WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 13, 2024 – 04:28 pm GMT

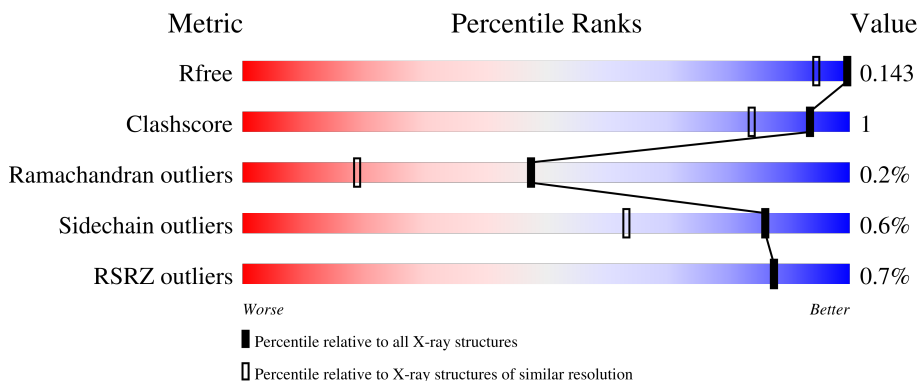|		
PDB ID	:	6SZK
Title	:	Hydrogenase-2 variant R479K - hydrogen reduced form treated with CO
Authors	:	Carr, S.B.; Beaton, S.E.; Evans, R.M.; Armstrong, F.A.
Deposited on	:	2019-10-02
Resolution	:	1.20 Å(reported)

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 1.20 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	Percentile Ranks	Value
Rfree		0.143
Clashscore		1
Ramachandran outliers		0.2%
Sidechain outliers		0.6%
RSRZ outliers		0.7%

Worse   *Better*

▮ Percentile relative to all X-ray structures

⍿ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1223 (1.22-1.18)
Clashscore	141614	1286 (1.22-1.18)
Ramachandran outliers	138981	1240 (1.22-1.18)
Sidechain outliers	138945	1239 (1.22-1.18)
RSRZ outliers	127900	1200 (1.22-1.18)

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	SSS	298	85% 5% 10%
1	TTT	298	85% 5% 10%
2	LLL	567	% 91% 5% ··
2	MMM	567	% 92% 5% ·

2 Entry composition ⓘ

There are 11 unique types of molecules in this entry. The entry contains 14308 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	SSS	268	Total	C	N	O	S	0	3	0
			2058	1304	363	378	13			
1	TTT	268	Total	C	N	O	S	0	3	0
			2056	1304	361	378	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SSS	291	HIS	-	expression tag	UNP P69741
SSS	292	HIS	-	expression tag	UNP P69741
SSS	293	HIS	-	expression tag	UNP P69741
SSS	294	HIS	-	expression tag	UNP P69741
SSS	295	HIS	-	expression tag	UNP P69741
SSS	296	HIS	-	expression tag	UNP P69741
TTT	291	HIS	-	expression tag	UNP P69741
TTT	292	HIS	-	expression tag	UNP P69741
TTT	293	HIS	-	expression tag	UNP P69741
TTT	294	HIS	-	expression tag	UNP P69741
TTT	295	HIS	-	expression tag	UNP P69741
TTT	296	HIS	-	expression tag	UNP P69741

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	LLL	551	Total	C	N	O	S	0	10	0
			4337	2761	740	818	18			
2	MMM	551	Total	C	N	O	S	0	7	0
			4319	2751	737	813	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LLL	479	LYS	ARG	engineered mutation	UNP V0V766
MMM	479	LYS	ARG	engineered mutation	UNP V0V766

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).
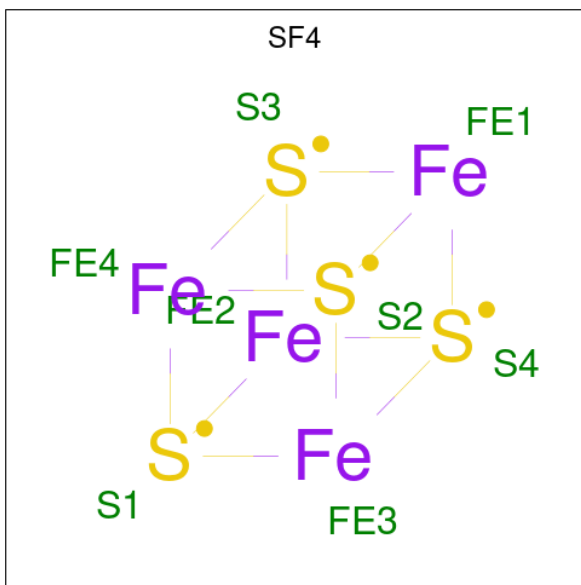
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	SSS	1	Total 8	Fe 4	S 4	0	0
3	SSS	1	Total 8	Fe 4	S 4	0	0
3	TTT	1	Total 8	Fe 4	S 4	0	0
3	TTT	1	Total 8	Fe 4	S 4	0	0

