wwPDB X-ray Structure Validation Summary Report (i)

Aug 23, 2026 – 07:20 am BST

PDB ID	:	6SYX / pdb_00006syx
Title	:	Hydrogenase-2 variant R479K - reduced sample exposed to pure oxygen
Authors	:	Carr, S.B.; Beaton, S.E.; Evans, R.M.; Armstrong, F.A.
Deposited on	:	2019-10-01
Resolution	:	1.30 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:

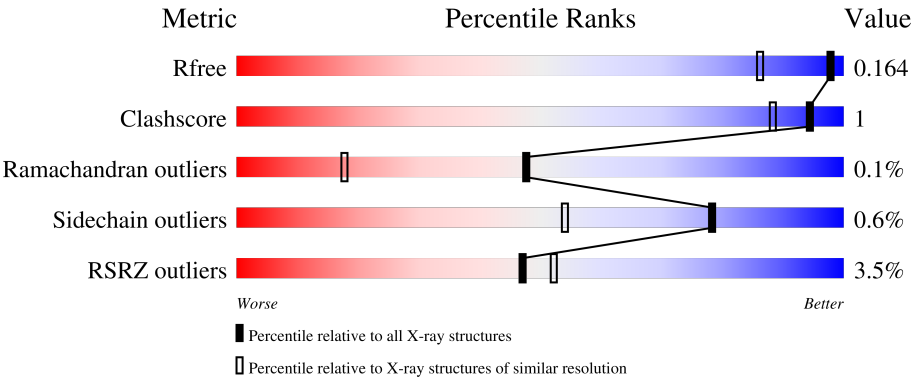
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

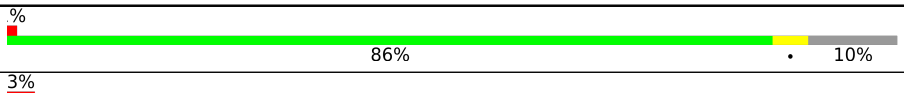
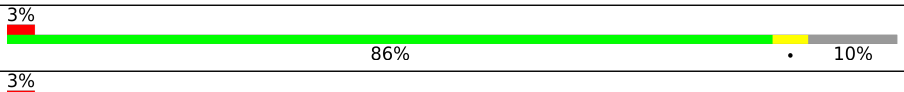
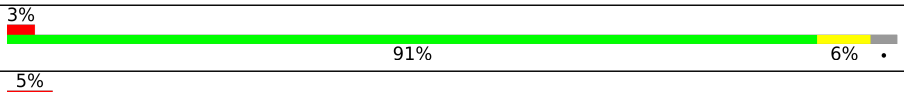
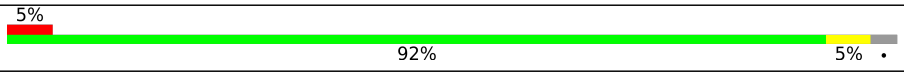
The reported resolution of this entry is 1.30 Å.

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}	180053	1553 (1.30-1.30)
Clashscore	190562	1595 (1.30-1.30)
Ramachandran outliers	187476	1551 (1.30-1.30)
Sidechain outliers	187428	1551 (1.30-1.30)
RSRZ outliers	180081	1549 (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	SSS	298	
1	TTT	298	
2	LLL	567	
2	MMM	567	

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 14669 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
			2064	1308	362	381	13			
1	TTT	268	Total	C	N	O	S	0	2	0
			2050	1300	361	376	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

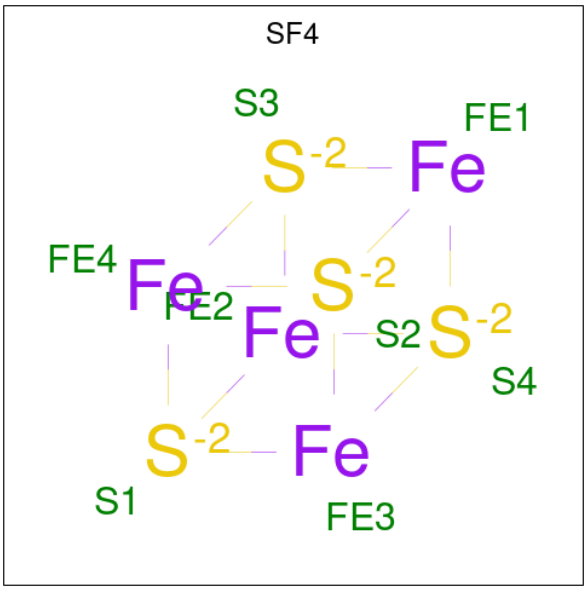
- Molecule 2 is a protein called Hydrogenase-2 large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	LLL	551	Total	C	N	O	S	0	6	0
			4313	2747	738	810	18			
2	MMM	551	Total	C	N	O	S	0	6	0
			4319	2750	741	810	18			

There are 2 discrepancies between the modelled and reference sequences:

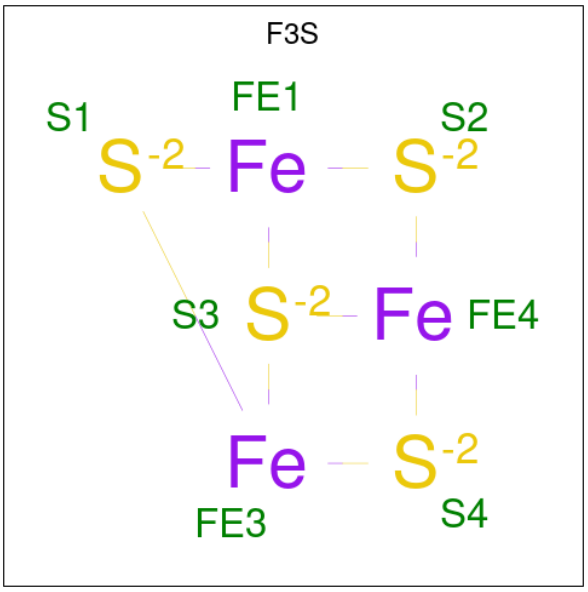
Chain	Residue	Modelled	Actual	Comment	Reference
LLL	479	LYS	ARG	engineered mutation	UNP V0V766
MMM	479	LYS	ARG	engineered mutation	UNP V0V766

