



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 13, 2025 – 06:14 PM JST

PDB ID : 8XXC
Title : DaCS-intermediate complex
Authors : Yang, L.; Fang, Y.J.
Deposited on : 2024-01-18
Resolution : 2.03 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

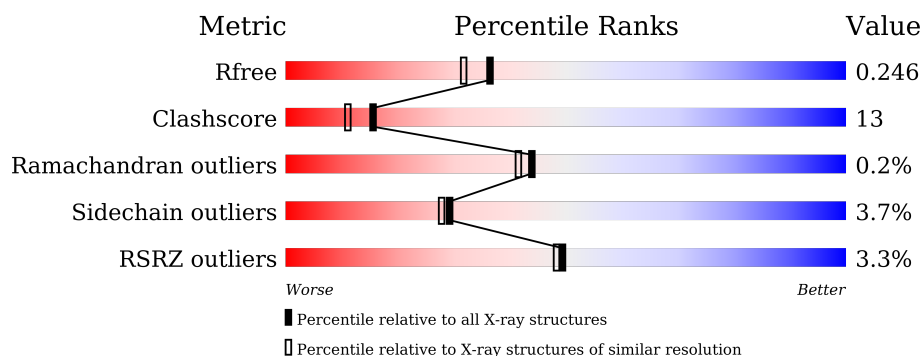
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	12358 (2.04-2.00)
Clashscore	180529	13897 (2.04-2.00)
Ramachandran outliers	177936	13770 (2.04-2.00)
Sidechain outliers	177891	13769 (2.04-2.00)
RSRZ outliers	164620	12358 (2.04-2.00)

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
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Mol	Chain	Length	Quality of chain
1	G	435	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>17%</div> <div></div> </div> </div>
1	H	435	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>18%</div> <div></div> </div> </div>

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
2	CIT	D	501	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 29531 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 Citrate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	0	0	0
			3435	2211	575	631	18			
1	B	434	Total	C	N	O	S	0	0	0
			3423	2202	572	631	18			
1	C	435	Total	C	N	O	S	0	0	0
			3431	2208	574	631	18			
1	D	435	Total	C	N	O	S	0	0	0
			3427	2205	573	631	18			
1	E	434	Total	C	N	O	S	0	0	0
			3423	2202	572	631	18			
1	F	434	Total	C	N	O	S	0	0	0
			3418	2199	571	630	18			
1	G	434	Total	C	N	O	S	0	0	0
			3422	2202	572	630	18			
1	H	434	Total	C	N	O	S	0	0	0
			3422	2202	572	630	18			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	SER	LYS	conflict	UNP A0A1G6J5C0
A	48	SER	CYS	conflict	UNP A0A1G6J5C0
A	99	VAL	ILE	conflict	UNP A0A1G6J5C0
A	180	ARG	LYS	conflict	UNP A0A1G6J5C0
A	309	SER	ALA	conflict	UNP A0A1G6J5C0
A	330	VAL	MET	conflict	UNP A0A1G6J5C0
A	353	TYR	PHE	conflict	UNP A0A1G6J5C0
B	24	SER	LYS	conflict	UNP A0A1G6J5C0
B	48	SER	CYS	conflict	UNP A0A1G6J5C0
B	99	VAL	ILE	conflict	UNP A0A1G6J5C0
B	180	ARG	LYS	conflict	UNP A0A1G6J5C0
B	309	SER	ALA	conflict	UNP A0A1G6J5C0
B	330	VAL	MET	conflict	UNP A0A1G6J5C0

