



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2026 – 12:17 AM JST

PDB ID : 7VXQ / pdb_00007vxq
Title : The Carbon Monoxide Complex of [NiFe]-hydrogenase (Hyb-type) from Citrobacter sp. S-77
Authors : Nishikawa, K.; Higuchi, K.; Imanishi, T.; Higuchi, Y.
Deposited on : 2021-11-13
Resolution : 1.77 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	:	1.8.5 (274361), 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

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 13403 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 [NiFe]-hydrogenase 2 large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	4	0
			4306	2735	744	807	20			
1	C	551	Total	C	N	O	S	0	2	0
			4292	2727	742	803	20			

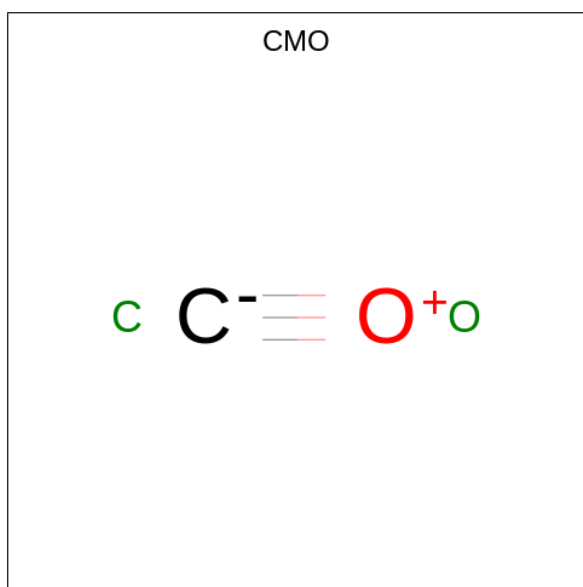
- Molecule 2 is a protein called NiFe hydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	268	Total	C	N	O	S	0	2	0
			2052	1300	365	373	14			
2	D	268	Total	C	N	O	S	0	0	0
			2037	1292	363	369	13			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

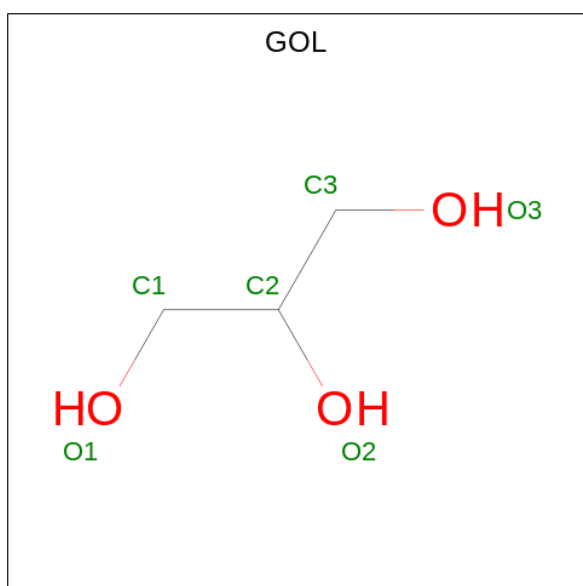
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			2	1	1		
4	C	1	Total	C	O	0	0
			2	1	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



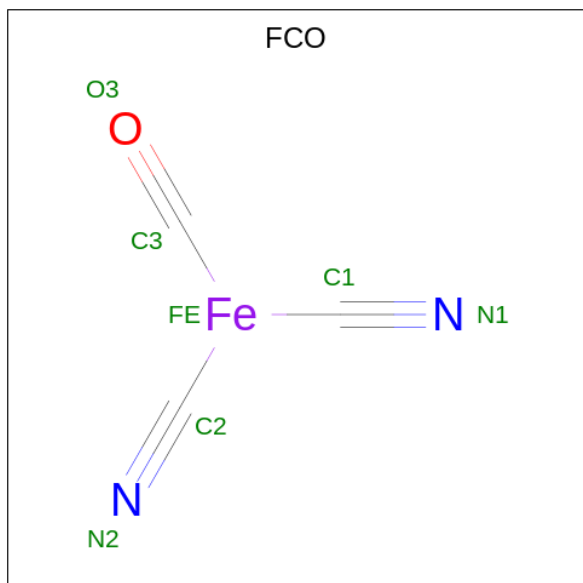
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	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).

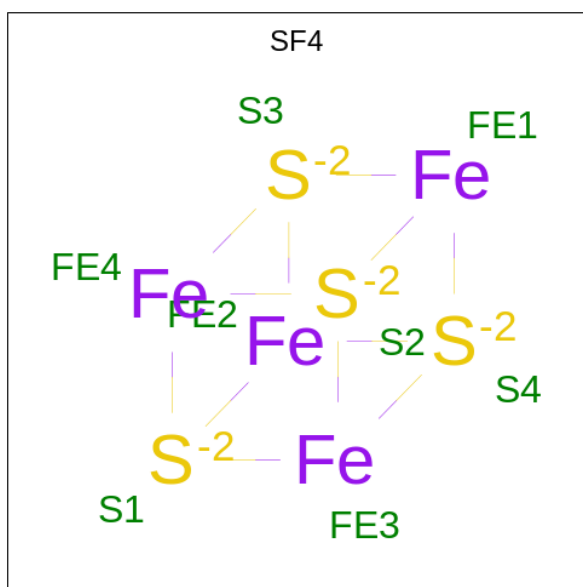


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
6	C	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		

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

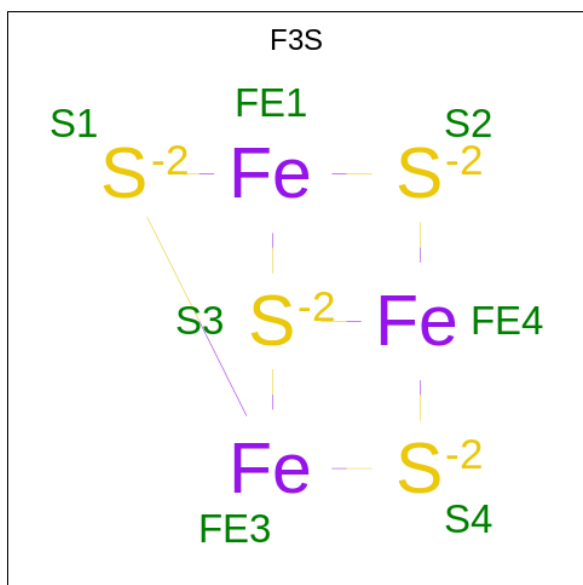
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ni	0	0
			1	1		
7	C	1	Total	Ni	0	0
			1	1		