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



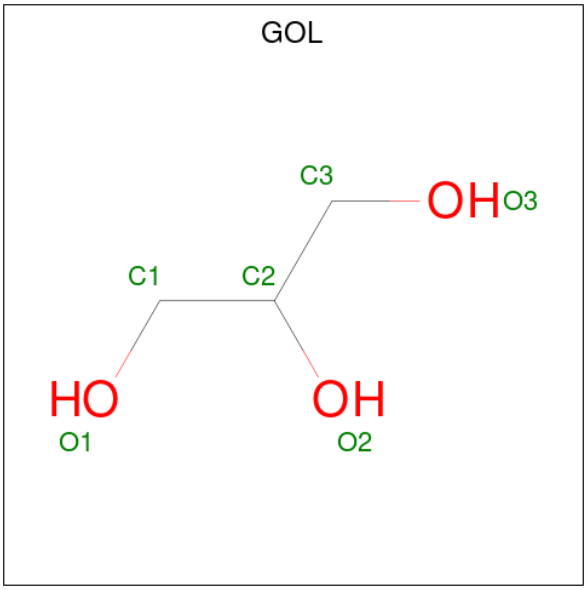
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	SSS	1	Total Fe S 8 4 4	0	0
3	SSS	1	Total Fe S 8 4 4	0	0
3	TTT	1	Total Fe S 8 4 4	0	0
3	TTT	1	Total Fe S 8 4 4	0	0

- Molecule 4 is FE3-S4 CLUSTER (CCD ID: 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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



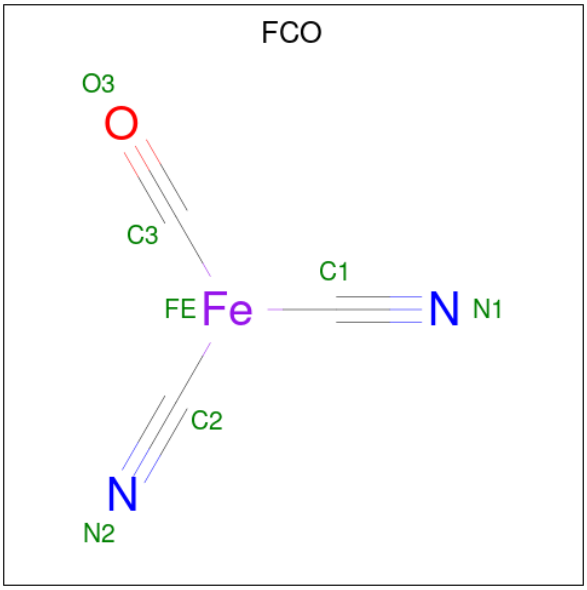
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	SSS	1	Total C O 6 3 3	0	0
5	SSS	1	Total C O 6 3 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	LLL	1	Total C O 6 3 3	0	0
5	LLL	1	Total C O 6 3 3	0	0
5	TTT	1	Total C O 6 3 3	0	0
5	MMM	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 (CCD ID: 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 (CCD ID: 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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	MMM	1	Total Ni 1 1	0	0

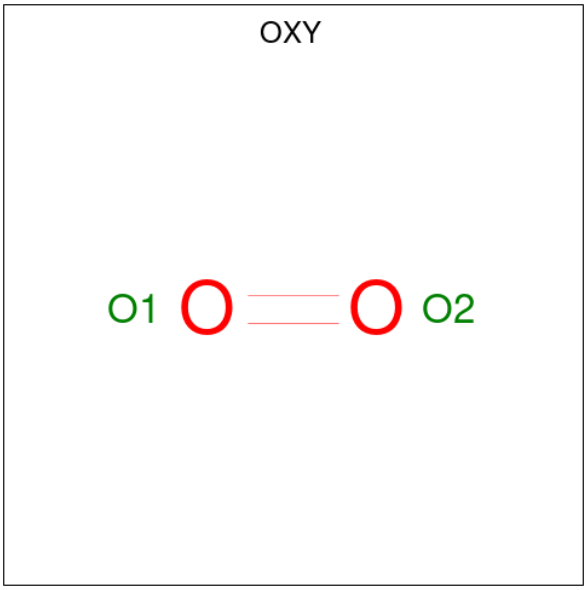
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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 CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 10 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O_2).



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

Continued on next page...

Continued from previous page...

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

- Molecule 11 is water.

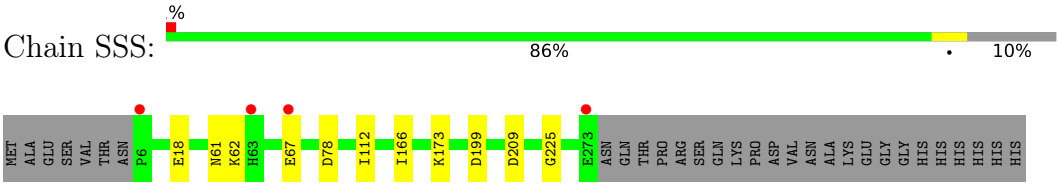
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	SSS	321	Total O 321 321	0	0
11	LLL	618	Total O 618 618	0	0
11	TTT	294	Total O 294 294	0	0
11	MMM	576	Total O 576 576	0	0

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.

