Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2025 – 12:55 pm GMT

PDB ID	:	9ERB
Title	:	Hydrogenase-2 Ni-B state
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Deposited on	:	2024-03-22
Resolution	:	1.30 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:

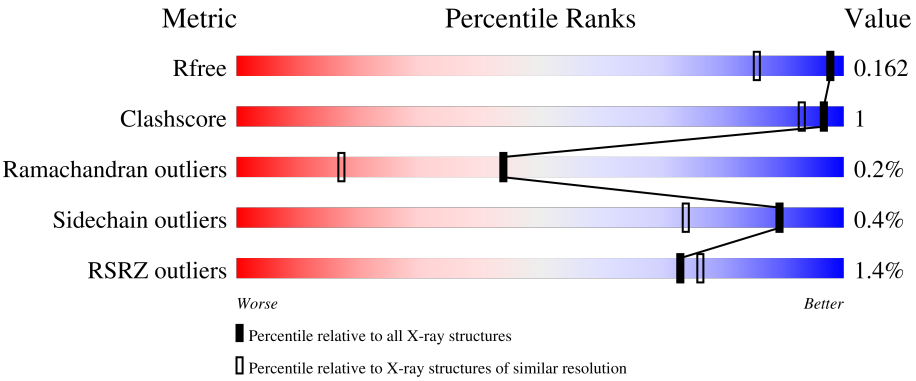
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.5

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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}	164625	1387 (1.30-1.30)
Clashscore	180529	1497 (1.30-1.30)
Ramachandran outliers	177936	1455 (1.30-1.30)
Sidechain outliers	177891	1455 (1.30-1.30)
RSRZ outliers	164620	1384 (1.30-1.30)

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 <=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	89% 10%
1	T	298	89% 10%
2	L	567	94%
2	M	567	93%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 27032 atoms, of which 12566 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	H	N	O	S	0	8	0
			4080	1314	2007	364	382	13			
1	T	268	Total	C	H	N	O	S	0	4	0
			4050	1306	1992	360	379	13			

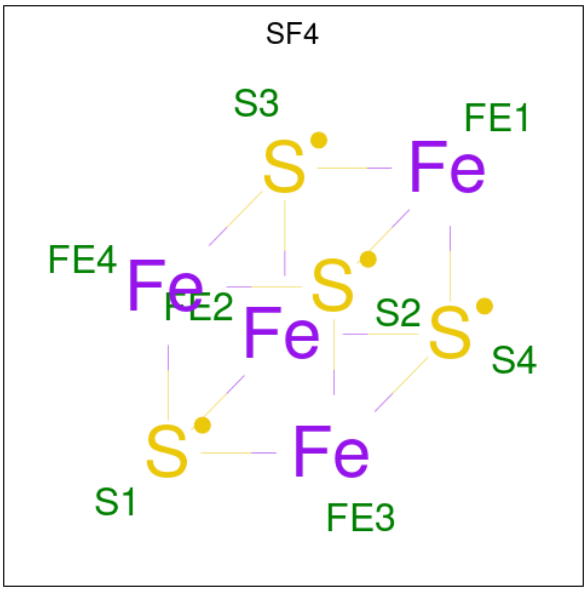
There are 12 discrepancies between the modelled and reference sequences:

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.

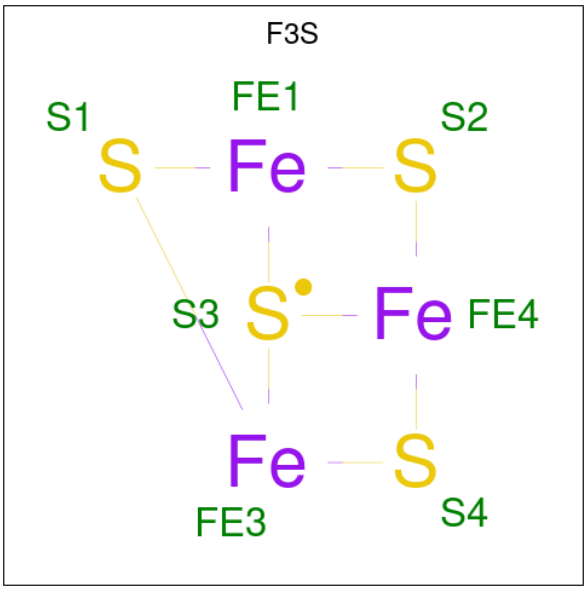
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	L	551	Total	C	H	N	O	S	0	8	0
			8588	2749	4264	743	814	18			
2	M	551	Total	C	H	N	O	S	0	9	0
			8608	2754	4279	742	815	18			

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



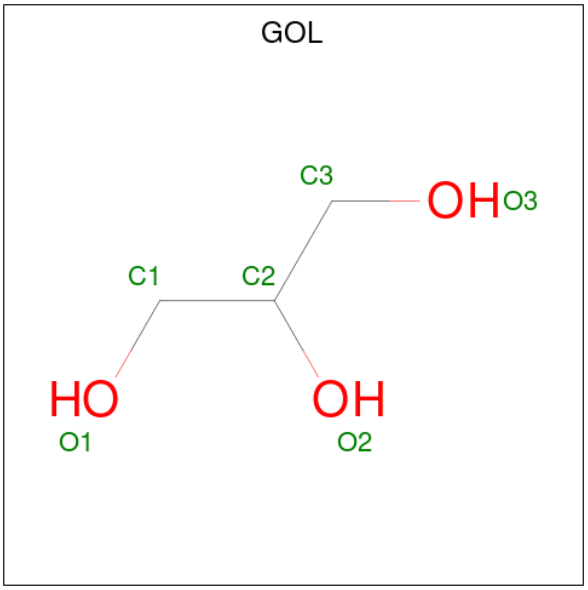
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	S	1	Total Fe S 8 4 4	0	0
3	S	1	Total Fe S 8 4 4	0	0
3	T	1	Total Fe S 8 4 4	0	0
3	T	1	Total Fe S 8 4 4	0	0

