



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:28 PM UTC

PDB ID : 9G7I / pdb_00009g7i
Title : Structure of carbon monoxide dehydrogenase/acetyl-CoA synthase (CODH/ACS) in complex with acetyl-Coenzyme A from *Clostridium autoethanogenum*
Authors : Lemaire, O.N.; Yin, M.D.; Murphy, B.J.; Wagner, T.
Deposited on : 2024-07-21
Resolution : 2.93 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

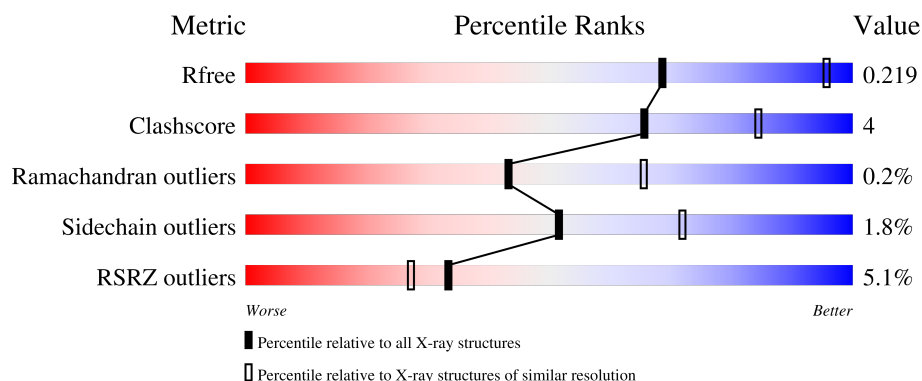
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.93 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	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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	A	708	15% 82% 15% ..
1	D	708	3% 92% 8% .
2	B	631	92% 7% .
2	C	631	% 92% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	B	717	-	-	-	X

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 20497 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.

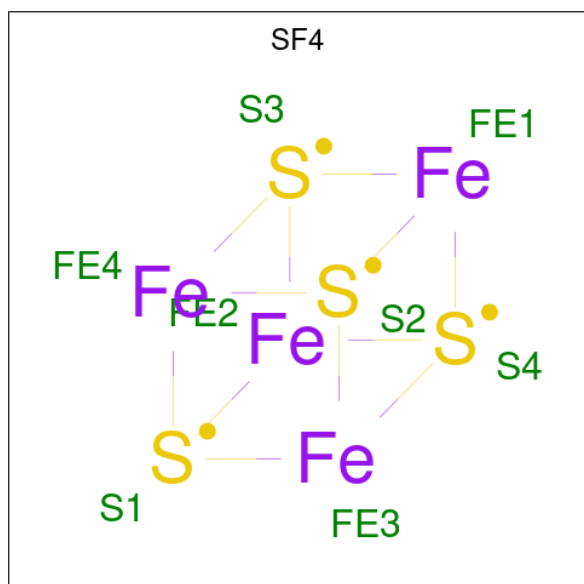
- Molecule 1 is a protein called CO-methylating acetyl-CoA synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	694	Total	C	N	O	S	0	1	0
			5284	3383	860	1006	35			
1	D	708	Total	C	N	O	S	0	0	0
			5392	3449	884	1023	36			

- Molecule 2 is a protein called Carbon monoxide dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	629	Total	C	N	O	S	0	0	0
			4723	2967	814	902	40			
2	C	630	Total	C	N	O	S	0	1	0
			4742	2978	818	906	40			

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).

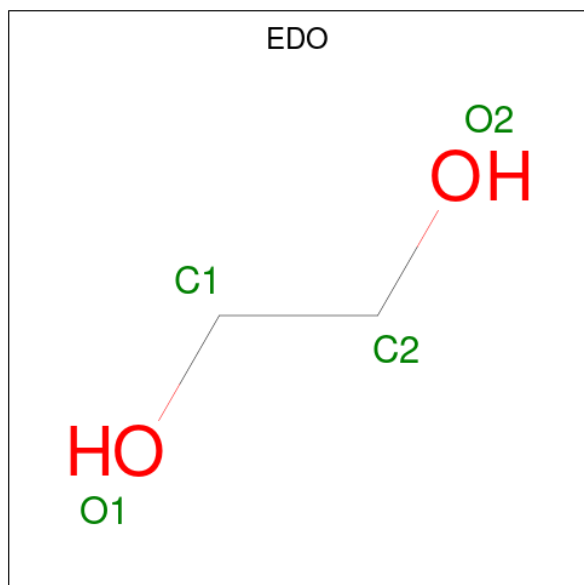


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is NICKEL (II) ION (CCD ID: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Ni	0	0
			2	2		
4	D	2	Total	Ni	0	0
			2	2		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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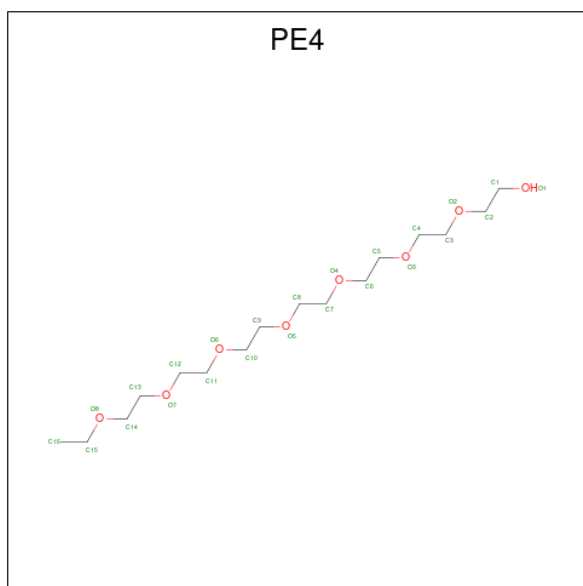
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0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

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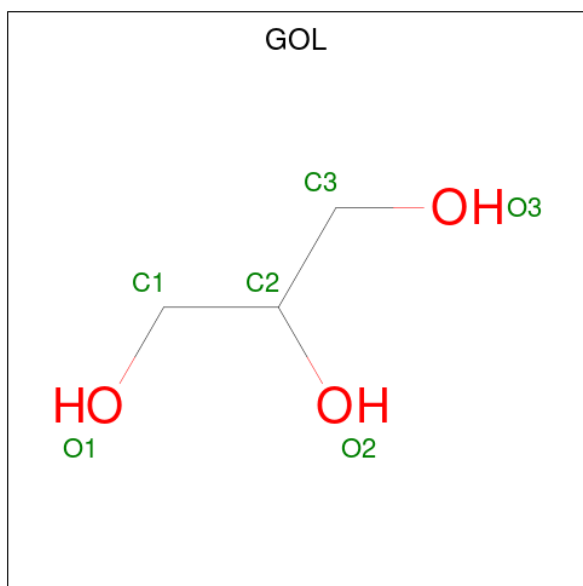
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0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

- Molecule 6 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (CCD ID: PE4) (formula: C₁₆H₃₄O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			7	4	3		
8	B	1	Total	C	O	0	0
			7	4	3		
8	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	4	Total	Ca	0	0
			4	4		
9	B	1	Total	Ca	0	0
			1	1		
9	C	3	Total	Ca	0	0
			3	3		
9	D	2	Total	Ca	0	0
			2	2		

- Molecule 10 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

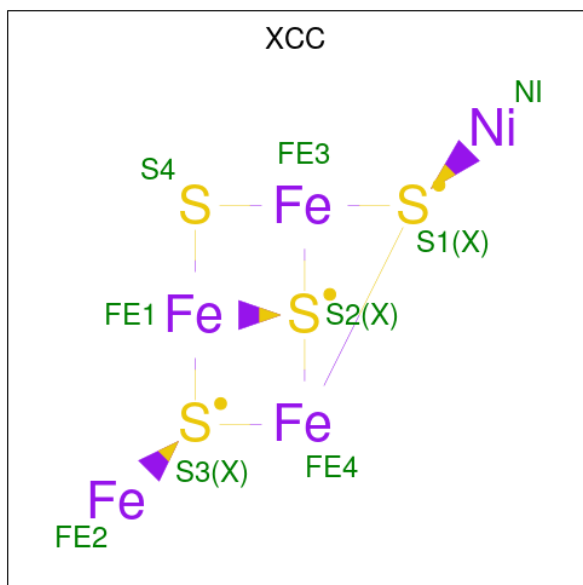
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	2	Total	Cl	0	0
			2	2		
10	B	5	Total	Cl	0	0
			5	5		

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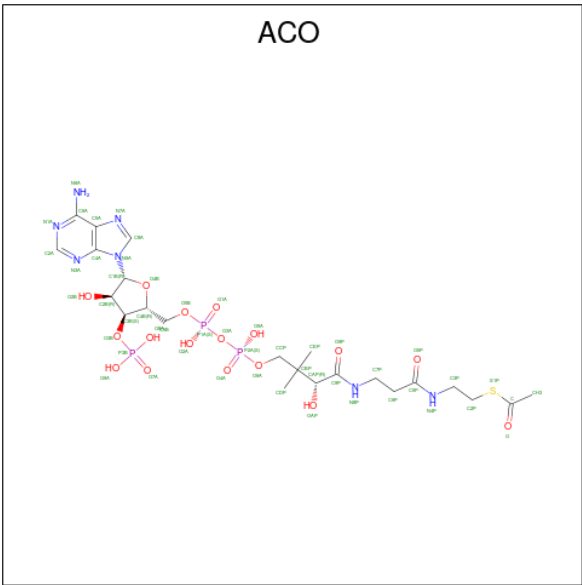
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	C	1	Total	Cl	0	0
			1	1		

- Molecule 11 is FE(4)-NI(1)-S(4) CLUSTER (CCD ID: XCC) (formula: Fe_4NiS_4) (labeled as "Ligand of Interest" by depositor).



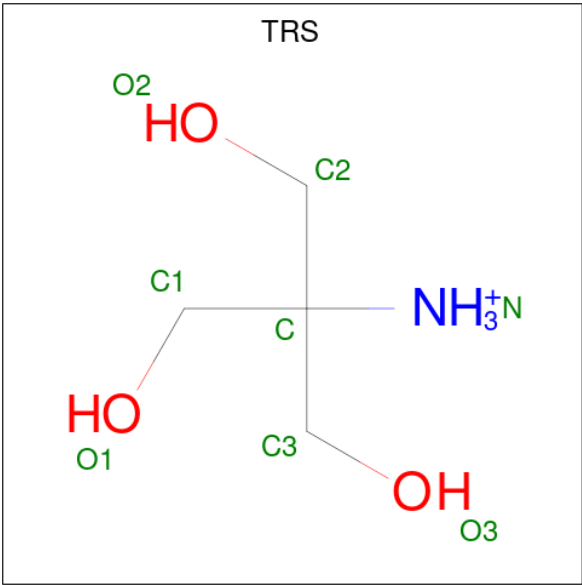
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
11	C	1	Total	Fe	Ni	S	0	0
			9	4	1	4		

- Molecule 12 is ACETYL COENZYME *A (CCD ID: ACO) (formula: $\text{C}_{23}\text{H}_{38}\text{N}_7\text{O}_{17}\text{P}_3\text{S}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
12	D	1	51	23	7	17	3	0	0

- Molecule 13 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
13	D	1	8	4	1	3	0	0

