wwPDB X-ray Structure Validation Summary Report (i)

Jan 14, 2024 – 02:53 am GMT

PDB ID	:	6SYO
Title	:	Hydrogenase-2 variant R479K - As Isolated form
Authors	:	Carr, S.B.; Beaton, S.E.; Evans, R.M.; Armstrong, F.A.
Deposited on	:	2019-09-30
Resolution	:	1.25 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 (i) 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 (i)) were used in the production of this report:

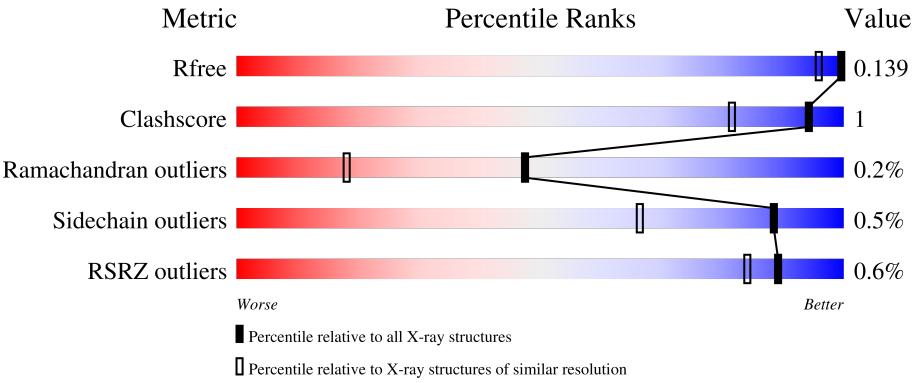
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.25 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}	130704	1023 (1.28-1.24)
Clashscore	141614	1060 (1.28-1.24)
Ramachandran outliers	138981	1029 (1.28-1.24)
Sidechain outliers	138945	1028 (1.28-1.24)
RSRZ outliers	127900	1004 (1.28-1.24)

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	86% · 10%
2	LLL	567	% 90% 7% ·
2	MMM	567	% 90% 7% ·

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 14582 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	4	0
			2066	1310	364	379	13			
1	TTT	268	Total	C	N	O	S	0	1	0
			2044	1295	360	376	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SSS	291	HIS	ASN	conflict	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	ASN	conflict	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

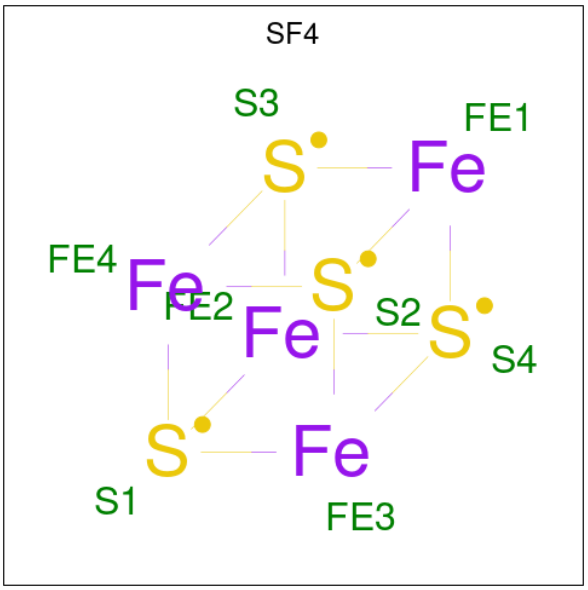
- Molecule 2 is a protein called Hydrogenase-2 large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	LLL	551	Total	C	N	O	S	0	7	0
			4325	2753	740	814	18			
2	MMM	551	Total	C	N	O	S	0	8	0
			4327	2755	741	813	18			

There are 2 discrepancies between the modelled and reference sequences:

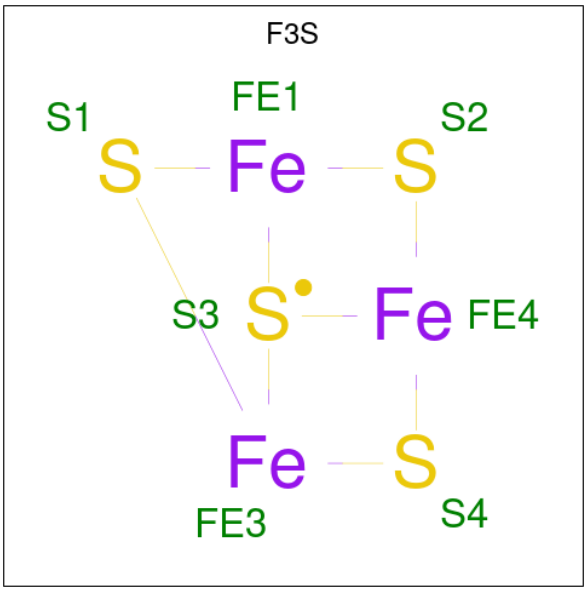
Chain	Residue	Modelled	Actual	Comment	Reference
LLL	479	LYS	ARG	engineered mutation	UNP P0ACE0
MMM	479	LYS	ARG	engineered mutation	UNP P0ACE0

