



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 02:25 PM UTC

PDB ID : 6SZK / pdb_00006szk
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)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

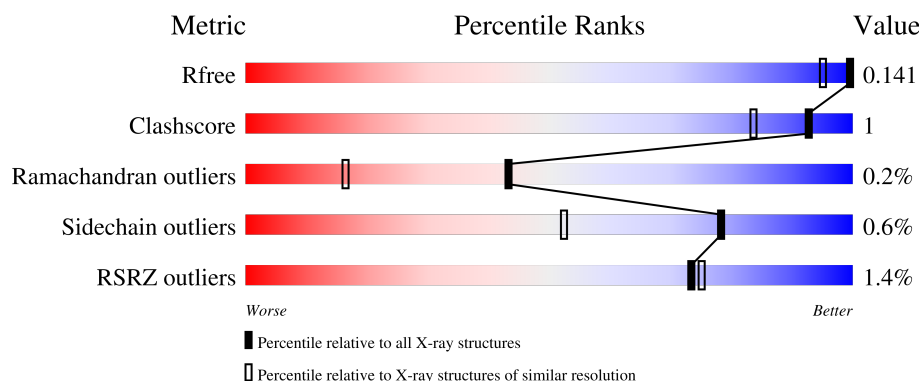
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.20 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1216 (1.20-1.20)
Clashscore	190562	1265 (1.20-1.20)
Ramachandran outliers	187476	1226 (1.20-1.20)
Sidechain outliers	187428	1226 (1.20-1.20)
RSRZ outliers	180081	1214 (1.20-1.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	SSS	298	 84% 6% 10%
1	TTT	298	 2% 81% 8% 10%
2	LLL	567	 2% 91% 5% ••
2	MMM	567	 2% 91% 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

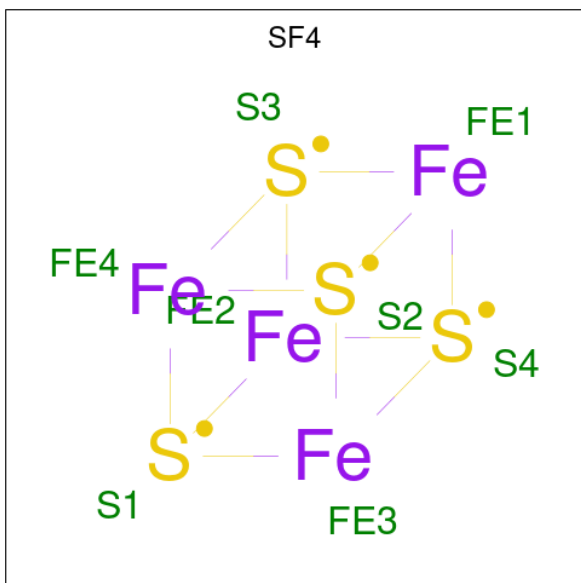
- Molecule 2 is a protein called Hydrogenase-2 large chain.

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:

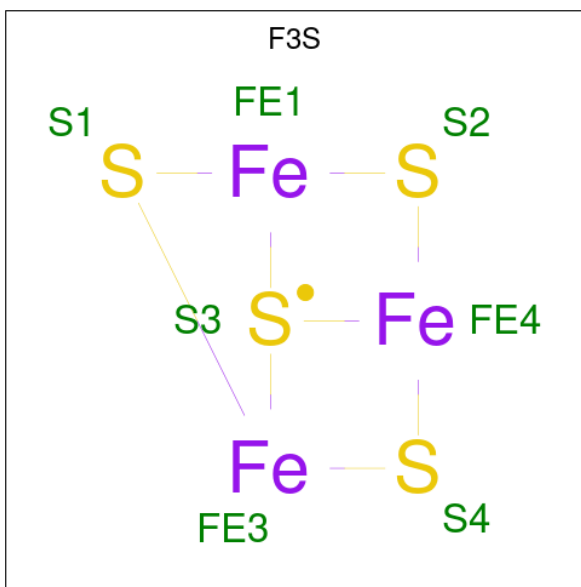
Chain	Residue	Modelled	Actual	Comment	Reference
LLL	479	LYS	ARG	engineered mutation	UNP V0V766
MMM	479	LYS	ARG	engineered mutation	UNP V0V766

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



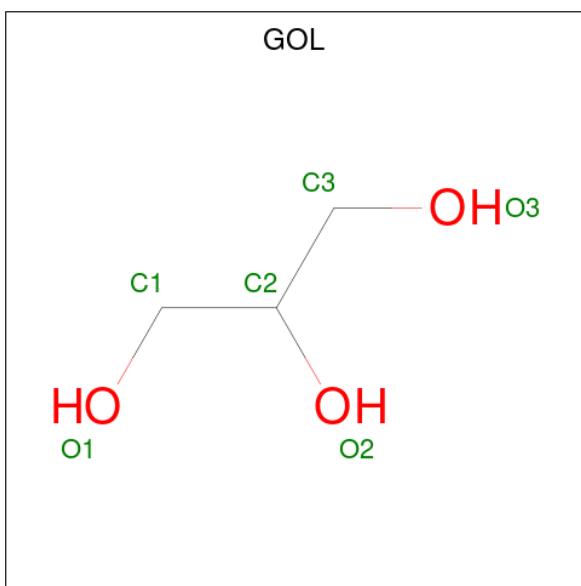
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	SSS	1	Total	Fe	S	0	0
			8	4	4		
3	SSS	1	Total	Fe	S	0	0
			8	4	4		
3	TTT	1	Total	Fe	S	0	0
			8	4	4		
3	TTT	1	Total	Fe	S	0	0
			8	4	4		