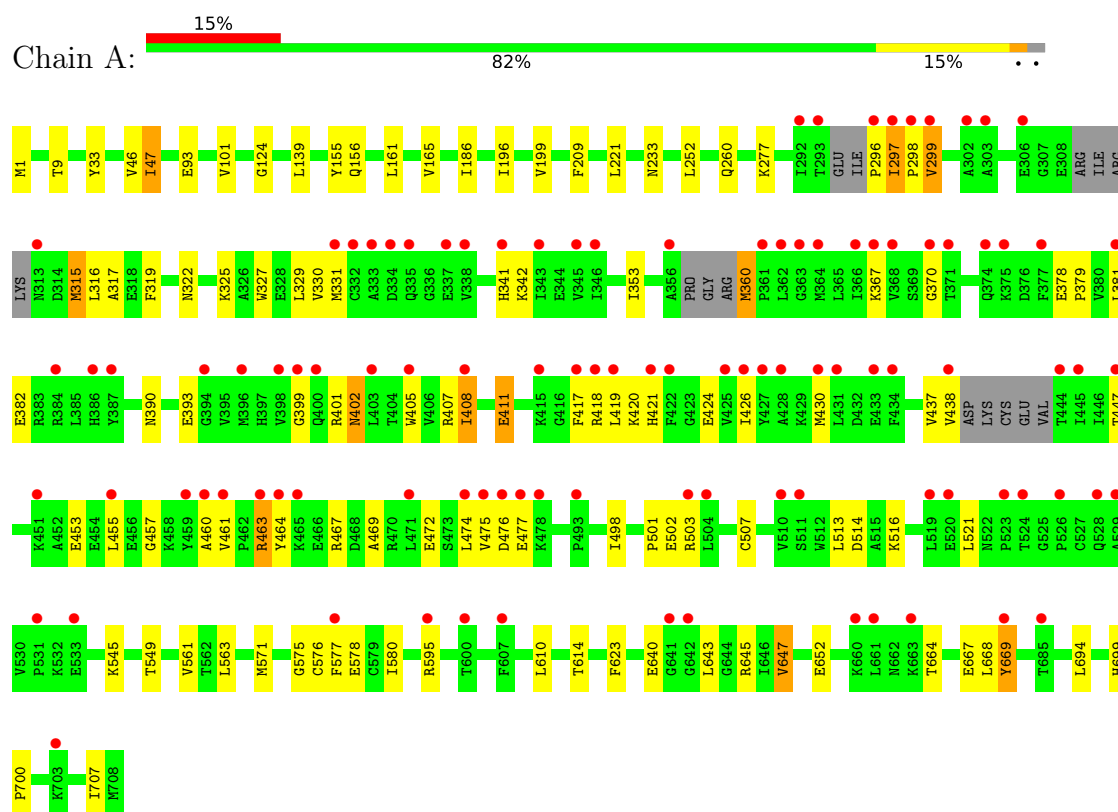
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	2	Total 2	O 2	0	0
14	B	5	Total 5	O 5	0	0
14	C	5	Total 5	O 5	0	0
14	D	2	Total 2	O 2	0	0

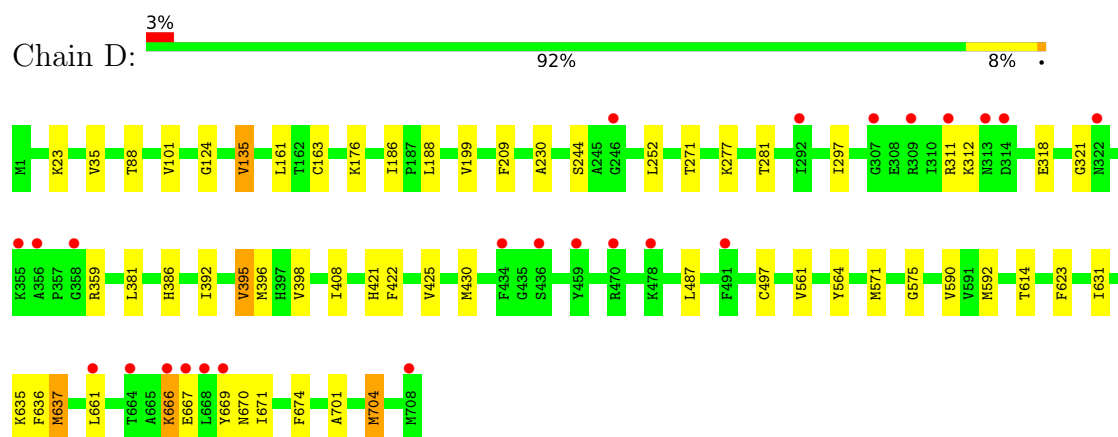
3 Residue-property plots

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: CO-methylating acetyl-CoA synthase

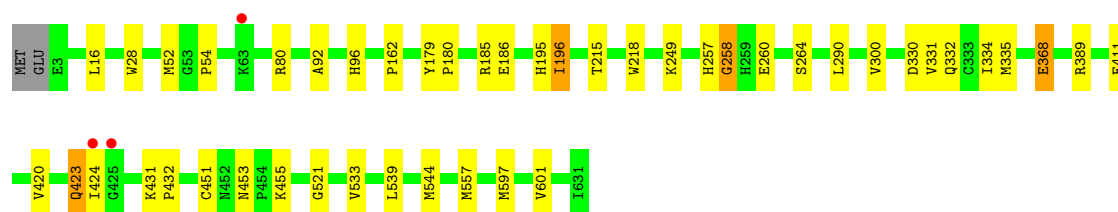


• Molecule 1: CO-methylating acetyl-CoA synthase



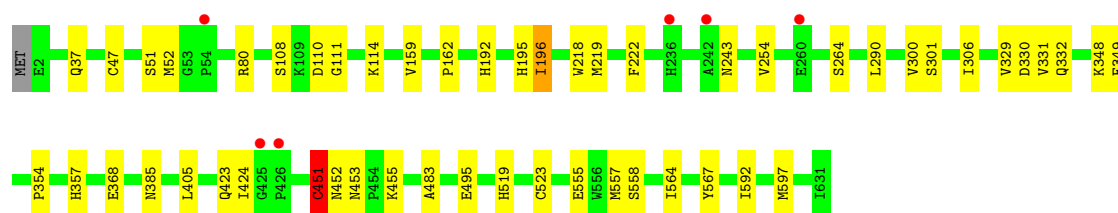
- Molecule 2: Carbon monoxide dehydrogenase

Chain B:  92% 7%



- Molecule 2: Carbon monoxide dehydrogenase

Chain C:  92% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	298.08Å 298.08Å 127.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.68 – 2.93 49.68 – 2.93	Depositor EDS
% Data completeness (in resolution range)	81.4 (49.68-2.93) 81.4 (49.68-2.93)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.190 , 0.220 0.190 , 0.219	Depositor DCC
R_{free} test set	5007 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å ²)	84.5	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 64.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20497	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% 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: XCC, PE4, GOL, PEG, SF4, CL, ACO, EDO, NI, CA, TRS

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	0.70	0/5375	0.97	5/7271 (0.1%)
1	D	0.64	0/5488	0.90	4/7428 (0.1%)
2	B	0.64	0/4797	0.96	5/6488 (0.1%)
2	C	0.65	0/4817	0.95	2/6515 (0.0%)
All	All	0.66	0/20477	0.95	16/27702 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	402	ASN	N-CA-C	-7.75	101.68	112.45
1	D	176	LYS	N-CA-C	7.14	121.25	111.39
2	B	521	GLY	N-CA-C	7.12	118.75	111.56
1	D	590	VAL	N-CA-C	6.35	118.54	108.89
2	B	52	MET	N-CA-C	-6.22	104.60	111.82
1	D	271	THR	CB-CA-C	-5.91	101.30	111.23
1	A	342	LYS	N-CA-C	-5.90	98.92	108.41
2	C	451	CYS	CB-CA-C	-5.86	107.08	114.40
2	C	110	ASP	N-CA-C	-5.75	103.54	110.44
1	A	399	GLY	CA-C-O	-5.58	117.77	122.29
2	B	424	ILE	N-CA-C	5.51	120.80	109.34
2	B	258	GLY	N-CA-C	5.41	117.03	111.56
1	D	271	THR	N-CA-C	5.38	118.51	107.69
1	A	341	HIS	N-CA-C	-5.31	102.46	110.70
2	B	257	HIS	CB-CA-C	5.15	119.64	109.66
1	A	514	ASP	N-CA-C	-5.02	105.88	111.36

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	5284	0	5365	70	0
1	D	5392	0	5489	33	0
2	B	4723	0	4803	31	0
2	C	4742	0	4818	32	0
3	A	8	0	0	1	0
3	B	8	0	0	1	0
3	C	16	0	0	1	0
3	D	8	0	0	1	0
4	A	2	0	0	0	0
4	D	2	0	0	0	0
5	A	32	0	48	0	0
5	B	60	0	90	0	0
5	C	28	0	42	0	0
5	D	16	0	24	0	0
6	A	10	0	12	0	0
7	A	6	0	8	0	0
7	B	24	0	32	0	0
7	D	6	0	8	0	0
8	A	7	0	10	0	0
8	B	7	0	10	0	0
8	D	7	0	10	0	0
9	A	4	0	0	0	0
9	B	1	0	0	0	0
9	C	3	0	0	0	0
9	D	2	0	0	0	0
10	A	2	0	0	0	0
10	B	5	0	0	0	0
10	C	1	0	0	0	0
11	B	9	0	0	0	0
11	C	9	0	0	0	0
12	D	51	0	34	2	0
13	D	8	0	12	0	0
14	A	2	0	0	0	0
14	B	5	0	0	0	0
14	C	5	0	0	0	0
14	D	2	0	0	0	0
All	All	20497	0	20815	157	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 4.

