Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2024 – 08:27 PM JST

PDB ID : 8ZHY
Title : Magnesium substituted Terephthalate 1,2-cis-dihydrodioldehydrogenase/Decarboxylase in complex with CO2.
Authors : Kumar, K.A.; Pahwa, D.; Kumar, P.
Deposited on : 2024-05-11
Resolution : 2.70 Å(reported)

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

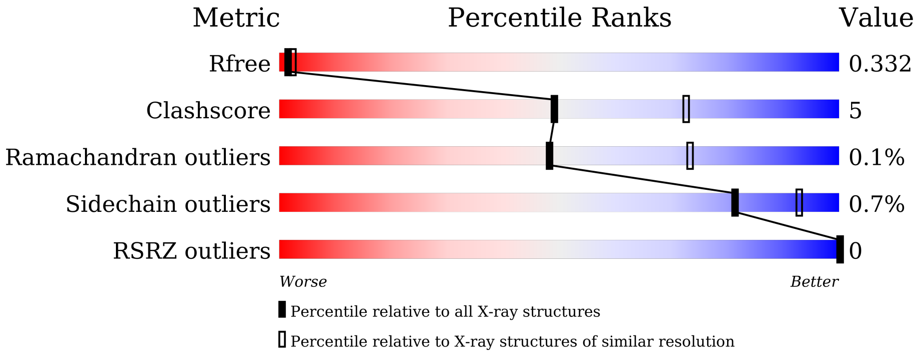
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.002 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.2

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 2.70 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}	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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	A	335	
1	B	335	
1	C	335	
1	D	335	

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 18775 atoms, of which 9442 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 4-hydroxythreonine-4-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	314	Total 4670	C 1445	H 2368	N 412	O 432	S 13	68	0	0
1	B	313	Total 4655	C 1441	H 2362	N 410	O 430	S 12	68	0	0
1	C	307	Total 4571	C 1414	H 2320	N 403	O 421	S 13	68	0	0
1	D	314	Total 4670	C 1445	H 2368	N 412	O 432	S 13	68	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP B7WRJ7
A	-18	GLY	-	expression tag	UNP B7WRJ7
A	-17	SER	-	expression tag	UNP B7WRJ7
A	-16	SER	-	expression tag	UNP B7WRJ7
A	-15	HIS	-	expression tag	UNP B7WRJ7
A	-14	HIS	-	expression tag	UNP B7WRJ7
A	-13	HIS	-	expression tag	UNP B7WRJ7
A	-12	HIS	-	expression tag	UNP B7WRJ7
A	-11	HIS	-	expression tag	UNP B7WRJ7
A	-10	HIS	-	expression tag	UNP B7WRJ7
A	-9	SER	-	expression tag	UNP B7WRJ7
A	-8	SER	-	expression tag	UNP B7WRJ7
A	-7	GLY	-	expression tag	UNP B7WRJ7
A	-6	LEU	-	expression tag	UNP B7WRJ7
A	-5	VAL	-	expression tag	UNP B7WRJ7
A	-4	PRO	-	expression tag	UNP B7WRJ7
A	-3	ARG	-	expression tag	UNP B7WRJ7
A	-2	GLY	-	expression tag	UNP B7WRJ7
A	-1	SER	-	expression tag	UNP B7WRJ7
A	0	HIS	-	expression tag	UNP B7WRJ7
B	-19	MET	-	initiating methionine	UNP B7WRJ7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP B7WRJ7
B	-17	SER	-	expression tag	UNP B7WRJ7
B	-16	SER	-	expression tag	UNP B7WRJ7
B	-15	HIS	-	expression tag	UNP B7WRJ7
B	-14	HIS	-	expression tag	UNP B7WRJ7
B	-13	HIS	-	expression tag	UNP B7WRJ7
B	-12	HIS	-	expression tag	UNP B7WRJ7
B	-11	HIS	-	expression tag	UNP B7WRJ7
B	-10	HIS	-	expression tag	UNP B7WRJ7
B	-9	SER	-	expression tag	UNP B7WRJ7
B	-8	SER	-	expression tag	UNP B7WRJ7
B	-7	GLY	-	expression tag	UNP B7WRJ7
B	-6	LEU	-	expression tag	UNP B7WRJ7
B	-5	VAL	-	expression tag	UNP B7WRJ7
B	-4	PRO	-	expression tag	UNP B7WRJ7
B	-3	ARG	-	expression tag	UNP B7WRJ7
B	-2	GLY	-	expression tag	UNP B7WRJ7
B	-1	SER	-	expression tag	UNP B7WRJ7
B	0	HIS	-	expression tag	UNP B7WRJ7
C	-19	MET	-	initiating methionine	UNP B7WRJ7
C	-18	GLY	-	expression tag	UNP B7WRJ7
C	-17	SER	-	expression tag	UNP B7WRJ7
C	-16	SER	-	expression tag	UNP B7WRJ7
C	-15	HIS	-	expression tag	UNP B7WRJ7
C	-14	HIS	-	expression tag	UNP B7WRJ7
C	-13	HIS	-	expression tag	UNP B7WRJ7
C	-12	HIS	-	expression tag	UNP B7WRJ7
C	-11	HIS	-	expression tag	UNP B7WRJ7
C	-10	HIS	-	expression tag	UNP B7WRJ7
C	-9	SER	-	expression tag	UNP B7WRJ7
C	-8	SER	-	expression tag	UNP B7WRJ7
C	-7	GLY	-	expression tag	UNP B7WRJ7
C	-6	LEU	-	expression tag	UNP B7WRJ7
C	-5	VAL	-	expression tag	UNP B7WRJ7
C	-4	PRO	-	expression tag	UNP B7WRJ7
C	-3	ARG	-	expression tag	UNP B7WRJ7
C	-2	GLY	-	expression tag	UNP B7WRJ7
C	-1	SER	-	expression tag	UNP B7WRJ7
C	0	HIS	-	expression tag	UNP B7WRJ7
D	-19	MET	-	initiating methionine	UNP B7WRJ7
D	-18	GLY	-	expression tag	UNP B7WRJ7
D	-17	SER	-	expression tag	UNP B7WRJ7

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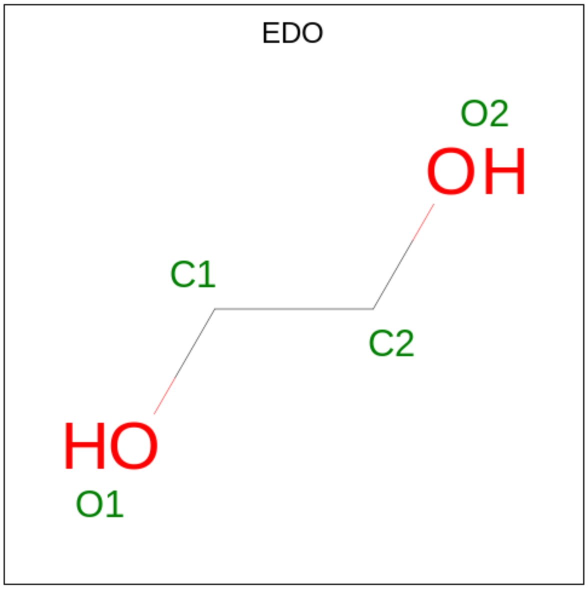
Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP B7WRJ7
D	-15	HIS	-	expression tag	UNP B7WRJ7
D	-14	HIS	-	expression tag	UNP B7WRJ7
D	-13	HIS	-	expression tag	UNP B7WRJ7
D	-12	HIS	-	expression tag	UNP B7WRJ7
D	-11	HIS	-	expression tag	UNP B7WRJ7
D	-10	HIS	-	expression tag	UNP B7WRJ7
D	-9	SER	-	expression tag	UNP B7WRJ7
D	-8	SER	-	expression tag	UNP B7WRJ7
D	-7	GLY	-	expression tag	UNP B7WRJ7
D	-6	LEU	-	expression tag	UNP B7WRJ7
D	-5	VAL	-	expression tag	UNP B7WRJ7
D	-4	PRO	-	expression tag	UNP B7WRJ7
D	-3	ARG	-	expression tag	UNP B7WRJ7
D	-2	GLY	-	expression tag	UNP B7WRJ7
D	-1	SER	-	expression tag	UNP B7WRJ7
D	0	HIS	-	expression tag	UNP B7WRJ7