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



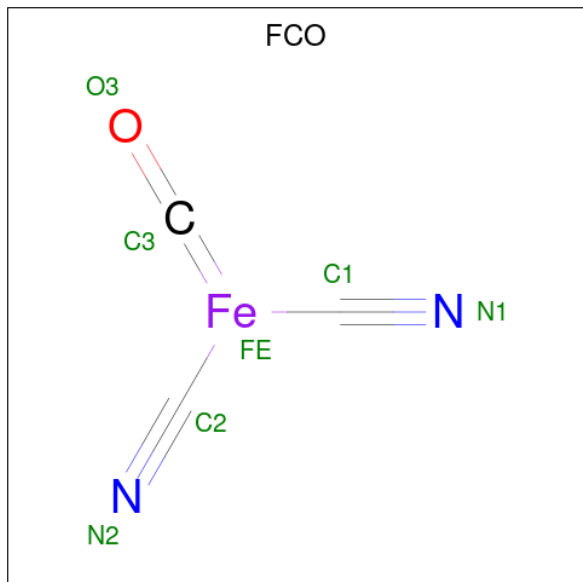
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	SSS	1	Total	Fe	S	0	0
			7	3	4		
4	TTT	1	Total	Fe	S	0	0
			7	3	4		

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



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

- Molecule 6 is CARBONMONOXIDE-(DICYANO) IRON (CCD ID: FCO) (formula: $\text{C}_3\text{FeN}_2\text{O}$) (labeled as "Ligand of Interest" by depositor).



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

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

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

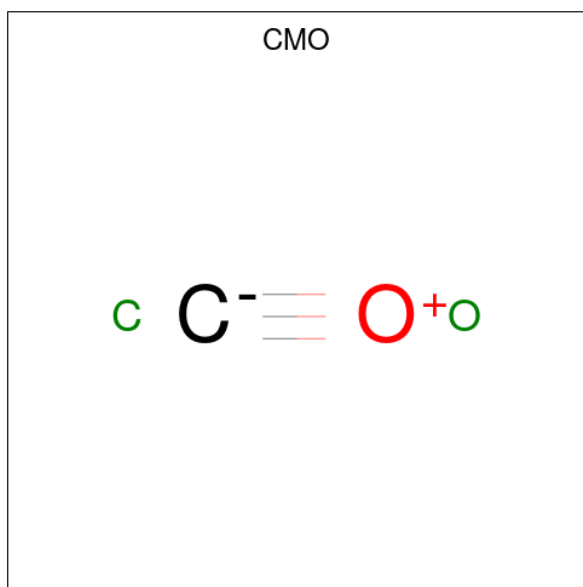
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- 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

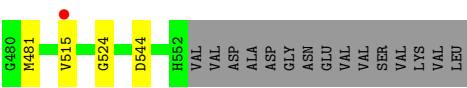
- Molecule 10 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO).



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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	SSS	256	Total O 256 256	0	0
11	LLL	496	Total O 496 496	0	0
11	TTT	234	Total O 234 234	0	0
11	MMM	467	Total O 467 467	0	0



4 Data and refinement statistics

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 86.70 – 1.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (86.70-1.20) 99.9 (86.70-1.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 1.20Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.121 , 0.141 0.121 , 0.141	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 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	SSS	1.55	11/2122 (0.5%)	1.17	3/2888 (0.1%)
1	TTT	1.64	17/2123 (0.8%)	1.25	11/2889 (0.4%)
2	LLL	1.47	10/4468 (0.2%)	1.18	13/6089 (0.2%)
2	MMM	1.50	11/4447 (0.2%)	1.20	9/6061 (0.1%)
All	All	1.52	49/13160 (0.4%)	1.20	36/17927 (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

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	TTT	83	LEU	C-O	11.85	1.39	1.24
1	TTT	60	GLU	CD-OE1	9.77	1.44	1.25
2	MMM	3	GLN	C-O	9.37	1.34	1.23
1	TTT	273	GLU	CD-OE1	8.54	1.41	1.25
1	SSS	191	HIS	CE1-NE2	7.83	1.40	1.32
1	TTT	6	PRO	N-CA	7.82	1.58	1.47
1	TTT	263	HIS	CE1-NE2	7.81	1.40	1.32
2	LLL	513	ASP	CG-OD2	-7.68	1.10	1.25
2	MMM	23	ILE	C-O	7.61	1.32	1.24
1	SSS	273	GLU	CD-OE1	7.37	1.39	1.25
2	LLL	107	HIS	CE1-NE2	7.27	1.39	1.32
2	LLL	174	HIS	N-CA	6.73	1.53	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	TTT	191	HIS	CE1-NE2	6.69	1.39	1.32
1	TTT	51	SER	CA-CB	6.54	1.63	1.53
1	TTT	16	ALA	CA-C	6.47	1.55	1.52
1	SSS	51	SER	CA-CB	6.37	1.63	1.53
1	SSS	127	GLY	C-N	-6.36	1.27	1.34
2	LLL	167	PHE	CA-C	6.30	1.61	1.52
1	SSS	220	HIS	CE1-NE2	6.21	1.38	1.32
2	MMM	3	GLN	CA-C	6.11	1.59	1.52
1	TTT	102	ARG	C-O	5.97	1.31	1.24
1	TTT	267	HIS	CG-ND1	5.94	1.44	1.38
2	MMM	107	HIS	CE1-NE2	5.93	1.38	1.32
2	MMM	28	VAL	C-O	5.92	1.29	1.24
1	TTT	6	PRO	N-CD	5.86	1.55	1.47
2	LLL	168	ALA	N-CA	5.83	1.53	1.45
1	SSS	212	HIS	CE1-NE2	5.78	1.38	1.32
2	MMM	134	LEU	C-O	5.76	1.31	1.24
2	LLL	515	VAL	C-O	5.70	1.30	1.24
2	LLL	424	ARG	NE-CZ	5.58	1.39	1.33
2	MMM	2	SER	N-CA	5.57	1.56	1.46
1	TTT	12	ILE	N-CA	5.49	1.52	1.46
1	TTT	47	HIS	CE1-NE2	5.45	1.38	1.32
2	MMM	469	PHE	N-CA	5.40	1.52	1.46
1	SSS	6	PRO	N-CA	5.38	1.55	1.47
2	MMM	420	SER	C-O	5.34	1.29	1.23
2	MMM	438	ILE	C-O	5.28	1.30	1.24
1	TTT	197	HIS	CE1-NE2	5.26	1.37	1.32
1	SSS	217	CYS	N-CA	5.22	1.52	1.46
1	SSS	56	HIS	CD2-NE2	5.21	1.43	1.37
2	LLL	6	THR	C-O	5.20	1.30	1.23
1	SSS	59	GLU	CD-OE2	-5.10	1.15	1.25
2	LLL	117	VAL	C-O	5.07	1.29	1.24
1	TTT	101	ILE	C-O	5.06	1.29	1.24
2	MMM	99	HIS	CE1-NE2	5.04	1.37	1.32
1	TTT	31	HIS	ND1-CE1	5.04	1.37	1.32
1	SSS	179	ARG	C-N	5.02	1.39	1.33
2	LLL	141	HIS	CD2-NE2	5.02	1.43	1.37
1	TTT	56	HIS	CD2-NE2	5.00	1.43	1.37

