



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 9ERS / pdb_00009ers
Title : Hydrogenase-2 Ni-C state
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Deposited on : 2024-03-25
Resolution : 1.59 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

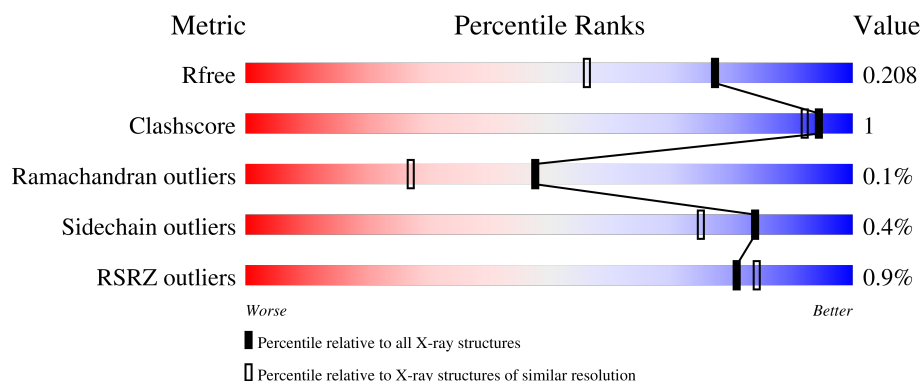
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.59 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	S	298	86% 10%
1	T	298	87% 10%
2	L	567	94% 10%
2	M	567	94% 10%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14239 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hydrogenase-2 small chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	S	268	Total	C	N	O	S	0	4	0
			2066	1308	363	382	13			
1	T	267	Total	C	N	O	S	0	7	0
			2079	1317	363	386	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	294	HIS	-	expression tag	UNP P69741
S	295	HIS	-	expression tag	UNP P69741
S	296	HIS	-	expression tag	UNP P69741
S	297	HIS	-	expression tag	UNP P69741
S	298	HIS	-	expression tag	UNP P69741
S	299	HIS	-	expression tag	UNP P69741
T	294	HIS	-	expression tag	UNP P69741
T	295	HIS	-	expression tag	UNP P69741
T	296	HIS	-	expression tag	UNP P69741
T	297	HIS	-	expression tag	UNP P69741
T	298	HIS	-	expression tag	UNP P69741
T	299	HIS	-	expression tag	UNP P69741

- Molecule 2 is a protein called Hydrogenase-2 large chain.

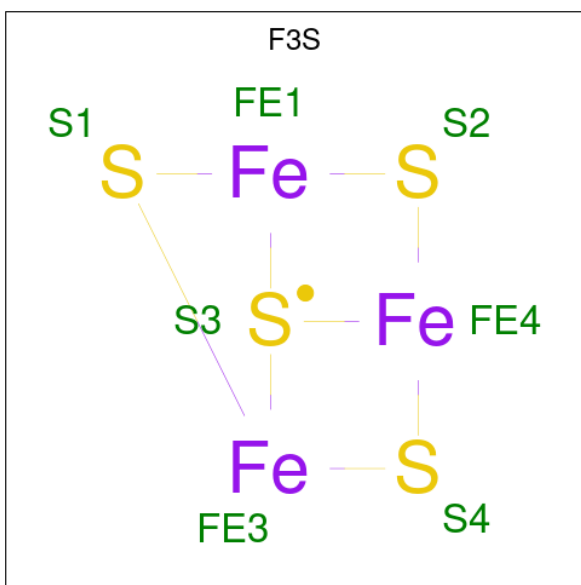
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	551	Total	C	N	O	S	0	6	0
			4320	2748	743	811	18			
2	M	551	Total	C	N	O	S	0	5	0
			4320	2747	744	811	18			

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	S	1	Total	Fe	S	0	0
			8	4	4		
3	S	1	Total	Fe	S	0	0
			8	4	4		
3	T	1	Total	Fe	S	0	0
			8	4	4		
3	T	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



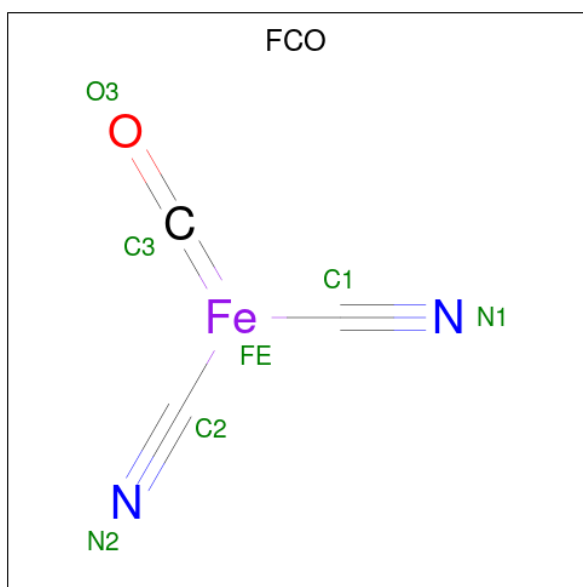
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	S	1	Total	Fe	S	0	0
			7	3	4		
4	T	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	S	1	Total	C	O	0	0
			6	3	3		
5	S	1	Total	C	O	0	0
			6	3	3		
5	T	1	Total	C	O	0	0
			6	3	3		
5	M	1	Total	C	O	0	0
			6	3	3		
5	M	1	Total	C	O	0	0
			6	3	3		
5	M	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is CARBONMONOXIDE-(DICYANO) IRON (CCD ID: FCO) (formula: C_3FeN_2O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
6	M	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		