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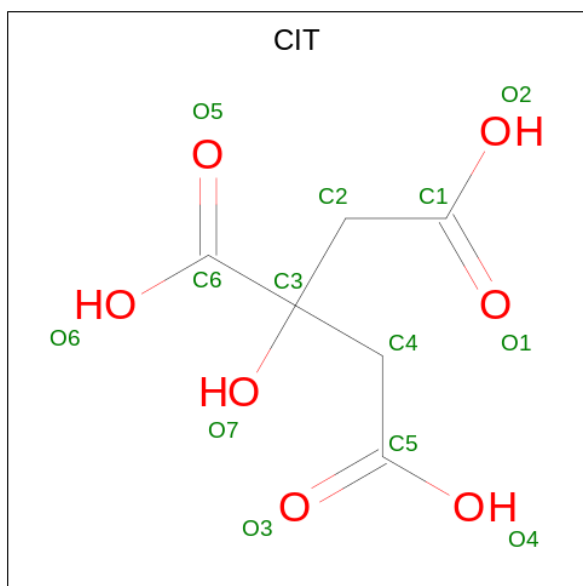
Chain	Residue	Modelled	Actual	Comment	Reference
B	353	TYR	PHE	conflict	UNP A0A1G6J5C0
C	24	SER	LYS	conflict	UNP A0A1G6J5C0
C	48	SER	CYS	conflict	UNP A0A1G6J5C0
C	99	VAL	ILE	conflict	UNP A0A1G6J5C0
C	180	ARG	LYS	conflict	UNP A0A1G6J5C0
C	309	SER	ALA	conflict	UNP A0A1G6J5C0
C	330	VAL	MET	conflict	UNP A0A1G6J5C0
C	353	TYR	PHE	conflict	UNP A0A1G6J5C0
D	24	SER	LYS	conflict	UNP A0A1G6J5C0
D	48	SER	CYS	conflict	UNP A0A1G6J5C0
D	99	VAL	ILE	conflict	UNP A0A1G6J5C0
D	180	ARG	LYS	conflict	UNP A0A1G6J5C0
D	309	SER	ALA	conflict	UNP A0A1G6J5C0
D	330	VAL	MET	conflict	UNP A0A1G6J5C0
D	353	TYR	PHE	conflict	UNP A0A1G6J5C0
E	24	SER	LYS	conflict	UNP A0A1G6J5C0
E	48	SER	CYS	conflict	UNP A0A1G6J5C0
E	99	VAL	ILE	conflict	UNP A0A1G6J5C0
E	180	ARG	LYS	conflict	UNP A0A1G6J5C0
E	309	SER	ALA	conflict	UNP A0A1G6J5C0
E	330	VAL	MET	conflict	UNP A0A1G6J5C0
E	353	TYR	PHE	conflict	UNP A0A1G6J5C0
F	24	SER	LYS	conflict	UNP A0A1G6J5C0
F	48	SER	CYS	conflict	UNP A0A1G6J5C0
F	99	VAL	ILE	conflict	UNP A0A1G6J5C0
F	180	ARG	LYS	conflict	UNP A0A1G6J5C0
F	309	SER	ALA	conflict	UNP A0A1G6J5C0
F	330	VAL	MET	conflict	UNP A0A1G6J5C0
F	353	TYR	PHE	conflict	UNP A0A1G6J5C0
G	24	SER	LYS	conflict	UNP A0A1G6J5C0
G	48	SER	CYS	conflict	UNP A0A1G6J5C0
G	99	VAL	ILE	conflict	UNP A0A1G6J5C0
G	180	ARG	LYS	conflict	UNP A0A1G6J5C0
G	309	SER	ALA	conflict	UNP A0A1G6J5C0
G	330	VAL	MET	conflict	UNP A0A1G6J5C0
G	353	TYR	PHE	conflict	UNP A0A1G6J5C0
H	24	SER	LYS	conflict	UNP A0A1G6J5C0
H	48	SER	CYS	conflict	UNP A0A1G6J5C0
H	99	VAL	ILE	conflict	UNP A0A1G6J5C0
H	180	ARG	LYS	conflict	UNP A0A1G6J5C0
H	309	SER	ALA	conflict	UNP A0A1G6J5C0
H	330	VAL	MET	conflict	UNP A0A1G6J5C0