- Molecule 4 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



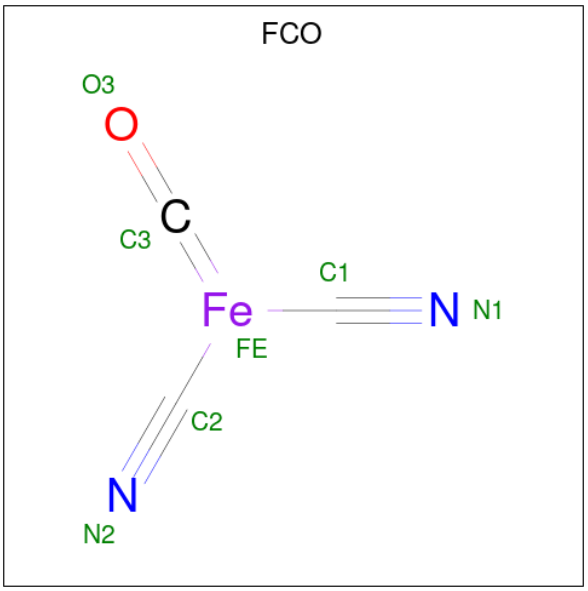
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	S	1	Total Fe S 7 3 4	0	0
4	T	1	Total Fe S 7 3 4	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: 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 7 3 1 2 1	0	0
6	M	1	Total C Fe N O 7 3 1 2 1	0	0

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

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

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

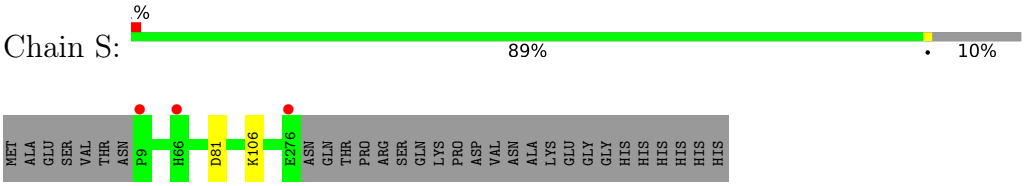
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	S	273	Total O 273 273	0	0
10	L	574	Total O 574 574	0	0
10	T	245	Total O 245 245	0	0
10	M	505	Total O 505 505	0	0

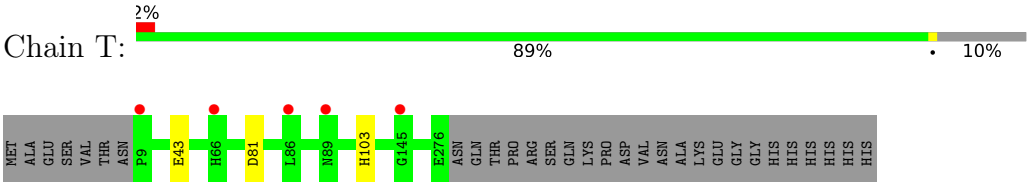
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

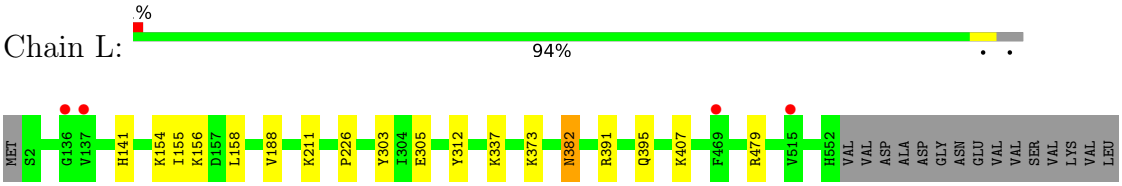
• Molecule 1: Hydrogenase-2 small chain



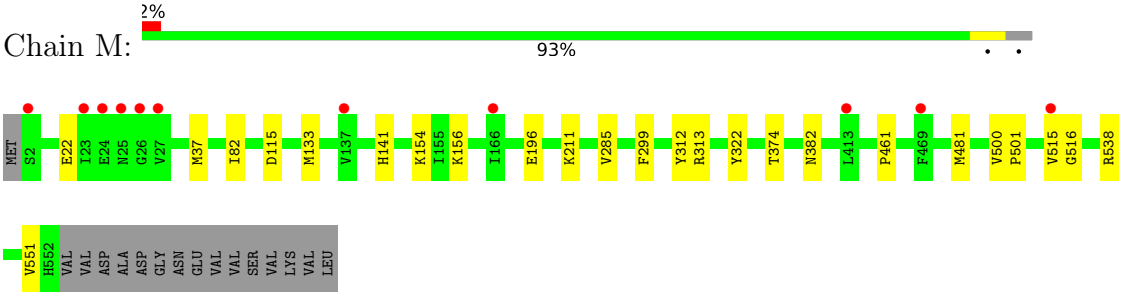
• Molecule 1: Hydrogenase-2 small chain



• Molecule 2: Hydrogenase-2 large chain



• Molecule 2: Hydrogenase-2 large chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	99.74Å 100.19Å 168.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.87 – 1.30 49.87 – 1.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.87-1.30) 99.9 (49.87-1.30)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 1.30Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.145 , 0.161 0.147 , 0.162	Depositor DCC
R_{free} test set	20477 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	10.8	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 36.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.006 for k,h,-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	27032	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.75% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: F3S, NI, GOL, MG, CL, SF4, FCO