- Molecule 7 is NICKEL (II) ION (CCD ID: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	L	1	Total	Ni	0	0
			1	1		
7	M	1	Total	Ni	0	0
			1	1		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	L	1	Total	Mg	0	0
			1	1		
8	M	2	Total	Mg	0	0
			2	2		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	S	225	Total	O	0	0
			225	225		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	L	500	Total 500	O 500	0	0
9	T	202	Total 202	O 202	0	0
9	M	426	Total 426	O 426	0	0

- Molecule 1: Hydrogenase-2 small chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.86Å 100.06Å 168.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.73 – 1.59 44.73 – 1.59	Depositor EDS
% Data completeness (in resolution range)	99.3 (44.73-1.59) 99.3 (44.73-1.59)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 1.59Å)	Xtriage
Refinement program	REFMAC 5.8.0405	Depositor
R, R_{free}	0.173 , 0.197 0.186 , 0.208	Depositor DCC
R_{free} test set	11098 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	18.8	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.010 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14239	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 4.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, FCO, SF4, NI, GOL, F3S

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	S	0.56	0/2127	0.86	3/2896 (0.1%)
1	T	0.57	0/2145	0.85	2/2922 (0.1%)
2	L	0.55	0/4439	0.87	1/6050 (0.0%)
2	M	0.55	0/4433	0.88	4/6041 (0.1%)
All	All	0.56	0/13144	0.87	10/17909 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	S	0	1
1	T	0	1
All	All	0	2

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	382	ASN	CA-CB-CG	7.59	120.19	112.60
2	L	99	HIS	CA-CB-CG	-6.83	106.97	113.80
2	M	99	HIS	CA-CB-CG	-6.28	107.52	113.80
1	S	212	ASP	CA-CB-CG	5.81	118.41	112.60
1	T	212	ASP	CA-CB-CG	5.33	117.93	112.60
2	M	544	ASP	CA-CB-CG	5.20	117.80	112.60
2	M	382	ASN	CB-CA-C	5.17	119.38	110.79
1	S	81	ASP	CA-CB-CG	5.07	117.67	112.60
1	S	89	ASN	CB-CA-C	-5.06	103.51	111.51
1	T	81	ASP	CA-CB-CG	5.04	117.64	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	S	198	ARG	Sidechain
1	T	198	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	S	2066	0	1985	7	0
1	T	2079	0	2001	4	0
2	L	4320	0	4261	12	0
2	M	4320	0	4255	10	0
3	S	16	0	0	0	0
3	T	16	0	0	0	0
4	S	7	0	0	0	0
4	T	7	0	0	0	0
5	M	18	0	24	1	0
5	S	12	0	16	3	0
5	T	6	0	8	0	0
6	L	7	0	0	0	0
6	M	7	0	0	0	0
7	L	1	0	0	0	0
7	M	1	0	0	0	0
8	L	1	0	0	0	0
8	M	2	0	0	0	0
9	L	500	0	0	4	3
9	M	426	0	0	1	2
9	S	225	0	0	2	1
9	T	202	0	0	2	0
All	All	14239	0	12550	32	3

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 1.