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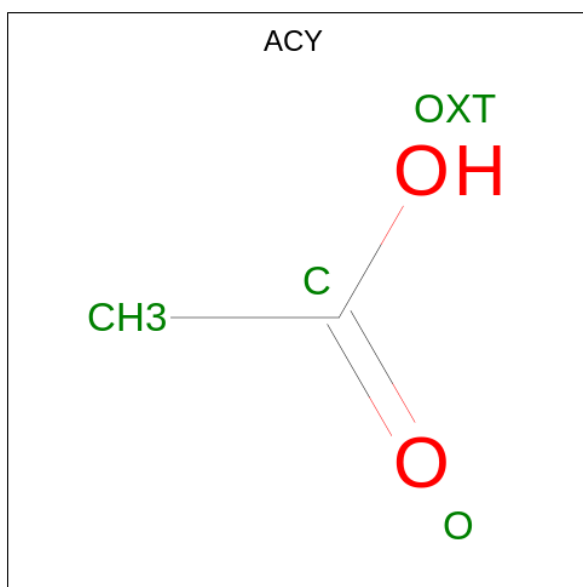
Chain	Residue	Modelled	Actual	Comment	Reference
H	353	TYR	PHE	conflict	UNP A0A1G6J5C0

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$) (labeled as "Ligand of Interest" by depositor).



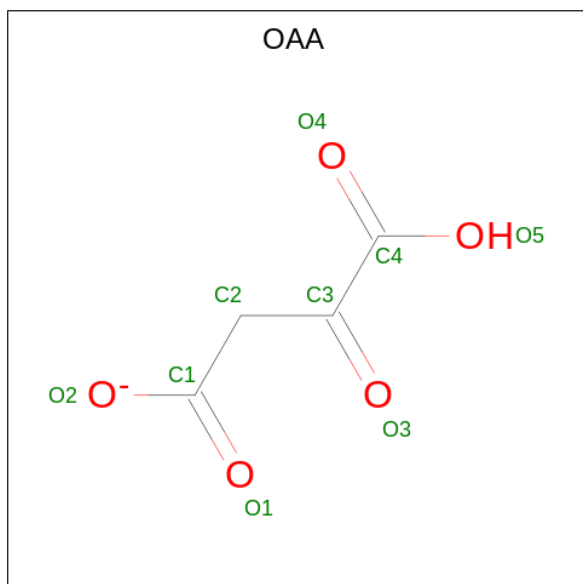
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		
2	C	1	Total	C	O	0	0
			13	6	7		
2	D	1	Total	C	O	0	0
			13	6	7		
2	G	1	Total	C	O	0	0
			13	6	7		
2	H	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is OXALOACETATE ION (three-letter code: OAA) (formula: $C_4H_3O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			9	4	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	C	O	0	0
			9	4	5		

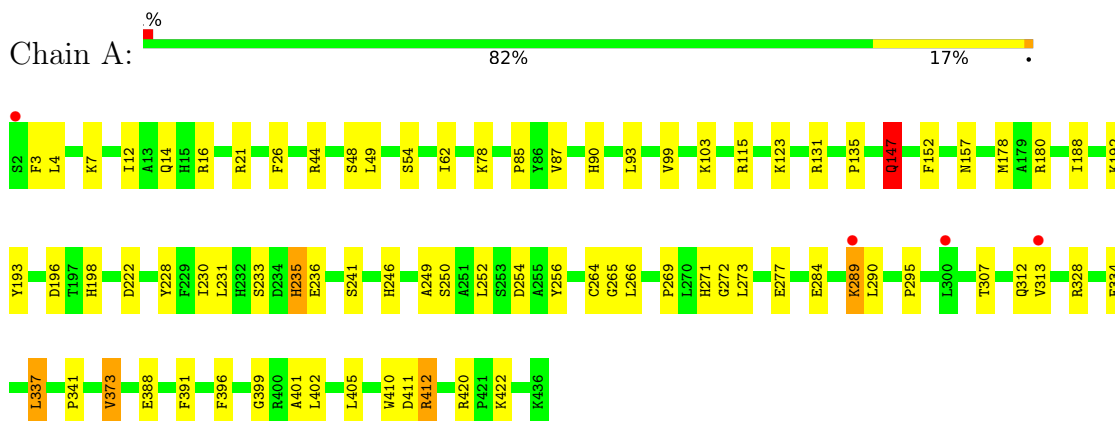
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	323	Total	O	0	0
			323	323		
5	B	320	Total	O	0	0
			320	320		
5	C	255	Total	O	0	0
			255	255		
5	D	221	Total	O	0	0
			221	221		
5	E	201	Total	O	0	0
			201	201		
5	F	173	Total	O	0	0
			173	173		
5	G	260	Total	O	0	0
			260	260		
5	H	273	Total	O	0	0
			273	273		