All (157) 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:C:424:ILE:HD11	1:D:281:THR:HB	1.64	0.79
1:A:299:VAL:HG23	1:A:393:GLU:HB3	1.73	0.71
1:A:316:LEU:HB3	1:A:408:ILE:HD11	1.73	0.71
1:D:277:LYS:O	1:D:281:THR:HG23	1.92	0.70
1:D:701:ALA:HA	1:D:704:MET:HE3	1.75	0.69
1:A:408:ILE:HG13	1:A:408:ILE:O	1.94	0.67
2:B:196:ILE:HD12	2:C:557:MET:HE1	1.78	0.65
1:A:315:MET:HE1	1:A:407:ARG:NH2	2.13	0.64
1:A:647:VAL:HG22	1:A:694:LEU:HD21	1.82	0.62
2:B:54:PRO:HD2	2:C:37:GLN:HB3	1.81	0.62
1:D:297:ILE:HG22	1:D:421:HIS:HB3	1.83	0.60
1:A:379:PRO:HG3	1:A:467:ARG:HD3	1.84	0.60
1:A:1:MET:HE1	1:A:9:THR:OG1	2.01	0.59
2:B:218:TRP:HZ2	2:B:544:MET:HE1	1.67	0.59
2:C:301:SER:C	2:C:405:LEU:HD11	2.30	0.57
1:A:463:ARG:HG3	1:A:467:ARG:HH21	1.72	0.55
1:A:647:VAL:CG2	1:A:694:LEU:HD21	2.38	0.54
1:A:317:ALA:HB3	1:A:408:ILE:HG12	1.90	0.53
2:C:423:GLN:HB2	1:D:281:THR:HG22	1.90	0.53
2:C:159:VAL:HG11	2:C:219:MET:SD	2.49	0.52
1:D:124:GLY:HA3	1:D:209:PHE:CZ	2.44	0.52
1:D:161:LEU:HD11	1:D:186:ILE:HD12	1.90	0.52
2:C:330:ASP:OD1	2:C:331:VAL:N	2.33	0.51
1:A:329:LEU:HD22	1:A:460:ALA:CA	2.39	0.51
1:D:592:MET:SD	1:D:631:ILE:HG12	2.51	0.51
1:A:405:TRP:HZ2	1:A:407:ARG:CZ	2.23	0.51
2:B:533:VAL:HG12	2:B:544:MET:HG2	1.93	0.51
2:B:557:MET:CE	2:C:52:MET:HG3	2.41	0.51
2:B:330:ASP:OD1	2:B:331:VAL:N	2.43	0.50
1:A:469:ALA:HA	1:A:472:GLU:HB2	1.92	0.50
1:D:408:ILE:HD11	1:D:422:PHE:HE2	1.76	0.50
1:A:640:GLU:O	1:A:645:ARG:NE	2.45	0.50
2:B:179:TYR:CG	2:B:180:PRO:HD2	2.47	0.50
1:A:664:THR:O	1:A:668:LEU:HG	2.12	0.50
1:A:513:LEU:HD23	1:A:516:LYS:HE2	1.94	0.49
2:C:195:HIS:CE1	2:C:196:ILE:HG22	2.47	0.49
1:A:664:THR:HA	1:A:667:GLU:CD	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:CYS:N	3:A:801:SF4:S1	2.86	0.49
2:C:300:VAL:HG23	2:C:306:ILE:HB	1.95	0.49
1:A:296:PRO:HB2	1:A:424:GLU:OE1	2.13	0.48
1:A:419:LEU:HD21	1:A:447:THR:HG21	1.95	0.48
1:D:636:PHE:CD2	1:D:637:MET:HG3	2.48	0.48
1:A:360:MET:HE3	1:A:360:MET:HB3	1.69	0.48
1:A:418:ARG:HG3	1:A:420:LYS:H	1.79	0.48
2:B:557:MET:HE2	2:B:557:MET:HB2	1.75	0.48
2:B:557:MET:HA	2:C:51:SER:OG	2.13	0.48
1:D:614:THR:HG22	1:D:623:PHE:HB3	1.95	0.48
2:B:249:LYS:O	2:B:389:ARG:NH1	2.46	0.48
2:B:264:SER:HB2	2:B:300:VAL:HG21	1.95	0.48
1:A:330:VAL:HG11	1:A:381:LEU:HD22	1.96	0.47
1:A:498:ILE:O	1:A:503:ARG:NH1	2.47	0.47
1:A:319:PHE:CE2	1:A:360:MET:HB2	2.49	0.47
1:A:297:ILE:HB	1:A:421:HIS:HB3	1.96	0.47
1:A:507:CYS:HB3	1:A:576:CYS:SG	2.54	0.47
1:D:381:LEU:HD12	1:D:430:MET:SD	2.55	0.47
1:A:402:ASN:HB2	1:A:464:TYR:HE2	1.80	0.47
2:B:368:GLU:CD	2:B:368:GLU:H	2.23	0.47
1:A:475:VAL:HB	1:A:477:GLU:HG2	1.95	0.47
1:D:321:GLY:HA2	12:D:805:ACO:H62A	1.80	0.46
2:C:557:MET:SD	2:C:558:SER:N	2.88	0.46
1:A:643:LEU:CD1	1:A:669:TYR:HE2	2.29	0.46
2:C:564:ILE:HA	2:C:567:TYR:CE2	2.51	0.46
1:D:661:LEU:HD21	1:D:674:PHE:HD2	1.80	0.46
2:C:453:ASN:OD1	2:C:455:LYS:HG3	2.16	0.46
1:A:417:PHE:CE1	1:A:421:HIS:HB2	2.50	0.46
2:B:258:GLY:HA3	2:B:330:ASP:OD1	2.15	0.46
2:B:557:MET:HE3	2:C:52:MET:HG3	1.98	0.46
2:B:162:PRO:HG2	2:B:218:TRP:HE3	1.82	0.45
1:A:353:ILE:HD11	1:A:360:MET:HG3	1.97	0.45
2:B:195:HIS:CE1	2:B:196:ILE:HG22	2.51	0.45
1:D:318:GLU:OE1	1:D:359:ARG:NE	2.49	0.45
1:D:88:THR:OG1	1:D:244:SER:HB3	2.16	0.45
1:D:135:VAL:HG22	1:D:230:ALA:HB2	1.97	0.45
1:D:163:CYS:HB3	1:D:188:LEU:HD11	1.99	0.45
1:A:437:VAL:HG11	1:A:521:LEU:CD2	2.47	0.45
2:C:254:VAL:HB	2:C:290:LEU:HD23	1.99	0.45
1:D:392:ILE:HB	1:D:395:VAL:HG22	1.98	0.45
1:A:411:GLU:H	1:A:411:GLU:CD	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:218:TRP:CZ2	2:B:544:MET:HE1	2.50	0.45
1:D:199:VAL:HG13	1:D:252:LEU:HD11	1.97	0.45
1:A:33:TYR:CD2	1:A:101:VAL:HG13	2.51	0.45
1:A:378:GLU:O	1:A:381:LEU:HB2	2.17	0.45
2:C:483:ALA:HB1	2:C:519:HIS:CD2	2.51	0.44
1:D:666:LYS:HB2	1:D:670:ASN:HB3	2.00	0.44
1:A:476:ASP:OD1	1:A:501:PRO:HB2	2.17	0.44
2:C:354:PRO:HA	2:C:357:HIS:CD2	2.53	0.44
1:D:135:VAL:HG22	1:D:230:ALA:CB	2.47	0.44
1:D:311:ARG:HH11	12:D:805:ACO:P2A	2.40	0.44
1:A:645:ARG:HD2	1:A:707:ILE:HD12	1.99	0.44
1:A:614:THR:HG22	1:A:623:PHE:HB3	2.00	0.44
2:C:162:PRO:HG2	2:C:218:TRP:HE3	1.82	0.44
1:D:637:MET:HE2	1:D:637:MET:HB3	1.70	0.44
1:A:325:LYS:NZ	1:A:453:GLU:HG2	2.32	0.44
2:C:264:SER:HB2	2:C:300:VAL:HG11	1.98	0.44
2:C:368:GLU:H	2:C:368:GLU:CD	2.26	0.44
1:A:463:ARG:HA	1:A:463:ARG:HD2	1.79	0.43
1:A:545:LYS:HE3	1:A:549:THR:HG23	2.00	0.43
1:D:35:VAL:HG12	1:D:101:VAL:HG21	2.00	0.43
1:A:277:LYS:HD2	2:B:423:GLN:HB3	1.99	0.43
1:A:298:PRO:HD2	1:A:421:HIS:CE1	2.53	0.43
1:A:699:HIS:CD2	1:A:700:PRO:HD2	2.53	0.43
2:B:597:MET:HG3	2:B:601:VAL:HG22	2.00	0.43
1:D:396:MET:HE3	1:D:398:VAL:HG23	2.01	0.43
1:A:370:GLY:HA3	1:A:438:VAL:C	2.43	0.43
1:A:460:ALA:O	1:A:461:VAL:C	2.61	0.43
1:A:460:ALA:HB1	1:A:464:TYR:CZ	2.54	0.43
1:D:667:GLU:HB2	1:D:669:TYR:CD1	2.54	0.43
2:B:411:GLU:HA	2:B:411:GLU:OE1	2.19	0.43
1:A:155:TYR:OH	1:A:233:ASN:ND2	2.52	0.43
2:B:186:GLU:HG3	2:B:215:THR:HG21	2.00	0.43
2:B:334:ILE:O	2:B:335:MET:C	2.62	0.43
2:B:431:LYS:HA	2:B:539:LEU:HD21	2.00	0.42
1:A:382:GLU:HG3	1:A:467:ARG:HH12	1.83	0.42
2:B:260:GLU:HG2	2:B:331:VAL:HG22	2.02	0.42
2:C:108:SER:OG	2:C:111:GLY:HA3	2.19	0.42
2:B:16:LEU:HD21	2:B:28:TRP:CE3	2.54	0.42
2:B:92:ALA:HA	2:C:192:HIS:CD2	2.54	0.42
2:C:592:ILE:O	2:C:597:MET:HB2	2.20	0.42
1:A:578:GLU:OE1	1:A:595:ARG:NH1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:ARG:NH2	3:B:702:SF4:S1	2.89	0.42
2:C:405:LEU:HD23	2:C:405:LEU:N	2.34	0.42
1:A:161:LEU:HD11	1:A:186:ILE:HD12	2.01	0.42
1:A:426:ILE:O	1:A:430:MET:HG2	2.20	0.42
2:B:290:LEU:HD23	2:B:290:LEU:HA	1.86	0.42
2:C:354:PRO:HA	2:C:357:HIS:NE2	2.35	0.42
1:A:46:VAL:HG21	1:A:196:ILE:HD11	2.02	0.41
1:A:47:ILE:HG13	1:A:93:GLU:OE1	2.20	0.41
1:A:476:ASP:OD1	1:A:502:GLU:HG3	2.20	0.41
1:A:322:ASN:ND2	1:A:652:GLU:OE2	2.53	0.41
1:A:457:GLY:HA2	1:A:461:VAL:HB	2.02	0.41
1:D:487:LEU:HD23	3:D:801:SF4:S2	2.60	0.41
1:D:614:THR:HG22	1:D:623:PHE:CB	2.51	0.41
2:C:52:MET:HE3	3:C:702:SF4:S4	2.60	0.41
1:D:561:VAL:HG13	1:D:571:MET:HG2	2.03	0.41
1:A:199:VAL:HG13	1:A:252:LEU:HD11	2.02	0.41
1:A:401:ARG:HB3	1:A:464:TYR:CE1	2.56	0.41
1:A:474:LEU:HD23	1:A:475:VAL:N	2.35	0.41
1:D:564:TYR:CD1	1:D:635:LYS:HB3	2.55	0.41
1:A:221:LEU:CD2	1:A:252:LEU:HD23	2.50	0.41
1:A:561:VAL:HG21	1:A:571:MET:SD	2.60	0.41
2:B:420:VAL:CG2	2:B:432:PRO:HG3	2.51	0.41
2:C:329:VAL:HG11	2:C:349:PHE:HE1	1.85	0.41
2:B:185:ARG:HG2	2:B:185:ARG:NH1	2.36	0.41
2:C:451:CYS:O	2:C:555:GLU:HB2	2.21	0.41
2:C:452:ASN:HD22	2:C:452:ASN:HA	1.75	0.40
1:A:124:GLY:HA3	1:A:209:PHE:CE2	2.55	0.40
1:A:124:GLY:HA3	1:A:209:PHE:CZ	2.56	0.40
1:A:401:ARG:HB3	1:A:464:TYR:CZ	2.55	0.40
2:C:47:CYS:SG	2:C:80:ARG:NH2	2.94	0.40
1:A:463:ARG:HA	1:A:463:ARG:HH11	1.86	0.40
2:C:348:LYS:HD2	2:C:385:ASN:ND2	2.37	0.40
1:D:386:HIS:CD2	1:D:386:HIS:C	2.99	0.40
1:D:631:ILE:HG22	1:D:661:LEU:HD12	2.03	0.40
1:A:327:TRP:CZ2	1:A:455:LEU:HB3	2.57	0.40
1:A:331:MET:HE2	1:A:463:ARG:HD3	2.04	0.40
1:A:577:PHE:CE1	1:A:580:ILE:HD11	2.57	0.40
2:B:453:ASN:OD1	2:B:455:LYS:HG3	2.22	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	685/708 (97%)	649 (95%)	35 (5%)	1 (0%)	48	71
1	D	706/708 (100%)	670 (95%)	35 (5%)	1 (0%)	48	71
2	B	627/631 (99%)	591 (94%)	35 (6%)	1 (0%)	43	65
2	C	629/631 (100%)	601 (96%)	26 (4%)	2 (0%)	36	59
All	All	2647/2678 (99%)	2511 (95%)	131 (5%)	5 (0%)	43	65

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	332	GLN
1	A	575	GLY
2	B	332	GLN
2	C	243	ASN
1	D	575	GLY

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	571/583 (98%)	553 (97%)	18 (3%)	34	59
1	D	583/583 (100%)	573 (98%)	10 (2%)	53	73
2	B	518/520 (100%)	513 (99%)	5 (1%)	68	81
2	C	520/520 (100%)	514 (99%)	6 (1%)	63	78
All	All	2192/2206 (99%)	2153 (98%)	39 (2%)	51	72

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ILE
1	A	139	LEU
1	A	156	GLN
1	A	165	VAL
1	A	260	GLN
1	A	297	ILE
1	A	299	VAL
1	A	315	MET
1	A	360	MET
1	A	367	LYS
1	A	390	ASN
1	A	408	ILE
1	A	411	GLU
1	A	463	ARG
1	A	563	LEU
1	A	610	LEU
1	A	647	VAL
1	A	669	TYR
2	B	96	HIS
2	B	196	ILE
2	B	368	GLU
2	B	423	GLN
2	B	451	CYS
2	C	114	LYS
2	C	196	ILE
2	C	222	PHE
2	C	451	CYS
2	C	495	GLU
2	C	523	CYS
1	D	23	LYS
1	D	135	VAL
1	D	312	LYS
1	D	395	VAL
1	D	425	VAL
1	D	497	CYS
1	D	637	MET
1	D	666	LYS
1	D	671	ILE
1	D	704	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	ASN
1	A	287	ASN
1	A	699	HIS
2	B	199	ASN
2	B	423	GLN
2	B	595	ASN
2	C	385	ASN
2	C	423	GLN
2	C	428	GLN
2	C	612	HIS
1	D	5	GLN
1	D	372	ASN
1	D	594	ASN

