



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 22, 2026 – 09:59 pm BST

PDB ID : 9SPZ / pdb_00009spz
Title : Crystal structure of the Molybdenum-containing nitrogenase from Methanocaldococcus infernus refined to 1.37 Å resolution - crystalline form A
Authors : Maslac, N.; Torer, M.R.; Bolte, P.; Wagner, T.
Deposited on : 2025-09-18
Resolution : 1.37 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

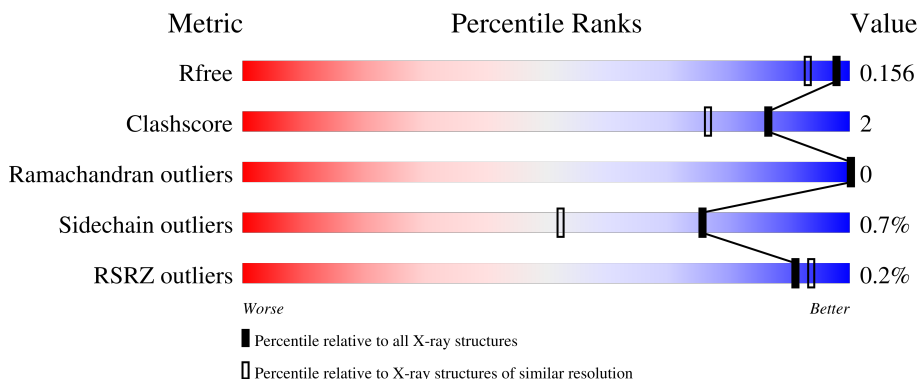
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.37 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	4403 (1.40-1.36)
Clashscore	190562	4528 (1.40-1.36)
Ramachandran outliers	187476	4459 (1.40-1.36)
Sidechain outliers	187428	4458 (1.40-1.36)
RSRZ outliers	180081	4399 (1.40-1.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	477	95% ..
1	C	477	% 94% 5% .
2	B	462	93% 7%
2	D	462	94% 6%

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 32198 atoms, of which 15347 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.

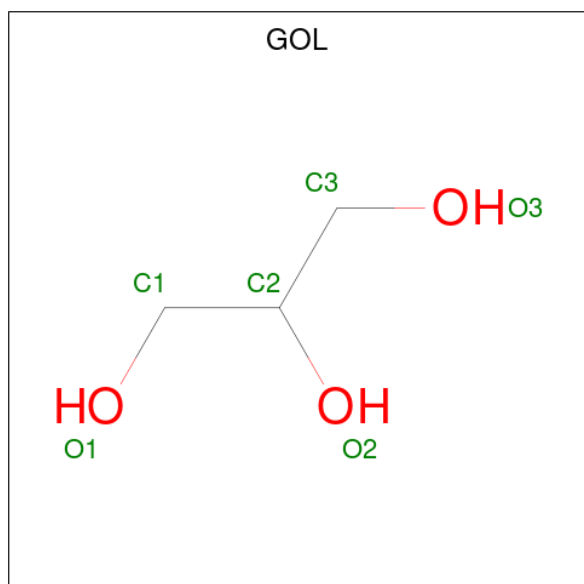
- Molecule 1 is a protein called Nitrogenase protein alpha chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	474	Total	C	H	N	O	S	0	14	0
			7768	2499	3883	658	702	26			
1	C	473	Total	C	H	N	O	S	0	2	0
			7623	2460	3802	644	692	25			

- Molecule 2 is a protein called Nitrogenase.

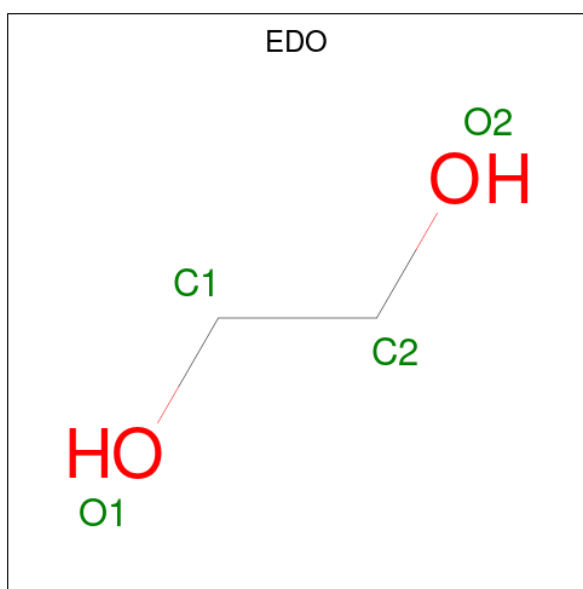
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	461	Total	C	H	N	O	S	0	28	0
			7555	2420	3793	632	692	18			
2	D	461	Total	C	H	N	O	S	0	11	0
			7406	2379	3710	619	680	18			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			13	3	7	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	C	1	Total	C	H	O	0	0
			14	3	8	3		
3	D	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



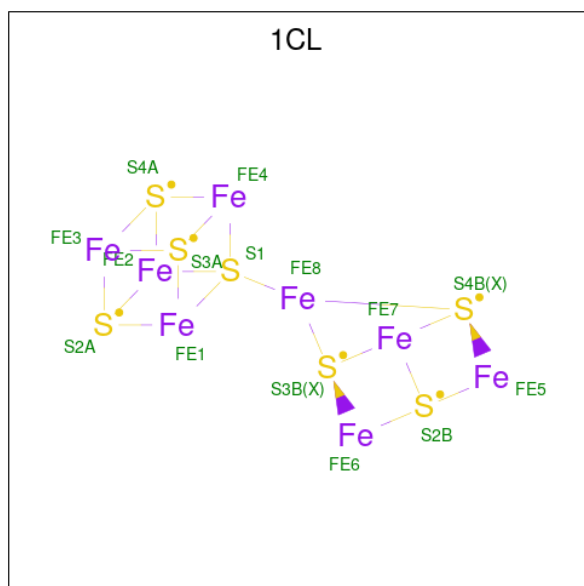
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		

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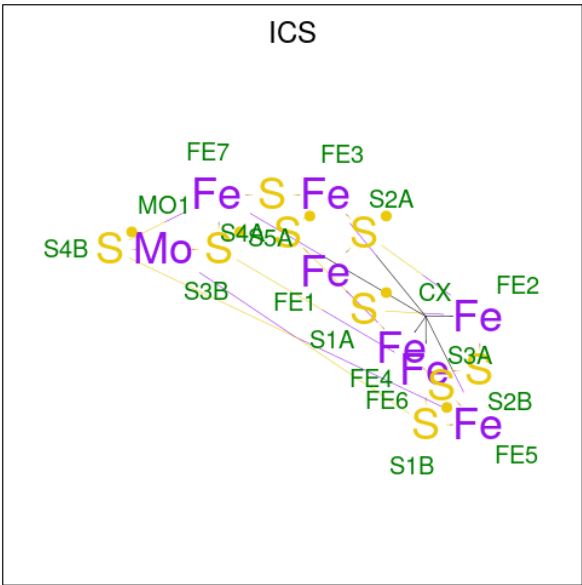
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	C	1	Total	C	H	O	0	0
			10	2	6	2		
4	C	1	Total	C	H	O	0	0
			10	2	6	2		
4	C	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 5 is FE(8)-S(7) CLUSTER, OXIDIZED (CCD ID: 1CL) (formula: Fe_8S_7) (labeled as "Ligand of Interest" by depositor).



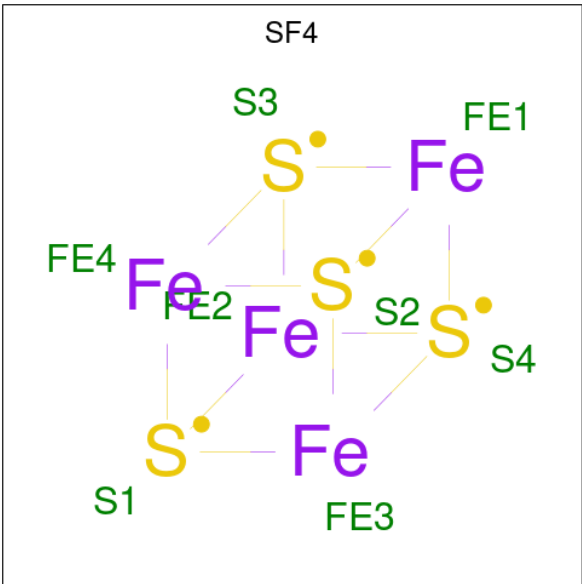
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Fe	S	0	1
			15	8	7		
5	C	1	Total	Fe	S	0	0
			15	8	7		

- Molecule 6 is iron-sulfur-molybdenum cluster with interstitial carbon (CCD ID: ICS) (formula: CFe_7MoS_9) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 7 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).

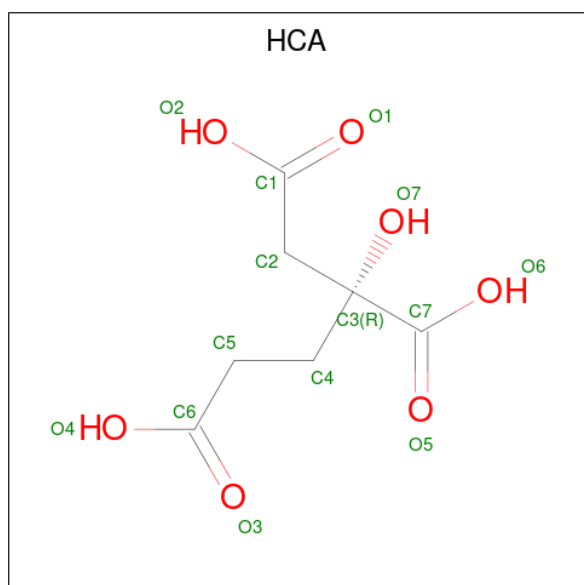


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	Fe	S	0	1
			8	4	4		

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

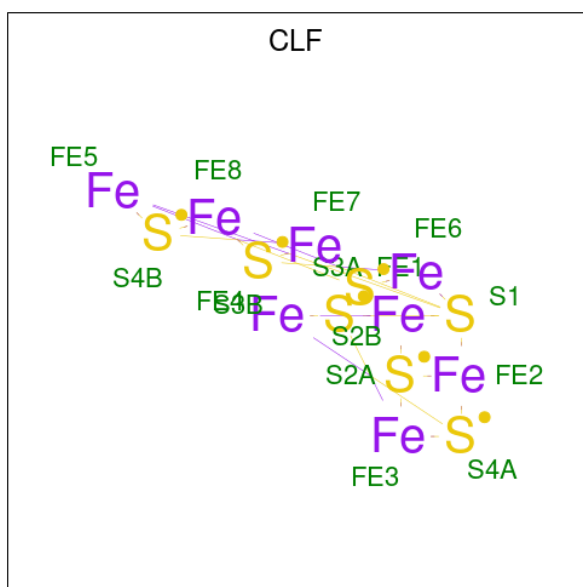
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl	0	0
			1	1		
8	B	2	Total	Cl	0	0
			2	2		
8	C	1	Total	Cl	0	0
			1	1		
8	D	1	Total	Cl	0	0
			1	1		

- Molecule 9 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (CCD ID: HCA) (formula: C₇H₁₀O₇) (labeled as "Ligand of Interest" by depositor).