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	0.53	0/2155	0.72	1/2933 (0.0%)
1	T	0.48	0/2128	0.72	1/2897 (0.0%)
2	L	0.51	0/4460	0.74	1/6079 (0.0%)
2	M	0.50	1/4462 (0.0%)	0.73	2/6082 (0.0%)
All	All	0.51	1/13205 (0.0%)	0.73	5/17991 (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
2	L	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	515	VAL	CB-CG1	-5.01	1.42	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	382	ASN	N-CA-CB	-5.80	100.17	110.60
1	T	81	ASP	CB-CG-OD1	5.74	123.47	118.30
1	S	81	ASP	CB-CG-OD1	5.43	123.19	118.30
2	L	382	ASN	N-CA-CB	-5.14	101.35	110.60
2	M	299	PHE	CB-CG-CD2	-5.08	117.25	120.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	479	ARG	Sidechain

5.2 Too-close contacts (i)

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	2073	2007	1987	0	0
1	T	2058	1992	1990	2	0
2	L	4324	4264	4237	9	0
2	M	4329	4279	4262	13	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	6	8	7	0	0
5	S	6	8	8	0	0
5	T	6	8	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	2	0	0	0	0
8	M	2	0	0	0	0
9	L	1	0	0	0	0
10	L	574	0	0	5	1
10	M	505	0	0	5	0
10	S	273	0	0	0	0
10	T	245	0	0	2	1
All	All	14466	12566	12499	24	1

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 (24) 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:T:103:HIS:O	10:T:401:HOH:O	1.76	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:337:LYS:NZ	10:L:704:HOH:O	2.04	0.86
2:L:154:LYS:NZ	10:L:703:HOH:O	2.03	0.81
2:L:156:LYS:NZ	10:L:701:HOH:O	1.87	0.78
2:M:22[A]:GLU:OE1	10:M:701:HOH:O	2.09	0.70
2:L:305[B]:GLU:CD	2:L:373:LYS:HZ2	2.06	0.59
2:M:156:LYS:NZ	10:M:708:HOH:O	2.42	0.52
2:L:407:LYS:HE3	10:L:1152:HOH:O	2.11	0.49
2:L:155:ILE:HD11	2:L:188:VAL:HG11	1.95	0.49
2:M:133:MET:HE1	10:M:779:HOH:O	2.13	0.48
2:M:374[B]:THR:HG21	2:M:516:GLY:HA2	1.96	0.48
1:T:43[A]:GLU:OE2	10:T:402:HOH:O	2.20	0.48
2:M:500:VAL:CG1	2:M:501:PRO:HD2	2.45	0.46
2:M:154:LYS:NZ	10:M:711:HOH:O	2.50	0.45
2:M:115:ASP:HB3	2:M:538:ARG:HG2	1.98	0.44
2:L:382:ASN:ND2	10:L:707:HOH:O	2.34	0.43
2:L:391:ARG:O	2:L:395[A]:GLN:HG3	2.18	0.42
2:M:285:VAL:HG13	2:M:481:MET:HG3	2.01	0.42
2:L:303:TYR:CE2	2:L:305[A]:GLU:CG	3.02	0.42
2:M:156:LYS:HB2	2:M:156:LYS:HE2	1.84	0.42
2:M:313:ARG:HD3	2:M:322:TYR:CE2	2.55	0.42
2:M:196[B]:GLU:HG3	10:M:725:HOH:O	2.20	0.41
2:M:82:ILE:HD11	2:M:461:PRO:HB3	2.02	0.41
2:M:37:MET:O	2:M:551:VAL:HG11	2.22	0.40

All (1) 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)
10:L:1209:HOH:O	10:T:459:HOH:O[2_455]	2.14	0.06

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	S	274/298 (92%)	266 (97%)	8 (3%)	0	100 100
1	T	270/298 (91%)	261 (97%)	9 (3%)	0	100 100
2	L	557/567 (98%)	532 (96%)	23 (4%)	2 (0%)	30 9
2	M	558/567 (98%)	537 (96%)	20 (4%)	1 (0%)	44 17
All	All	1659/1730 (96%)	1596 (96%)	60 (4%)	3 (0%)	44 17

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	211	LYS
2	L	211	LYS
2	L	226	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	S	220/239 (92%)	219 (100%)	1 (0%)	86 67
1	T	217/239 (91%)	217 (100%)	0	100 100
2	L	473/479 (99%)	470 (99%)	3 (1%)	84 62
2	M	473/479 (99%)	471 (100%)	2 (0%)	89 74
All	All	1383/1436 (96%)	1377 (100%)	6 (0%)	89 74

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

Mol	Chain	Res	Type
1	S	106	LYS
2	L	141	HIS
2	L	158	LEU
2	L	312	TYR
2	M	141	HIS
2	M	312	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such

sidechains are listed below:

Mol	Chain	Res	Type
2	L	25	ASN
2	L	531	ASN
2	M	47	ASN
2	M	531	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 7 are monoatomic - leaving 11 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	M	605	-	5,5,5	1.46	1 (20%)	5,5,5	1.17	0
5	GOL	S	304	-	5,5,5	1.49	1 (20%)	5,5,5	0.65	0
3	SF4	S	301	1	0,12,12	-	-	-		
4	F3S	S	302	1	0,9,9	-	-	-		
3	SF4	T	301	1	0,12,12	-	-	-		
3	SF4	S	303	1	0,12,12	-	-	-		
5	GOL	T	304	-	5,5,5	1.33	1 (20%)	5,5,5	0.71	0
6	FCO	M	601	2,10	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SF4	T	303	1	0,12,12	-	-	-		
4	F3S	T	302	1	0,9,9	-	-	-		
6	FCO	L	601	2,10	0,6,6	-	-	-		

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	M	605	-	-	4/4/4/4	-
5	GOL	S	304	-	-	0/4/4/4	-
3	SF4	S	301	1	-	-	0/6/5/5
3	SF4	T	301	1	-	-	0/6/5/5
4	F3S	S	302	1	-	-	0/3/3/3
3	SF4	S	303	1	-	-	0/6/5/5
5	GOL	T	304	-	-	0/4/4/4	-
3	SF4	T	303	1	-	-	0/6/5/5
4	F3S	T	302	1	-	-	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	605	GOL	O2-C2	-3.03	1.34	1.43
5	S	304	GOL	C3-C2	2.59	1.62	1.51
5	T	304	GOL	C3-C2	2.24	1.60	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

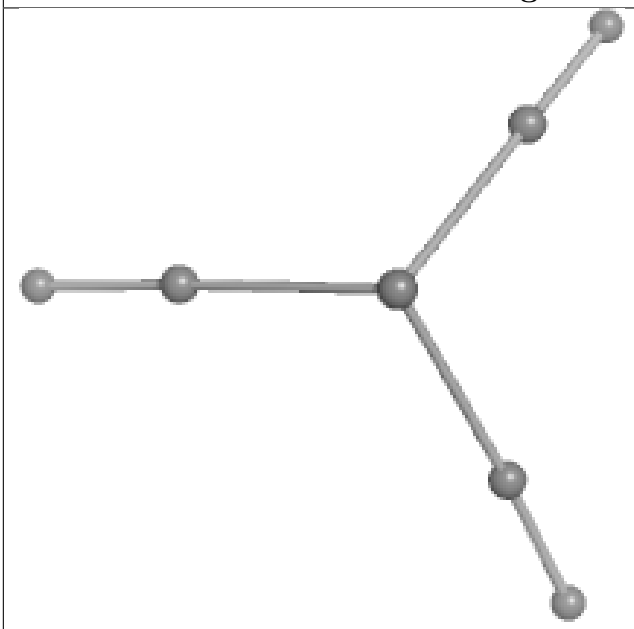
There are no ring outliers.

No monomer is involved in short contacts.

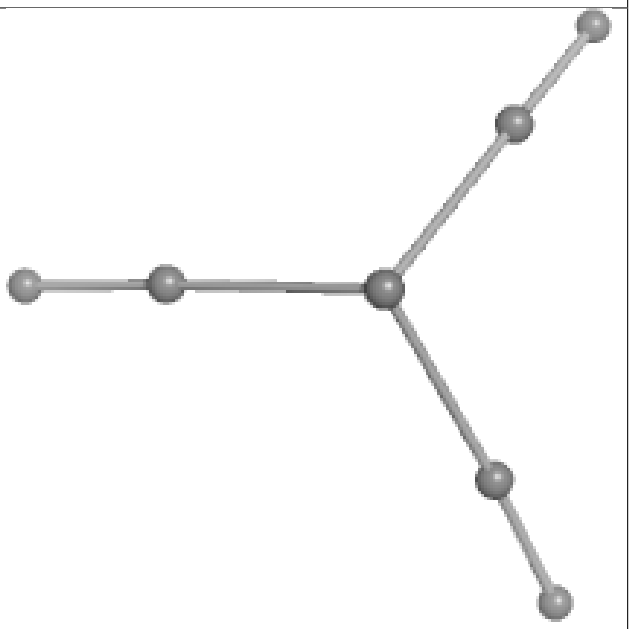
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 then 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.