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 75 ligands modelled in this entry, 22 are monoatomic - leaving 53 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	$\# Z > 2$
12	ACO	D	805	-	51,53,53	2.20	13 (25%)	73,79,79	2.24	12 (16%)
5	EDO	B	717	-	3,3,3	0.15	0	2,2,2	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	A	806	-	3,3,3	0.34	0	2,2,2	0.15	0
5	EDO	B	716	-	3,3,3	0.23	0	2,2,2	0.33	0
8	PEG	D	804	-	6,6,6	0.20	0	5,5,5	0.20	0
5	EDO	C	712	-	3,3,3	0.33	0	2,2,2	0.21	0
5	EDO	B	721	-	3,3,3	0.06	0	2,2,2	0.11	0
7	GOL	B	707	-	5,5,5	0.09	0	5,5,5	0.32	0
5	EDO	A	818	-	3,3,3	0.37	0	2,2,2	0.14	0
5	EDO	A	804	-	3,3,3	0.18	0	2,2,2	0.09	0
5	EDO	A	816	-	3,3,3	0.24	0	2,2,2	0.36	0
5	EDO	B	726	-	3,3,3	0.06	0	2,2,2	0.12	0
3	SF4	B	702	2	0,12,12	-	-	-	-	-
7	GOL	B	706	-	5,5,5	0.09	0	5,5,5	0.31	0
5	EDO	C	711	-	3,3,3	0.23	0	2,2,2	0.36	0
5	EDO	A	819	-	3,3,3	0.06	0	2,2,2	0.11	0
3	SF4	C	701	2	0,12,12	-	-	-	-	-
6	PE4	A	805	-	9,9,23	0.50	0	8,8,22	0.63	0
11	XCC	C	704	2	0,11,11	-	-	-	-	-
3	SF4	C	702	2	0,12,12	-	-	-	-	-
5	EDO	C	713	-	3,3,3	0.06	0	2,2,2	0.12	0
7	GOL	B	701	-	5,5,5	0.07	0	5,5,5	0.19	0
5	EDO	C	710	-	3,3,3	0.27	0	2,2,2	0.24	0
5	EDO	B	722	-	3,3,3	0.04	0	2,2,2	0.05	0
5	EDO	B	723	-	3,3,3	0.07	0	2,2,2	0.14	0
3	SF4	D	801	1	0,12,12	-	-	-	-	-
8	PEG	B	703	-	6,6,6	0.25	0	5,5,5	0.27	0
5	EDO	B	714	-	3,3,3	0.29	0	2,2,2	0.27	0
5	EDO	D	810	-	3,3,3	0.28	0	2,2,2	0.26	0
3	SF4	A	801	1	0,12,12	-	-	-	-	-
5	EDO	A	815	-	3,3,3	0.27	0	2,2,2	0.37	0
5	EDO	B	718	-	3,3,3	0.07	0	2,2,2	0.12	0
5	EDO	B	728	-	3,3,3	0.07	0	2,2,2	0.12	0
5	EDO	D	811	-	3,3,3	0.21	0	2,2,2	0.48	0
5	EDO	D	813	-	3,3,3	0.06	0	2,2,2	0.11	0
5	EDO	B	725	-	3,3,3	0.05	0	2,2,2	0.11	0
5	EDO	B	719	-	3,3,3	0.07	0	2,2,2	0.13	0
13	TRS	D	807	-	7,7,7	0.14	0	9,9,9	0.23	0
5	EDO	A	820	-	3,3,3	0.06	0	2,2,2	0.11	0
5	EDO	B	727	-	3,3,3	0.07	0	2,2,2	0.11	0
5	EDO	C	703	-	3,3,3	0.30	0	2,2,2	0.23	0
8	PEG	A	808	-	6,6,6	0.17	0	5,5,5	0.18	0
7	GOL	B	704	-	5,5,5	0.04	0	5,5,5	0.19	0
5	EDO	C	714	-	3,3,3	0.05	0	2,2,2	0.11	0
5	EDO	B	715	-	3,3,3	0.30	0	2,2,2	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	D	812	-	3,3,3	0.27	0	2,2,2	0.26	0
7	GOL	A	807	-	5,5,5	0.04	0	5,5,5	0.16	0
7	GOL	D	806	-	5,5,5	0.09	0	5,5,5	0.31	0
5	EDO	B	724	-	3,3,3	0.06	0	2,2,2	0.14	0
5	EDO	A	817	-	3,3,3	0.26	0	2,2,2	0.27	0
5	EDO	C	709	-	3,3,3	0.30	0	2,2,2	0.25	0
11	XCC	B	705	2	0,11,11	-	-	-	-	-
5	EDO	B	720	-	3,3,3	0.07	0	2,2,2	0.11	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
12	ACO	D	805	-	-	25/51/67/67	0/3/3/3
5	EDO	B	717	-	-	0/1/1/1	-
5	EDO	A	806	-	-	1/1/1/1	-
5	EDO	B	716	-	-	0/1/1/1	-
8	PEG	D	804	-	-	1/4/4/4	-
5	EDO	C	712	-	-	1/1/1/1	-
5	EDO	B	721	-	-	0/1/1/1	-
7	GOL	B	707	-	-	1/4/4/4	-
5	EDO	A	818	-	-	1/1/1/1	-
5	EDO	A	816	-	-	0/1/1/1	-
5	EDO	A	804	-	-	1/1/1/1	-
5	EDO	B	726	-	-	0/1/1/1	-
3	SF4	B	702	2	-	-	0/6/5/5
7	GOL	B	706	-	-	0/4/4/4	-
5	EDO	C	711	-	-	0/1/1/1	-
5	EDO	A	819	-	-	1/1/1/1	-
3	SF4	C	701	2	-	-	0/6/5/5
6	PE4	A	805	-	-	3/7/7/21	-
11	XCC	C	704	2	-	-	0/3/3/3
3	SF4	C	702	2	-	-	0/6/5/5
5	EDO	C	713	-	-	0/1/1/1	-
7	GOL	B	701	-	-	0/4/4/4	-
5	EDO	C	710	-	-	0/1/1/1	-
5	EDO	B	722	-	-	1/1/1/1	-
5	EDO	B	723	-	-	0/1/1/1	-
3	SF4	D	801	1	-	-	0/6/5/5
8	PEG	B	703	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	714	-	-	1/1/1/1	-
5	EDO	D	810	-	-	1/1/1/1	-
5	EDO	B	718	-	-	1/1/1/1	-
5	EDO	A	815	-	-	0/1/1/1	-
3	SF4	A	801	1	-	-	0/6/5/5
5	EDO	B	728	-	-	1/1/1/1	-
5	EDO	D	811	-	-	0/1/1/1	-
5	EDO	D	813	-	-	1/1/1/1	-
5	EDO	B	725	-	-	0/1/1/1	-
5	EDO	B	719	-	-	1/1/1/1	-
13	TRS	D	807	-	-	8/9/9/9	-
5	EDO	A	820	-	-	0/1/1/1	-
5	EDO	B	727	-	-	0/1/1/1	-
5	EDO	C	703	-	-	1/1/1/1	-
8	PEG	A	808	-	-	1/4/4/4	-
7	GOL	B	704	-	-	0/4/4/4	-
5	EDO	C	714	-	-	1/1/1/1	-
5	EDO	B	715	-	-	1/1/1/1	-
5	EDO	D	812	-	-	1/1/1/1	-
7	GOL	A	807	-	-	0/4/4/4	-
7	GOL	D	806	-	-	2/4/4/4	-
5	EDO	B	724	-	-	1/1/1/1	-
5	EDO	A	817	-	-	0/1/1/1	-
5	EDO	C	709	-	-	1/1/1/1	-
11	XCC	B	705	2	-	-	0/3/3/3
5	EDO	B	720	-	-	0/1/1/1	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	805	ACO	C5P-N4P	5.41	1.46	1.33
12	D	805	ACO	C9P-N8P	5.40	1.46	1.33
12	D	805	ACO	P1A-O3A	5.37	1.65	1.59
12	D	805	ACO	P2A-O3A	5.36	1.65	1.59
12	D	805	ACO	C1B-N9A	-4.73	1.33	1.46
12	D	805	ACO	C6A-N6A	4.43	1.45	1.34
12	D	805	ACO	C3B-C4B	4.08	1.63	1.52
12	D	805	ACO	P3B-O3B	3.10	1.65	1.59
12	D	805	ACO	C8A-N9A	-2.78	1.32	1.37
12	D	805	ACO	C5A-C4A	-2.72	1.34	1.39
12	D	805	ACO	O9P-C9P	-2.27	1.19	1.23
12	D	805	ACO	O5P-C5P	-2.21	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	805	ACO	O2B-C2B	2.20	1.48	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	805	ACO	C4A-N9A-C8A	9.54	115.75	105.74
12	D	805	ACO	N9A-C8A-N7A	-8.14	102.39	113.94
12	D	805	ACO	N3A-C2A-N1A	-5.76	119.86	128.58
12	D	805	ACO	N3A-C4A-N9A	5.45	136.44	127.17
12	D	805	ACO	C1B-N9A-C8A	-5.38	115.15	127.09
12	D	805	ACO	C5A-C4A-N3A	-4.44	120.61	126.72
12	D	805	ACO	C5A-N7A-C8A	4.10	109.90	103.45
12	D	805	ACO	C2A-N3A-C4A	3.33	119.96	111.83
12	D	805	ACO	C5A-C4A-N9A	-2.63	102.94	105.81
12	D	805	ACO	C2P-C3P-N4P	-2.16	107.91	112.41
12	D	805	ACO	P3B-O3B-C3B	-2.14	117.71	123.43
12	D	805	ACO	C6P-C5P-N4P	2.02	120.02	116.34

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	D	805	ACO	O4B-C4B-C5B-O5B
12	D	805	ACO	C5B-O5B-P1A-O1A
12	D	805	ACO	C5B-O5B-P1A-O2A
12	D	805	ACO	C5B-O5B-P1A-O3A
12	D	805	ACO	OAP-CAP-CBP-CCP
12	D	805	ACO	C9P-CAP-CBP-CCP
12	D	805	ACO	OAP-CAP-CBP-CDP
12	D	805	ACO	C9P-CAP-CBP-CDP
12	D	805	ACO	OAP-CAP-CBP-CEP
12	D	805	ACO	C9P-CAP-CBP-CEP
12	D	805	ACO	CAP-C9P-N8P-C7P
12	D	805	ACO	S1P-C2P-C3P-N4P
13	D	807	TRS	N-C-C2-O2
13	D	807	TRS	C1-C-C3-O3
13	D	807	TRS	C2-C-C3-O3
13	D	807	TRS	N-C-C3-O3
12	D	805	ACO	O9P-C9P-N8P-C7P
12	D	805	ACO	C3B-C4B-C5B-O5B
5	A	806	EDO	O1-C1-C2-O2
7	D	806	GOL	C1-C2-C3-O3