- Molecule 4 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).
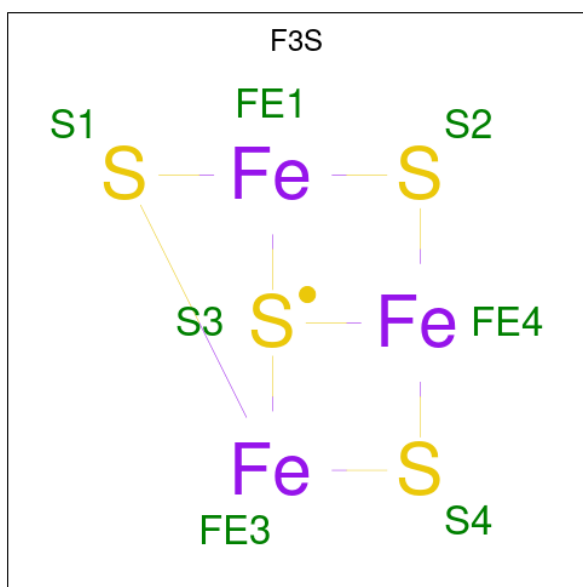
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	SSS	1	Total Fe S 7 3 4		0	0
4	TTT	1	Total Fe S 7 3 4		0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	SSS	1	Total C O 6 3 3		0	0
5	MMM	1	Total C O 6 3 3		0	0

- Molecule 6 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula: C_3FeN_2O) (labeled as "Ligand of Interest" by depositor).
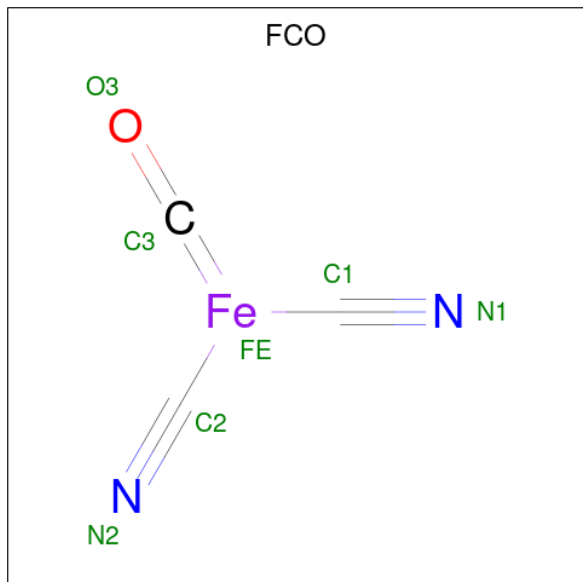
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	LLL	1	Total 7	C 3	Fe 1	N 2	O 1	0	0
6	MMM	1	Total 7	C 3	Fe 1	N 2	O 1	0	0

- 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	LLL	1	Total 1	Ni 1	0	0
7	MMM	1	Total 1	Ni 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	LLL	2	Total 2	Mg 2	0	0
8	TTT	2	Total 2	Mg 2	0	0
8	MMM	1	Total 1	Mg 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	LLL	1	Total 1	Cl 1	0	0
9	MMM	1	Total 1	Cl 1	0	0

• Molecule 10 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).
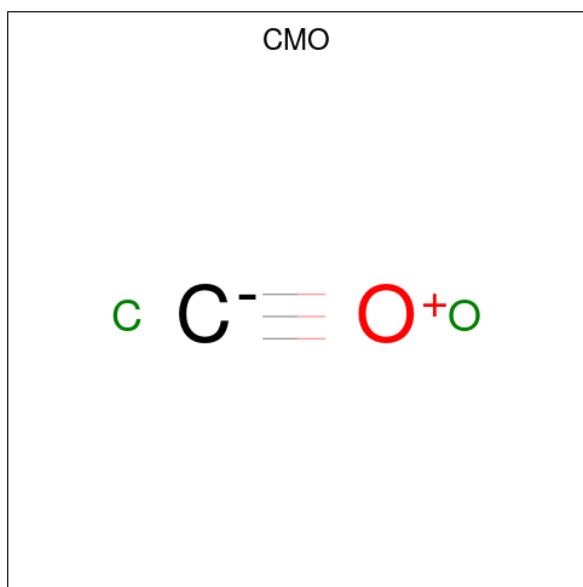
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	LLL	1	Total 2	C 1	O 1	0	0
10	MMM	1	Total 2	C 1	O 1	0	0

• Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	SSS	256	Total 256	O 256	0	0
11	LLL	496	Total 496	O 496	0	0
11	TTT	234	Total 234	O 234	0	0
11	MMM	467	Total 467	O 467	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: Hydrogenase-2 small chain
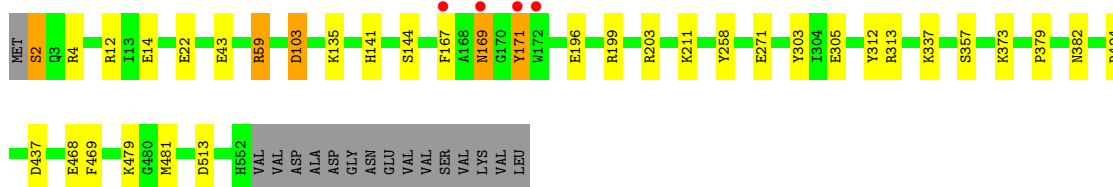
Chain SSS:
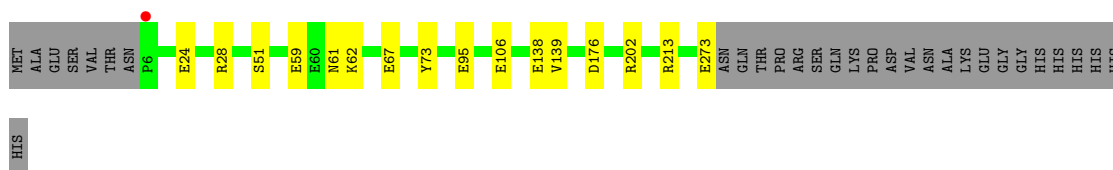
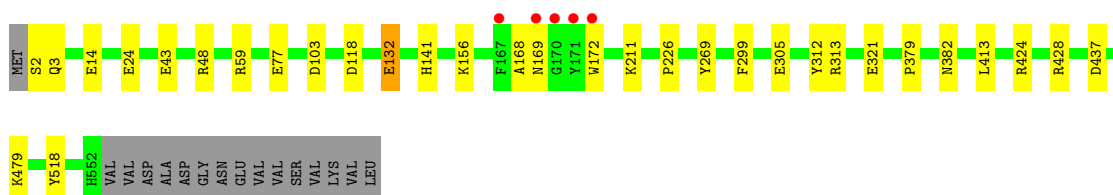- Molecule 1: Hydrogenase-2 small chain

Chain TTT:

- Molecule 2: Hydrogenase-2 large chain

Chain LLL:

- Molecule 2: Hydrogenase-2 large chain

Chain MMM:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	100.67Å 101.21Å 170.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	86.70 – 1.20 85.41 – 1.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (86.70-1.20) 99.9 (85.41-1.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 1.20Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.121 , 0.141 0.123 , 0.143	Depositor DCC
R_{free} test set	27288 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	11.5	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 55.3	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	14308	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: FCO, NI, SF4, MG, CL, F3S, CMO, 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	SSS	1.22	9/2122 (0.4%)	1.00	7/2888 (0.2%)
1	TTT	1.31	13/2123 (0.6%)	1.04	5/2889 (0.2%)
2	LLL	1.12	8/4468 (0.2%)	1.01	16/6089 (0.3%)
2	MMM	1.13	10/4447 (0.2%)	1.00	10/6061 (0.2%)
All	All	1.17	40/13160 (0.3%)	1.01	38/17927 (0.2%)

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	LLL	0	2
2	MMM	0	1
All	All	0	3

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	TTT	60	GLU	CD-OE1	16.60	1.44	1.25
1	TTT	273	GLU	CD-OE1	14.47	1.41	1.25
1	SSS	273	GLU	CD-OE1	12.46	1.39	1.25
1	SSS	59	GLU	CD-OE2	-9.08	1.15	1.25
1	TTT	83	LEU	C-O	8.35	1.39	1.23

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	TTT	273	GLU	OE1-CD-OE2	9.48	134.68	123.30
1	TTT	202	ARG	NE-CZ-NH2	-9.25	115.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	LLL	2	SER	N-CA-CB	-8.78	97.33	110.50
2	LLL	313	ARG	NE-CZ-NH2	-8.45	116.07	120.30
2	LLL	12	ARG	NE-CZ-NH1	8.05	124.32	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	LLL	171	TYR	Sidechain
2	LLL	59	ARG	Sidechain
2	MMM	59	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	SSS	2058	0	1986	6	0
1	TTT	2056	0	1987	4	0
2	LLL	4337	0	4285	23	0
2	MMM	4319	0	4268	9	0
3	SSS	16	0	0	0	0
3	TTT	16	0	0	0	0
4	SSS	7	0	0	0	0
4	TTT	7	0	0	0	0
5	MMM	6	0	8	1	0
5	SSS	6	0	8	0	0
6	LLL	7	0	0	0	0
6	MMM	7	0	0	0	0
7	LLL	1	0	0	0	0
7	MMM	1	0	0	0	0
8	LLL	2	0	0	0	0
8	MMM	1	0	0	0	0
8	TTT	2	0	0	0	0
9	LLL	1	0	0	0	0
9	MMM	1	0	0	0	0
10	LLL	2	0	0	0	0
10	MMM	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	LLL	496	0	0	12	0
11	MMM	467	0	0	5	0
11	SSS	256	0	0	1	0
11	TTT	234	0	0	3	0
All	All	14308	0	12542	36	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 1.

The worst 5 of 36 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:LLL:22[B]:GLU:OE2	11:LLL:701:HOH:O	1.58	1.18
2:MMM:379:PRO:HB2	11:MMM:931:HOH:O	1.74	0.87
2:LLL:22[B]:GLU:OE2	11:LLL:702:HOH:O	1.96	0.84
2:LLL:103:ASP:CG	11:LLL:703:HOH:O	2.16	0.83
2:LLL:2:SER:OG	2:LLL:22[B]:GLU:OE1	1.96	0.82

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	SSS	269/298 (90%)	259 (96%)	10 (4%)	0	100	100
1	TTT	269/298 (90%)	259 (96%)	10 (4%)	0	100	100
2	LLL	559/567 (99%)	535 (96%)	23 (4%)	1 (0%)	47	19
2	MMM	556/567 (98%)	533 (96%)	21 (4%)	2 (0%)	34	11
All	All	1653/1730 (96%)	1586 (96%)	64 (4%)	3 (0%)	47	19