All (32) 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:S:130:GLY:HA3	9:S:490:HOH:O	1.89	0.71
2:M:313:ARG:HD3	2:M:322:TYR:CE2	2.34	0.63
1:S:141:GLU:HG3	9:S:401:HOH:O	2.04	0.56
1:S:202:ASP:OD2	1:T:202:ASP:OD2	2.23	0.56
2:L:313:ARG:HD3	2:L:322:TYR:CE2	2.42	0.54
1:T:66:HIS:HB3	9:T:580:HOH:O	2.10	0.52
2:M:77:GLU:HB2	5:M:605:GOL:H12	1.92	0.50
2:M:155:ILE:HD11	2:M:188:VAL:HG11	1.93	0.50
2:L:6[A]:THR:HG21	9:L:820:HOH:O	2.12	0.50
2:M:455:HIS:HD2	9:M:972:HOH:O	1.95	0.49
2:L:155:ILE:HD11	2:L:188:VAL:HG11	1.94	0.48
1:T:106:LYS:HD3	9:T:560:HOH:O	2.14	0.47
1:S:209:GLU:OE1	5:S:304:GOL:H2	2.15	0.47
2:M:115:ASP:HB3	2:M:538:ARG:HG2	1.97	0.47
2:L:356:TRP:CD1	2:L:356:TRP:C	2.94	0.45
2:L:489:LYS:NZ	9:L:716:HOH:O	2.50	0.45
2:L:69:ALA:HB1	2:L:218:LEU:HD12	2.00	0.44
1:S:270:HIS:ND1	5:S:304:GOL:H11	2.32	0.43
2:M:356:TRP:C	2:M:356:TRP:CD1	2.96	0.43
2:L:530:PRO:HD3	9:L:1052:HOH:O	2.18	0.43
1:S:228:GLY:N	1:S:229:PRO:CD	2.82	0.43
2:M:99:HIS:CD2	2:M:99:HIS:C	2.96	0.42
2:M:69:ALA:HB1	2:M:218:LEU:HD12	2.01	0.42
2:L:379:PRO:HA	2:L:382[B]:ASN:HB3	2.02	0.42
1:T:228:GLY:N	1:T:229:PRO:CD	2.83	0.42
1:S:271:GLN:OE1	5:S:305:GOL:H2	2.19	0.42
2:M:500:VAL:CG1	2:M:501:PRO:HD2	2.50	0.41
2:L:115:ASP:HB3	2:L:538:ARG:HG2	2.01	0.41
2:M:212:THR:HA	2:M:213:PRO:C	2.44	0.41
2:L:212:THR:HA	2:L:213:PRO:C	2.46	0.41
2:L:357:SER:HB3	9:L:876:HOH:O	2.20	0.40
2:L:99:HIS:CD2	2:L:99:HIS:C	2.97	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:1143:HOH:O	9:M:892:HOH:O[3_544]	1.97	0.23
9:S:490:HOH:O	9:L:737:HOH:O[4_445]	2.04	0.16
9:L:1032:HOH:O	9:M:1093:HOH:O[3_544]	2.17	0.03

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	S	270/298 (91%)	261 (97%)	9 (3%)	0	100	100
1	T	272/298 (91%)	265 (97%)	7 (3%)	0	100	100
2	L	554/567 (98%)	531 (96%)	22 (4%)	1 (0%)	43	24
2	M	553/567 (98%)	530 (96%)	22 (4%)	1 (0%)	43	24
All	All	1649/1730 (95%)	1587 (96%)	60 (4%)	2 (0%)	48	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	211	LYS
2	M	211	LYS

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	S	217/239 (91%)	216 (100%)	1 (0%)	81	70
1	T	219/239 (92%)	218 (100%)	1 (0%)	81	70
2	L	471/479 (98%)	468 (99%)	3 (1%)	78	66
2	M	470/479 (98%)	469 (100%)	1 (0%)	87	81
All	All	1377/1436 (96%)	1371 (100%)	6 (0%)	84	75

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	251	ILE
2	L	102	HIS
2	L	382[A]	ASN
2	L	382[B]	ASN
1	T	251	ILE
2	M	382	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	20	GLN
1	S	274	ASN
2	L	87	ASN
2	L	449	ASN
2	L	520	GLN
1	T	10	GLN
1	T	75	GLN
1	T	274	ASN
2	M	411	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 5 are monoatomic - leaving 14 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	GOL	S	305	-	5,5,5	0.13	0	5,5,5	0.36	0
5	GOL	M	606	-	5,5,5	0.10	0	5,5,5	0.21	0
4	F3S	T	302	1	0,9,9	-	-	-		
3	SF4	T	303	1	0,12,12	-	-	-		
5	GOL	T	304	-	5,5,5	0.23	0	5,5,5	0.48	0
3	SF4	S	303	1	0,12,12	-	-	-		
5	GOL	S	304	-	5,5,5	0.26	0	5,5,5	0.83	0
5	GOL	M	601	-	5,5,5	0.23	0	5,5,5	0.44	0
6	FCO	L	601	2	0,6,6	-	-	-		
4	F3S	S	302	1	0,9,9	-	-	-		
6	FCO	M	602	2	0,6,6	-	-	-		
5	GOL	M	605	-	5,5,5	0.22	0	5,5,5	0.54	0
3	SF4	T	301	1	0,12,12	-	-	-		
3	SF4	S	301	1	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	S	305	-	-	1/4/4/4	-
5	GOL	M	606	-	-	0/4/4/4	-
4	F3S	T	302	1	-	-	0/3/3/3
5	GOL	M	601	-	-	2/4/4/4	-
5	GOL	T	304	-	-	0/4/4/4	-
3	SF4	S	303	1	-	-	0/6/5/5
5	GOL	S	304	-	-	2/4/4/4	-
3	SF4	T	303	1	-	-	0/6/5/5
4	F3S	S	302	1	-	-	0/3/3/3
5	GOL	M	605	-	-	2/4/4/4	-
3	SF4	T	301	1	-	-	0/6/5/5
3	SF4	S	301	1	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