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C H O 10 2 6 2	2	0
2	A	1	Total C H O 10 2 6 2	2	0
2	A	1	Total C H O 10 2 6 2	2	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	C	1	10	2	6	2	2	0

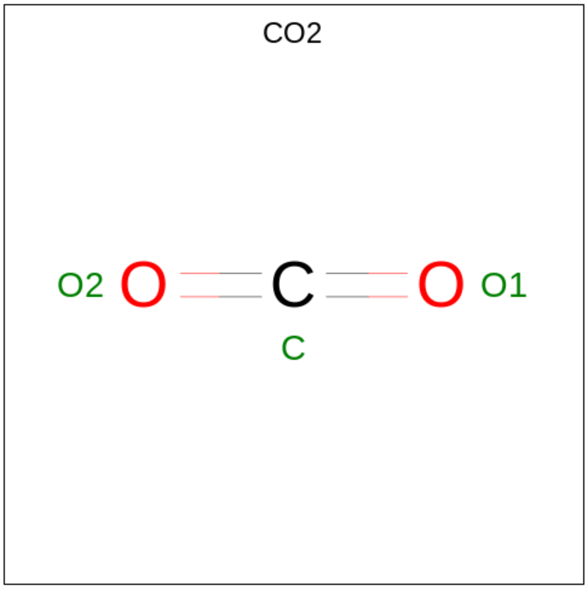
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Na 1	0	0
4	D	1	Total 1	Na 1	0	0

- Molecule 5 is CARBON DIOXIDE (three-letter code: CO2) (formula: CO_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 3 1 2	0	0
5	C	1	Total C O 3 1 2	0	0
5	C	1	Total C O 3 1 2	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Mg 1 1	0	0
6	D	1	Total Mg 1 1	0	0

- Molecule 7 is water.

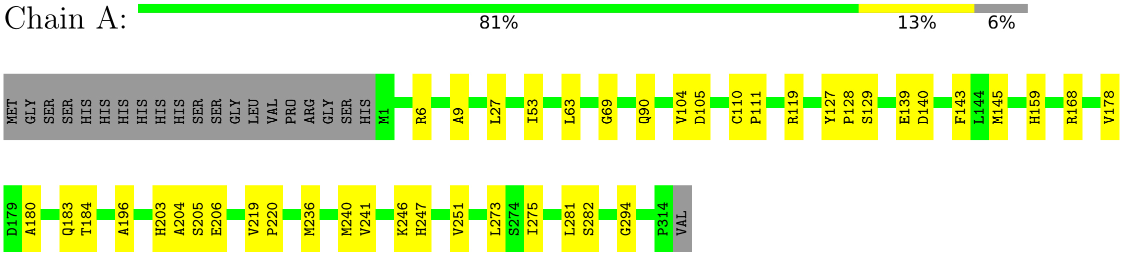
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	47	Total O 47 47	0	0
7	B	27	Total O 27 27	0	0
7	C	36	Total O 36 36	0	0
7	D	43	Total O 43 43	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

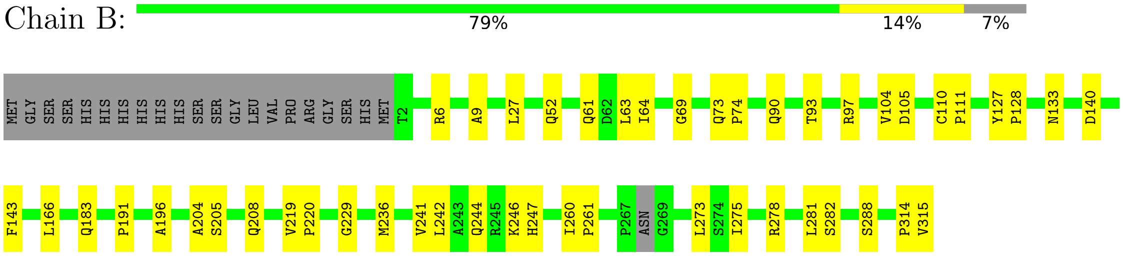
- Molecule 1: 4-hydroxythreonine-4-phosphate dehydrogenase

Chain A:



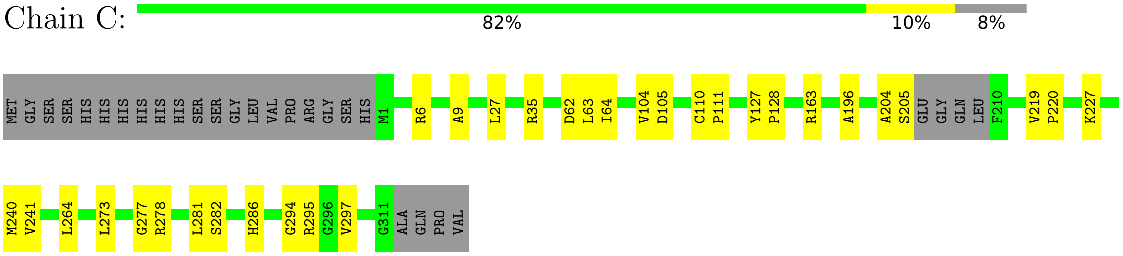
- Molecule 1: 4-hydroxythreonine-4-phosphate dehydrogenase

Chain B:



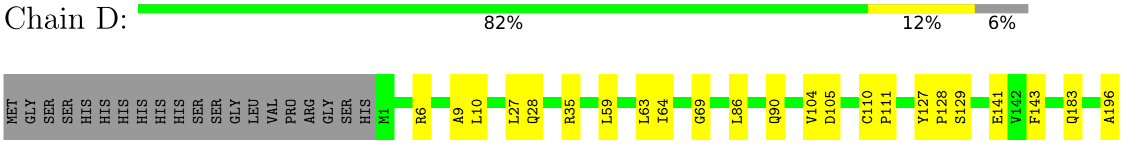
- Molecule 1: 4-hydroxythreonine-4-phosphate dehydrogenase

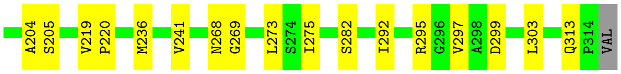
Chain C:



- Molecule 1: 4-hydroxythreonine-4-phosphate dehydrogenase

Chain D:




A204
S205
V219
P220
M236
V241
N268
G269
L273
S274
I275
S282
I292
R295
G296
V297
A298
D299
L303
Q313
P314
VAL

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	86.73Å 93.78Å 166.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 20.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-2.70) 80.0 (20.00-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.18 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.283 , 0.330 0.284 , 0.332	Depositor DCC
R_{free} test set	1853 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	31.1	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 17.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	18775	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4732e-03.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CO2, ZN, EDO, MG, NA

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	0.39	0/2339	0.71	0/3183
1	B	0.38	0/2329	0.70	0/3169
1	C	0.38	0/2286	0.71	0/3109
1	D	0.38	0/2339	0.72	0/3183
All	All	0.38	0/9293	0.71	0/12644

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**
1	C	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	**Chain**	**Res**	**Type**	**Group**
1	C	295	ARG	Sidechain
1	D	35	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	A	2302	2368	2357	27	0
1	B	2293	2362	2347	25	0
1	C	2251	2320	2308	24	0
1	D	2302	2368	2356	31	0
2	A	12	18	18	0	0
2	C	4	6	6	1	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
5	B	3	0	0	0	0
5	C	6	0	0	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	A	47	0	0	3	0
7	B	27	0	0	0	0
7	C	36	0	0	2	0
7	D	43	0	0	5	0
All	All	9333	9442	9392	99	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 5.

