



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 30, 2026 – 07:20 am BST

PDB ID : 29UN / pdb_000029un
Title : Mo-Nitrogenase, MoFe protein, P1+ redox state, -200 mV
Authors : Laxmi, S.; Seefeldt, L.C.; Carr, S.B.; Vincent, K.A.
Deposited on : 2026-04-08
Resolution : 2.00 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

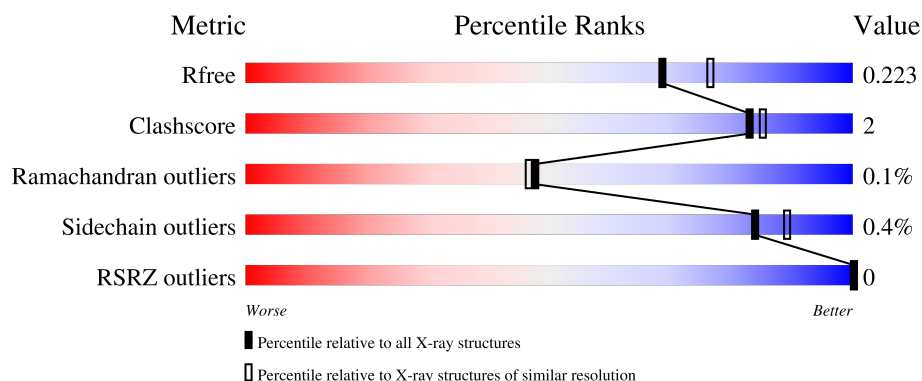
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

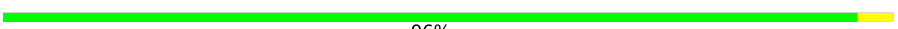
The reported resolution of this entry is 2.00 Å.

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.



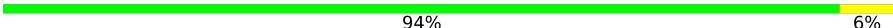
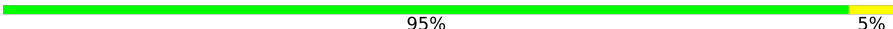
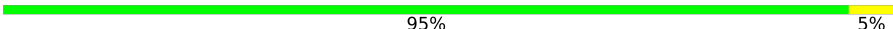
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	 87% 7% 6%
1	C	505	 87% 8% 6%
1	E	505	 88% 7% 6%
1	G	505	 88% 6% 6%
2	B	523	 96% .

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Mol	Chain	Length	Quality of chain
2	D	523	 94%6%
2	F	523	 95%5%
2	H	523	 95%5%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 65162 atoms, of which 31484 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	2	0
			7532	2413	3736	647	710	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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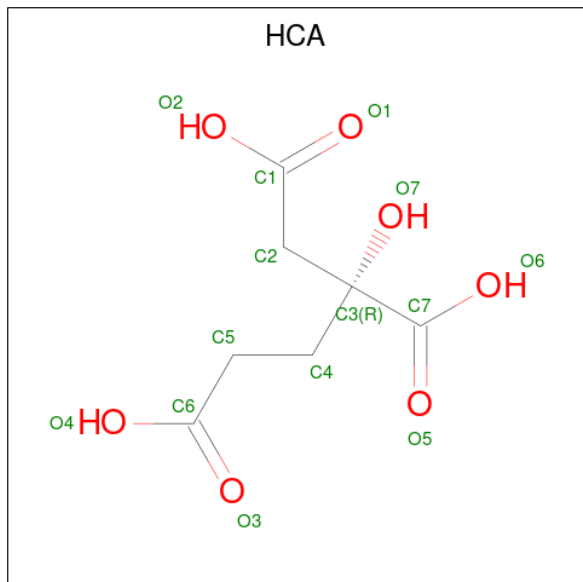
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	PRO	-	expression tag	UNP P07328
A	-3	GLN	-	expression tag	UNP P07328
A	-2	PHE	-	expression tag	UNP P07328
A	-1	GLU	-	expression tag	UNP P07328
A	0	LYS	-	expression tag	UNP P07328
C	-12	MET	-	initiating 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.

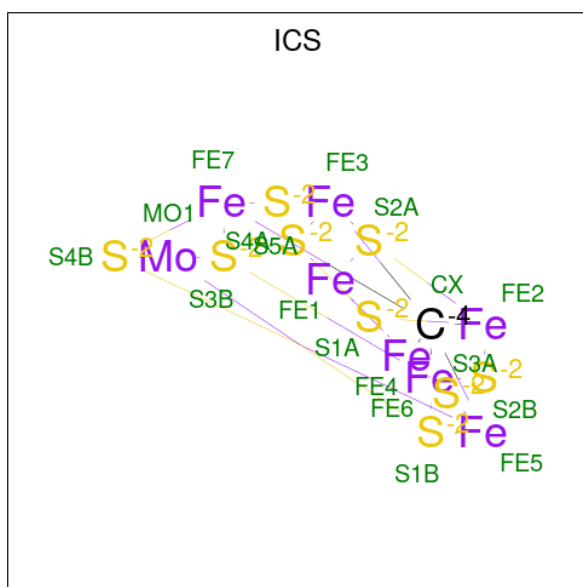
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	F	522	Total	C	H	N	O	S	0	2	0
			8271	2668	4093	706	776	28			
2	B	522	Total	C	H	N	O	S	0	0	0
			8262	2666	4088	705	775	28			
2	D	522	Total	C	H	N	O	S	0	0	0
			8264	2666	4090	705	775	28			
2	H	522	Total	C	H	N	O	S	0	0	0
			8263	2666	4089	705	775	28			

- 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).

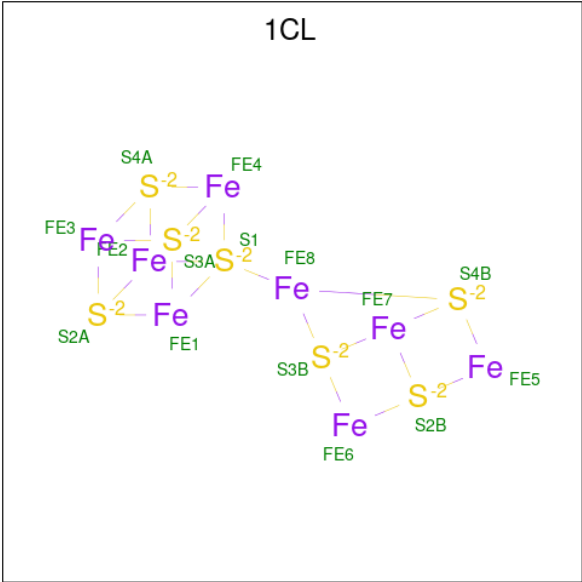


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total	C	Fe	Mo	S	
			18	1	7	1	9	0
4	A	1	Total	C	Fe	Mo	S	
			18	1	7	1	9	0
4	C	1	Total	C	Fe	Mo	S	
			18	1	7	1	9	0
4	G	1	Total	C	Fe	Mo	S	
			18	1	7	1	9	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

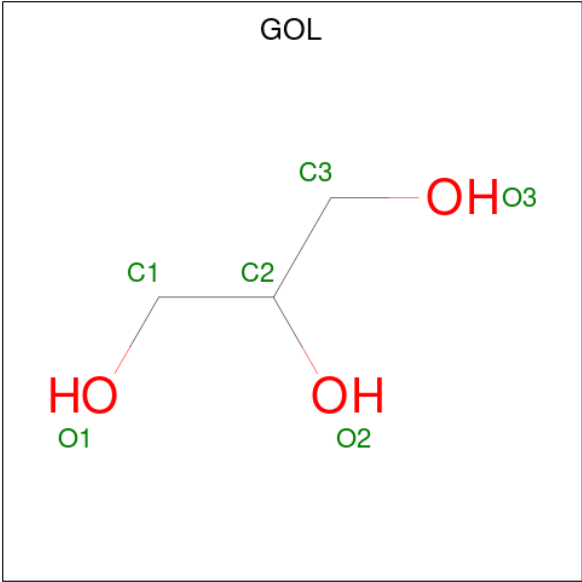
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	1	Total	Cl	0	0
			1	1		
5	A	1	Total	Cl	0	0
			1	1		
5	C	1	Total	Cl	0	0
			1	1		
5	G	1	Total	Cl	0	0
			1	1		

- Molecule 6 is FE(8)-S(7) CLUSTER, OXIDIZED (CCD ID: 1CL) (formula: Fe₈S₇) (labeled as "Ligand of Interest" by depositor).



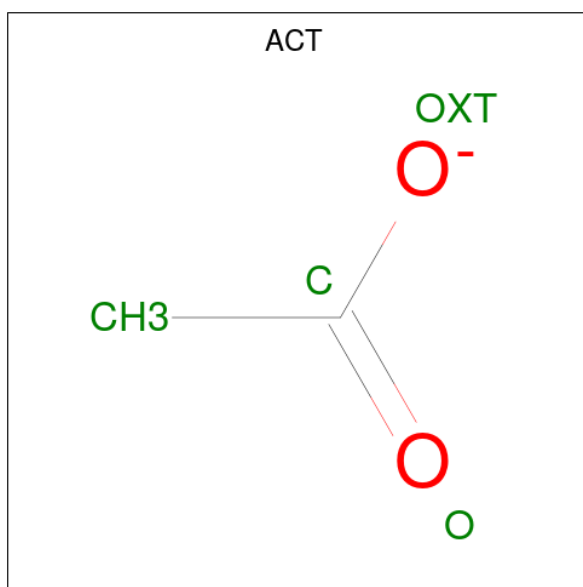
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	F	1	Total	Fe	S	0	0
			15	8	7		
6	B	1	Total	Fe	S	0	0
			15	8	7		
6	D	1	Total	Fe	S	0	0
			15	8	7		
6	H	1	Total	Fe	S	0	0
			15	8	7		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 8 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	E	194	Total	O	0	0
			194	194		
9	F	227	Total	O	0	0
			227	227		

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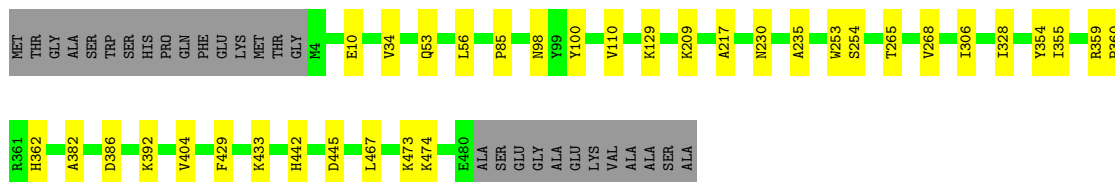
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	113	Total 113	O 113	0	0
9	B	198	Total 198	O 198	0	0
9	C	202	Total 202	O 202	0	0
9	D	228	Total 228	O 228	0	0
9	G	106	Total 106	O 106	0	0
9	H	198	Total 198	O 198	0	0

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.