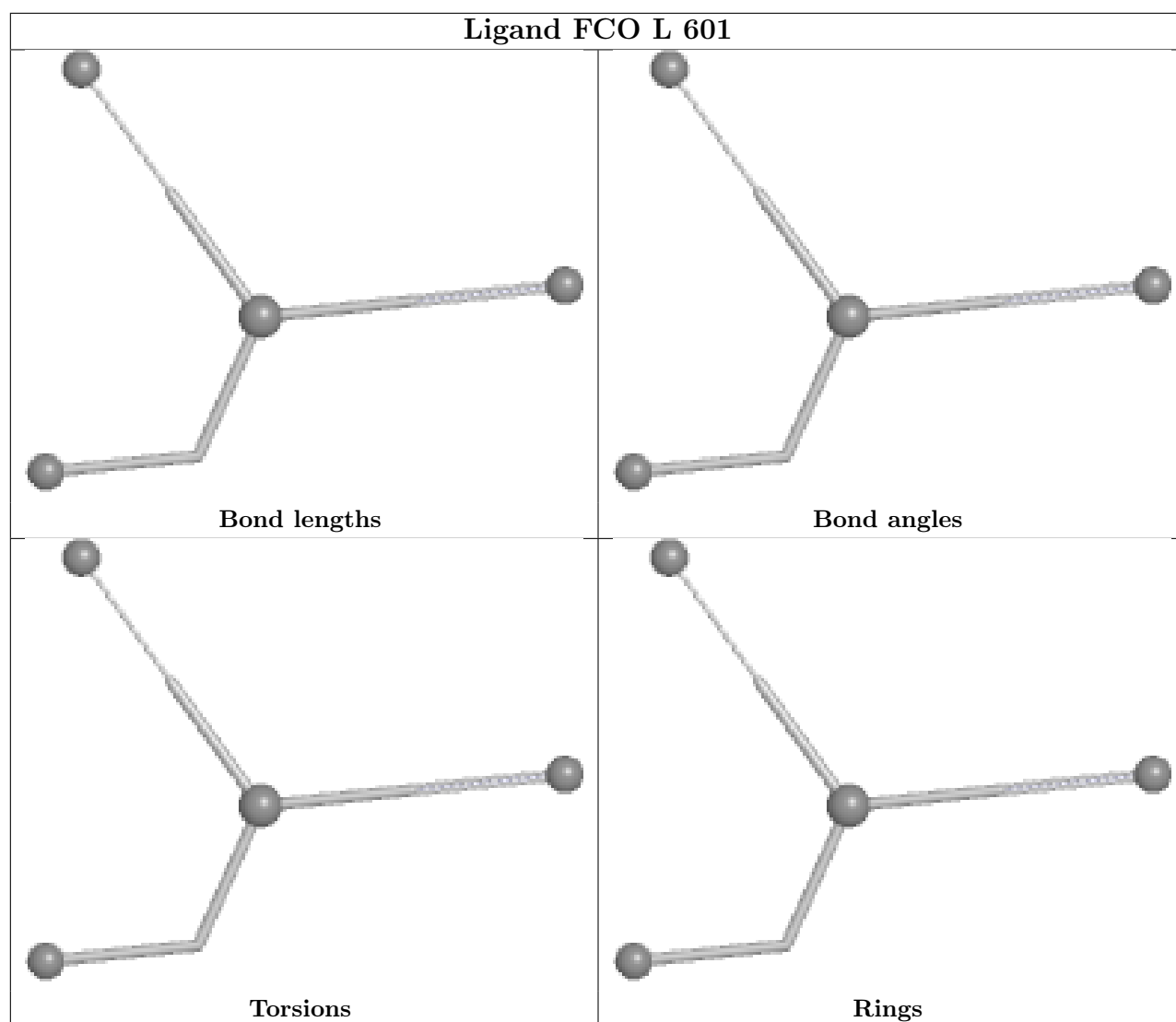
Mol	Chain	Res	Type	Atoms
5	S	304	GOL	C1-C2-C3-O3
5	S	304	GOL	O2-C2-C3-O3
5	M	601	GOL	C1-C2-C3-O3
5	M	605	GOL	O1-C1-C2-C3
5	M	601	GOL	O2-C2-C3-O3
5	M	605	GOL	O1-C1-C2-O2
5	S	305	GOL	O1-C1-C2-O2