All (99) 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:C:297:VAL:O	1:D:299:ASP:HB3	1.48	1.14
1:C:62:ASP:HB3	7:C:501:HOH:O	1.75	0.86
1:A:119:ARG:NH1	1:B:229:GLY:O	2.26	0.68
1:A:27:LEU:HD13	1:A:63:LEU:HD11	1.76	0.67
1:C:297:VAL:C	1:D:299:ASP:HB3	2.18	0.63
1:B:27:LEU:HD13	1:B:63:LEU:HD11	1.79	0.62
1:A:246:LYS:HG3	1:A:247:HIS:CE1	2.34	0.61
1:C:27:LEU:HD13	1:C:63:LEU:HD11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:PRO:HG2	1:B:315:VAL:HG22	1.83	0.60
1:D:27:LEU:HD13	1:D:63:LEU:HD11	1.83	0.60
1:D:269:GLY:N	7:D:504:HOH:O	2.36	0.58
1:B:244:GLN:HB3	1:B:246:LYS:HE3	1.86	0.58
1:C:219:VAL:HB	1:C:220:PRO:HD3	1.86	0.57
1:C:294:GLY:O	1:D:268:ASN:ND2	2.39	0.56
1:A:206:GLU:HG3	7:A:536:HOH:O	2.04	0.55
1:B:219:VAL:HB	1:B:220:PRO:HD3	1.89	0.54
1:B:143:PHE:O	1:B:275:ILE:HG12	2.07	0.54
1:A:143:PHE:O	1:A:275:ILE:HG12	2.08	0.54
1:A:140:ASP:HB3	1:A:168:ARG:HH11	1.73	0.54
1:C:273:LEU:HD22	1:C:282:SER:HB2	1.90	0.54
1:D:143:PHE:O	1:D:275:ILE:HG12	2.08	0.54
1:A:273:LEU:HD22	1:A:282:SER:HB2	1.91	0.53
1:D:219:VAL:HB	1:D:220:PRO:HD3	1.89	0.53
1:A:219:VAL:HB	1:A:220:PRO:HD3	1.90	0.53
1:C:286:HIS:CD2	1:D:297:VAL:HG11	2.44	0.53
1:D:6:ARG:HD3	1:D:105:ASP:HB2	1.91	0.53
1:A:180:ALA:O	1:A:183:GLN:HG3	2.08	0.52
1:C:35:ARG:NE	7:C:501:HOH:O	2.40	0.52
1:B:273:LEU:HD22	1:B:282:SER:HB2	1.92	0.52
1:B:6:ARG:HD3	1:B:105:ASP:HB2	1.92	0.52
1:B:246:LYS:HG3	1:B:247:HIS:CE1	2.45	0.52
1:B:196:ALA:HB1	1:B:241:VAL:HG11	1.92	0.51
1:A:6:ARG:HD3	1:A:105:ASP:HB2	1.92	0.51
7:A:504:HOH:O	1:D:86:LEU:HD13	2.10	0.51
1:B:166:LEU:HB3	1:C:163:ARG:NH1	2.26	0.51
1:A:145:MET:HE2	1:A:184:THR:HG21	1.92	0.50
1:D:273:LEU:HD22	1:D:282:SER:HB2	1.93	0.49
1:D:196:ALA:HB1	1:D:241:VAL:HG11	1.94	0.49
1:C:196:ALA:HB1	1:C:241:VAL:HG11	1.95	0.49
1:D:295:ARG:HH21	1:D:295:ARG:HG3	1.77	0.49
1:B:93:THR:O	1:B:97:ARG:HG3	2.13	0.48
1:B:9:ALA:HB2	1:B:104:VAL:HG21	1.96	0.48
1:D:141:GLU:HA	7:D:535:HOH:O	2.14	0.48
1:D:69:GLY:HA2	1:D:90:GLN:OE1	2.14	0.47
1:A:69:GLY:HA2	1:A:90:GLN:OE1	2.15	0.47
1:A:196:ALA:HB1	1:A:241:VAL:HG11	1.95	0.47
1:B:242:LEU:HB3	1:C:264:LEU:HD13	1.97	0.46
1:B:69:GLY:HA2	1:B:90:GLN:OE1	2.15	0.46
1:D:28:GLN:HE21	1:D:59:LEU:HD22	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:GLN:HB2	1:B:74:PRO:HD2	1.98	0.46
1:A:203:HIS:HB2	1:A:206:GLU:HG2	1.99	0.45
1:A:9:ALA:HB2	1:A:104:VAL:HG21	1.98	0.45
1:C:6:ARG:HD3	1:C:105:ASP:HB2	1.97	0.45
1:A:204:ALA:O	1:A:205:SER:HB2	2.17	0.45
1:D:204:ALA:O	1:D:205:SER:HB2	2.17	0.45
1:D:64:ILE:HD12	1:D:64:ILE:N	2.31	0.45
1:B:204:ALA:O	1:B:205:SER:HB2	2.17	0.45
1:D:9:ALA:HB2	1:D:104:VAL:HG21	1.99	0.45
1:A:203:HIS:CB	1:A:206:GLU:HG2	2.47	0.44
1:D:236:MET:HB2	1:D:241:VAL:CG2	2.48	0.44
1:A:129:SER:HB2	1:A:139:GLU:OE2	2.18	0.44
1:A:281:LEU:C	1:A:281:LEU:HD23	2.39	0.44
1:C:9:ALA:HB2	1:C:104:VAL:HG21	2.00	0.43
1:C:297:VAL:O	1:D:299:ASP:CB	2.41	0.43
1:D:110:CYS:HB3	1:D:111:PRO:CD	2.48	0.43
1:D:127:TYR:N	1:D:128:PRO:HD2	2.33	0.43
1:D:292:ILE:HB	1:D:297:VAL:HG22	1.99	0.43
1:D:64:ILE:CD1	7:D:515:HOH:O	2.66	0.43
1:A:127:TYR:N	1:A:128:PRO:CD	2.82	0.43
1:A:236:MET:HB2	1:A:241:VAL:CG2	2.49	0.43
1:C:6:ARG:HH12	2:C:402:EDO:H21	1.83	0.43
1:C:64:ILE:N	1:C:64:ILE:HD12	2.34	0.43
1:B:64:ILE:HD12	1:B:64:ILE:N	2.34	0.42
1:C:127:TYR:N	1:C:128:PRO:CD	2.82	0.42
1:D:10:LEU:HD11	1:D:303:LEU:HD11	2.01	0.42
1:A:53:ILE:HD13	1:A:294:GLY:HA2	2.01	0.42
1:B:127:TYR:N	1:B:128:PRO:CD	2.82	0.42
1:A:110:CYS:HB3	1:A:111:PRO:CD	2.49	0.42
1:C:281:LEU:C	1:C:281:LEU:HD23	2.39	0.42
1:B:281:LEU:HD23	1:B:281:LEU:C	2.40	0.42
1:D:28:GLN:HG2	1:D:59:LEU:HD22	2.01	0.42
1:C:204:ALA:O	1:C:205:SER:HB2	2.18	0.41
1:C:227:LYS:HD3	1:C:227:LYS:HA	1.90	0.41
1:A:159:HIS:HB2	7:A:502:HOH:O	2.20	0.41
1:B:236:MET:HB2	1:B:241:VAL:CG2	2.51	0.41
1:D:127:TYR:N	1:D:128:PRO:CD	2.83	0.41
1:B:111:PRO:HB2	1:B:288:SER:HA	2.02	0.41
1:A:236:MET:HB3	1:A:240:MET:HE1	2.02	0.41
1:B:183:GLN:OE1	1:B:278:ARG:HG3	2.21	0.41
1:C:277:GLY:O	1:C:278:ARG:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:GLN:HG2	7:D:518:HOH:O	2.21	0.41
1:B:260:ILE:N	1:B:261:PRO:HD2	2.36	0.41
1:C:110:CYS:HB3	1:C:111:PRO:CD	2.50	0.41
1:A:178:VAL:HG22	1:A:251:VAL:HG21	2.02	0.40
1:B:110:CYS:HB3	1:B:111:PRO:CD	2.51	0.40
1:A:140:ASP:CB	1:A:168:ARG:HH11	2.34	0.40
1:C:127:TYR:N	1:C:128:PRO:HD2	2.36	0.40
1:D:273:LEU:CD2	1:D:282:SER:HB2	2.51	0.40
1:D:313:GLN:HG2	7:D:526:HOH:O	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	312/335 (93%)	298 (96%)	14 (4%)	0	100	100
1	B	309/335 (92%)	297 (96%)	11 (4%)	1 (0%)	37	61
1	C	303/335 (90%)	292 (96%)	11 (4%)	0	100	100
1	D	312/335 (93%)	299 (96%)	13 (4%)	0	100	100
All	All	1236/1340 (92%)	1186 (96%)	49 (4%)	1 (0%)	48	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	208	GLN

