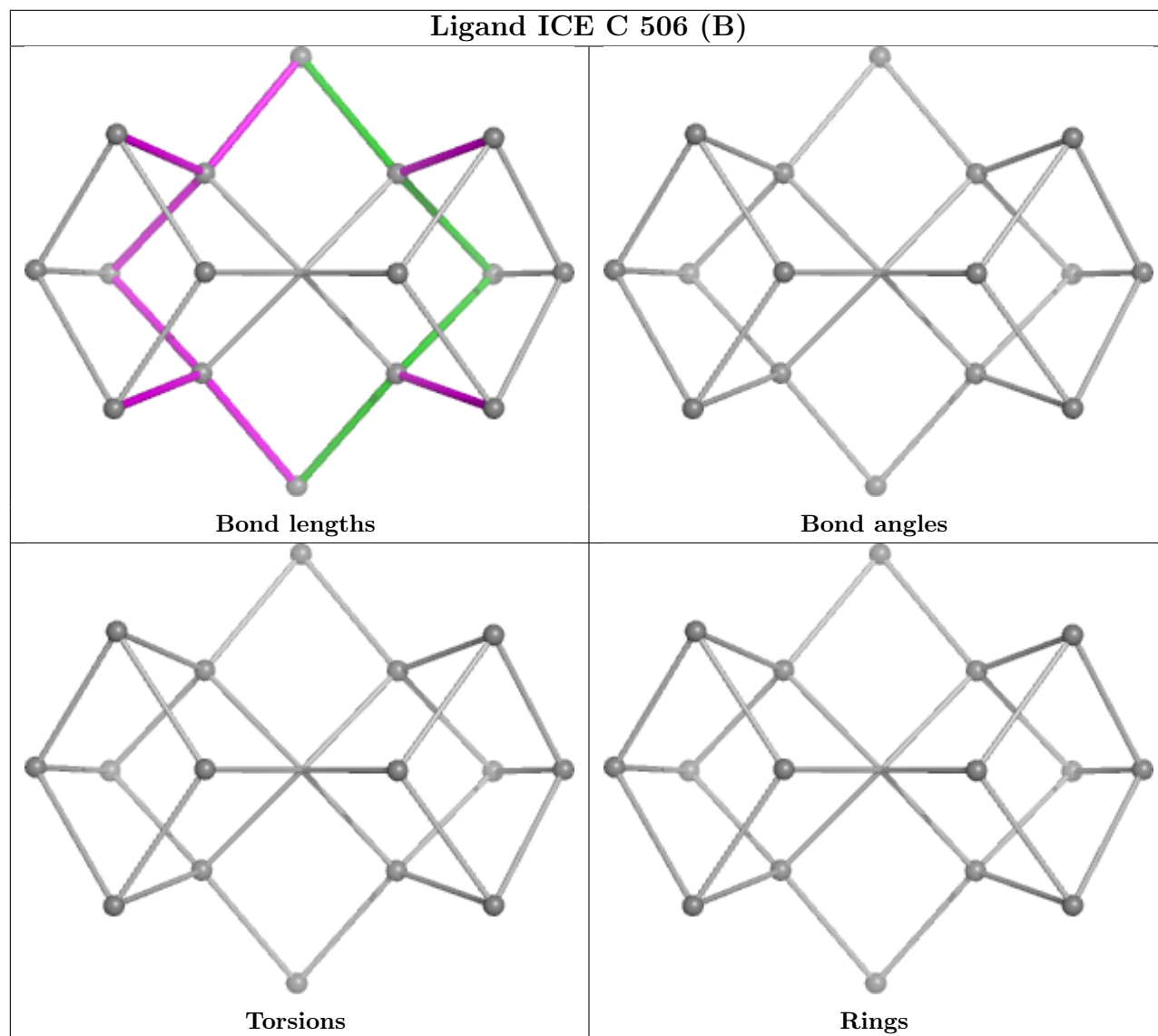
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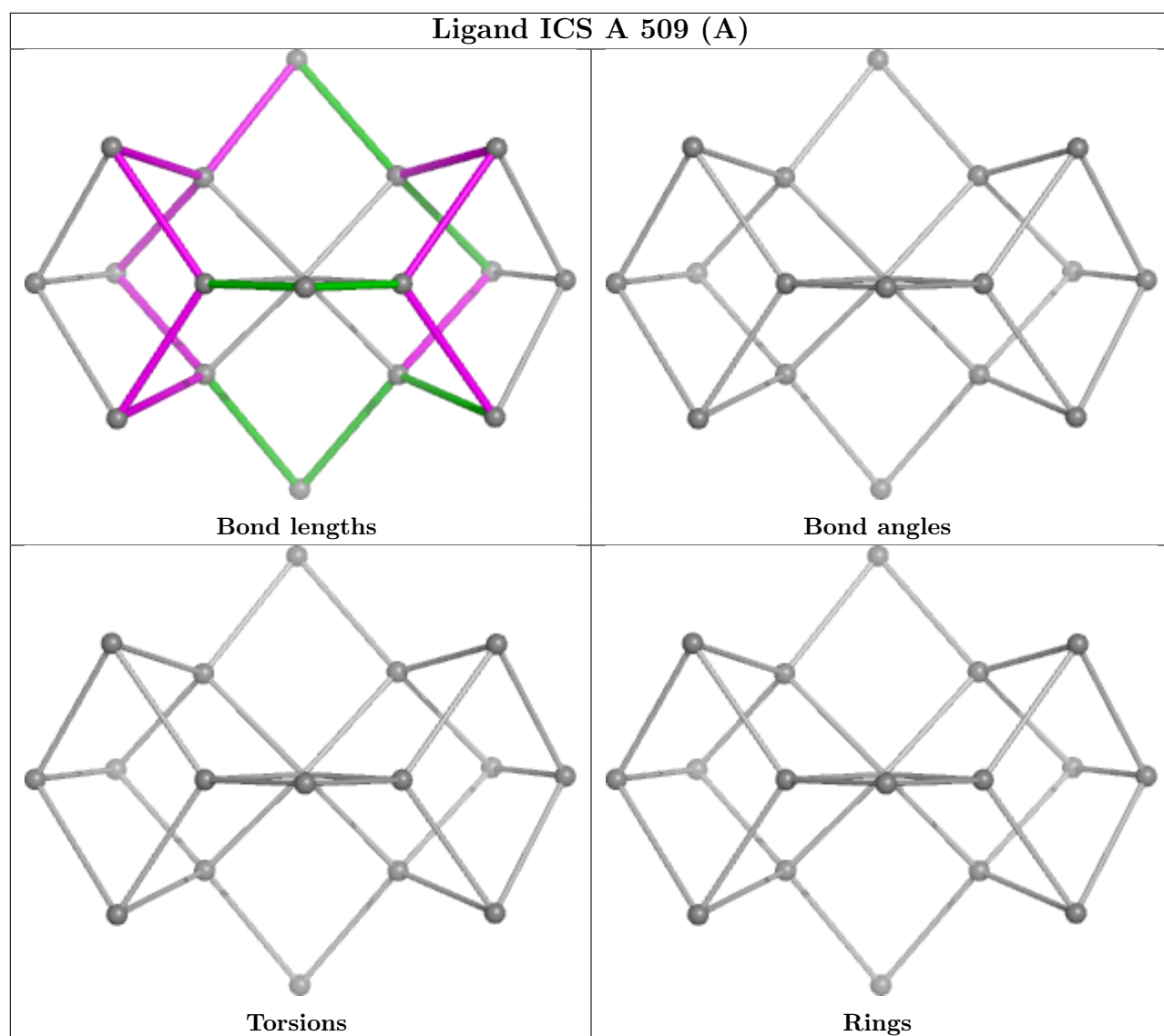
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	509[A]	ICS	2	0
7	A	510[B]	ICE	1	0
8	A	511[B]	A1JPX	1	0
11	B	502[A]	A1JPW	1	0
3	C	501	HCA	3	0
11	D	503[A]	A1JPW	1	0
10	D	502	MPD	3	0
3	A	501	HCA	2	0
6	C	505[A]	ICS	1	0
10	B	501	MPD	2	0

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

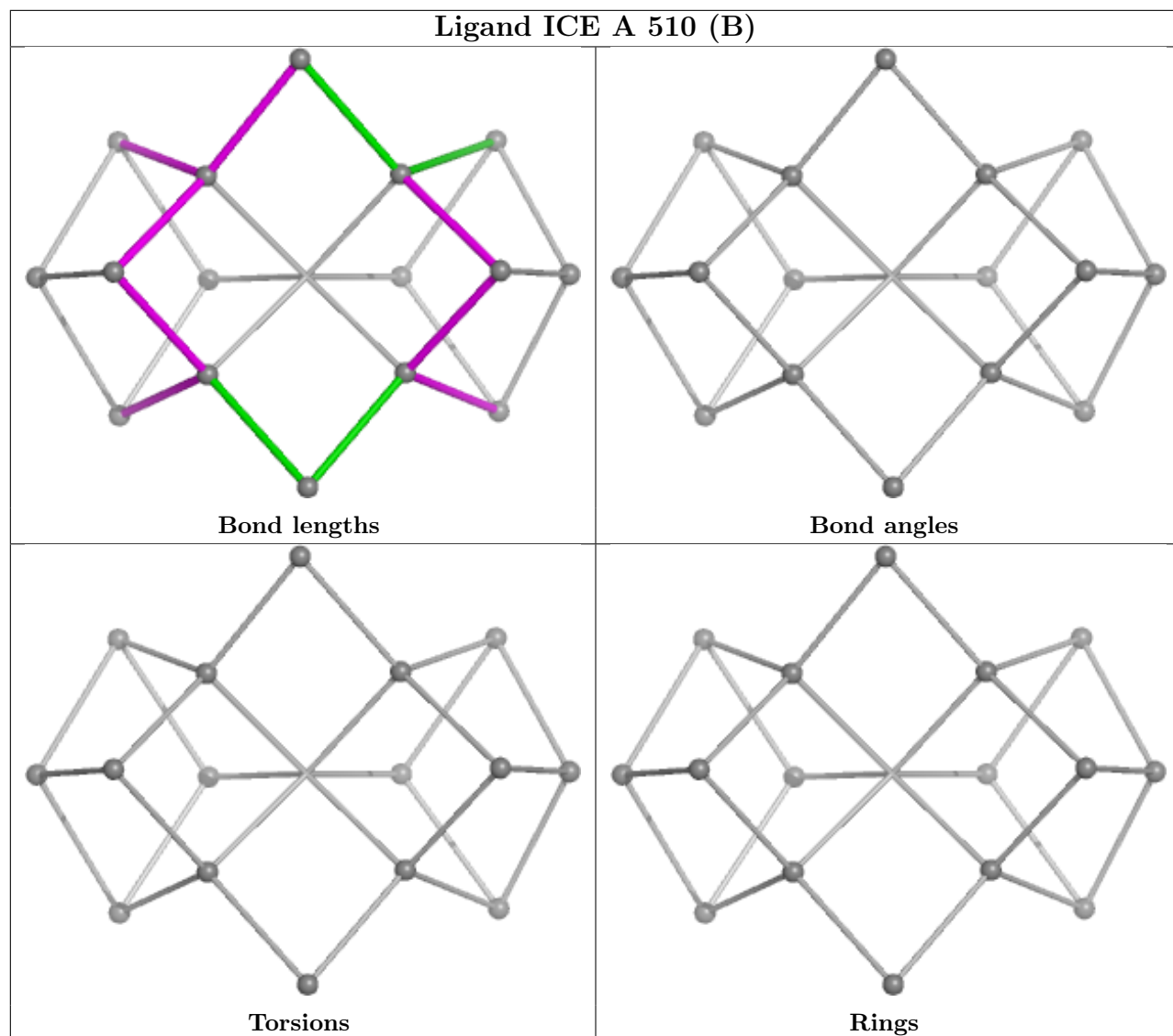
Ligand A1JPX C 507 (B)