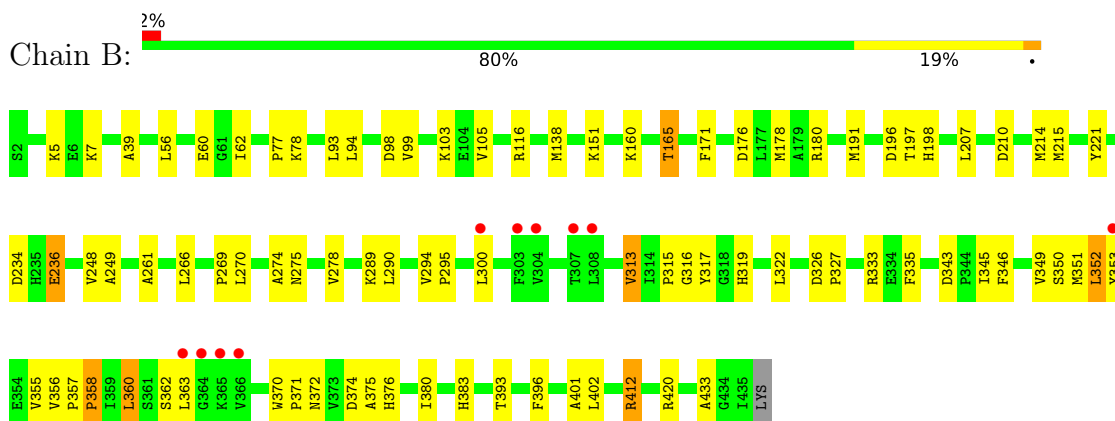
3 Residue-property plots

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.