- Molecule 8 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			8	4	4		
8	B	1	Total	Fe	S	0	0
			8	4	4		
8	D	1	Total	Fe	S	0	0
			8	4	4		
8	D	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 9 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total 7	Fe 3	S 4	0	0
9	D	1	Total 7	Fe 3	S 4	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	212	Total 212	O 212	0	0
10	B	104	Total 104	O 104	0	0
10	C	209	Total 209	O 209	0	0
10	D	99	Total 99	O 99	0	0

VAL	GLY	LEU	LEU	GLY	GLY	VAL	VAL	GLY	LEU	VAL	ALA	GLY	VAL	SER	VAL	VAL	MET	ALA	VAL	VAL	ARG	GLU	LEU	GLY	ARG	GLN	GLN	LYS	LYS	ASP	ASN	ALA	ASP	SER	ARG	GLY	GLU
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.39Å 122.32Å 99.91Å 90.00° 103.11° 90.00°	Depositor
Resolution (Å)	34.49 – 1.77 34.49 – 1.77	Depositor EDS
% Data completeness (in resolution range)	98.4 (34.49-1.77) 98.5 (34.49-1.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 1.77Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.161 , 0.193 0.161 , 0.193	Depositor DCC
R_{free} test set	7429 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 30.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	13403	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	A	1.08	0/4415	1.29	9/6017 (0.1%)
1	C	1.08	3/4398 (0.1%)	1.30	6/5994 (0.1%)
2	B	1.11	0/2111	1.31	3/2874 (0.1%)
2	D	1.10	1/2096 (0.0%)	1.29	3/2854 (0.1%)
All	All	1.09	4/13020 (0.0%)	1.30	21/17739 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	193	GLN	C-O	5.83	1.30	1.24
1	C	431	HIS	CE1-NE2	5.26	1.37	1.32
1	C	68	HIS	CE1-NE2	5.22	1.37	1.32
2	D	34	HIS	CE1-NE2	5.05	1.37	1.32

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	212	ASP	CA-CB-CG	7.55	120.15	112.60
1	A	99	HIS	CA-CB-CG	-6.66	107.14	113.80
1	C	63	VAL	N-CA-C	-6.32	104.99	110.74
2	B	81	ASP	CA-CB-CG	6.28	118.88	112.60
1	A	28	VAL	N-CA-CB	6.21	117.29	110.53
1	A	63	VAL	N-CA-C	-5.88	105.11	110.82
1	C	232	LEU	CB-CA-C	5.87	119.21	109.53
2	D	66	HIS	CB-CA-C	5.84	120.78	110.85
1	A	467	GLY	CA-C-O	-5.67	118.37	122.45
1	C	467	GLY	CA-C-O	-5.46	118.52	122.45
1	A	280	VAL	N-CA-C	-5.44	107.68	112.90
1	C	99	HIS	CA-CB-CG	-5.41	108.39	113.80
1	A	170	GLY	CA-C-O	-5.38	116.74	122.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	208	LYS	CB-CA-C	5.35	118.06	109.07
1	A	382	ASN	CB-CA-C	5.32	120.89	110.67
1	C	382	ASN	CA-CB-CG	5.29	117.89	112.60
1	C	107	HIS	CA-CB-CG	-5.24	108.56	113.80
2	D	44	THR	CB-CA-C	5.19	118.12	109.56
2	B	22	CYS	N-CA-C	-5.02	107.16	113.28
1	A	202	ASN	CA-CB-CG	-5.01	107.59	112.60
1	A	107	HIS	CA-CB-CG	-5.01	108.79	113.80

There are no chirality outliers.

There are no planarity outliers.

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	A	4306	0	4238	20	0
1	C	4292	0	4227	30	0
2	B	2052	0	1973	9	0
2	D	2037	0	1964	9	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	2	0	0	1	0
4	C	2	0	0	1	0
5	A	12	0	16	0	0
5	B	12	0	16	0	0
6	A	7	0	0	0	0
6	C	7	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	16	0	0	0	0
8	D	16	0	0	0	0
9	B	7	0	0	0	0
9	D	7	0	0	0	0
10	A	212	0	0	4	0
10	B	104	0	0	1	0
10	C	209	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	D	99	0	0	0	0
All	All	13403	0	12434	62	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 2.