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



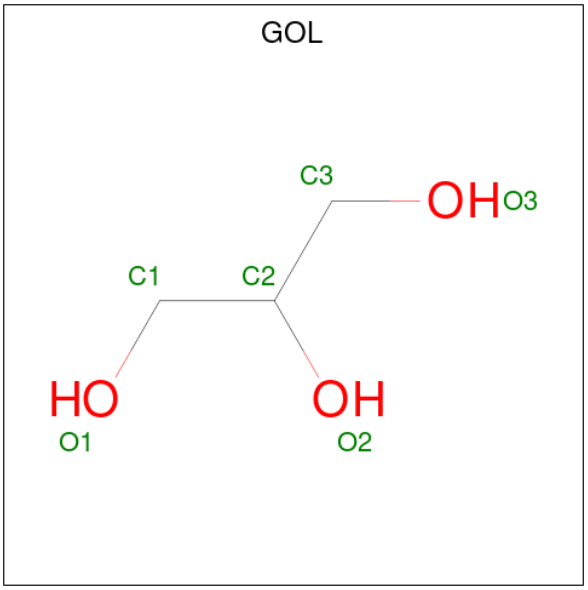
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	SSS	1	Total Fe S 8 4 4	0	0
3	SSS	1	Total Fe S 8 4 4	0	0
3	TTT	1	Total Fe S 8 4 4	0	0
3	TTT	1	Total Fe S 8 4 4	0	0

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



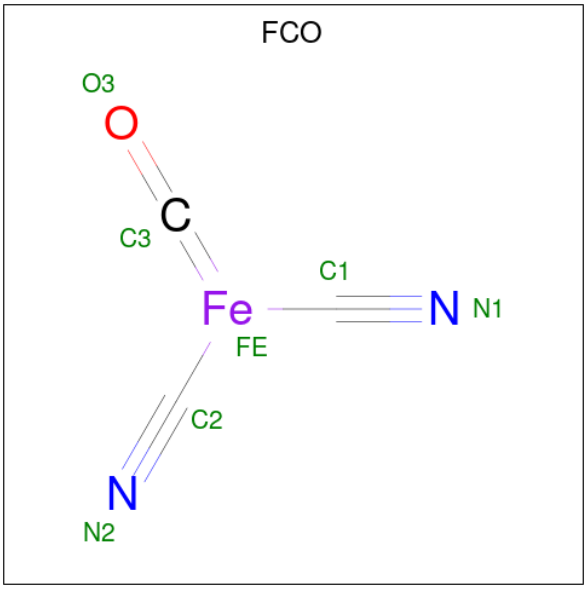
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	SSS	1	Total Fe S 7 3 4	0	0
4	TTT	1	Total Fe S 7 3 4	0	0

- 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	LLL	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 C Fe N O 7 3 1 2 1	0	0
6	MMM	1	Total C Fe N O 7 3 1 2 1	0	0

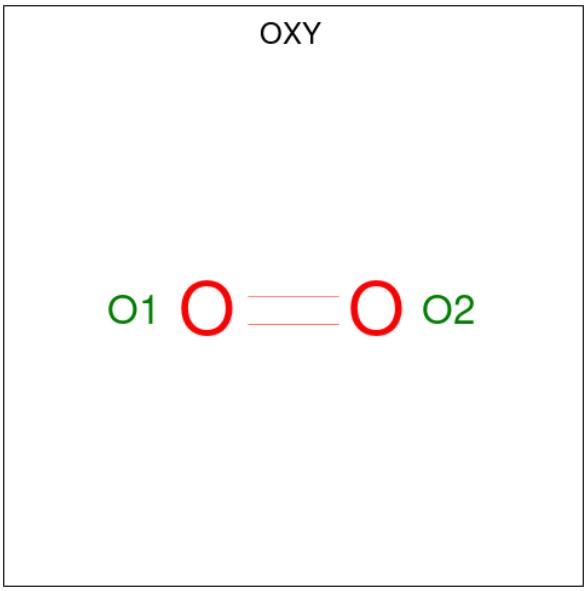
- Molecule 7 is NICKEL (II) ION (three-letter code: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 9 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	LLL	1	Total O 2 2	0	0
9	MMM	1	Total O 2 2	0	0

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	MMM	1	Total Cl 1 1	0	0

- Molecule 11 is water.

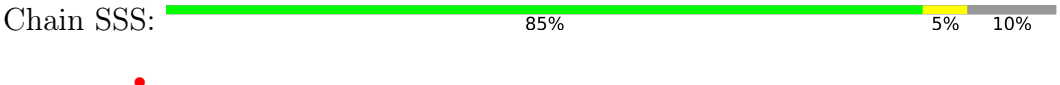
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	SSS	297	Total O 297 297	0	0
11	LLL	613	Total O 613 613	0	0
11	TTT	272	Total O 272 272	0	0
11	MMM	555	Total O 555 555	0	0

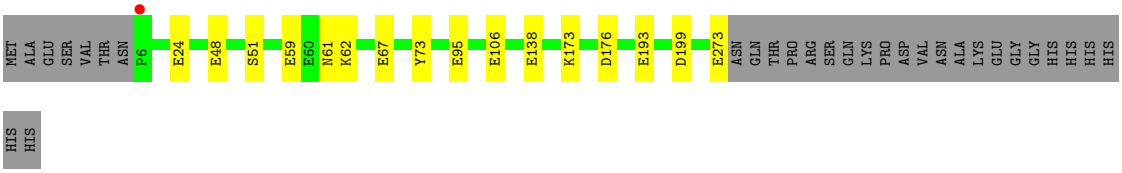
3 Residue-property plots (i)

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

Chain SSS:



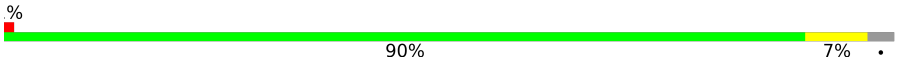


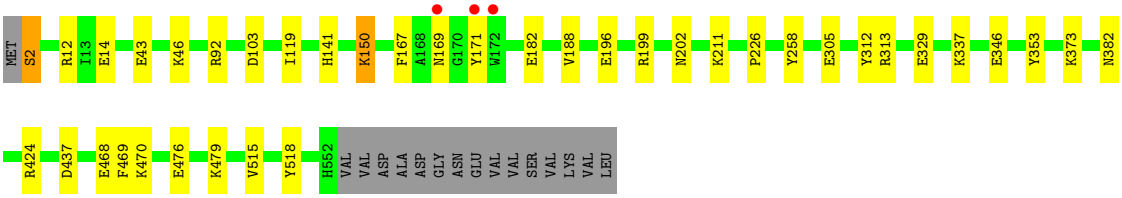
• Molecule 1: Hydrogenase-2 small chain

Chain TTT:

• Molecule 2: Hydrogenase-2 large chain

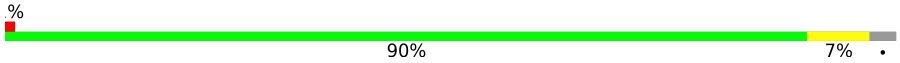
Chain LLL:

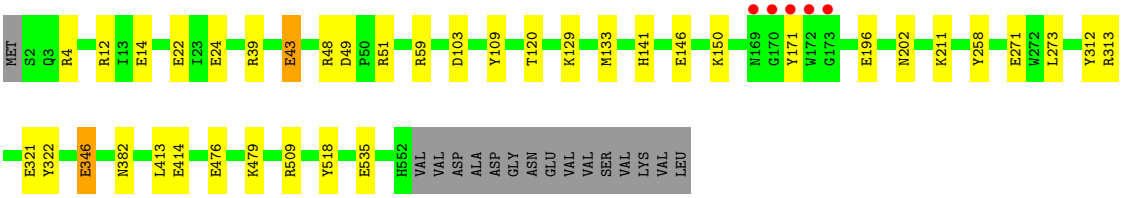




• Molecule 2: Hydrogenase-2 large chain

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)	85.56 – 1.25 85.41 – 1.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (85.56-1.25) 99.9 (85.41-1.25)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 1.25Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.114 , 0.136 0.117 , 0.139	Depositor DCC
R_{free} test set	23819 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	11.9	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.5	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	14582	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 4.76% 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: CL, NI, F3S, SF4, OXY, GOL, MG, 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	SSS	1.25	10/2130 (0.5%)	1.03	5/2899 (0.2%)
1	TTT	1.24	8/2105 (0.4%)	1.07	2/2866 (0.1%)
2	LLL	1.13	12/4447 (0.3%)	1.02	14/6059 (0.2%)
2	MMM	1.17	11/4455 (0.2%)	1.03	14/6071 (0.2%)
All	All	1.18	41/13137 (0.3%)	1.03	35/17895 (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 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	MMM	196	GLU	CD-OE2	14.52	1.41	1.25
1	SSS	59	GLU	CD-OE2	-11.49	1.13	1.25
1	TTT	95	GLU	CD-OE2	11.29	1.38	1.25
2	LLL	43	GLU	CD-OE1	9.96	1.36	1.25
1	SSS	273	GLU	CD-OE1	9.68	1.36	1.25

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	MMM	48	ARG	NE-CZ-NH2	-8.80	115.90	120.30
2	MMM	12	ARG	NE-CZ-NH1	7.75	124.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	TTT	202	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	TTT	195	ARG	NE-CZ-NH1	7.36	123.98	120.30
2	LLL	313	ARG	NE-CZ-NH2	-7.16	116.72	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	515	VAL	Mainchain
2	MMM	59	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	SSS	2066	0	1996	9	0
1	TTT	2044	0	1968	3	0
2	LLL	4325	0	4271	17	0
2	MMM	4327	0	4279	10	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	LLL	6	0	8	0	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	1	0	0	0	0
9	LLL	2	0	0	0	0
9	MMM	2	0	0	0	0
10	MMM	1	0	0	0	0
11	LLL	613	0	0	6	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	MMM	555	0	0	5	0
11	SSS	297	0	0	3	0
11	TTT	272	0	0	3	1
All	All	14582	0	12530	33	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.

The worst 5 of 33 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:SSS:61[A]:ASN:HD21	2:LLL:169:ASN:HB3	1.09	1.18
1:SSS:61[A]:ASN:HD21	2:LLL:169:ASN:CB	1.65	1.08
2:MMM:150:LYS:HE3	11:MMM:820:HOH:O	1.69	0.90
1:SSS:61[A]:ASN:ND2	2:LLL:169:ASN:HB3	1.93	0.82
1:SSS:61[A]:ASN:ND2	2:LLL:169:ASN:CB	2.44	0.79

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)
11:LLL:883:HOH:O	11:TTT:649:HOH:O[2_675]	1.95	0.25

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	SSS	270/298 (91%)	259 (96%)	11 (4%)	0	100 100
1	TTT	267/298 (90%)	257 (96%)	10 (4%)	0	100 100
2	LLL	556/567 (98%)	533 (96%)	21 (4%)	2 (0%)	34 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	MMM	557/567 (98%)	535 (96%)	21 (4%)	1 (0%)	47 18
All	All	1650/1730 (95%)	1584 (96%)	63 (4%)	3 (0%)	47 18