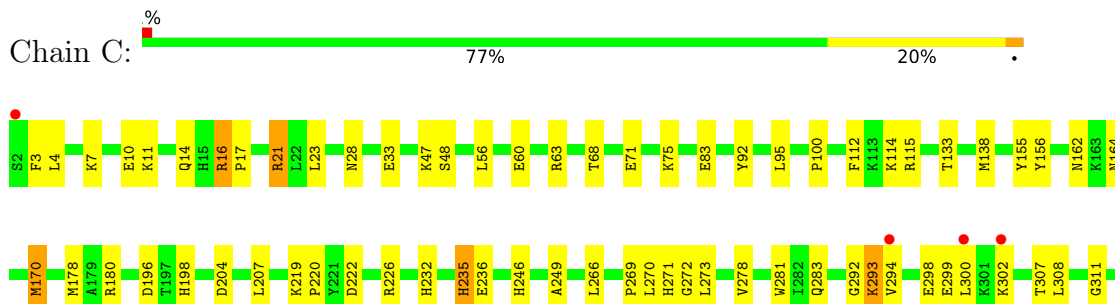
• Molecule 1: Citrate synthase

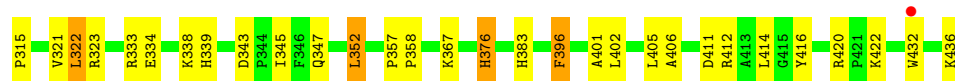


• Molecule 1: Citrate synthase

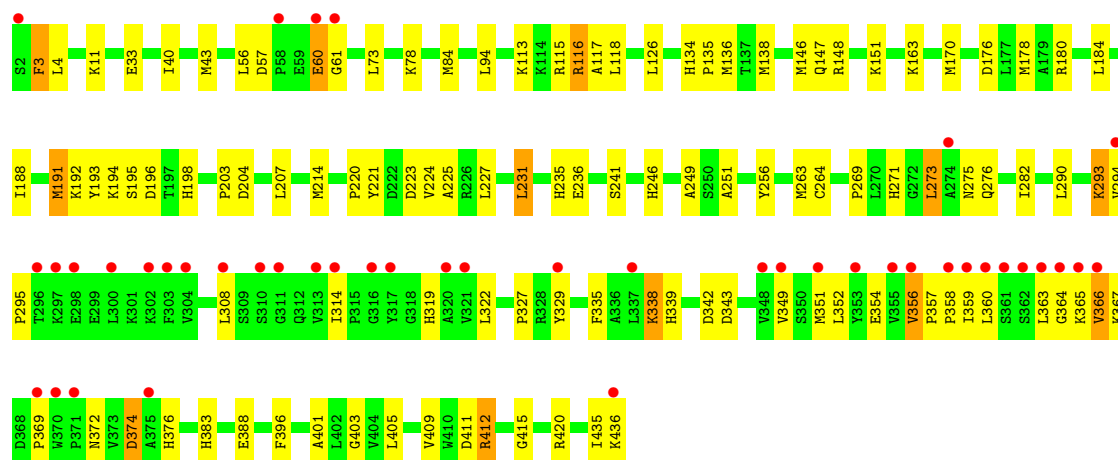
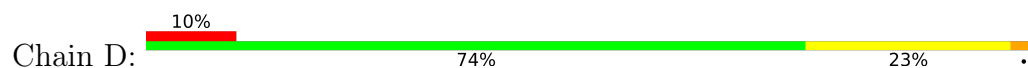


• Molecule 1: Citrate synthase

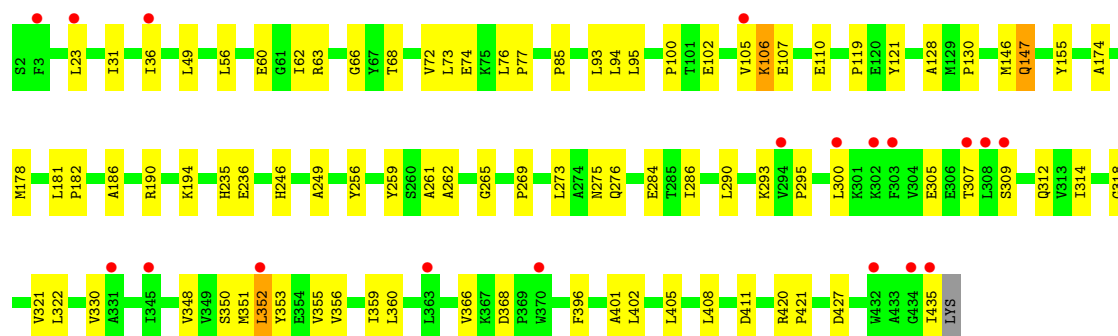
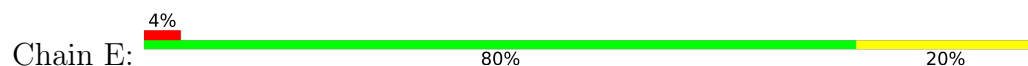




