



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 30, 2026 – 11:01 am BST

PDB ID : 29UP / pdb_000029up
Title : Mo-Nitrogenase, MoFe protein, P2+ redox state, +50 mV
Authors : Laxmi, S.; Seefeldt, L.C.; Carr, S.B.; Vincent, K.A.
Deposited on : 2026-04-08
Resolution : 1.90 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

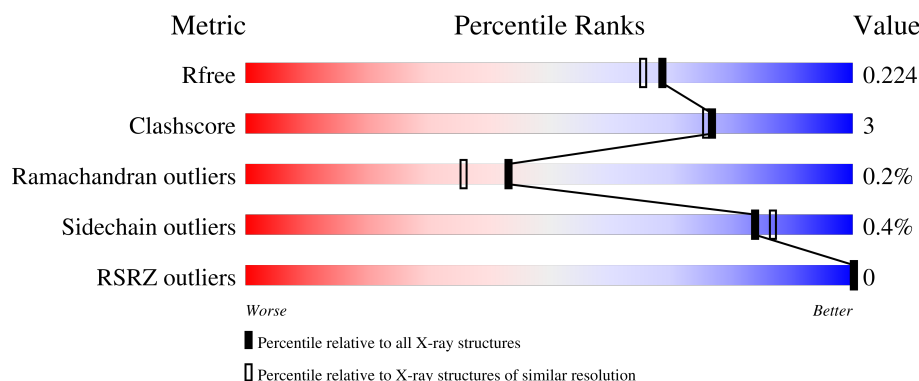
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

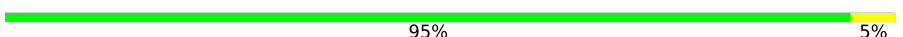
The reported resolution of this entry is 1.90 Å.

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.



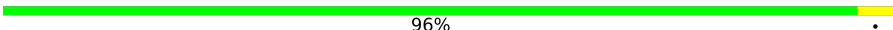
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	505	
1	C	505	
1	E	505	
1	G	505	
2	B	523	

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Mol	Chain	Length	Quality of chain
2	D	523	 96% .
2	F	523	 94% 6%
2	H	523	 92% 8%

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
7	ACT	F	602	-	X	X	-
7	ACT	F	603	-	X	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 64989 atoms, of which 31510 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 molybdenum-iron protein alpha chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	E	477	Total	C	H	N	O	S	0	4	0
			7544	2416	3742	648	712	26			
1	A	477	Total	C	H	N	O	S	0	2	0
			7531	2413	3735	647	710	26			
1	C	477	Total	C	H	N	O	S	0	2	0
			7532	2413	3736	647	710	26			
1	G	477	Total	C	H	N	O	S	0	2	0
			7531	2413	3735	647	710	26			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-12	MET	-	initiating methionine	UNP P07328
E	-11	THR	-	expression tag	UNP P07328
E	-10	GLY	-	expression tag	UNP P07328
E	-9	ALA	-	expression tag	UNP P07328
E	-8	SER	-	expression tag	UNP P07328
E	-7	TRP	-	expression tag	UNP P07328
E	-6	SER	-	expression tag	UNP P07328
E	-5	HIS	-	expression tag	UNP P07328
E	-4	PRO	-	expression tag	UNP P07328
E	-3	GLN	-	expression tag	UNP P07328
E	-2	PHE	-	expression tag	UNP P07328
E	-1	GLU	-	expression tag	UNP P07328
E	0	LYS	-	expression tag	UNP P07328
A	-12	MET	-	initiating methionine	UNP P07328
A	-11	THR	-	expression tag	UNP P07328
A	-10	GLY	-	expression tag	UNP P07328
A	-9	ALA	-	expression tag	UNP P07328
A	-8	SER	-	expression tag	UNP P07328
A	-7	TRP	-	expression tag	UNP P07328
A	-6	SER	-	expression tag	UNP P07328
A	-5	HIS	-	expression tag	UNP P07328

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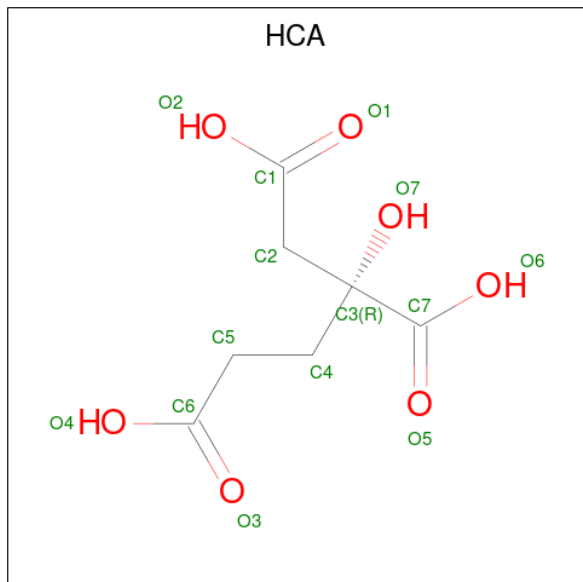
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	PRO	-	expression tag	UNP P07328
A	-3	GLN	-	expression tag	UNP P07328
A	-2	PHE	-	expression tag	UNP P07328
A	-1	GLU	-	expression tag	UNP P07328
A	0	LYS	-	expression tag	UNP P07328
C	-12	MET	-	initiating methionine	UNP P07328
C	-11	THR	-	expression tag	UNP P07328
C	-10	GLY	-	expression tag	UNP P07328
C	-9	ALA	-	expression tag	UNP P07328
C	-8	SER	-	expression tag	UNP P07328
C	-7	TRP	-	expression tag	UNP P07328
C	-6	SER	-	expression tag	UNP P07328
C	-5	HIS	-	expression tag	UNP P07328
C	-4	PRO	-	expression tag	UNP P07328
C	-3	GLN	-	expression tag	UNP P07328
C	-2	PHE	-	expression tag	UNP P07328
C	-1	GLU	-	expression tag	UNP P07328
C	0	LYS	-	expression tag	UNP P07328
G	-12	MET	-	initiating methionine	UNP P07328
G	-11	THR	-	expression tag	UNP P07328
G	-10	GLY	-	expression tag	UNP P07328
G	-9	ALA	-	expression tag	UNP P07328
G	-8	SER	-	expression tag	UNP P07328
G	-7	TRP	-	expression tag	UNP P07328
G	-6	SER	-	expression tag	UNP P07328
G	-5	HIS	-	expression tag	UNP P07328
G	-4	PRO	-	expression tag	UNP P07328
G	-3	GLN	-	expression tag	UNP P07328
G	-2	PHE	-	expression tag	UNP P07328
G	-1	GLU	-	expression tag	UNP P07328
G	0	LYS	-	expression tag	UNP P07328

- Molecule 2 is a protein called Nitrogenase molybdenum-iron protein beta chain.

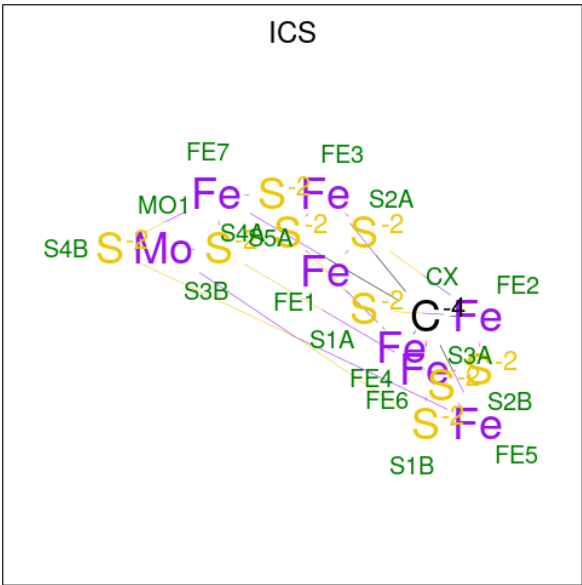
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	F	522	Total	C	H	N	O	S	0	2	0
			8270	2668	4092	706	776	28			
2	B	522	Total	C	H	N	O	S	0	0	0
			8262	2666	4088	705	775	28			
2	D	522	Total	C	H	N	O	S	0	0	0
			8262	2666	4088	705	775	28			
2	H	522	Total	C	H	N	O	S	0	0	0
			8262	2666	4088	705	775	28			

- Molecule 3 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (CCD ID: HCA) (formula: $C_7H_{10}O_7$).



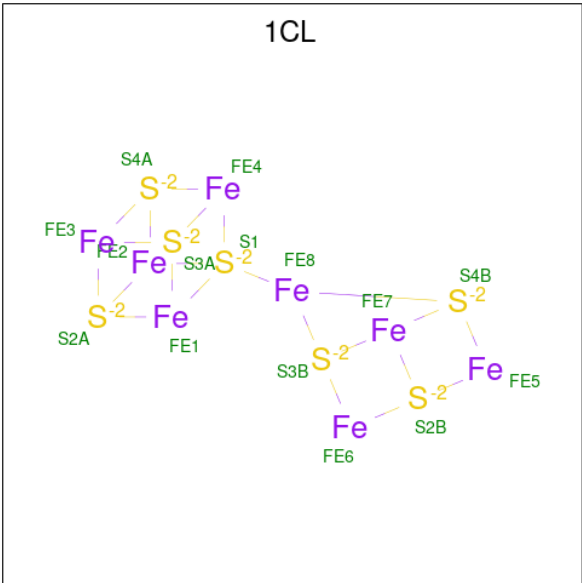
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total	C	H	O	0	0
			20	7	6	7		
3	A	1	Total	C	H	O	0	0
			20	7	6	7		
3	C	1	Total	C	H	O	0	0
			20	7	6	7		
3	G	1	Total	C	H	O	0	0
			20	7	6	7		

- Molecule 4 is iron-sulfur-molybdenum cluster with interstitial carbon (CCD ID: ICS) (formula: CFe_7MoS_9) (labeled as "Ligand of Interest" by depositor).