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	243/261 (93%)	243 (100%)	0	100	100
1	B	242/261 (93%)	237 (98%)	5 (2%)	48	76
1	C	238/261 (91%)	237 (100%)	1 (0%)	89	96
1	D	243/261 (93%)	242 (100%)	1 (0%)	89	96
All	All	966/1044 (92%)	959 (99%)	7 (1%)	81	93

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	52	GLN
1	B	61	GLN
1	B	133	ASN
1	B	140	ASP
1	B	314	PRO
1	C	240	MET
1	D	129	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	49	GLN
1	C	29	GLN
1	C	286	HIS
1	D	28	GLN
1	D	133	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
2	EDO	A	402	-	3,3,3	0.25	0	2,2,2	0.44	0
2	EDO	A	401	-	3,3,3	0.27	0	2,2,2	0.47	0
2	EDO	A	403	-	3,3,3	0.63	0	2,2,2	0.44	0
5	CO2	C	403	-	2,2,2	0.36	0	1,1,1	0.49	0
5	CO2	C	401	-	2,2,2	0.97	0	1,1,1	0.08	0
2	EDO	C	402	-	3,3,3	0.25	0	2,2,2	0.16	0
5	CO2	B	401	-	2,2,2	0.43	0	1,1,1	0.09	0

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
2	EDO	A	402	-	-	1/1/1/1	-
2	EDO	A	401	-	-	1/1/1/1	-
2	EDO	A	403	-	-	0/1/1/1	-
2	EDO	C	402	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	EDO	O1-C1-C2-O2
2	C	402	EDO	O1-C1-C2-O2
2	A	402	EDO	O1-C1-C2-O2

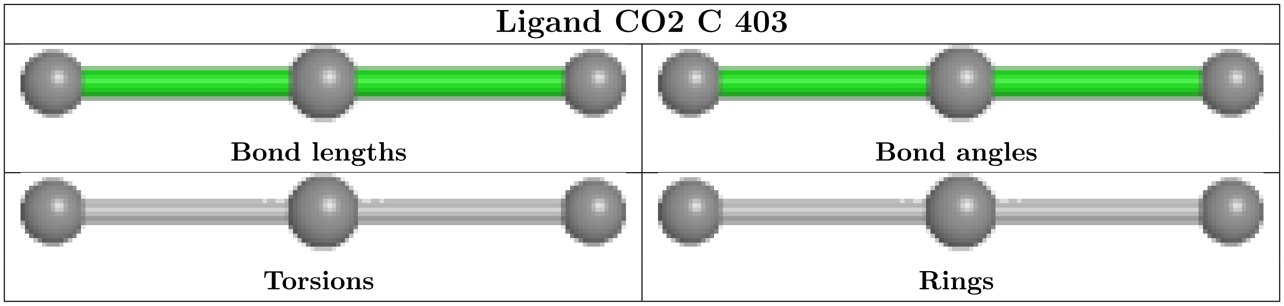
There are no ring outliers.

1 monomer is involved in 1 short contact:

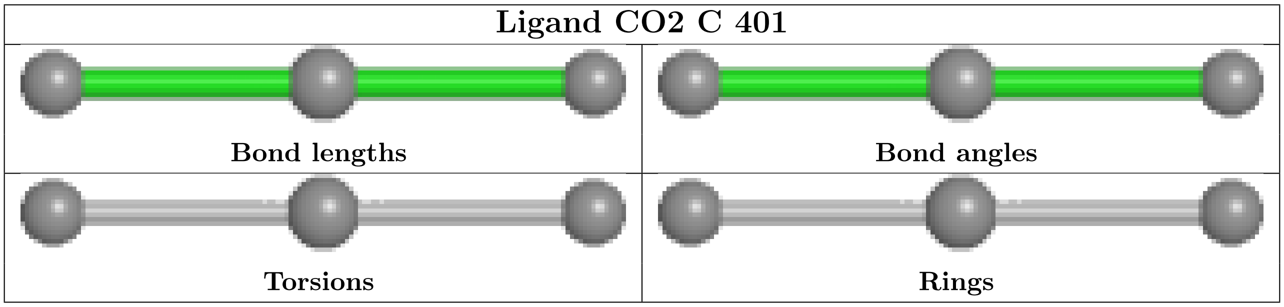
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	402	EDO	1	0

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.