All (62) 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:D:40:LEU:HA	2:D:44:THR:HG23	1.63	0.81
1:A:456[B]:THR:HG22	10:A:996:HOH:O	1.89	0.71
1:C:514:GLU:OE1	10:C:801:HOH:O	2.15	0.65
1:C:479:ARG:CZ	4:C:703:CMO:O	2.49	0.61
1:A:500:VAL:CG1	1:A:501:PRO:HD2	2.32	0.60
1:A:479:ARG:CZ	4:A:703:CMO:O	2.50	0.59
1:C:210:GLY:CA	2:D:251:ILE:HG12	2.35	0.57
2:B:202:ASP:OD2	2:D:202:ASP:OD2	2.23	0.56
1:C:210:GLY:HA3	2:D:251:ILE:HG12	1.88	0.55
1:A:500:VAL:HG12	1:A:501:PRO:HD2	1.90	0.54
2:B:185:PHE:O	1:C:232:LEU:HB2	2.08	0.53
1:A:373:LYS:HE2	10:A:981:HOH:O	2.08	0.52
2:B:213:GLU:O	10:B:501:HOH:O	2.19	0.52
1:C:80:LEU:CD1	1:C:463:ILE:HD13	2.40	0.52
1:C:80:LEU:HD13	1:C:463:ILE:HD13	1.92	0.51
1:C:291:ASP:OD2	1:C:296:SER:OG	2.20	0.50
1:A:120:THR:O	1:A:123:LEU:HB2	2.13	0.49
1:C:303:TYR:CE2	1:C:305:THR:HG23	2.48	0.48
1:C:232:LEU:HD12	1:C:232:LEU:C	2.39	0.48
10:A:938:HOH:O	1:C:150:LYS:HE2	2.14	0.47
1:C:212:THR:HA	1:C:213:PRO:C	2.39	0.47
1:A:373:LYS:HD2	10:A:831:HOH:O	2.15	0.47
1:A:500:VAL:HG11	1:A:549:CYS:HB3	1.96	0.47
1:A:544:ASP:N	1:A:545:PRO:HD3	2.30	0.47
2:D:247:TRP:CH2	2:D:249:VAL:HB	2.51	0.46
1:A:212:THR:HA	1:A:213:PRO:C	2.41	0.46
1:C:27:VAL:CG1	1:C:524:GLY:HA2	2.45	0.46
1:C:133:MET:HE1	1:C:183:VAL:HG22	1.99	0.45
1:C:136:GLY:O	1:C:407:LYS:NZ	2.43	0.45
2:D:23:THR:HG22	2:D:23:THR:O	2.17	0.45
1:C:283:LEU:HB2	1:C:375:VAL:HG11	1.98	0.45
2:B:230:GLU:HG3	2:B:273:ALA:HB1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:TYR:N	1:A:270:PRO:CD	2.80	0.44
1:C:80:LEU:HD11	1:C:463:ILE:CD1	2.47	0.44
1:C:82:ILE:HD11	1:C:461:PRO:HB3	1.99	0.44
1:C:537:VAL:CG1	1:C:541:HIS:CE1	3.01	0.44
1:C:69:ALA:HB1	1:C:218:LEU:HD12	1.99	0.44
1:C:80:LEU:CD1	1:C:463:ILE:CD1	2.96	0.43
1:A:69:ALA:HB1	1:A:218:LEU:HD12	1.99	0.43
2:B:253:HIS:CG	2:B:254:PRO:HD2	2.53	0.43
1:A:166:ILE:HD12	1:A:166:ILE:HA	1.90	0.43
1:C:506:SER:HB3	1:C:518:TYR:CE2	2.54	0.42
1:C:303:TYR:CE2	1:C:305:THR:CG2	3.02	0.42
1:C:380:LEU:HB2	1:C:424:ARG:HA	2.01	0.42
1:C:155:ILE:HD11	1:C:188:VAL:HG11	2.01	0.42
1:A:12:ARG:HA	2:B:52:VAL:O	2.20	0.42
2:B:247:TRP:CH2	2:B:249:VAL:HB	2.55	0.42
1:C:30:LYS:HE2	1:C:32:TRP:CZ2	2.54	0.42
1:A:8:ASP:HA	1:A:9:PRO:HA	1.91	0.41
1:C:374[A]:THR:HG21	1:C:514:GLU:HG2	2.02	0.41
1:A:418:LEU:O	1:A:423:GLY:HA3	2.20	0.41
1:C:123:LEU:HD11	1:C:159:VAL:HG21	2.02	0.41
2:D:247:TRP:CZ2	2:D:249:VAL:HB	2.55	0.41
1:A:337:LYS:HA	1:A:337:LYS:HD2	1.88	0.41
1:C:374[B]:THR:HG21	10:C:809:HOH:O	2.20	0.41
1:A:166:ILE:HG22	1:A:167:PHE:CD2	2.55	0.41
1:C:500:VAL:CG1	1:C:501:PRO:HD2	2.51	0.41
2:D:251:ILE:C	2:D:251:ILE:HD12	2.46	0.41
2:D:49:TYR:OH	2:D:51:GLU:OE1	2.23	0.40
1:A:500:VAL:HG13	1:A:501:PRO:HD2	2.02	0.40
2:B:228:GLY:N	2:B:229:PRO:CD	2.84	0.40
1:A:227:ILE:O	2:B:216:ARG:HD2	2.20	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	A	553/552 (100%)	530 (96%)	22 (4%)	1 (0%)	43	29
1	C	551/552 (100%)	530 (96%)	20 (4%)	1 (0%)	43	29
2	B	268/335 (80%)	258 (96%)	10 (4%)	0	100	100
2	D	266/335 (79%)	258 (97%)	8 (3%)	0	100	100
All	All	1638/1774 (92%)	1576 (96%)	60 (4%)	2 (0%)	48	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	211	LYS
1	C	211	LYS

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	A	464/461 (101%)	458 (99%)	6 (1%)	61	46
1	C	462/461 (100%)	454 (98%)	8 (2%)	53	36
2	B	212/261 (81%)	207 (98%)	5 (2%)	43	24
2	D	210/261 (80%)	208 (99%)	2 (1%)	68	55
All	All	1348/1444 (93%)	1327 (98%)	21 (2%)	55	38

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	VAL
1	A	123	LEU
1	A	156	LYS
1	A	164	LEU
1	A	166	ILE
1	A	382	ASN

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Mol	Chain	Res	Type
2	B	21	GLU
2	B	63	GLU
2	B	73	LYS
2	B	142	VAL
2	B	251	ILE
1	C	46	LYS
1	C	81	ASN
1	C	119	ILE
1	C	129	LYS
1	C	232	LEU
1	C	306	ASP
1	C	346	GLU
1	C	382	ASN
2	D	44	THR
2	D	173	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	395	HIS
1	A	455	HIS
2	B	59	HIS
2	B	67	ASN
2	B	140	GLN
2	B	223	HIS
1	C	202	ASN
2	D	10	GLN
2	D	75	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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
8	SF4	D	401	2	0,12,12	-	-	-		
4	CMO	C	703	-	0,1,1	-	-	-		
4	CMO	A	703	-	0,1,1	-	-	-		
5	GOL	A	705	-	5,5,5	0.12	0	5,5,5	0.37	0
8	SF4	B	403	2	0,12,12	-	-	-		
8	SF4	B	405	2	0,12,12	-	-	-		
9	F3S	B	404	2	0,9,9	-	-	-		
5	GOL	B	402	-	5,5,5	0.17	0	5,5,5	0.34	0
6	FCO	A	706	1,7	1,6,6	4.05	1 (100%)	-		
9	F3S	D	402	2	0,9,9	-	-	-		
5	GOL	B	401	-	5,5,5	0.14	0	5,5,5	0.40	0
5	GOL	A	704	-	5,5,5	0.13	0	5,5,5	0.33	0
8	SF4	D	403	2	0,12,12	-	-	-		
6	FCO	C	704	1,7	1,6,6	2.53	1 (100%)	-		