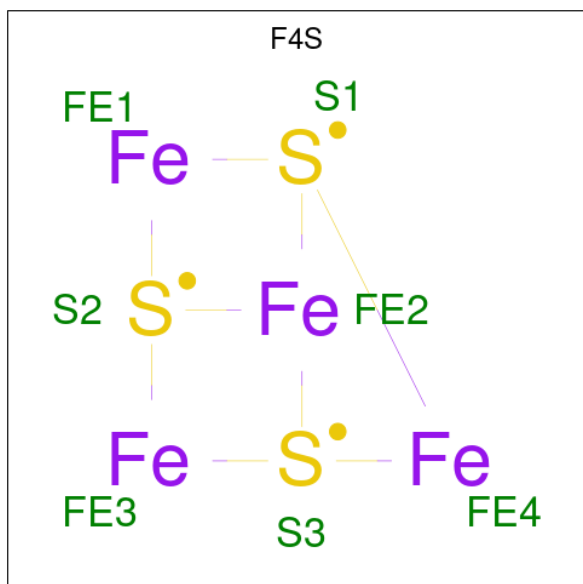
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	H	O	0	0
			20	7	6	7		
9	C	1	Total	C	H	O	0	0
			20	7	6	7		

- Molecule 10 is FE(8)-S(7) CLUSTER (CCD ID: CLF) (formula: Fe₈S₇) (labeled as "Ligand of Interest" by depositor).



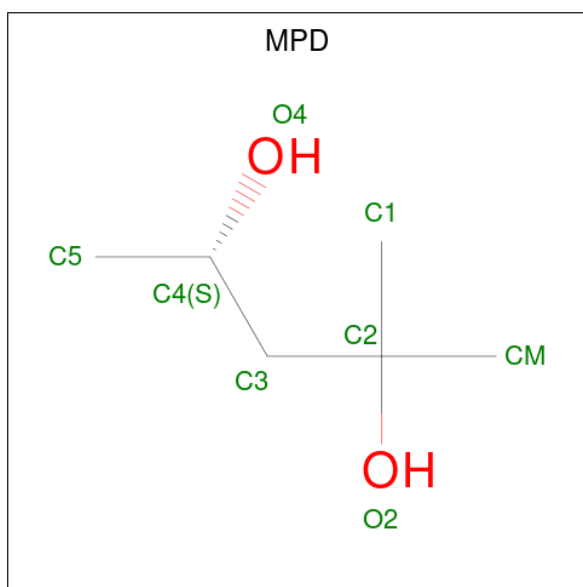
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	Fe	S	0	1
			15	8	7		

- Molecule 11 is FE4-S3 CLUSTER (CCD ID: F4S) (formula: Fe_4S_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	Fe	S	0	1
			7	4	3		

- Molecule 12 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $\text{C}_6\text{H}_{14}\text{O}_2$).



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

- Molecule 13 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

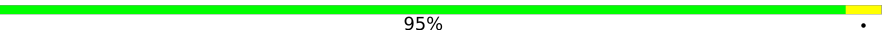
- Molecule 14 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	418	Total O 418 418	0	8
14	B	443	Total O 443 443	0	27
14	C	245	Total O 245 245	0	10
14	D	348	Total O 348 348	0	13

3 Residue-property plots [i](#)

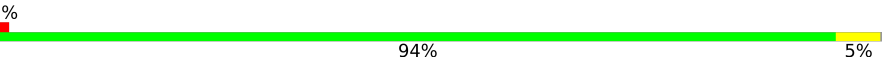
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

Chain A:  95% ..

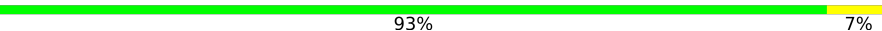


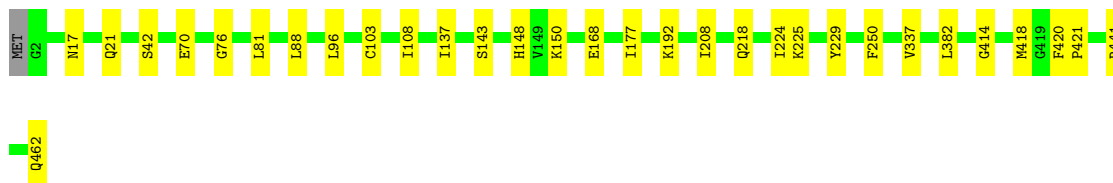
- Molecule 1: Nitrogenase protein alpha chain

Chain C:  94% 5% .

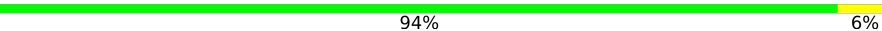


- Molecule 2: Nitrogenase

Chain B:  93% 7%



- Molecule 2: Nitrogenase

Chain D:  94% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.43Å 117.18Å 106.63Å 90.00° 91.48° 90.00°	Depositor
Resolution (Å)	21.91 – 1.37 21.91 – 1.37	Depositor EDS
% Data completeness (in resolution range)	67.9 (21.91-1.37) 68.0 (21.91-1.37)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 1.37Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.123 , 0.156 0.124 , 0.156	Depositor DCC
R_{free} test set	13626 reflections (3.39%)	wwPDB-VP
Wilson B-factor (Å ²)	16.0	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	32198	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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: MG, EDO, MPD, 1CL, GOL, F4S, CLF, HCA, SF4, CL, ICS

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	0.48	0/4041	0.71	0/5442
1	C	0.50	0/3927	0.74	0/5296
2	B	0.49	1/3955 (0.0%)	0.71	2/5349 (0.0%)
2	D	0.49	0/3818	0.71	0/5166
All	All	0.49	1/15741 (0.0%)	0.72	2/21253 (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	1
1	C	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	70	GLU	C-N	-6.22	1.25	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	225[A]	LYS	N-CA-C	-5.04	108.16	114.56
2	B	225[B]	LYS	N-CA-C	-5.04	108.16	114.56

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	80[A]	ARG	Sidechain
1	C	80	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	3885	3883	3811	16	0
1	C	3821	3802	3788	17	0
2	B	3762	3793	3680	17	0
2	D	3696	3710	3672	16	0
3	A	30	40	40	0	0
3	B	12	15	15	0	0
3	C	6	8	8	0	0
3	D	6	8	8	0	0
4	A	8	12	12	0	0
4	B	12	18	18	1	0
4	C	12	18	18	0	0
5	A	15	0	0	2	0
5	C	15	0	0	0	0
6	A	18	0	0	0	0
6	C	18	0	0	1	0
7	A	8	0	0	1	0
8	A	1	0	0	0	0
8	B	2	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	1	0
9	A	14	6	6	2	0
9	C	14	6	6	2	0
10	B	15	0	0	2	0
11	B	7	0	0	1	0
12	B	16	28	28	0	0
13	B	2	0	0	0	0
14	A	418	0	0	0	0
14	B	443	0	0	0	0
14	C	245	0	0	0	0
14	D	348	0	0	0	0
All	All	16851	15347	15110	64	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 64 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:20:CYS:HB2	2:D:143:SER:HB2	1.83	0.60
1:A:430:HIS:HB3	9:A:512:HCA:O5	2.08	0.53
2:B:224[B]:ILE:HD13	2:B:229:TYR:CD1	2.43	0.53
2:D:337:VAL:HG21	2:D:418[A]:MET:SD	2.49	0.52
1:C:224:LYS:HB3	1:C:225:PRO:HD3	1.92	0.52

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	486/477 (102%)	467 (96%)	19 (4%)	0	100	100
1	C	473/477 (99%)	453 (96%)	20 (4%)	0	100	100
2	B	487/462 (105%)	476 (98%)	11 (2%)	0	100	100
2	D	470/462 (102%)	460 (98%)	10 (2%)	0	100	100
All	All	1916/1878 (102%)	1856 (97%)	60 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	420/410 (102%)	418 (100%)	2 (0%)	81	62
1	C	408/410 (100%)	406 (100%)	2 (0%)	81	62
2	B	414/391 (106%)	409 (99%)	5 (1%)	63	33
2	D	399/391 (102%)	395 (99%)	4 (1%)	68	40
All	All	1641/1602 (102%)	1628 (99%)	13 (1%)	76	48

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	82	ASN
1	C	339	VAL
2	D	462	GLN
2	D	441[A]	ARG
2	D	441[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	434	GLN
2	B	43	GLN
1	C	162	ASN
1	C	445	ASN
2	D	80	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 35 ligands modelled in this entry, 7 are monoatomic - leaving 28 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$
4	EDO	C	503	-	3,3,3	0.11	0	2,2,2	0.08	0
12	MPD	B	509	-	7,7,7	0.37	0	9,10,10	0.64	0
4	EDO	C	502	-	3,3,3	0.07	0	2,2,2	0.21	0
3	GOL	A	506	-	5,5,5	0.09	0	5,5,5	0.33	0
5	1CL	A	507[A]	1,2	0,22,22	-	-	-	-	-
4	EDO	B	505	-	3,3,3	0.06	0	2,2,2	0.18	0
6	ICS	C	506	9,1	18,30,30	2.55	11 (61%)	-	-	-
3	GOL	C	504	-	5,5,5	0.08	0	5,5,5	0.30	0
3	GOL	A	505	-	5,5,5	0.09	0	5,5,5	0.30	0
6	ICS	A	508	9,1	18,30,30	2.93	12 (66%)	-	-	-
11	F4S	B	502[C]	1,2,14	0,9,9	-	-	-	-	-
3	GOL	A	501	-	5,5,5	0.89	0	5,5,5	0.66	0
3	GOL	A	503	-	5,5,5	0.81	0	5,5,5	0.97	0
4	EDO	C	501	-	3,3,3	0.48	0	2,2,2	0.53	0
3	GOL	B	504	-	5,5,5	1.35	1 (20%)	5,5,5	0.98	0
7	SF4	A	509[C]	1,2	0,12,12	-	-	-	-	-
3	GOL	A	502	-	5,5,5	0.78	0	5,5,5	0.63	0
3	GOL	D	501	-	5,5,5	0.09	0	5,5,5	0.33	0
4	EDO	A	510	-	3,3,3	0.06	0	2,2,2	0.25	0
4	EDO	B	506	-	3,3,3	0.07	0	2,2,2	0.21	0
12	MPD	B	503	-	7,7,7	0.34	0	9,10,10	0.39	0
4	EDO	B	507	-	3,3,3	0.06	0	2,2,2	0.17	0
10	CLF	B	501[B]	1,2	0,24,24	-	-	-	-	-
9	HCA	A	512	6	13,13,13	1.18	2 (15%)	14,18,18	1.51	2 (14%)
5	1CL	C	505	1,2	0,22,22	-	-	-	-	-
3	GOL	B	508	-	5,5,5	0.09	0	5,5,5	0.31	0
4	EDO	A	504	-	3,3,3	0.08	0	2,2,2	0.18	0
9	HCA	C	508	6	13,13,13	1.18	2 (15%)	14,18,18	1.57	3 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	C	503	-	-	1/1/1/1	-
12	MPD	B	509	-	-	0/5/5/5	-
4	EDO	C	502	-	-	1/1/1/1	-
3	GOL	A	506	-	-	2/4/4/4	-
5	1CL	A	507[A]	1,2	-	-	0/10/8/8
4	EDO	B	505	-	-	0/1/1/1	-
3	GOL	C	504	-	-	1/4/4/4	-
3	GOL	A	505	-	-	4/4/4/4	-
11	F4S	B	502[C]	1,2,14	-	-	0/4/3/3
3	GOL	A	501	-	-	4/4/4/4	-
3	GOL	A	503	-	-	0/4/4/4	-
4	EDO	C	501	-	-	1/1/1/1	-
3	GOL	B	504	-	-	2/4/4/4	-
7	SF4	A	509[C]	1,2	-	-	0/6/5/5
3	GOL	A	502	-	-	2/4/4/4	-
3	GOL	D	501	-	-	4/4/4/4	-
4	EDO	A	510	-	-	1/1/1/1	-
4	EDO	B	506	-	-	0/1/1/1	-
12	MPD	B	503	-	-	0/5/5/5	-
4	EDO	B	507	-	-	1/1/1/1	-
10	CLF	B	501[B]	1,2	-	-	0/12/10/10
9	HCA	A	512	6	-	4/17/17/17	-
5	1CL	C	505	1,2	-	-	0/10/8/8
3	GOL	B	508	-	-	4/4/4/4	-
4	EDO	A	504	-	-	0/1/1/1	-
9	HCA	C	508	6	-	4/17/17/17	-