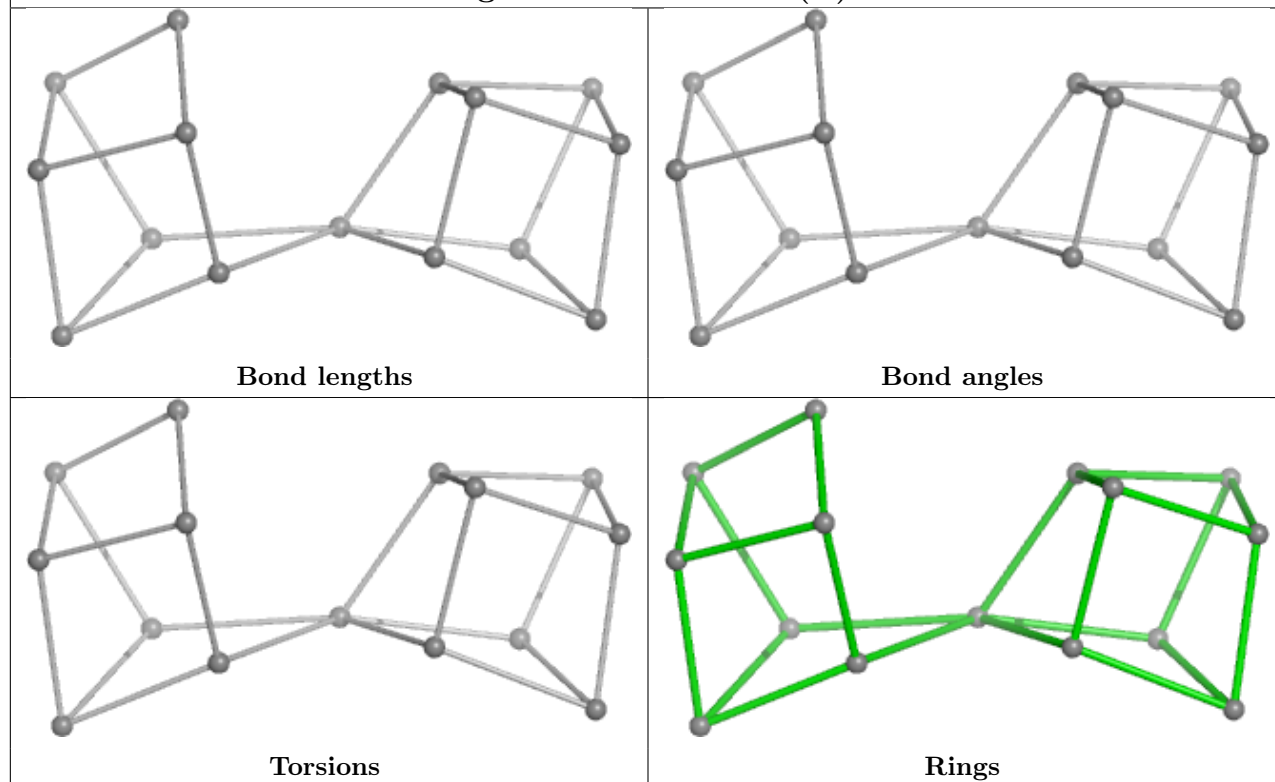




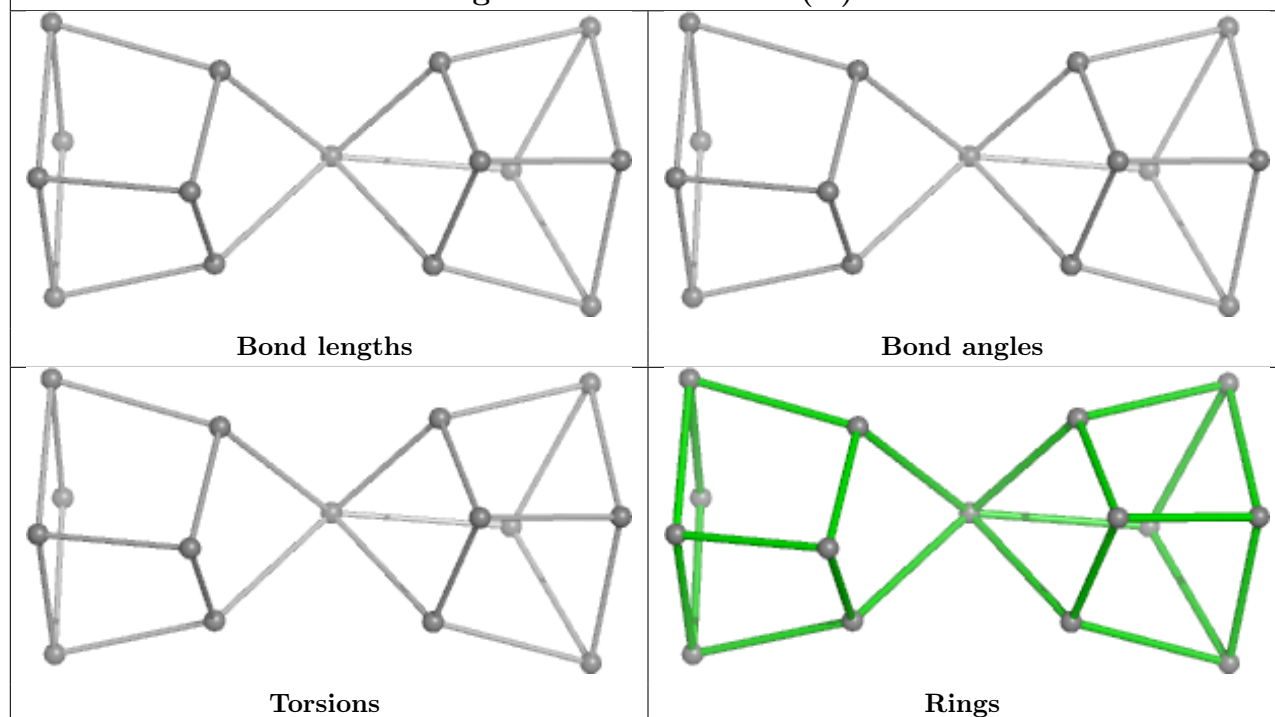
Ligand ICE A 510 (B)