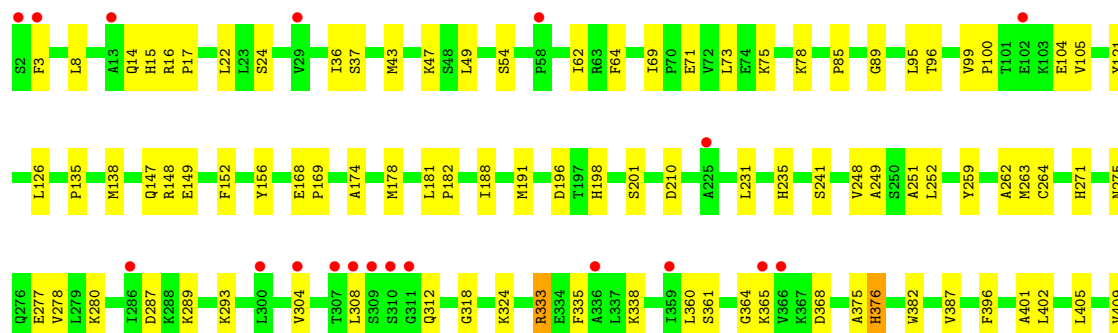
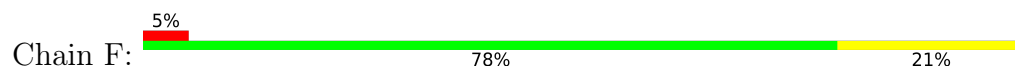
● Molecule 1: Citrate synthase



● Molecule 1: Citrate synthase

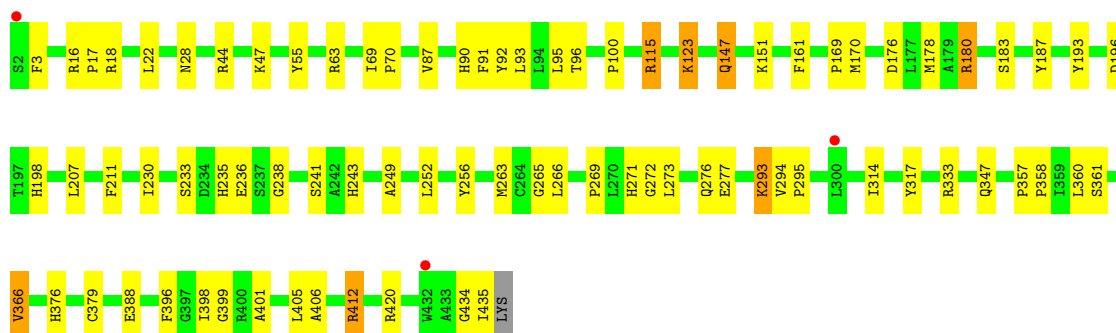
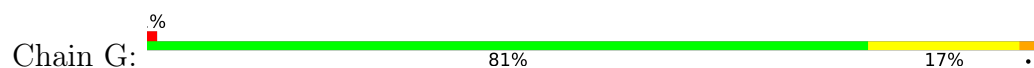


● Molecule 1: Citrate synthase

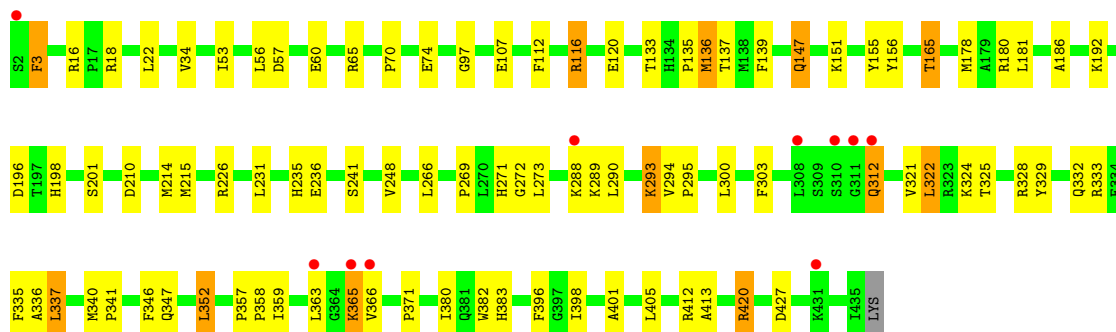
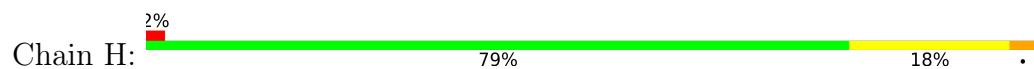