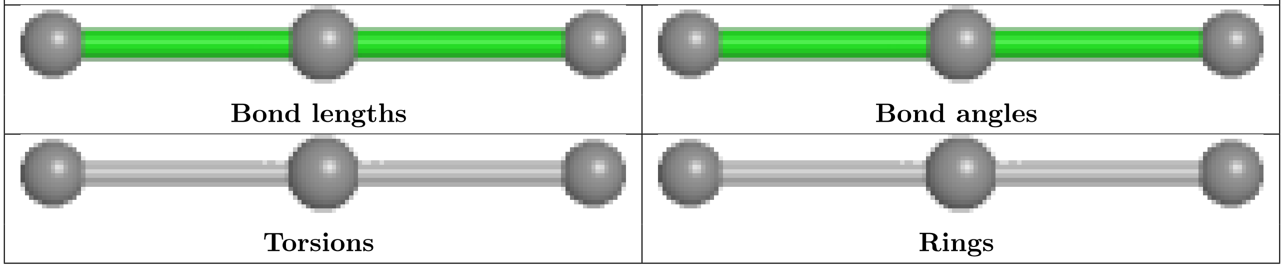
Ligand CO2 C 403



Ligand CO2 C 401



Ligand CO2 B 401



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	314/335 (93%)	-1.62	0	100	100	13, 26, 42, 68	0
1	B	313/335 (93%)	-1.50	0	100	100	19, 34, 54, 79	0
1	C	307/335 (91%)	-1.51	0	100	100	20, 33, 48, 59	0
1	D	314/335 (93%)	-1.62	0	100	100	13, 25, 42, 58	0
All	All	1248/1340 (93%)	-1.57	0	100	100	13, 29, 48, 79	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	B	402	1/1	0.93	0.05	30,30,30,30	0
5	CO2	B	401	3/3	0.97	0.04	20,20,20,20	0
4	NA	A	405	1/1	0.97	0.08	30,30,30,30	0
3	ZN	A	404	1/1	0.98	0.03	58,58,58,58	0

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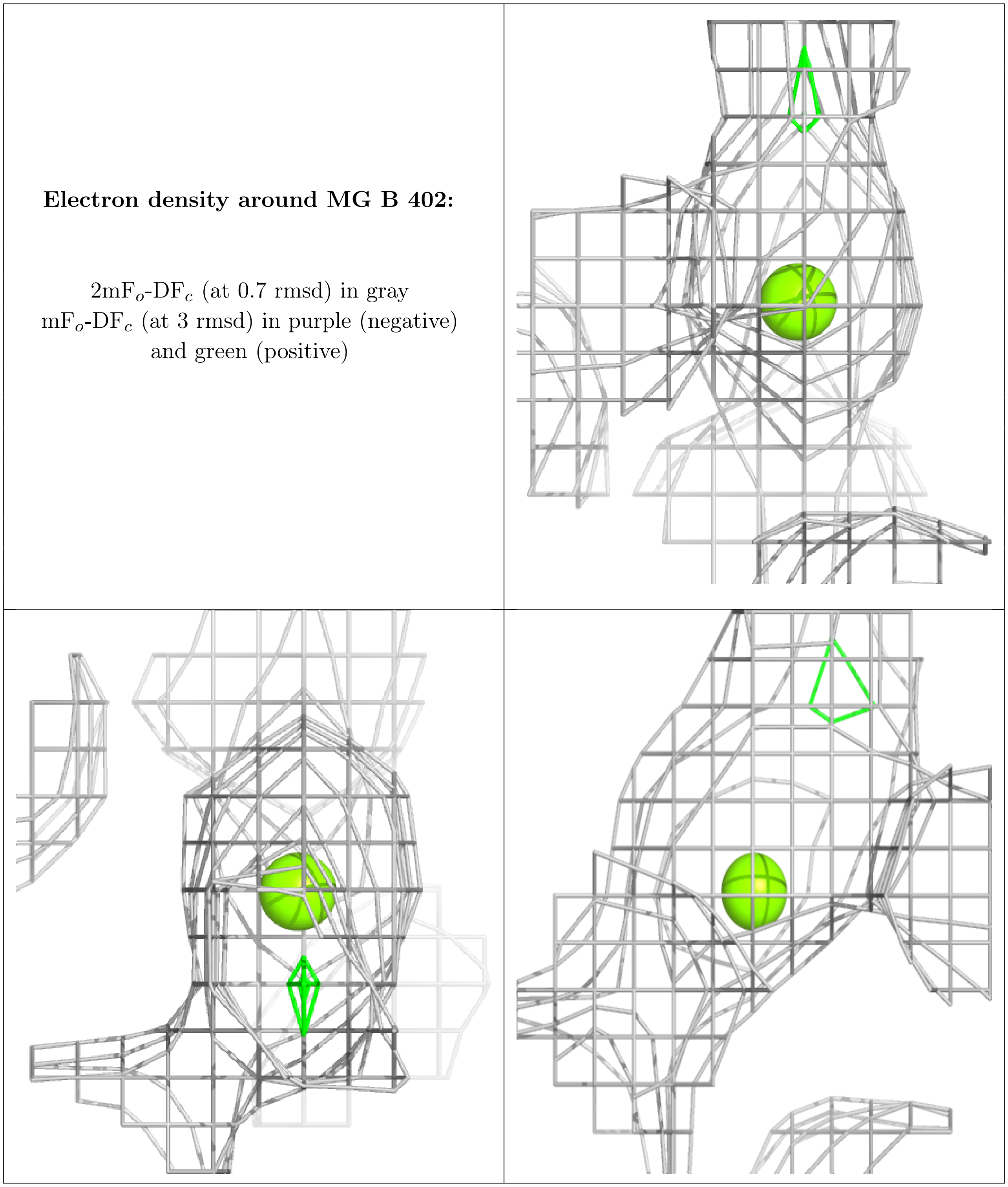
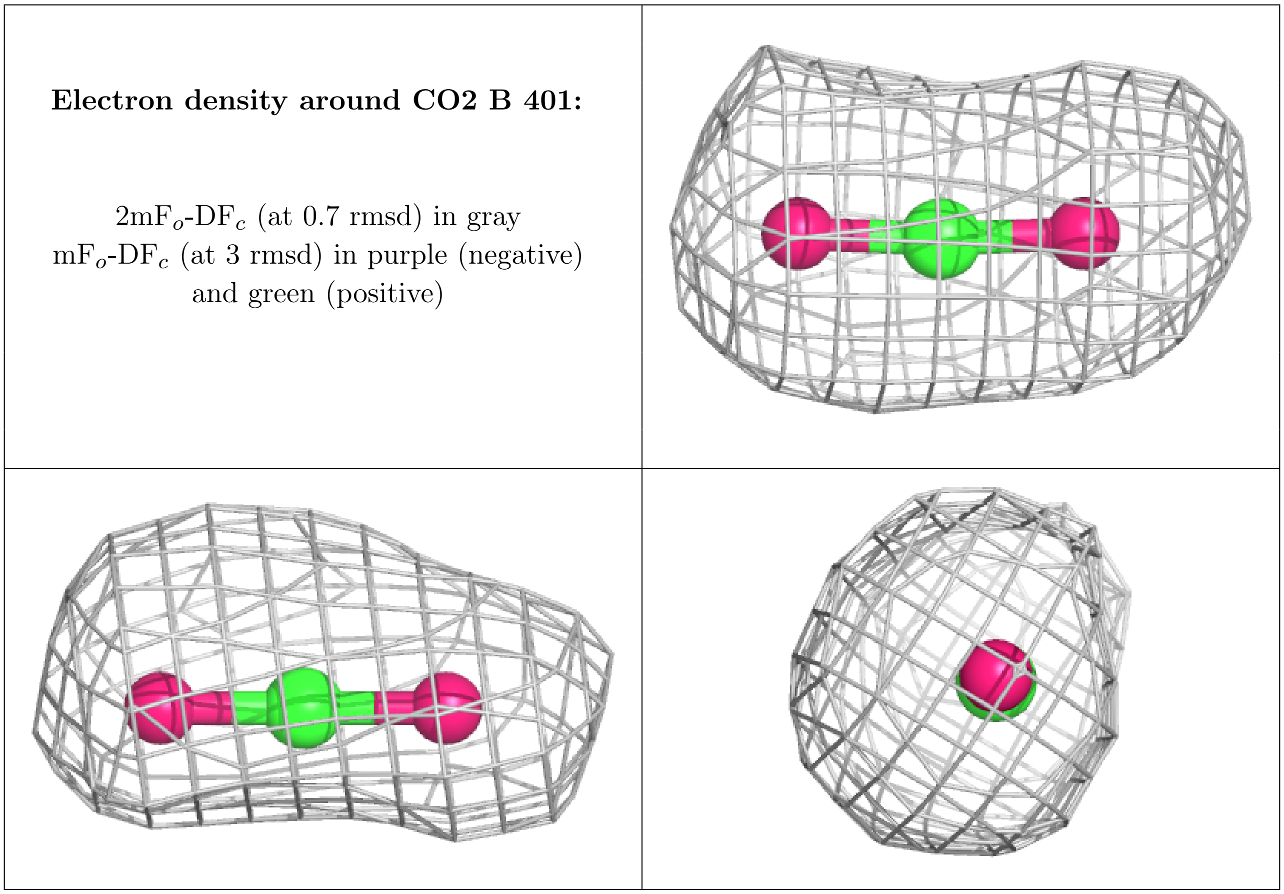
Mol	**Type**	**Chain**	**Res**	**Atoms**	**RSCC**	**RSR**	**B-factors($\mathring{A}^2$)**	**Q<0.9**
2	EDO	A	401	4/4	0.98	0.04	20,20,20,20	2
2	EDO	A	402	4/4	0.98	0.05	20,20,20,20	2
5	CO2	C	403	3/3	0.98	0.04	20,20,20,20	0
2	EDO	C	402	4/4	0.98	0.03	20,20,20,20	2
4	NA	D	403	1/1	0.99	0.02	30,30,30,30	0
3	ZN	C	404	1/1	0.99	0.02	58,58,58,58	0
5	CO2	C	401	3/3	0.99	0.03	20,20,20,20	0
3	ZN	D	401	1/1	0.99	0.03	73,73,73,73	0
2	EDO	A	403	4/4	0.99	0.04	20,20,20,20	2
6	MG	D	402	1/1	0.99	0.03	30,30,30,30	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.