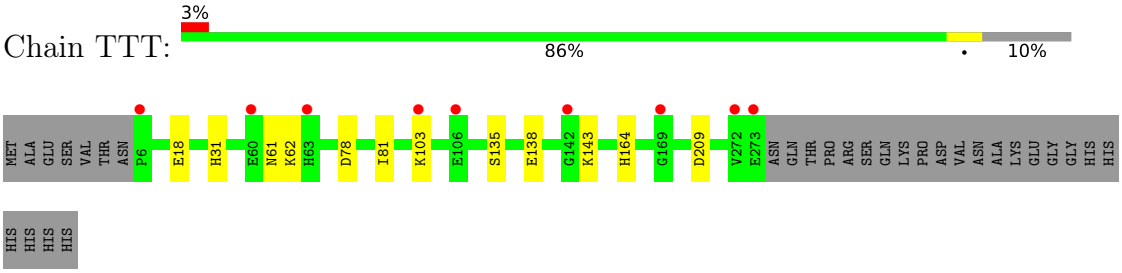
• Molecule 1: Hydrogenase-2 small chain

Chain SSS:



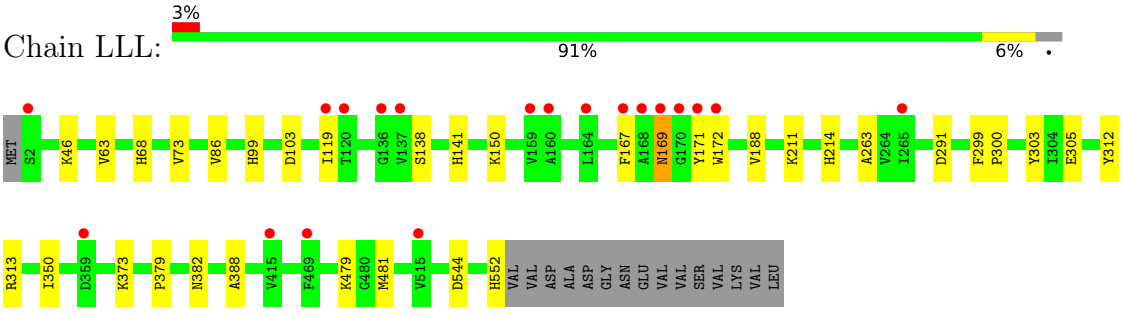
• Molecule 1: Hydrogenase-2 small chain

Chain TTT:



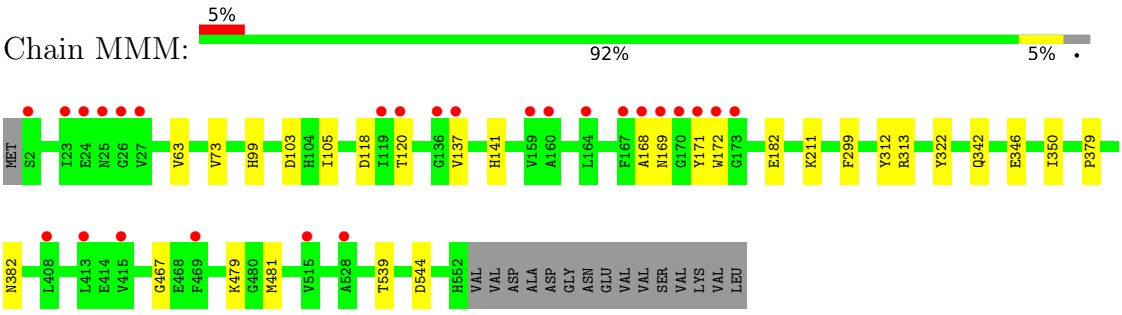
• Molecule 2: Hydrogenase-2 large chain

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	100.73Å 101.33Å 170.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.13 – 1.30 87.13 – 1.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (87.13-1.30) 99.5 (87.13-1.30)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 1.30Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.147 , 0.163 0.148 , 0.164	Depositor DCC
R_{free} test set	20792 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å^2)	9.7	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.007 for k,h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	14669	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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, OXY, CL, SF4, FCO, MG, NI, 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	1.44	5/2131 (0.2%)	1.17	2/2900 (0.1%)
1	TTT	1.44	4/2114 (0.2%)	1.22	4/2877 (0.1%)
2	LLL	1.34	9/4438 (0.2%)	1.20	12/6047 (0.2%)
2	MMM	1.35	5/4441 (0.1%)	1.21	11/6052 (0.2%)
All	All	1.38	23/13124 (0.2%)	1.20	29/17876 (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	1

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	TTT	138	GLU	C-O	7.18	1.32	1.24
1	SSS	225	GLY	N-CA	6.52	1.50	1.45
2	LLL	544	ASP	C-O	6.43	1.26	1.23
2	LLL	544	ASP	N-CA	6.21	1.50	1.46
2	LLL	263	ALA	C-O	6.15	1.31	1.24

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	MMM	171	TYR	CB-CA-C	7.23	121.19	111.14
2	LLL	382	ASN	N-CA-CB	-6.77	100.19	110.01
2	MMM	299	PHE	CA-CB-CG	6.55	120.36	113.80
2	LLL	544	ASP	CA-CB-CG	6.53	119.13	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	LLL	167	PHE	CB-CA-C	6.50	121.70	110.01

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	LLL	171	TYR	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	2064	0	1990	8	0
1	TTT	2050	0	1981	4	0
2	LLL	4313	0	4267	16	0
2	MMM	4319	0	4270	8	0
3	SSS	16	0	0	1	0
3	TTT	16	0	0	0	0
4	SSS	7	0	0	0	0
4	TTT	7	0	0	0	0
5	LLL	12	0	16	0	0
5	MMM	12	0	16	0	0
5	SSS	12	0	16	0	0
5	TTT	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	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
11	LLL	618	0	0	8	0
11	MMM	576	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	SSS	321	0	0	5	0
11	TTT	294	0	0	2	0
All	All	14669	0	12564	32	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 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)
2:MMM:379:PRO:HB2	11:MMM:907:HOH:O	1.71	0.89
1:TTT:61:ASN:HD21	2:MMM:169:ASN:HB3	1.39	0.86
2:LLL:379:PRO:HB2	11:LLL:938:HOH:O	1.83	0.76
1:TTT:62:LYS:HE2	11:TTT:829:HOH:O	1.89	0.72
2:LLL:305[A]:GLU:CD	2:LLL:373:LYS:NZ	2.48	0.71