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	508	ICS	S4B-FE7	-4.90	2.20	2.32
6	A	508	ICS	S3B-FE7	-4.50	2.21	2.32
6	A	508	ICS	S1B-FE6	-4.41	2.21	2.32
6	A	508	ICS	S1B-FE5	-4.26	2.21	2.32
6	C	506	ICS	S1B-FE5	-4.16	2.22	2.32

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	512	HCA	O5-C7-C3	-3.71	117.00	122.25
9	C	508	HCA	O6-C7-C3	3.54	119.19	113.05
9	A	512	HCA	O6-C7-C3	2.69	117.72	113.05
9	C	508	HCA	O5-C7-C3	-2.66	118.49	122.25
9	C	508	HCA	O4-C6-C5	2.08	120.72	114.03

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

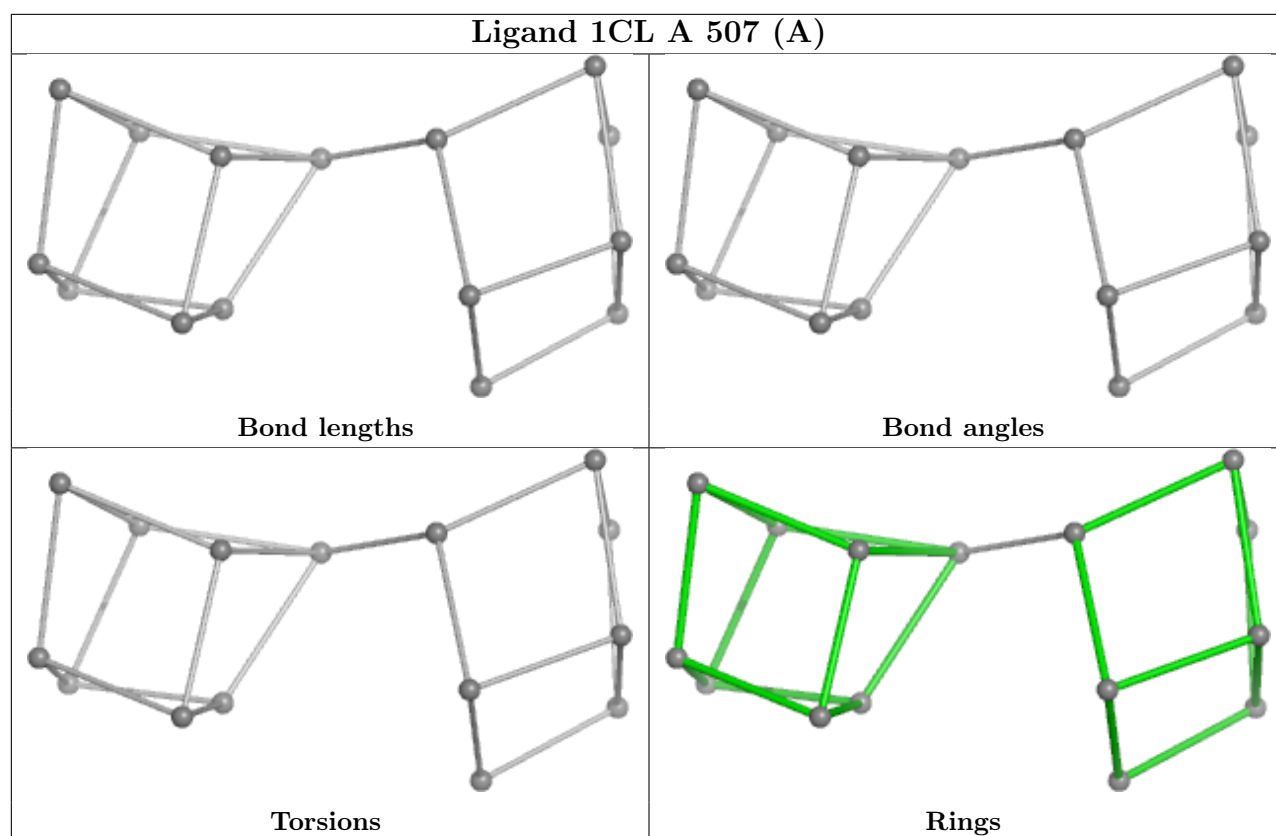
Mol	Chain	Res	Type	Atoms
3	A	501	GOL	C1-C2-C3-O3
3	A	502	GOL	C1-C2-C3-O3
3	A	506	GOL	C1-C2-C3-O3
3	A	506	GOL	O2-C2-C3-O3
3	B	508	GOL	C1-C2-C3-O3

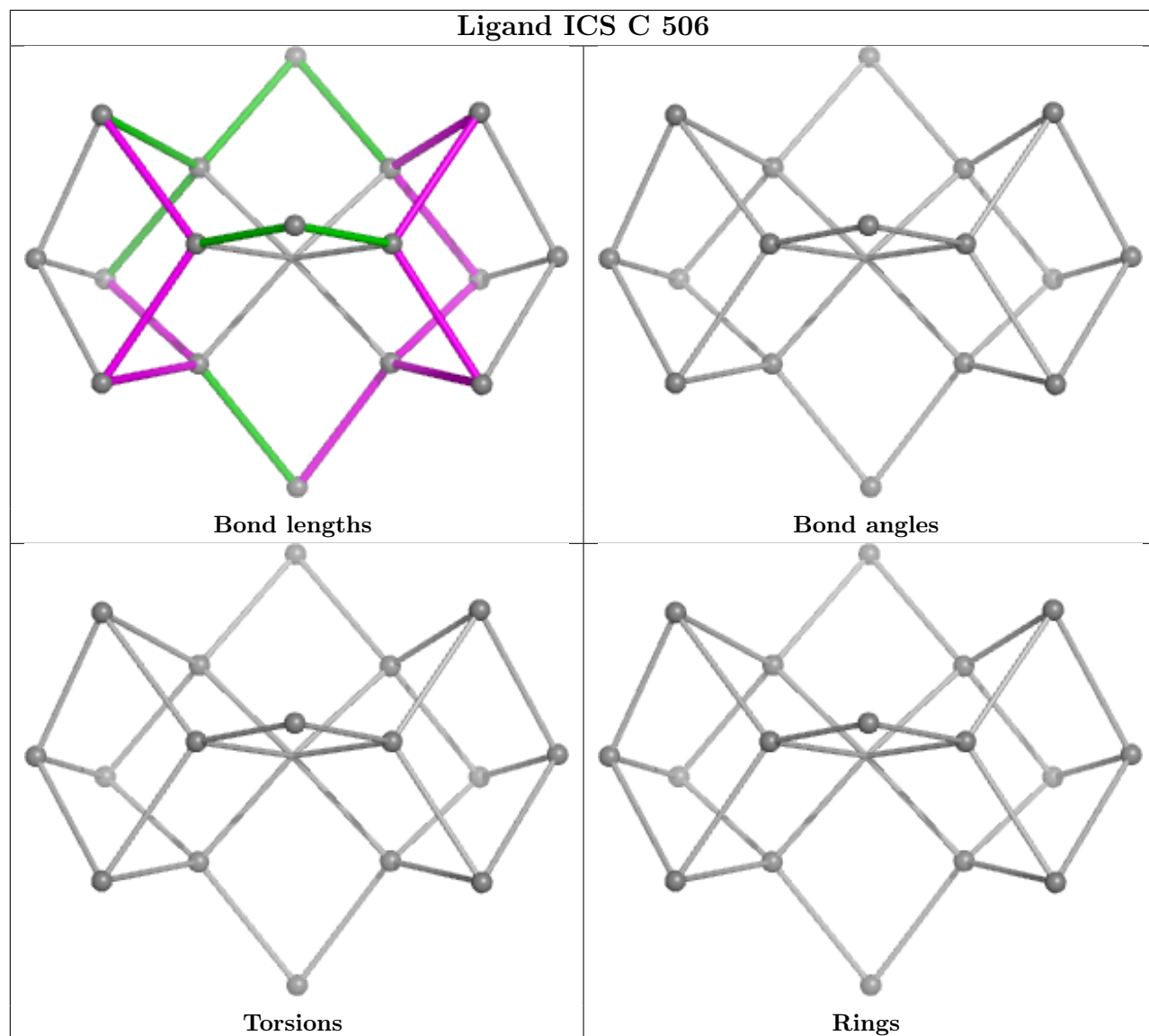
There are no ring outliers.

8 monomers are involved in 12 short contacts:

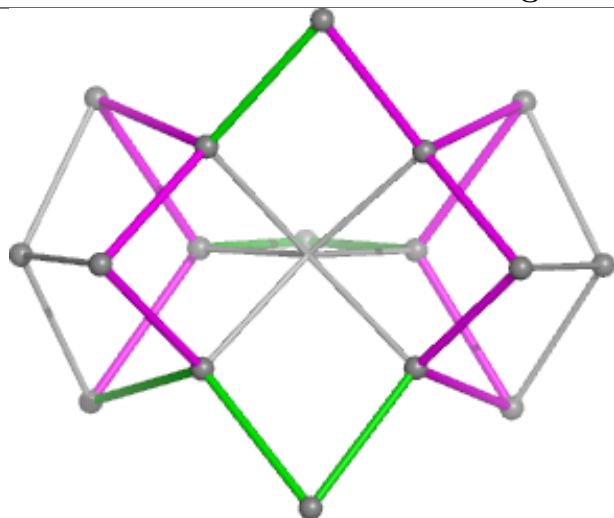
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	507[A]	1CL	2	0
6	C	506	ICS	1	0
11	B	502[C]	F4S	1	0
7	A	509[C]	SF4	1	0
4	B	507	EDO	1	0
10	B	501[B]	CLF	2	0
9	A	512	HCA	2	0
9	C	508	HCA	2	0

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.