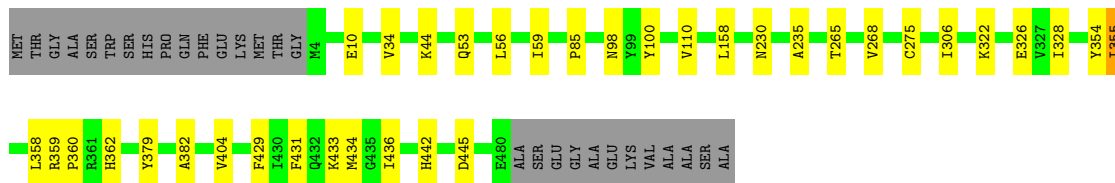
- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

Chain E: 



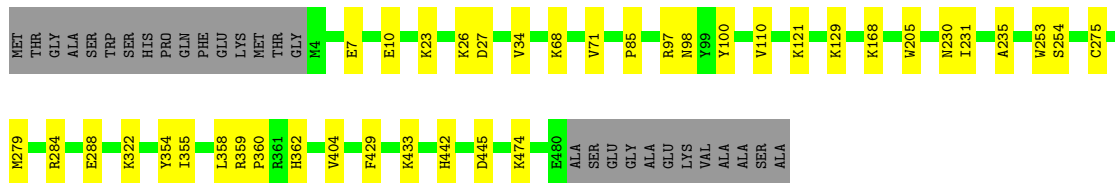
- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

Chain A: 



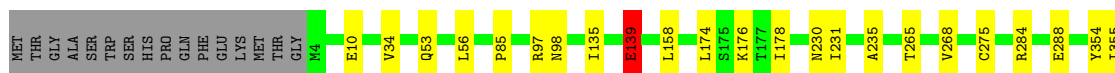
- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

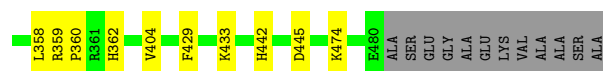
Chain C: 



- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

Chain G: 





- Molecule 2: Nitrogenase molybdenum-iron protein beta chain

Chain F: 95% 5%



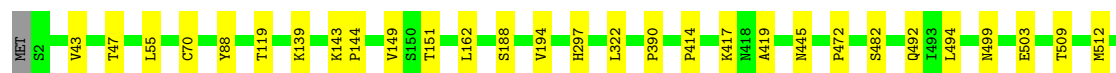
- Molecule 2: Nitrogenase molybdenum-iron protein beta chain

Chain B: 96% 4%



- Molecule 2: Nitrogenase molybdenum-iron protein beta chain

Chain D: 94% 6%



- Molecule 2: Nitrogenase molybdenum-iron protein beta chain

Chain H: 95% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.14Å 156.82Å 202.32Å 90.00° 89.98° 90.00°	Depositor
Resolution (Å)	77.68 – 2.00 77.68 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (77.68-2.00) 98.4 (77.68-2.00)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.196 , 0.222 0.196 , 0.223	Depositor DCC
R_{free} test set	17553 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.824	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 28.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.477 for h,-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	65162	wwPDB-VP
Average B, all atoms (Å ²)	45.0	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 47.10 % 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 1.0412e-04. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, GOL, CL, HCA, ICS, 1CL

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	0.28	0/3891	0.46	0/5247
1	C	0.30	0/3891	0.46	0/5247
1	E	0.30	0/3891	0.46	0/5247
1	G	0.27	0/3891	0.45	1/5247 (0.0%)
2	B	0.30	0/4280	0.45	0/5786
2	D	0.29	0/4280	0.44	0/5786
2	F	0.30	0/4292	0.45	0/5803
2	H	0.30	0/4280	0.46	0/5786
All	All	0.29	0/32696	0.46	1/44149 (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	G	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	G	139	GLU	CB-CG-CD	-5.48	103.29	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	139	GLU	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	20	0
1	C	3796	3736	3725	25	0
1	E	3796	3736	3725	20	0
1	G	3796	3735	3725	17	0
2	B	4174	4088	4088	21	0
2	D	4174	4090	4088	18	0
2	F	4178	4093	4087	16	0
2	H	4174	4089	4088	24	0
3	A	14	6	6	1	0
3	C	14	6	6	1	0
3	E	14	6	6	1	0
3	G	14	6	6	1	0
4	A	18	0	0	0	0
4	C	18	0	0	1	0
4	E	18	0	0	0	0
4	G	18	0	0	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
6	B	15	0	0	1	0
6	D	15	0	0	1	0
6	F	15	0	0	1	0
6	H	15	0	0	1	0
7	A	6	8	8	0	0
7	B	30	40	40	0	0
7	D	24	32	32	0	0
7	F	12	16	16	0	0
7	H	24	32	32	0	0
8	A	4	3	3	0	0
8	B	4	3	3	1	0
8	D	12	9	9	2	0
8	F	12	9	9	0	0
8	H	8	6	6	0	0
9	A	113	0	0	0	0
9	B	198	0	0	0	0
9	C	202	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	D	228	0	0	0	0
9	E	194	0	0	0	0
9	F	227	0	0	0	0
9	G	106	0	0	0	0
9	H	198	0	0	0	0
All	All	33678	31484	31433	155	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 155 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:B:118:MET:HB2	2:B:154:MET:HE1	1.61	0.80
1:C:129:LYS:HA	1:C:129:LYS:HE2	1.69	0.74
2:B:118:MET:HE2	2:B:154:MET:HE3	1.71	0.72
1:E:129:LYS:HA	1:E:129:LYS:HE2	1.71	0.71
2:B:50:LYS:N	2:B:50:LYS:HD3	2.10	0.66

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	477/505 (94%)	459 (96%)	17 (4%)	1 (0%)	43	42
1	C	477/505 (94%)	459 (96%)	17 (4%)	1 (0%)	43	42
1	E	477/505 (94%)	459 (96%)	17 (4%)	1 (0%)	43	42
1	G	477/505 (94%)	459 (96%)	17 (4%)	1 (0%)	43	42
2	B	520/523 (99%)	510 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	520/523 (99%)	508 (98%)	12 (2%)	0	100	100
2	F	522/523 (100%)	512 (98%)	9 (2%)	1 (0%)	43	42
2	H	520/523 (99%)	510 (98%)	10 (2%)	0	100	100
All	All	3990/4112 (97%)	3876 (97%)	109 (3%)	5 (0%)	48	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	355	ILE
1	E	355	ILE
2	F	255	SER
1	A	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%)	405 (99%)	4 (1%)	68	75
1	C	409/426 (96%)	406 (99%)	3 (1%)	76	82
1	E	409/426 (96%)	406 (99%)	3 (1%)	76	82
1	G	409/426 (96%)	406 (99%)	3 (1%)	76	82
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%)	455 (100%)	0	100	100
2	H	454/455 (100%)	454 (100%)	0	100	100
All	All	3453/3524 (98%)	3440 (100%)	13 (0%)	84	89