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	LLL	211	LYS
2	MMM	211	LYS
2	MMM	226	PRO

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	SSS	216/239 (90%)	216 (100%)	0	100	100
1	TTT	216/239 (90%)	216 (100%)	0	100	100
2	LLL	475/479 (99%)	471 (99%)	4 (1%)	81	55
2	MMM	472/479 (98%)	468 (99%)	4 (1%)	81	55
All	All	1379/1436 (96%)	1371 (99%)	8 (1%)	86	63

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	MMM	479	LYS
2	MMM	413	LEU
2	MMM	141	HIS
2	LLL	479	LYS
2	MMM	312	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 9 are monoatomic - leaving 12 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	#$\|Z\| > 2$
3	SF4	TTT	401	1	0,12,12	-	-	-		
5	GOL	SSS	404	-	5,5,5	0.63	0	5,5,5	1.30	1 (20%)
6	FCO	MMM	601	2	0,6,6	-	-	-		
4	F3S	SSS	402	1	0,9,9	-	-	-		
6	FCO	LLL	601	2	0,6,6	-	-	-		
10	CMO	LLL	606	-	0,1,1	-	-	-		
10	CMO	MMM	605	-	0,1,1	-	-	-		
5	GOL	MMM	606	-	5,5,5	0.25	0	5,5,5	0.47	0
3	SF4	TTT	403	1	0,12,12	-	-	-		
3	SF4	SSS	403	1	0,12,12	-	-	-		
4	F3S	TTT	402	1	0,9,9	-	-	-		
3	SF4	SSS	401	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
3	SF4	TTT	401	1	-	-	0/6/5/5
5	GOL	SSS	404	-	-	0/4/4/4	-
4	F3S	SSS	402	1	-	-	0/3/3/3
5	GOL	MMM	606	-	-	0/4/4/4	-
3	SF4	TTT	403	1	-	-	0/6/5/5
3	SF4	SSS	403	1	-	-	0/6/5/5
4	F3S	TTT	402	1	-	-	0/3/3/3
3	SF4	SSS	401	1	-	-	0/6/5/5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

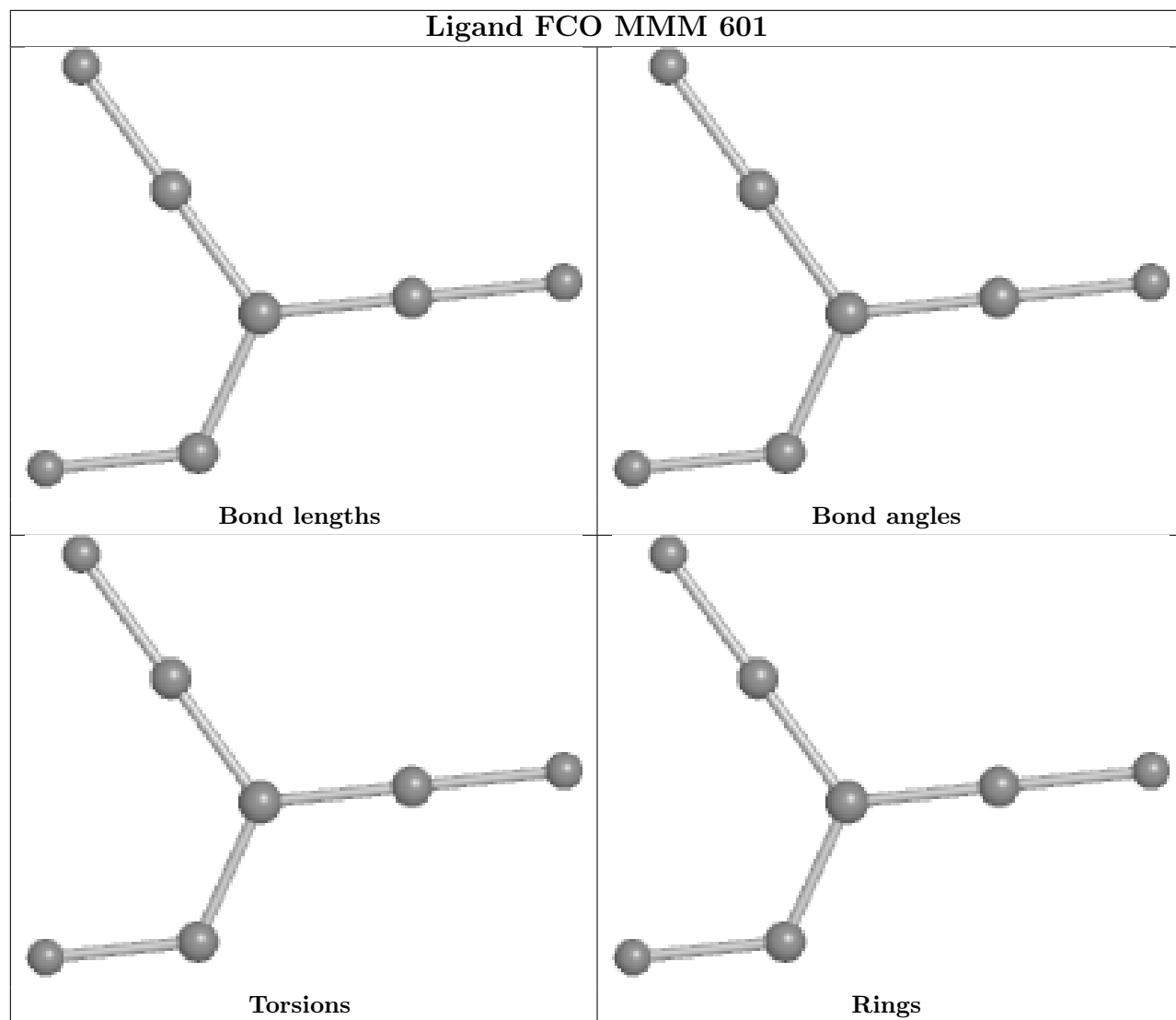| Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	SSS	404	GOL	O1-C1-C2	2.14	120.45	110.20