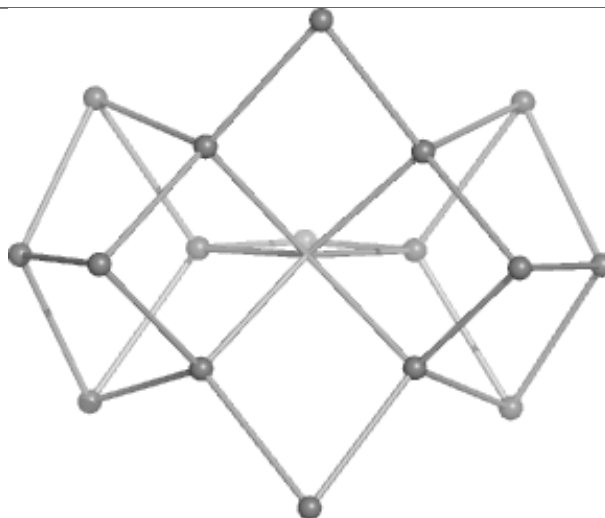




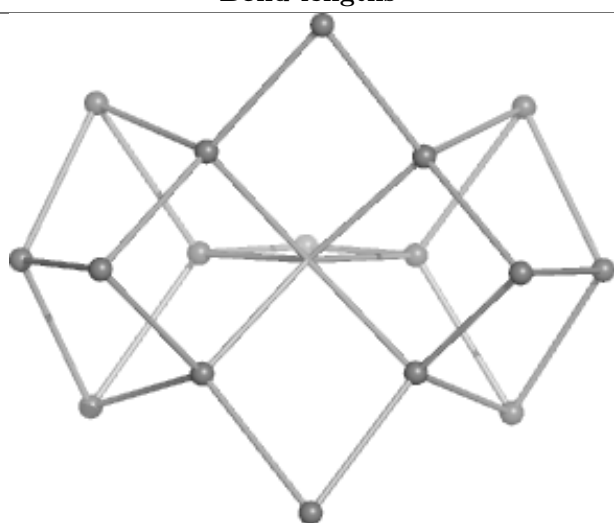
Ligand ICS A 508



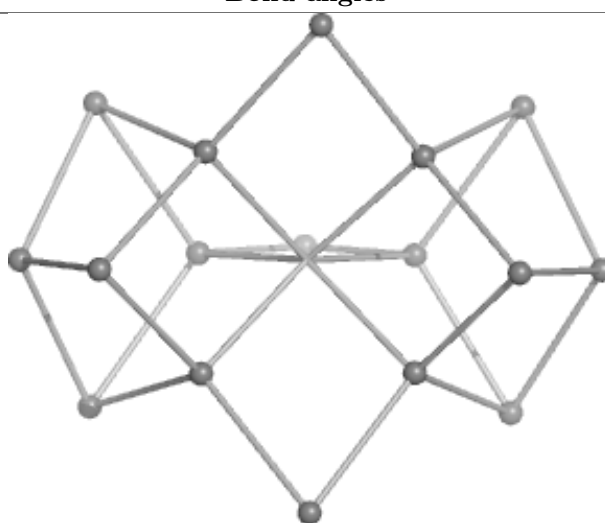
Bond lengths



Bond angles

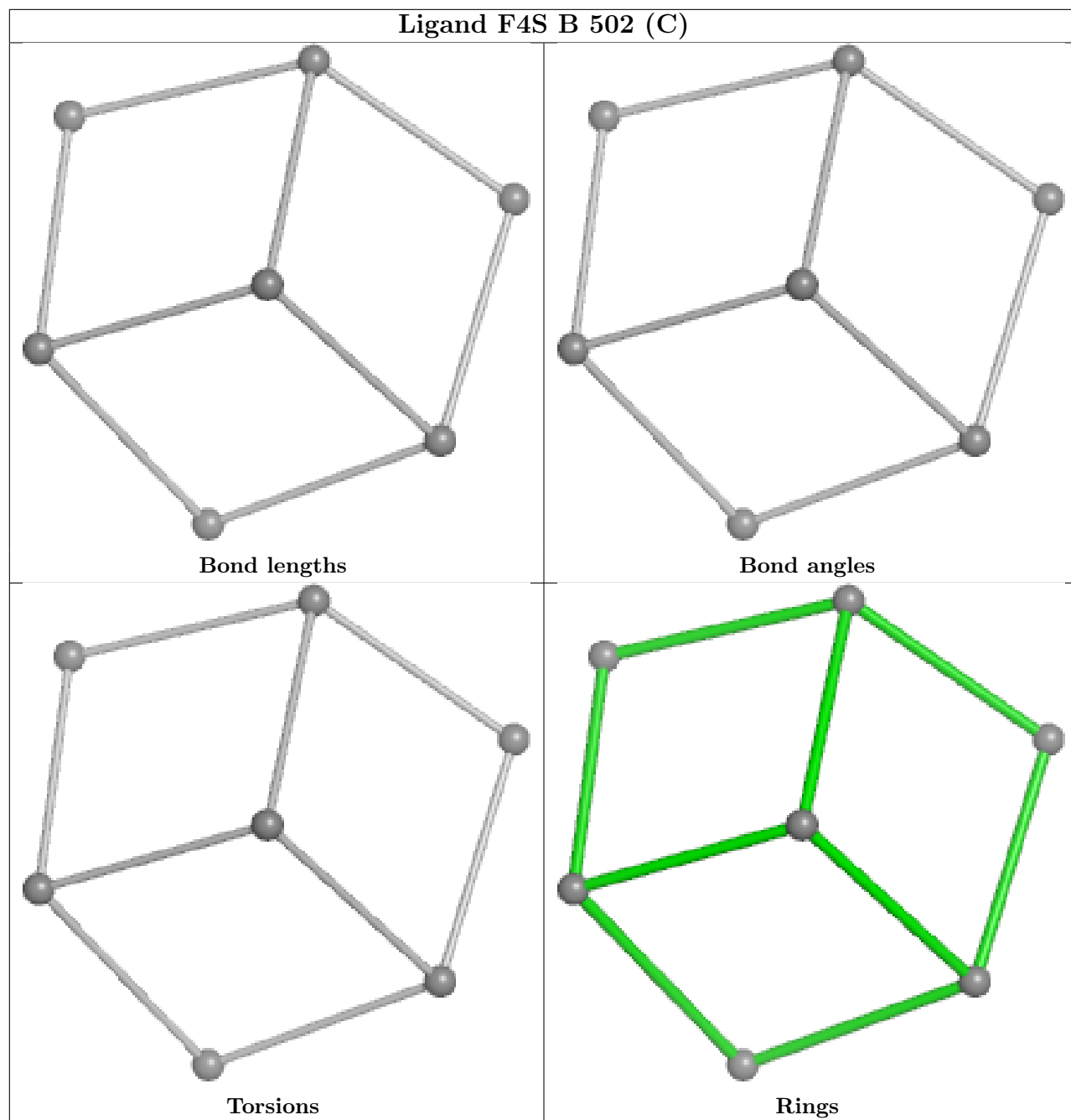


Torsions

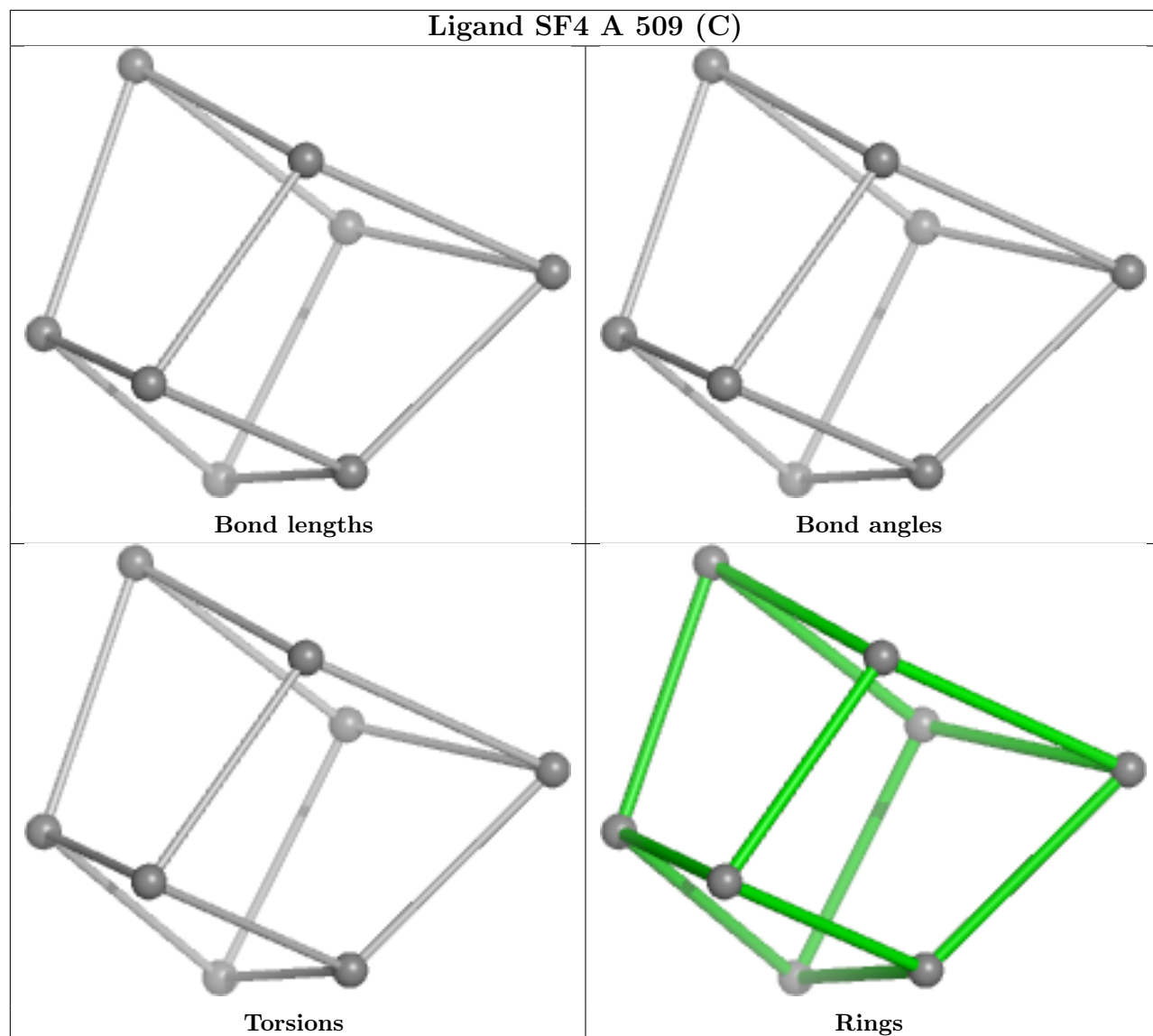


Rings

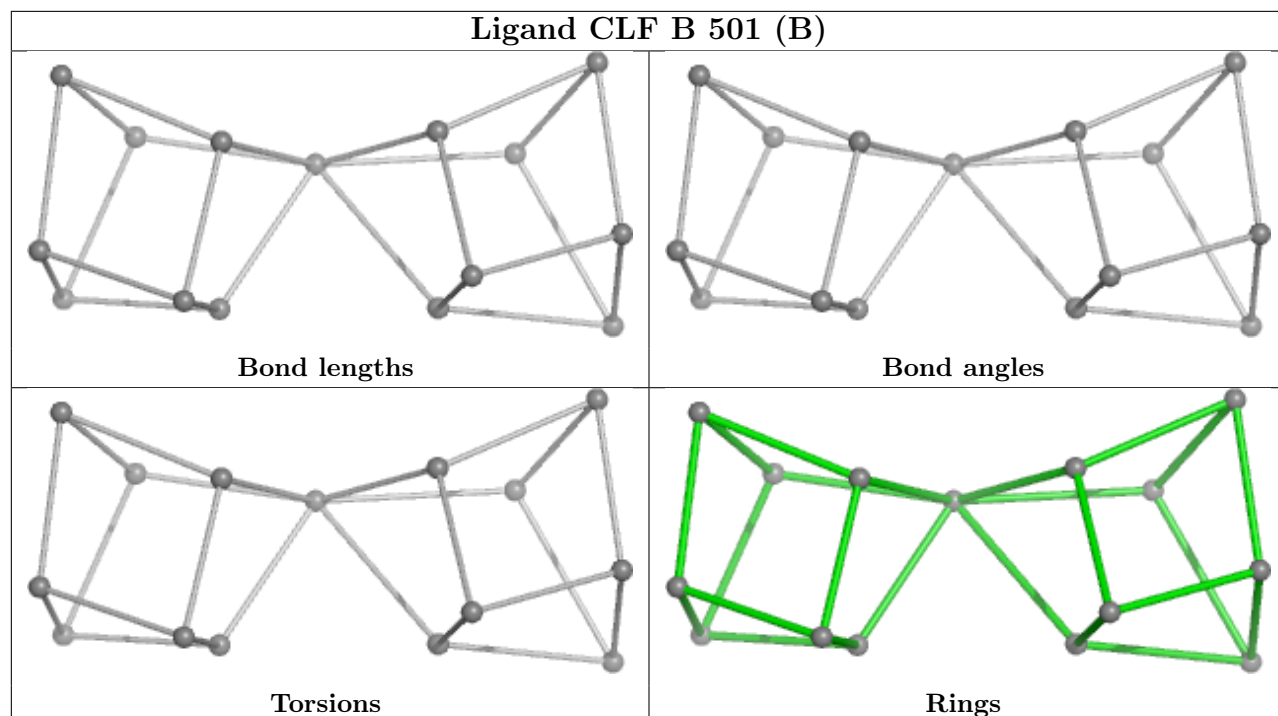
Ligand F4S B 502 (C)