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	SSS	270/298 (91%)	261 (97%)	9 (3%)	0	100	100
1	TTT	268/298 (90%)	260 (97%)	8 (3%)	0	100	100
2	LLL	555/567 (98%)	531 (96%)	23 (4%)	1 (0%)	43	17
2	MMM	555/567 (98%)	531 (96%)	23 (4%)	1 (0%)	43	17
All	All	1648/1730 (95%)	1583 (96%)	63 (4%)	2 (0%)	48	18

All (2) Ramachandran outliers are listed below:

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

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	215/239 (90%)	214 (100%)	1 (0%)	81	60
2	LLL	471/479 (98%)	467 (99%)	4 (1%)	73	45
2	MMM	471/479 (98%)	468 (99%)	3 (1%)	78	54
All	All	1374/1436 (96%)	1366 (99%)	8 (1%)	78	54

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

Mol	Chain	Res	Type
2	MMM	479	LYS
2	MMM	312	TYR
1	TTT	143	LYS
2	LLL	479	LYS
2	MMM	141	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 25 ligands modelled in this entry, 8 are monoatomic - leaving 17 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	MMM	601	-	5,5,5	0.35	0	5,5,5	0.76	0
10	OXY	LLL	608	7	1,1,1	0.19	0	-		
3	SF4	TTT	604	1	0,12,12	-	-	-		
5	GOL	MMM	605	-	5,5,5	0.29	0	5,5,5	1.01	0
6	FCO	MMM	602	2	1,6,6	0.01	0	-		
5	GOL	SSS	404	-	5,5,5	0.41	0	5,5,5	0.81	0
4	F3S	TTT	603	1	0,9,9	-	-	-		
6	FCO	LLL	602	2	1,6,6	2.75	1 (100%)	-		
5	GOL	LLL	601	-	5,5,5	0.29	0	5,5,5	0.49	0
5	GOL	TTT	601	-	5,5,5	0.26	0	5,5,5	0.69	0
5	GOL	LLL	605	-	5,5,5	0.15	0	5,5,5	0.32	0
5	GOL	SSS	405	-	5,5,5	0.25	0	5,5,5	0.39	0
3	SF4	TTT	602	1	0,12,12	-	-	-		
4	F3S	SSS	402	1	0,9,9	-	-	-		
3	SF4	SSS	401	1	0,12,12	-	-	-		
10	OXY	MMM	607	7	1,1,1	0.14	0	-		
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	MMM	601	-	-	0/4/4/4	-
3	SF4	TTT	604	1	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	MMM	605	-	-	3/4/4/4	-
5	GOL	SSS	404	-	-	1/4/4/4	-
4	F3S	TTT	603	1	-	-	0/3/3/3
5	GOL	LLL	601	-	-	2/4/4/4	-
5	GOL	TTT	601	-	-	2/4/4/4	-
5	GOL	LLL	605	-	-	0/4/4/4	-
5	GOL	SSS	405	-	-	0/4/4/4	-
3	SF4	TTT	602	1	-	-	0/6/5/5
4	F3S	SSS	402	1	-	-	0/3/3/3
3	SF4	SSS	401	1	-	-	0/6/5/5
3	SF4	SSS	403	1	-	-	0/6/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	LLL	602	FCO	O3-C3	-2.75	1.12	1.16

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	LLL	601	GOL	C1-C2-C3-O3
5	TTT	601	GOL	C1-C2-C3-O3
5	MMM	605	GOL	O1-C1-C2-C3
5	MMM	605	GOL	O1-C1-C2-O2
5	LLL	601	GOL	O2-C2-C3-O3

There are no ring outliers.