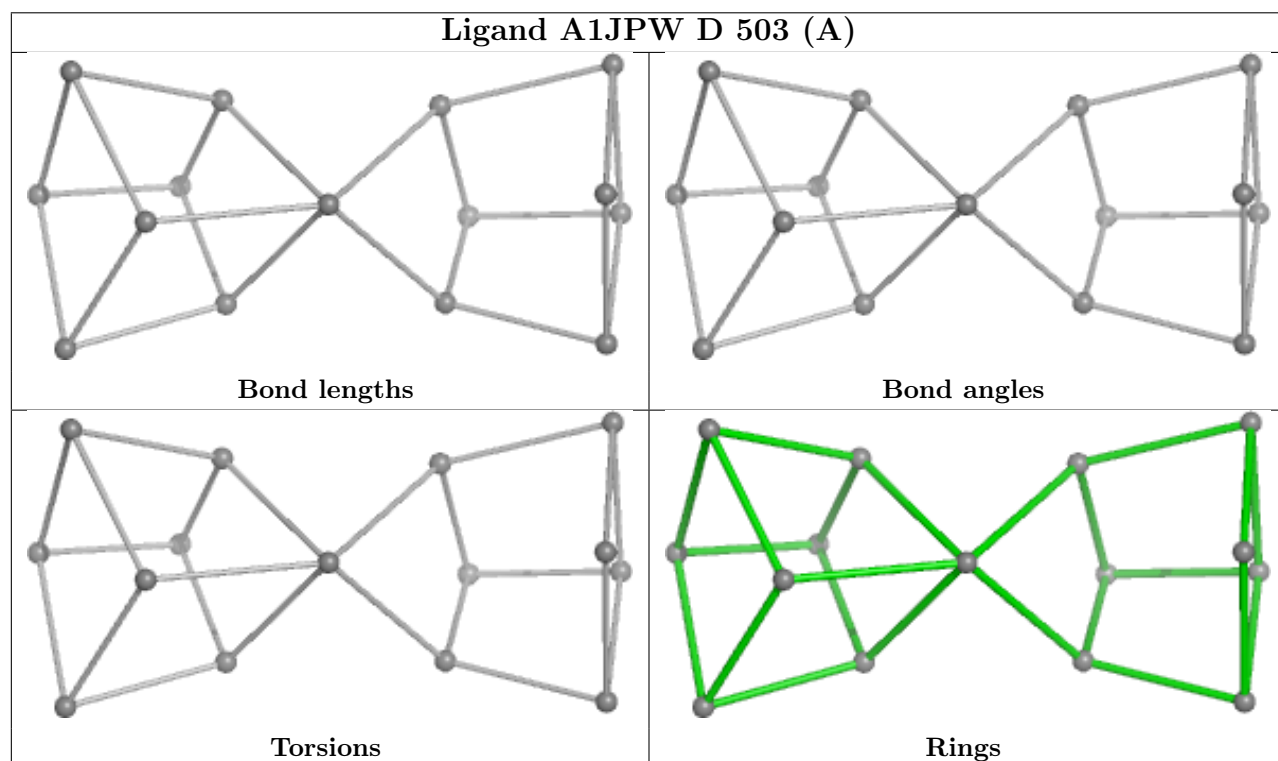
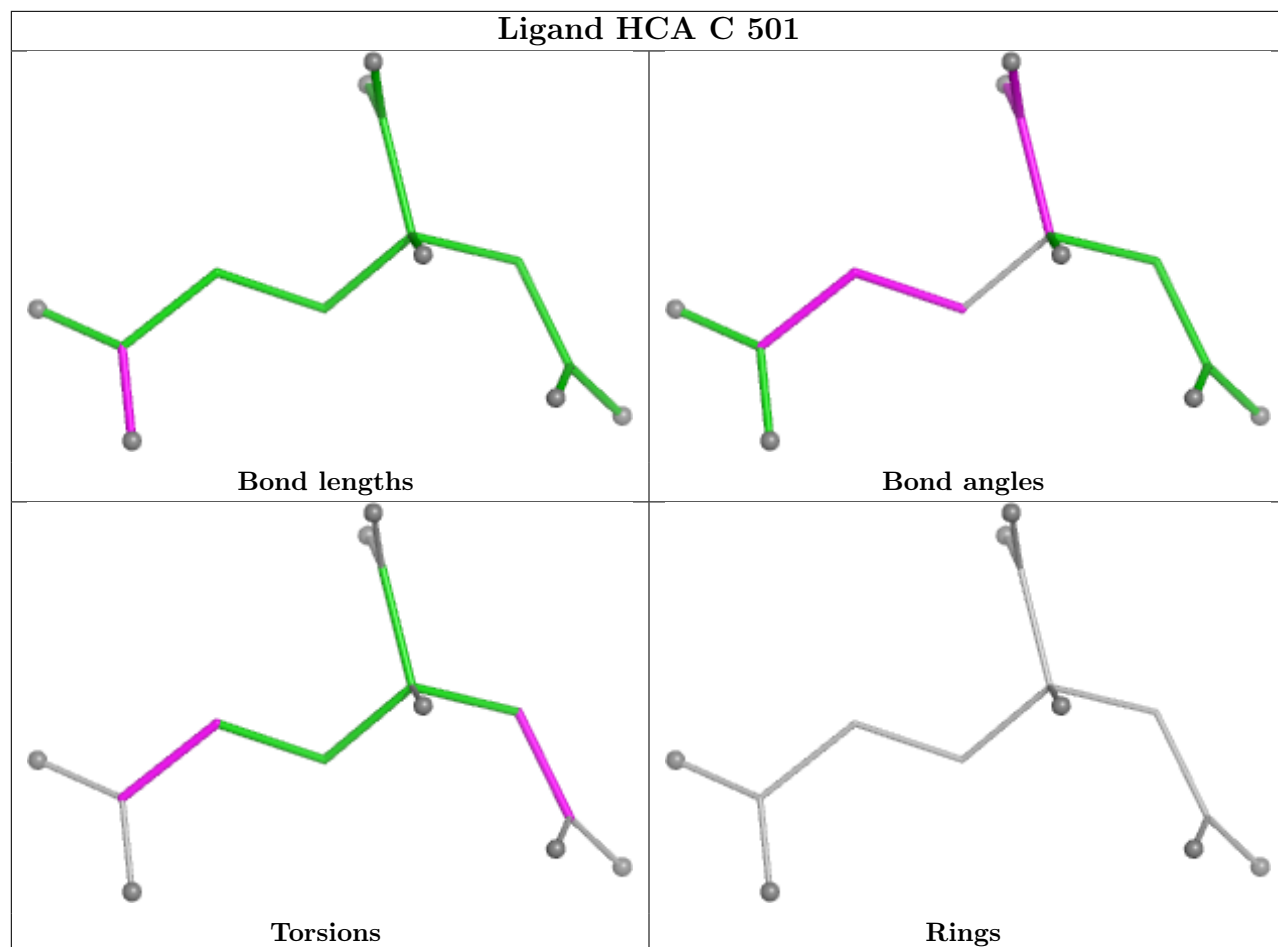


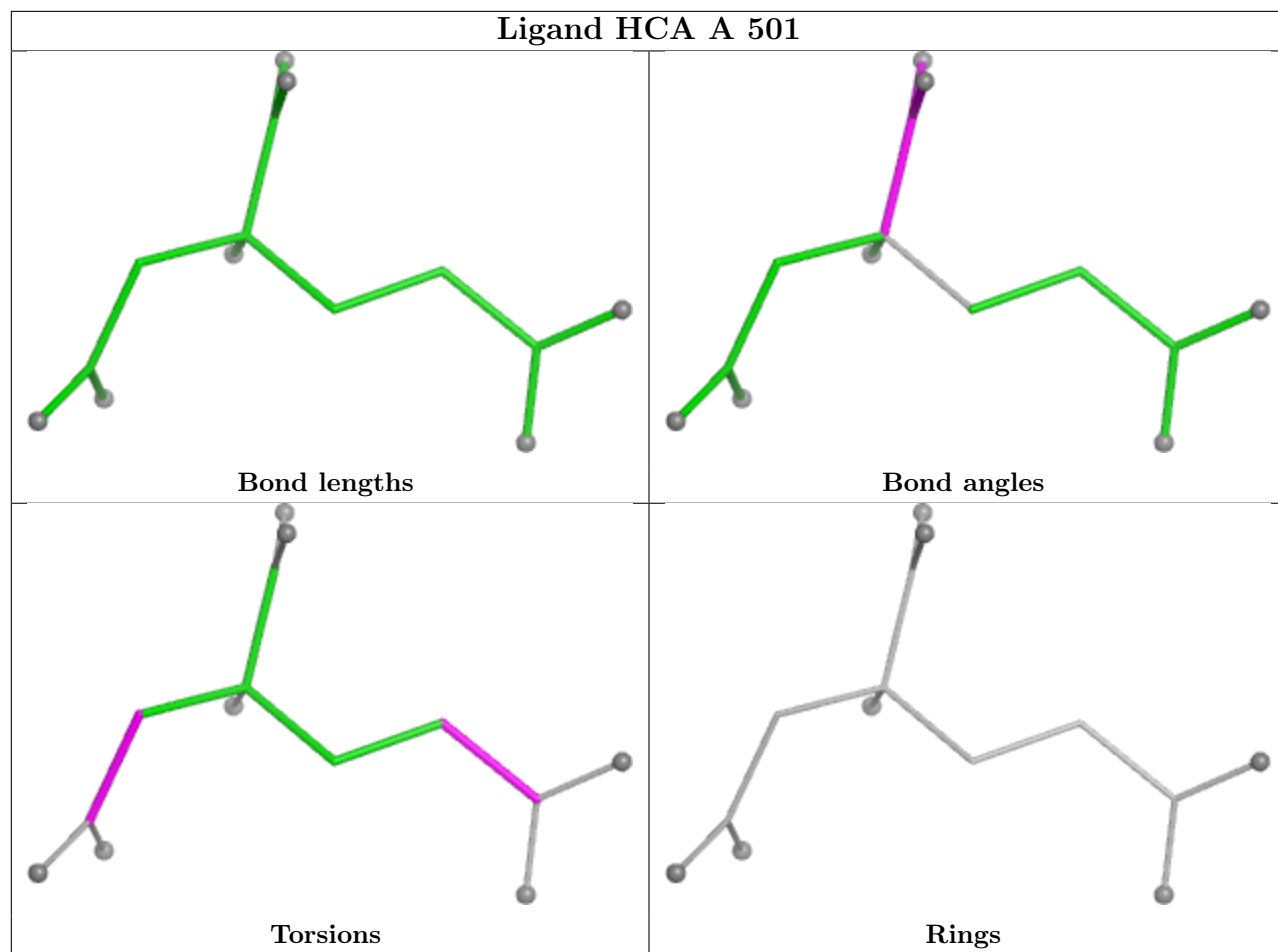
Ligand A1JPX A 511 (B)

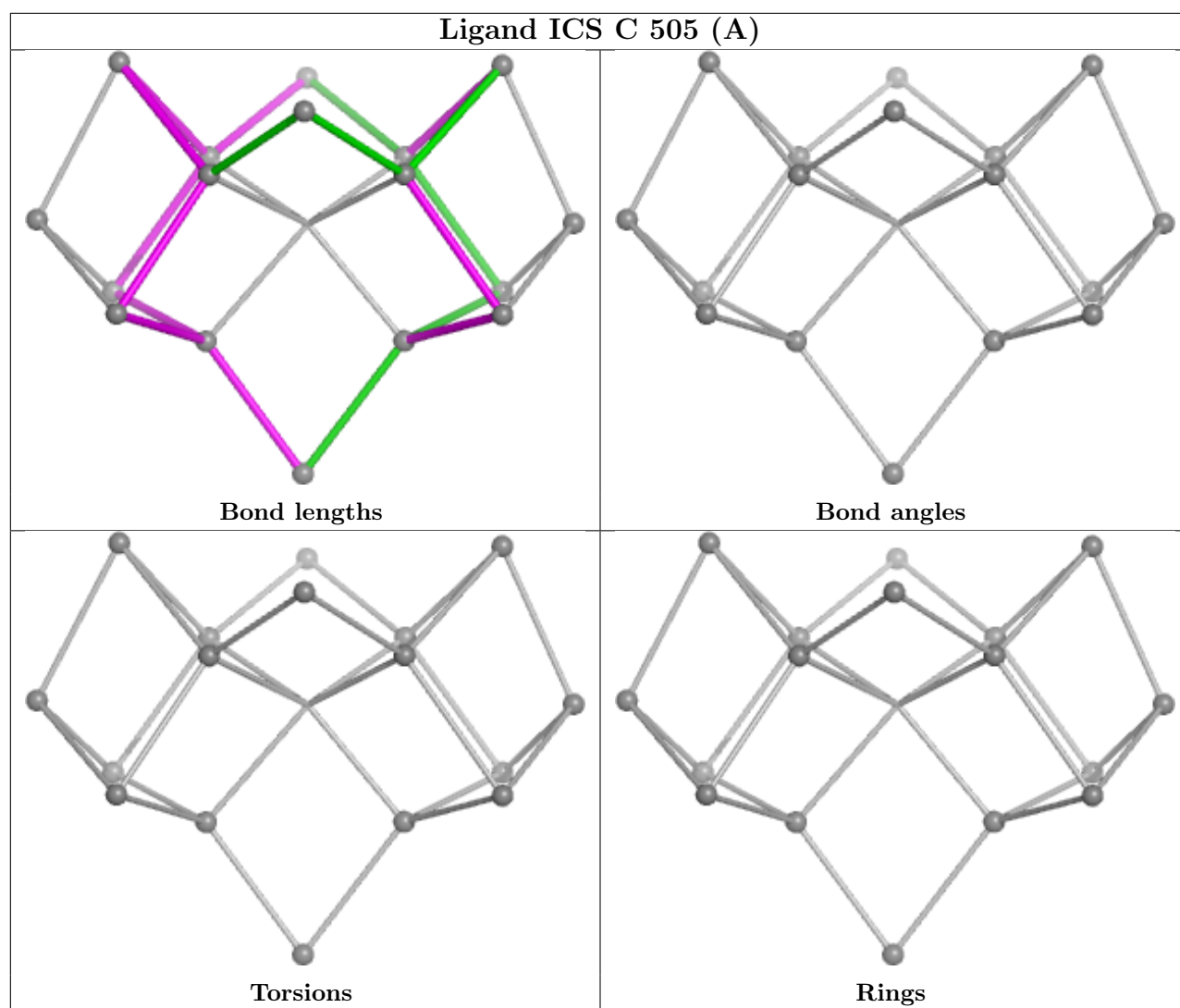


Ligand A1JPW B 502 (A)









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	473/477 (99%)	-0.13	3 (0%) 85 88	8, 18, 32, 44	8 (1%)
1	C	473/477 (99%)	-0.36	2 (0%) 88 91	6, 15, 29, 42	11 (2%)
2	B	461/462 (99%)	-0.23	4 (0%) 81 84	6, 15, 30, 45	22 (4%)
2	D	461/462 (99%)	-0.34	5 (1%) 78 80	6, 14, 26, 48	20 (4%)
All	All	1868/1878 (99%)	-0.26	14 (0%) 84 87	6, 15, 30, 48	61 (3%)

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	169	GLU	3.6
2	D	170	LYS	3.4
1	A	28	ILE	2.7
2	B	129	GLU	2.7
2	D	168	GLU	2.5

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.