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	LLL	211	LYS
2	MMM	211	LYS
2	LLL	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	SSS	217/239 (91%)	217 (100%)	0	100 100
1	TTT	214/239 (90%)	214 (100%)	0	100 100
2	LLL	472/479 (98%)	468 (99%)	4 (1%)	81 53
2	MMM	473/479 (99%)	470 (99%)	3 (1%)	86 62
All	All	1376/1436 (96%)	1369 (100%)	7 (0%)	88 66

5 of 7 residues with a non-rotameric sidechain are listed below:

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

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

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 7 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	$\#\|Z\| > 2$
9	OXY	MMM	605	7	1,1,1	0.02	0	-		
5	GOL	LLL	606	-	5,5,5	0.28	0	5,5,5	1.34	0
9	OXY	LLL	605	7	1,1,1	0.16	0	-		
5	GOL	SSS	404	-	5,5,5	0.77	0	5,5,5	1.17	0
4	F3S	SSS	402	1	0,9,9	-	-	-		
3	SF4	SSS	401	1	0,12,12	-	-	-		
3	SF4	TTT	403	1	0,12,12	-	-	-		
4	F3S	TTT	402	1	0,9,9	-	-	-		
6	FCO	MMM	601	2	0,6,6	-	-	-		
6	FCO	LLL	601	2	0,6,6	-	-	-		
3	SF4	TTT	401	1	0,12,12	-	-	-		
3	SF4	SSS	403	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	LLL	606	-	-	4/4/4/4	-
5	GOL	SSS	404	-	-	0/4/4/4	-
4	F3S	SSS	402	1	-	-	0/3/3/3
3	SF4	SSS	401	1	-	-	0/6/5/5
3	SF4	TTT	403	1	-	-	0/6/5/5
4	F3S	TTT	402	1	-	-	0/3/3/3
3	SF4	TTT	401	1	-	-	0/6/5/5
3	SF4	SSS	403	1	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

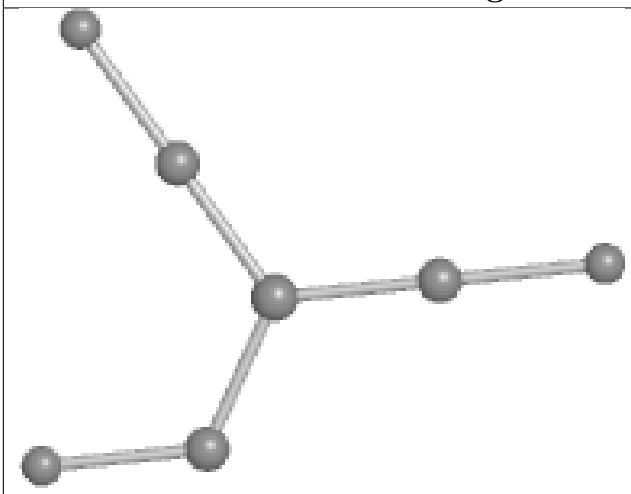
Mol	Chain	Res	Type	Atoms
5	LLL	606	GOL	O1-C1-C2-C3
5	LLL	606	GOL	C1-C2-C3-O3
5	LLL	606	GOL	O1-C1-C2-O2
5	LLL	606	GOL	O2-C2-C3-O3

There are no ring outliers.

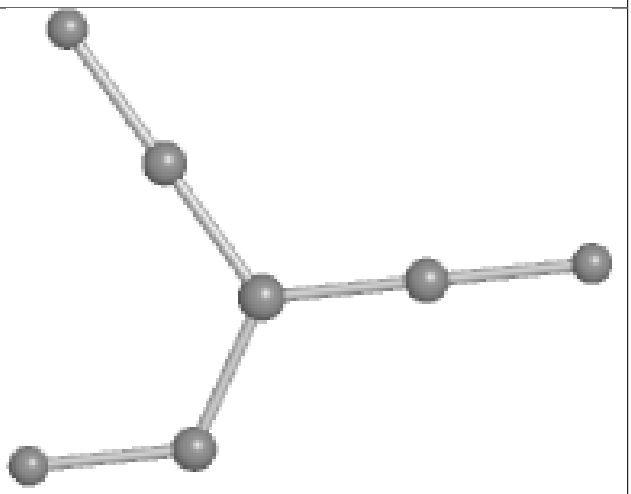
No monomer is involved in short contacts.

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.