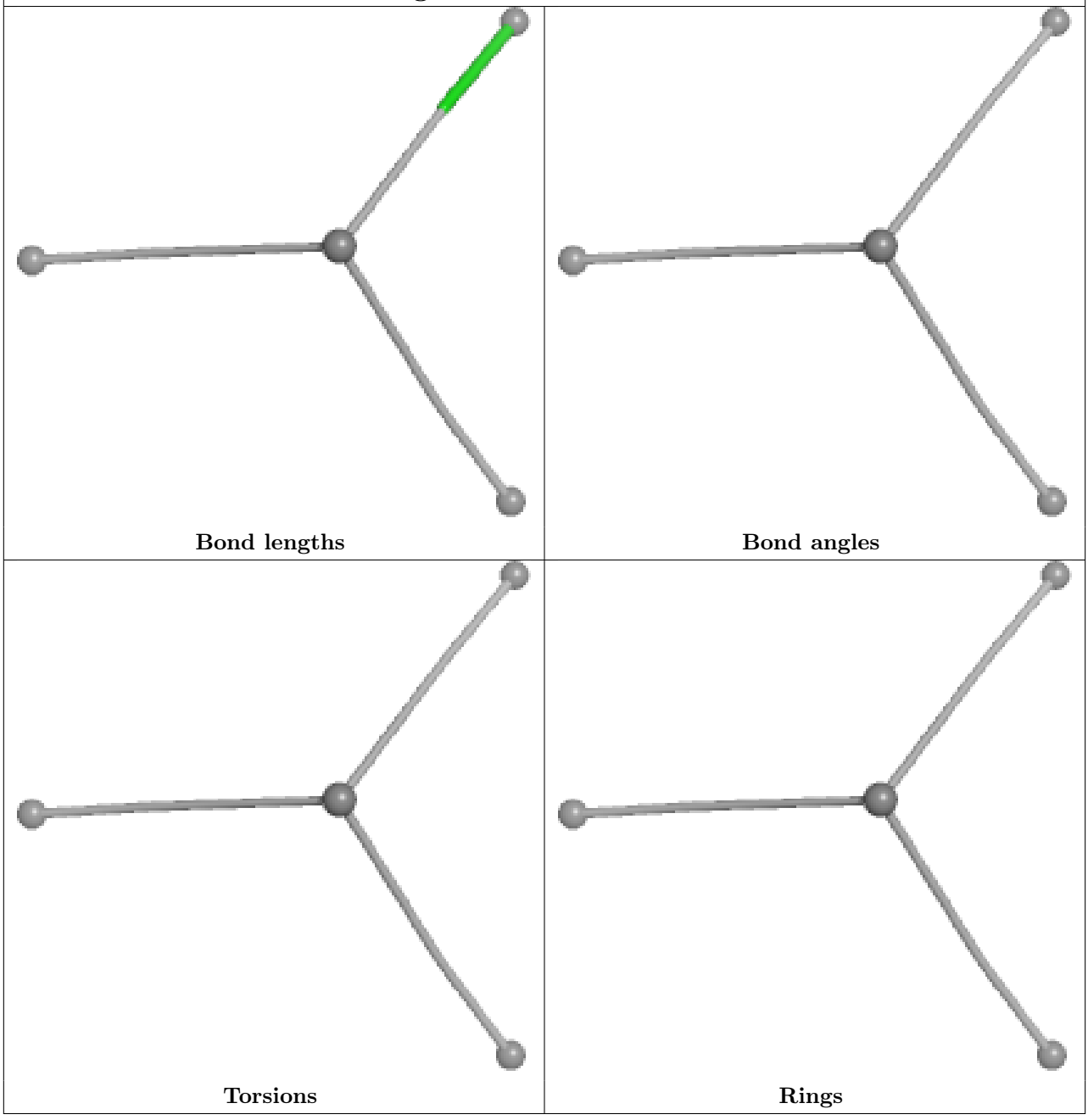
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	SSS	403	SF4	1	0

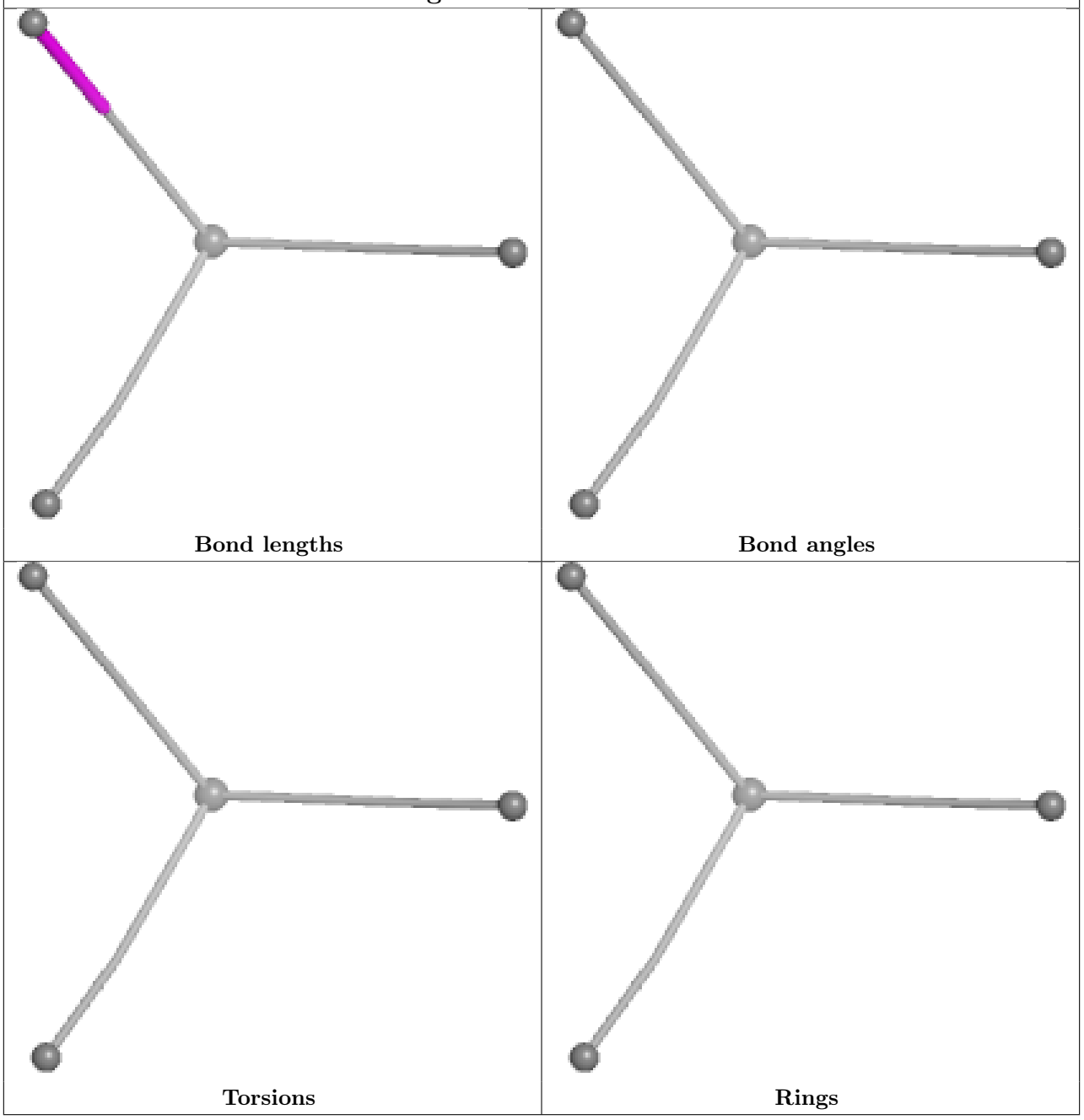
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 602