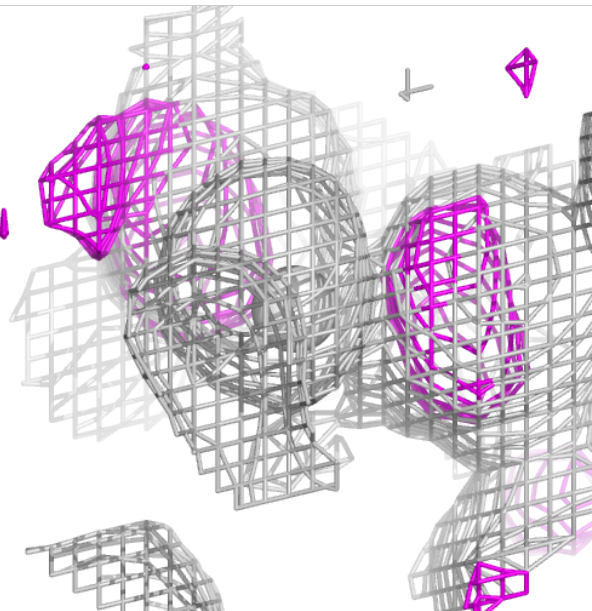
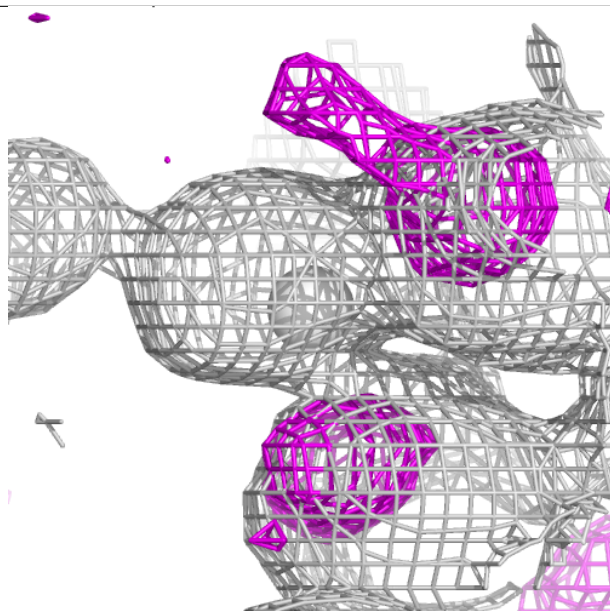
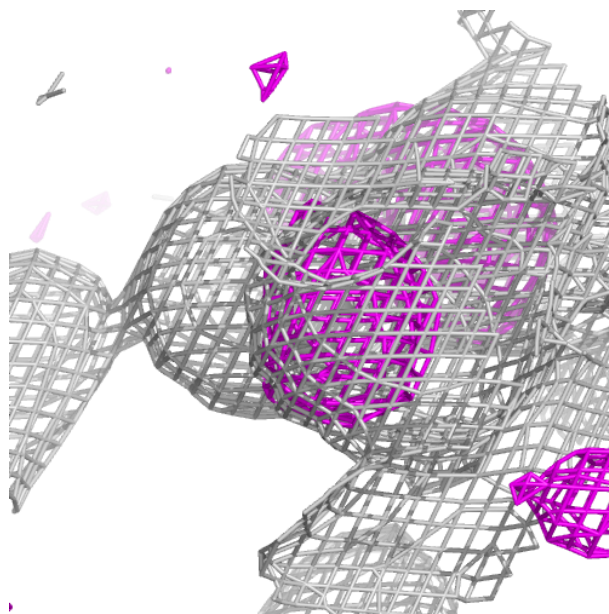
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	D	505	6/6	0.56	0.17	50,60,60,60	0
5	GOL	A	503	6/6	0.61	0.18	47,56,57,58	0
5	GOL	D	509	6/6	0.64	0.17	45,54,57,58	0
5	GOL	A	508[A]	6/6	0.65	0.25	24,29,30,32	14
5	GOL	D	507	6/6	0.66	0.17	43,51,52,54	0
5	GOL	C	504	6/6	0.66	0.16	45,54,56,57	0
5	GOL	A	507	6/6	0.67	0.13	47,57,58,58	0
5	GOL	D	504	6/6	0.68	0.21	45,54,59,59	0
5	GOL	B	504	6/6	0.69	0.18	46,55,56,57	0
5	GOL	D	506	6/6	0.70	0.15	46,55,56,56	0
5	GOL	A	505	6/6	0.74	0.15	46,55,56,57	0
5	GOL	B	503	6/6	0.75	0.14	43,51,52,54	0
5	GOL	A	506	6/6	0.76	0.15	45,54,55,55	0
5	GOL	C	503	6/6	0.80	0.12	34,41,46,47	0
10	MPD	D	502	8/8	0.81	0.13	30,36,41,43	0
5	GOL	D	508	6/6	0.84	0.13	35,42,47,47	0
10	MPD	B	501	8/8	0.85	0.11	32,40,42,43	0
5	GOL	A	504	6/6	0.85	0.11	36,43,49,51	0
10	MPD	D	501	8/8	0.90	0.10	30,36,37,37	0
9	UNX	A	512[B]	1/1	0.96	0.08	11,11,11,11	1
3	HCA	A	501	14/14	0.97	0.05	11,12,14,14	0
4	H2S	C	502[B]	1/1	0.97	0.04	10,10,10,10	1
4	H2S	A	502[B]	1/1	0.98	0.04	15,15,15,15	1
3	HCA	C	501	14/14	0.98	0.04	9,10,12,12	0
12	MG	B	506	1/1	0.98	0.04	9,9,9,9	0
13	CL	D	512	1/1	0.98	0.07	25,25,25,25	0
12	MG	B	505	1/1	0.99	0.04	11,11,11,11	0
8	A1JPX	A	511[B]	15/15	0.99	0.03	11,11,13,13	15
13	CL	B	508	1/1	0.99	0.05	18,18,18,18	0
13	CL	B	509	1/1	0.99	0.10	32,32,32,32	0
13	CL	D	511	1/1	0.99	0.06	22,22,22,22	0
11	A1JPW	B	502[A]	15/15	0.99	0.03	13,13,14,14	15
11	A1JPW	D	503[A]	15/15	1.00	0.01	9,10,11,11	15
6	ICS	C	505[A]	18/18	1.00	0.02	9,10,11,11	18
9	UNX	C	508[B]	1/1	1.00	0.03	10,10,10,10	1
13	CL	B	507	1/1	1.00	0.03	15,15,15,15	0
7	ICE	A	510[B]	17/17	1.00	0.02	12,12,13,13	17
7	ICE	C	506[B]	17/17	1.00	0.02	9,10,10,11	17
13	CL	D	510	1/1	1.00	0.06	20,20,20,20	0
6	ICS	A	509[A]	18/18	1.00	0.02	11,12,13,13	18
8	A1JPX	C	507[B]	15/15	1.00	0.01	9,9,10,10	15
14	NA	D	513	1/1	1.00	0.02	16,16,16,16	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.

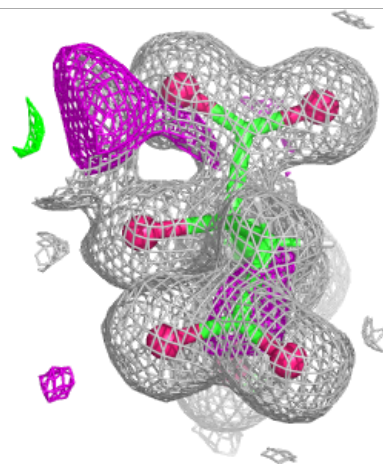
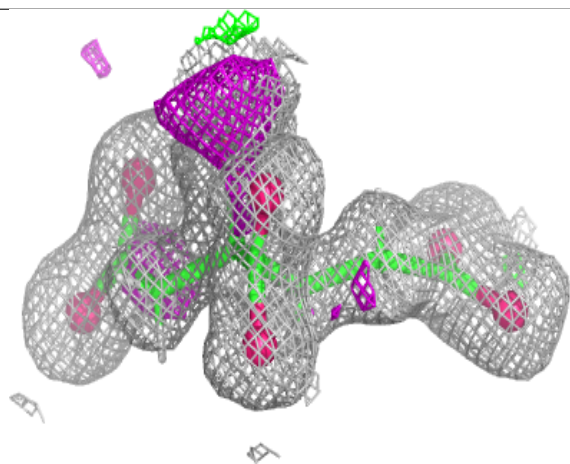
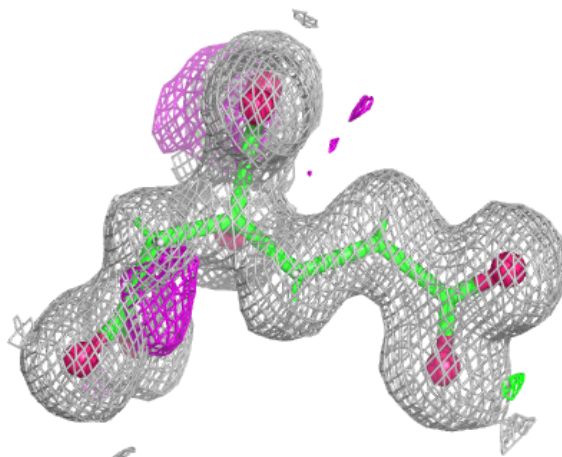
Electron density around UNX A 512 (B):