• Molecule 1: Citrate synthase



• Molecule 1: Citrate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	361.42Å 361.42Å 77.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.07 – 2.03 25.07 – 2.03	Depositor EDS
% Data completeness (in resolution range)	96.2 (25.07-2.03) 96.3 (25.07-2.03)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.8.0411	Depositor
R, R_{free}	0.196 , 0.239 0.204 , 0.246	Depositor DCC
R_{free} test set	12273 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.035 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	29531	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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 25.62 % 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 3.0653e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: OAA, ACY, CIT

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	0.44	0/3523	0.76	2/4773 (0.0%)
1	B	0.43	0/3511	0.74	0/4759
1	C	0.39	0/3519	0.73	0/4769
1	D	0.40	0/3515	0.73	0/4765
1	E	0.34	0/3511	0.68	0/4759
1	F	0.35	1/3506 (0.0%)	0.62	0/4754
1	G	0.41	0/3510	0.75	2/4758 (0.0%)
1	H	0.42	2/3510 (0.1%)	0.74	1/4758 (0.0%)
All	All	0.40	3/28105 (0.0%)	0.72	5/38095 (0.0%)

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	A	0	2
1	B	0	1
1	C	0	3
1	D	0	3
1	E	0	1
1	F	0	2
1	G	0	3
1	H	0	3
All	All	0	18

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	107	GLU	CD-OE1	5.96	1.32	1.25
1	F	304	VAL	C-N	-5.49	1.21	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	120	GLU	CD-OE2	-5.12	1.20	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	GLN	CB-CA-C	5.91	122.22	110.40
1	H	136	MET	CG-SD-CE	-5.75	91.00	100.20
1	G	123	LYS	CB-CA-C	5.54	121.49	110.40
1	A	412	ARG	CB-CG-CD	5.42	125.69	111.60
1	G	236	GLU	CB-CA-C	5.06	120.53	110.40

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	ARG	Sidechain
1	A	44	ARG	Sidechain
1	B	180	ARG	Sidechain
1	C	16	ARG	Sidechain
1	C	323	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3435	0	3416	92	0
1	B	3423	0	3395	87	0
1	C	3431	0	3405	94	0
1	D	3427	0	3394	126	0
1	E	3423	0	3395	77	0
1	F	3418	0	3380	78	0
1	G	3422	0	3392	93	0
1	H	3422	0	3392	100	0
2	A	13	0	5	1	0
2	B	13	0	5	0	0
2	C	13	0	5	1	0
2	D	13	0	5	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	13	0	5	1	0
2	H	13	0	5	1	0
3	E	4	0	3	0	0
3	F	4	0	3	0	0
4	E	9	0	2	0	0
4	F	9	0	2	0	0
5	A	323	0	0	51	0
5	B	320	0	0	44	0
5	C	255	0	0	50	0
5	D	221	0	0	49	0
5	E	201	0	0	40	0
5	F	173	0	0	38	0
5	G	260	0	0	54	0
5	H	273	0	0	49	0
All	All	29531	0	27209	724	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 13.

The worst 5 of 724 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:D:409:VAL:HG22	5:D:727:HOH:O	1.15	1.31
1:G:412:ARG:HB2	5:G:611:HOH:O	1.13	1.26
1:G:3:PHE:CG	5:G:795:HOH:O	1.80	1.25
1:B:178:MET:SD	5:B:857:HOH:O	1.96	1.24
1:F:263:MET:HE2	5:F:602:HOH:O	1.37	1.22