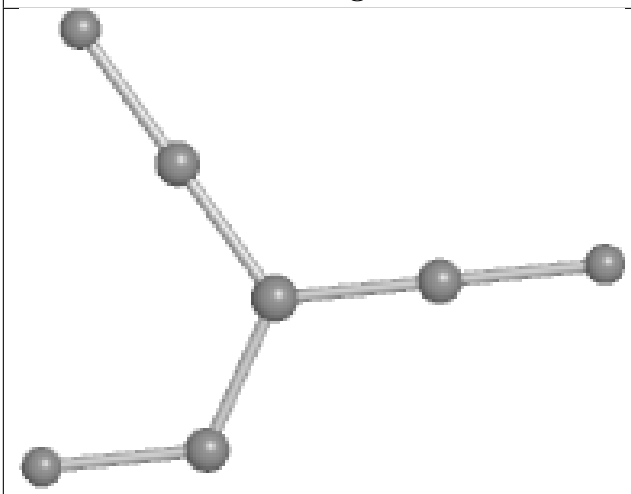
Ligand FCO MMM 601



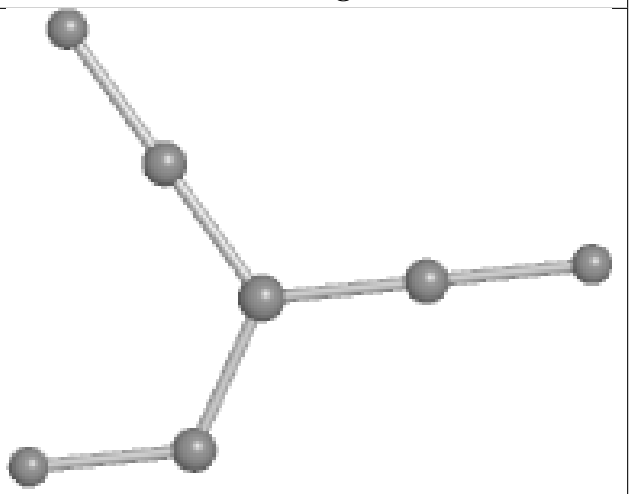
Bond lengths



Bond angles

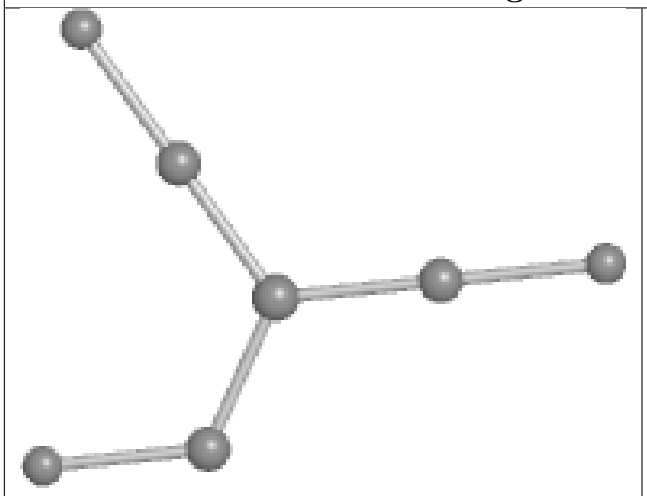


Torsions

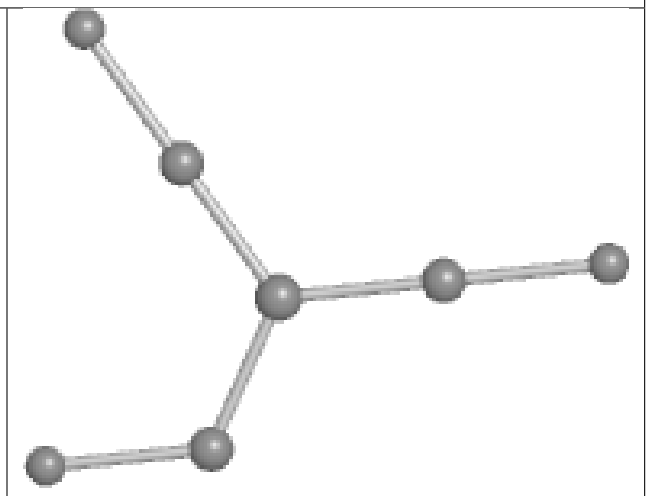


Rings

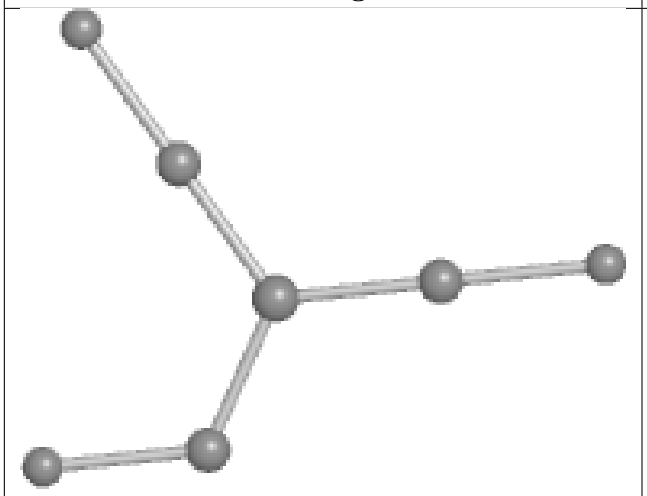
Ligand FCO LLL 601



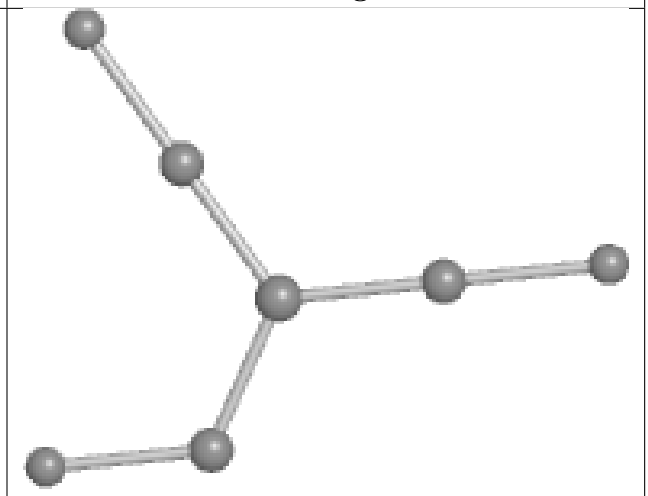
Bond lengths



Bond angles



Torsions



Rings

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	SSS	268/298 (89%)	-0.50	1 (0%)	92	87	8, 12, 26, 44	0
1	TTT	268/298 (89%)	-0.50	1 (0%)	92	87	9, 14, 29, 57	0
2	LLL	551/567 (97%)	-0.53	3 (0%)	91	85	8, 12, 26, 40	0
2	MMM	551/567 (97%)	-0.46	5 (0%)	84	76	8, 14, 29, 63	0
All	All	1638/1730 (94%)	-0.50	10 (0%)	89	84	8, 13, 28, 63	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	MMM	172	TRP	6.3
2	LLL	172	TRP	5.6
2	MMM	171	TYR	4.6
1	TTT	6	PRO	4.1
2	LLL	171	TYR	3.7

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

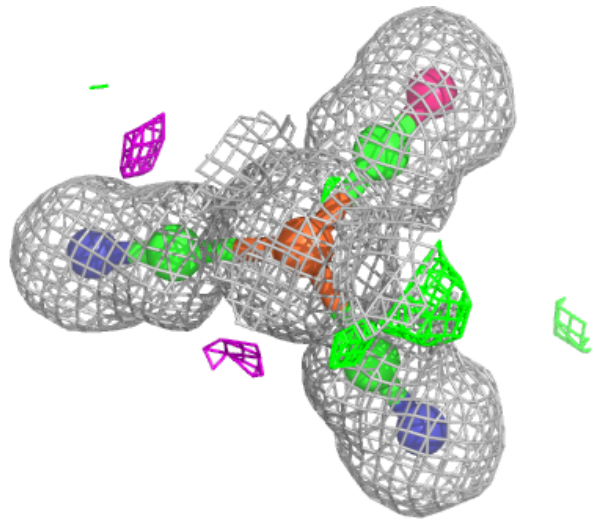
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