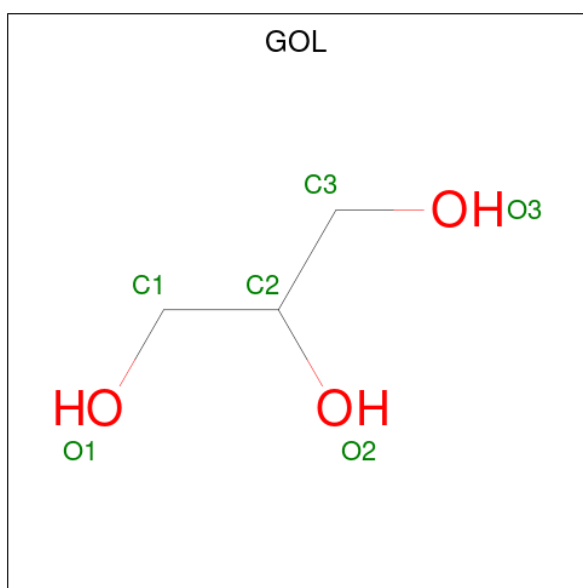
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total	C	Fe	Mo	S	
			18	1	7	1	9	0
4	A	1	Total	C	Fe	Mo	S	
			18	1	7	1	9	0
4	C	1	Total	C	Fe	Mo	S	
			18	1	7	1	9	0
4	G	1	Total	C	Fe	Mo	S	
			18	1	7	1	9	0

- Molecule 5 is FE(8)-S(7) CLUSTER, OXIDIZED (CCD ID: 1CL) (formula: Fe₈S₇) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



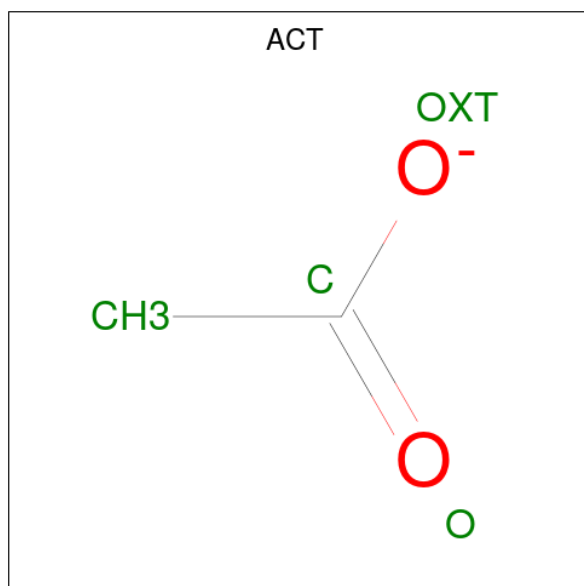
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	F	1	Total	C	H	O	0	0
			14	3	8	3		
6	F	1	Total	C	H	O	0	0
			14	3	8	3		
6	F	1	Total	C	H	O	0	0
			14	3	8	3		
6	A	1	Total	C	H	O	0	0
			14	3	8	3		
6	B	1	Total	C	H	O	0	0
			14	3	8	3		
6	B	1	Total	C	H	O	0	0
			14	3	8	3		
6	B	1	Total	C	H	O	0	0
			14	3	8	3		

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

- Molecule 7 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



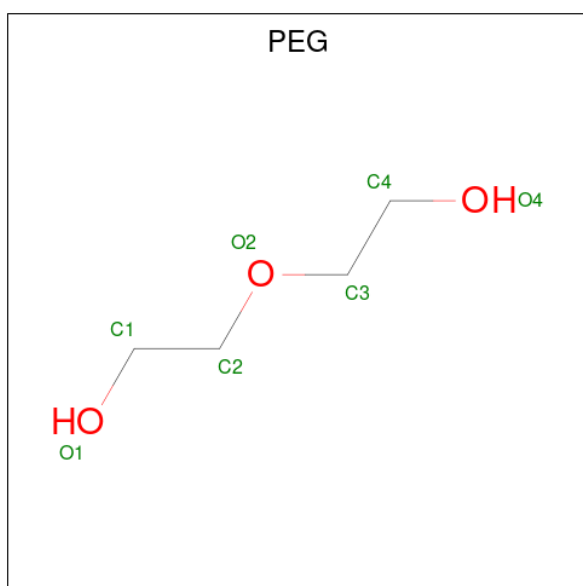
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	F	1	Total	C	H	O	0	0
			7	2	3	2		
7	F	1	Total	C	H	O	0	0
			7	2	3	2		
7	B	1	Total	C	H	O	0	0
			7	2	3	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	H	O	0	0
			7	2	3	2		
7	D	1	Total	C	H	O	0	0
			7	2	3	2		
7	D	1	Total	C	H	O	0	0
			7	2	3	2		
7	H	1	Total	C	H	O	0	0
			7	2	3	2		
7	H	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	F	1	Total	C	H	O	0	0
			17	4	10	3		
8	D	1	Total	C	H	O	0	0
			17	4	10	3		
8	H	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	F	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total 1	Cl 1	0	0
9	C	1	Total 1	Cl 1	0	0
9	G	1	Total 1	Cl 1	0	0

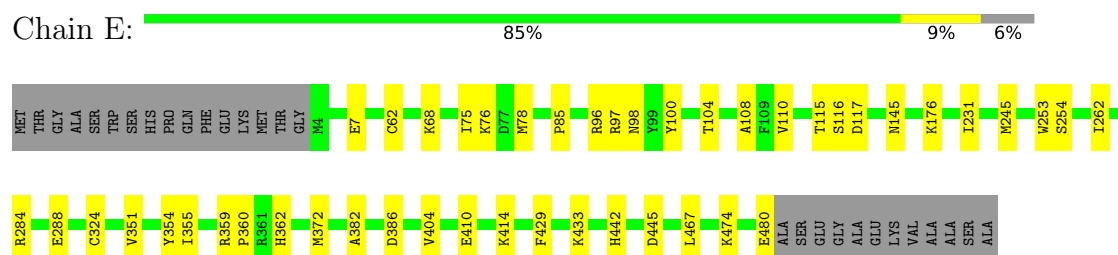
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	E	176	Total 176	O 176	0	0
10	F	195	Total 195	O 195	0	0
10	A	82	Total 82	O 82	0	0
10	B	176	Total 176	O 176	0	0
10	C	172	Total 172	O 172	0	0
10	D	203	Total 203	O 203	0	0
10	G	87	Total 87	O 87	0	0
10	H	157	Total 157	O 157	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.

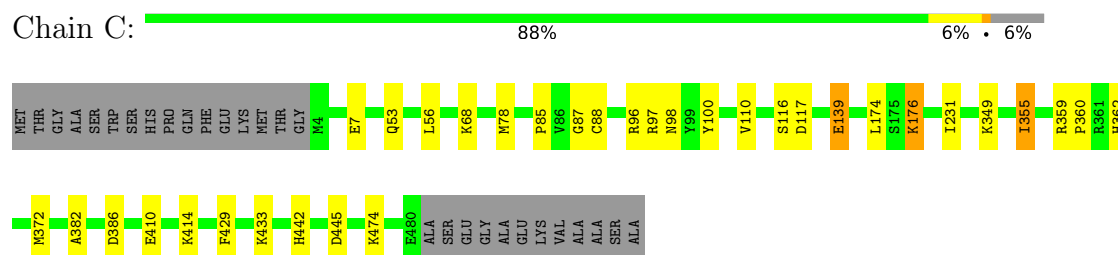
- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain



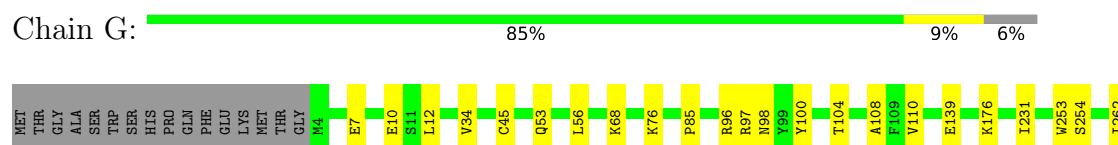
- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain



- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain



- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain





- Molecule 2: Nitrogenase molybdenum-iron protein beta chain

Chain F: 94% 6%



- Molecule 2: Nitrogenase molybdenum-iron protein beta chain

Chain B: 95% 5%



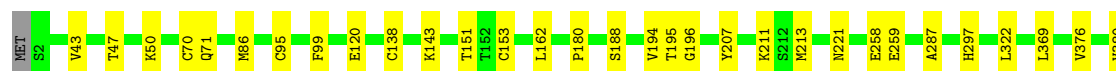
- Molecule 2: Nitrogenase molybdenum-iron protein beta chain

Chain D: 96% 0%



- Molecule 2: Nitrogenase molybdenum-iron protein beta chain

Chain H: 92% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.01Å 156.85Å 202.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.43 – 1.90 67.43 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.1 (67.43-1.90) 97.1 (67.43-1.90)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.197 , 0.226 0.195 , 0.224	Depositor DCC
R_{free} test set	20118 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.733	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 25.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.479 for h,-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	64989	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.55 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.7630e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 1CL, PEG, HCA, CL, ICS, ACT, GOL

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	0.67	0/3891	0.72	0/5247
1	C	0.77	1/3891 (0.0%)	0.78	2/5247 (0.0%)
1	E	0.76	1/3903 (0.0%)	0.75	0/5263
1	G	0.67	0/3891	0.70	0/5247
2	B	0.70	0/4280	0.70	0/5786
2	D	0.74	1/4280 (0.0%)	0.75	0/5786
2	F	0.73	0/4292	0.73	0/5803
2	H	0.78	3/4280 (0.1%)	0.72	0/5786
All	All	0.73	6/32708 (0.0%)	0.73	2/44165 (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
1	E	0	2
1	G	0	1
All	All	0	5

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	143	LYS	C-O	-13.16	1.17	1.23
1	C	78	MET	SD-CE	7.40	1.98	1.79
2	D	143	LYS	C-O	-6.69	1.20	1.23
2	H	143	LYS	CA-C	5.46	1.57	1.53
1	E	78	MET	SD-CE	5.22	1.92	1.79

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	176	LYS	CD-CE-NZ	-5.42	94.55	111.90
1	C	139	GLU	CB-CG-CD	-5.16	103.82	112.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	96	ARG	Sidechain
1	C	96	ARG	Sidechain
1	E	75	ILE	Peptide
1	E	96	ARG	Sidechain
1	G	96	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	3796	3735	3725	33	0
1	C	3796	3736	3725	21	0
1	E	3802	3742	3725	28	0
1	G	3796	3735	3725	25	0
2	B	4174	4088	4087	22	0
2	D	4174	4088	4087	13	0
2	F	4178	4092	4086	18	0
2	H	4174	4088	4087	28	0
3	A	14	6	6	2	0
3	C	14	6	6	2	0
3	E	14	6	6	3	0
3	G	14	6	6	2	0
4	A	18	0	0	1	0
4	C	18	0	0	0	0
4	E	18	0	0	0	0
4	G	18	0	0	0	0
5	A	15	0	0	1	0
5	D	15	0	0	1	0
5	E	15	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	15	0	0	1	0
6	A	6	8	8	0	0
6	B	24	32	32	1	0
6	C	6	8	8	0	0
6	D	24	32	32	0	0
6	F	18	24	24	0	0
6	H	18	24	24	0	0
7	B	8	6	6	0	0
7	D	8	6	6	0	0
7	F	8	6	6	2	0
7	H	8	6	6	0	0
8	D	7	10	10	1	0
8	F	7	10	10	1	0
8	H	7	10	10	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	F	1	0	0	0	0
9	G	1	0	0	0	0
10	A	82	0	0	1	0
10	B	176	0	0	0	0
10	C	172	0	0	0	0
10	D	203	0	0	0	0
10	E	176	0	0	0	0
10	F	195	0	0	2	0
10	G	87	0	0	1	0
10	H	157	0	0	0	0
All	All	33479	31510	31453	184	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 3.