There are no chirality outliers.

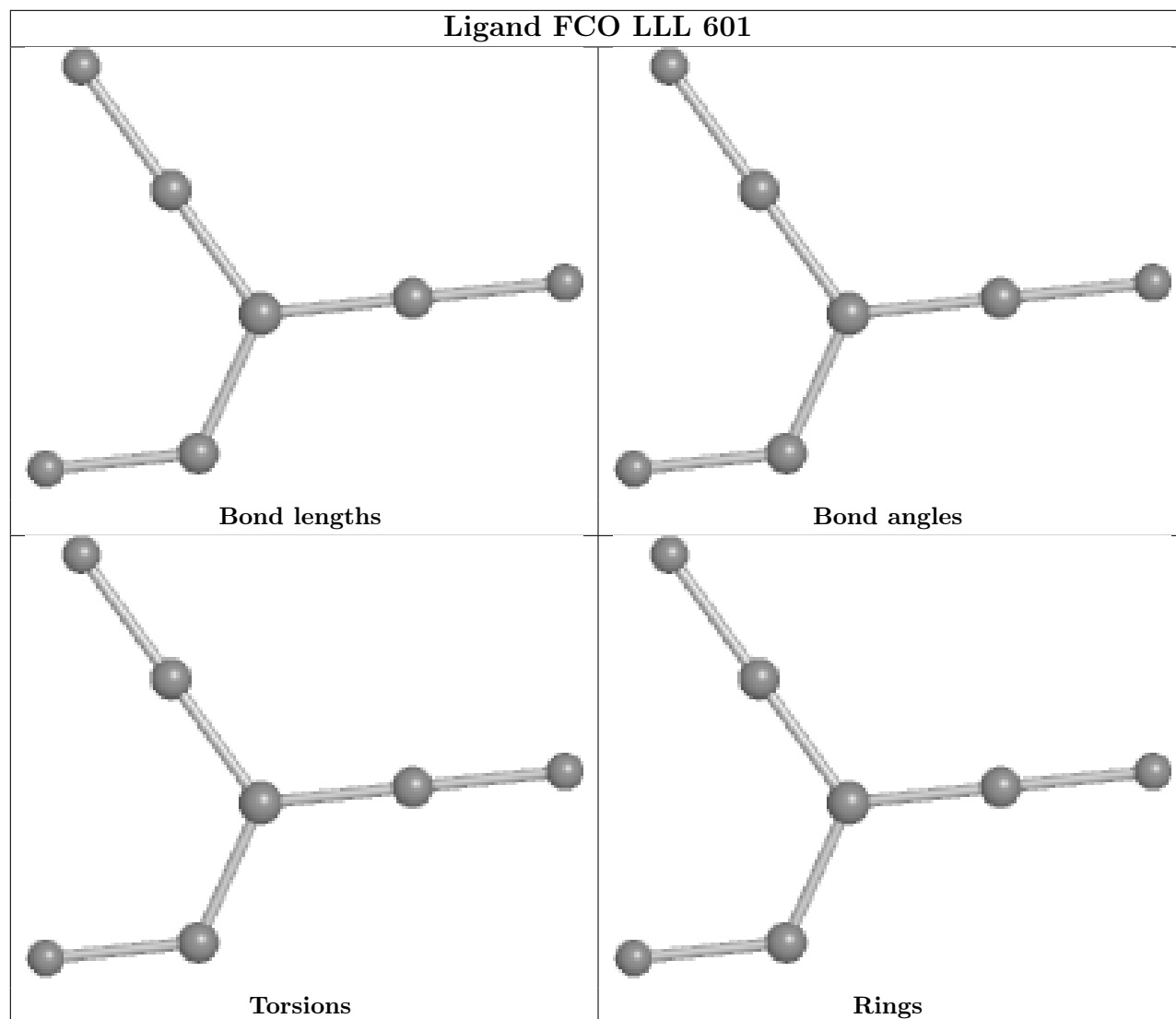There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	MMM	606	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 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 MMM 601