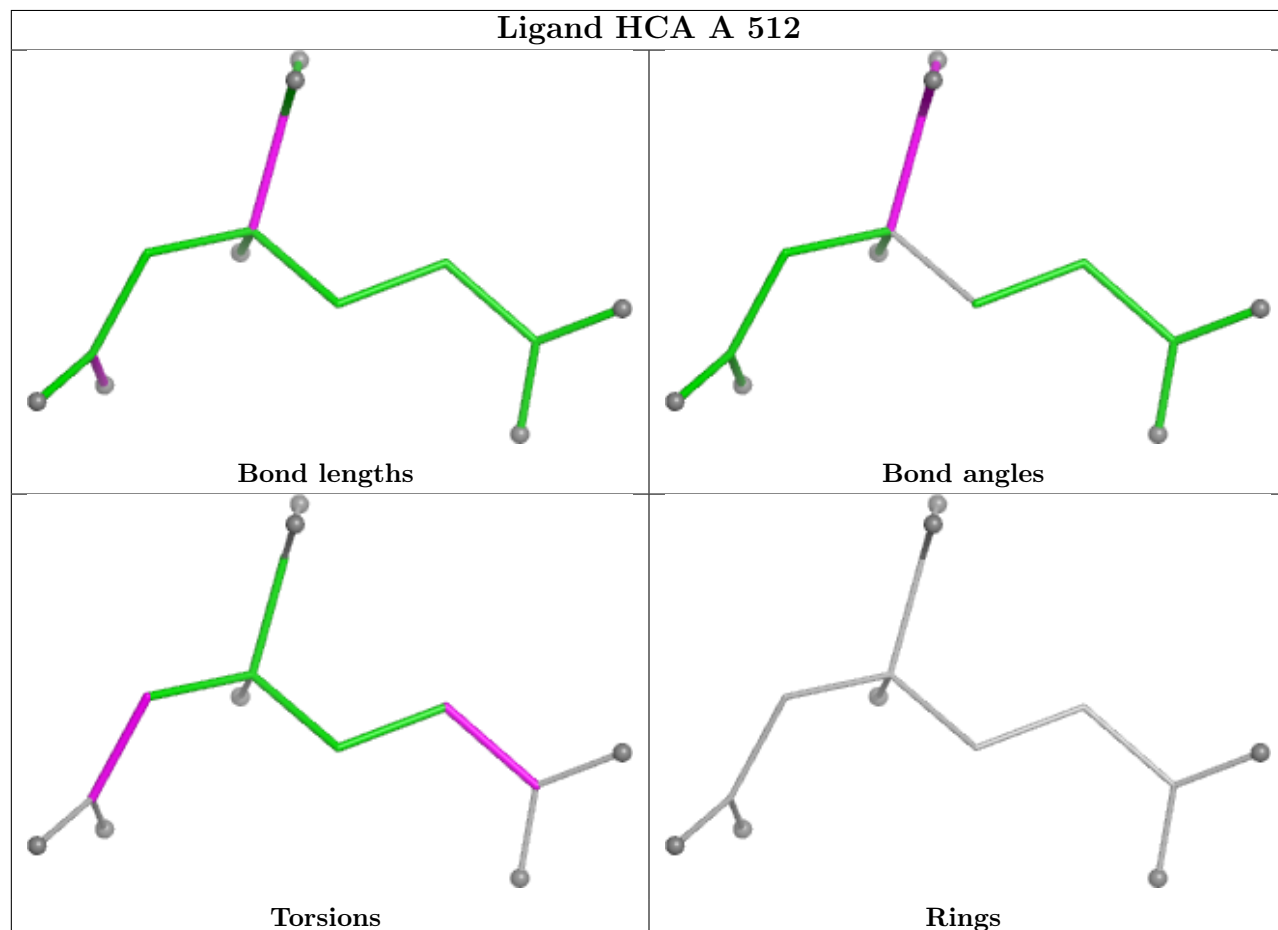
Ligand SF4 A 509 (C)

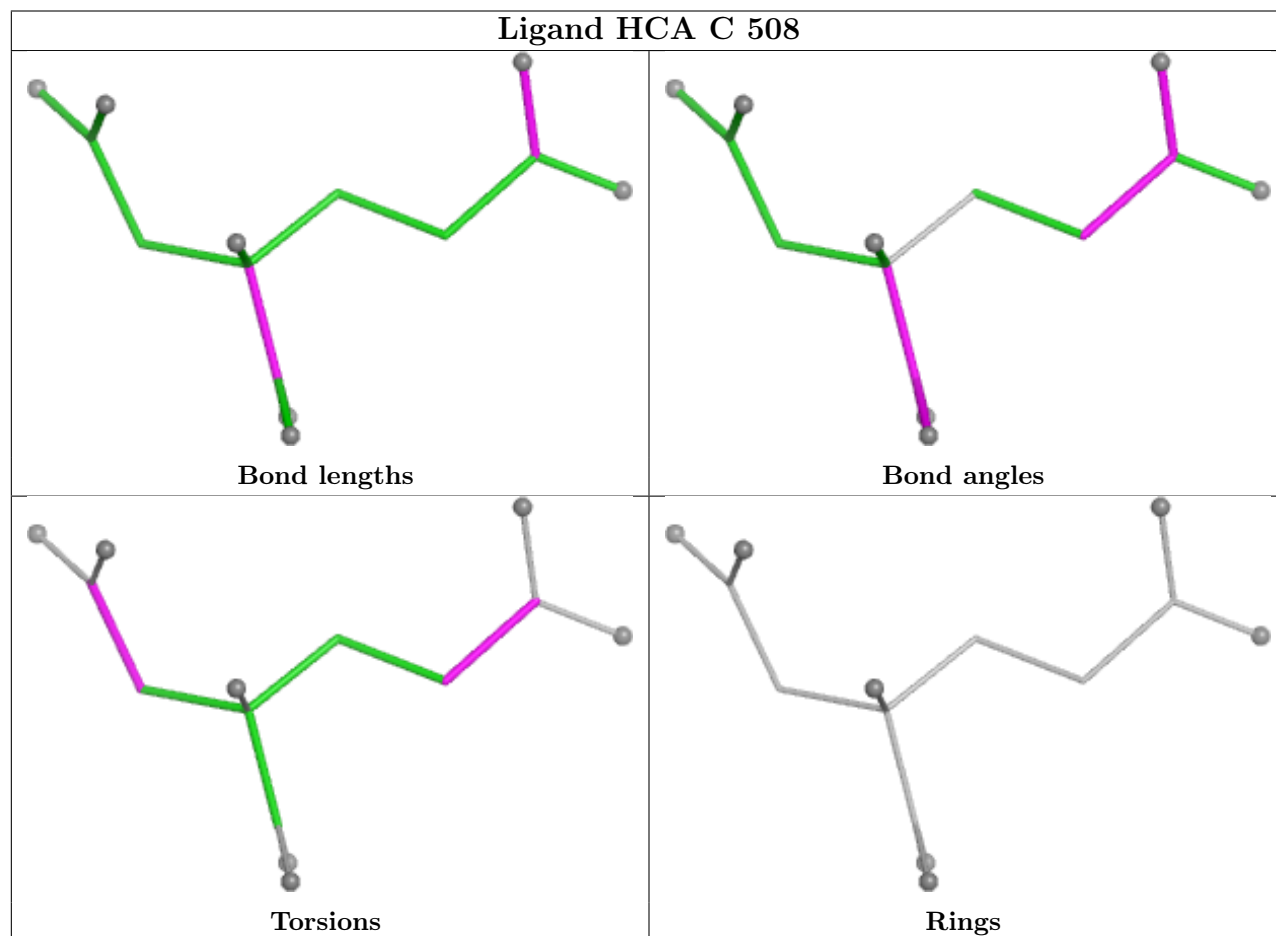
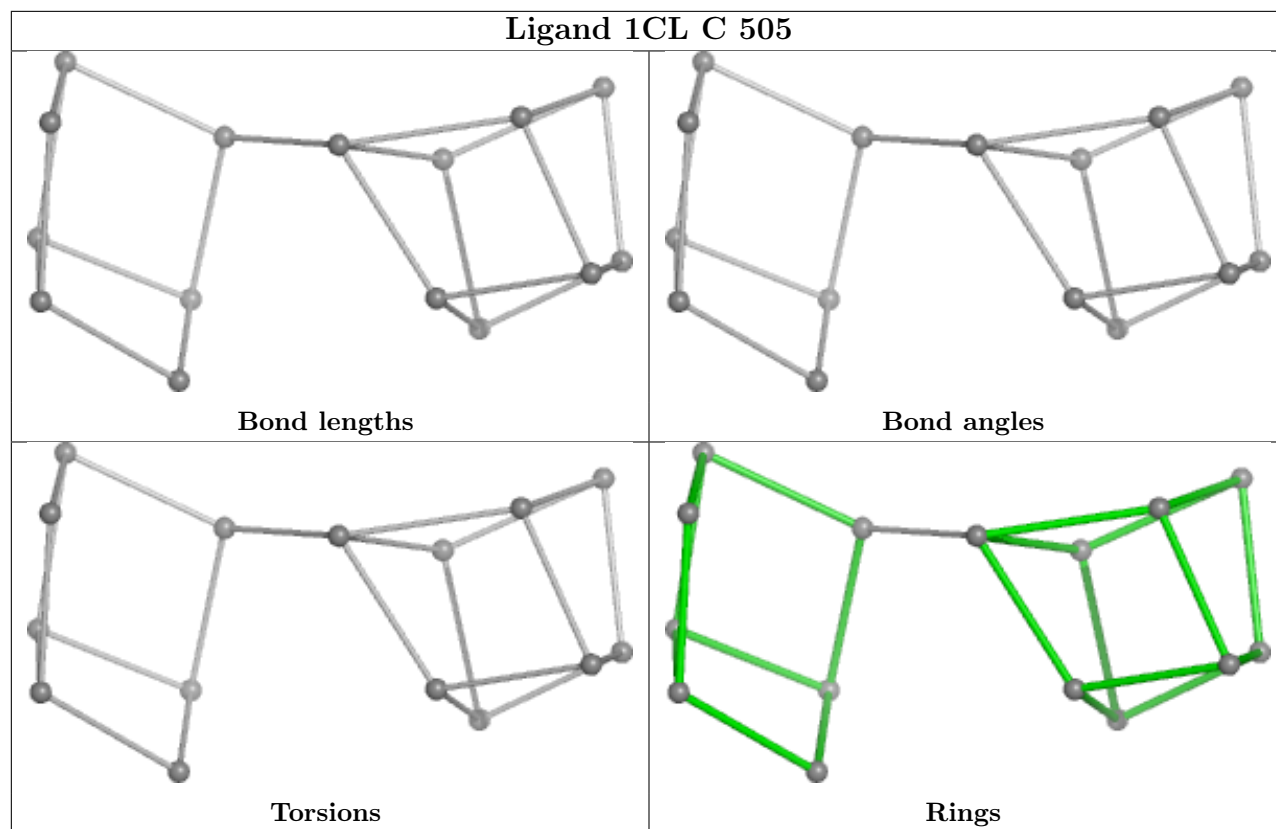


Ligand CLF B 501 (B)



Ligand HCA A 512





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	474/477 (99%)	-0.75	0 100 100	7, 19, 34, 43	7 (1%)
1	C	473/477 (99%)	-0.08	3 (0%) 85 89	15, 31, 50, 68	1 (0%)
2	B	461/462 (99%)	-0.78	0 100 100	7, 16, 32, 50	14 (3%)
2	D	461/462 (99%)	-0.41	1 (0%) 91 93	8, 25, 45, 67	6 (1%)
All	All	1869/1878 (99%)	-0.51	4 (0%) 91 93	7, 23, 43, 68	28 (1%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	248	PHE	2.4
2	D	108	ILE	2.4
1	C	26	GLU	2.4
1	C	34	ILE	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](#)