The worst 5 of 184 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:A:42:SER:HA	1:A:391:MET:HE1	1.65	0.79
1:A:174:LEU:O	1:A:176:LYS:HG2	1.89	0.73
1:C:139:GLU:CD	1:C:176:LYS:HZ1	1.98	0.72
1:C:174:LEU:O	1:C:176:LYS:HG2	1.89	0.71
1:G:349:LYS:HB2	1:G:372:MET:HE3	1.76	0.67

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	477/505 (94%)	457 (96%)	19 (4%)	1 (0%)	43	36
1	C	477/505 (94%)	457 (96%)	19 (4%)	1 (0%)	43	36
1	E	479/505 (95%)	458 (96%)	20 (4%)	1 (0%)	43	36
1	G	477/505 (94%)	456 (96%)	20 (4%)	1 (0%)	43	36
2	B	520/523 (99%)	507 (98%)	13 (2%)	0	100	100
2	D	520/523 (99%)	508 (98%)	11 (2%)	1 (0%)	43	36
2	F	522/523 (100%)	512 (98%)	9 (2%)	1 (0%)	43	36
2	H	520/523 (99%)	507 (98%)	13 (2%)	0	100	100
All	All	3992/4112 (97%)	3862 (97%)	124 (3%)	6 (0%)	43	36

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	255	SER
2	D	255	SER
1	A	355	ILE
1	C	355	ILE
1	G	355	ILE

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	409/426 (96%)	406 (99%)	3 (1%)	76	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	409/426 (96%)	406 (99%)	3 (1%)	76	78
1	E	411/426 (96%)	408 (99%)	3 (1%)	76	78
1	G	409/426 (96%)	406 (99%)	3 (1%)	76	78
2	B	454/455 (100%)	454 (100%)	0	100	100
2	D	454/455 (100%)	454 (100%)	0	100	100
2	F	455/455 (100%)	454 (100%)	1 (0%)	87	90
2	H	454/455 (100%)	453 (100%)	1 (0%)	87	90
All	All	3455/3524 (98%)	3441 (100%)	14 (0%)	84	87

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	98	ASN
1	C	362	HIS
2	H	195	THR
1	G	362	HIS
1	G	445	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	163	ASN
2	H	317	ASN
2	H	418	ASN
2	H	163	ASN
2	B	93	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 43 ligands modelled in this entry, 4 are monoatomic - leaving 39 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
6	GOL	B	601	-	5,5,5	0.41	0	5,5,5	0.60	0
8	PEG	F	606	-	6,6,6	0.62	0	5,5,5	0.82	0
7	ACT	D	606	-	3,3,3	2.31	1 (33%)	3,3,3	1.36	0
8	PEG	D	607	-	6,6,6	0.55	0	5,5,5	0.64	0
4	ICS	A	503	3,1	18,30,30	2.45	10 (55%)	-		
4	ICS	E	602	3,1	18,30,30	2.95	11 (61%)	-		
6	GOL	F	605	-	5,5,5	0.45	0	5,5,5	0.70	0
7	ACT	F	603	-	3,3,3	2.14	1 (33%)	3,3,3	1.69	2 (66%)
5	1CL	D	601	2,1	0,22,22	-	-	-		
6	GOL	F	601	-	5,5,5	0.56	0	5,5,5	0.96	0
3	HCA	C	601	4	13,13,13	1.73	3 (23%)	14,18,18	1.89	3 (21%)
6	GOL	D	608	-	5,5,5	0.29	0	5,5,5	0.38	0
4	ICS	C	602	3,1	18,30,30	3.20	10 (55%)	-		
7	ACT	D	605	-	3,3,3	1.73	2 (66%)	3,3,3	0.89	0
6	GOL	D	602	-	5,5,5	0.12	0	5,5,5	0.84	0
4	ICS	G	602	3,1	18,30,30	2.68	12 (66%)	-		
6	GOL	D	604	-	5,5,5	0.55	0	5,5,5	0.86	0
7	ACT	F	602	-	3,3,3	1.93	2 (66%)	3,3,3	1.41	1 (33%)
3	HCA	E	601	4	13,13,13	2.06	5 (38%)	14,18,18	1.88	3 (21%)
8	PEG	H	605	-	6,6,6	0.72	0	5,5,5	0.65	0
6	GOL	B	605	-	5,5,5	0.28	0	5,5,5	0.80	0
7	ACT	B	603	-	3,3,3	1.76	1 (33%)	3,3,3	1.55	0
6	GOL	C	603	-	5,5,5	0.58	0	5,5,5	0.99	0
6	GOL	B	604	-	5,5,5	0.07	0	5,5,5	0.57	0
6	GOL	H	606	-	5,5,5	0.29	0	5,5,5	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	B	602	-	5,5,5	0.42	0	5,5,5	0.68	0
6	GOL	D	603	-	5,5,5	0.51	0	5,5,5	0.64	0
5	1CL	A	504	2,1	0,22,22	-	-	-	-	-
7	ACT	H	604	-	3,3,3	1.62	1 (33%)	3,3,3	1.08	0
6	GOL	F	604	-	5,5,5	0.74	0	5,5,5	0.41	0
6	GOL	H	603	-	5,5,5	0.42	0	5,5,5	0.77	0
7	ACT	H	607	-	3,3,3	1.91	1 (33%)	3,3,3	1.49	0
5	1CL	E	603	2,1	0,22,22	-	-	-	-	-
7	ACT	B	606	-	3,3,3	2.02	1 (33%)	3,3,3	1.47	0
5	1CL	H	601	2,1	0,22,22	-	-	-	-	-
6	GOL	A	501	-	5,5,5	0.46	0	5,5,5	0.70	0
3	HCA	G	601	4	13,13,13	1.69	3 (23%)	14,18,18	1.86	4 (28%)
6	GOL	H	602	-	5,5,5	0.39	0	5,5,5	0.56	0
3	HCA	A	502	4	13,13,13	1.82	4 (30%)	14,18,18	1.92	5 (35%)

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
6	GOL	B	601	-	-	3/4/4/4	-
8	PEG	F	606	-	-	1/4/4/4	-
8	PEG	D	607	-	-	2/4/4/4	-
6	GOL	F	605	-	-	0/4/4/4	-
5	1CL	D	601	2,1	-	-	0/10/8/8
6	GOL	F	601	-	-	1/4/4/4	-
3	HCA	C	601	4	-	4/17/17/17	-
6	GOL	D	608	-	-	0/4/4/4	-
6	GOL	D	602	-	-	0/4/4/4	-
6	GOL	D	604	-	-	2/4/4/4	-
3	HCA	E	601	4	-	4/17/17/17	-
8	PEG	H	605	-	-	0/4/4/4	-
6	GOL	B	605	-	-	0/4/4/4	-
6	GOL	C	603	-	-	0/4/4/4	-
6	GOL	B	604	-	-	0/4/4/4	-
6	GOL	H	606	-	-	4/4/4/4	-
6	GOL	B	602	-	-	2/4/4/4	-
6	GOL	D	603	-	-	0/4/4/4	-
5	1CL	A	504	2,1	-	-	0/10/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	F	604	-	-	0/4/4/4	-
6	GOL	H	603	-	-	2/4/4/4	-
5	1CL	E	603	2,1	-	-	0/10/8/8
5	1CL	H	601	2,1	-	-	0/10/8/8
6	GOL	A	501	-	-	3/4/4/4	-
3	HCA	G	601	4	-	2/17/17/17	-
6	GOL	H	602	-	-	0/4/4/4	-
3	HCA	A	502	4	-	3/17/17/17	-

The worst 5 of 68 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	602	ICS	S2A-FE2	-5.82	2.18	2.32
4	C	602	ICS	S2A-FE2	-5.69	2.18	2.32
4	C	602	ICS	S3B-FE7	-5.22	2.19	2.32
4	C	602	ICS	S1B-FE6	-5.05	2.20	2.32
4	C	602	ICS	S4B-FE7	-4.76	2.20	2.32

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	601	HCA	O6-C7-C3	4.89	121.55	113.05
3	C	601	HCA	O6-C7-C3	4.59	121.03	113.05
3	A	502	HCA	O5-C7-C3	-4.10	116.44	122.25
3	G	601	HCA	O5-C7-C3	-3.78	116.90	122.25
3	A	502	HCA	O6-C7-C3	3.63	119.36	113.05

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	601	HCA	C2-C3-C4-C5
6	B	601	GOL	O1-C1-C2-C3
6	B	602	GOL	C1-C2-C3-O3
6	D	604	GOL	O1-C1-C2-C3
6	H	603	GOL	C1-C2-C3-O3

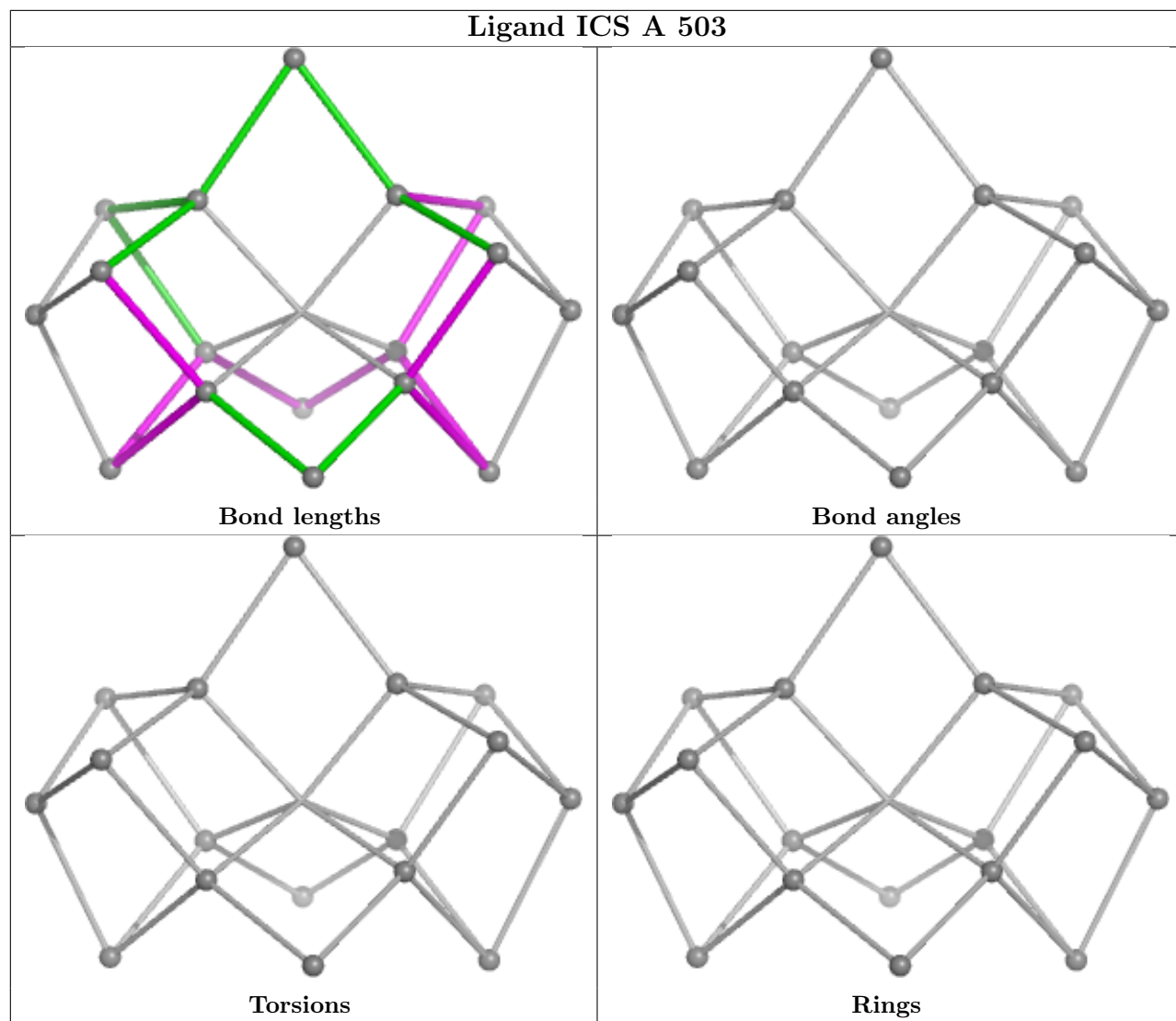
There are no ring outliers.