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	LLL	2	SER	N-CA-CB	-7.75	97.33	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	MMM	382	ASN	N-CA-CB	-7.45	99.21	110.01
2	LLL	382	ASN	N-CA-CB	-7.43	99.24	110.01
1	TTT	20	THR	CB-CA-C	7.33	117.08	109.83
1	TTT	6	PRO	CA-N-CD	-7.00	102.21	112.00
2	LLL	515	VAL	N-CA-CB	-6.79	102.84	110.99
2	MMM	544	ASP	CA-CB-CG	6.79	119.39	112.60
1	SSS	20	THR	CB-CA-C	6.79	116.55	109.83
1	SSS	18	GLU	CB-CG-CD	6.78	124.12	112.60
2	MMM	103	ASP	CA-CB-CG	6.57	119.17	112.60
2	MMM	515	VAL	N-CA-CB	-6.44	101.67	110.56
2	MMM	172	TRP	CB-CA-C	6.41	119.88	110.26
1	TTT	6	PRO	N-CA-C	-6.39	96.11	112.10
2	LLL	299	PHE	CA-CB-CG	6.38	120.18	113.80
2	LLL	544	ASP	CA-CB-CG	6.32	118.92	112.60
1	TTT	176	ASP	CA-CB-CG	6.29	118.89	112.60
2	MMM	382	ASN	OD1-CG-ND2	6.07	128.67	122.60
2	LLL	167	PHE	CB-CA-C	6.03	120.86	110.01
2	LLL	169	ASN	CA-CB-CG	5.97	118.57	112.60
1	TTT	62	LYS	CG-CD-CE	5.96	125.01	111.30
2	LLL	99	HIS	CA-CB-CG	-5.87	107.93	113.80
2	LLL	382	ASN	OD1-CG-ND2	5.86	128.46	122.60
2	LLL	468	GLU	CB-CG-CD	5.84	122.54	112.60
2	LLL	103	ASP	CA-CB-CG	5.67	118.27	112.60
1	TTT	243	VAL	N-CA-C	5.59	114.78	106.85
2	MMM	102	HIS	CE1-NE2-CD2	-5.58	103.42	109.00
1	TTT	95	GLU	CB-CG-CD	5.57	122.08	112.60
1	TTT	60	GLU	CB-CG-CD	5.56	122.05	112.60
1	TTT	193	GLU	CB-CG-CD	5.33	121.67	112.60
1	TTT	199	ASP	CA-CB-CG	5.33	117.93	112.60
2	LLL	168	ALA	O-C-N	5.26	128.79	122.79
2	LLL	135	LYS	CA-C-O	-5.12	114.81	120.70
2	MMM	469	PHE	CA-CB-CG	-5.09	108.71	113.80
1	SSS	78	ASP	CA-CB-CG	5.08	117.68	112.60
2	MMM	169	ASN	CA-CB-CG	5.04	117.64	112.60
1	TTT	267	HIS	CG-CD2-NE2	5.00	112.20	107.20

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
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	7	0
1	TTT	2056	0	1987	5	0
2	LLL	4337	0	4285	21	0
2	MMM	4319	0	4268	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	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
11	LLL	496	0	0	10	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	37	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.