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

Mol	Chain	Res	Type
1	C	98	ASN

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Mol	Chain	Res	Type
1	C	362	HIS
1	G	445	ASP
1	G	98	ASN
1	G	362	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	128	GLN
2	D	268	GLN
2	D	168	ASN
2	D	363	HIS
2	F	363	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 4 are monoatomic - leaving 38 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
8	ACT	D	605	-	3,3,3	1.56	1 (33%)	3,3,3	0.51	0
8	ACT	D	608	-	3,3,3	1.64	1 (33%)	3,3,3	1.52	1 (33%)
8	ACT	B	605	-	3,3,3	1.57	1 (33%)	3,3,3	0.47	0
8	ACT	A	504	-	3,3,3	1.62	1 (33%)	3,3,3	0.43	0
8	ACT	H	606	-	3,3,3	1.48	1 (33%)	3,3,3	1.04	0
8	ACT	D	606	-	3,3,3	1.50	1 (33%)	3,3,3	0.61	0
7	GOL	D	603	-	5,5,5	0.33	0	5,5,5	0.39	0
6	1CL	B	602	2,1	0,22,22	-	-	-	-	-
7	GOL	D	604	-	5,5,5	0.31	0	5,5,5	0.68	0
8	ACT	F	603	-	3,3,3	1.55	1 (33%)	3,3,3	0.58	0
7	GOL	B	603	-	5,5,5	0.31	0	5,5,5	0.52	0
7	GOL	B	604	-	5,5,5	0.27	0	5,5,5	0.43	0
7	GOL	D	602	-	5,5,5	0.32	0	5,5,5	0.72	0
7	GOL	A	501	-	5,5,5	0.31	0	5,5,5	0.41	0
4	ICS	C	602	1,3	18,30,30	2.38	10 (55%)	-	-	-
7	GOL	B	601	-	5,5,5	0.28	0	5,5,5	0.42	0
7	GOL	F	605	-	5,5,5	0.32	0	5,5,5	0.50	0
7	GOL	B	606	-	5,5,5	0.29	0	5,5,5	0.27	0
7	GOL	H	604	-	5,5,5	0.32	0	5,5,5	0.36	0
3	HCA	G	601	4	13,13,13	1.74	2 (15%)	14,18,18	1.83	2 (14%)
8	ACT	F	606	-	3,3,3	1.60	1 (33%)	3,3,3	0.65	0
8	ACT	H	602	-	3,3,3	1.60	1 (33%)	3,3,3	0.45	0
6	1CL	F	601	2,1	0,22,22	-	-	-	-	-
3	HCA	C	601	4	13,13,13	1.77	3 (23%)	14,18,18	2.02	3 (21%)
4	ICS	G	602	1,3	18,30,30	2.39	9 (50%)	-	-	-
7	GOL	H	603	-	5,5,5	0.35	0	5,5,5	0.70	0
4	ICS	A	503	1,3	18,30,30	2.44	9 (50%)	-	-	-
7	GOL	D	607	-	5,5,5	0.26	0	5,5,5	0.33	0
7	GOL	H	607	-	5,5,5	0.30	0	5,5,5	0.33	0
8	ACT	F	604	-	3,3,3	1.63	1 (33%)	3,3,3	0.20	0
7	GOL	F	602	-	5,5,5	0.31	0	5,5,5	0.54	0
3	HCA	A	502	4	13,13,13	1.76	2 (15%)	14,18,18	1.94	3 (21%)
7	GOL	B	607	-	5,5,5	0.34	0	5,5,5	0.61	0
7	GOL	H	605	-	5,5,5	0.33	0	5,5,5	0.46	0
6	1CL	H	601	2,1	0,22,22	-	-	-	-	-
4	ICS	E	602	1,3	18,30,30	2.47	10 (55%)	-	-	-
6	1CL	D	601	2,1	0,22,22	-	-	-	-	-
3	HCA	E	601	4	13,13,13	1.67	2 (15%)	14,18,18	1.86	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
7	GOL	D	603	-	-	2/4/4/4	-
7	GOL	D	604	-	-	0/4/4/4	-
6	1CL	B	602	2,1	-	-	0/10/8/8
7	GOL	B	603	-	-	2/4/4/4	-
7	GOL	B	604	-	-	1/4/4/4	-
7	GOL	D	602	-	-	0/4/4/4	-
7	GOL	A	501	-	-	0/4/4/4	-
7	GOL	H	604	-	-	4/4/4/4	-
7	GOL	B	601	-	-	2/4/4/4	-
7	GOL	F	605	-	-	0/4/4/4	-
7	GOL	B	606	-	-	0/4/4/4	-
3	HCA	G	601	4	-	4/17/17/17	-
6	1CL	F	601	2,1	-	-	0/10/8/8
7	GOL	H	603	-	-	0/4/4/4	-
3	HCA	C	601	4	-	4/17/17/17	-
7	GOL	D	607	-	-	0/4/4/4	-
7	GOL	H	607	-	-	0/4/4/4	-
7	GOL	F	602	-	-	2/4/4/4	-
3	HCA	A	502	4	-	4/17/17/17	-
7	GOL	B	607	-	-	0/4/4/4	-
7	GOL	H	605	-	-	2/4/4/4	-
6	1CL	H	601	2,1	-	-	0/10/8/8
6	1CL	D	601	2,1	-	-	0/10/8/8
3	HCA	E	601	4	-	4/17/17/17	-

The worst 5 of 57 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	602	ICS	S3B-FE6	-4.30	2.21	2.32
4	A	503	ICS	S4B-FE7	-4.30	2.21	2.32
3	C	601	HCA	C3-C7	4.30	1.57	1.53
4	E	602	ICS	S3B-FE6	-4.21	2.22	2.32
3	G	601	HCA	C3-C7	4.13	1.57	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	HCA	O5-C7-C3	-4.95	115.24	122.25
3	A	502	HCA	O6-C7-C3	4.38	120.65	113.05
3	A	502	HCA	O5-C7-C3	-4.31	116.14	122.25
3	C	601	HCA	O6-C7-C3	4.14	120.23	113.05
3	E	601	HCA	O5-C7-C3	-4.08	116.47	122.25

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	601	GOL	C1-C2-C3-O3
7	D	603	GOL	C1-C2-C3-O3
7	D	603	GOL	O2-C2-C3-O3
7	H	604	GOL	C1-C2-C3-O3
7	H	604	GOL	O2-C2-C3-O3

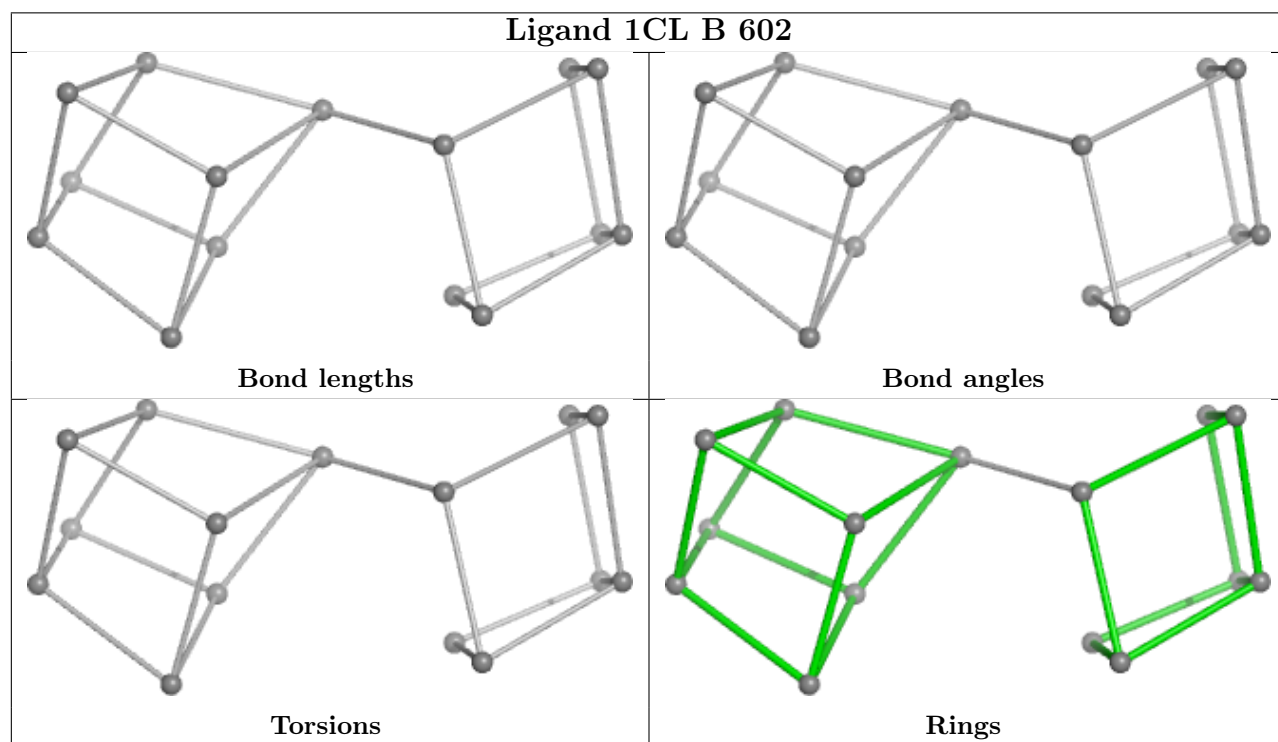
There are no ring outliers.