13 monomers are involved in 19 short contacts:

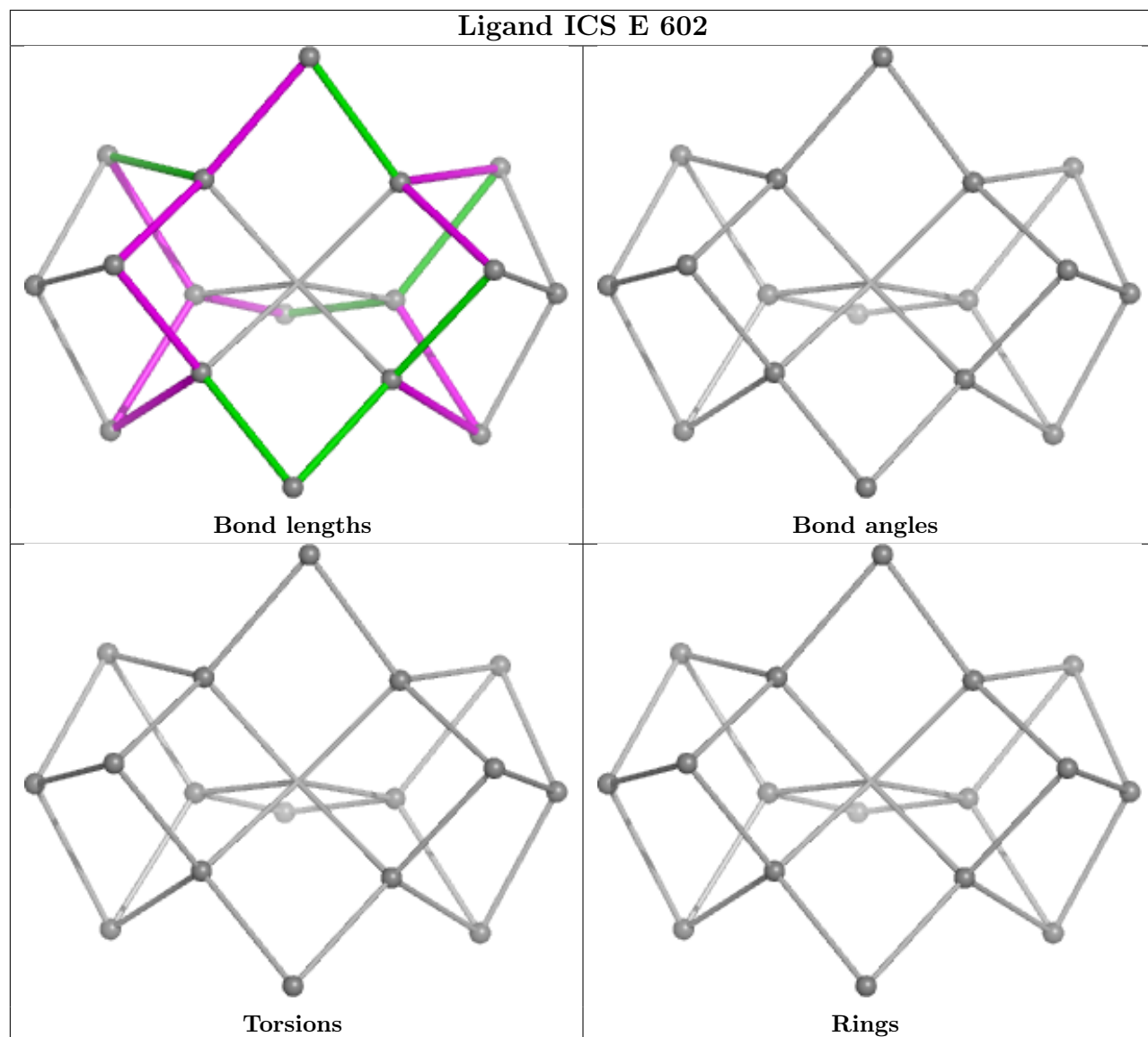
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	606	PEG	1	0
8	D	607	PEG	1	0
4	A	503	ICS	1	0
5	D	601	1CL	1	0
3	C	601	HCA	2	0
7	F	602	ACT	2	0
3	E	601	HCA	3	0
6	B	602	GOL	1	0
5	A	504	1CL	1	0
5	E	603	1CL	1	0
5	H	601	1CL	1	0
3	G	601	HCA	2	0
3	A	502	HCA	2	0

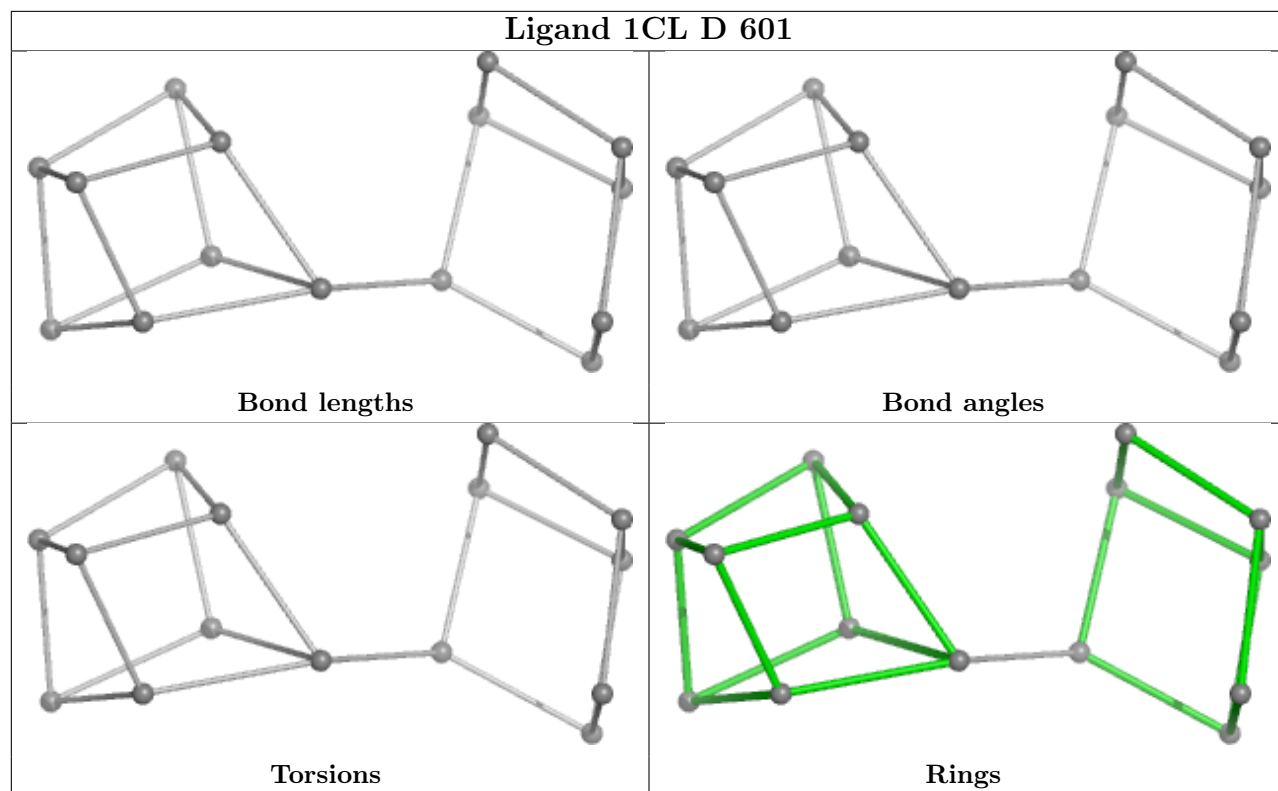
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 503