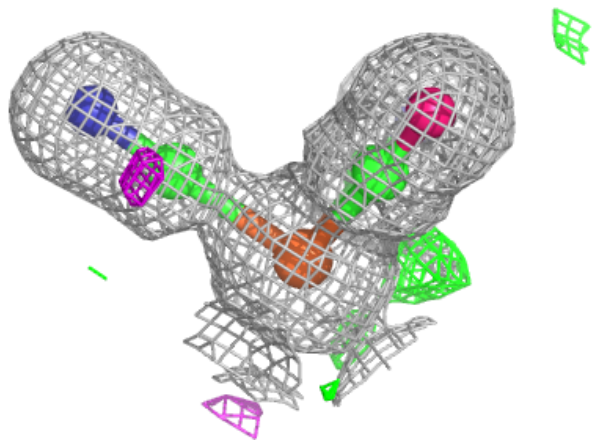
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	SSS	404	6/6	0.88	0.14	20,27,31,31	0
5	GOL	LLL	606	6/6	0.93	0.12	24,31,38,42	0
9	OXY	MMM	605	2/2	0.95	0.16	16,16,16,18	2
9	OXY	LLL	605	2/2	0.96	0.18	13,13,13,16	2
8	MG	LLL	603	1/1	0.98	0.28	32,32,32,32	0
8	MG	TTT	404	1/1	0.99	0.18	22,22,22,22	0
3	SF4	SSS	401	8/8	1.00	0.06	10,10,10,10	0
3	SF4	SSS	403	8/8	1.00	0.06	8,8,9,9	0
6	FCO	LLL	601	7/7	1.00	0.06	7,8,9,9	0
6	FCO	MMM	601	7/7	1.00	0.06	9,9,10,11	0
7	NI	LLL	602	1/1	1.00	0.05	9,9,9,9	0
7	NI	MMM	602	1/1	1.00	0.05	10,10,10,10	0
3	SF4	TTT	401	8/8	1.00	0.06	10,10,10,11	0
8	MG	LLL	604	1/1	1.00	0.09	7,7,7,7	0
3	SF4	TTT	403	8/8	1.00	0.06	9,10,10,10	0
8	MG	MMM	603	1/1	1.00	0.06	8,8,8,8	0
4	F3S	SSS	402	7/7	1.00	0.06	8,9,9,9	0
4	F3S	TTT	402	7/7	1.00	0.06	9,9,9,10	0
10	CL	MMM	604	1/1	1.00	0.05	17,17,17,17	0

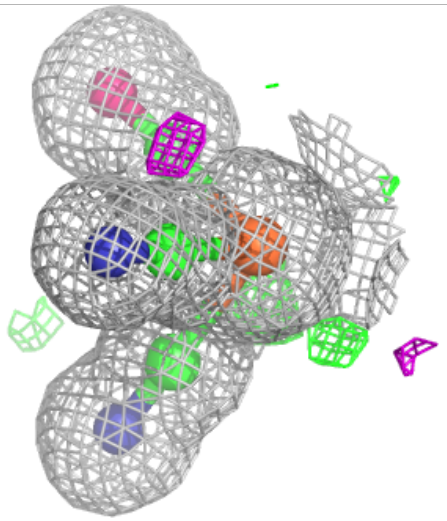
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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)