Ligand FCO LLL 602



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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%)	-0.09	4 (1%)	72	76	4, 10, 23, 38	4 (1%)
1	TTT	268/298 (89%)	0.16	9 (3%)	48	54	7, 12, 26, 51	2 (0%)
2	LLL	551/567 (97%)	-0.07	19 (3%)	48	54	6, 10, 23, 40	6 (1%)
2	MMM	551/567 (97%)	0.17	26 (4%)	36	42	5, 12, 27, 64	6 (1%)
All	All	1638/1730 (94%)	0.04	58 (3%)	47	52	4, 11, 25, 64	18 (1%)

The worst 5 of 58 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	MMM	172	TRP	9.9
2	LLL	172	TRP	7.2
1	TTT	6	PRO	6.1
2	LLL	171	TYR	5.5
2	MMM	171	TYR	4.8

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 oligosaccharides in this entry.

6.4 Ligands

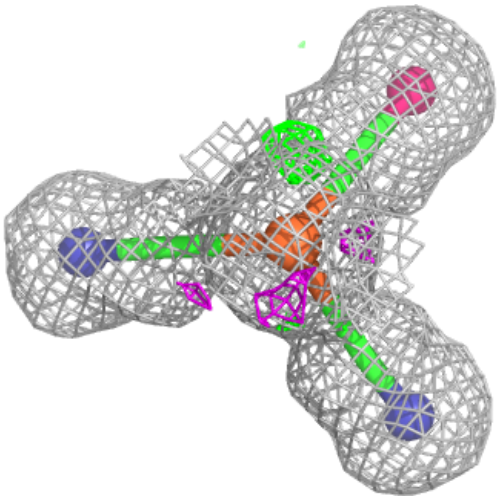
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

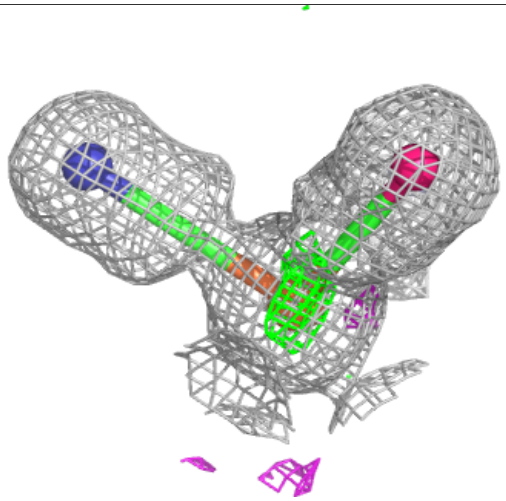
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	MMM	605	6/6	0.82	0.16	31,33,34,37	0
5	GOL	TTT	601	6/6	0.83	0.16	26,31,32,34	0
5	GOL	LLL	601	6/6	0.84	0.15	18,28,33,44	0
5	GOL	LLL	605	6/6	0.84	0.14	25,29,33,36	0
5	GOL	SSS	404	6/6	0.86	0.14	20,27,29,30	0
5	GOL	SSS	405	6/6	0.89	0.11	23,28,28,33	0
5	GOL	MMM	601	6/6	0.91	0.11	18,23,29,37	0
8	MG	LLL	606	1/1	0.92	0.24	29,29,29,29	0
8	MG	TTT	605	1/1	0.98	0.19	18,18,18,18	0
9	CL	LLL	607	1/1	0.98	0.05	16,16,16,16	0
10	OXY	LLL	608	2/2	0.98	0.16	12,12,12,14	2
9	CL	MMM	606	1/1	0.99	0.04	15,15,15,15	0
8	MG	MMM	604	1/1	0.99	0.02	6,6,6,6	0
10	OXY	MMM	607	2/2	0.99	0.12	14,14,14,17	2
6	FCO	MMM	602	7/7	1.00	0.02	7,7,7,8	0
7	NI	LLL	603	1/1	1.00	0.01	7,7,7,7	0
7	NI	MMM	603	1/1	1.00	0.02	8,8,8,8	0
8	MG	LLL	604	1/1	1.00	0.02	5,5,5,5	0
3	SF4	SSS	403	8/8	1.00	0.01	6,6,6,7	0
3	SF4	TTT	602	8/8	1.00	0.02	7,8,8,9	0
3	SF4	TTT	604	8/8	1.00	0.02	7,7,8,8	0
4	F3S	SSS	402	7/7	1.00	0.01	6,7,7,7	0
4	F3S	TTT	603	7/7	1.00	0.01	7,7,7,7	0
3	SF4	SSS	401	8/8	1.00	0.02	8,8,8,8	0
6	FCO	LLL	602	7/7	1.00	0.02	6,6,7,8	0

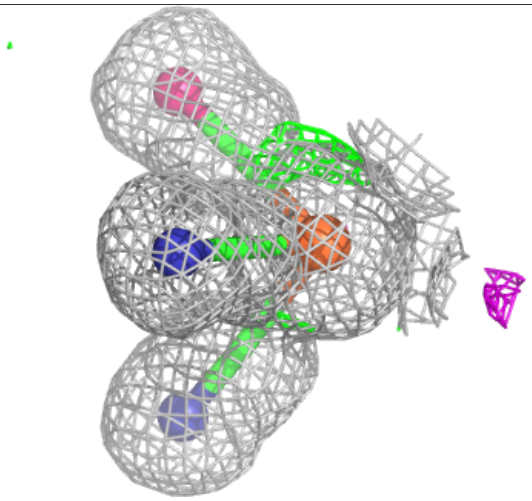
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FCO 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)