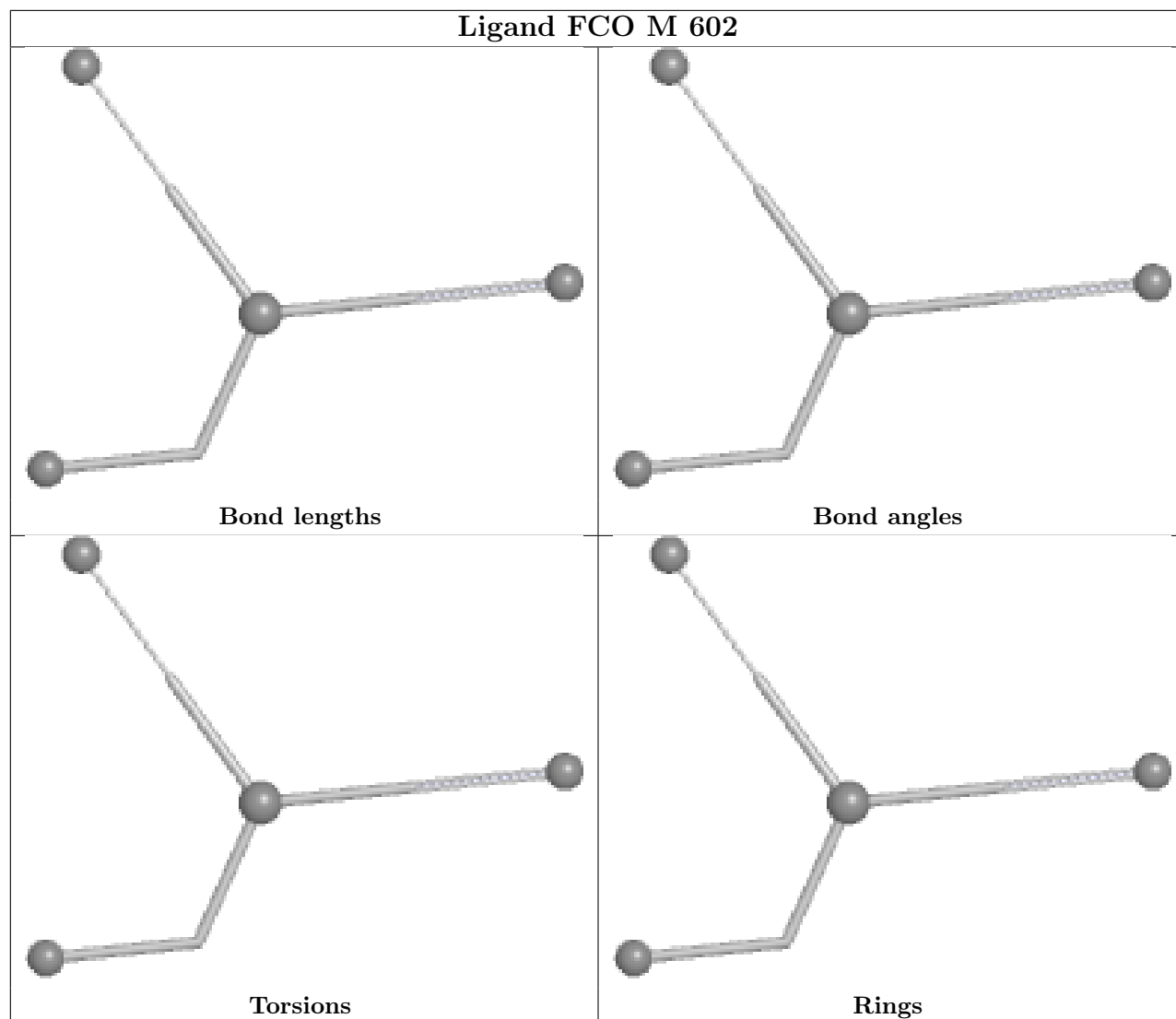
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	S	305	GOL	1	0
5	S	304	GOL	2	0
5	M	605	GOL	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	S	268/298 (89%)	-0.11	3 (1%) 78 82	10, 21, 37, 58	4 (1%)
1	T	267/298 (89%)	0.03	2 (0%) 84 87	11, 23, 39, 55	7 (2%)
2	L	551/567 (97%)	-0.20	3 (0%) 87 90	8, 21, 33, 44	6 (1%)
2	M	551/567 (97%)	0.05	6 (1%) 78 82	8, 23, 40, 63	5 (0%)
All	All	1637/1730 (94%)	-0.06	14 (0%) 81 84	8, 22, 38, 63	22 (1%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	27	VAL	3.3
1	S	9	PRO	3.3
2	M	137	VAL	3.0
1	S	66	HIS	3.0
2	M	515	VAL	2.7
1	T	66	HIS	2.7
2	M	2	SER	2.6
2	M	23	ILE	2.5
2	M	413	LEU	2.3
1	S	275	VAL	2.3
1	T	145	GLY	2.1
2	L	515	VAL	2.0
2	L	172	TRP	2.0
2	L	137	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