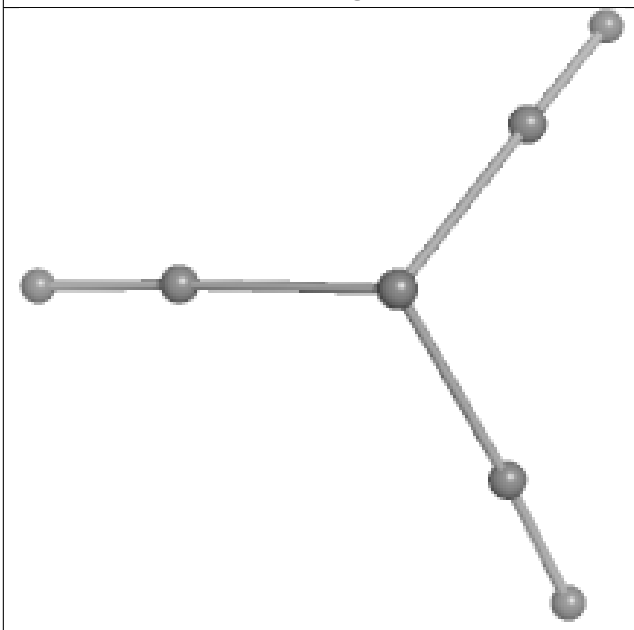
Ligand FCO M 601



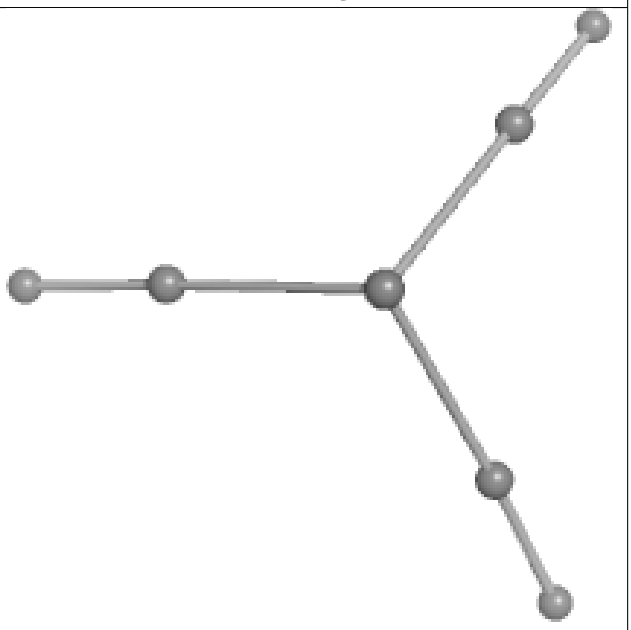
Bond lengths



Bond angles

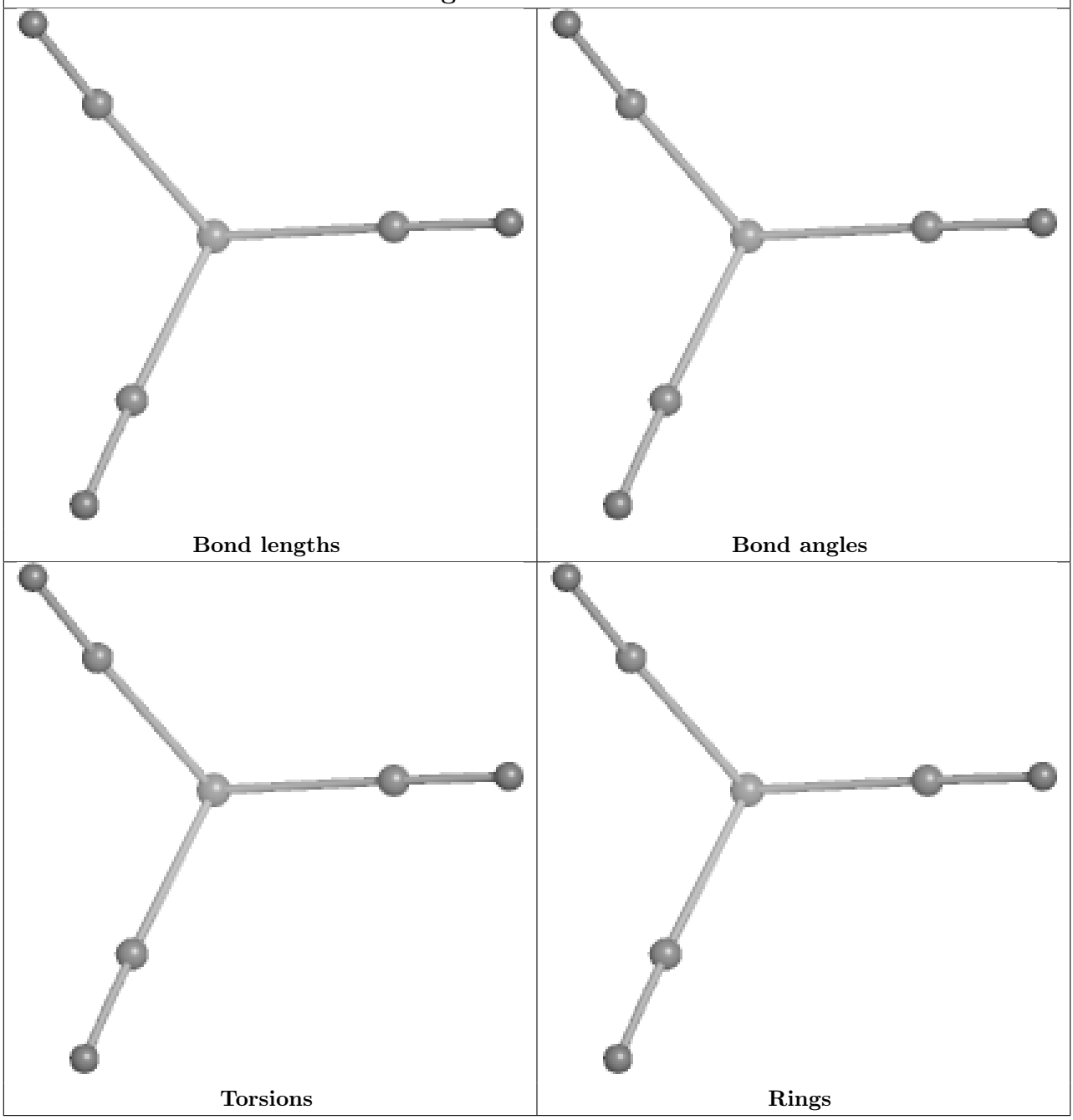


Torsions



Rings

Ligand FCO L 601



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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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%)	-0.43	3 (1%)	77	80	5, 12, 27, 41	5 (1%)
1	T	268/298 (89%)	-0.17	5 (1%)	66	69	7, 14, 30, 41	4 (1%)
2	L	551/567 (97%)	-0.47	4 (0%)	84	87	6, 12, 23, 36	5 (0%)
2	M	551/567 (97%)	-0.24	11 (1%)	64	69	6, 14, 28, 42	7 (1%)
All	All	1638/1730 (94%)	-0.34	23 (1%)	73	76	5, 13, 27, 42	21 (1%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	137	VAL	4.0
1	T	9	PRO	3.6
2	M	515	VAL	3.5
2	M	27	VAL	3.2
2	L	136	GLY	3.2
2	M	2	SER	3.2
2	L	137	VAL	2.9
2	L	469	PHE	2.8
2	M	23	ILE	2.8
2	M	166	ILE	2.8
2	M	413	LEU	2.7
2	L	515	VAL	2.6
2	M	469	PHE	2.6
1	T	66	HIS	2.5
1	S	66	HIS	2.2
2	M	24	GLU	2.1
1	T	89	ASN	2.1
1	T	86	LEU	2.1
2	M	25	ASN	2.1
1	S	9	PRO	2.1
1	S	276	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	T	145	GLY	2.0