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
8	SF4	D	401	2	-	-	0/6/5/5
8	SF4	B	403	2	-	-	0/6/5/5
8	SF4	B	405	2	-	-	0/6/5/5
5	GOL	A	705	-	-	0/4/4/4	-
9	F3S	B	404	2	-	-	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	402	-	-	0/4/4/4	-
9	F3S	D	402	2	-	-	0/3/3/3
5	GOL	B	401	-	-	3/4/4/4	-
5	GOL	A	704	-	-	0/4/4/4	-
8	SF4	D	403	2	-	-	0/6/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	706	FCO	O3-C3	-4.05	1.10	1.16
6	C	704	FCO	O3-C3	-2.53	1.12	1.16

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

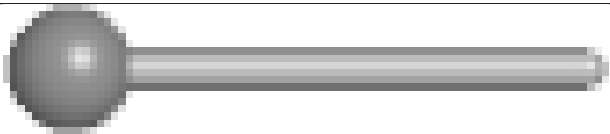
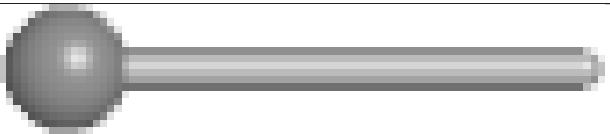
Mol	Chain	Res	Type	Atoms
5	B	401	GOL	O1-C1-C2-C3
5	B	401	GOL	C1-C2-C3-O3
5	B	401	GOL	O2-C2-C3-O3

There are no ring outliers.

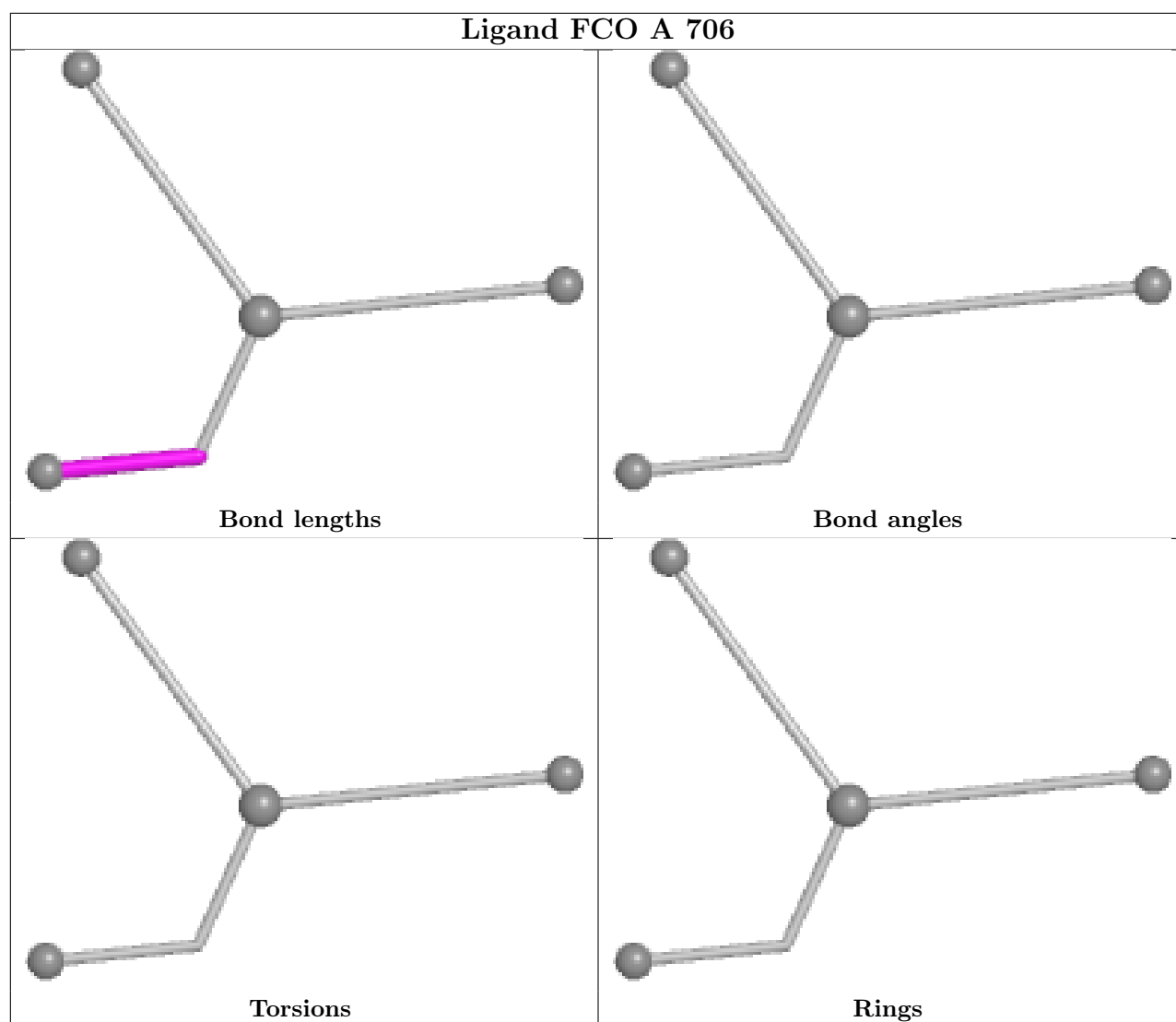
2 monomers are involved in 2 short contacts:

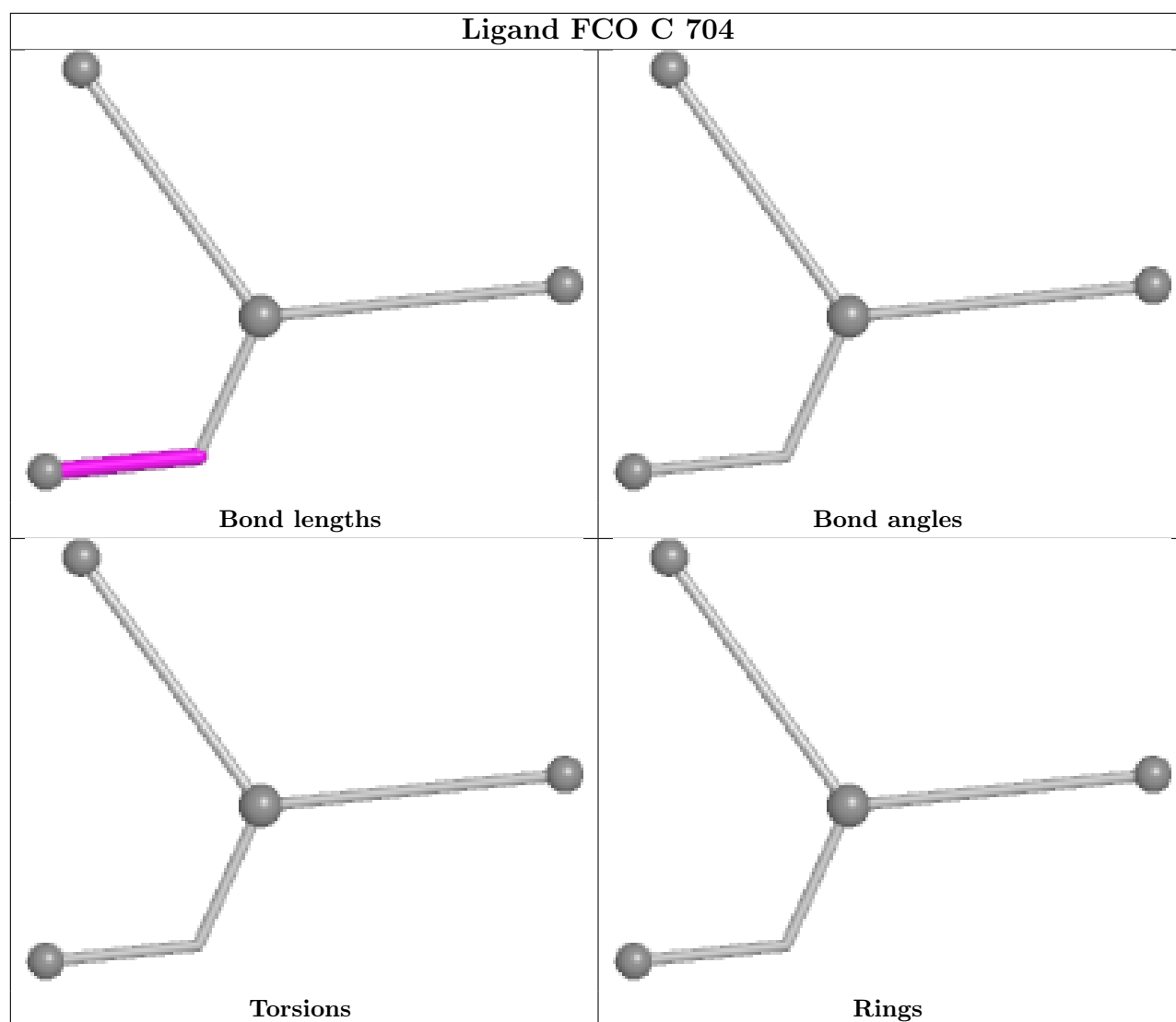
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	703	CMO	1	0
4	A	703	CMO	1	0

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.

Ligand CMO C 703	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CMO A 703	
 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	A	551/552 (99%)	0.05	6 (1%) 78 84	16, 32, 50, 71	4 (0%)
1	C	551/552 (99%)	0.07	4 (0%) 84 88	16, 32, 47, 75	2 (0%)
2	B	268/335 (80%)	0.14	2 (0%) 84 88	15, 34, 51, 67	2 (0%)
2	D	268/335 (80%)	0.14	1 (0%) 88 92	25, 34, 49, 74	0
All	All	1638/1774 (92%)	0.09	13 (0%) 82 87	15, 33, 50, 75	8 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	9	PRO	4.1
2	B	9	PRO	3.3
1	A	310	SER	2.9
1	C	307	ALA	2.9
1	A	309	LEU	2.8
1	A	166	ILE	2.7
1	C	309	LEU	2.4
2	B	66	HIS	2.4
1	A	307	ALA	2.3
1	C	459	VAL	2.3
1	A	311	THR	2.2
1	C	310	SER	2.1
1	A	415	VAL	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