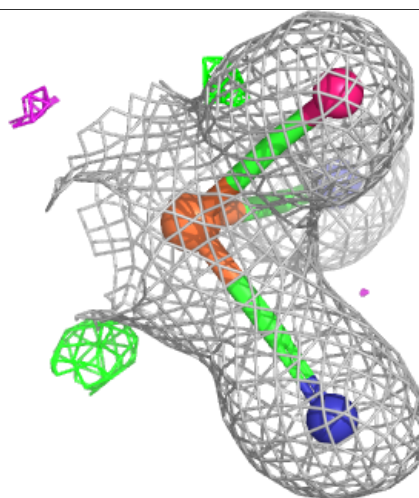
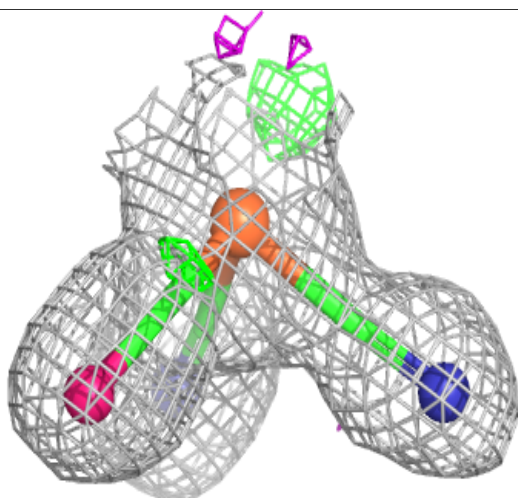
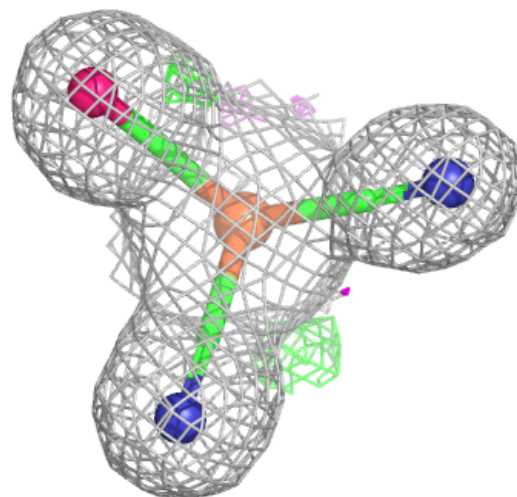
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	M	606	6/6	0.85	0.12	49,50,53,54	0
5	GOL	S	305	6/6	0.87	0.13	44,46,47,49	0
5	GOL	M	601	6/6	0.90	0.12	27,32,38,43	0
8	MG	M	607	1/1	0.92	0.10	74,74,74,74	0
5	GOL	M	605	6/6	0.93	0.10	25,37,40,43	0
5	GOL	S	304	6/6	0.94	0.08	24,25,28,28	0
5	GOL	T	304	6/6	0.97	0.06	24,26,27,29	0
6	FCO	M	602	7/7	0.99	0.05	14,17,19,19	0
3	SF4	T	301	8/8	1.00	0.02	18,20,21,21	0
3	SF4	T	303	8/8	1.00	0.03	18,19,20,21	0
4	F3S	S	302	7/7	1.00	0.03	16,16,17,18	0
4	F3S	T	302	7/7	1.00	0.02	16,17,18,18	0
6	FCO	L	601	7/7	1.00	0.04	15,16,17,18	0
3	SF4	S	301	8/8	1.00	0.02	18,19,21,21	0
7	NI	L	602	1/1	1.00	0.01	19,19,19,19	0
7	NI	M	603	1/1	1.00	0.02	21,21,21,21	0
8	MG	L	603	1/1	1.00	0.03	12,12,12,12	0
8	MG	M	604	1/1	1.00	0.04	15,15,15,15	0
3	SF4	S	303	8/8	1.00	0.03	16,17,19,19	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.