2	M	26	GLY	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 monosaccharides 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, 95^{th} 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.

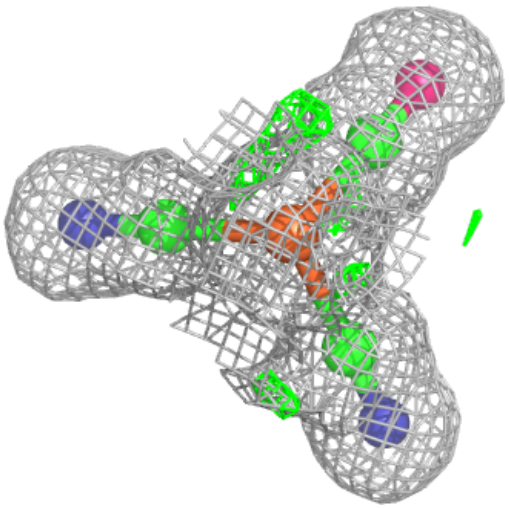
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	MG	L	604	1/1	0.73	0.18	42,42,42,42	0
5	GOL	M	605	6/6	0.89	0.14	14,31,46,46	0
5	GOL	S	304	6/6	0.95	0.07	15,21,26,26	0
5	GOL	T	304	6/6	0.95	0.07	15,21,27,27	0
8	MG	M	604	1/1	0.97	0.22	27,27,27,27	0
9	CL	L	605	1/1	0.99	0.06	18,18,18,18	0
3	SF4	S	301	8/8	1.00	0.02	9,9,9,9	0
3	SF4	S	303	8/8	1.00	0.01	8,8,8,8	0
3	SF4	T	301	8/8	1.00	0.02	9,9,9,10	0
6	FCO	L	601	7/7	1.00	0.03	7,8,8,9	0
6	FCO	M	601	7/7	1.00	0.03	8,8,9,10	0
7	NI	L	602	1/1	1.00	0.02	9,9,9,9	0
7	NI	M	602	1/1	1.00	0.02	10,10,10,10	0
8	MG	L	603	1/1	1.00	0.07	4,4,4,4	0
3	SF4	T	303	8/8	1.00	0.02	8,9,10,10	0
8	MG	M	603	1/1	1.00	0.08	6,6,6,6	0
4	F3S	S	302	7/7	1.00	0.01	8,8,8,9	0
4	F3S	T	302	7/7	1.00	0.02	8,8,9,9	0

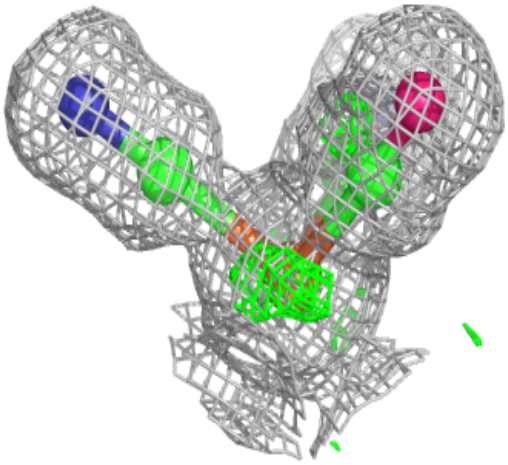
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

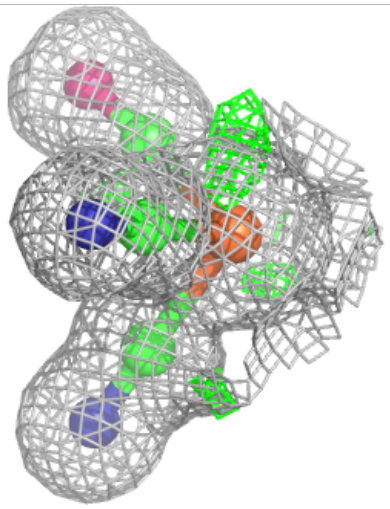
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FCO 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)