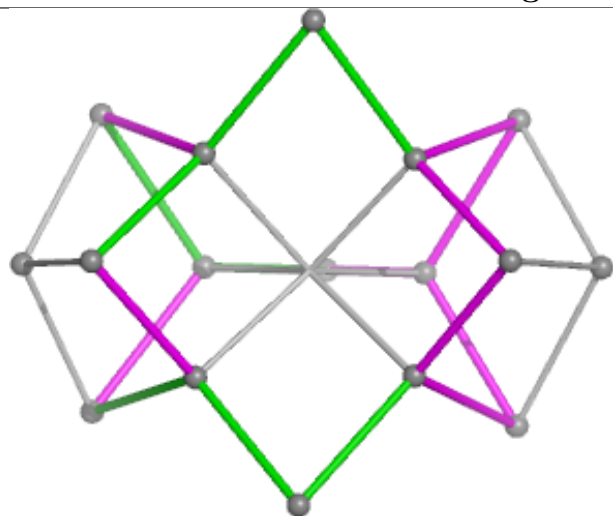


Ligand ICS E 602

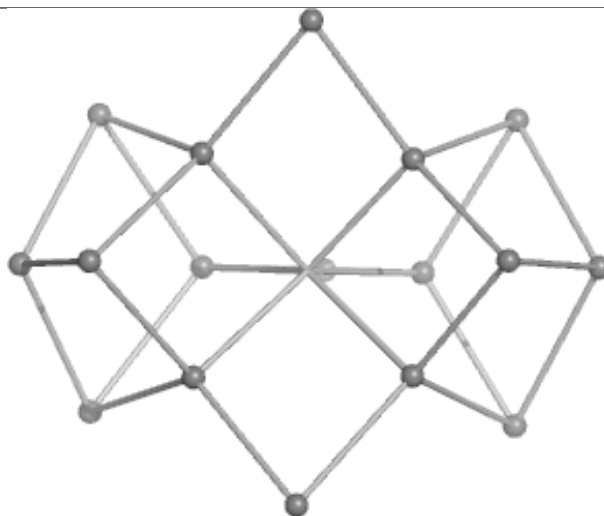




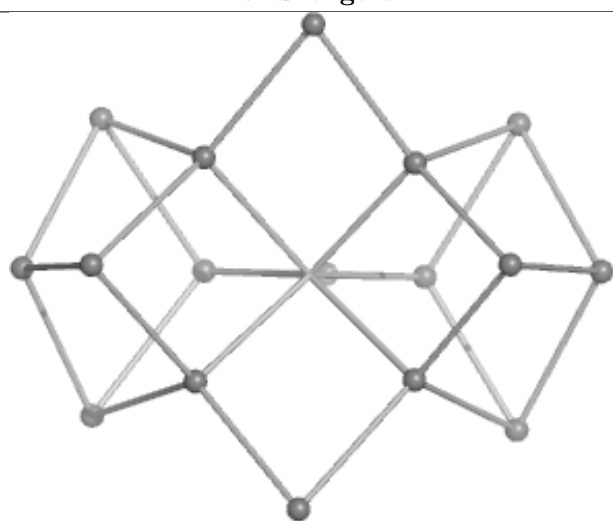
Ligand ICS C 602



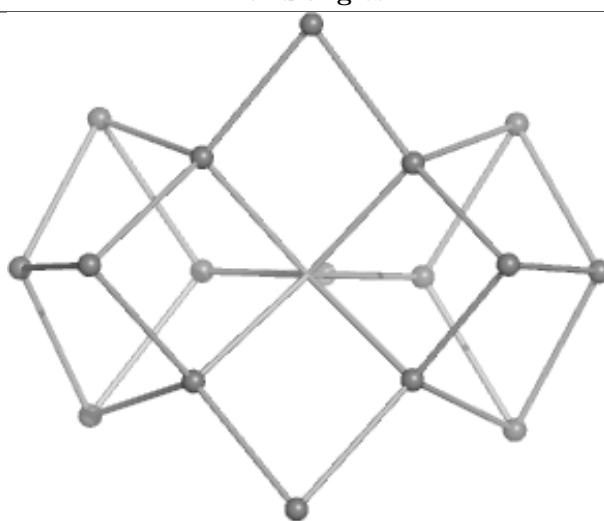
Bond lengths



Bond angles

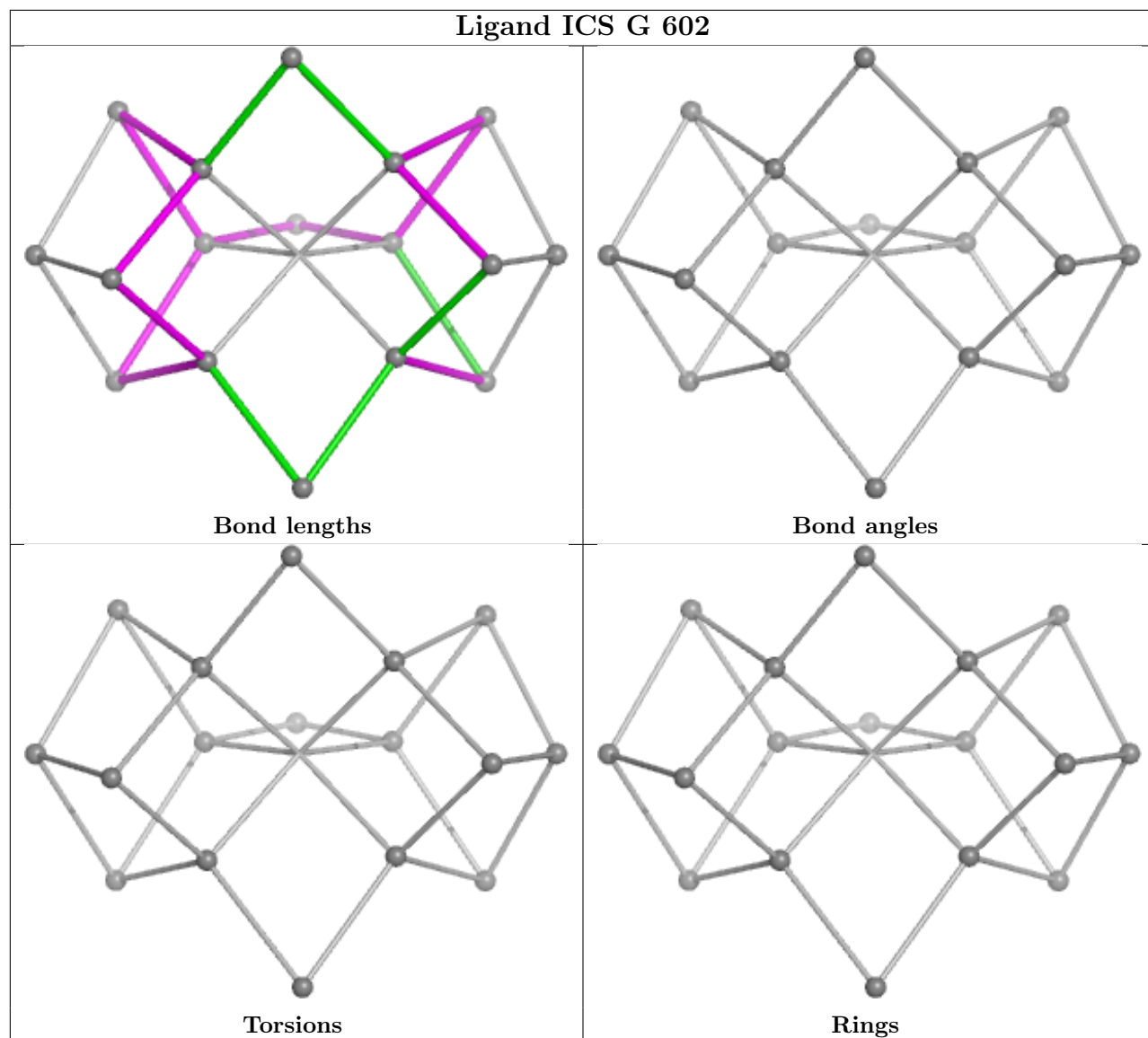


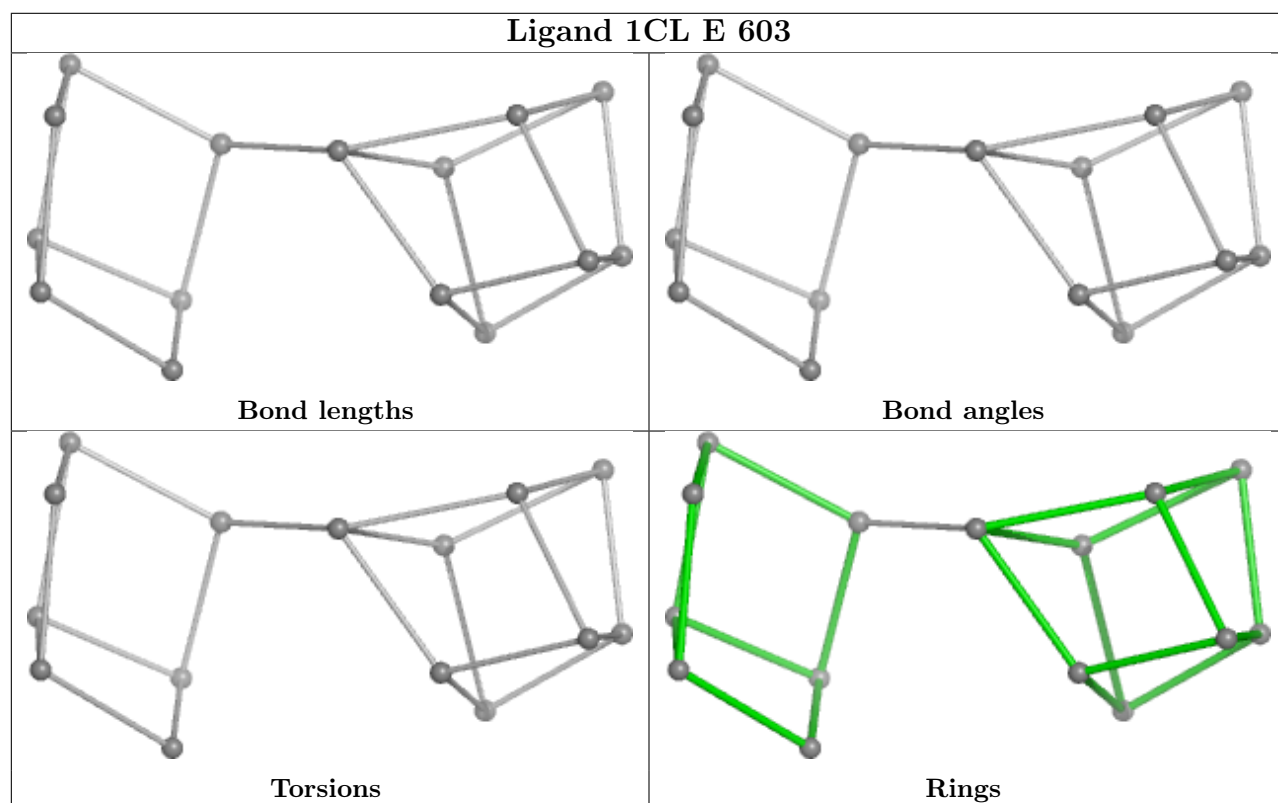
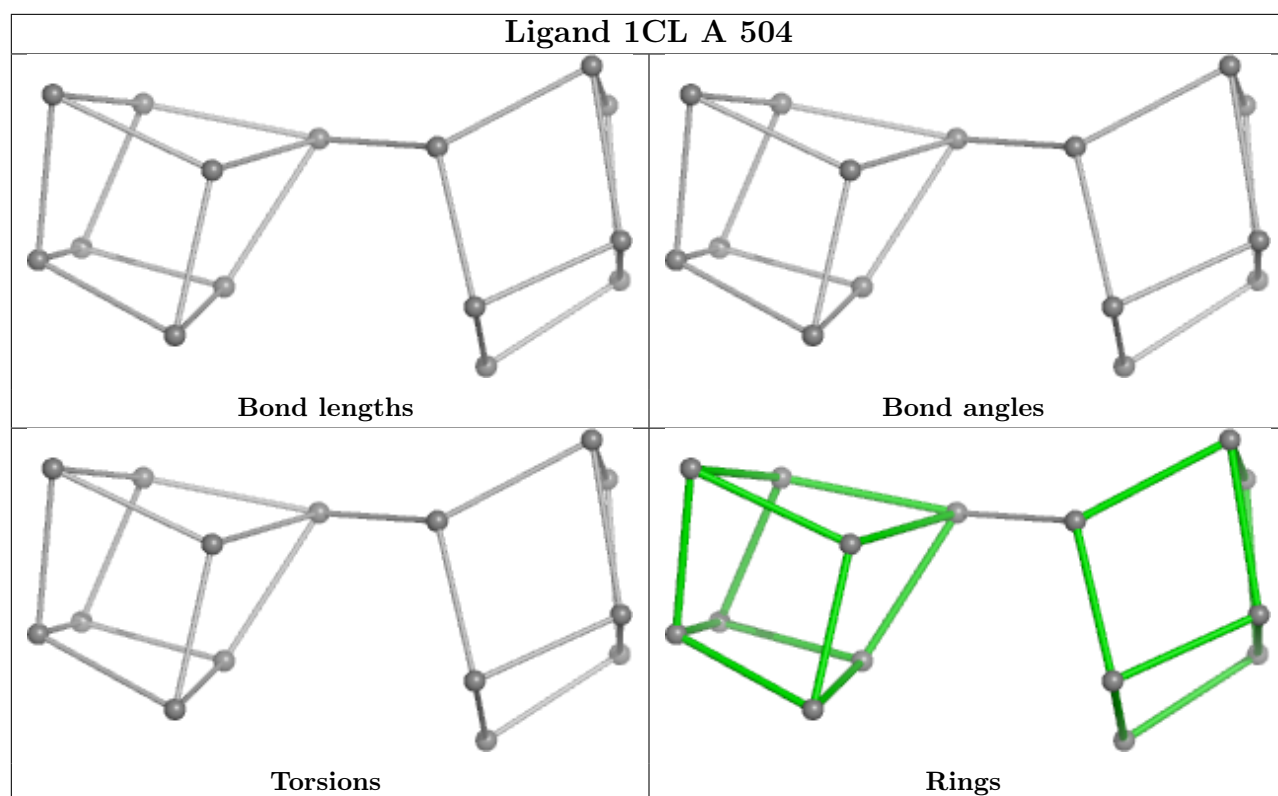
Torsions