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



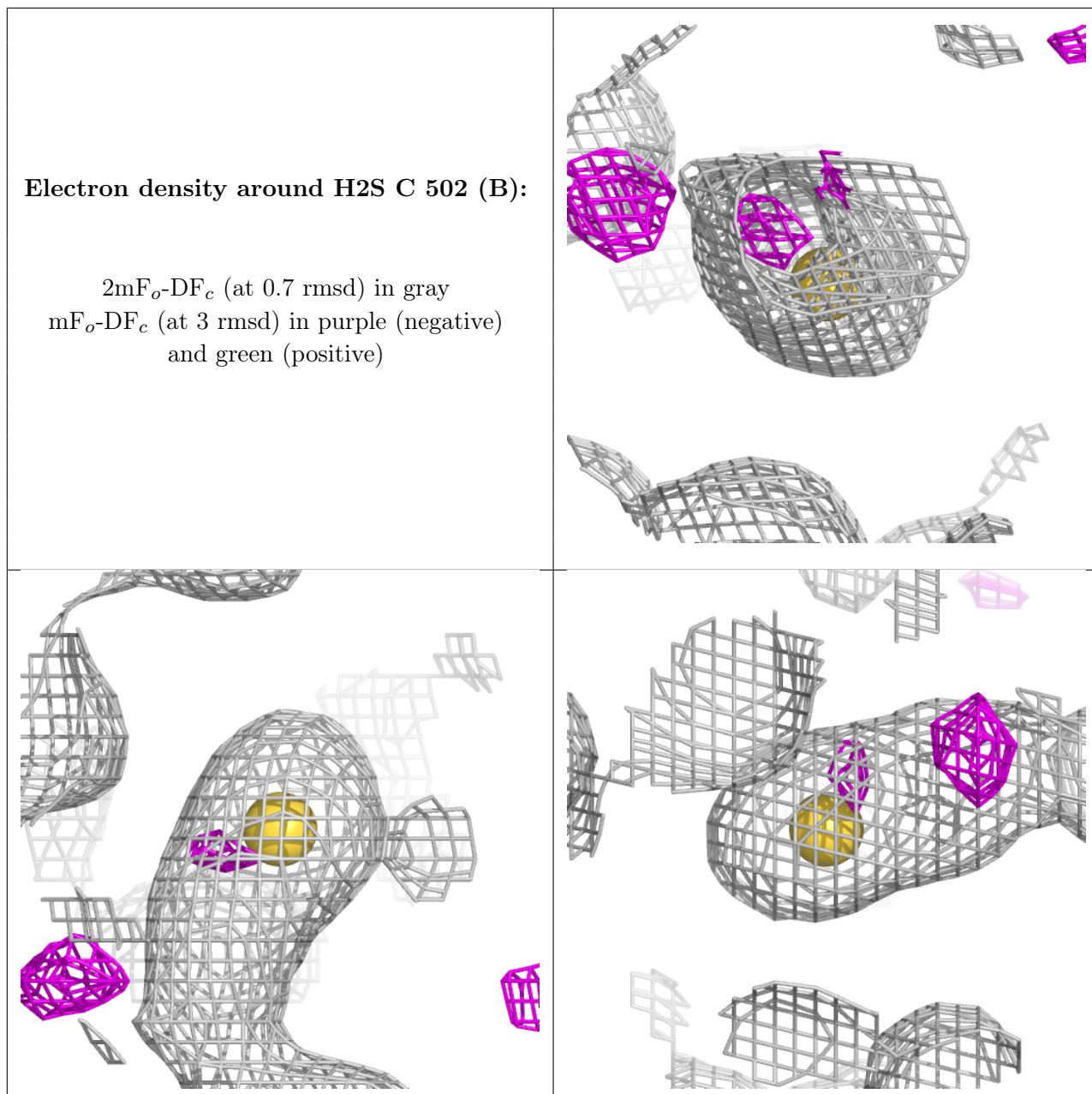
Electron density around HCA A 501:

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



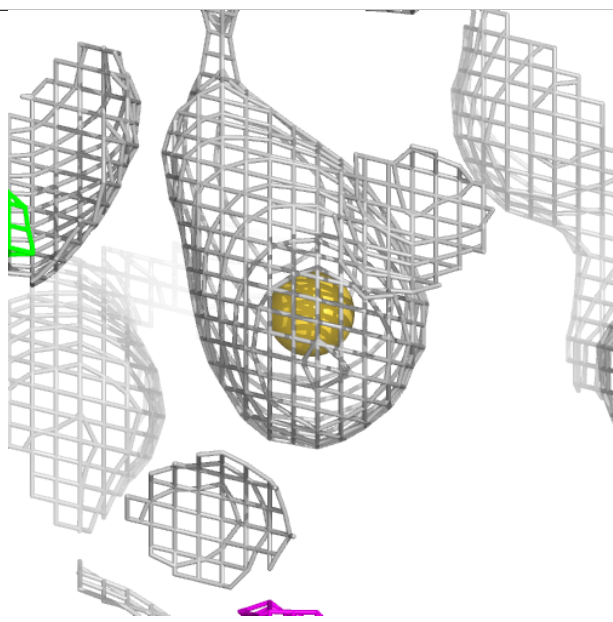
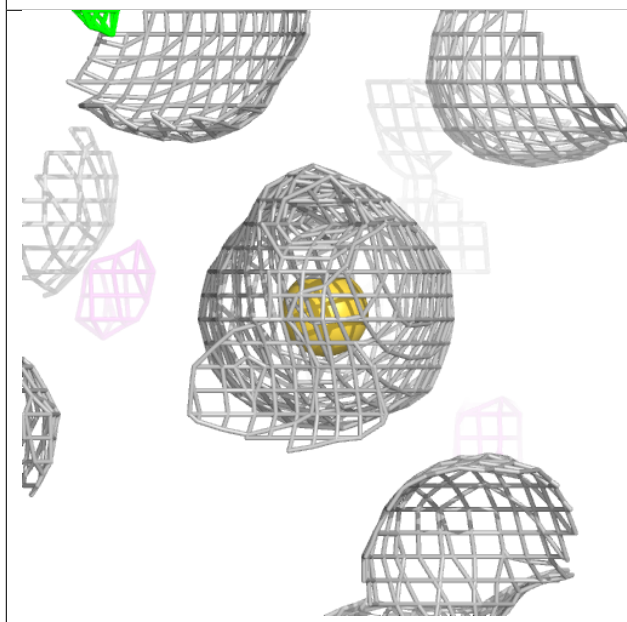
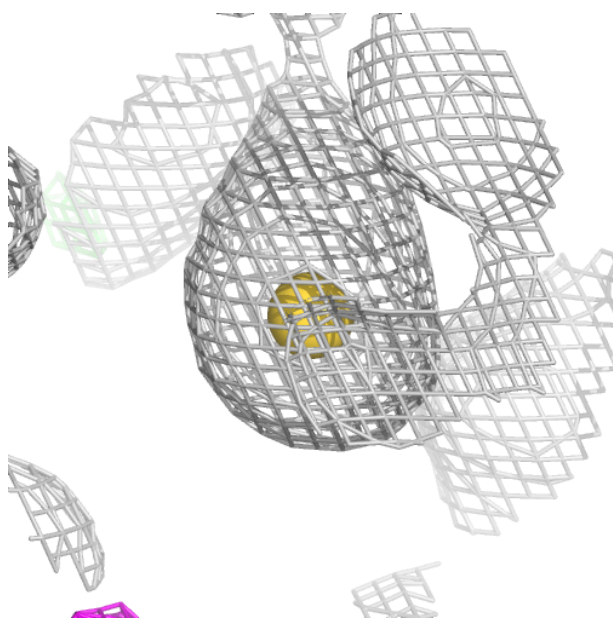
Electron density around H2S C 502 (B):

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



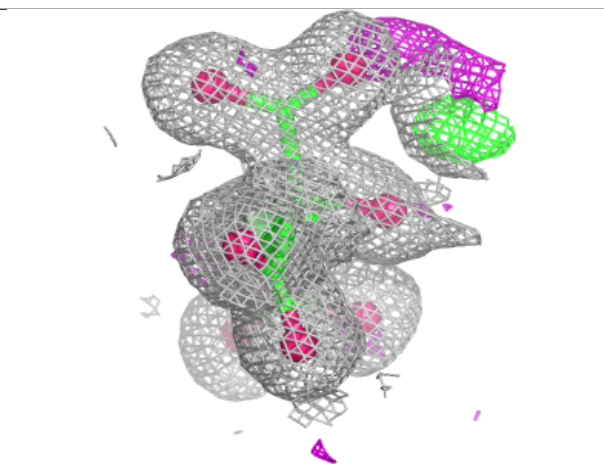
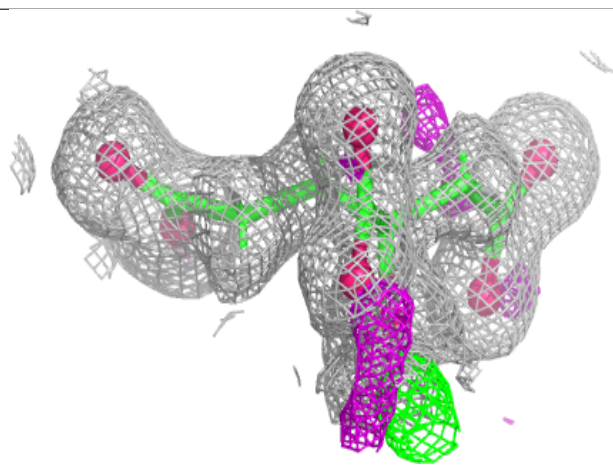
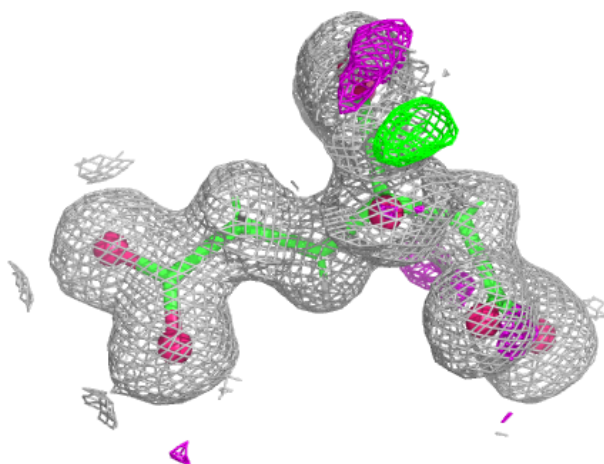
Electron density around H2S A 502 (B):