Bond lengths

Bond angles

Torsions

Rings

Ligand FCO LLL 601

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 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	SSS	268/298 (89%)	-0.25	1 (0%)	92	92	8, 13, 26, 52	0
1	TTT	268/298 (89%)	-0.25	1 (0%)	92	92	9, 14, 31, 83	0
2	LLL	551/567 (97%)	-0.26	4 (0%)	87	87	8, 13, 27, 59	0
2	MMM	551/567 (97%)	-0.22	5 (0%)	84	84	9, 14, 30, 68	0
All	All	1638/1730 (94%)	-0.24	11 (0%)	87	87	8, 13, 30, 83	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	MMM	172	TRP	6.6
2	LLL	172	TRP	6.3
1	TTT	6	PRO	5.3
2	LLL	171	TYR	4.7
2	MMM	171	TYR	4.4

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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(Å^2)	Q<0.9
8	MG	TTT	405	1/1	0.81	0.13	42,42,42,42	0
5	GOL	SSS	404	6/6	0.89	0.14	18,25,27,28	6
5	GOL	MMM	606	6/6	0.94	0.10	29,32,36,39	0
8	MG	LLL	604	1/1	0.98	0.33	30,30,30,30	0
8	MG	TTT	404	1/1	0.99	0.20	23,23,23,23	0
10	CMO	LLL	606	2/2	0.99	0.11	10,10,10,14	2
10	CMO	MMM	605	2/2	0.99	0.17	10,10,10,15	2
3	SF4	SSS	403	8/8	1.00	0.07	8,9,9,9	0
6	FCO	LLL	601	7/7	1.00	0.07	8,9,9,9	0
6	FCO	MMM	601	7/7	1.00	0.06	9,10,10,11	0
7	NI	LLL	602	1/1	1.00	0.06	9,9,9,9	0
7	NI	MMM	602	1/1	1.00	0.06	10,10,10,10	0
8	MG	LLL	603	1/1	1.00	0.09	8,8,8,8	0
3	SF4	TTT	401	8/8	1.00	0.07	10,10,11,11	0
3	SF4	TTT	403	8/8	1.00	0.06	9,10,10,10	0
4	F3S	SSS	402	7/7	1.00	0.07	8,9,9,9	0
8	MG	MMM	603	1/1	1.00	0.07	9,9,9,9	0
9	CL	LLL	605	1/1	1.00	0.06	18,18,18,18	0
9	CL	MMM	604	1/1	1.00	0.06	17,17,17,17	0
4	F3S	TTT	402	7/7	1.00	0.07	9,9,10,10	0
3	SF4	SSS	401	8/8	1.00	0.07	10,10,10,10	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.