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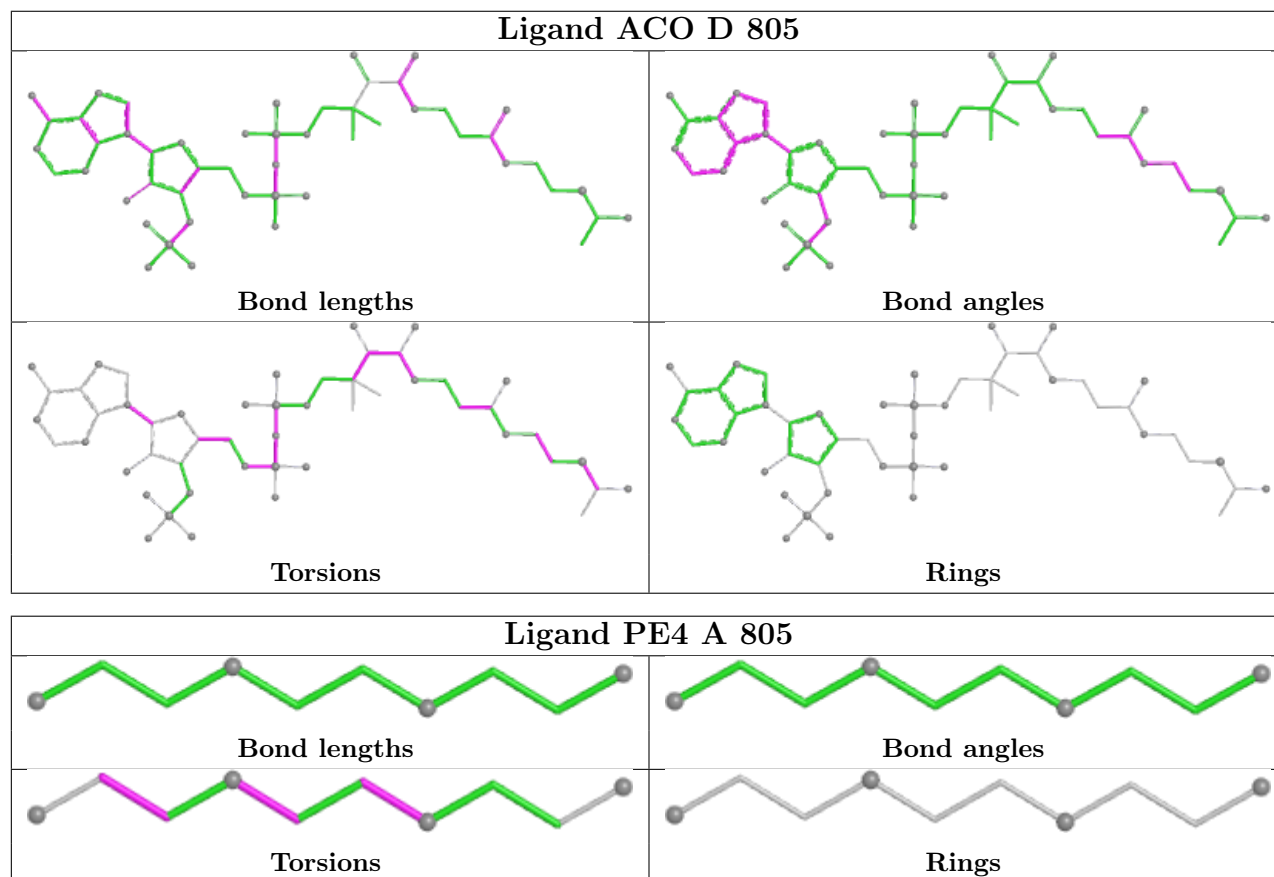
Mol	Chain	Res	Type	Atoms
8	B	703	PEG	O1-C1-C2-O2
12	D	805	ACO	O-C-S1P-C2P
5	A	818	EDO	O1-C1-C2-O2
5	B	722	EDO	O1-C1-C2-O2
8	B	703	PEG	O2-C3-C4-O4
12	D	805	ACO	C2B-C1B-N9A-C4A
5	A	819	EDO	O1-C1-C2-O2
5	C	703	EDO	O1-C1-C2-O2
5	C	712	EDO	O1-C1-C2-O2
5	C	714	EDO	O1-C1-C2-O2
5	D	810	EDO	O1-C1-C2-O2
12	D	805	ACO	C2B-C1B-N9A-C8A
12	D	805	ACO	P2A-O3A-P1A-O1A
6	A	805	PE4	O7-C13-C14-O8
7	B	707	GOL	O2-C2-C3-O3
13	D	807	TRS	C2-C-C1-O1
12	D	805	ACO	CH3-C-S1P-C2P
12	D	805	ACO	P2A-O3A-P1A-O5B
6	A	805	PE4	C12-C11-O6-C10
5	B	714	EDO	O1-C1-C2-O2
13	D	807	TRS	C3-C-C1-O1
5	C	709	EDO	O1-C1-C2-O2
5	D	812	EDO	O1-C1-C2-O2
6	A	805	PE4	C11-C12-O7-C13
5	B	715	EDO	O1-C1-C2-O2
5	B	719	EDO	O1-C1-C2-O2
13	D	807	TRS	N-C-C1-O1
13	D	807	TRS	C3-C-C2-O2
5	D	813	EDO	O1-C1-C2-O2
12	D	805	ACO	O5P-C5P-C6P-C7P
12	D	805	ACO	P1A-O3A-P2A-O4A
12	D	805	ACO	P1A-O3A-P2A-O5A
8	D	804	PEG	O1-C1-C2-O2
7	D	806	GOL	O2-C2-C3-O3
5	A	804	EDO	O1-C1-C2-O2
5	B	728	EDO	O1-C1-C2-O2
12	D	805	ACO	N4P-C5P-C6P-C7P
5	B	718	EDO	O1-C1-C2-O2
5	B	724	EDO	O1-C1-C2-O2
12	D	805	ACO	N8P-C9P-CAP-OAP
8	A	808	PEG	C4-C3-O2-C2

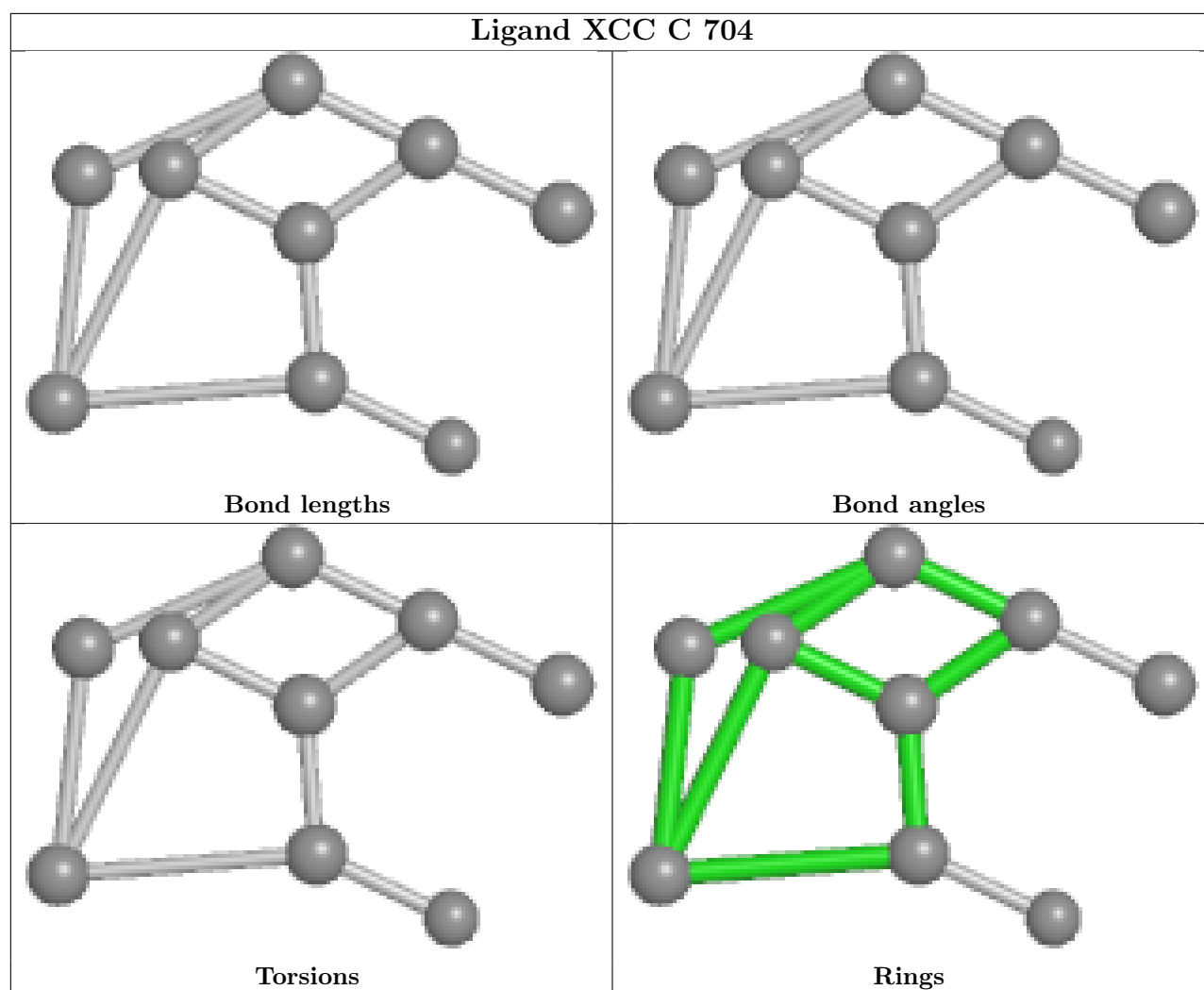
There are no ring outliers.

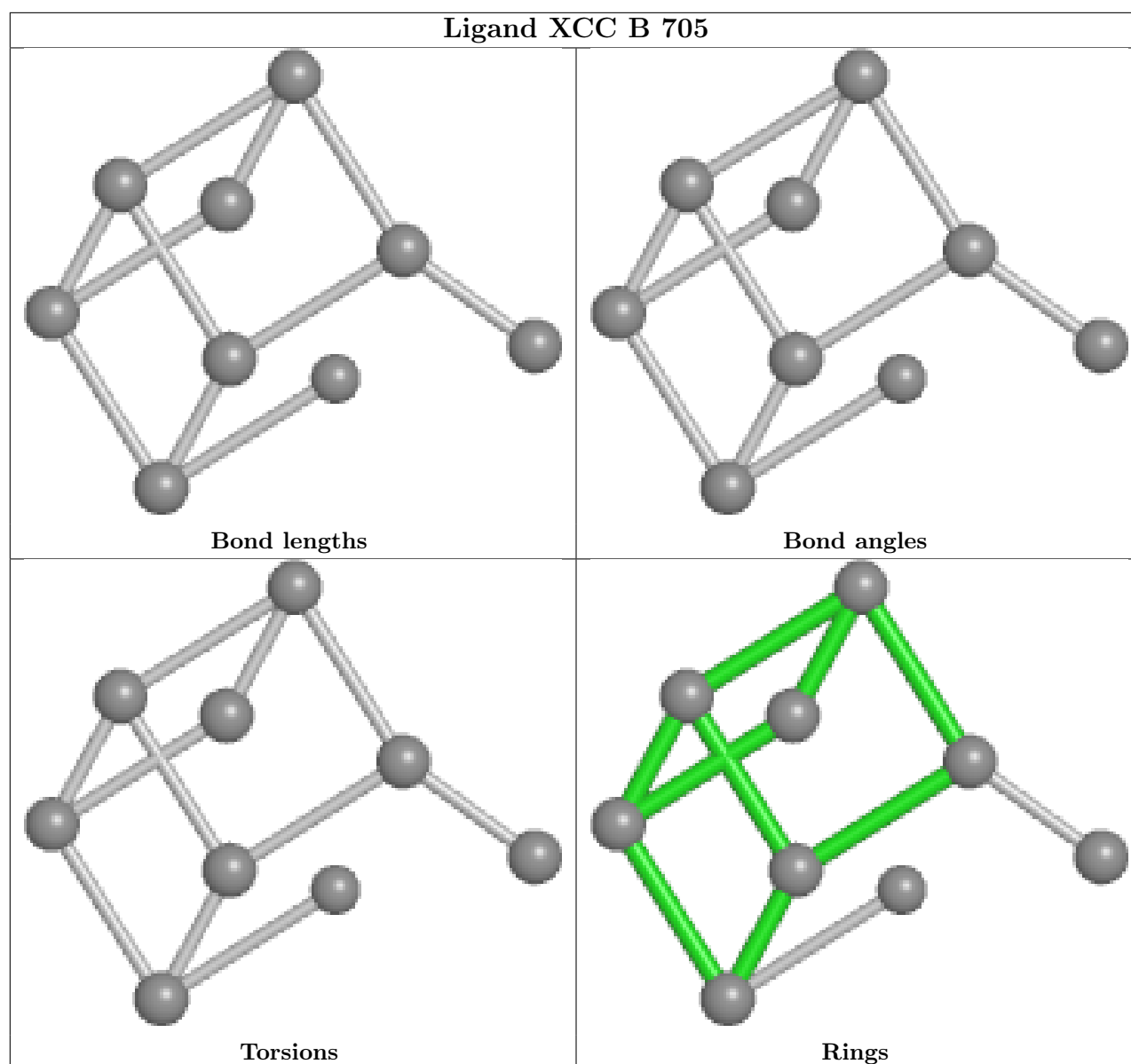
5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	D	805	ACO	2	0
3	B	702	SF4	1	0
3	C	702	SF4	1	0
3	D	801	SF4	1	0
3	A	801	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 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	A	694/708 (98%)	0.58	104 (14%) 5 5	42, 112, 196, 245	1 (0%)
1	D	708/708 (100%)	0.11	24 (3%) 48 40	63, 93, 159, 220	0
2	B	629/631 (99%)	-0.47	3 (0%) 87 83	39, 57, 82, 133	0
2	C	630/631 (99%)	-0.27	6 (0%) 79 74	39, 72, 104, 157	1 (0%)
All	All	2661/2678 (99%)	0.01	137 (5%) 33 27	39, 76, 169, 245	2 (0%)