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



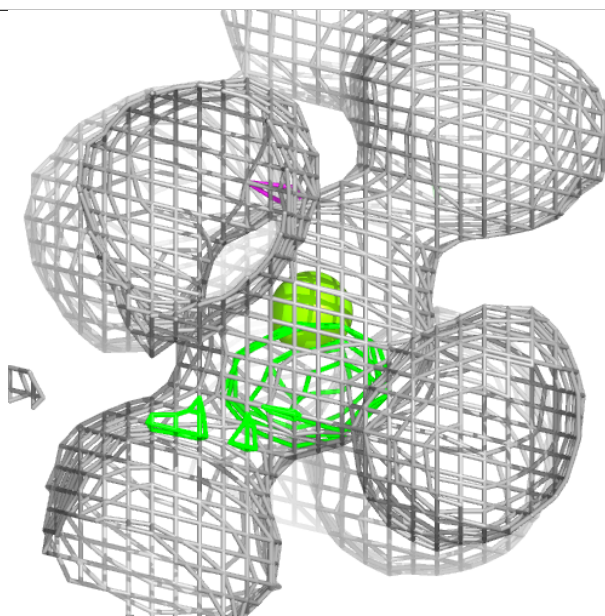
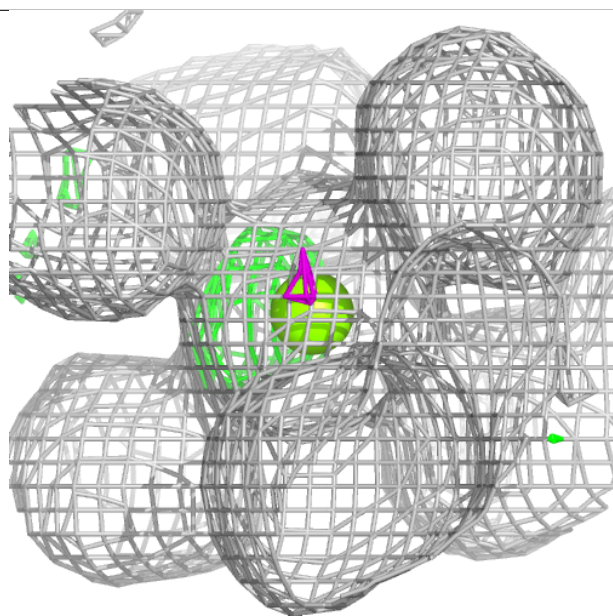
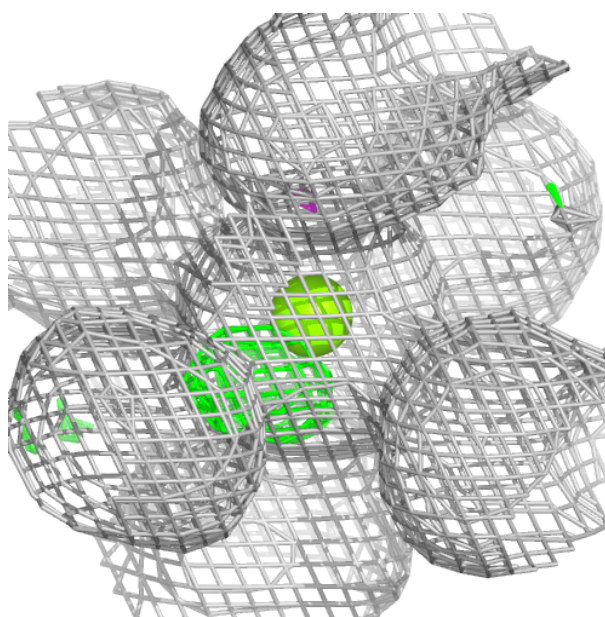
Electron density around HCA C 501:

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and green (positive)



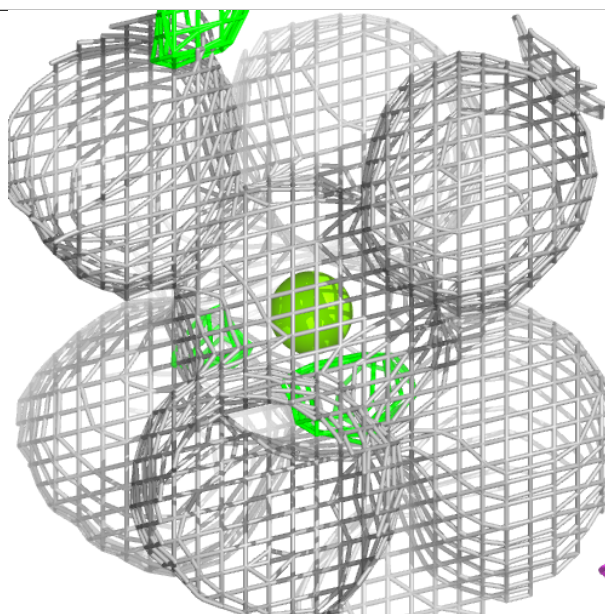
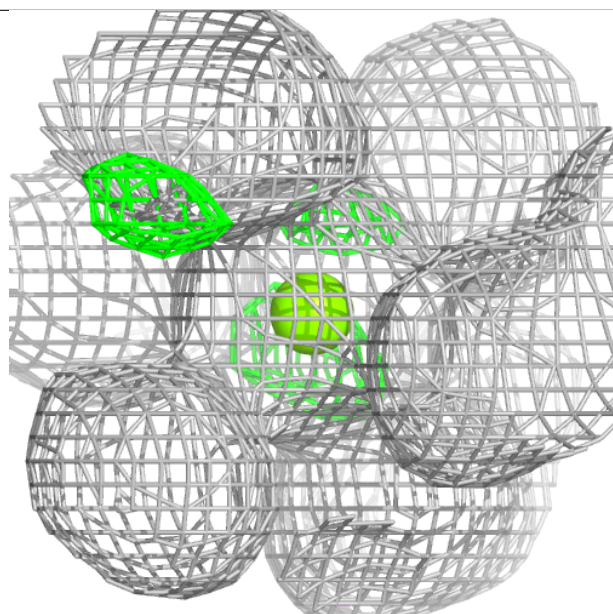
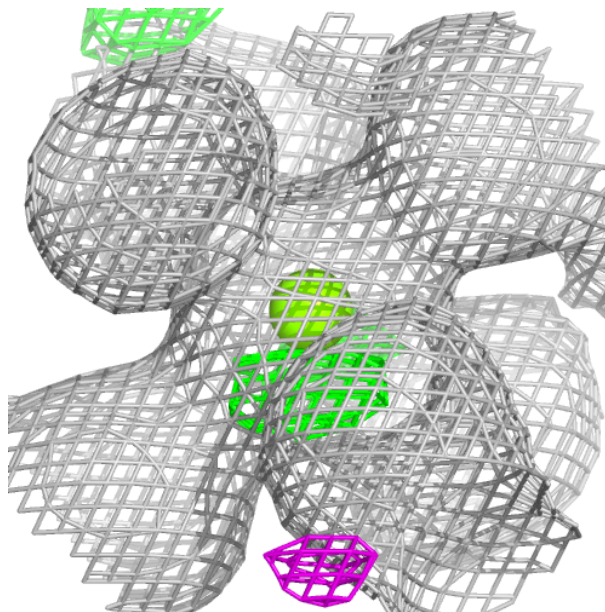
Electron density around MG B 506:

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and green (positive)



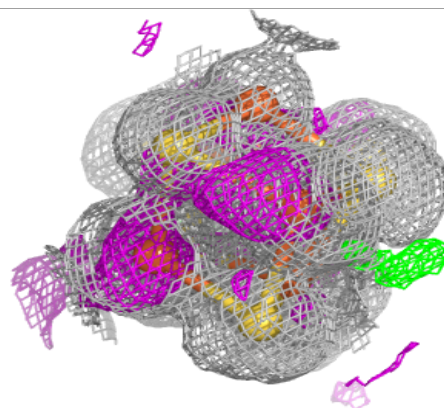
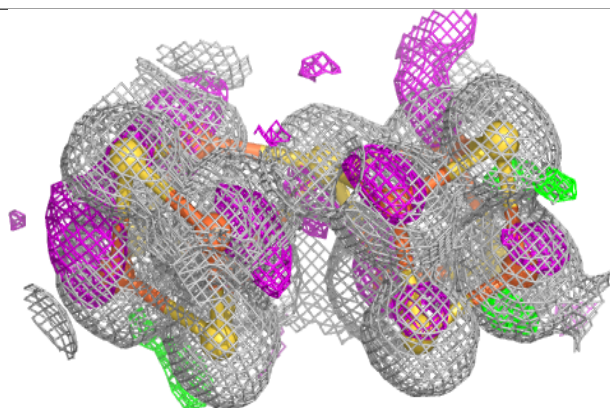
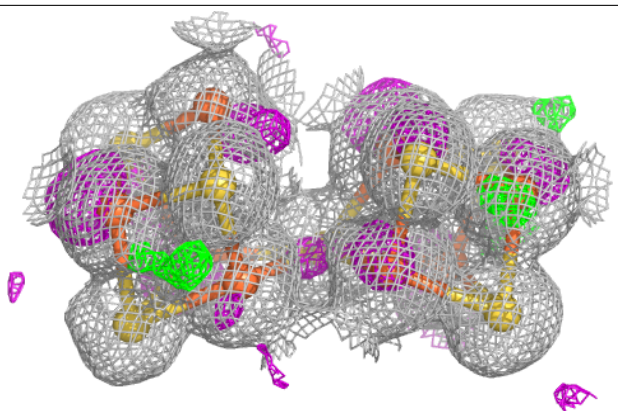
Electron density around MG B 505:

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and green (positive)