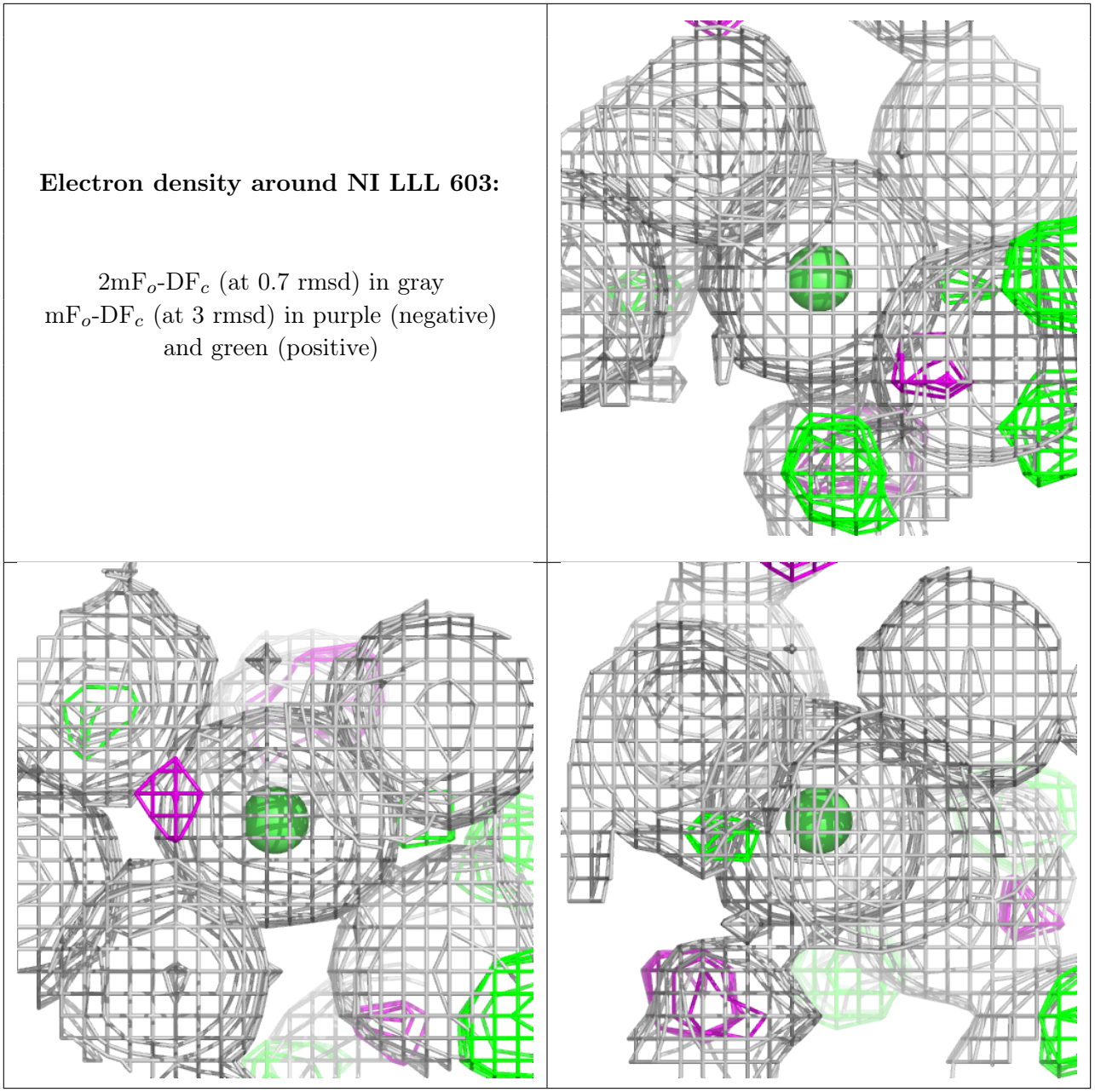






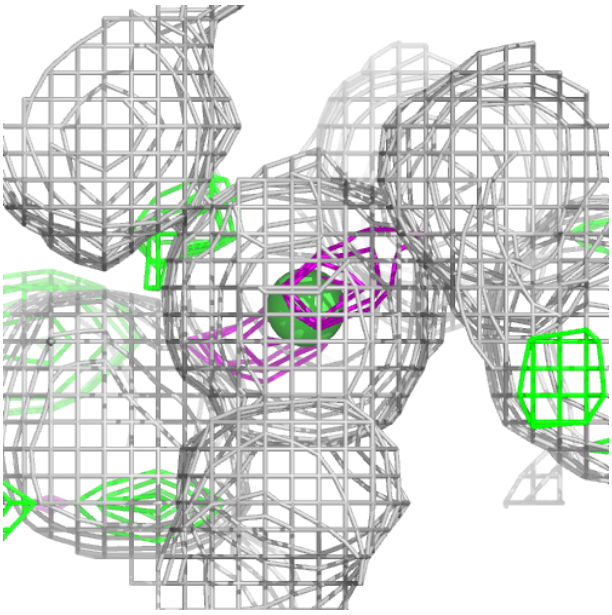
Electron density around NI LLL 603:

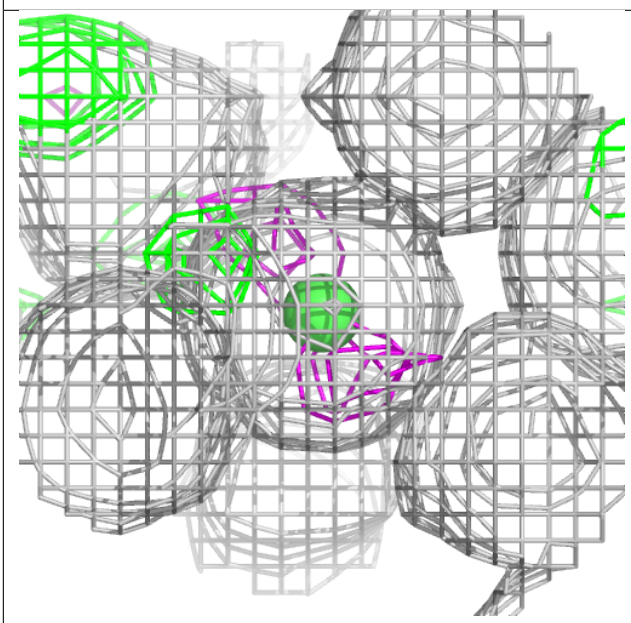
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