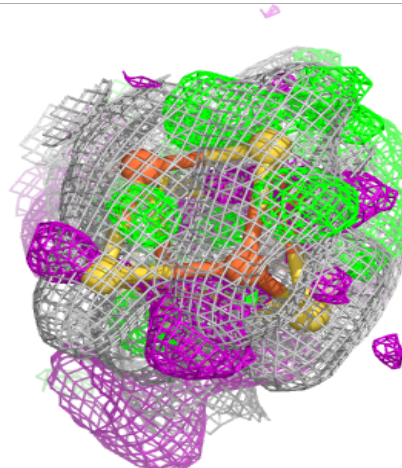
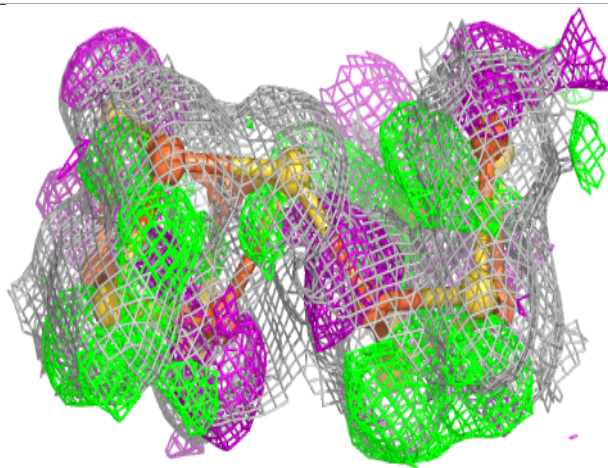
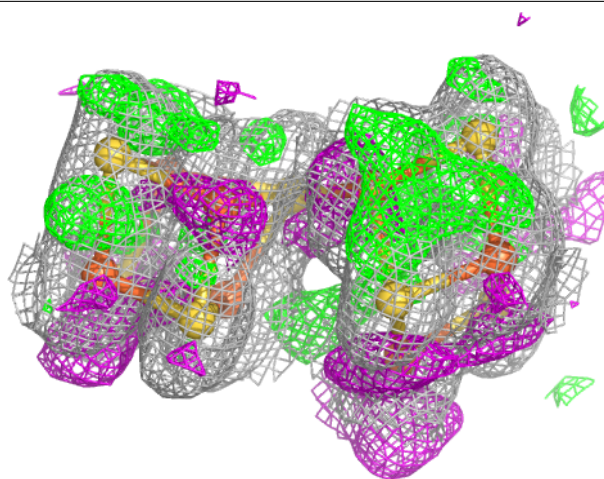
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	D	501	6/6	0.67	0.14	43,52,55,57	0
4	EDO	A	510	4/4	0.68	0.13	48,58,58,58	0
3	GOL	B	504	6/6	0.72	0.15	41,45,52,54	0
3	GOL	B	508	6/6	0.72	0.12	37,45,49,49	0
3	GOL	A	505	6/6	0.72	0.14	36,44,53,53	0
3	GOL	A	506	6/6	0.72	0.15	44,53,54,55	0
4	EDO	C	503	4/4	0.72	0.13	44,54,54,55	0
4	EDO	C	502	4/4	0.75	0.12	45,54,55,55	0
4	EDO	B	506	4/4	0.75	0.15	46,55,56,58	0
4	EDO	B	505	4/4	0.76	0.13	48,57,58,59	0
3	GOL	A	502	6/6	0.76	0.14	49,59,60,60	0
3	GOL	C	504	6/6	0.78	0.14	43,52,54,55	0
4	EDO	B	507	4/4	0.78	0.14	38,46,48,50	0
4	EDO	A	504	4/4	0.82	0.11	46,55,55,56	0
4	EDO	C	501	4/4	0.86	0.10	45,55,55,56	0
12	MPD	B	503	8/8	0.87	0.10	32,38,44,45	0
8	CL	A	511	1/1	0.90	0.11	65,65,65,65	0
3	GOL	A	501	6/6	0.90	0.10	29,41,50,53	0
3	GOL	A	503	6/6	0.91	0.08	32,39,43,44	0
8	CL	C	507	1/1	0.92	0.13	66,66,66,66	0
12	MPD	B	509	8/8	0.93	0.07	33,41,43,45	0
5	1CL	C	505	15/15	0.98	0.05	27,30,33,33	0
9	HCA	C	508	14/14	0.98	0.04	19,22,27,27	0
6	ICS	C	506	18/18	0.99	0.03	21,24,26,27	0
8	CL	D	502	1/1	0.99	0.04	44,44,44,44	0
9	HCA	A	512	14/14	0.99	0.03	9,11,12,12	0
7	SF4	A	509[C]	8/8	0.99	0.02	11,12,12,13	8
10	CLF	B	501[B]	15/15	0.99	0.03	10,11,13,13	15
11	F4S	B	502[C]	7/7	0.99	0.03	12,13,13,14	7
5	1CL	A	507[A]	15/15	0.99	0.02	11,12,14,16	15
8	CL	B	513	1/1	0.99	0.03	36,36,36,36	0
8	CL	B	512	1/1	1.00	0.03	19,19,19,19	0
6	ICS	A	508	18/18	1.00	0.02	9,11,13,13	0
13	MG	B	510	1/1	1.00	0.01	10,10,10,10	0
13	MG	B	511	1/1	1.00	0.01	15,15,15,15	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.

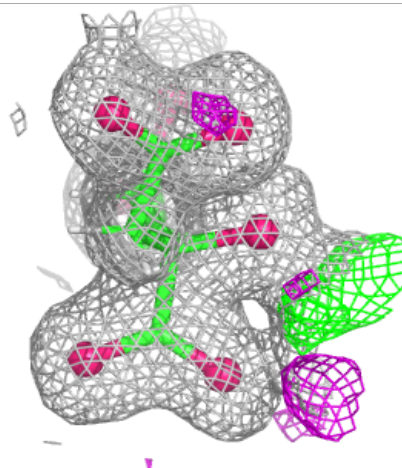
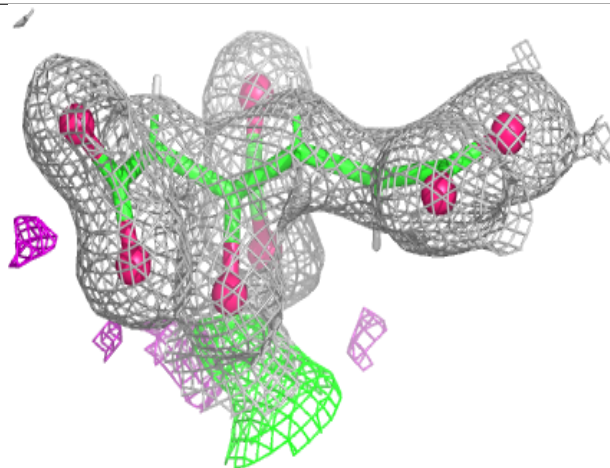
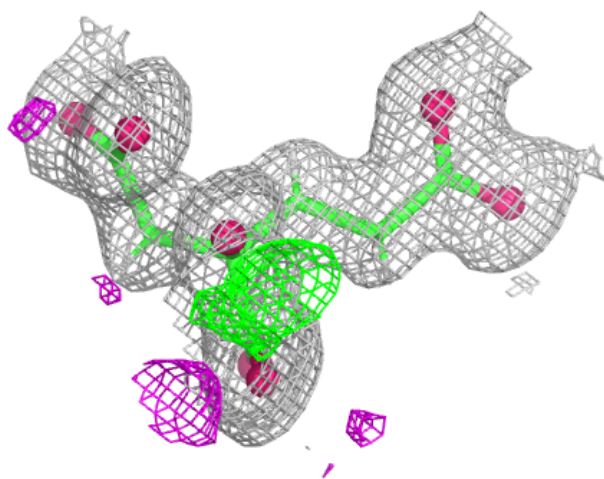
Electron density around 1CL C 505:

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



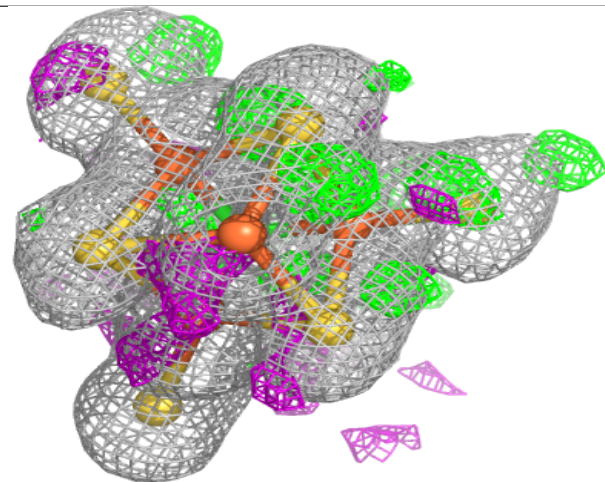
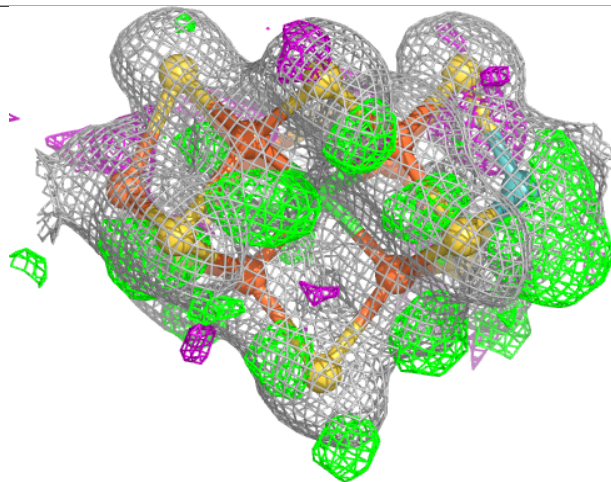
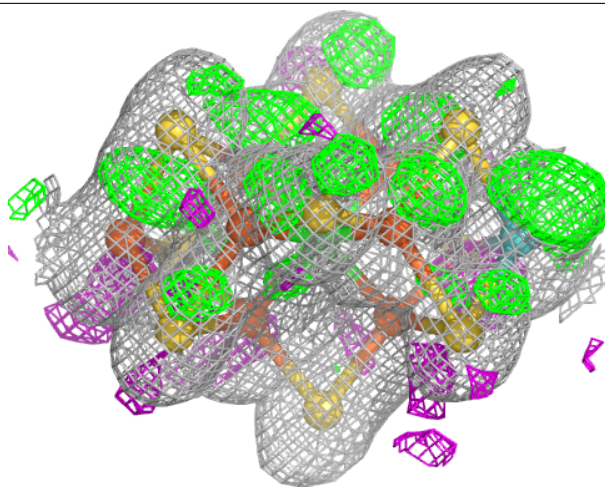
Electron density around HCA C 508:

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



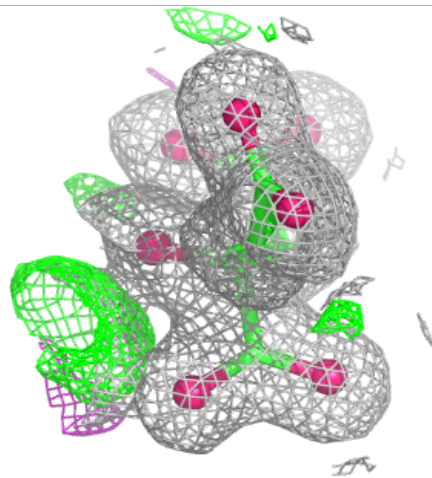
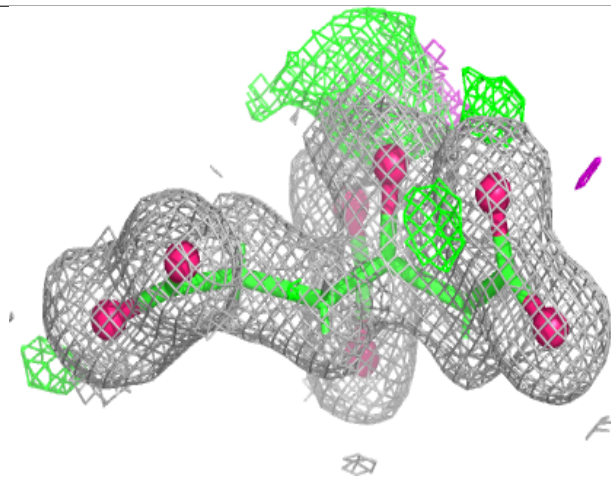
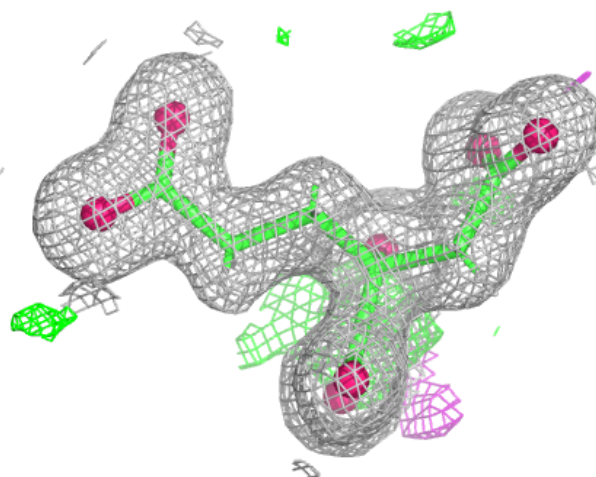
Electron density around ICS C 506:

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



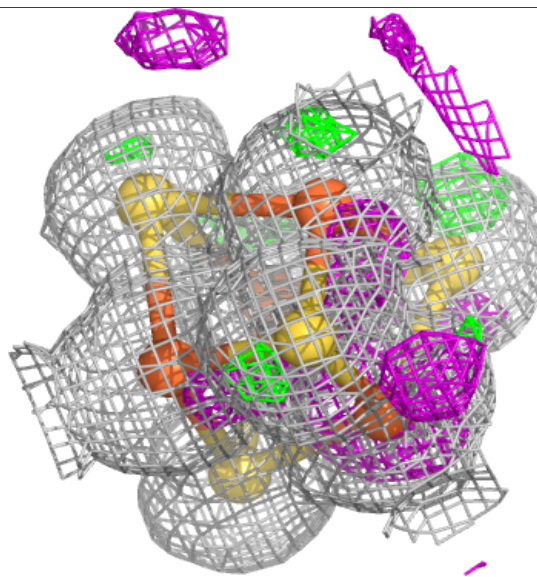
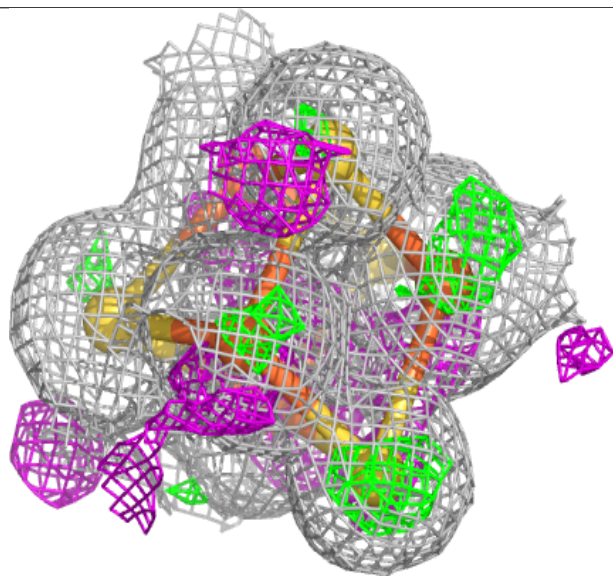
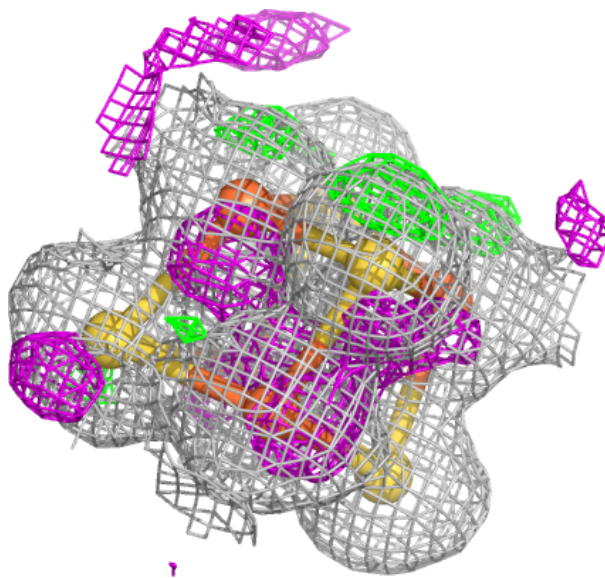
Electron density around HCA A 512:

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



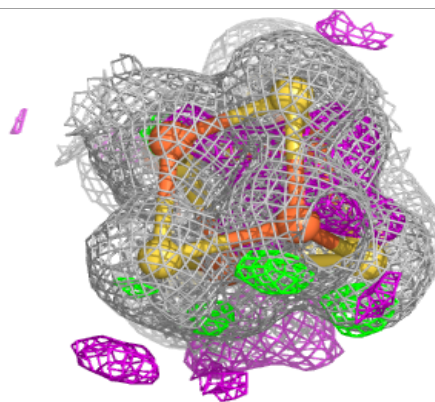
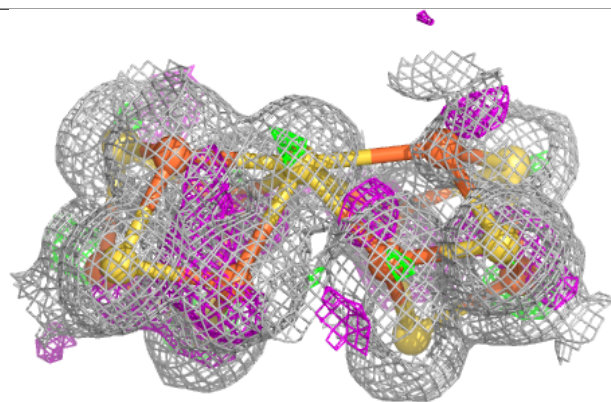
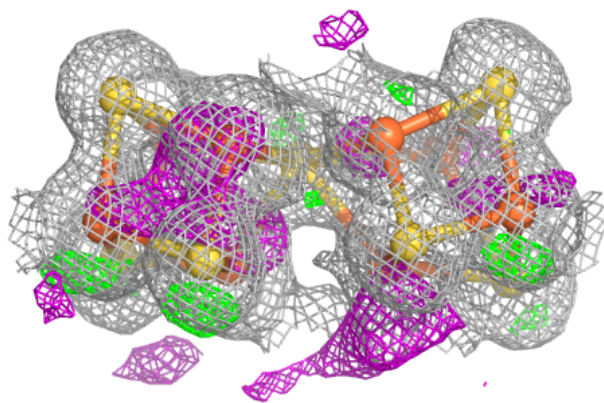
Electron density around SF4 A 509 (C):

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



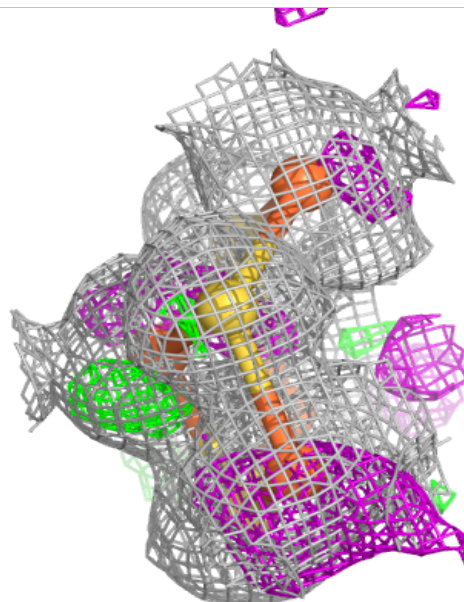
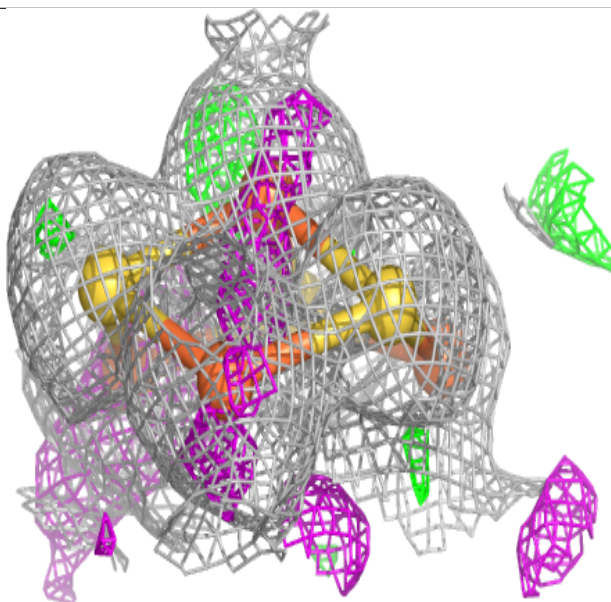
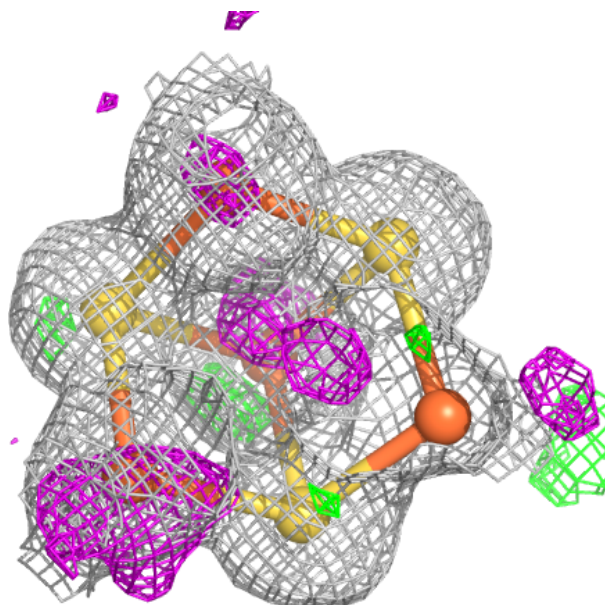
Electron density around CLF B 501 (B):