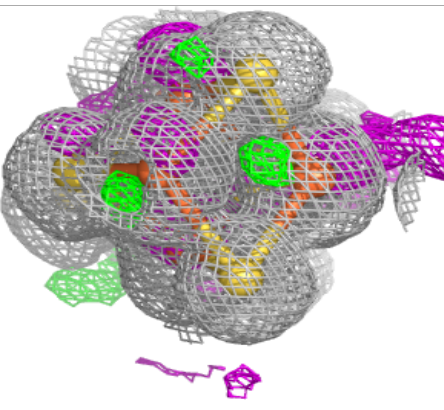
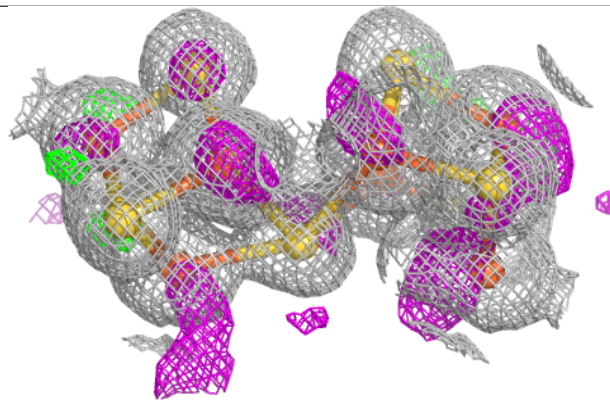
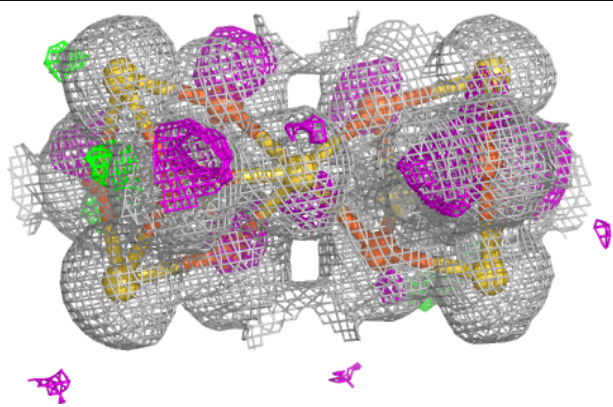


Electron density around A1JPX A 511 (B):

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

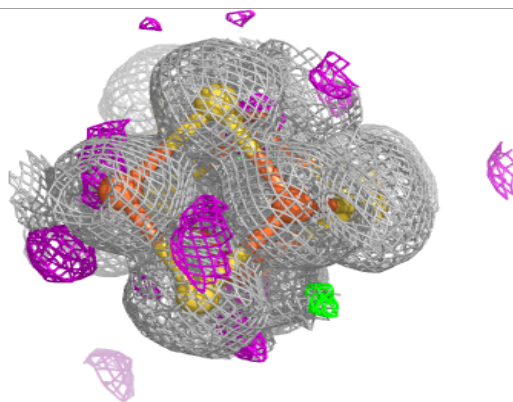
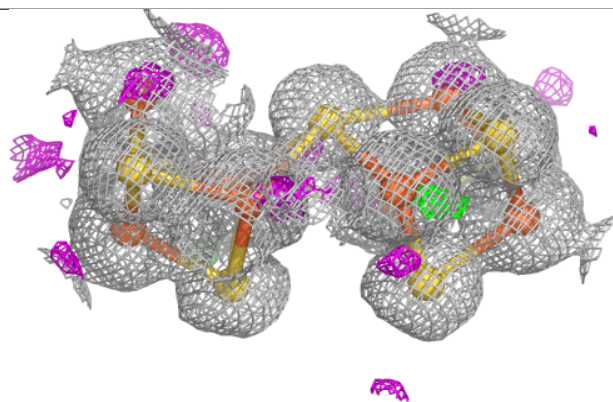
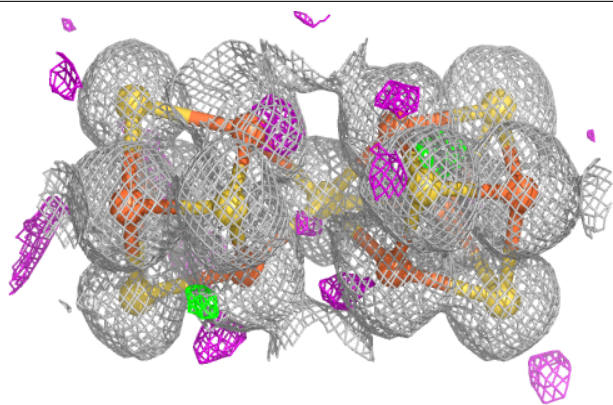
**Electron density around A1JPW B 502 (A):**

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



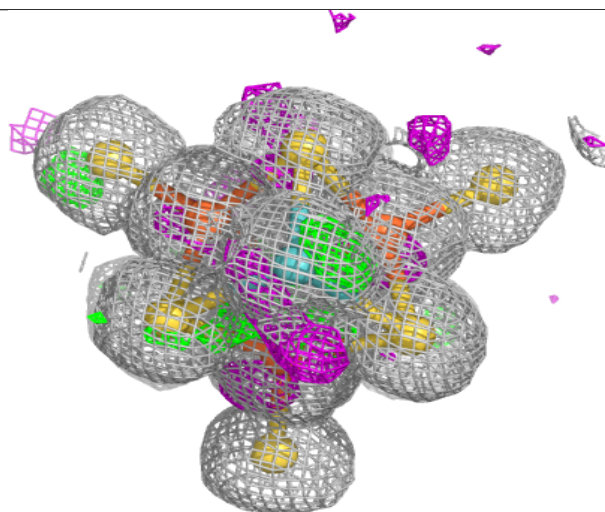
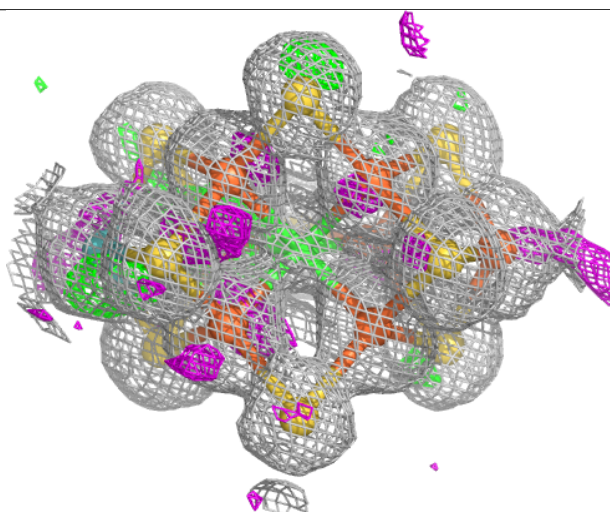
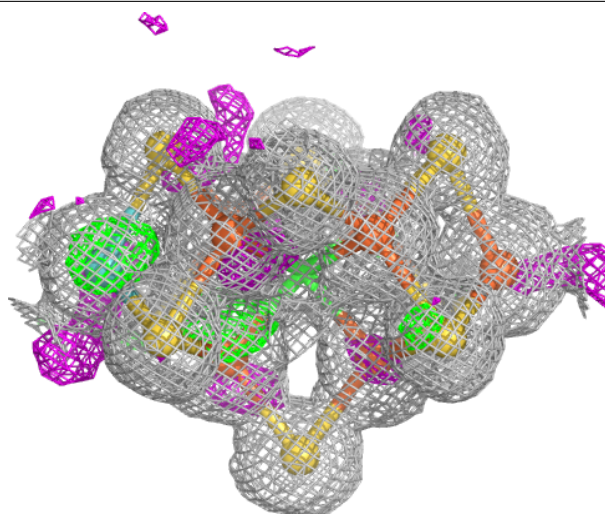
Electron density around A1JPW D 503 (A):

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



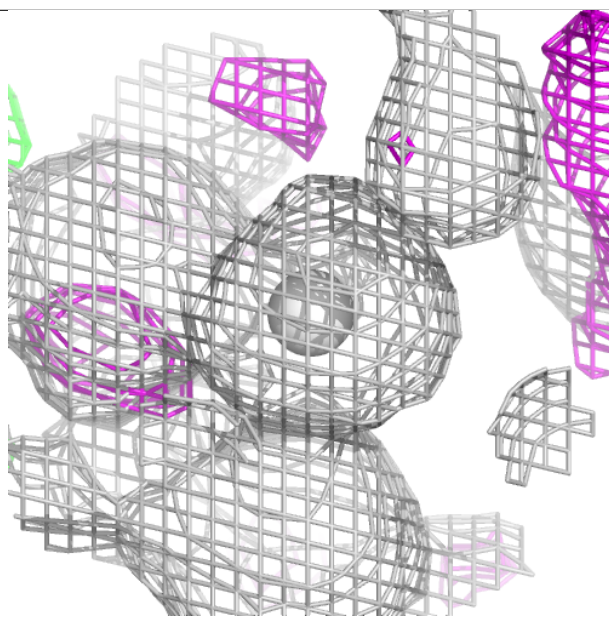
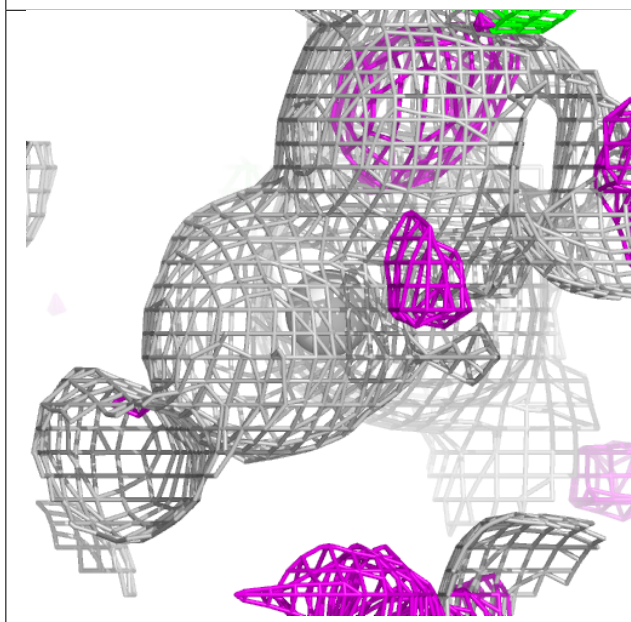
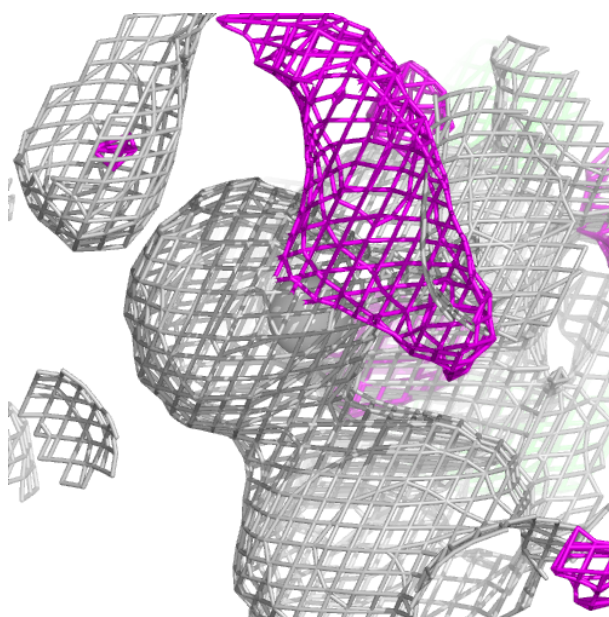
Electron density around ICS C 505 (A):