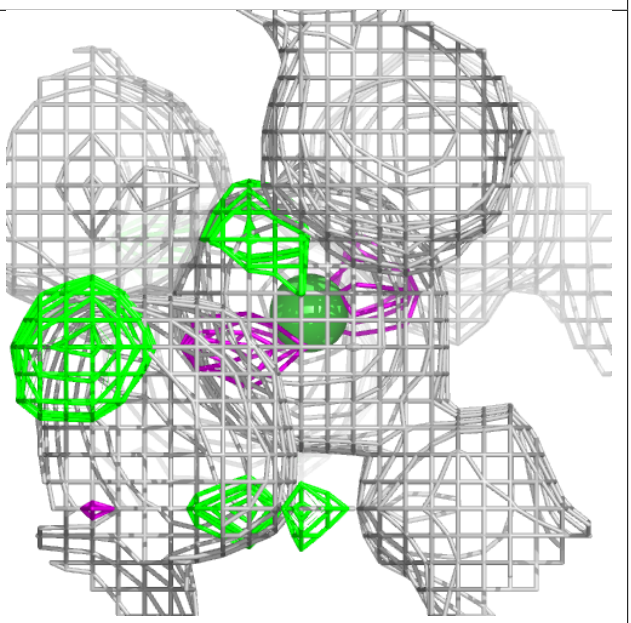


Electron density around NI MMM 603:

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

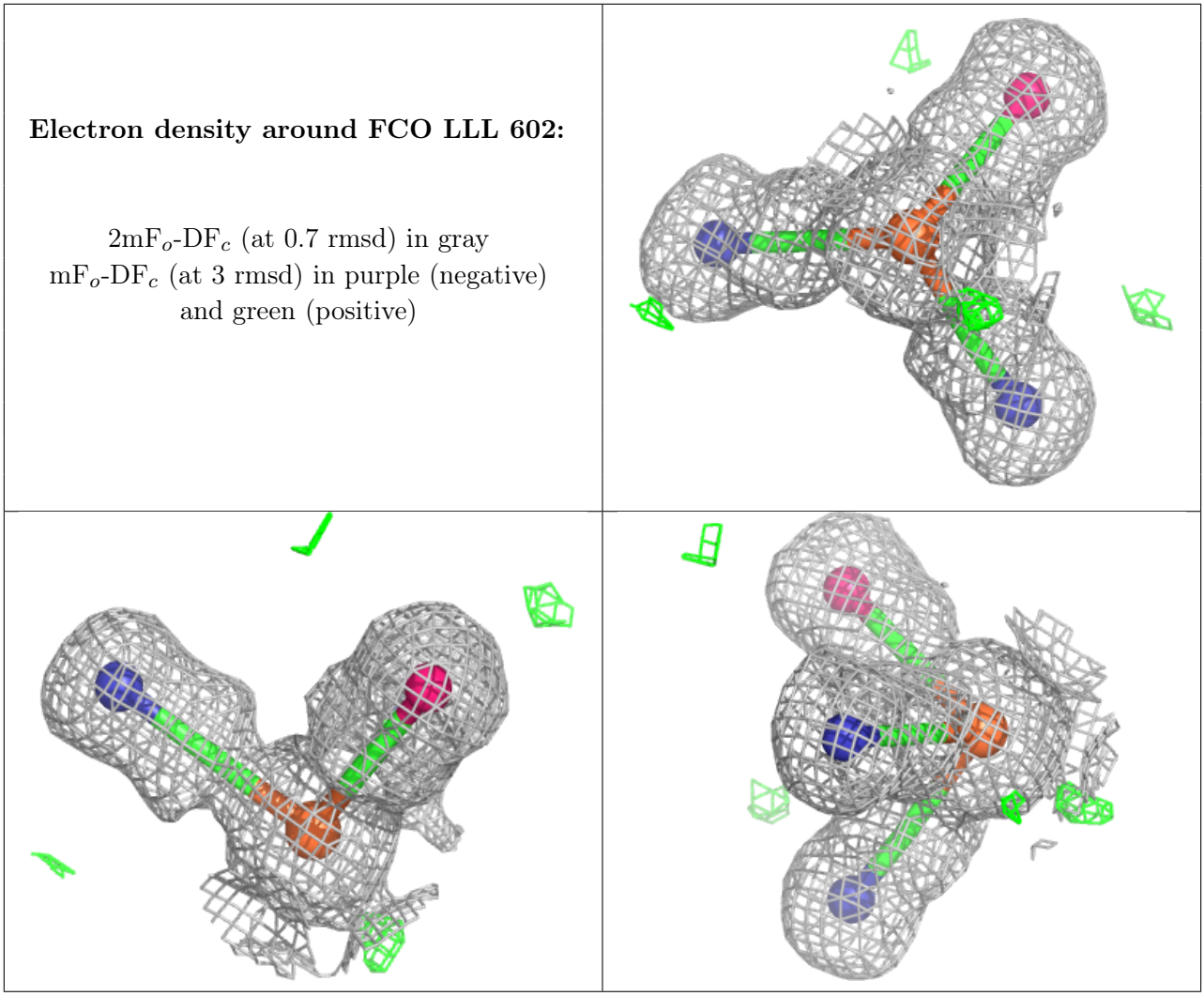






Electron density around FCO LLL 602:

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



6.5 Other polymers

There are no such residues in this entry.