All (37) 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:103:ASP:CG	11:LLL:703:HOH:O	2.16	0.87
2:MMM:379:PRO:HB2	11:MMM:931:HOH:O	1.74	0.87
2:LLL:2:SER:OG	2:LLL:22[B]:GLU:OE1	1.96	0.82
2:LLL:379:PRO:HB2	11:LLL:884:HOH:O	1.79	0.81
2:LLL:305[A]:GLU:CD	2:LLL:373:LYS:HZ2	1.92	0.78
2:LLL:305[A]:GLU:CD	2:LLL:373:LYS:NZ	2.43	0.77
1:SSS:61[A]:ASN:OD1	2:LLL:169:ASN:HB3	1.87	0.73
1:SSS:61[A]:ASN:OD1	2:LLL:169:ASN:CB	2.40	0.69
1:TTT:62:LYS:HE2	11:TTT:638:HOH:O	1.97	0.65
2:LLL:103:ASP:OD2	11:LLL:703:HOH:O	2.13	0.64
1:SSS:61[A]:ASN:HD21	2:LLL:169:ASN:CG	2.06	0.63
1:SSS:61[A]:ASN:ND2	2:LLL:169:ASN:OD1	2.27	0.63
2:MMM:481:MET:HE3	11:MMM:740:HOH:O	2.03	0.57
2:LLL:144:SER:HB3	11:LLL:814:HOH:O	2.05	0.57
1:SSS:62:LYS:HE2	11:SSS:505:HOH:O	2.07	0.55
2:MMM:437[A]:ASP:CG	11:MMM:730:HOH:O	2.49	0.54
2:LLL:103:ASP:CB	11:LLL:703:HOH:O	2.53	0.54
2:LLL:481:MET:HE3	11:LLL:737:HOH:O	2.08	0.54
2:MMM:132:GLU:HG3	11:MMM:1090:HOH:O	2.08	0.53
1:TTT:103:LYS:CD	11:TTT:682:HOH:O	2.57	0.53
1:TTT:103:LYS:HD3	11:TTT:682:HOH:O	2.10	0.52
2:MMM:156:LYS:HE2	11:MMM:952:HOH:O	2.09	0.51
2:LLL:437[B]:ASP:CG	11:LLL:732:HOH:O	2.52	0.51
2:MMM:118:ASP:HA	2:MMM:172:TRP:CE3	2.48	0.49
2:LLL:303:TYR:CE2	2:LLL:305[B]:GLU:CG	2.98	0.47
1:TTT:61:ASN:OD1	2:MMM:169:ASN:HB3	2.16	0.46
2:LLL:172:TRP:CD1	11:LLL:715:HOH:O	2.68	0.46
2:MMM:27:VAL:HG13	2:MMM:524:GLY:C	2.42	0.44
2:LLL:337:LYS:HD2	11:LLL:1181:HOH:O	2.17	0.43
1:SSS:61[A]:ASN:OD1	2:LLL:169:ASN:HB2	2.17	0.42
1:SSS:88:ILE:C	1:SSS:88:ILE:HD12	2.44	0.42
2:LLL:135:LYS:HA	2:LLL:135:LYS:HD3	1.92	0.42
2:LLL:144:SER:CB	11:LLL:814:HOH:O	2.65	0.42
2:MMM:168:ALA:HB2	5:MMM:606:GOL:H31	2.02	0.42
1:TTT:88:ILE:C	1:TTT:88:ILE:HD12	2.45	0.41
2:LLL:305[A]:GLU:OE1	2:LLL:373:LYS:NZ	2.54	0.40
2:MMM:118:ASP:HA	2:MMM:172:TRP:CZ3	2.56	0.40

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%)	43	16
2	MMM	556/567 (98%)	533 (96%)	21 (4%)	2 (0%)	30	10
All	All	1653/1730 (96%)	1586 (96%)	64 (4%)	3 (0%)	43	16

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%)	73	44
2	MMM	472/479 (98%)	468 (99%)	4 (1%)	73	44
All	All	1379/1436 (96%)	1371 (99%)	8 (1%)	78	52

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	LLL	141	HIS
2	LLL	169	ASN
2	LLL	312	TYR
2	LLL	479	LYS
2	MMM	141	HIS
2	MMM	312	TYR
2	MMM	413	LEU
2	MMM	479	LYS

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 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	403	1	0,12,12	-	-	-		
3	SF4	SSS	401	1	0,12,12	-	-	-		
5	GOL	MMM	606	-	5,5,5	0.26	0	5,5,5	0.49	0
10	CMO	LLL	606	-	0,1,1	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CMO	MMM	605	-	0,1,1	-	-	-		
4	F3S	SSS	402	1	0,9,9	-	-	-		
3	SF4	TTT	401	1	0,12,12	-	-	-		
6	FCO	MMM	601	2	0,6,6	-	-	-		
4	F3S	TTT	402	1	0,9,9	-	-	-		
5	GOL	SSS	404	-	5,5,5	0.65	0	5,5,5	1.36	1 (20%)
3	SF4	SSS	403	1	0,12,12	-	-	-		
6	FCO	LLL	601	2	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
3	SF4	TTT	403	1	-	-	0/6/5/5
5	GOL	MMM	606	-	-	0/4/4/4	-
3	SF4	SSS	401	1	-	-	0/6/5/5
3	SF4	TTT	401	1	-	-	0/6/5/5
4	F3S	SSS	402	1	-	-	0/3/3/3
4	F3S	TTT	402	1	-	-	0/3/3/3
5	GOL	SSS	404	-	-	0/4/4/4	-
3	SF4	SSS	403	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(°)	Ideal(°)
5	SSS	404	GOL	O1-C1-C2	2.24	120.45	110.38

There are no chirality outliers.

There are no torsion outliers.