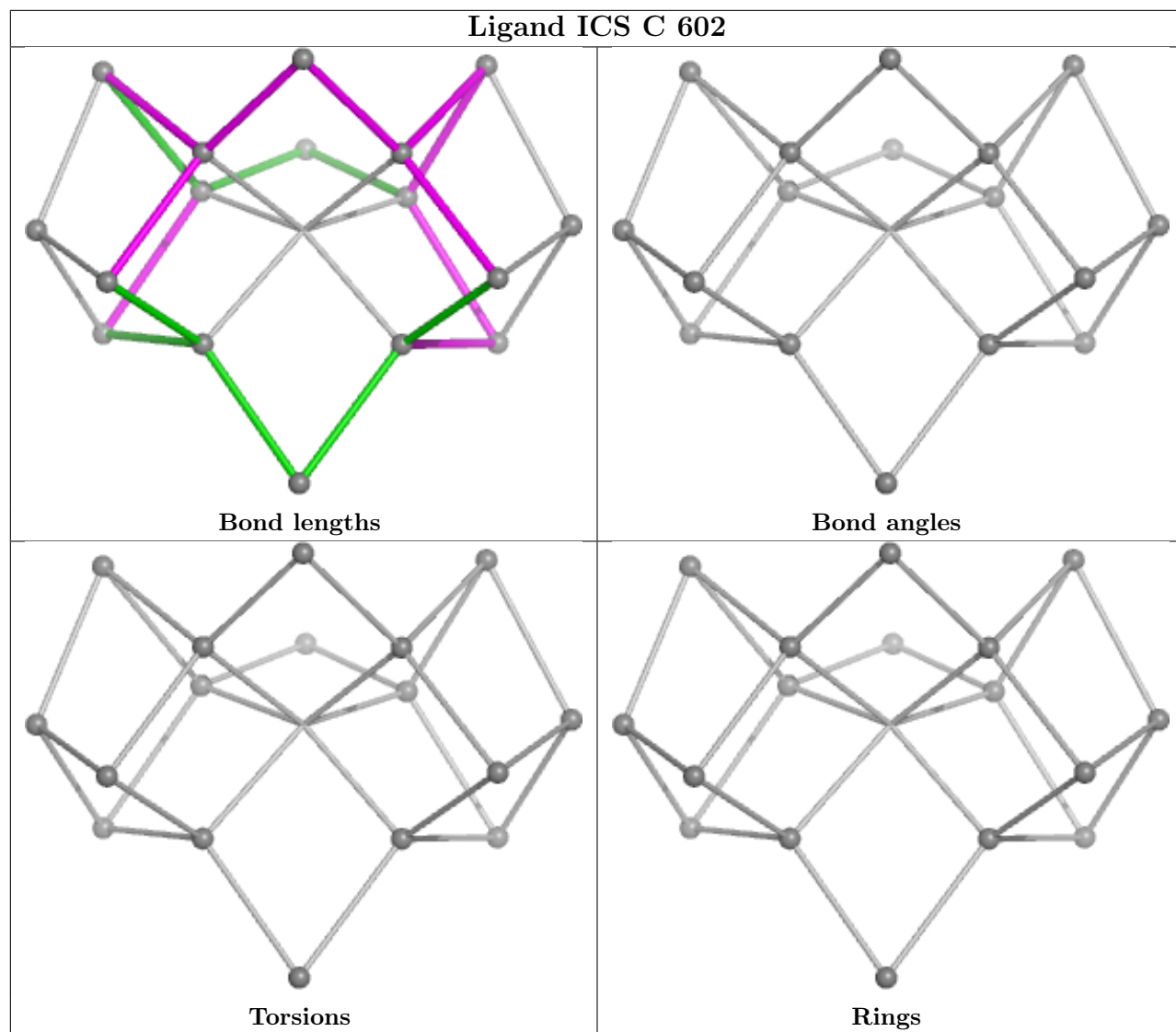
12 monomers are involved in 12 short contacts:

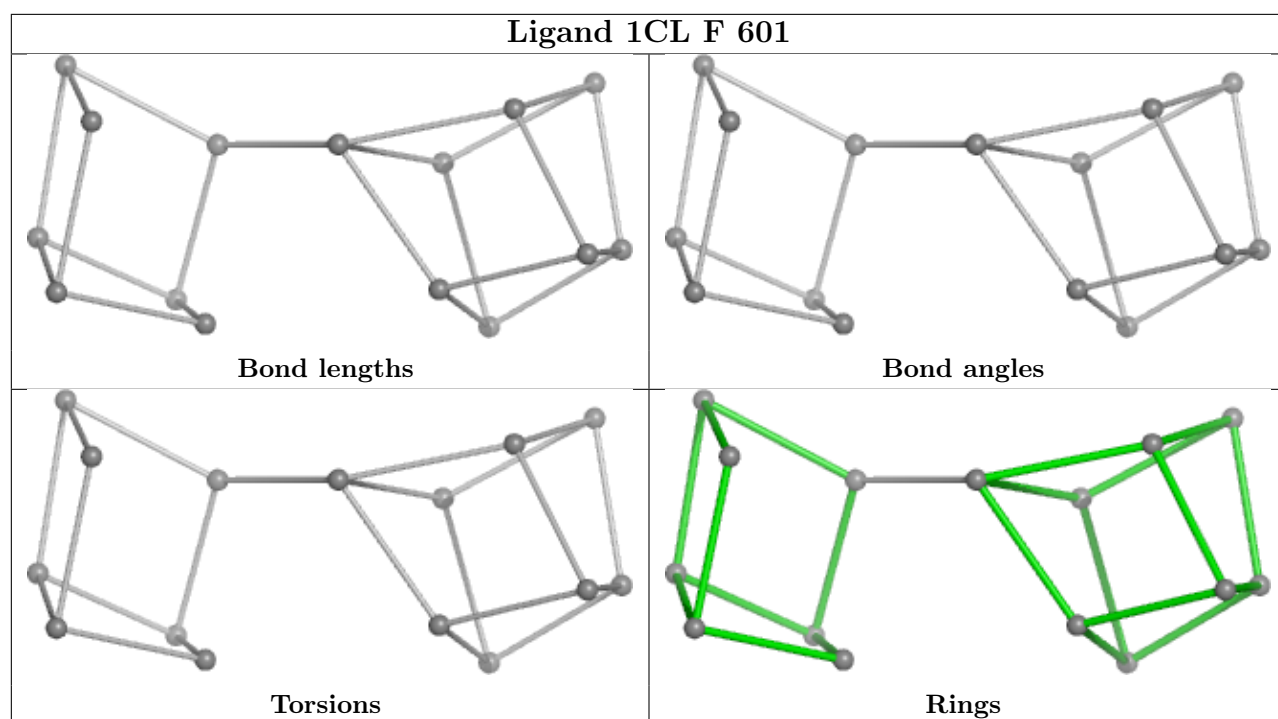
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	608	ACT	1	0
8	B	605	ACT	1	0
8	D	606	ACT	1	0
6	B	602	1CL	1	0
4	C	602	ICS	1	0
3	G	601	HCA	1	0
6	F	601	1CL	1	0
3	C	601	HCA	1	0
3	A	502	HCA	1	0
6	H	601	1CL	1	0
6	D	601	1CL	1	0
3	E	601	HCA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

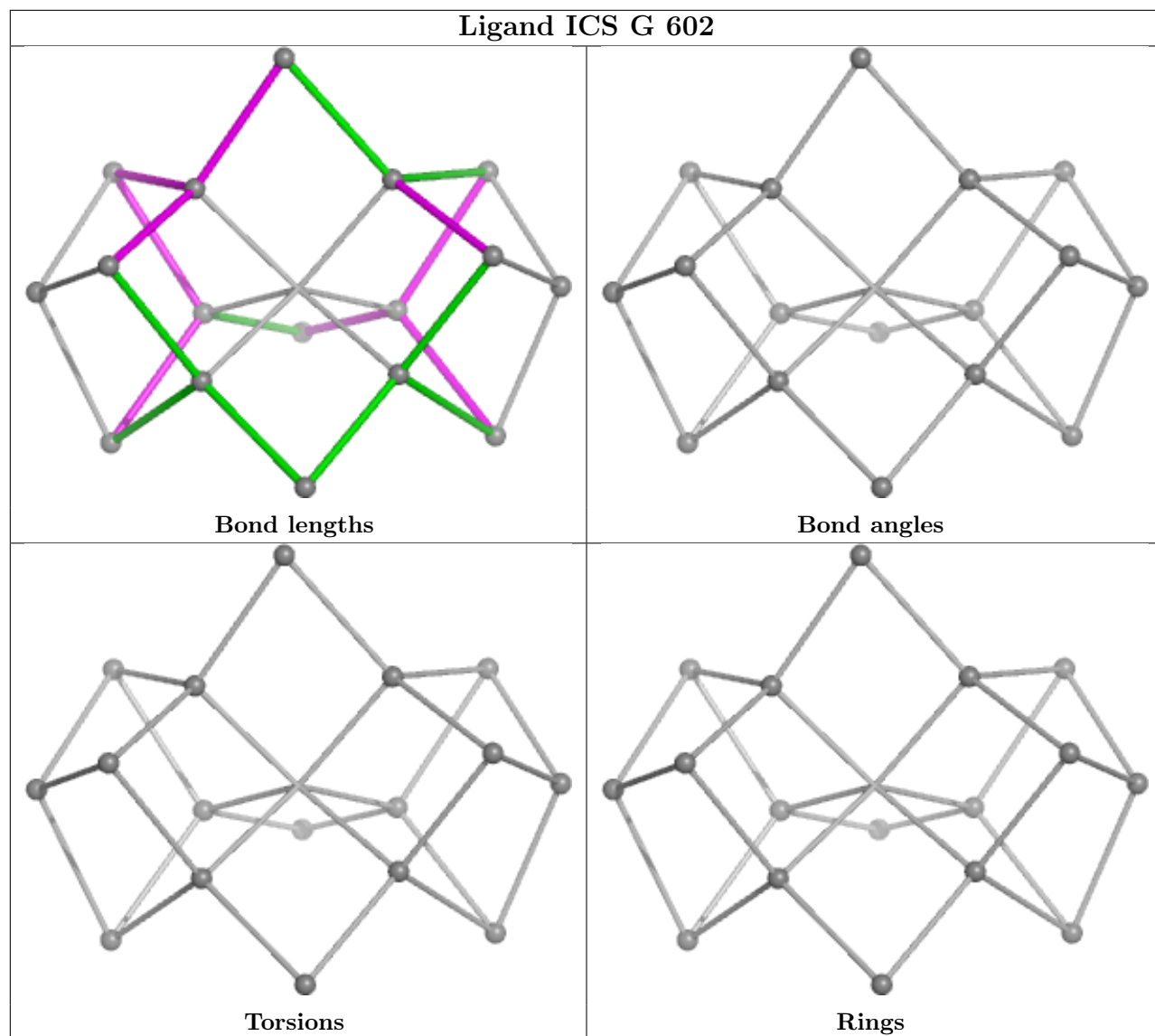
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