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	371	THR	8.1
1	A	438	VAL	6.4
1	A	431	LEU	6.4
1	A	427	TYR	5.5
1	A	368	VAL	5.4
1	A	331	MET	5.1
1	A	361	PRO	5.1
1	A	338	VAL	5.0
1	A	362	LEU	4.7
1	A	471	LEU	4.6
1	A	292	ILE	4.5
1	A	425	VAL	4.5
2	B	63	LYS	4.4
1	A	341	HIS	4.3
1	A	356	ALA	4.3
1	D	491	PHE	4.2
1	A	296	PRO	4.2
1	A	332	CYS	4.2
1	A	434	PHE	4.1
1	A	475	VAL	4.0
1	A	459	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	504	LEU	3.8
1	A	661	LEU	3.7
1	A	461	VAL	3.7
1	D	668	LEU	3.7
2	C	425	GLY	3.5
1	A	444	THR	3.5
1	A	374	GLN	3.4
1	A	377	PHE	3.4
1	A	531	PRO	3.4
1	A	343	ILE	3.4
1	A	367	LYS	3.4
1	A	524	THR	3.4
1	A	299	VAL	3.3
1	A	398	VAL	3.3
1	D	708	MET	3.2
2	C	242	ALA	3.1
1	D	313	ASN	3.1
1	A	375	LYS	3.1
1	D	322	ASN	3.1
1	D	292	ILE	3.1
1	D	307	GLY	3.1
1	A	600	THR	3.1
1	A	333	ALA	3.0
1	A	400	GLN	3.0
1	D	358	GLY	3.0
1	A	387	TYR	3.0
1	D	246	GLY	3.0
1	A	460	ALA	3.0
1	D	470	ARG	3.0
1	A	303	ALA	3.0
1	A	399	GLY	2.9
1	A	533	GLU	2.9
1	A	405	TRP	2.9
1	A	464	TYR	2.9
1	D	669	TYR	2.9
2	C	260	GLU	2.9
1	A	403	LEU	2.9
1	D	666	LYS	2.8
1	A	428	ALA	2.8
1	A	422	PHE	2.8
1	A	366	ILE	2.8
1	A	396	MET	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	425	GLY	2.8
1	A	478	LYS	2.8
1	A	685	THR	2.8
1	A	394	GLY	2.7
1	A	408	ILE	2.7
1	A	293	THR	2.6
1	D	314	ASP	2.6
1	D	309	ARG	2.6
1	A	523	PRO	2.6
1	A	381	LEU	2.6
1	A	334	ASP	2.6
1	A	386	HIS	2.6
1	A	418	ARG	2.6
1	A	445	ILE	2.6
1	A	298	PRO	2.6
1	A	669	TYR	2.6
1	D	355	LYS	2.6
1	A	430	MET	2.6
1	A	337	GLU	2.6
1	A	607	PHE	2.6
1	A	503	ARG	2.5
2	C	236[A]	HIS	2.5
1	A	384	ARG	2.5
1	A	421	HIS	2.5
1	A	419	LEU	2.5
2	C	426	PRO	2.5
1	A	417	PHE	2.5
1	D	356	ALA	2.5
1	A	511	SER	2.5
1	D	667	GLU	2.5
1	A	476	ASP	2.4
1	A	528	GLN	2.4
1	A	663	LYS	2.4
1	D	459	TYR	2.4
1	A	433	GLU	2.4
1	A	493	PRO	2.4
1	A	529	ALA	2.4
1	A	370	GLY	2.4
1	A	426	ILE	2.4
1	A	346	ILE	2.3
1	A	641	GLY	2.3
1	A	335	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	519	LEU	2.3
1	D	436	SER	2.3
1	A	455	LEU	2.3
1	D	664	THR	2.3
1	A	477	GLU	2.2
1	A	302	ALA	2.2
1	A	447	THR	2.2
1	A	363	GLY	2.2
1	A	642	GLY	2.2
1	D	434	PHE	2.2
1	A	520	GLU	2.2
1	A	510	VAL	2.2
1	D	661	LEU	2.1
1	D	311	ARG	2.1
1	A	415	LYS	2.1
2	C	54	PRO	2.1
1	A	345	VAL	2.1
1	A	660	LYS	2.1
1	A	577	PHE	2.1
1	A	463	ARG	2.1
1	A	595	ARG	2.1
2	B	424	ILE	2.1
1	A	451	LYS	2.0
1	A	703	LYS	2.0
1	D	478	LYS	2.0
1	A	474	LEU	2.0
1	A	364	MET	2.0
1	A	526	PRO	2.0
1	A	313	ASN	2.0
1	A	297	ILE	2.0
1	A	306	GLU	2.0
1	A	465	LYS	2.0

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, 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
5	EDO	A	815	4/4	0.52	0.20	99,104,118,120	0
5	EDO	B	723	4/4	0.52	0.26	97,98,106,108	0
5	EDO	B	717	4/4	0.53	0.43	73,78,86,94	0
7	GOL	A	807	6/6	0.54	0.12	121,132,134,137	0
12	ACO	D	805	51/51	0.54	0.22	53,160,214,232	0
7	GOL	B	707	6/6	0.56	0.23	79,103,116,118	0
5	EDO	A	816	4/4	0.60	0.36	72,74,85,100	0
5	EDO	C	711	4/4	0.60	0.27	74,80,81,85	0
5	EDO	D	813	4/4	0.60	0.38	87,101,117,121	0
5	EDO	D	811	4/4	0.61	0.15	101,109,109,120	0
5	EDO	D	812	4/4	0.63	0.13	99,111,116,119	0
10	CL	B	712	1/1	0.65	0.16	122,122,122,122	0
5	EDO	B	724	4/4	0.67	0.26	89,96,100,112	0
9	CA	D	808	1/1	0.67	0.12	126,126,126,126	0
9	CA	A	810	1/1	0.68	0.11	136,136,136,136	0
5	EDO	B	721	4/4	0.68	0.30	99,102,105,122	0
10	CL	B	713	1/1	0.71	0.17	98,98,98,98	0
5	EDO	B	718	4/4	0.71	0.15	92,94,100,108	0
5	EDO	C	710	4/4	0.72	0.23	105,108,111,121	0
5	EDO	A	806	4/4	0.72	0.20	91,96,102,106	0
8	PEG	D	804	7/7	0.72	0.29	94,111,120,121	0
5	EDO	C	713	4/4	0.72	0.14	100,101,110,111	0
9	CA	D	809	1/1	0.74	0.15	163,163,163,163	0
9	CA	C	707	1/1	0.74	0.32	123,123,123,123	0
13	TRS	D	807	8/8	0.74	0.24	60,85,102,103	0
7	GOL	B	701	6/6	0.75	0.21	79,87,110,114	0
7	GOL	B	706	6/6	0.75	0.12	88,96,103,107	0
5	EDO	B	725	4/4	0.75	0.19	82,89,105,110	0
5	EDO	A	820	4/4	0.76	0.30	92,99,107,117	0
5	EDO	A	804	4/4	0.76	0.19	80,82,92,94	0
5	EDO	B	714	4/4	0.78	0.19	87,88,93,120	0
5	EDO	B	727	4/4	0.78	0.30	66,91,92,101	0
7	GOL	D	806	6/6	0.78	0.24	93,115,117,119	0
5	EDO	C	709	4/4	0.79	0.22	84,90,98,104	0
5	EDO	D	810	4/4	0.80	0.20	80,100,104,110	0
6	PE4	A	805	10/24	0.80	0.19	94,110,120,121	0
8	PEG	B	703	7/7	0.81	0.19	83,87,108,116	0

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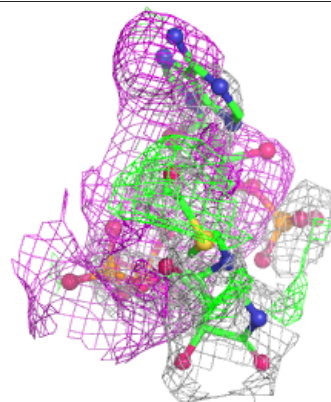
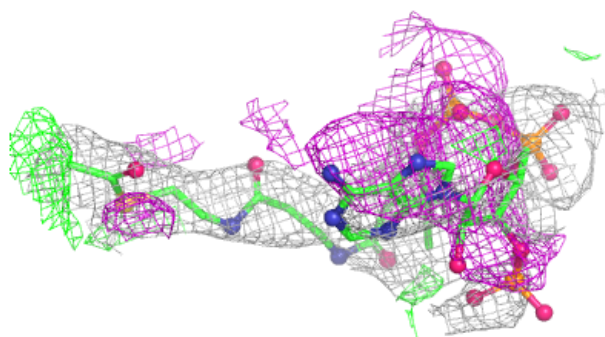
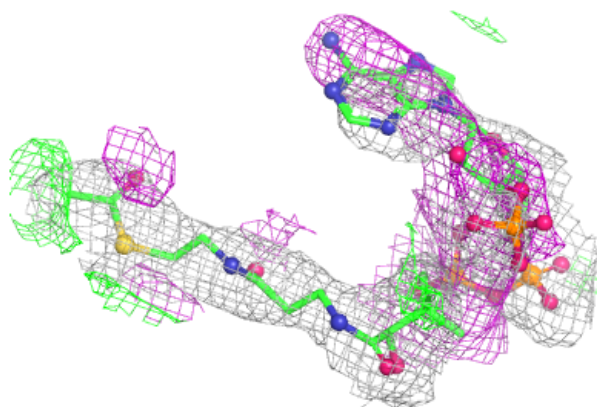
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	C	712	4/4	0.82	0.29	98,100,108,111	0
7	GOL	B	704	6/6	0.82	0.19	90,96,98,104	0
5	EDO	B	715	4/4	0.82	0.22	74,91,94,100	0
9	CA	A	809	1/1	0.83	0.14	125,125,125,125	0
9	CA	C	705	1/1	0.84	0.14	103,103,103,103	0
5	EDO	A	819	4/4	0.84	0.17	83,96,97,100	0
5	EDO	B	719	4/4	0.85	0.21	97,104,106,108	0
5	EDO	B	722	4/4	0.85	0.31	71,75,75,93	0
8	PEG	A	808	7/7	0.86	0.19	83,99,110,130	0
5	EDO	B	716	4/4	0.87	0.15	63,72,77,80	0
10	CL	A	814	1/1	0.87	0.22	105,105,105,105	0
5	EDO	C	703	4/4	0.87	0.26	91,93,94,96	0
5	EDO	B	728	4/4	0.88	0.28	72,73,83,89	0
9	CA	A	812	1/1	0.89	0.12	124,124,124,124	0
10	CL	A	813	1/1	0.89	0.15	94,94,94,94	0
5	EDO	A	817	4/4	0.89	0.28	88,91,108,124	0
10	CL	B	710	1/1	0.89	0.19	78,78,78,78	0
9	CA	B	708	1/1	0.91	0.13	122,122,122,122	0
5	EDO	C	714	4/4	0.91	0.18	81,82,83,83	0
10	CL	B	709	1/1	0.91	0.12	68,68,68,68	0
9	CA	C	706	1/1	0.91	0.11	123,123,123,123	0
9	CA	A	811	1/1	0.92	0.08	118,118,118,118	0
5	EDO	B	720	4/4	0.92	0.14	56,72,80,88	0
5	EDO	B	726	4/4	0.93	0.15	89,93,93,113	0
5	EDO	A	818	4/4	0.93	0.13	86,93,97,100	0
10	CL	B	711	1/1	0.94	0.12	96,96,96,96	0
11	XCC	C	704	9/9	0.94	0.08	55,81,126,128	0
10	CL	C	708	1/1	0.95	0.10	83,83,83,83	0
3	SF4	A	801	8/8	0.97	0.06	99,149,172,181	0
4	NI	A	803	1/1	0.98	0.06	183,183,183,183	0
3	SF4	B	702	8/8	0.99	0.04	53,55,72,74	0
11	XCC	B	705	9/9	0.99	0.04	45,60,75,88	0
4	NI	D	802	1/1	0.99	0.03	75,75,75,75	0
4	NI	D	803	1/1	0.99	0.02	53,53,53,53	0
4	NI	A	802	1/1	0.99	0.04	117,117,117,117	0
3	SF4	C	702	8/8	1.00	0.06	43,52,66,71	0
3	SF4	D	801	8/8	1.00	0.02	70,73,93,94	0
3	SF4	C	701	8/8	1.00	0.04	44,53,59,60	0