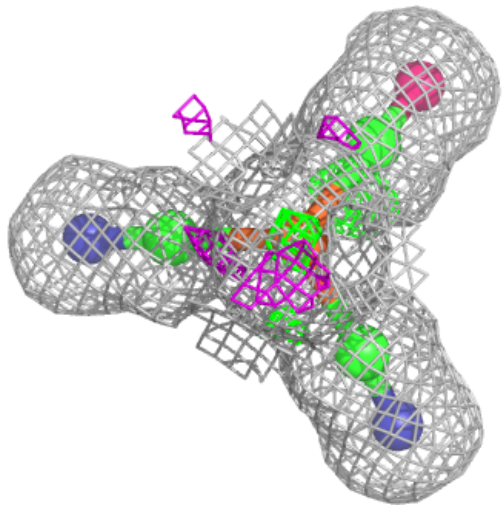


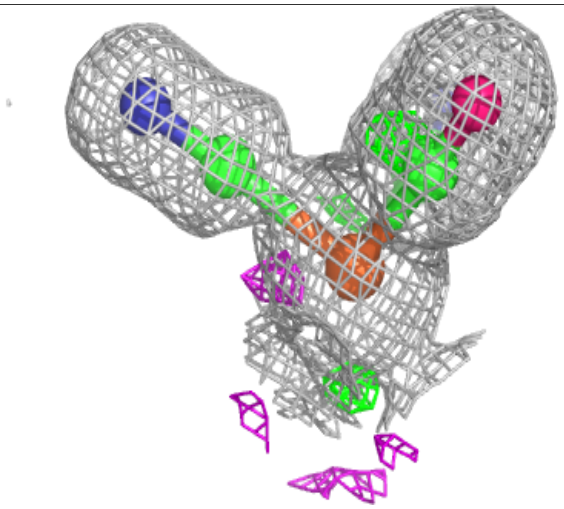


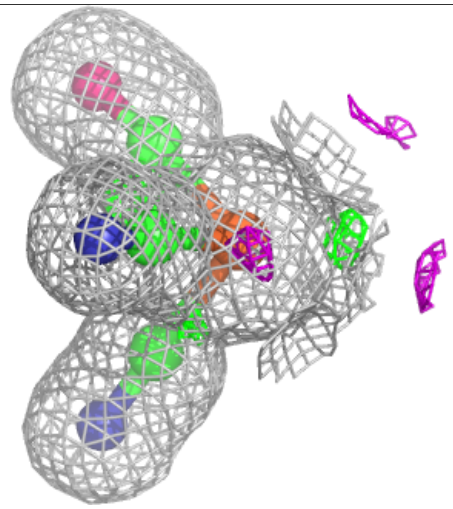


Electron density around FCO M 601:

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

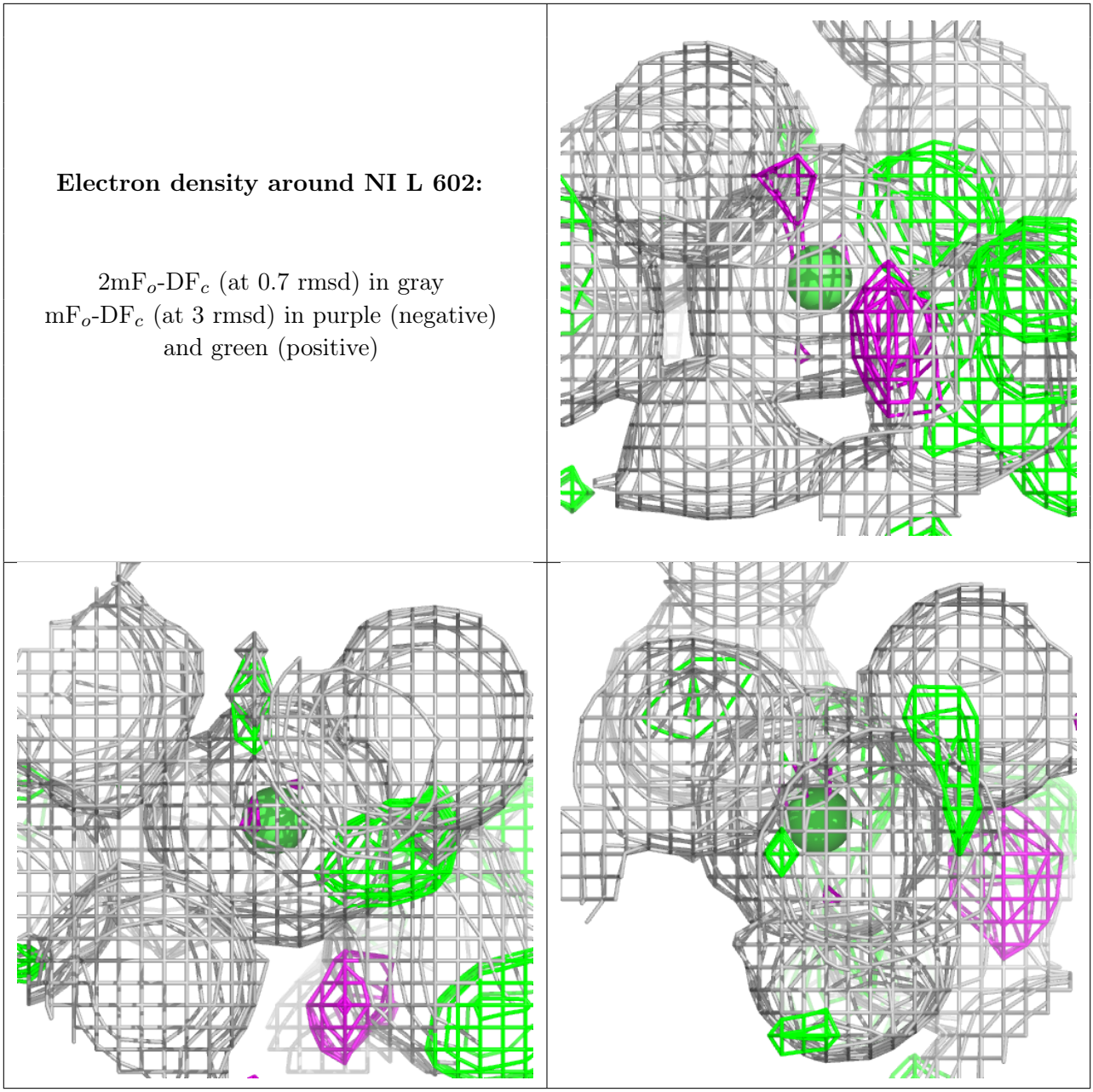






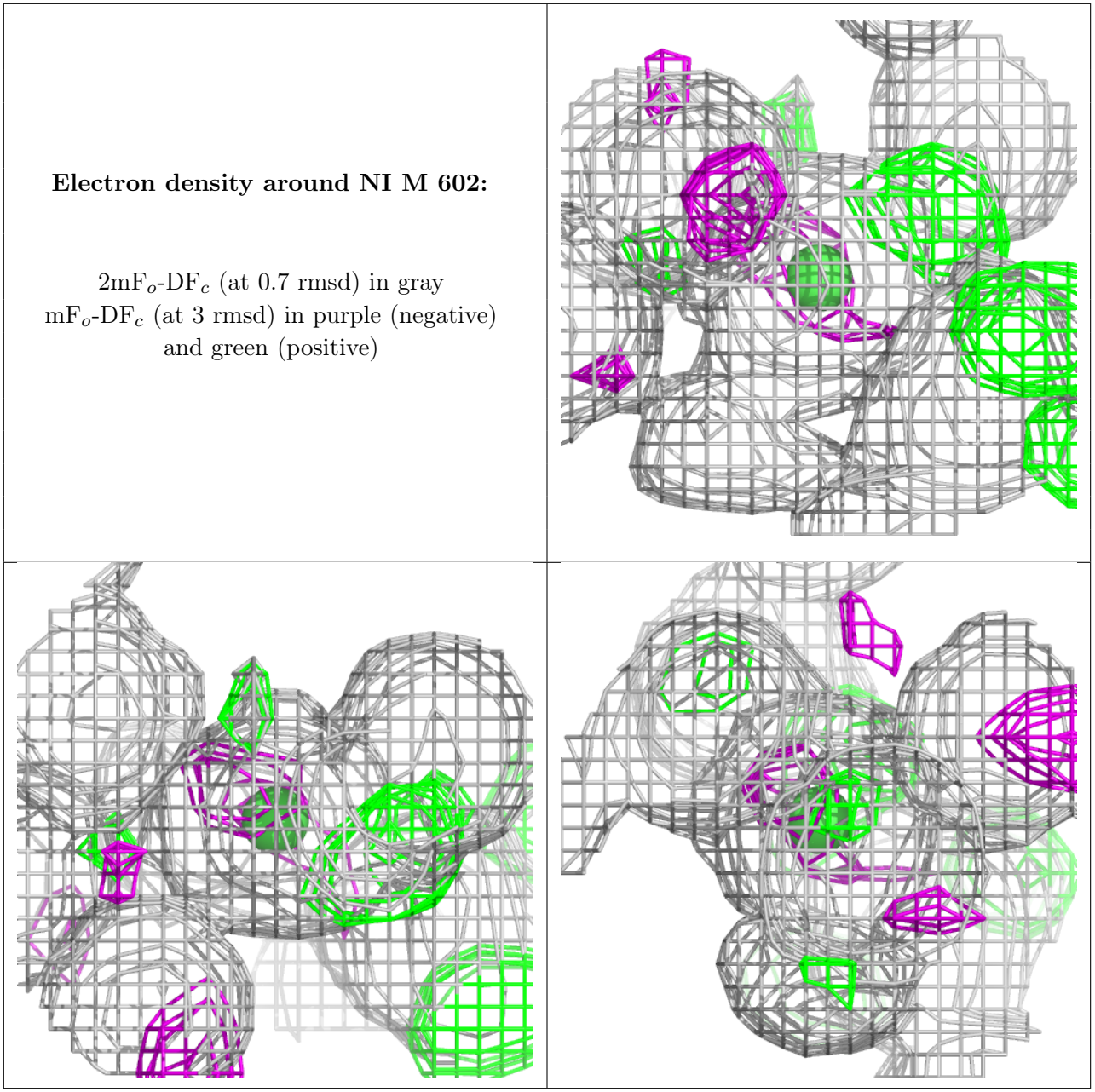
Electron density around NI L 602:

$2mF_o$-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 602:

$2mF_o$-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.