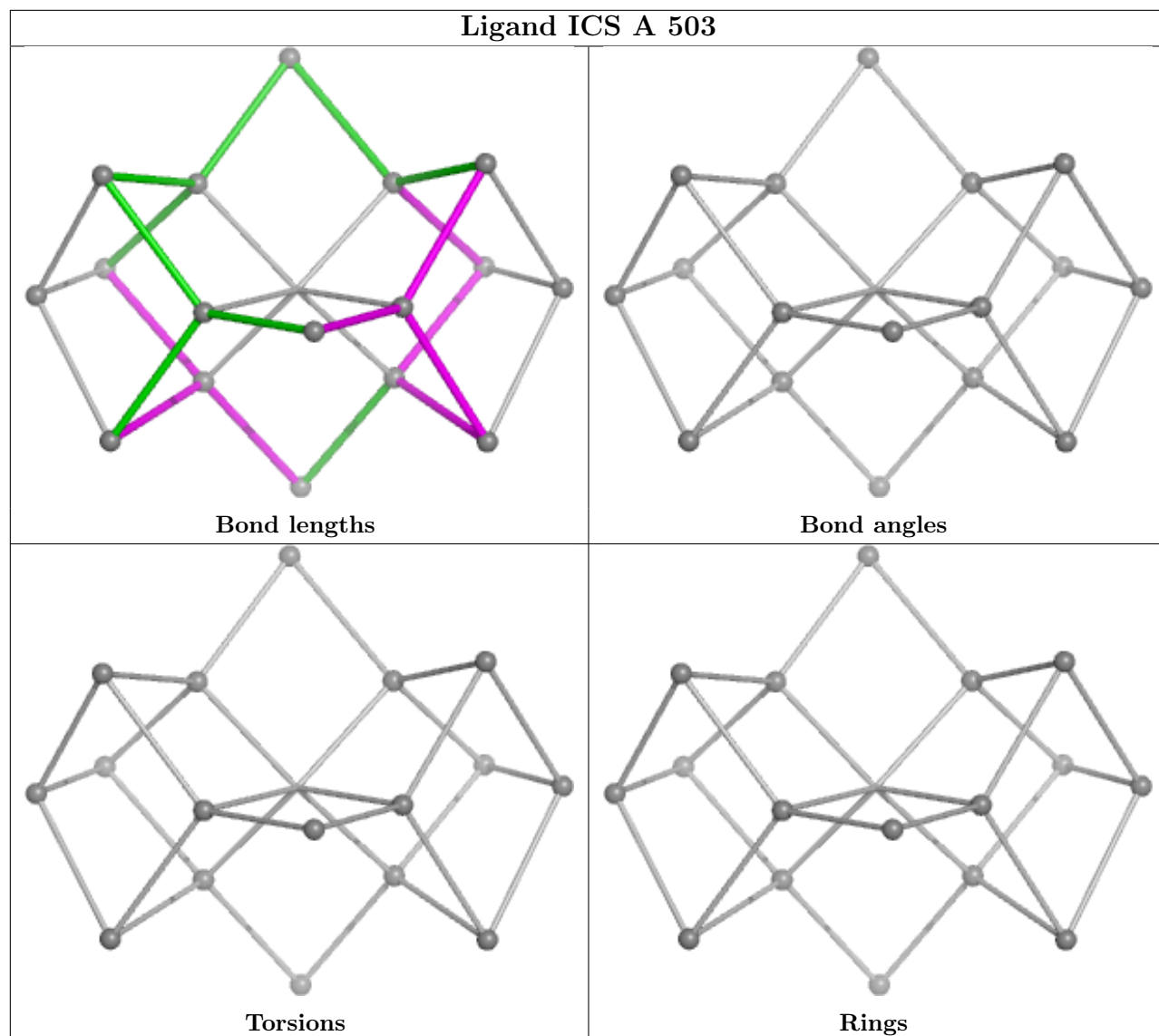


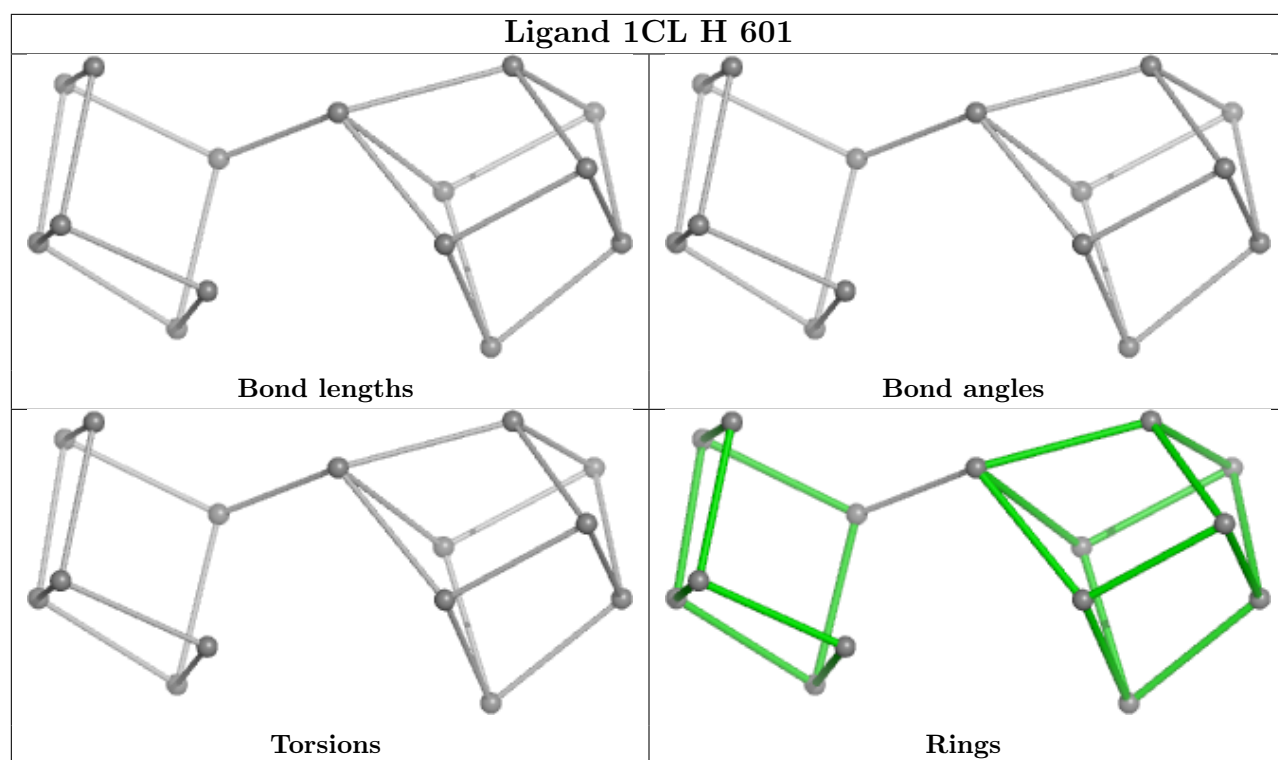


Ligand ICS G 602

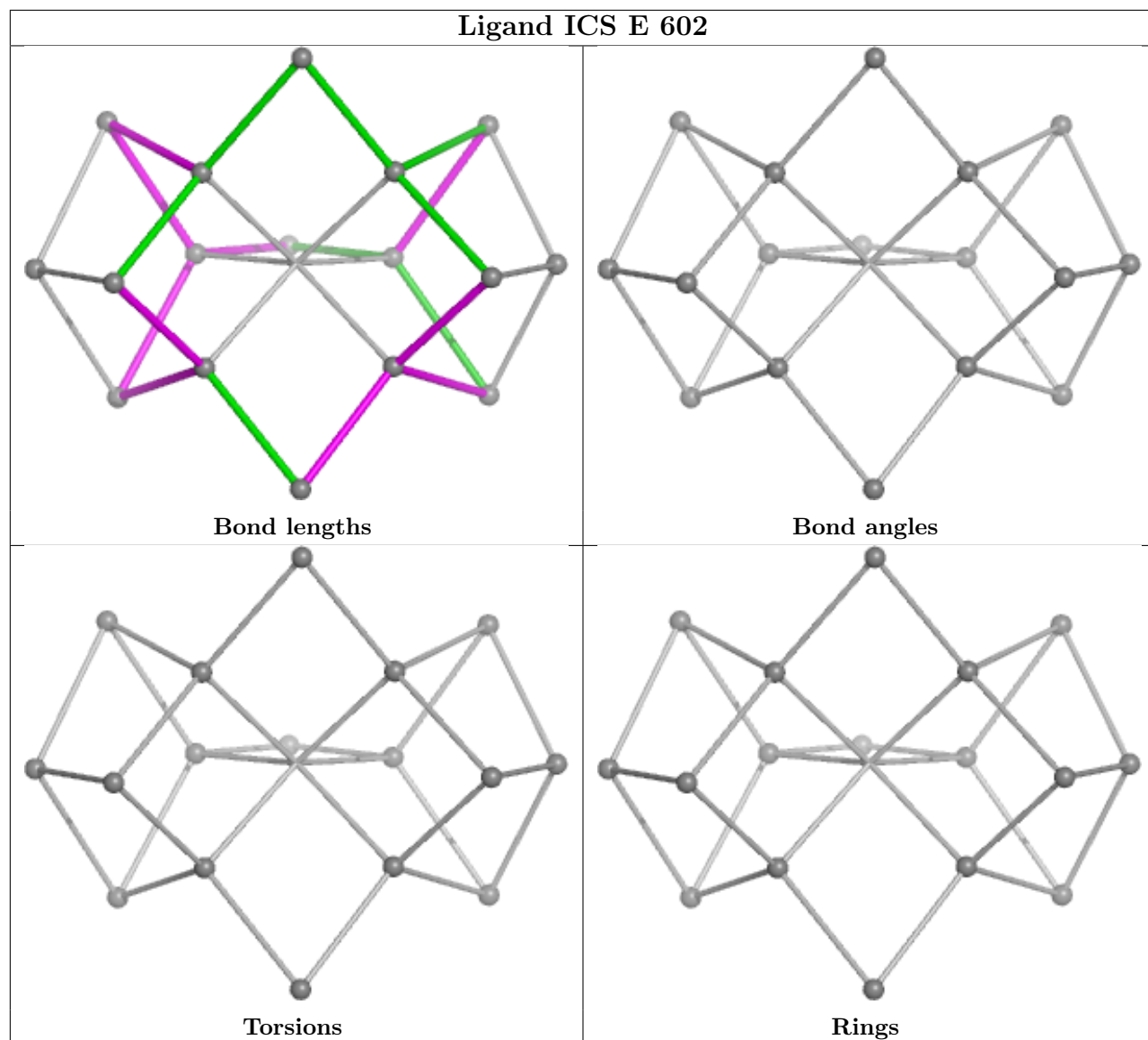


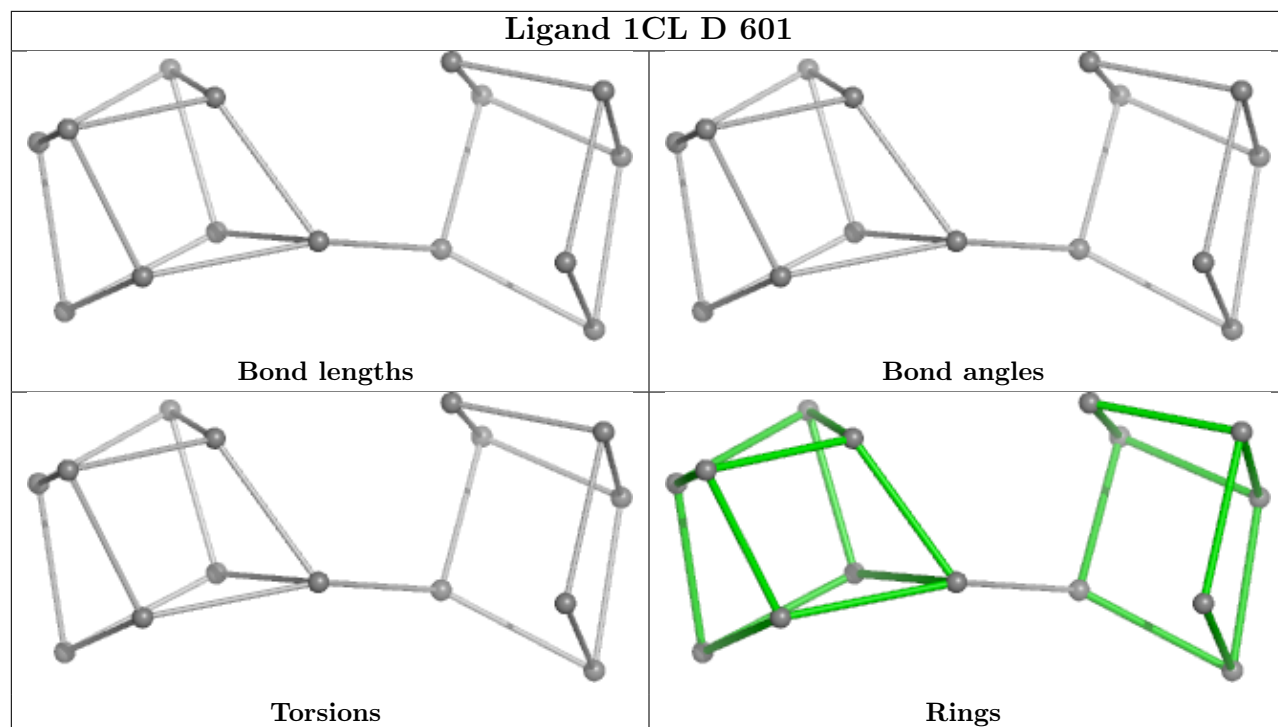
Ligand ICS A 503





Ligand ICS E 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%)	-1.49	0 100 100	29, 52, 74, 101	1 (0%)
1	C	477/505 (94%)	-1.63	0 100 100	20, 37, 55, 75	1 (0%)
1	E	477/505 (94%)	-1.63	0 100 100	20, 38, 55, 76	1 (0%)
1	G	477/505 (94%)	-1.49	0 100 100	29, 51, 74, 99	1 (0%)
2	B	522/523 (99%)	-1.55	0 100 100	29, 46, 65, 88	0
2	D	522/523 (99%)	-1.63	0 100 100	27, 40, 58, 73	0
2	F	522/523 (99%)	-1.61	0 100 100	17, 40, 57, 75	1 (0%)
2	H	522/523 (99%)	-1.57	0 100 100	29, 46, 67, 85	0
All	All	3996/4112 (97%)	-1.57	0 100 100	17, 43, 66, 101	5 (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.

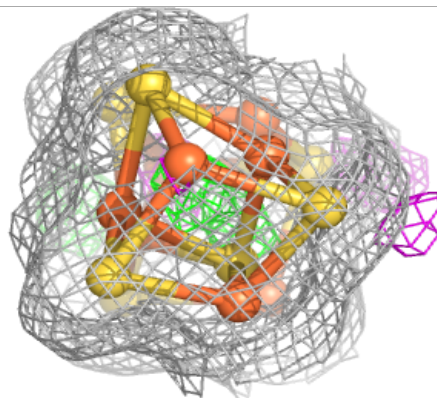
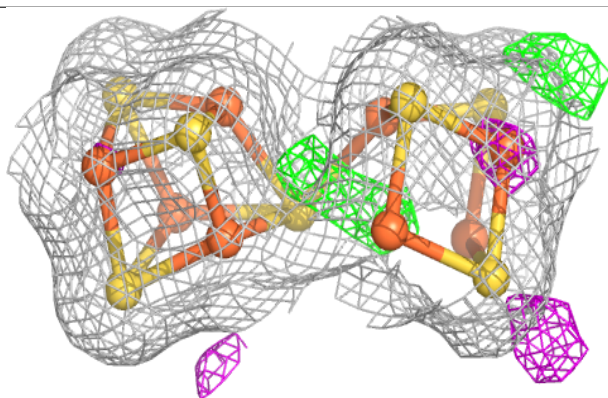
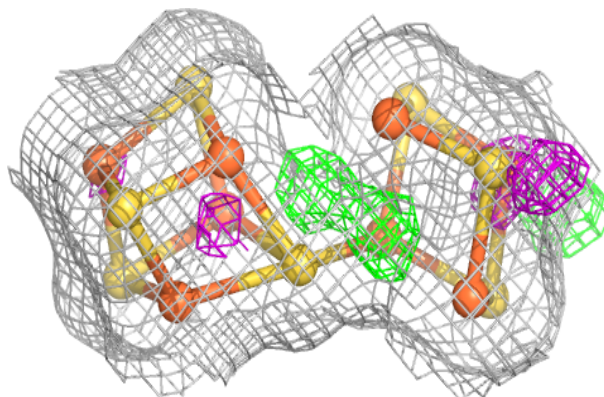
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	GOL	H	605	6/6	0.98	0.05	51,61,67,68	0
8	ACT	F	604	4/4	0.98	0.08	45,50,56,56	0
8	ACT	F	606	4/4	0.98	0.06	41,48,52,52	0
8	ACT	A	504	4/4	0.98	0.08	50,56,63,63	0
8	ACT	D	606	4/4	0.98	0.06	38,45,49,53	0
8	ACT	D	608	4/4	0.98	0.06	39,46,50,50	0
8	ACT	H	602	4/4	0.98	0.10	49,56,63,63	0
7	GOL	B	604	6/6	0.99	0.04	51,61,63,66	0
7	GOL	B	606	6/6	0.99	0.03	46,55,61,66	0
7	GOL	B	607	6/6	0.99	0.03	33,45,52,55	0