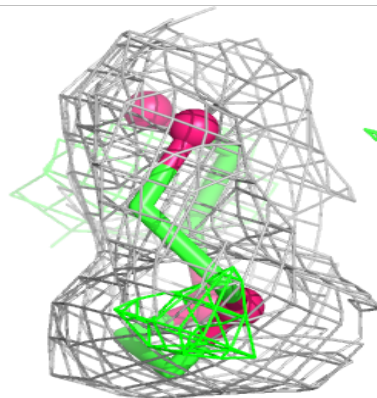
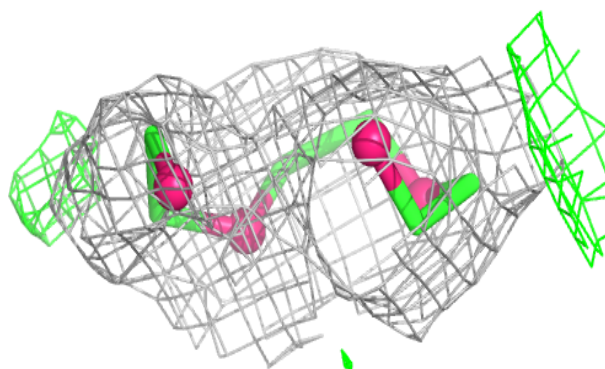
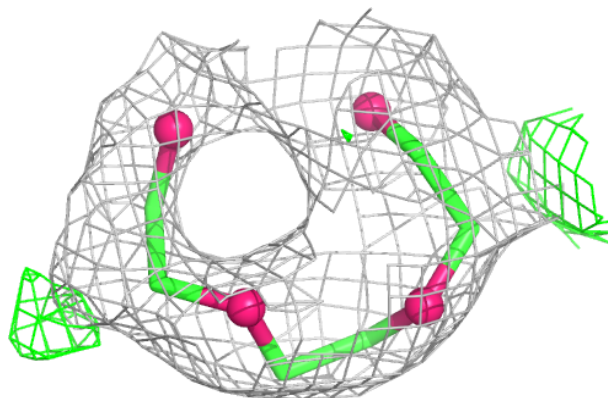
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACO D 805:

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

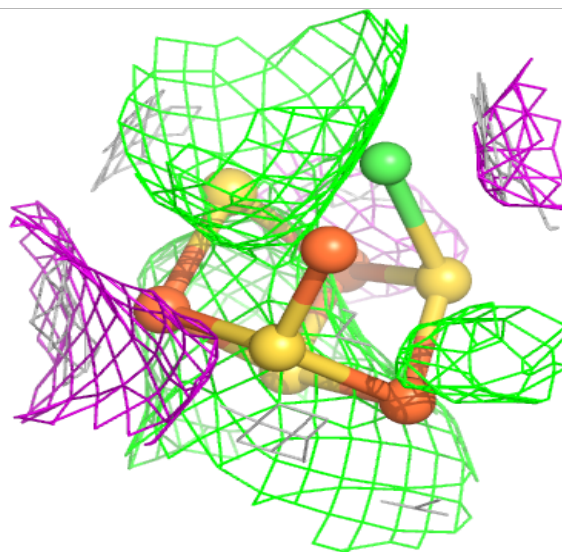
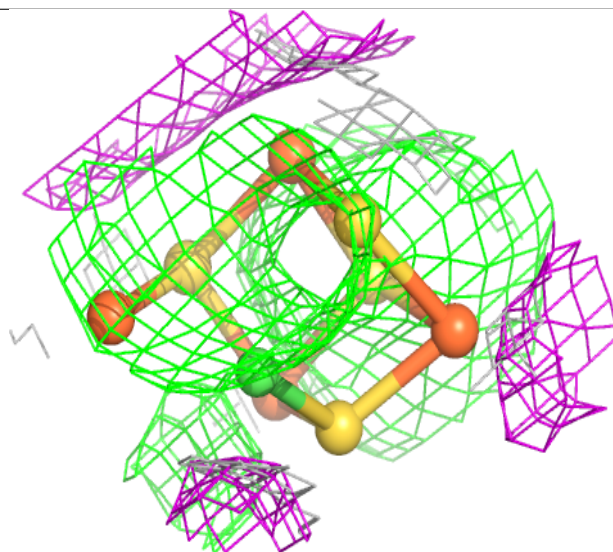
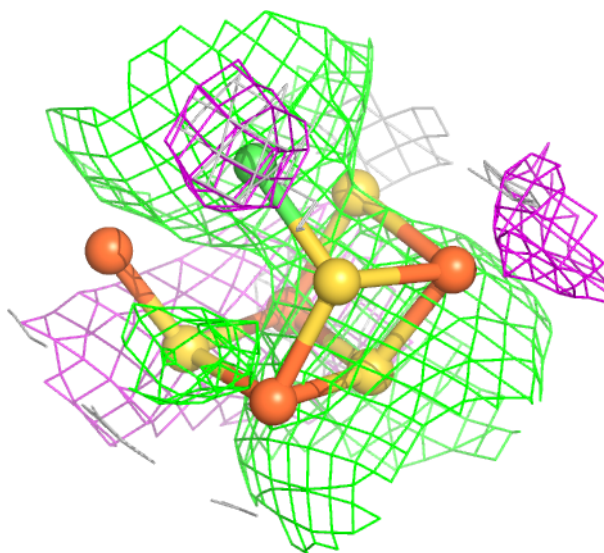
**Electron density around PE4 A 805:**

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



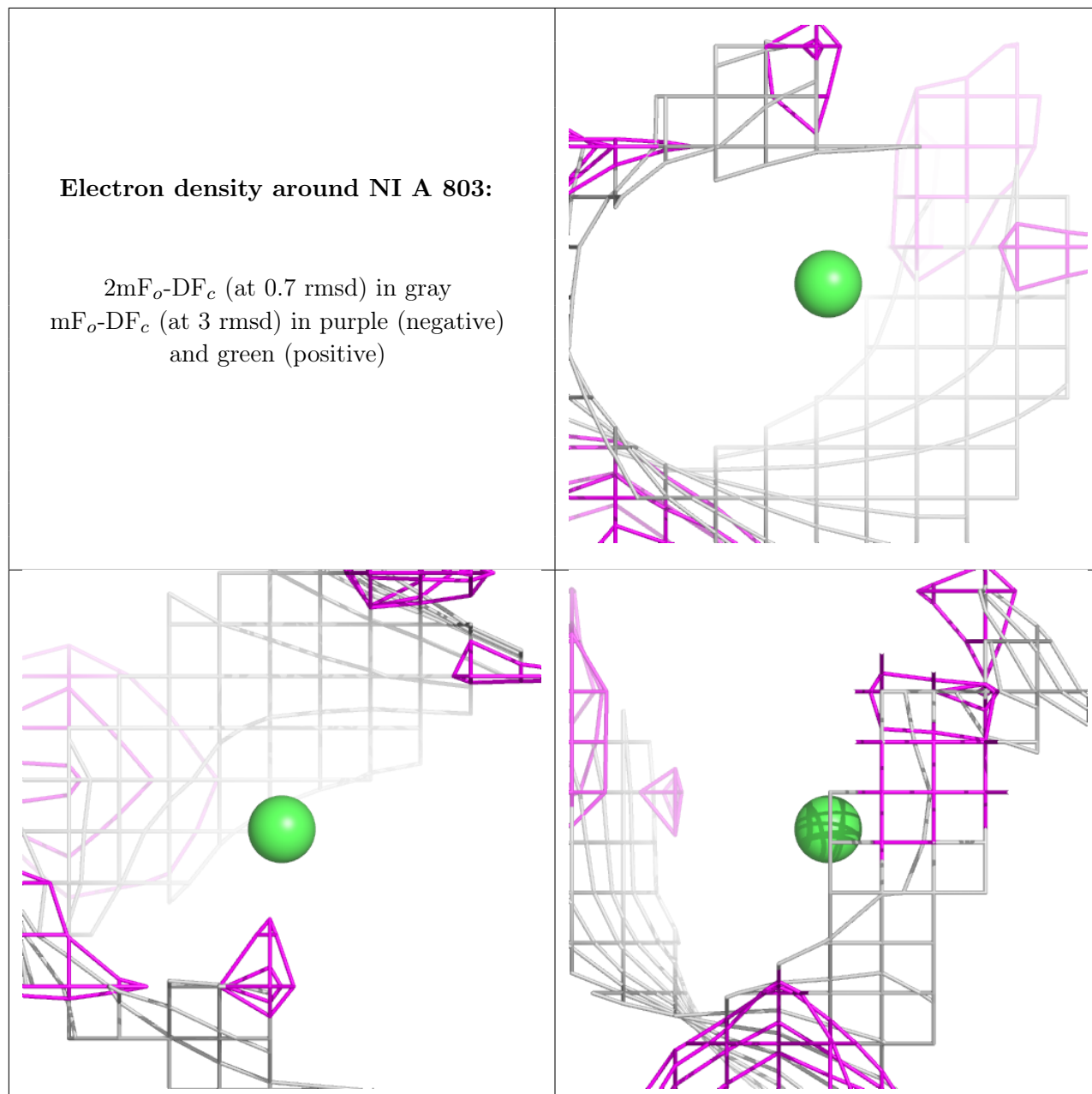
Electron density around XCC C 704:

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



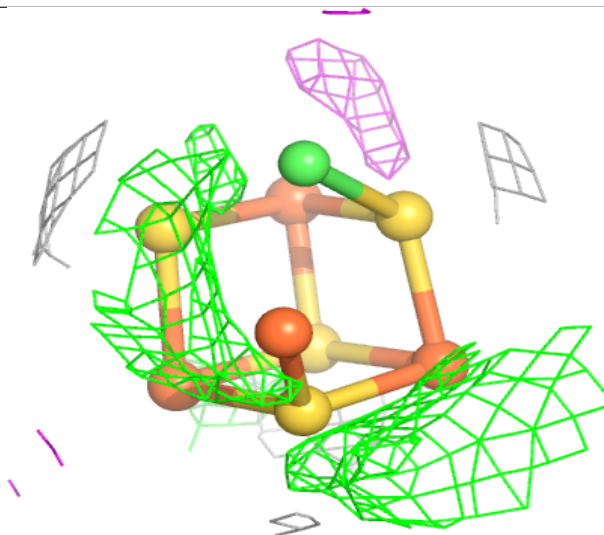
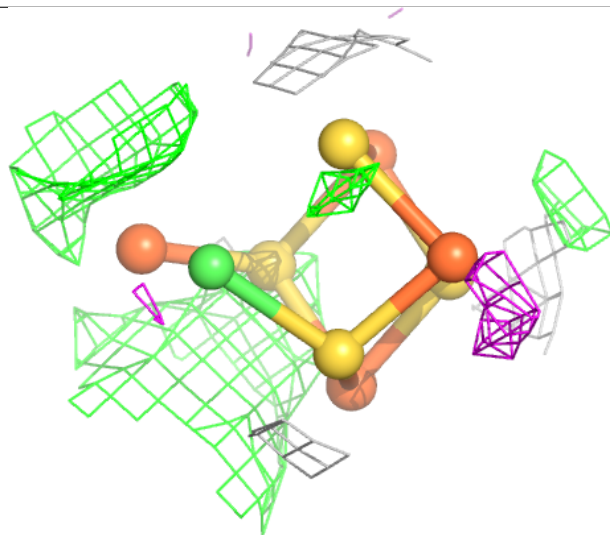
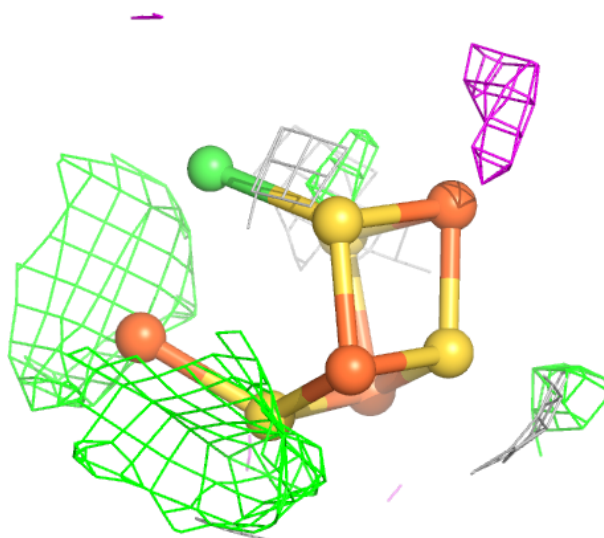
Electron density around NI A 803:

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



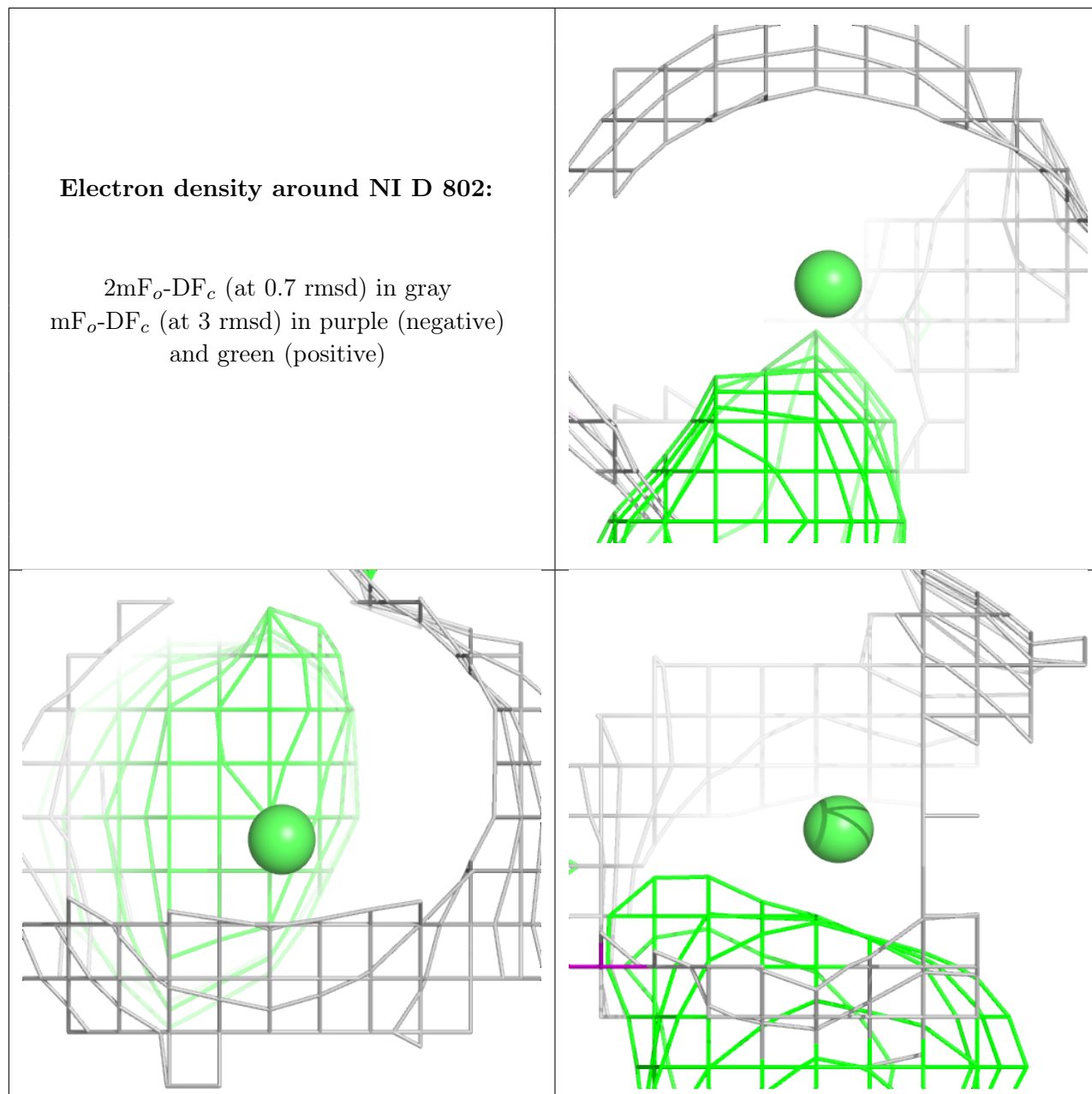
Electron density around XCC B 705:

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



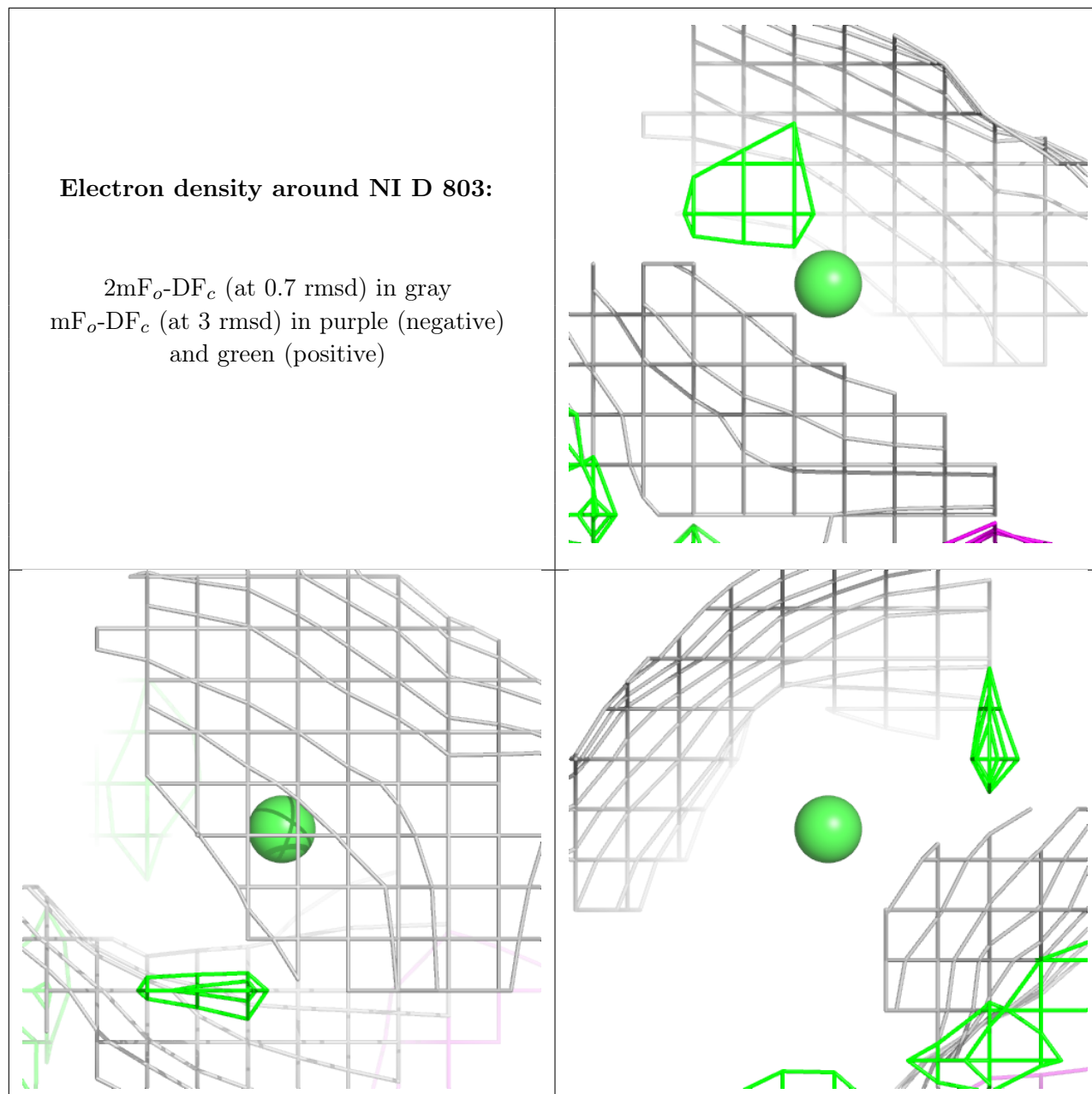
Electron density around NI D 802:

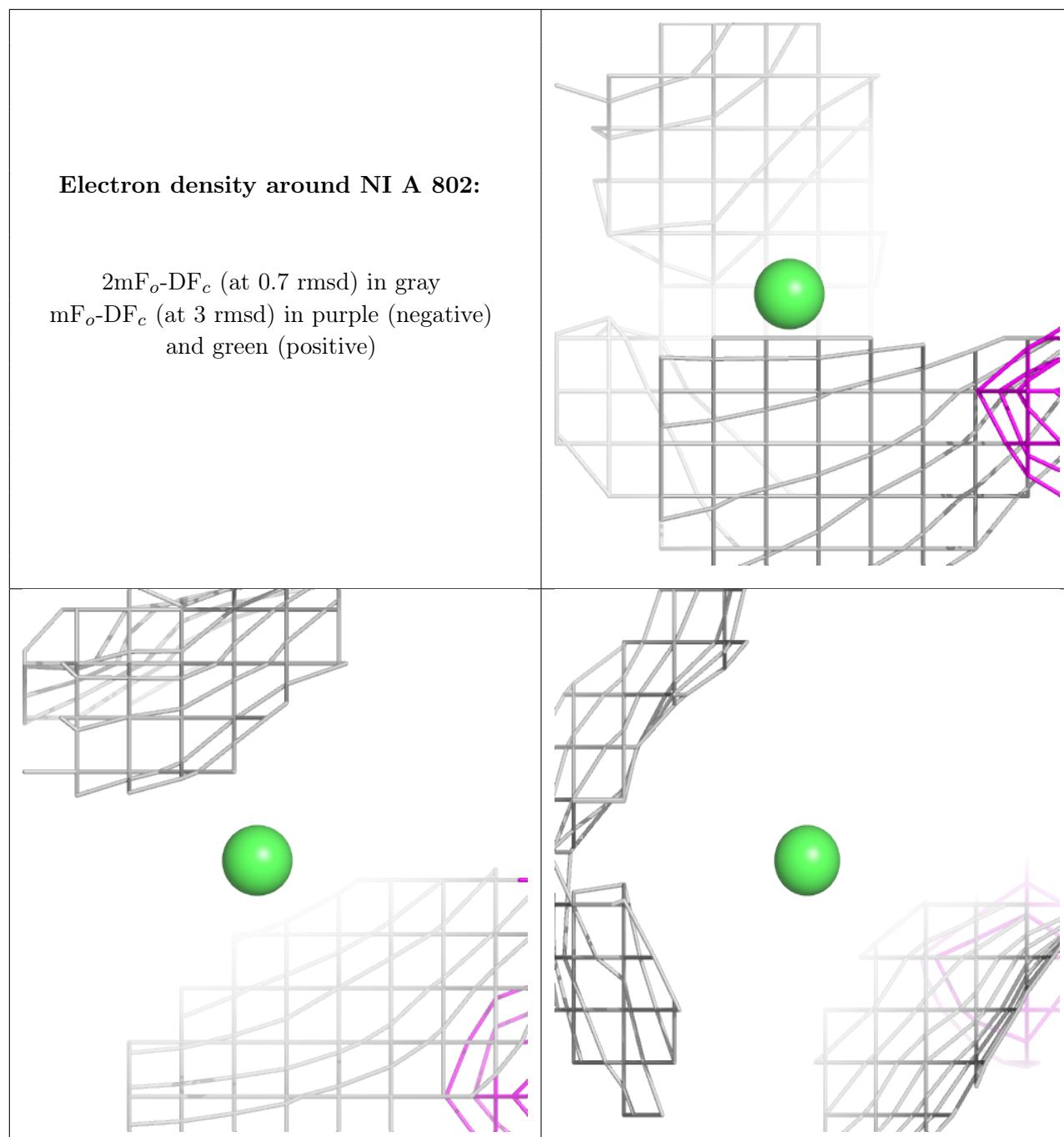
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NI D 803:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.