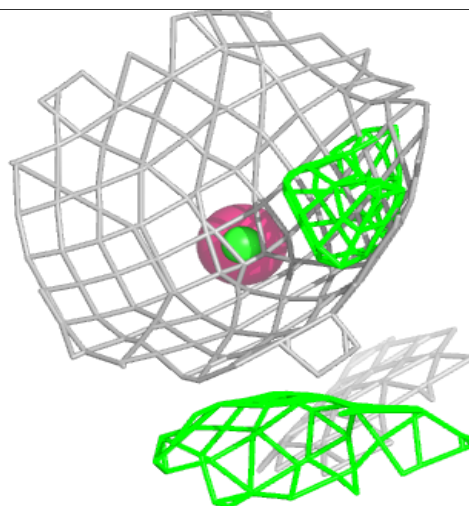
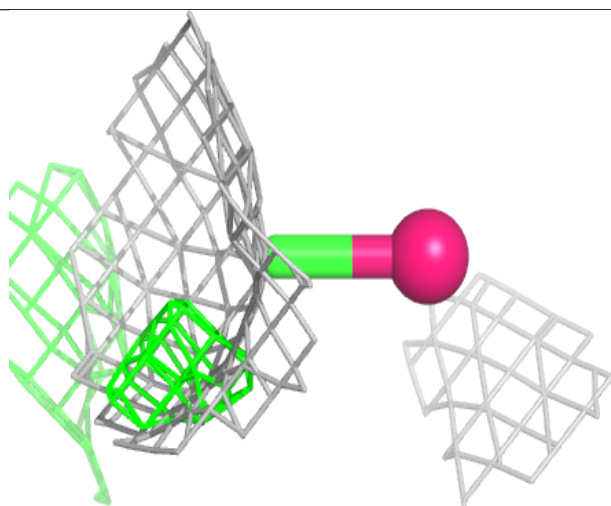
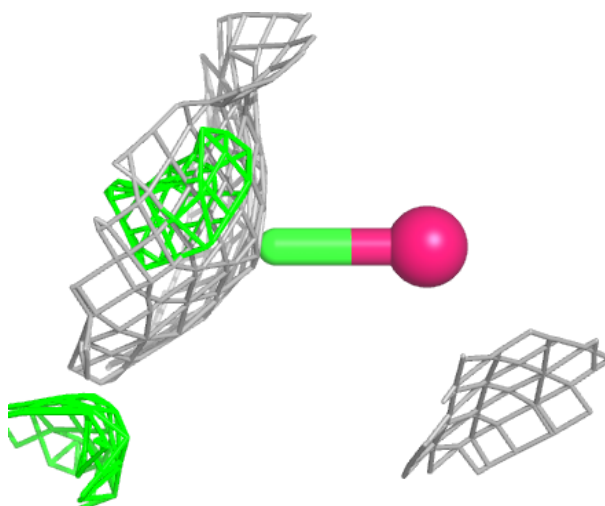
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	A	704	6/6	0.88	0.11	48,54,57,57	0
5	GOL	B	402	6/6	0.89	0.11	43,45,46,47	6
5	GOL	A	705	6/6	0.90	0.09	36,38,44,44	6
4	CMO	C	703	2/2	0.91	0.23	26,26,26,28	2
4	CMO	A	703	2/2	0.92	0.22	25,25,25,26	2
5	GOL	B	401	6/6	0.93	0.09	34,38,43,47	6
8	SF4	D	401	8/8	0.97	0.05	30,31,35,35	0
8	SF4	B	403	8/8	0.98	0.04	29,29,31,35	0
6	FCO	A	706	7/7	0.99	0.05	21,23,25,25	0
6	FCO	C	704	7/7	0.99	0.06	24,24,28,28	0
7	NI	A	707	1/1	0.99	0.02	27,27,27,27	0
7	NI	C	705	1/1	0.99	0.02	28,28,28,28	0
3	MG	A	701	1/1	0.99	0.03	25,25,25,25	0
8	SF4	B	405	8/8	0.99	0.03	24,27,29,30	0
3	MG	C	701	1/1	0.99	0.03	26,26,26,26	0
8	SF4	D	403	8/8	0.99	0.03	23,28,29,30	0
9	F3S	B	404	7/7	0.99	0.03	22,25,27,28	0
9	F3S	D	402	7/7	0.99	0.04	27,28,29,31	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.

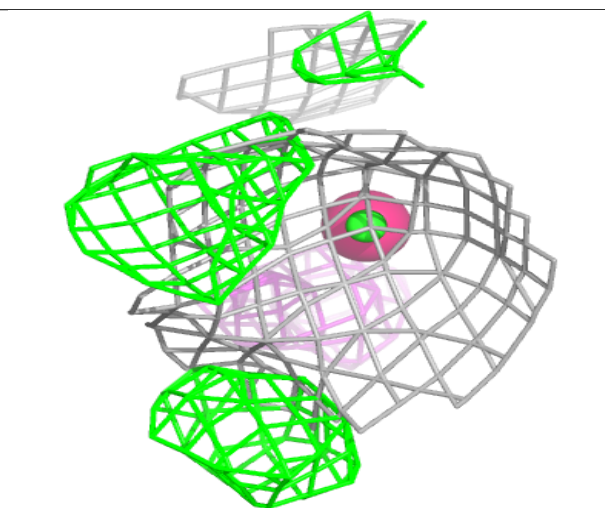
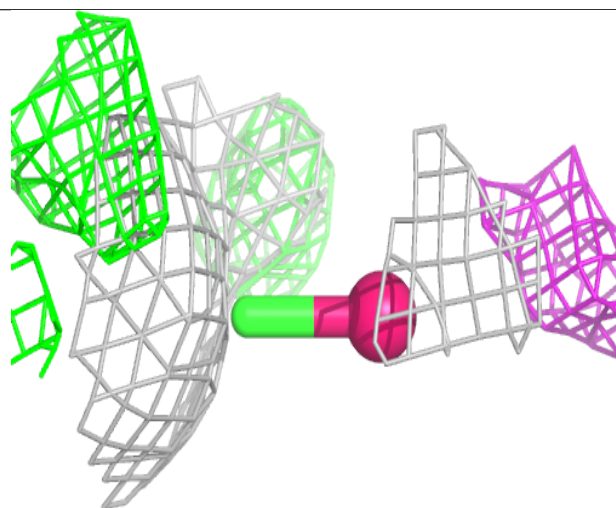
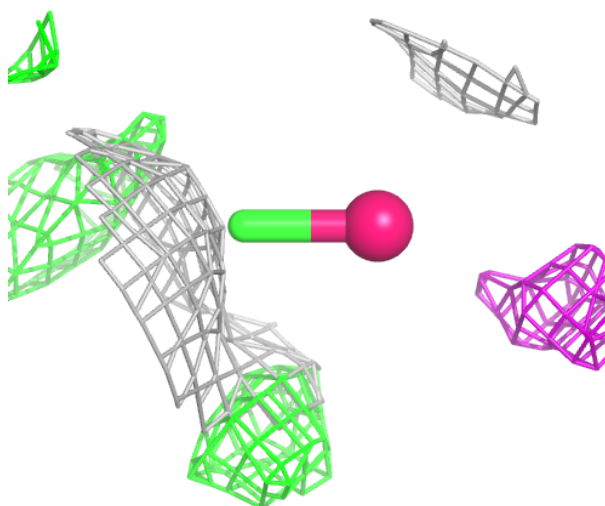
Electron density around CMO C 703:

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



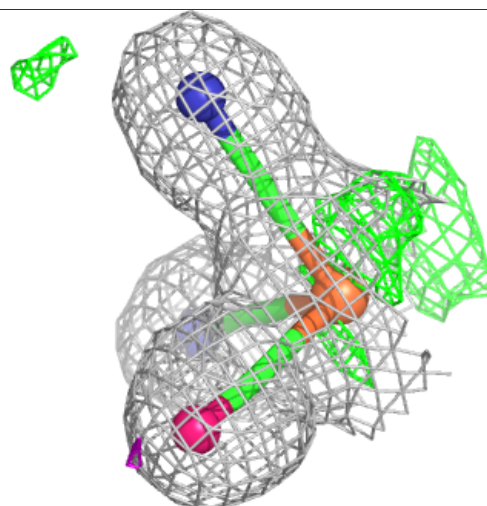
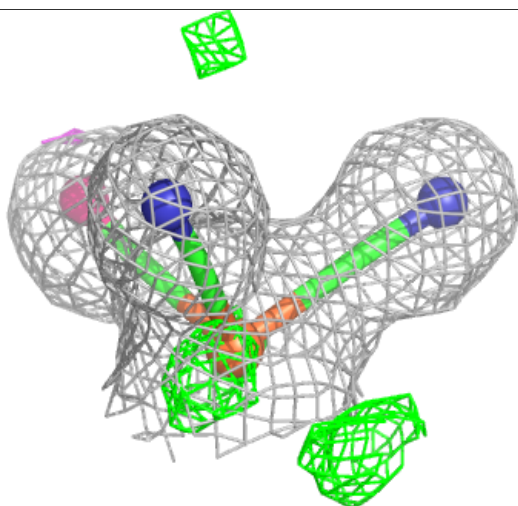
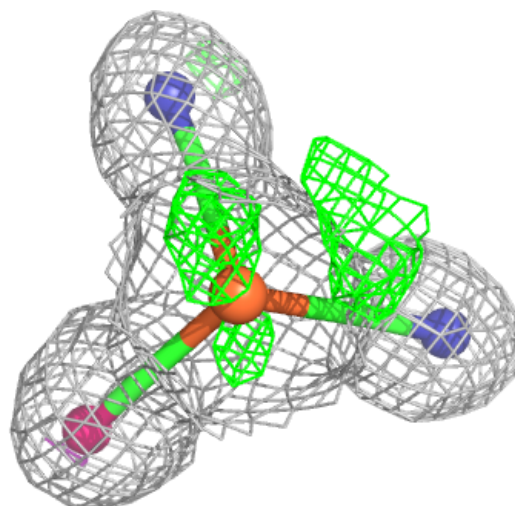
Electron density around CMO A 703:

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



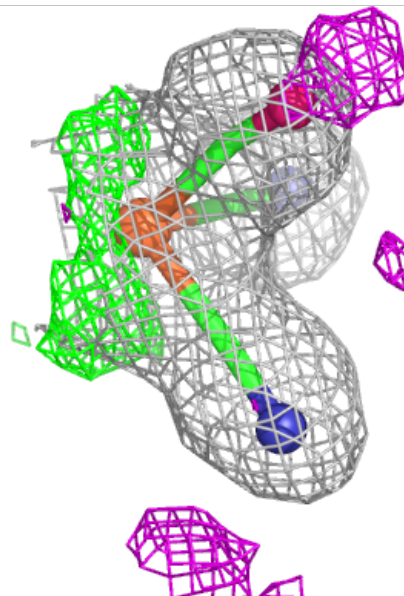
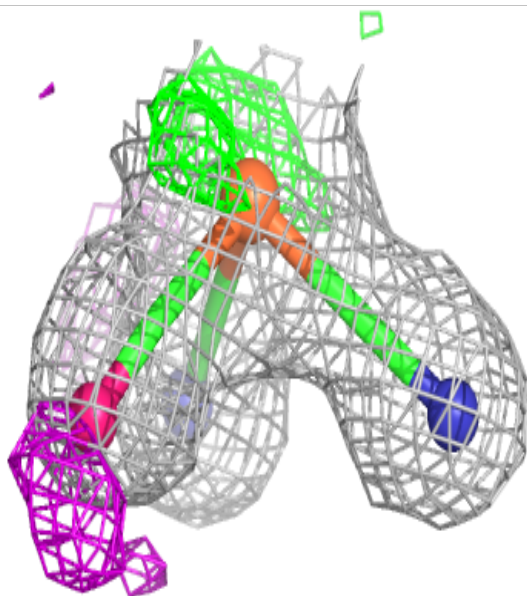
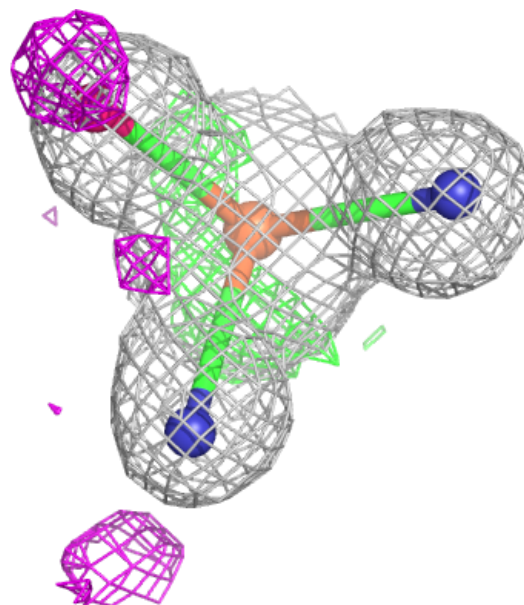
Electron density around FCO A 706:

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



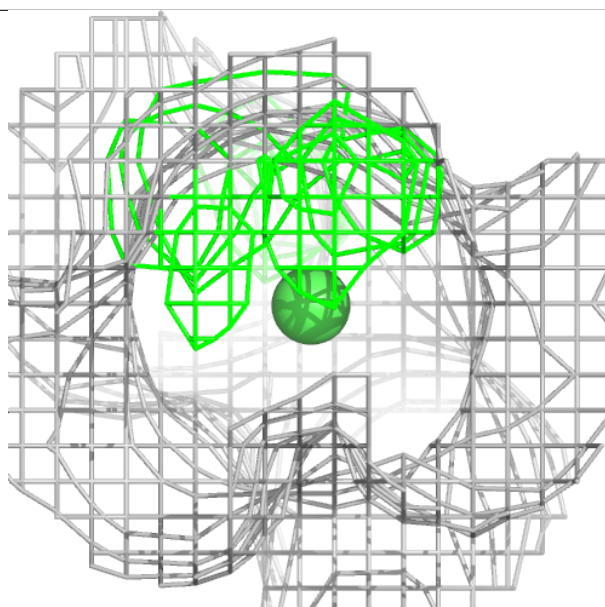
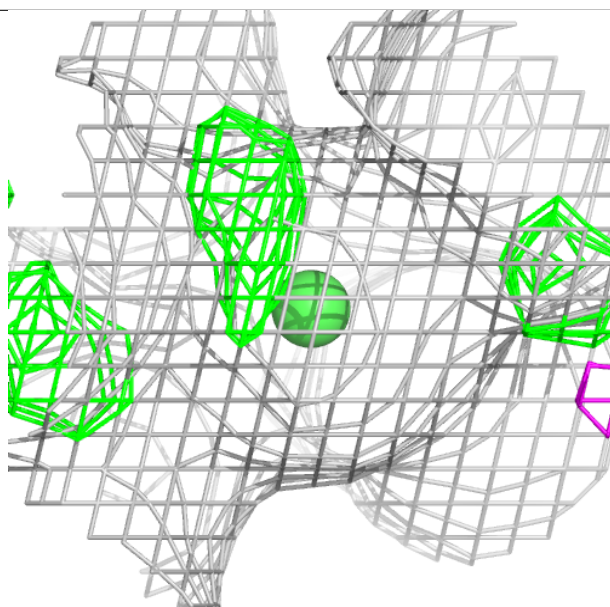
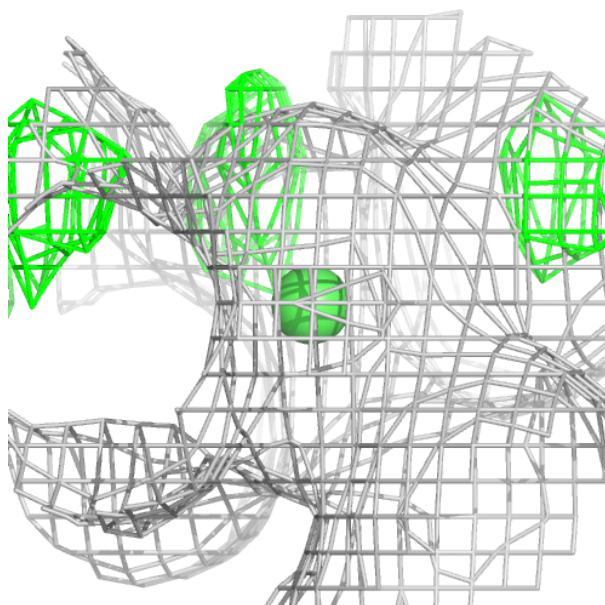
Electron density around FCO C 704:

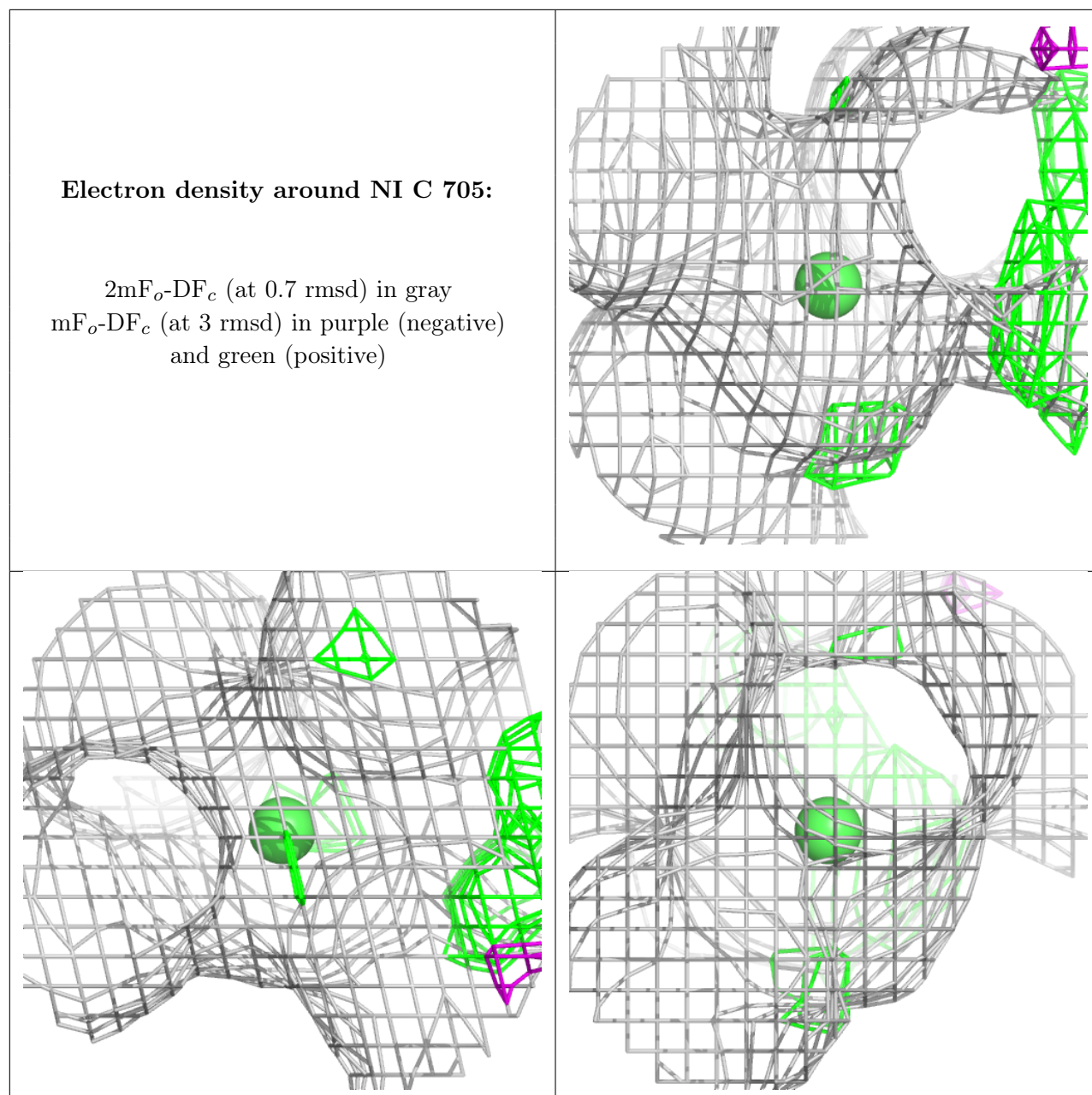
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NI A 707:

$2mF_o-DF_c$ (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.