7	GOL	D	602	6/6	0.99	0.05	34,41,45,46	0
7	GOL	D	603	6/6	0.99	0.03	37,46,52,62	0
7	GOL	D	604	6/6	0.99	0.04	44,53,60,60	0
7	GOL	D	607	6/6	0.99	0.03	37,45,55,55	0
7	GOL	H	603	6/6	0.99	0.05	36,43,49,50	0
3	HCA	A	502	14/14	0.99	0.03	29,32,39,39	0
7	GOL	H	607	6/6	0.99	0.03	45,55,62,65	0
8	ACT	F	603	4/4	0.99	0.03	33,38,40,41	0
3	HCA	C	601	14/14	0.99	0.03	24,27,32,32	0
7	GOL	F	602	6/6	0.99	0.04	41,49,59,63	0
7	GOL	F	605	6/6	0.99	0.03	34,41,43,46	0
8	ACT	B	605	4/4	0.99	0.04	37,41,45,45	0
8	ACT	D	605	4/4	0.99	0.03	33,39,40,42	0
7	GOL	A	501	6/6	0.99	0.06	38,46,54,58	0
7	GOL	B	601	6/6	0.99	0.04	41,50,57,63	0
7	GOL	B	603	6/6	0.99	0.04	33,40,45,54	0
8	ACT	H	606	4/4	0.99	0.04	36,40,44,44	0
6	1CL	B	602	15/15	1.00	0.01	29,33,43,44	0
6	1CL	D	601	15/15	1.00	0.01	23,27,38,39	0
7	GOL	H	604	6/6	1.00	0.03	34,42,47,57	0
6	1CL	H	601	15/15	1.00	0.01	28,33,44,45	0
3	HCA	E	601	14/14	1.00	0.02	24,28,32,32	0
3	HCA	G	601	14/14	1.00	0.03	28,33,40,40	0
4	ICS	E	602	18/18	1.00	0.01	23,25,27,27	0
4	ICS	A	503	18/18	1.00	0.01	25,31,33,34	0
4	ICS	C	602	18/18	1.00	0.01	22,24,26,28	0
4	ICS	G	602	18/18	1.00	0.01	27,31,34,34	0
5	CL	E	603	1/1	1.00	0.03	32,32,32,32	0
5	CL	A	505	1/1	1.00	0.04	38,38,38,38	0
5	CL	C	603	1/1	1.00	0.03	33,33,33,33	0
5	CL	G	603	1/1	1.00	0.04	38,38,38,38	0
6	1CL	F	601	15/15	1.00	0.01	23,28,38,38	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.