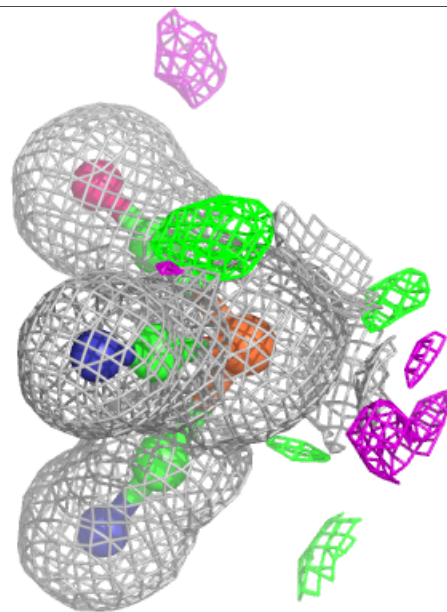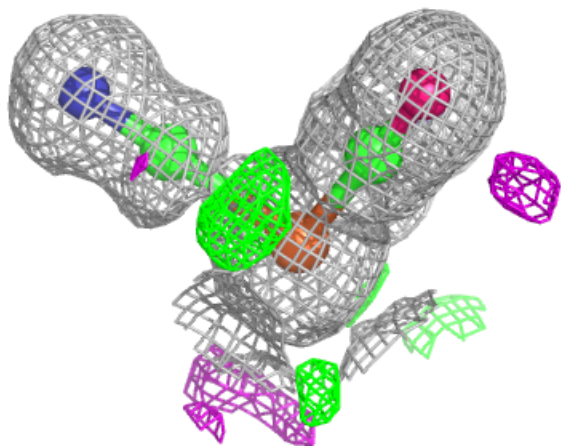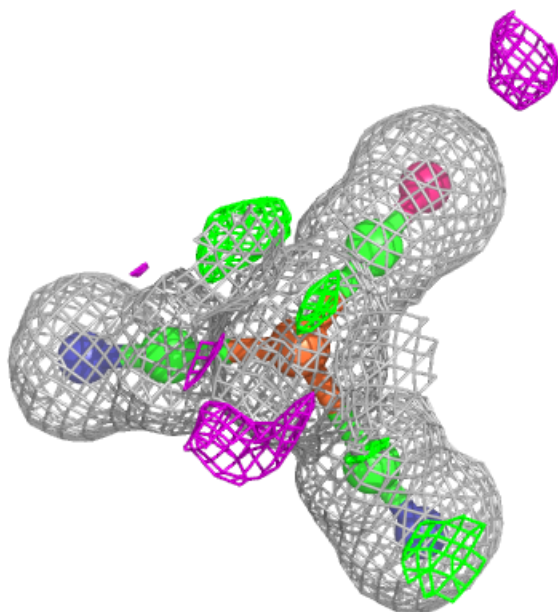
Electron density around FCO LLL 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
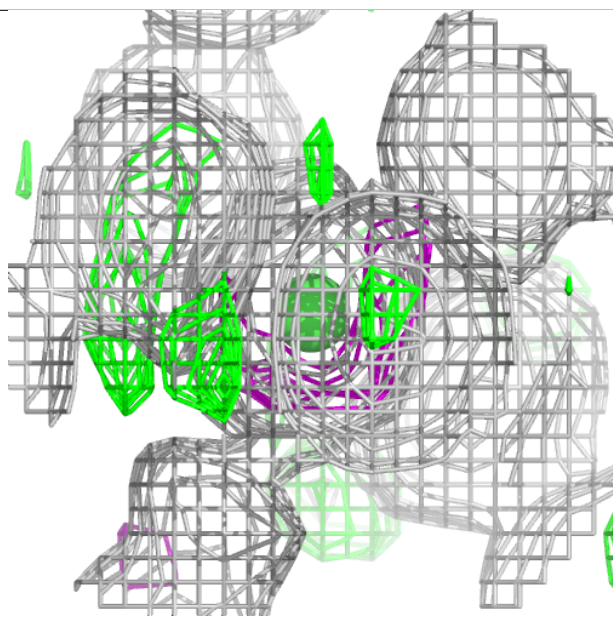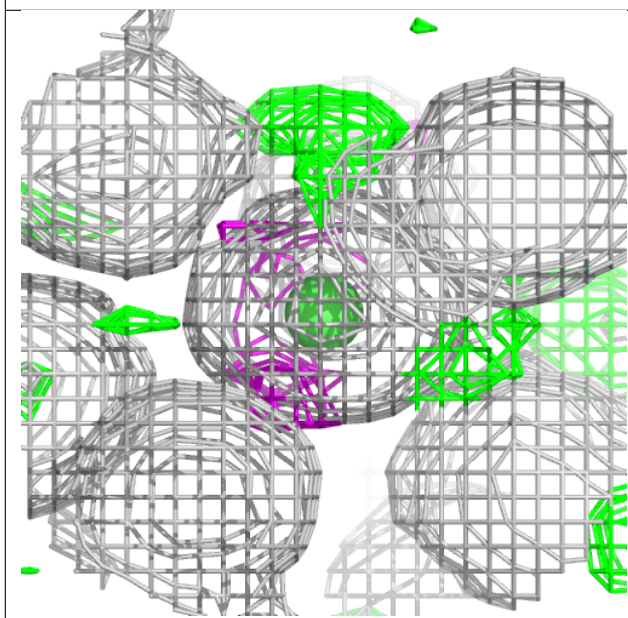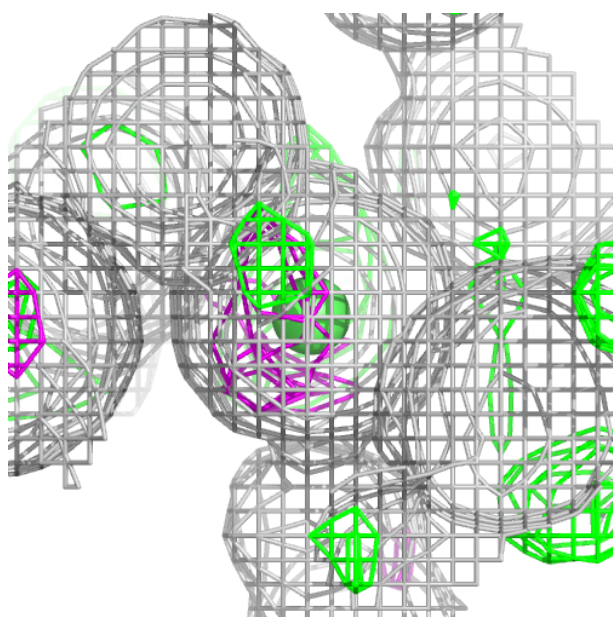mF_o-DF_c (at 3 rmsd) in purple (negative)
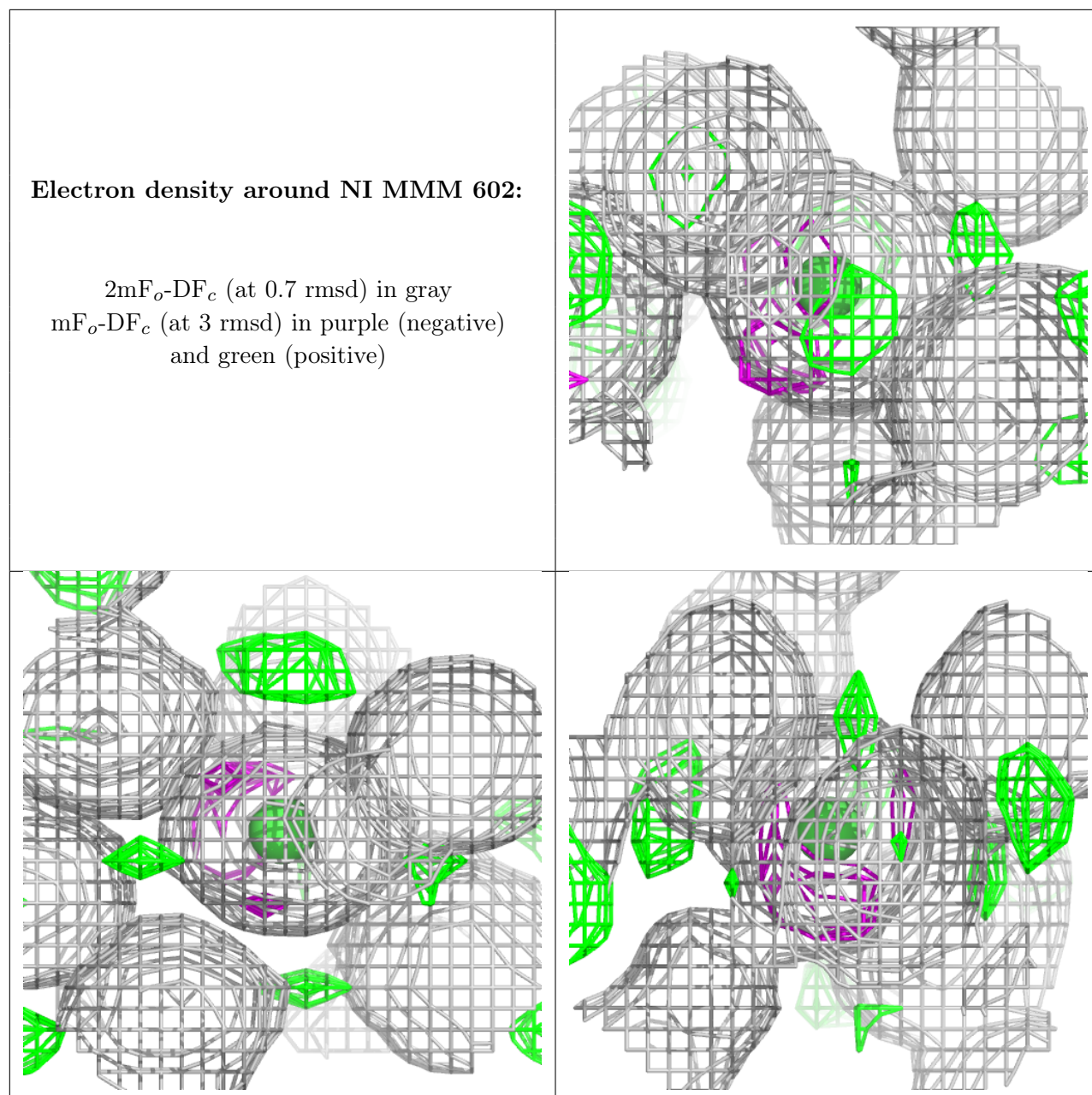and green (positive)
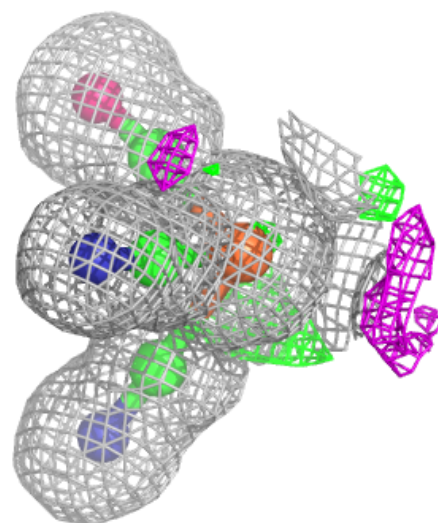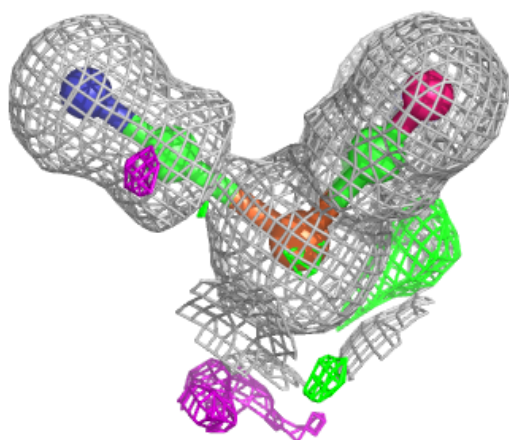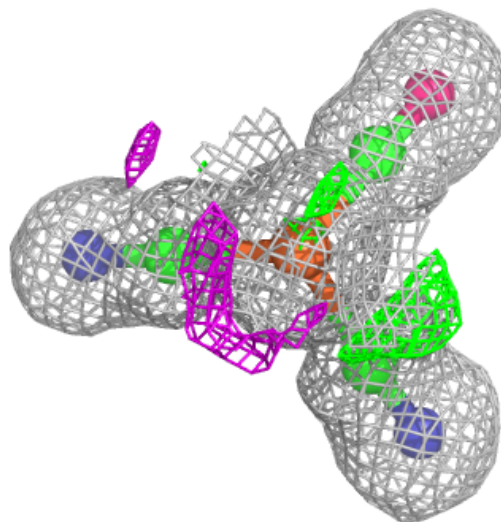
Electron density around FCO MMM 601:

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

Electron density around NI LLL 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 MMM 602:

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

6.5   Other polymers ⓘ

There are no such residues in this entry.