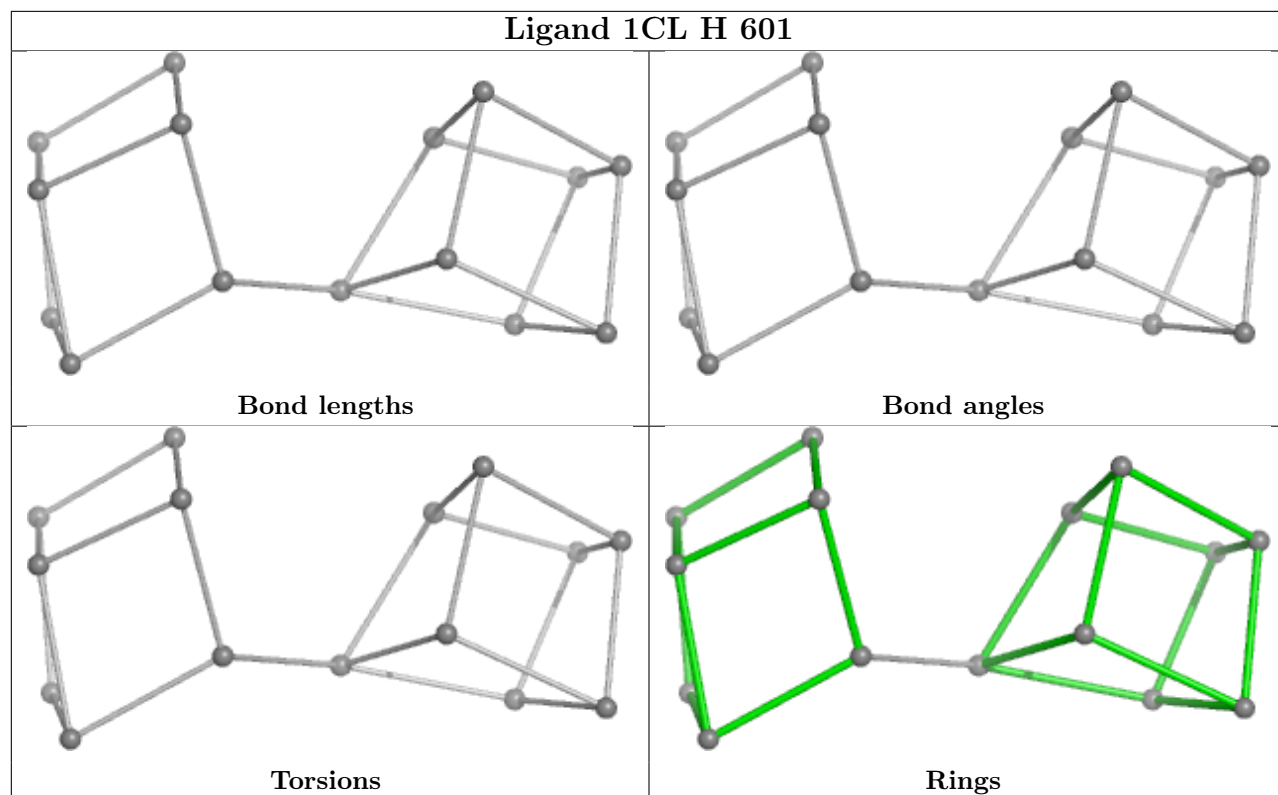


Rings

Ligand ICS G 602







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	477/505 (94%)	-1.20	0 100 100	30, 51, 75, 97	1 (0%)
1	C	477/505 (94%)	-1.47	0 100 100	20, 37, 55, 73	1 (0%)
1	E	477/505 (94%)	-1.46	0 100 100	17, 37, 55, 69	2 (0%)
1	G	477/505 (94%)	-1.22	0 100 100	30, 52, 73, 100	1 (0%)
2	B	522/523 (99%)	-1.38	0 100 100	27, 45, 67, 89	0
2	D	522/523 (99%)	-1.48	0 100 100	24, 39, 58, 74	0
2	F	522/523 (99%)	-1.46	0 100 100	16, 39, 56, 69	1 (0%)
2	H	522/523 (99%)	-1.38	0 100 100	28, 41, 55, 68	0
All	All	3996/4112 (97%)	-1.38	0 100 100	16, 42, 65, 100	6 (0%)

There are no RSRZ outliers to report.

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](#)

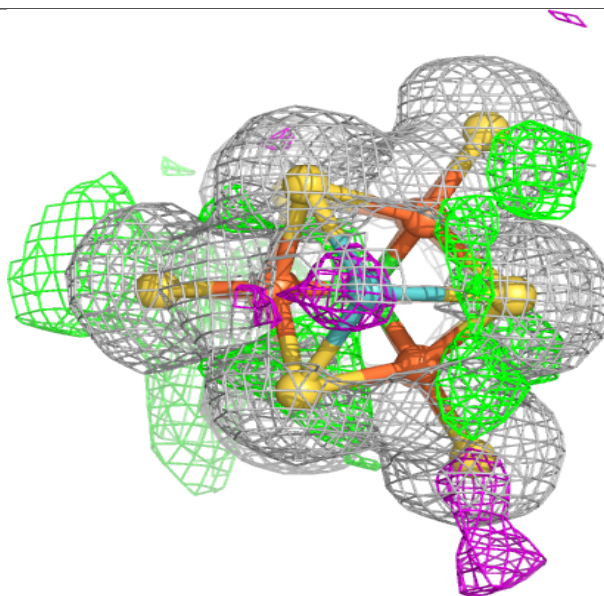
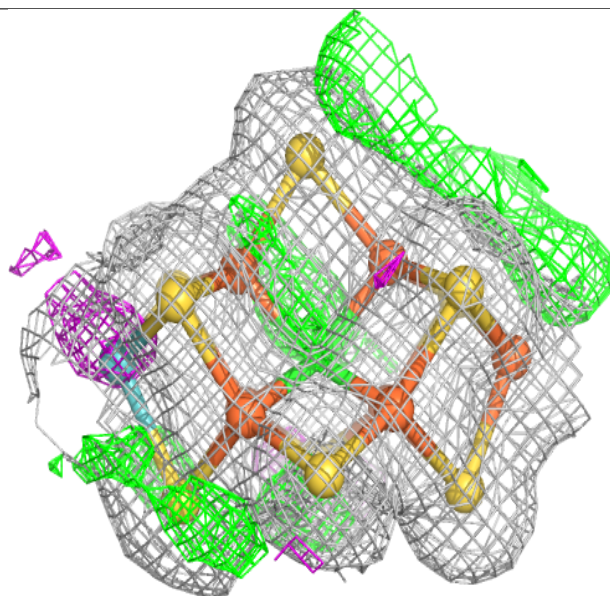
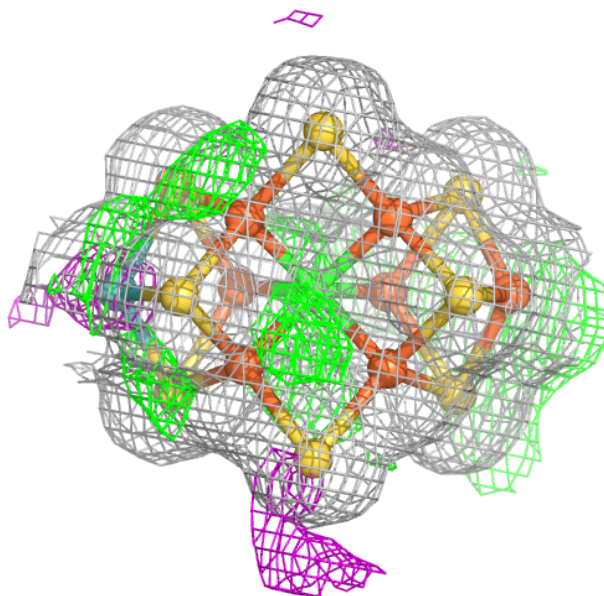
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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
7	ACT	D	606	4/4	0.97	0.07	40,48,55,56	0
6	GOL	H	603	6/6	0.98	0.05	47,57,66,68	0
7	ACT	F	603	4/4	0.98	0.07	41,50,57,60	0
6	GOL	B	602	6/6	0.98	0.05	61,74,81,84	0
7	ACT	H	607	4/4	0.98	0.08	43,52,54,54	0
8	PEG	H	605	7/7	0.98	0.06	44,54,66,66	0
3	HCA	A	502	14/14	0.99	0.03	33,36,44,44	0
6	GOL	B	604	6/6	0.99	0.04	50,61,66,66	0
6	GOL	B	605	6/6	0.99	0.03	37,46,55,55	0
6	GOL	C	603	6/6	0.99	0.03	32,41,45,54	0
6	GOL	D	602	6/6	0.99	0.03	33,40,46,47	0
6	GOL	D	603	6/6	0.99	0.04	49,59,63,71	0
6	GOL	D	604	6/6	0.99	0.04	50,60,69,69	0
6	GOL	D	608	6/6	0.99	0.04	46,55,62,62	0
6	GOL	H	602	6/6	0.99	0.04	40,49,56,57	0
6	GOL	F	601	6/6	0.99	0.04	43,53,62,66	0
6	GOL	H	606	6/6	0.99	0.04	47,60,67,73	0
7	ACT	F	602	4/4	0.99	0.06	36,41,44,45	0
6	GOL	F	604	6/6	0.99	0.04	41,49,53,58	0
7	ACT	B	603	4/4	0.99	0.07	42,48,51,51	0
7	ACT	B	606	4/4	0.99	0.05	43,52,58,60	0
7	ACT	D	605	4/4	0.99	0.04	33,37,39,41	0
6	GOL	F	605	6/6	0.99	0.04	34,41,46,50	0
7	ACT	H	604	4/4	0.99	0.06	36,42,43,43	0
6	GOL	A	501	6/6	0.99	0.04	46,55,63,69	0
8	PEG	F	606	7/7	0.99	0.05	40,48,56,56	0
8	PEG	D	607	7/7	0.99	0.04	40,51,65,65	0
6	GOL	B	601	6/6	0.99	0.03	36,44,50,57	0
4	ICS	C	602	18/18	1.00	0.01	21,24,26,26	0
4	ICS	G	602	18/18	1.00	0.01	37,39,41,41	0
5	1CL	E	603	15/15	1.00	0.01	25,26,30,32	0
5	1CL	A	504	15/15	1.00	0.01	36,39,41,42	0
5	1CL	D	601	15/15	1.00	0.01	24,25,28,32	0
5	1CL	H	601	15/15	1.00	0.01	36,38,41,42	0
3	HCA	E	601	14/14	1.00	0.03	22,27,33,33	0
3	HCA	C	601	14/14	1.00	0.02	21,27,33,33	0
3	HCA	G	601	14/14	1.00	0.03	34,36,44,44	0
4	ICS	E	602	18/18	1.00	0.01	21,24,27,27	0
4	ICS	A	503	18/18	1.00	0.01	36,38,40,41	0
9	CL	F	607	1/1	1.00	0.02	33,33,33,33	0
9	CL	B	607	1/1	1.00	0.01	35,35,35,35	0
9	CL	C	604	1/1	1.00	0.03	32,32,32,32	0
9	CL	G	603	1/1	1.00	0.04	35,35,35,35	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.