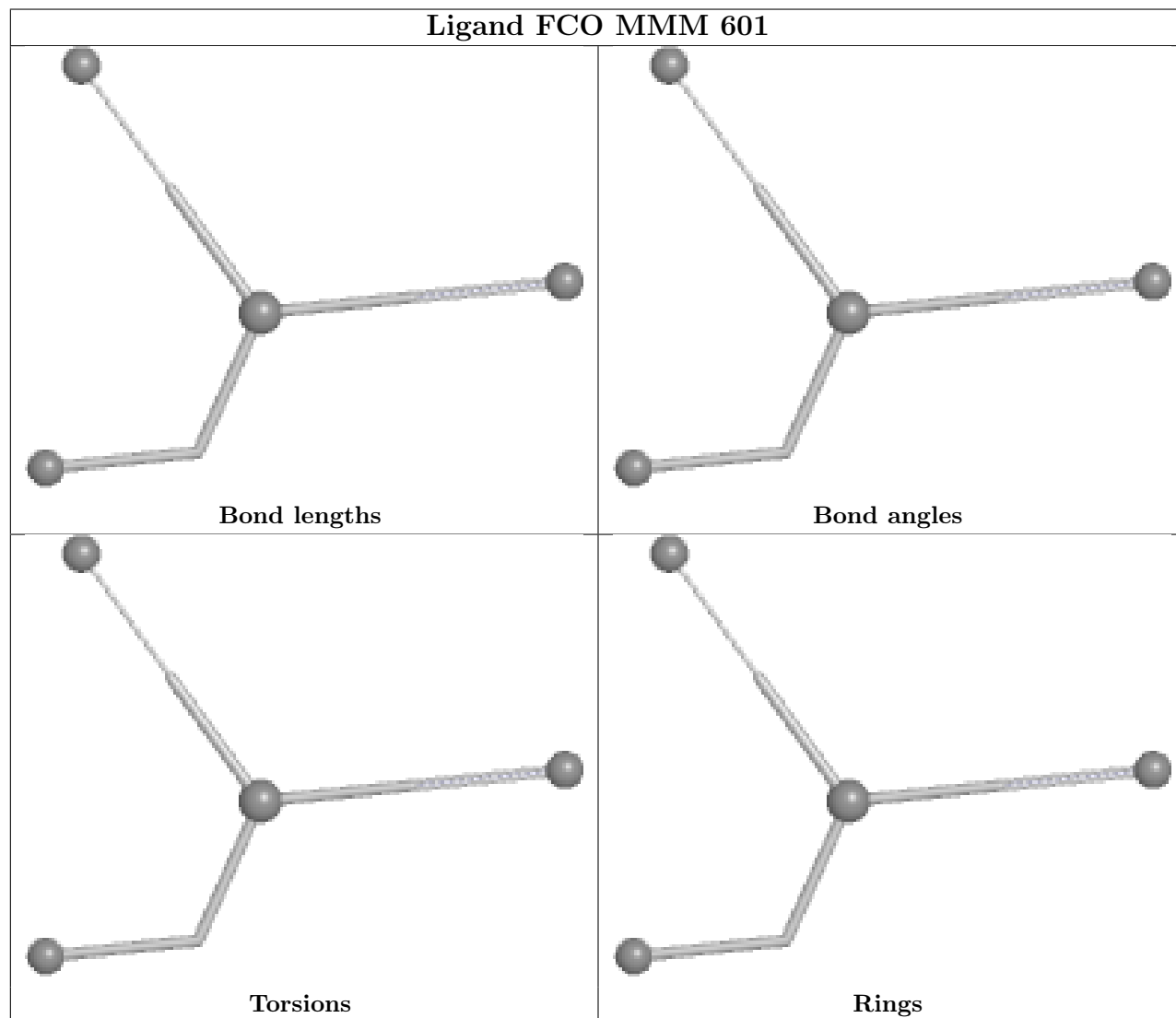
There are no ring outliers.

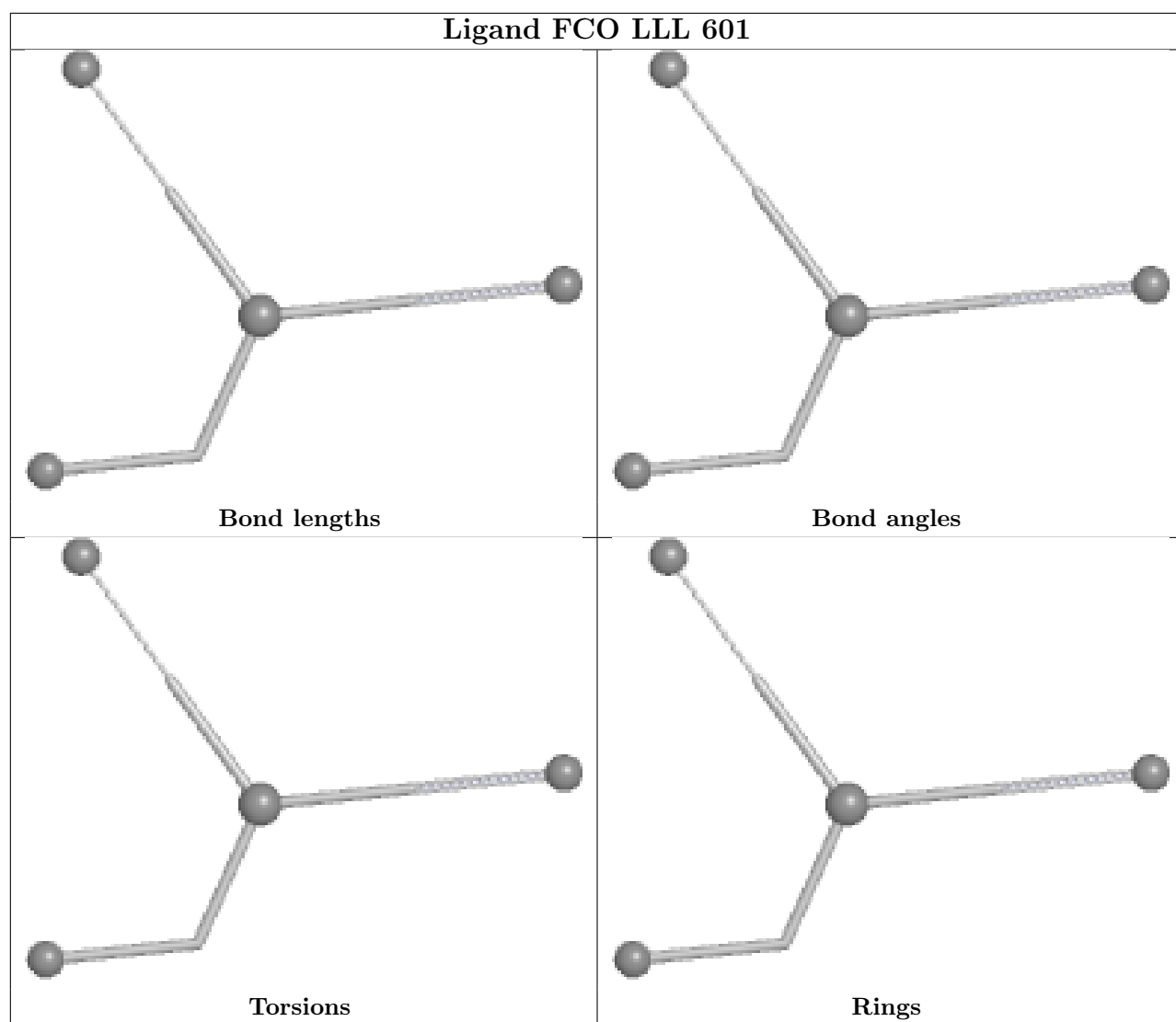
1 monomer is involved in 1 short contact:

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	-0.31	1 (0%) 88 91	8, 12, 26, 52	3 (1%)
1	TTT	268/298 (89%)	-0.16	3 (1%) 78 79	9, 14, 30, 83	3 (1%)
2	LLL	551/567 (97%)	-0.31	8 (1%) 72 73	7, 12, 27, 59	10 (1%)
2	MMM	551/567 (97%)	-0.20	11 (1%) 65 65	7, 14, 30, 68	7 (1%)
All	All	1638/1730 (94%)	-0.25	23 (1%) 73 75	7, 13, 29, 83	23 (1%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	TTT	6	PRO	8.4
2	MMM	172	TRP	7.5
2	LLL	172	TRP	7.4
1	SSS	6	PRO	5.4
2	MMM	170	GLY	4.5
2	LLL	168	ALA	3.9
2	LLL	171	TYR	3.8
2	MMM	171	TYR	3.7
2	LLL	136	GLY	3.4
2	LLL	167	PHE	3.0
2	LLL	169	ASN	3.0
2	MMM	27	VAL	2.9
2	MMM	169	ASN	2.8
2	MMM	2	SER	2.5
2	MMM	136	GLY	2.4
2	MMM	515	VAL	2.4
2	LLL	170	GLY	2.3
2	MMM	164	LEU	2.2
2	MMM	25	ASN	2.2
2	MMM	413	LEU	2.2
1	TTT	60	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	TTT	273	GLU	2.0
2	LLL	120	THR	2.0

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

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

6.3 Carbohydrates [i](#)

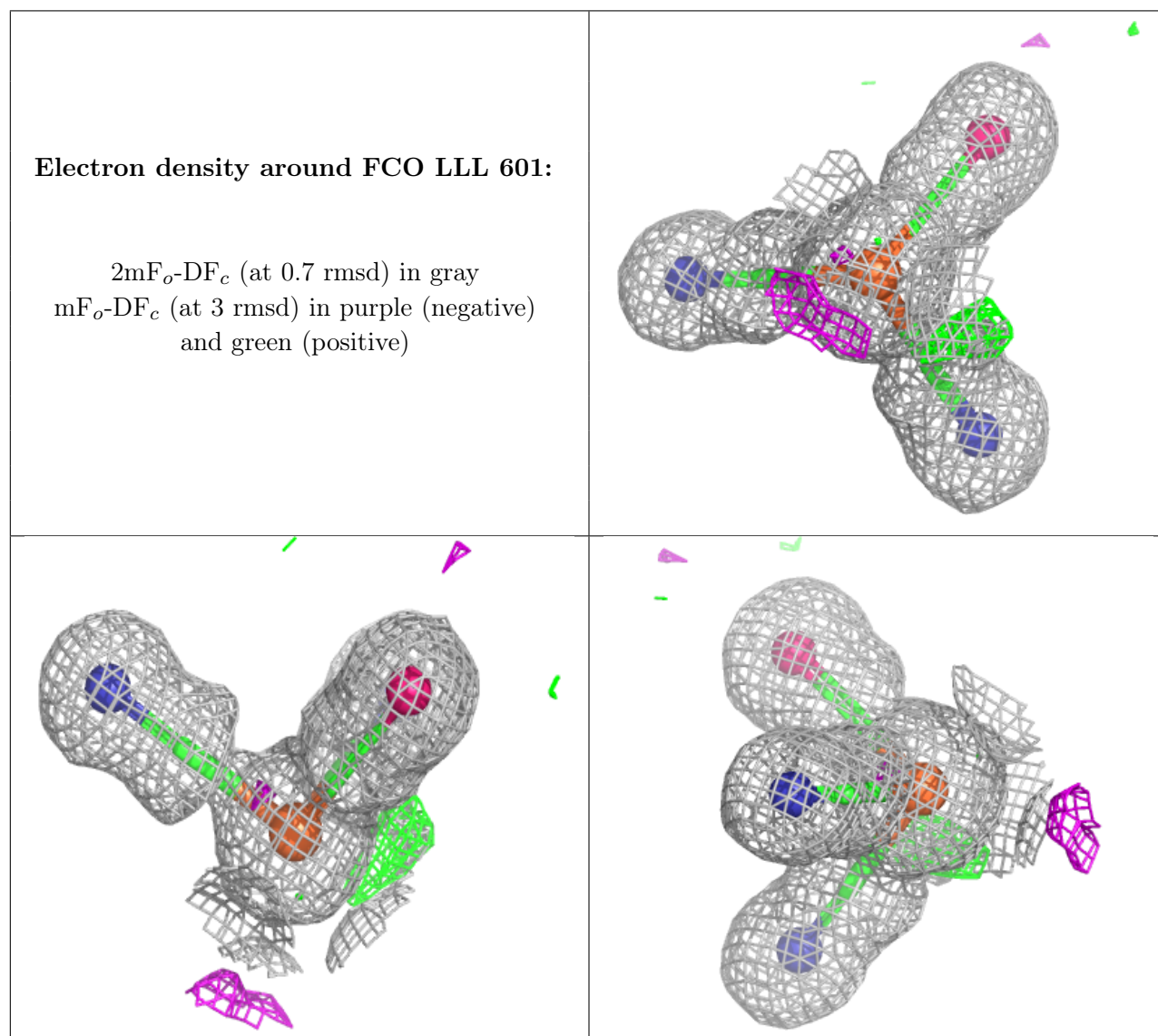
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