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



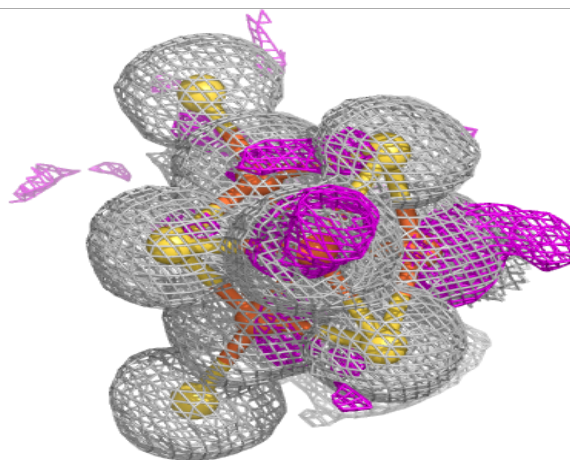
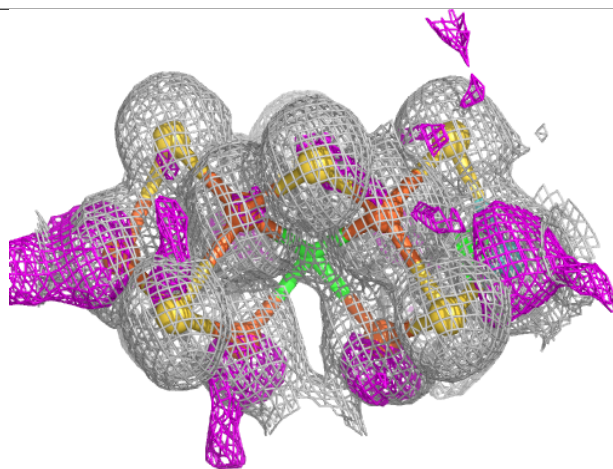
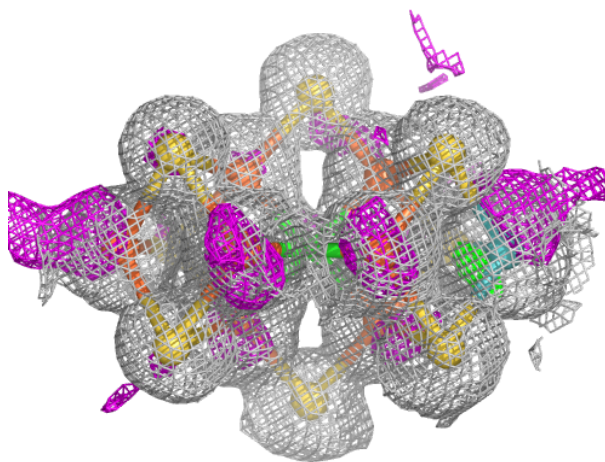
Electron density around UNX C 508 (B):

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



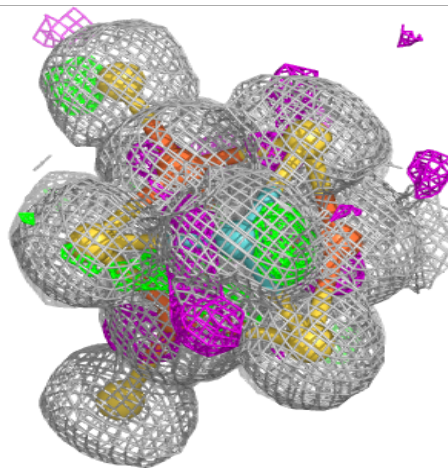
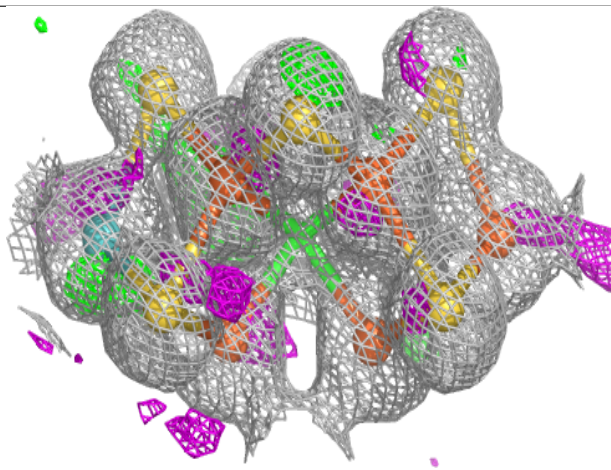
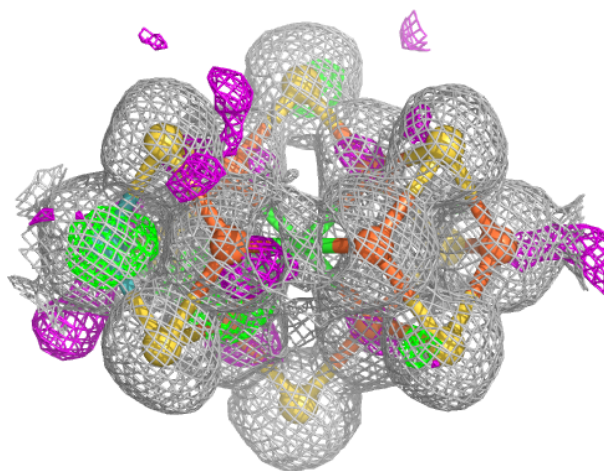
Electron density around ICE A 510 (B):

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



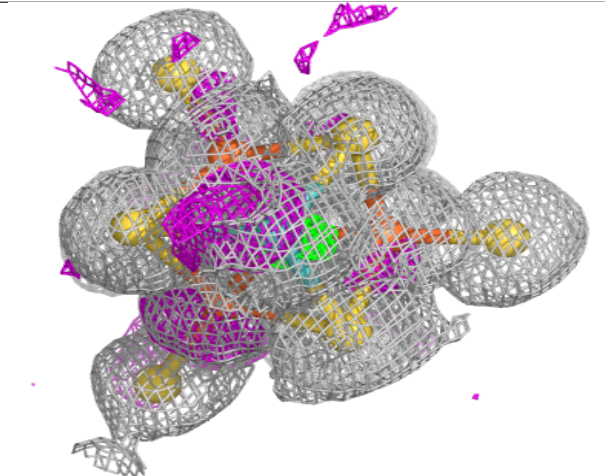
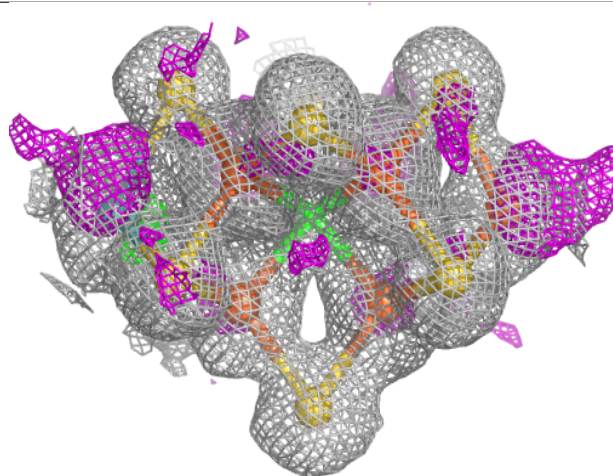
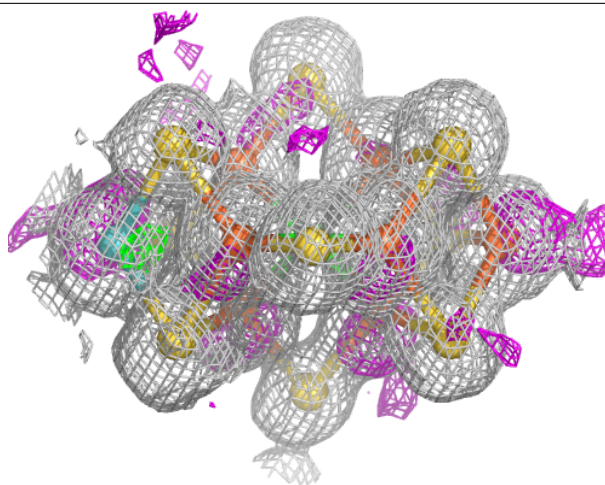
Electron density around ICE C 506 (B):

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



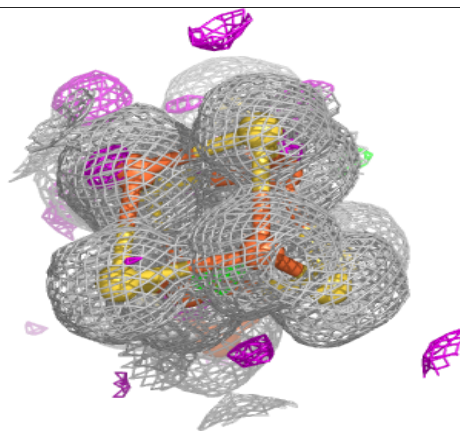
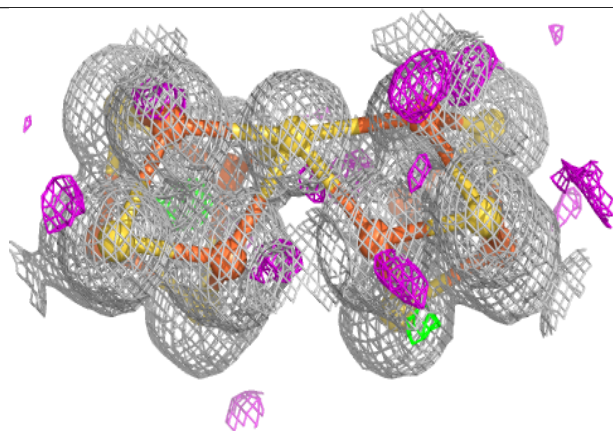
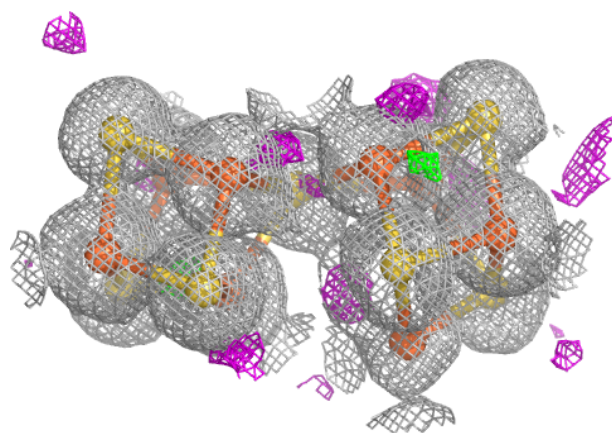
Electron density around ICS A 509 (A):

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



Electron density around A1JPX C 507 (B):

$2mF_o-DF_c$ (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.