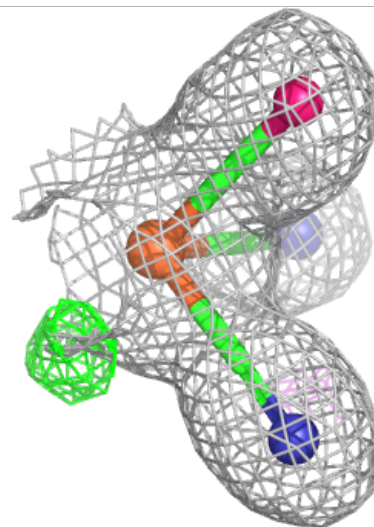
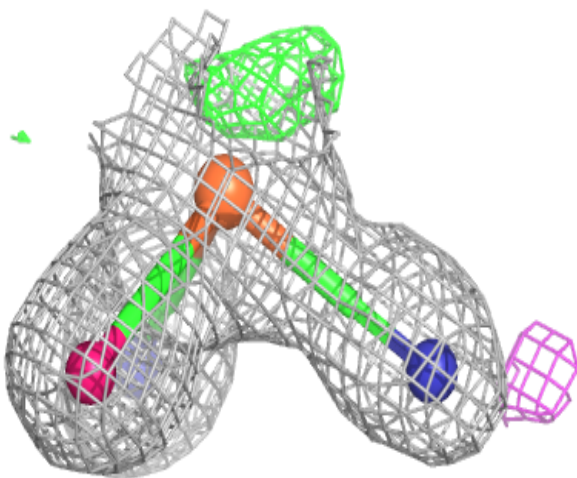
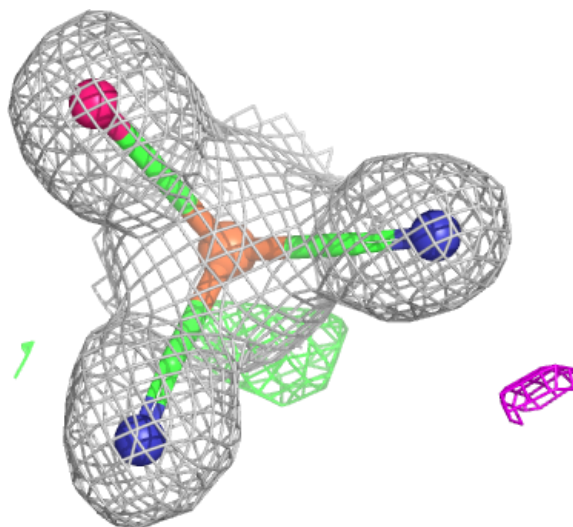
Electron density around FCO M 602:

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



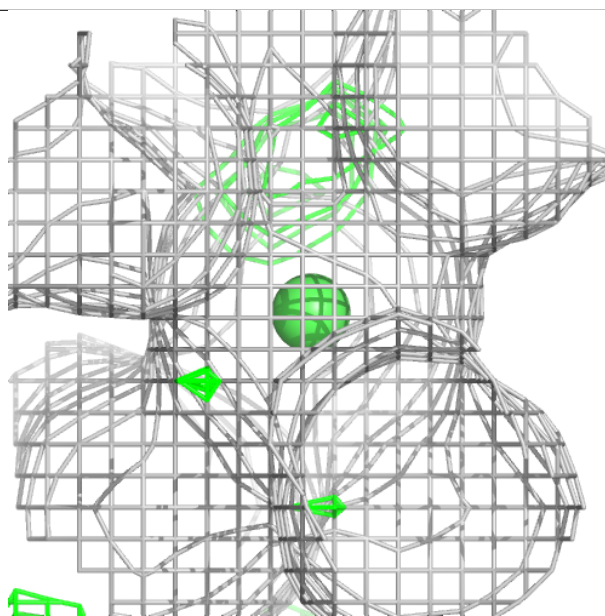
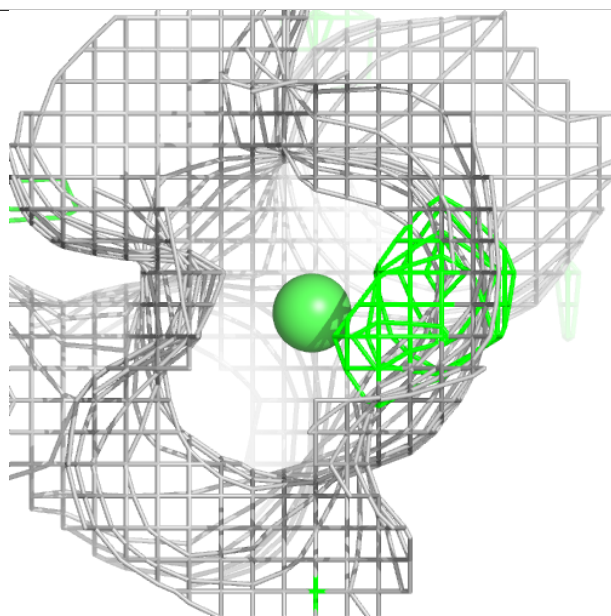
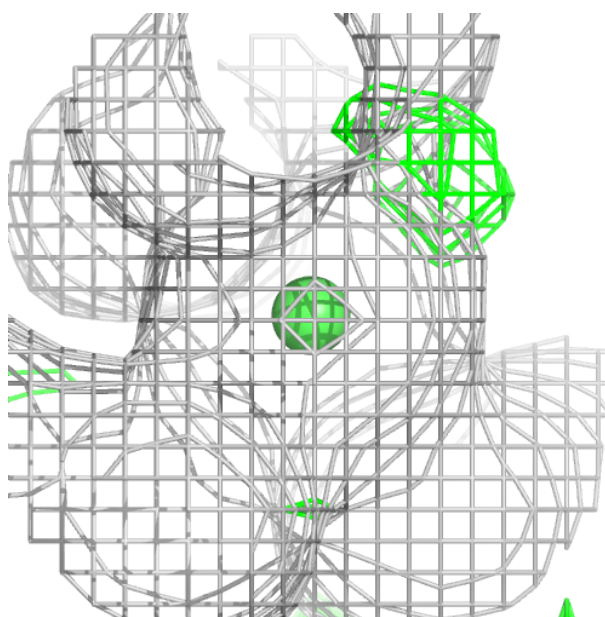
Electron density around FCO L 601:

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



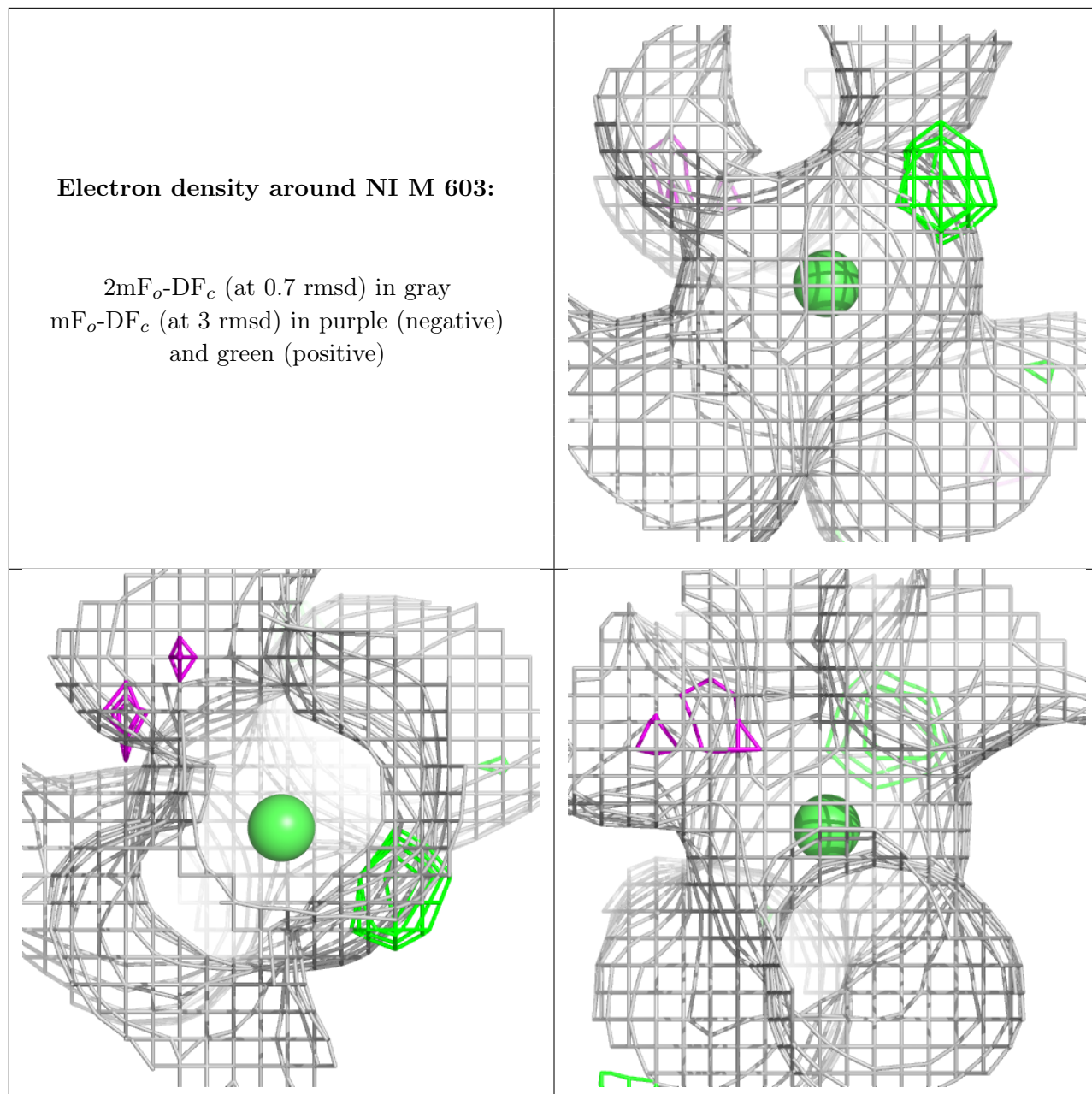
Electron density around NI L 602:

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



Electron density around NI M 603:

$2mF_o-DF_c$ (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.