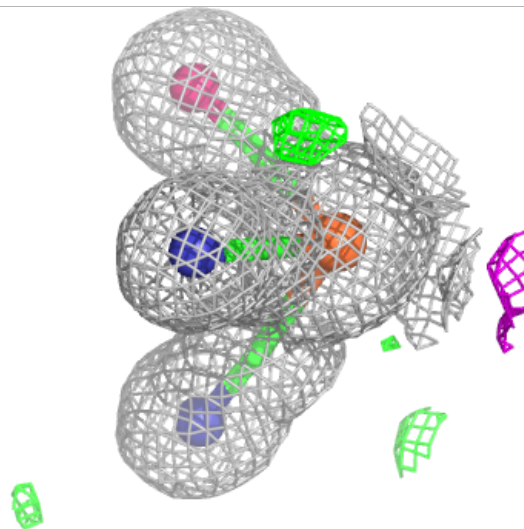
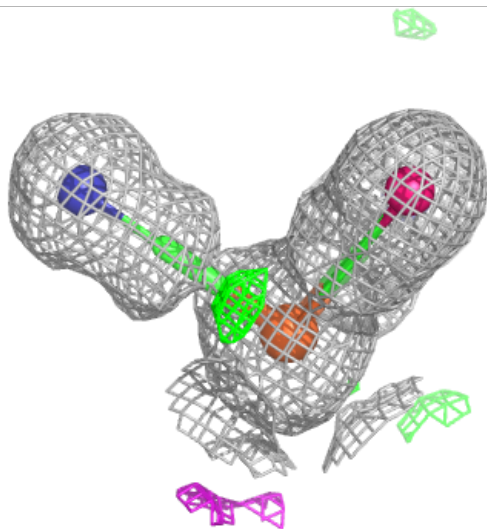
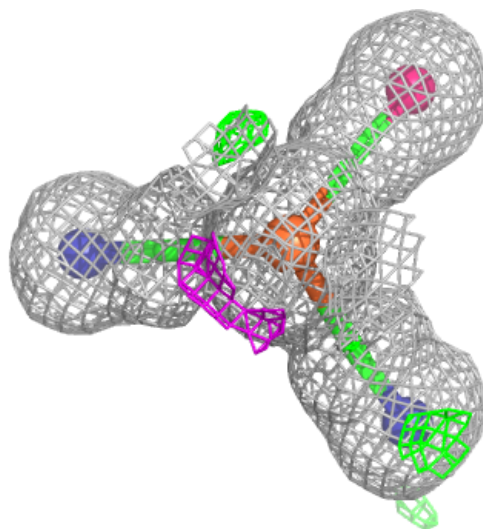
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	MG	TTT	405	1/1	0.89	0.12	42,42,42,42	0
5	GOL	MMM	606	6/6	0.94	0.09	29,32,36,39	0
5	GOL	SSS	404	6/6	0.94	0.10	18,25,27,28	6
8	MG	LLL	604	1/1	0.96	0.29	30,30,30,30	0
10	CMO	LLL	606	2/2	0.98	0.10	10,10,10,14	2
10	CMO	MMM	605	2/2	0.98	0.10	10,10,10,15	2
8	MG	TTT	404	1/1	0.99	0.21	23,23,23,23	0
3	SF4	SSS	403	8/8	1.00	0.01	8,9,9,9	0
6	FCO	LLL	601	7/7	1.00	0.02	8,9,9,9	0
6	FCO	MMM	601	7/7	1.00	0.02	9,10,10,11	0
7	NI	LLL	602	1/1	1.00	0.02	9,9,9,9	0
7	NI	MMM	602	1/1	1.00	0.02	10,10,10,10	0
8	MG	LLL	603	1/1	1.00	0.02	8,8,8,8	0
3	SF4	TTT	401	8/8	1.00	0.01	10,10,11,11	0
3	SF4	TTT	403	8/8	1.00	0.01	9,10,10,10	0
4	F3S	SSS	402	7/7	1.00	0.01	8,9,9,9	0
8	MG	MMM	603	1/1	1.00	0.02	9,9,9,9	0
9	CL	LLL	605	1/1	1.00	0.03	18,18,18,18	0
9	CL	MMM	604	1/1	1.00	0.02	17,17,17,17	0
4	F3S	TTT	402	7/7	1.00	0.01	9,9,10,10	0
3	SF4	SSS	401	8/8	1.00	0.01	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.