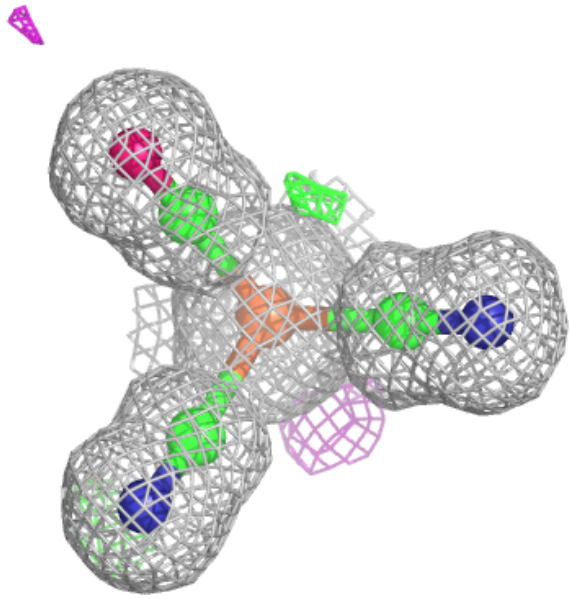


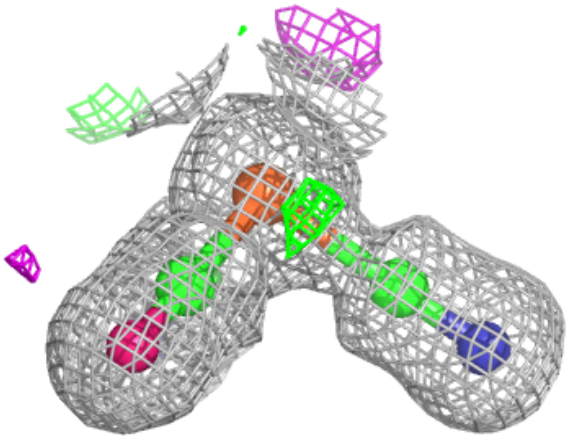


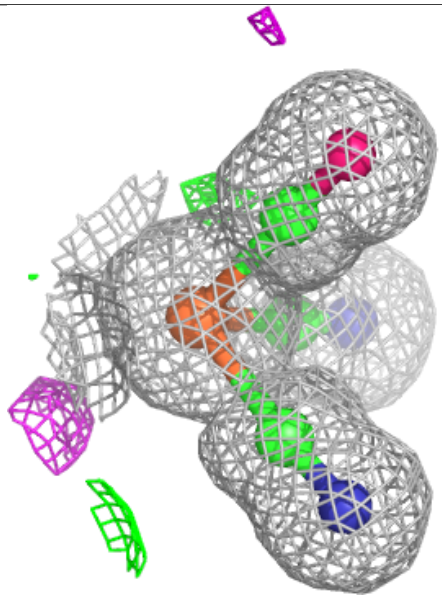


Electron density around FCO MMM 601:

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

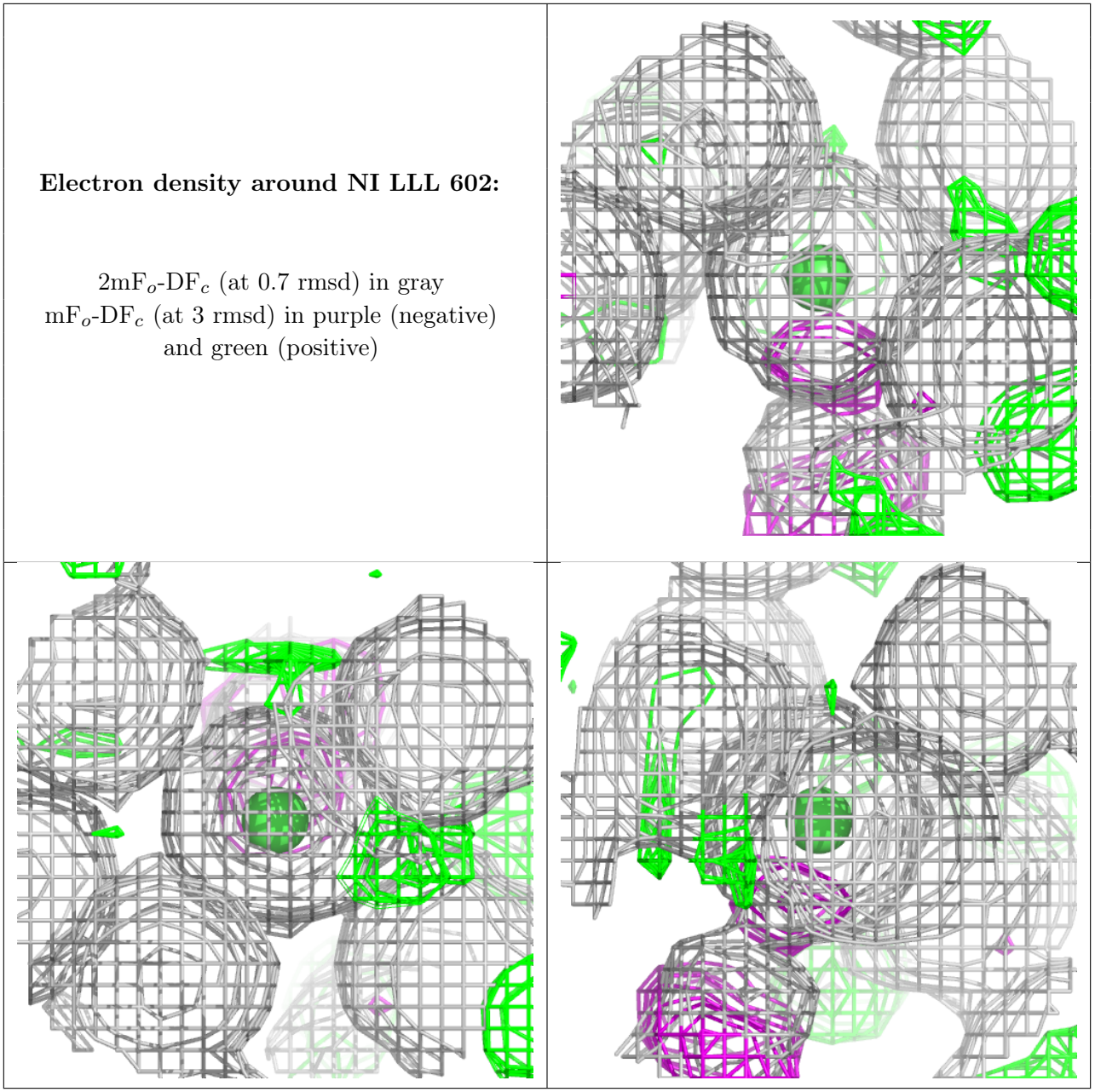






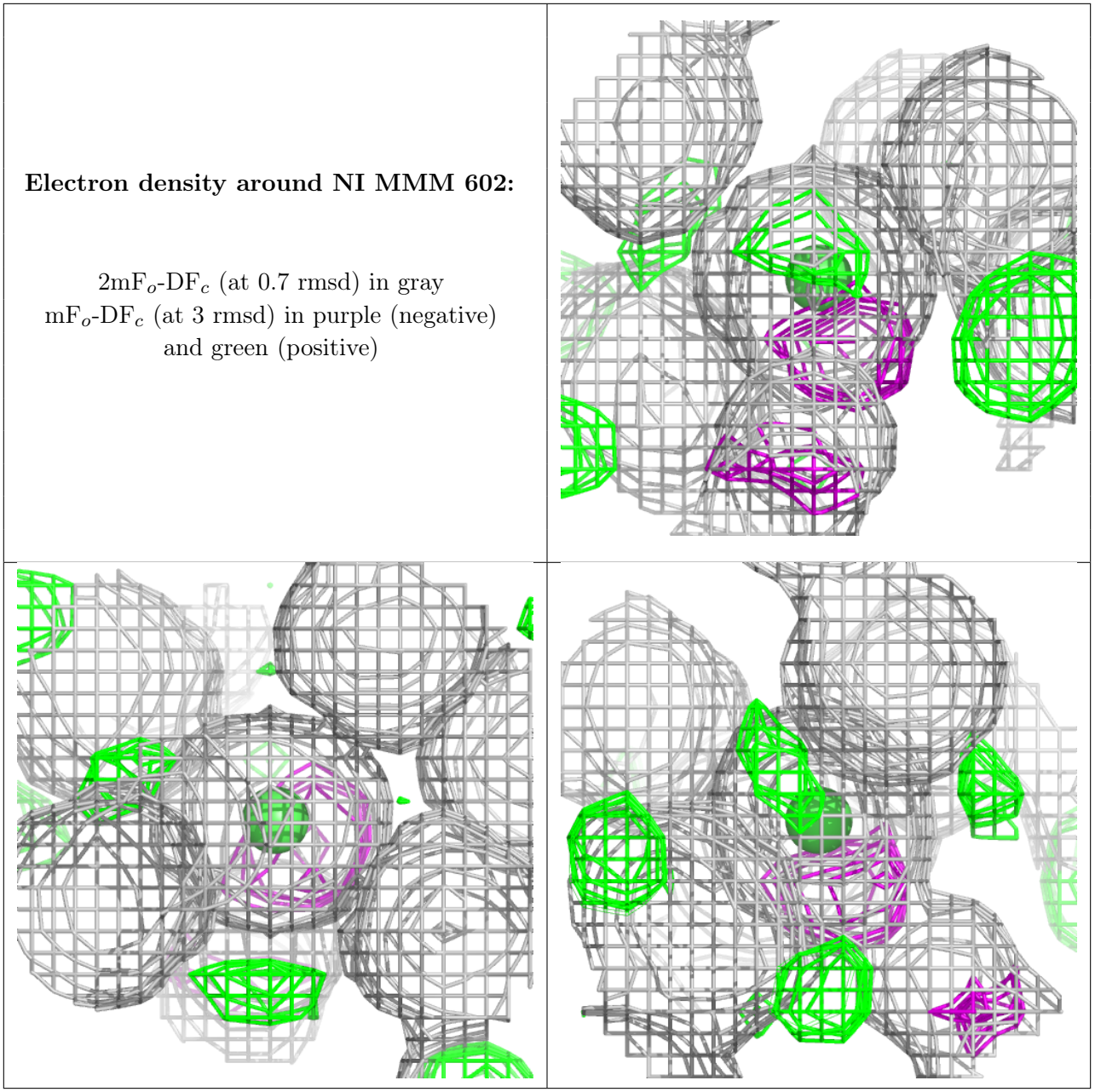
Electron density around NI LLL 602:

$2mF_o$-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:

$2mF_o$-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.