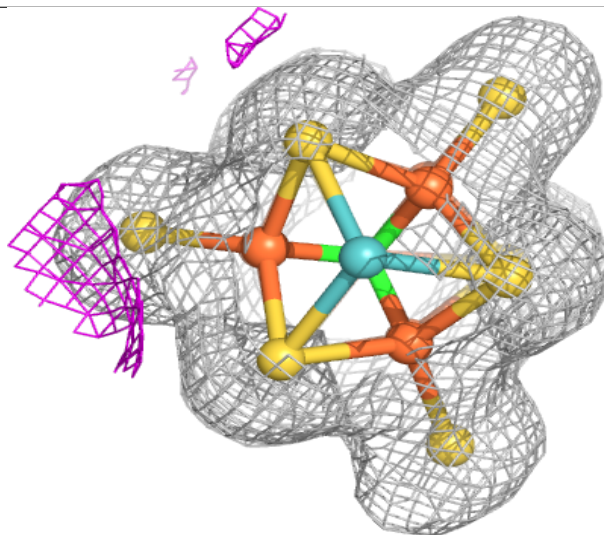
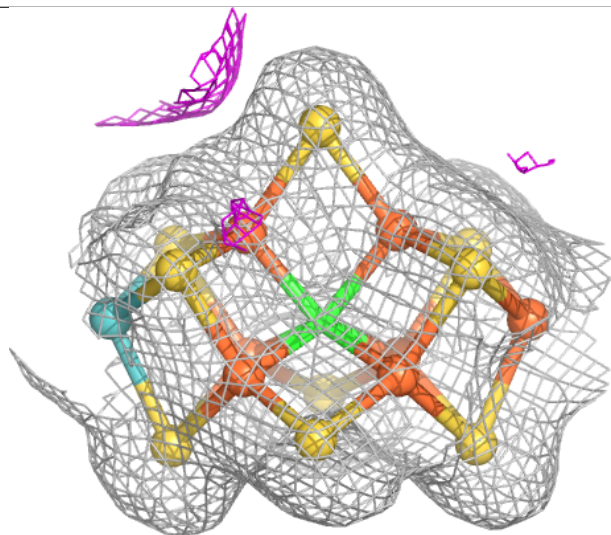
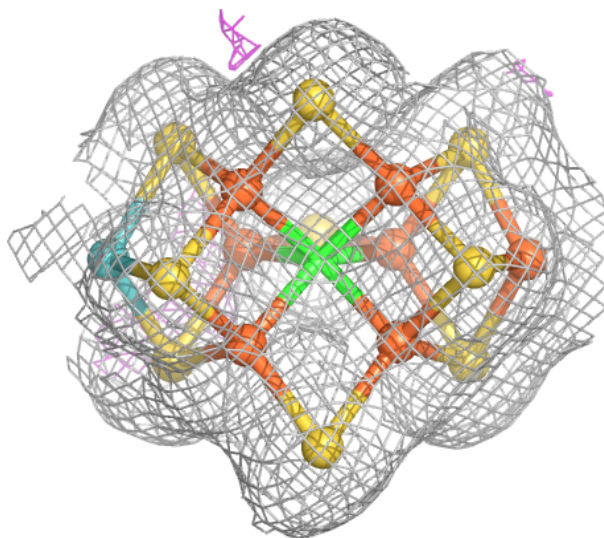
Electron density around ICS C 602:

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



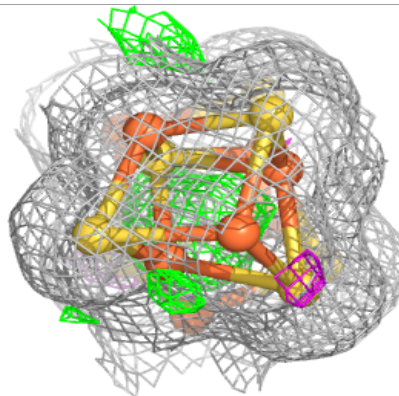
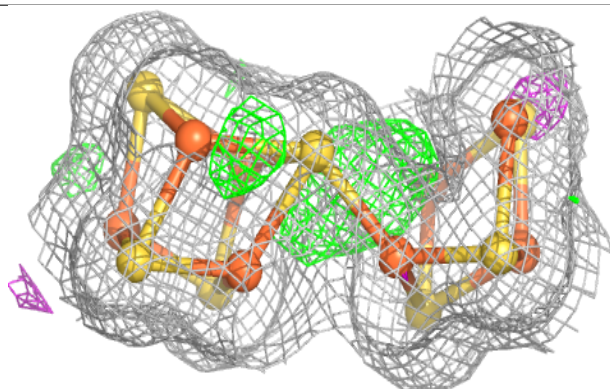
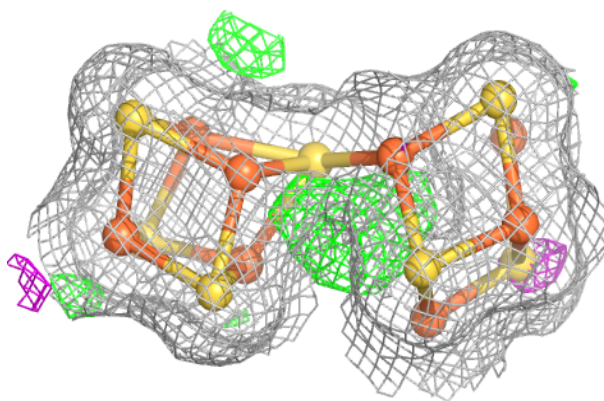
Electron density around ICS G 602:

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

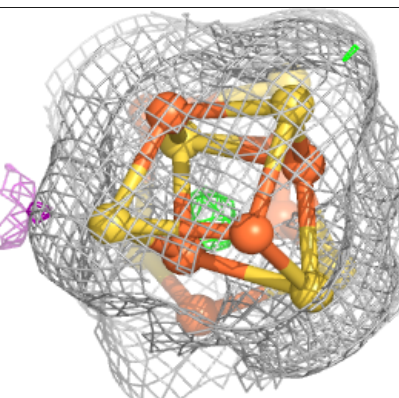
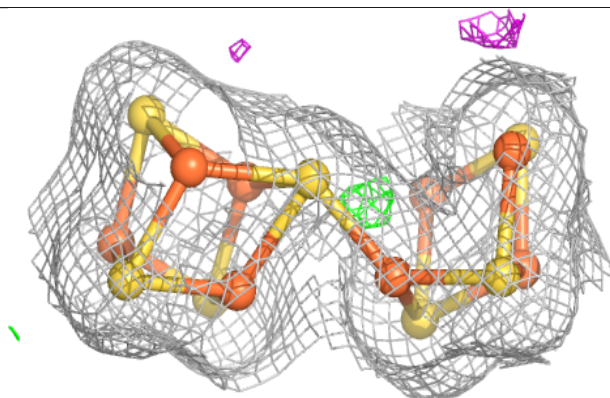
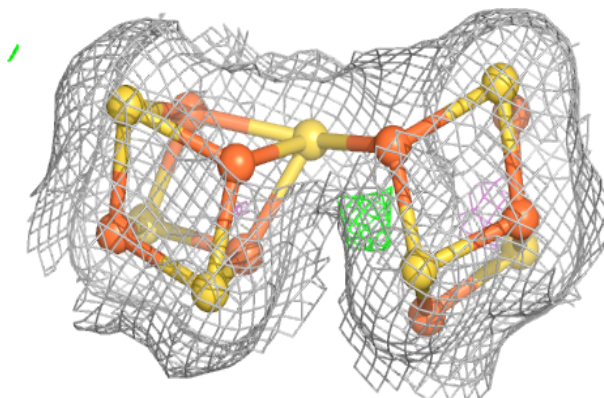


Electron density around 1CL E 603:

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

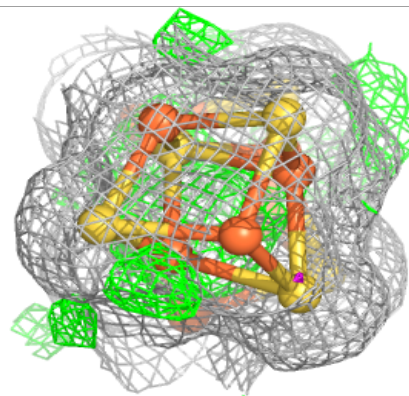
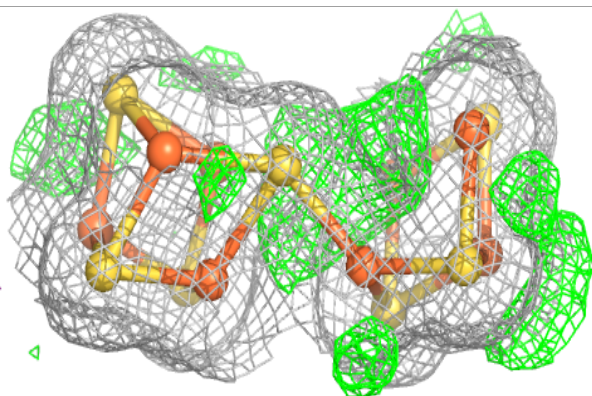
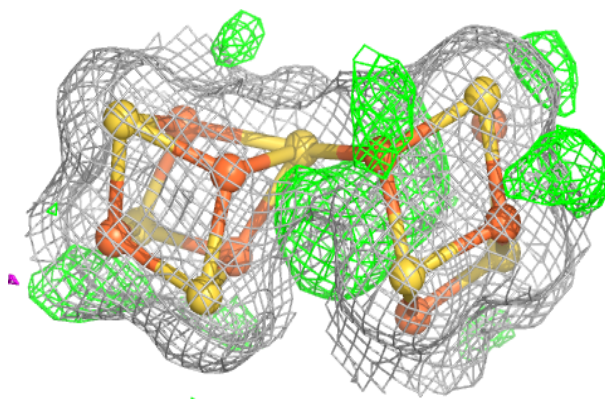
**Electron density around 1CL A 504:**

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

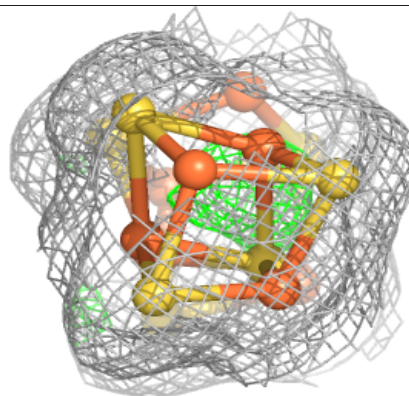
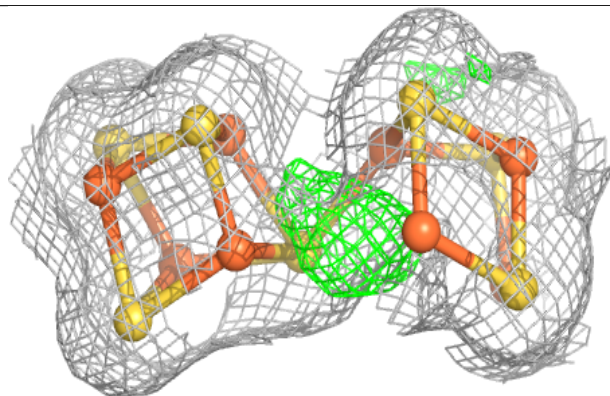
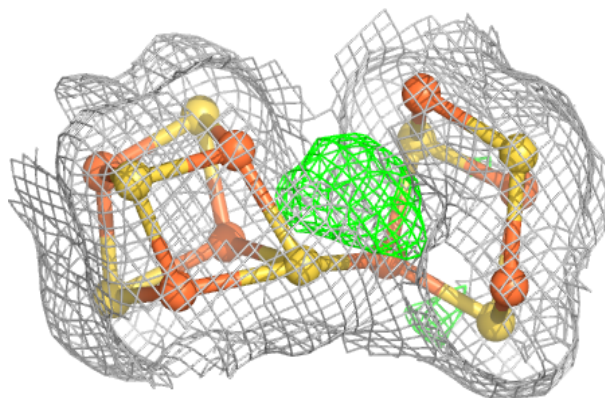


Electron density around 1CL D 601:

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

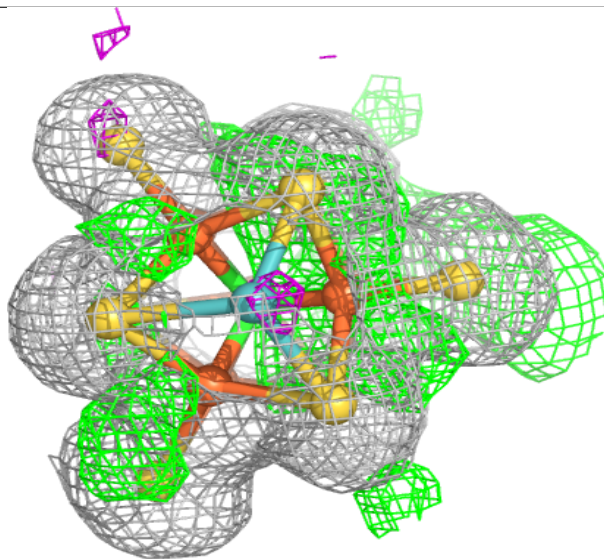
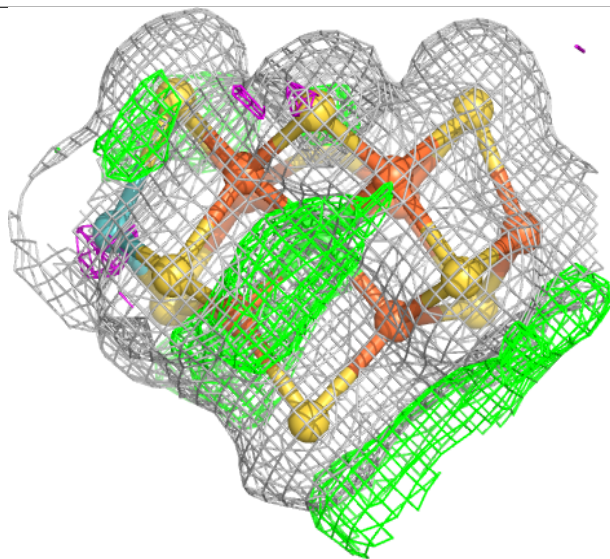
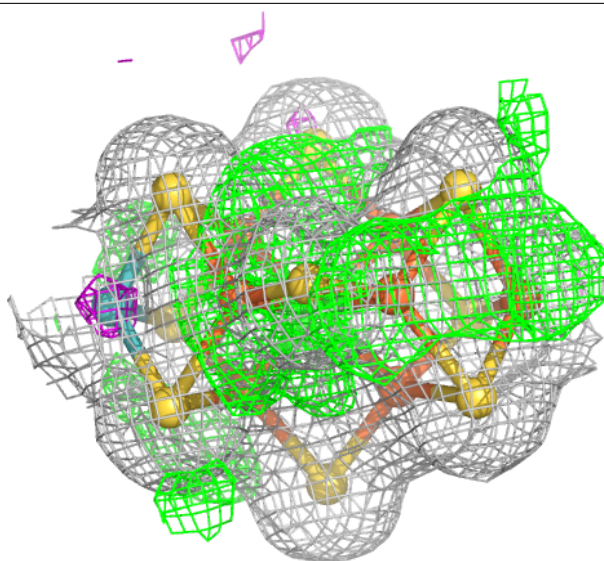
**Electron density around 1CL H 601:**

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



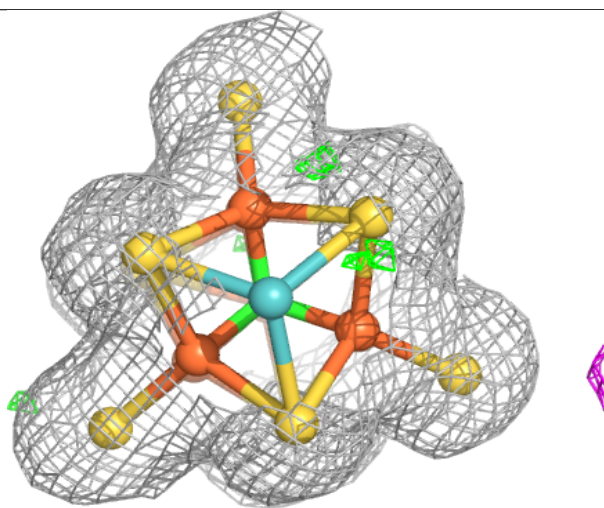
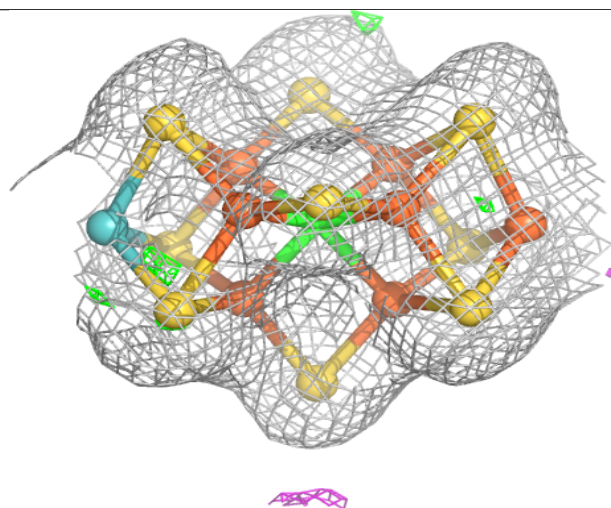
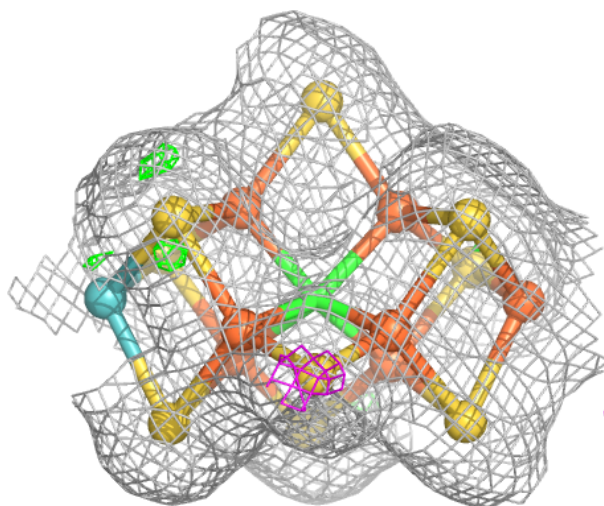
Electron density around ICS E 602:

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



Electron density around ICS A 503:

$2mF_o-DF_c$ (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.