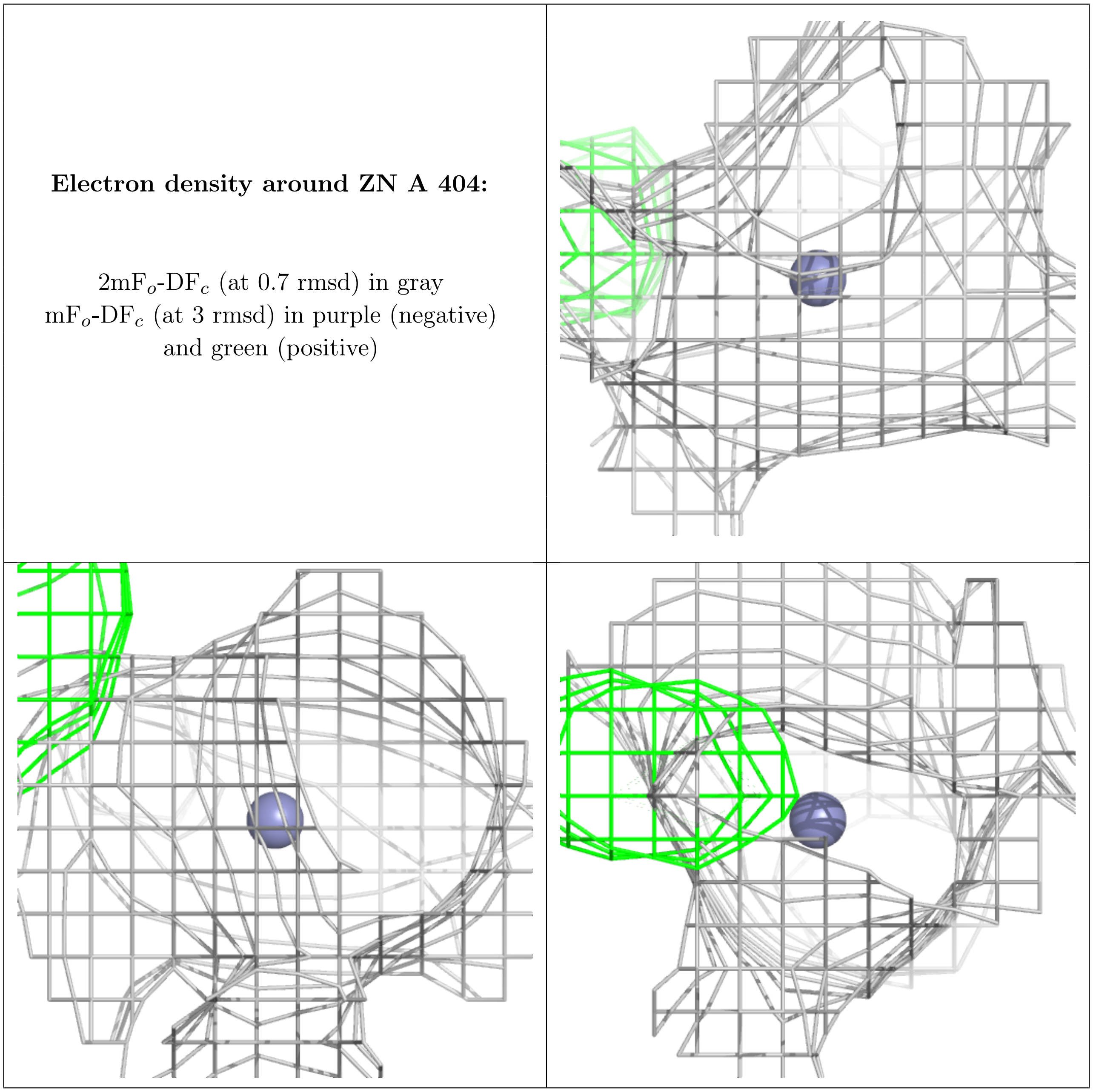
Electron density around MG B 402:

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 CO2 B 401:

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

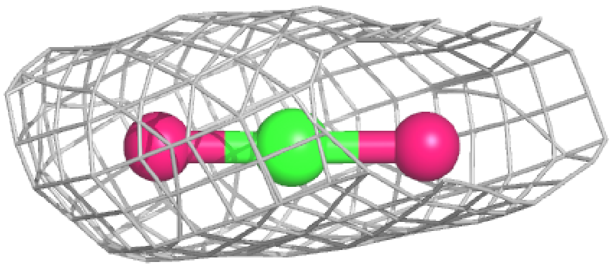


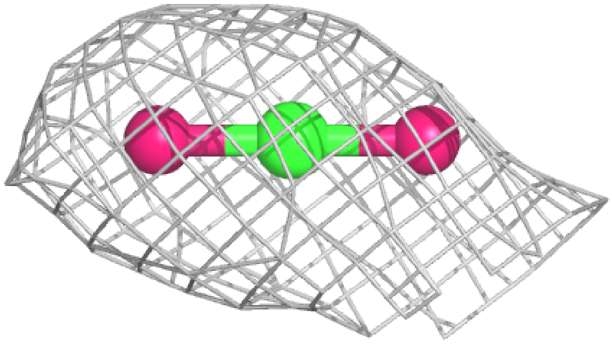
Electron density around ZN A 404:

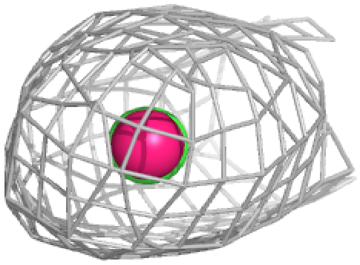
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

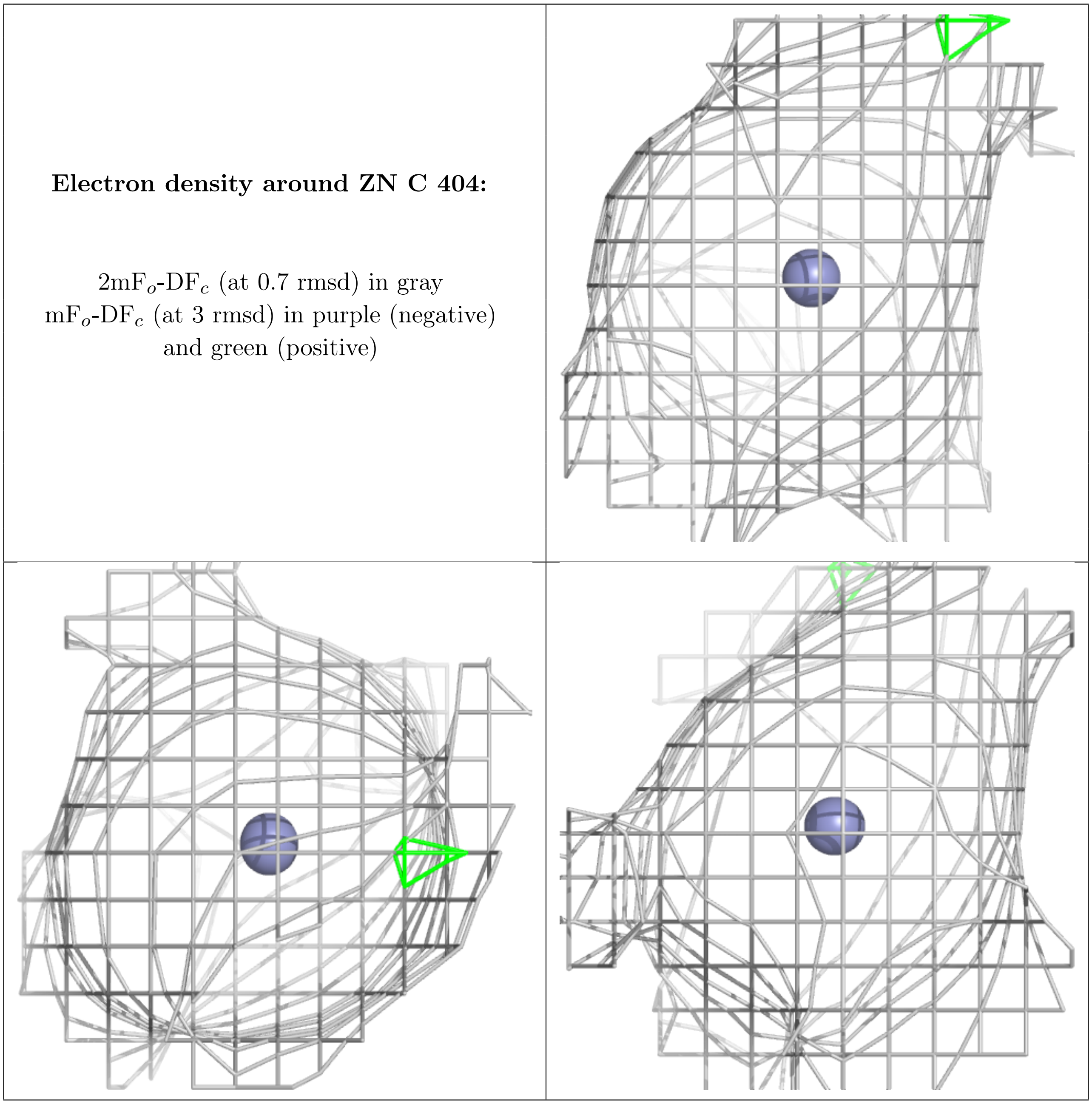
Electron density around CO2 C 403:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)







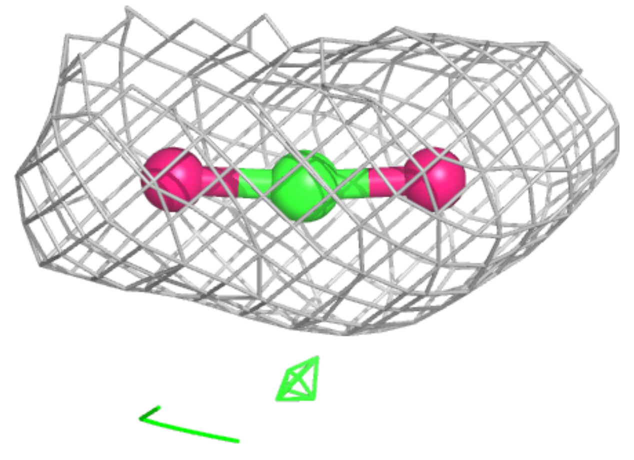


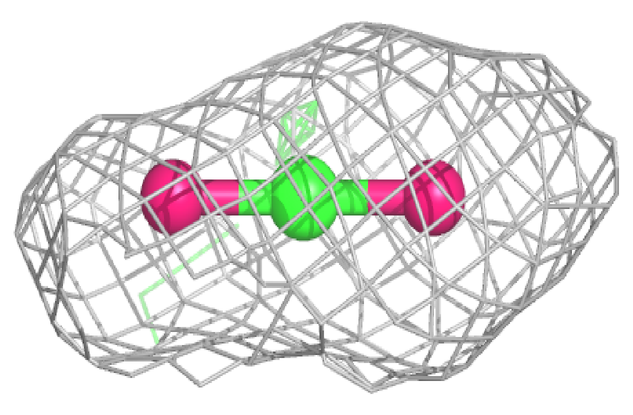
Electron density around ZN C 404:

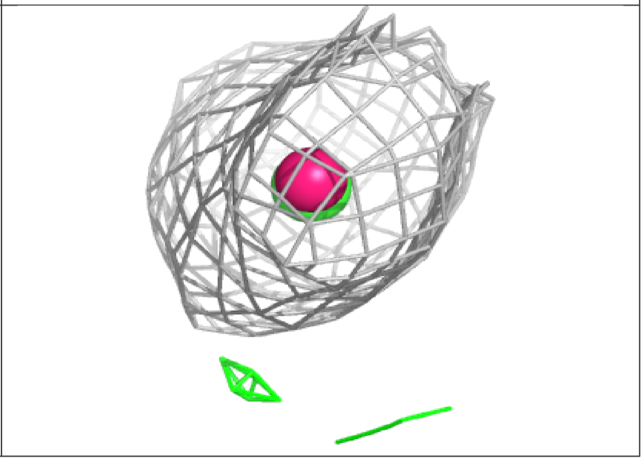
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