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



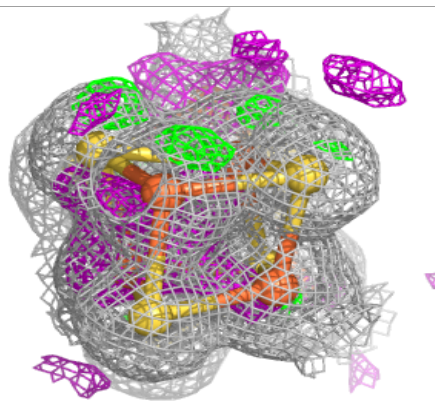
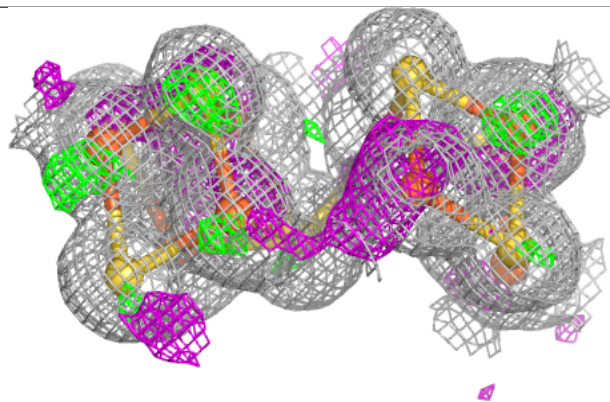
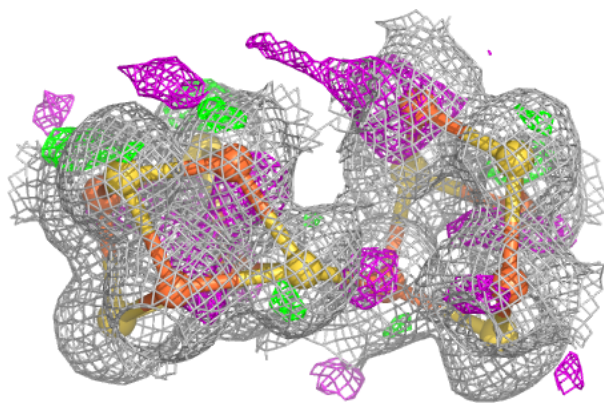
Electron density around F4S B 502 (C):

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and green (positive)



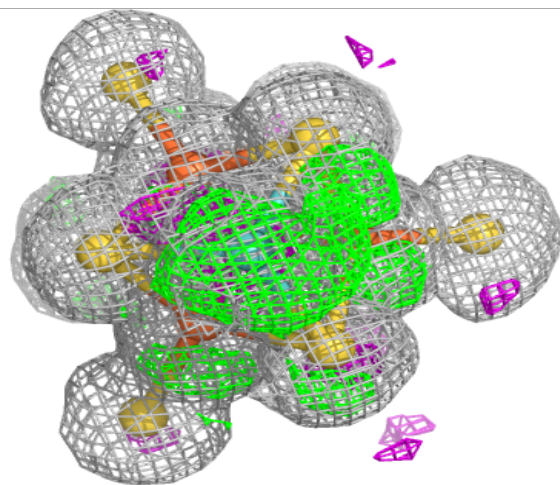
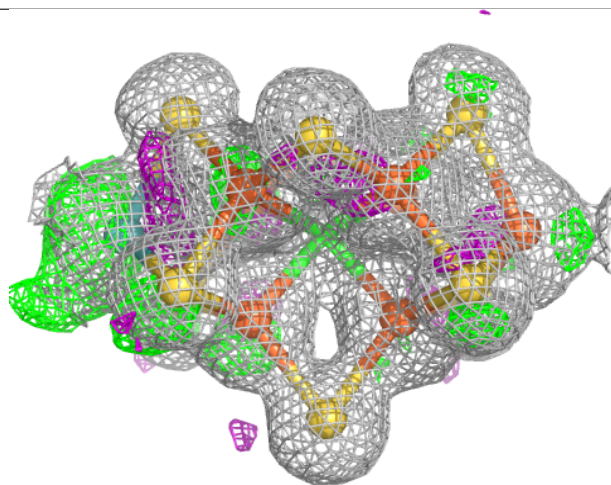
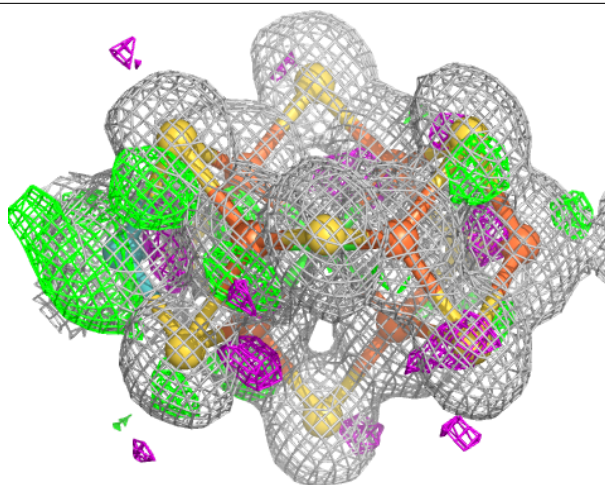
Electron density around 1CL A 507 (A):

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



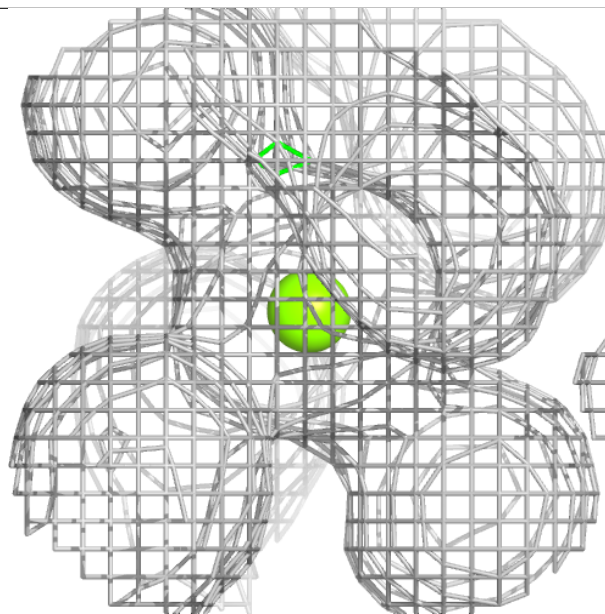
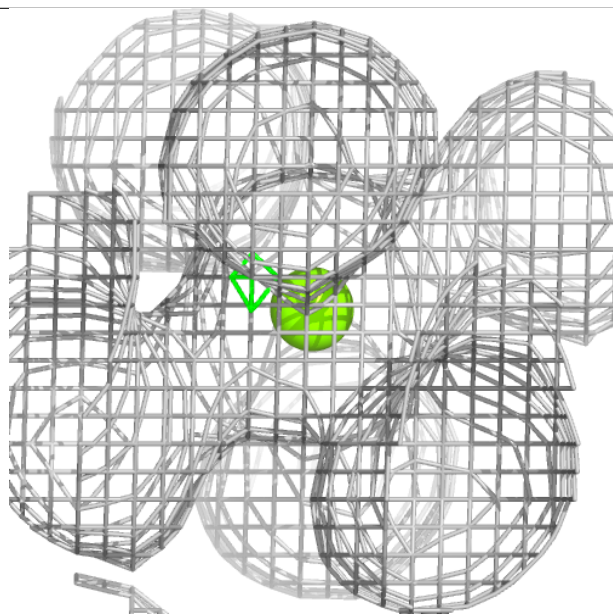
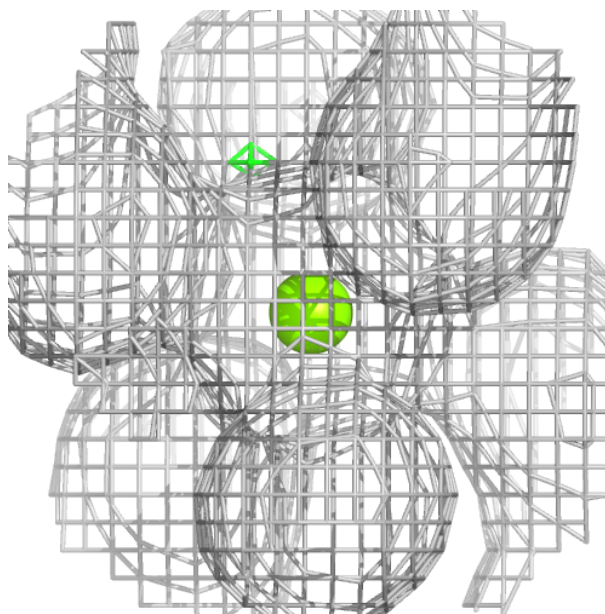
Electron density around ICS A 508:

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



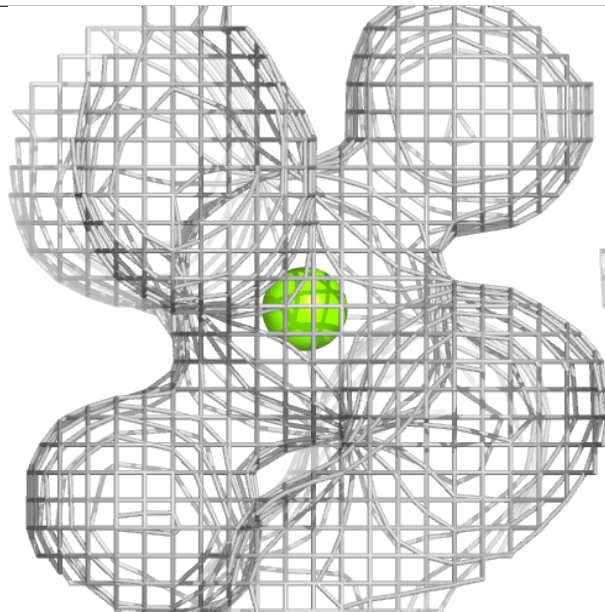
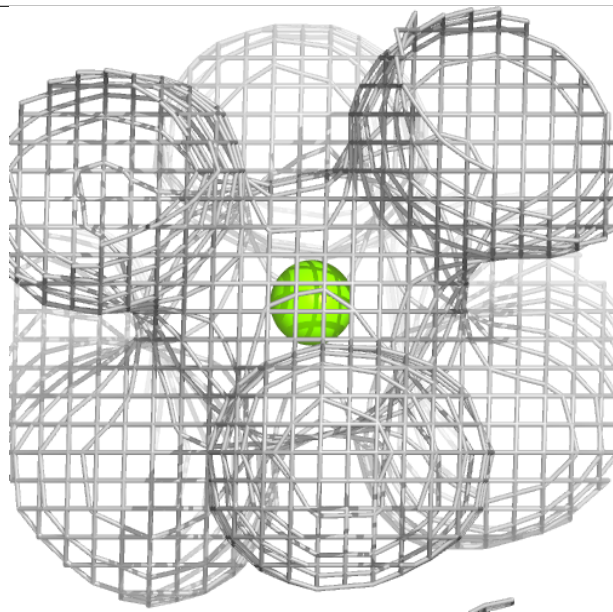
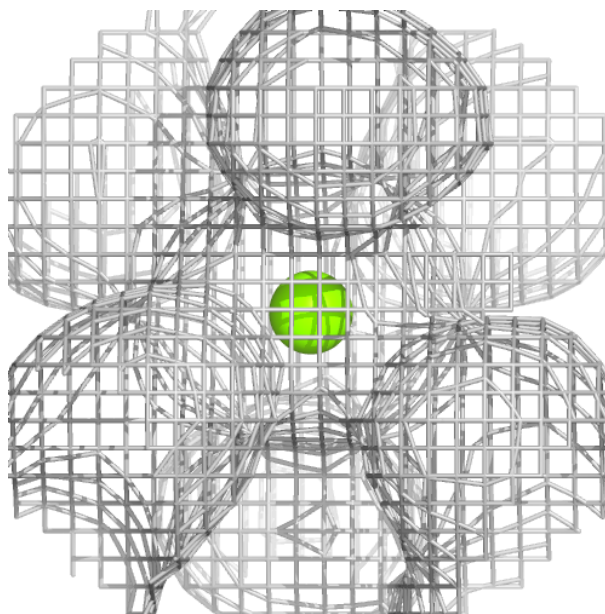
Electron density around MG B 510:

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



Electron density around MG B 511:

$2mF_o-DF_c$ (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.