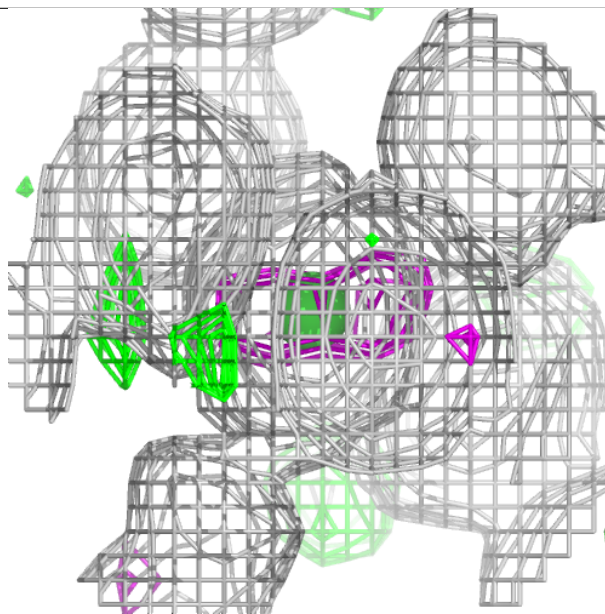
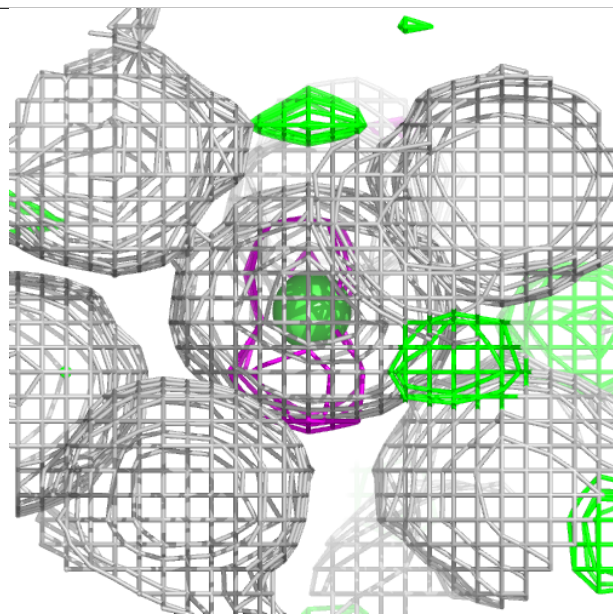
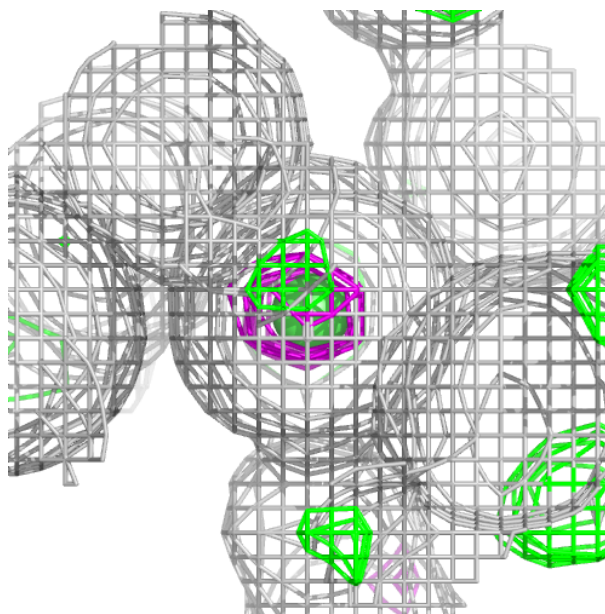
Electron density around FCO MMM 601:

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



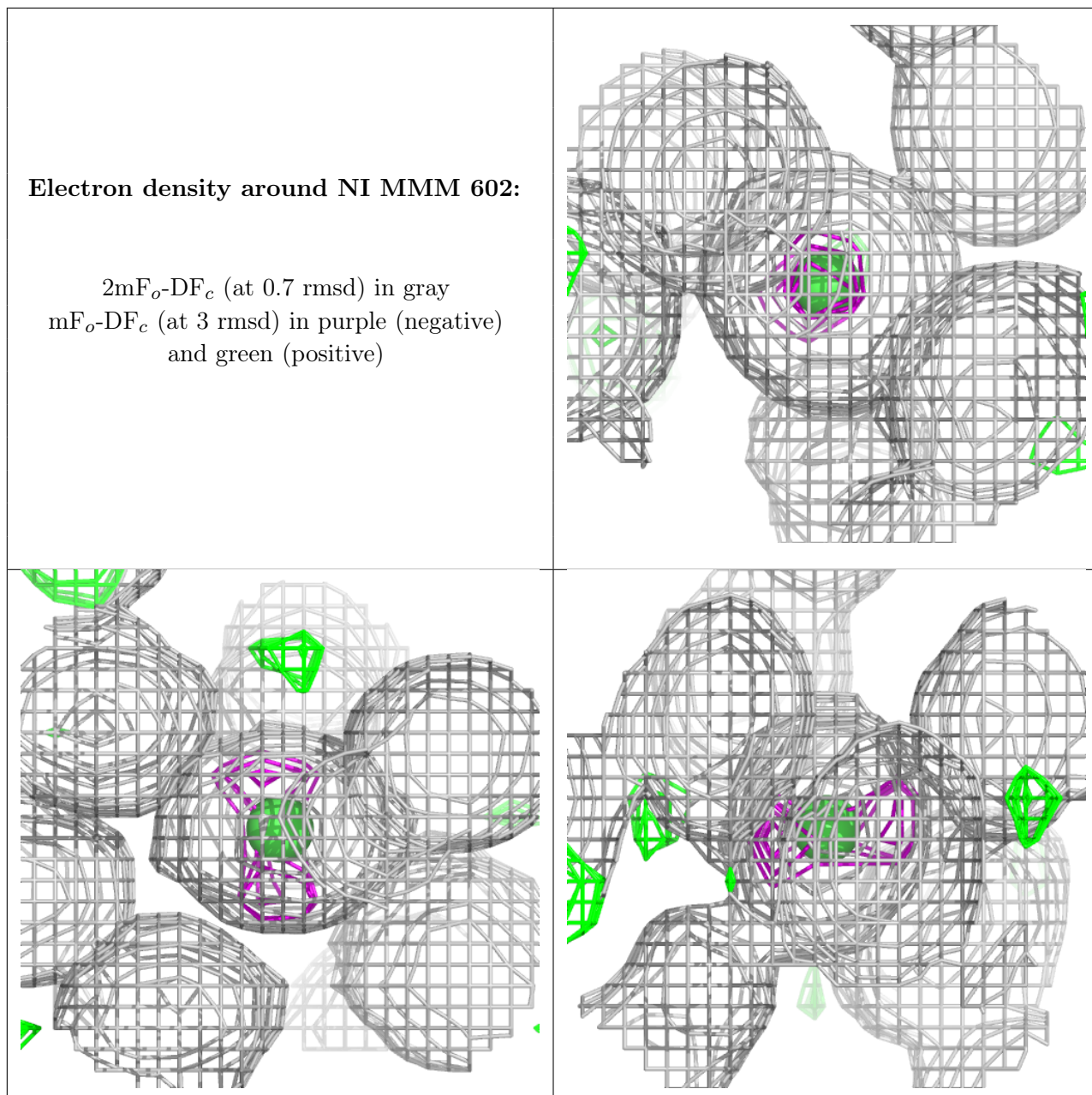
Electron density around NI LLL 602:

$2mF_o-DF_c$ (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.