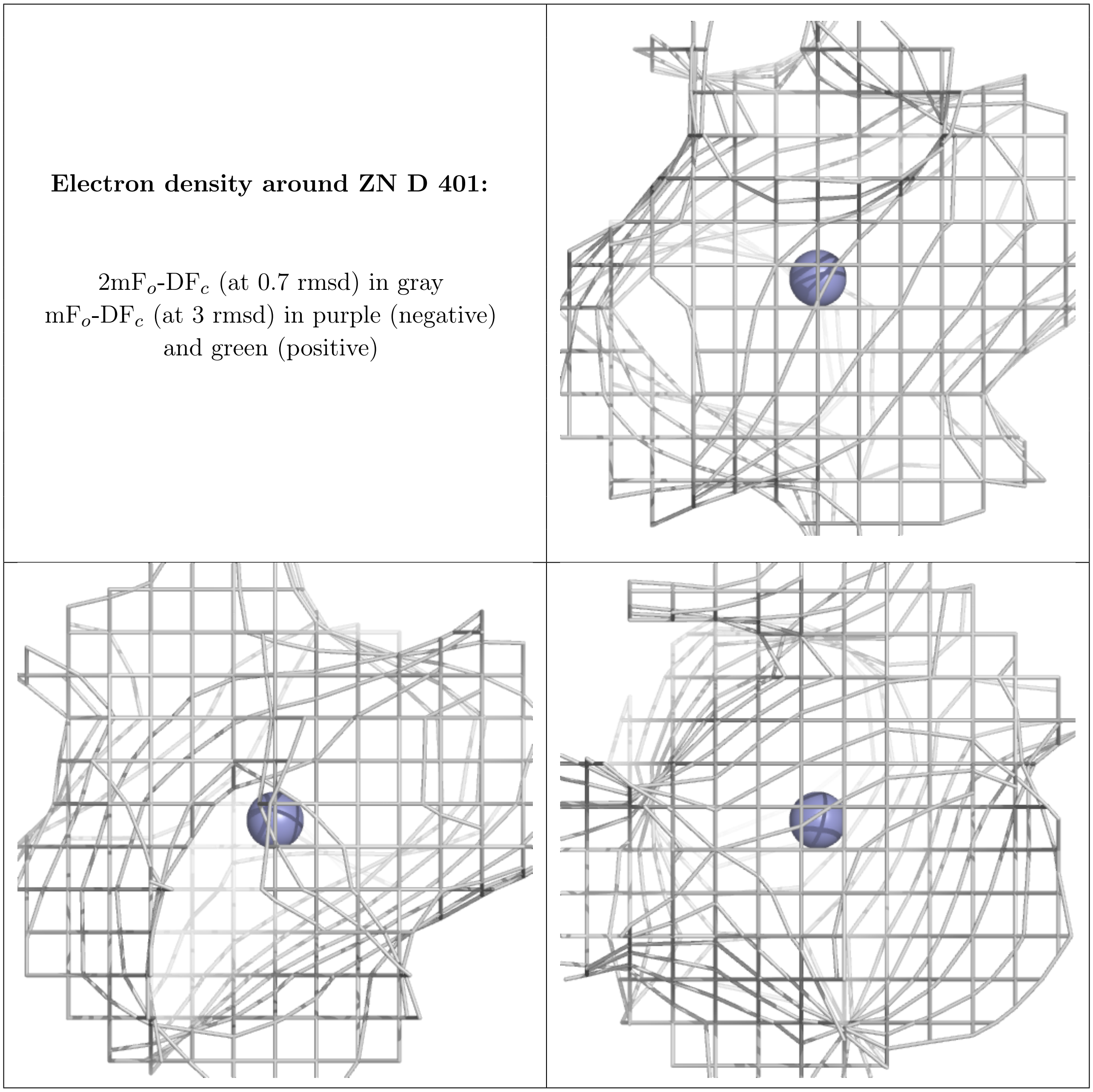
Electron density around CO2 C 401:

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



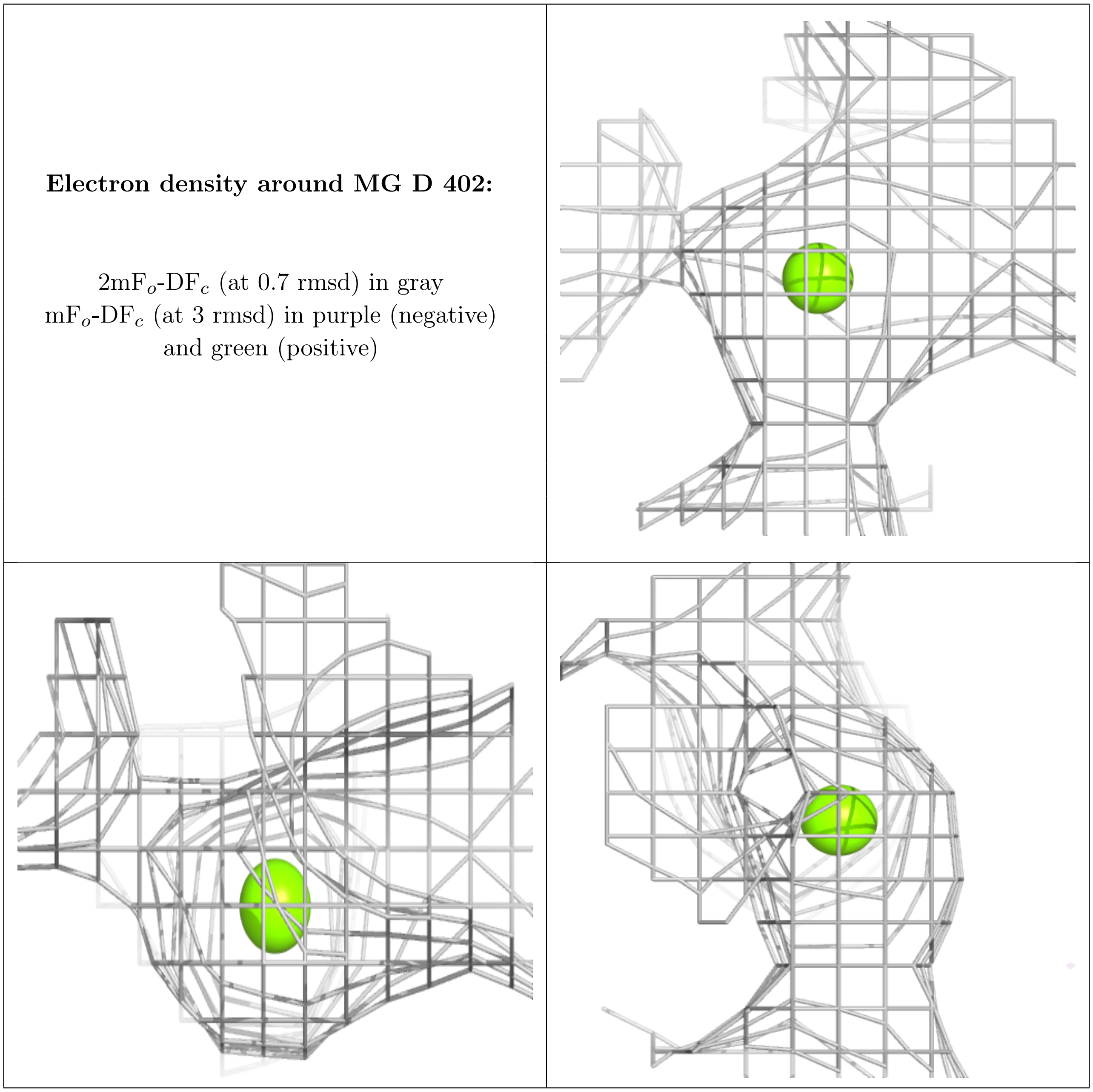






Electron density around ZN D 401:

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



Electron density around MG D 402:

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.