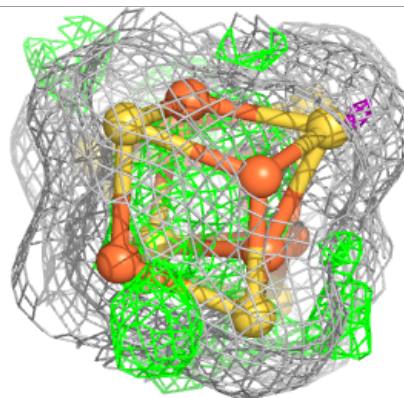
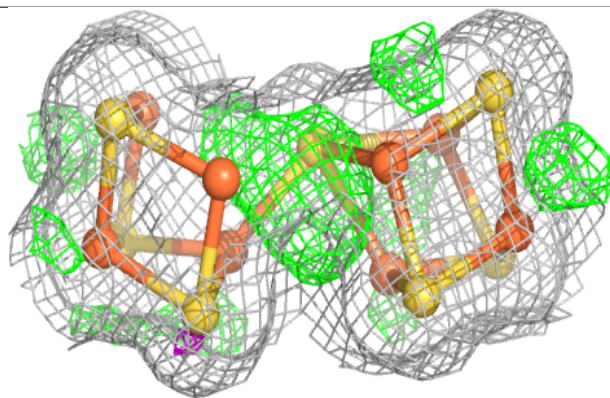
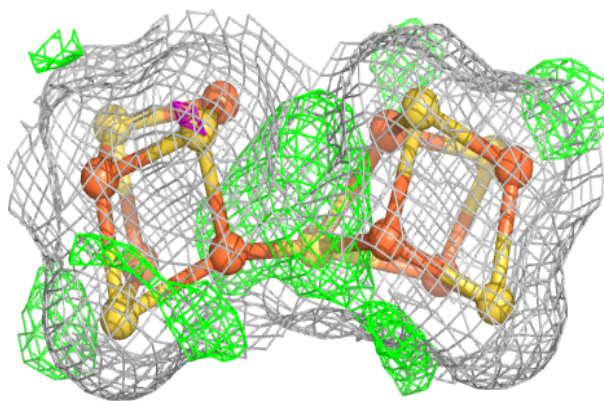
Electron density around 1CL B 602:

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

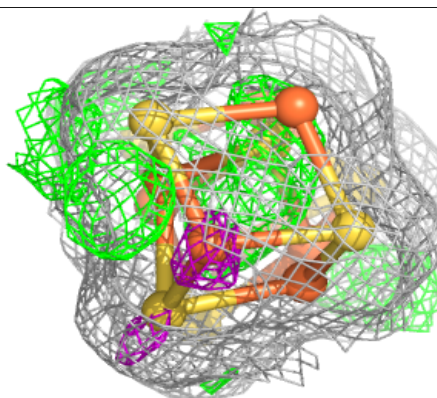
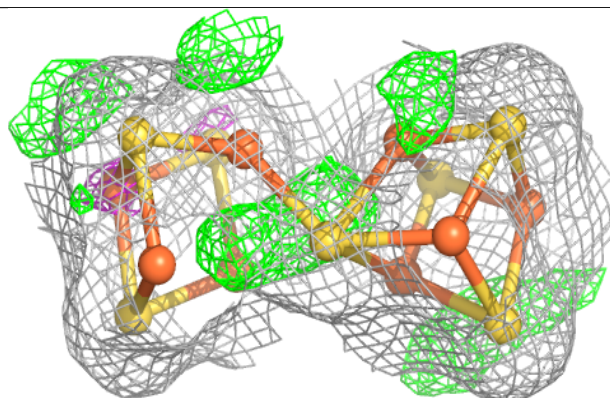
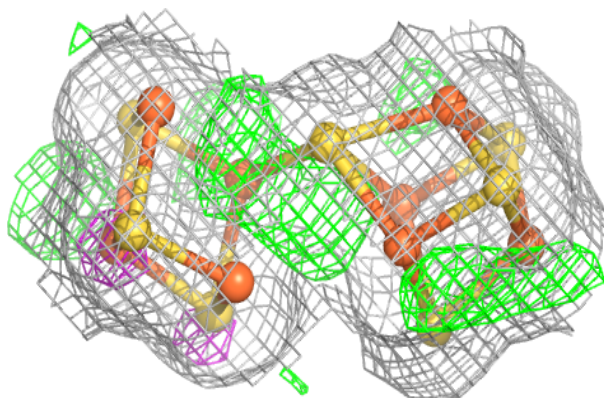


Electron density around 1CL D 601:

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

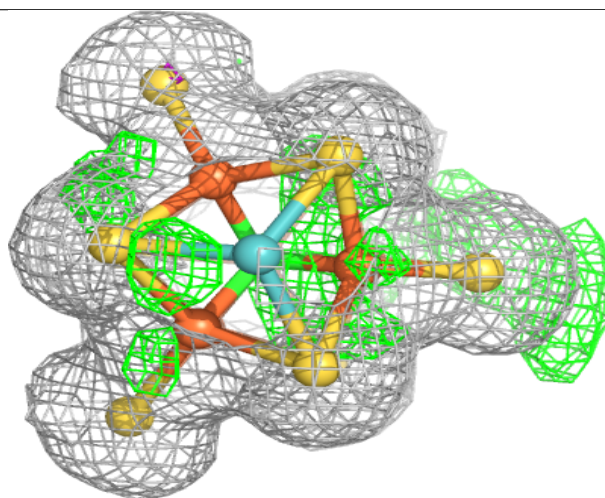
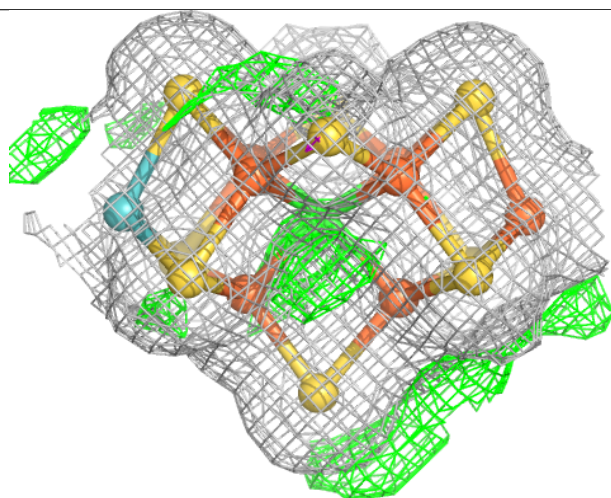
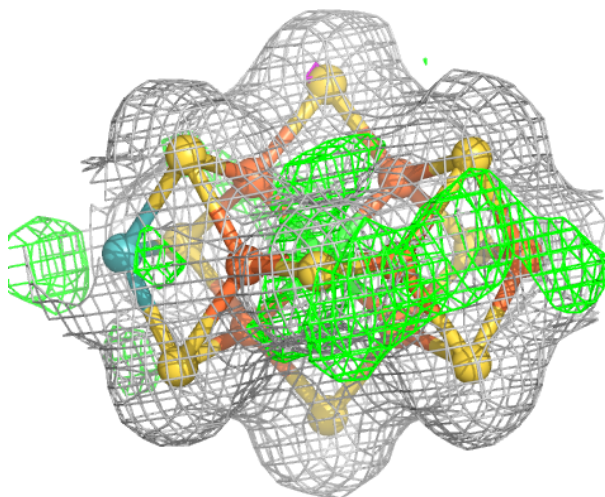
**Electron density around 1CL H 601:**

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



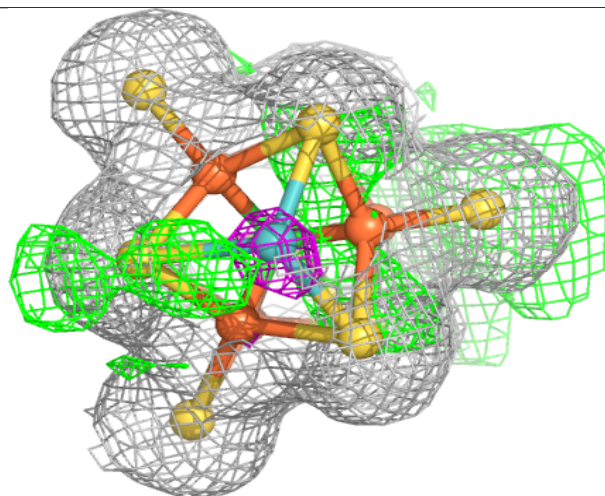
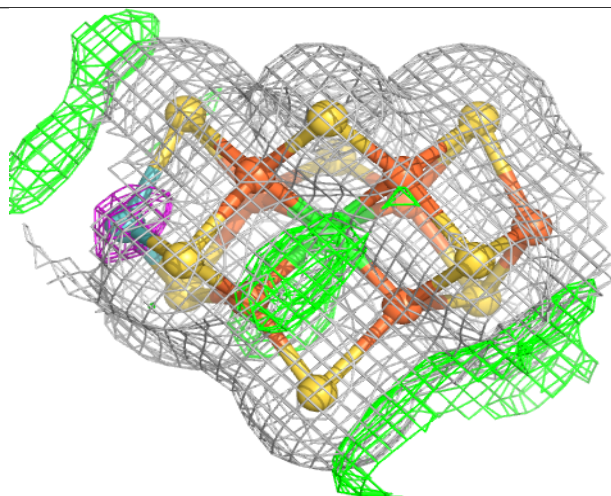
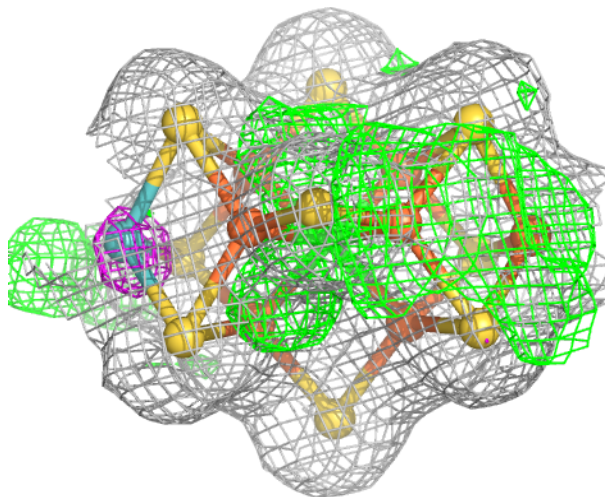
Electron density around ICS E 602:

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



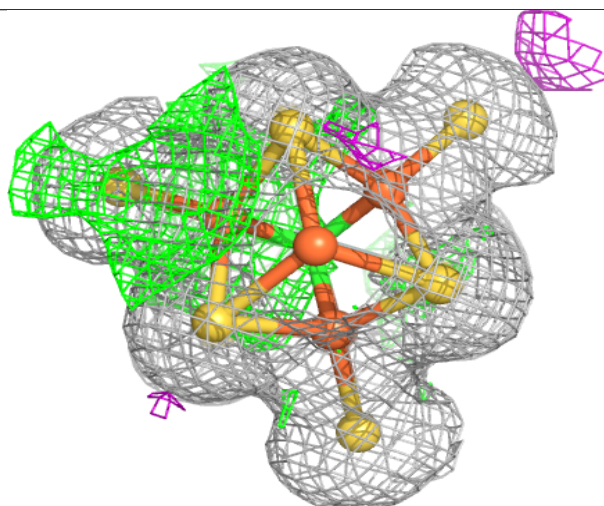
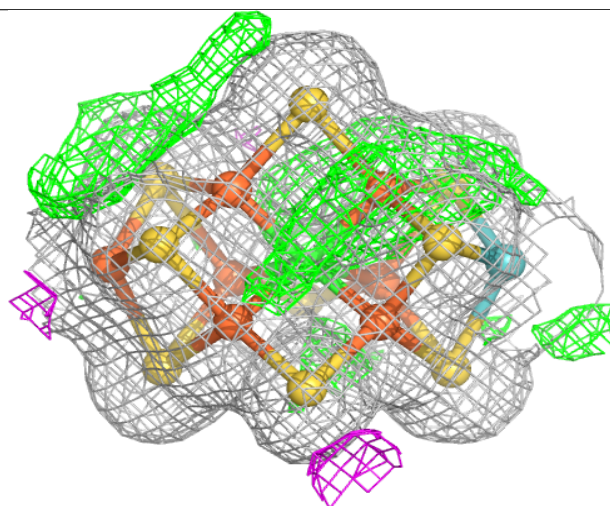
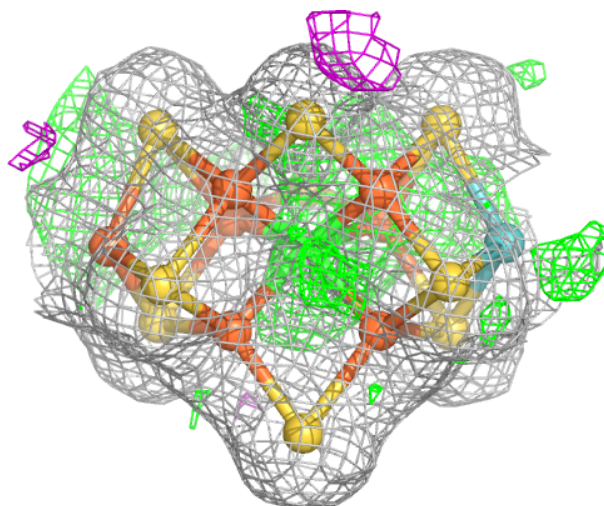
Electron density around ICS A 503:

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



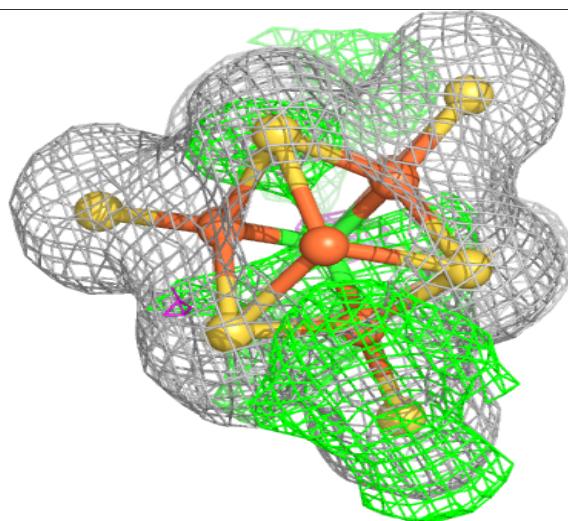
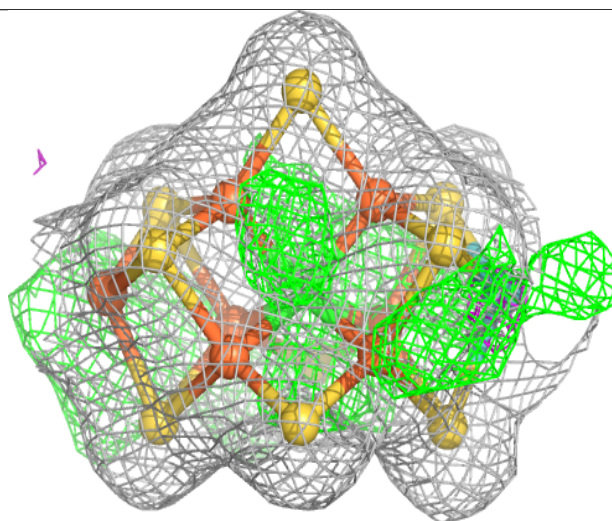
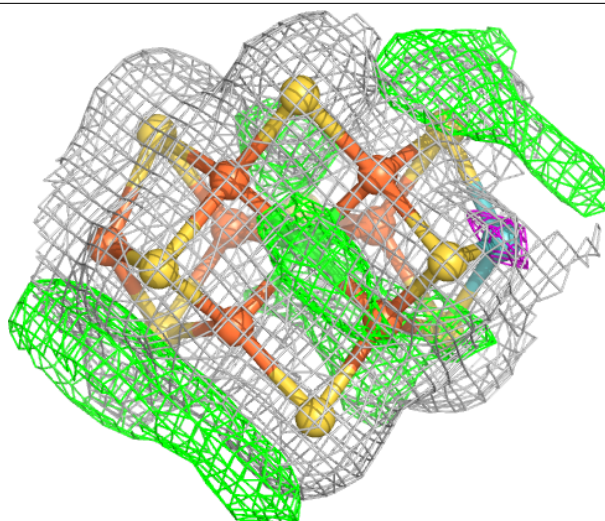
Electron density around ICS C 602:

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



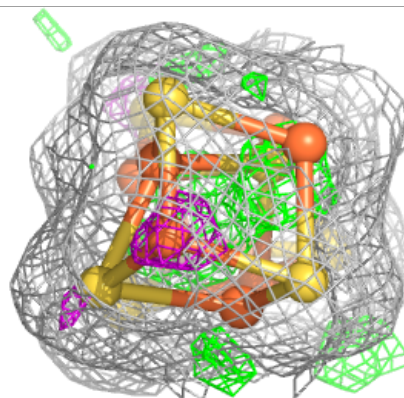
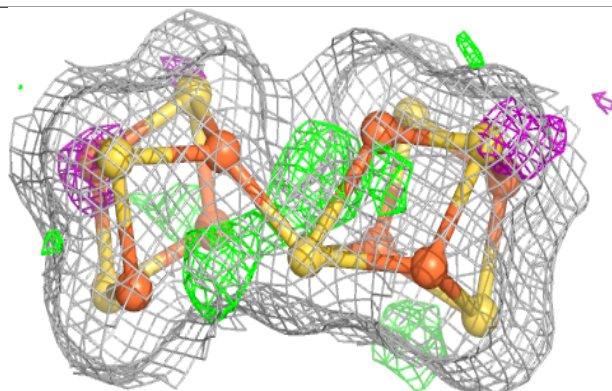
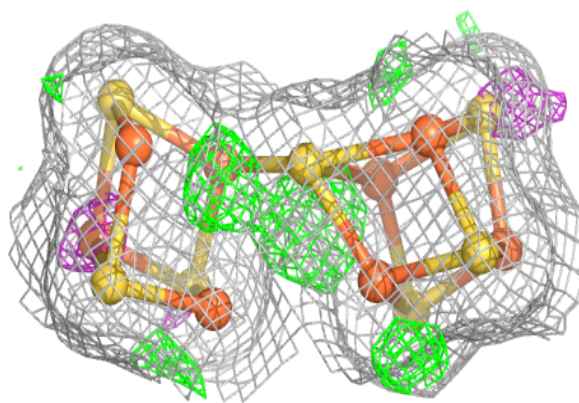
Electron density around ICS G 602:

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



Electron density around 1CL F 601:

$2mF_o - DF_c$ (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.