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	433/435 (100%)	424 (98%)	8 (2%)	1 (0%)	44	41
1	B	432/435 (99%)	420 (97%)	11 (2%)	1 (0%)	44	41
1	C	433/435 (100%)	424 (98%)	8 (2%)	1 (0%)	44	41
1	D	433/435 (100%)	412 (95%)	19 (4%)	2 (0%)	25	20
1	E	432/435 (99%)	417 (96%)	14 (3%)	1 (0%)	44	41
1	F	432/435 (99%)	416 (96%)	16 (4%)	0	100	100
1	G	432/435 (99%)	425 (98%)	7 (2%)	0	100	100
1	H	432/435 (99%)	422 (98%)	9 (2%)	1 (0%)	44	41
All	All	3459/3480 (99%)	3360 (97%)	92 (3%)	7 (0%)	44	41

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	GLU
1	C	236	GLU
1	D	366	VAL
1	H	236	GLU
1	B	236	GLU

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	363/365 (100%)	353 (97%)	10 (3%)	38	39
1	B	362/365 (99%)	350 (97%)	12 (3%)	33	32
1	C	362/365 (99%)	350 (97%)	12 (3%)	33	32
1	D	361/365 (99%)	344 (95%)	17 (5%)	22	19
1	E	362/365 (99%)	346 (96%)	16 (4%)	24	21
1	F	360/365 (99%)	345 (96%)	15 (4%)	25	23
1	G	361/365 (99%)	352 (98%)	9 (2%)	42	44
1	H	361/365 (99%)	344 (95%)	17 (5%)	22	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2892/2920 (99%)	2784 (96%)	108 (4%)	29	28

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	106	LYS
1	F	147	GLN
1	H	324	LYS
1	E	155	TYR
1	E	396	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	383	HIS
1	G	198	HIS
1	F	147	GLN
1	F	347	GLN
1	G	271	HIS

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](#)

10 ligands are modelled in this entry.

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	CIT	D	501	-	12,12,12	1.15	0	17,17,17	1.07	1 (5%)
3	ACY	E	501	-	3,3,3	1.05	0	3,3,3	0.87	0
4	OAA	E	502	-	8,8,8	4.98	2 (25%)	9,10,10	2.05	3 (33%)
2	CIT	B	501	-	12,12,12	1.30	2 (16%)	17,17,17	1.29	2 (11%)
4	OAA	F	502	-	8,8,8	6.09	2 (25%)	9,10,10	1.58	1 (11%)
2	CIT	C	501	-	12,12,12	1.19	0	17,17,17	1.79	4 (23%)
2	CIT	G	501	-	12,12,12	1.12	1 (8%)	17,17,17	1.78	5 (29%)
2	CIT	A	501	-	12,12,12	1.05	1 (8%)	17,17,17	1.48	3 (17%)
3	ACY	F	501	-	3,3,3	1.34	0	3,3,3	0.55	0
2	CIT	H	501	-	12,12,12	1.13	0	17,17,17	1.47	3 (17%)

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	CIT	D	501	-	-	4/16/16/16	-
4	OAA	E	502	-	-	1/8/8/8	-
2	CIT	B	501	-	-	6/16/16/16	-
4	OAA	F	502	-	-	0/8/8/8	-
2	CIT	C	501	-	-	9/16/16/16	-
2	CIT	G	501	-	-	9/16/16/16	-
2	CIT	A	501	-	-	9/16/16/16	-
2	CIT	H	501	-	-	0/16/16/16	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	502	OAA	C3-C4	-16.87	1.30	1.53
4	E	502	OAA	C3-C4	-13.83	1.34	1.53
2	B	501	CIT	O6-C6	-2.48	1.21	1.30
2	B	501	CIT	C3-C6	2.27	1.55	1.53
4	F	502	OAA	O5-C4	-2.17	1.24	1.30

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	CIT	O5-C6-C3	-4.29	116.17	122.25
2	G	501	CIT	O5-C6-C3	-3.93	116.69	122.25
2	H	501	CIT	O5-C6-C3	-3.69	117.03	122.25
2	A	501	CIT	O5-C6-C3	-3.53	117.26	122.25
2	C	501	CIT	O6-C6-C3	3.24	118.67	113.05

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

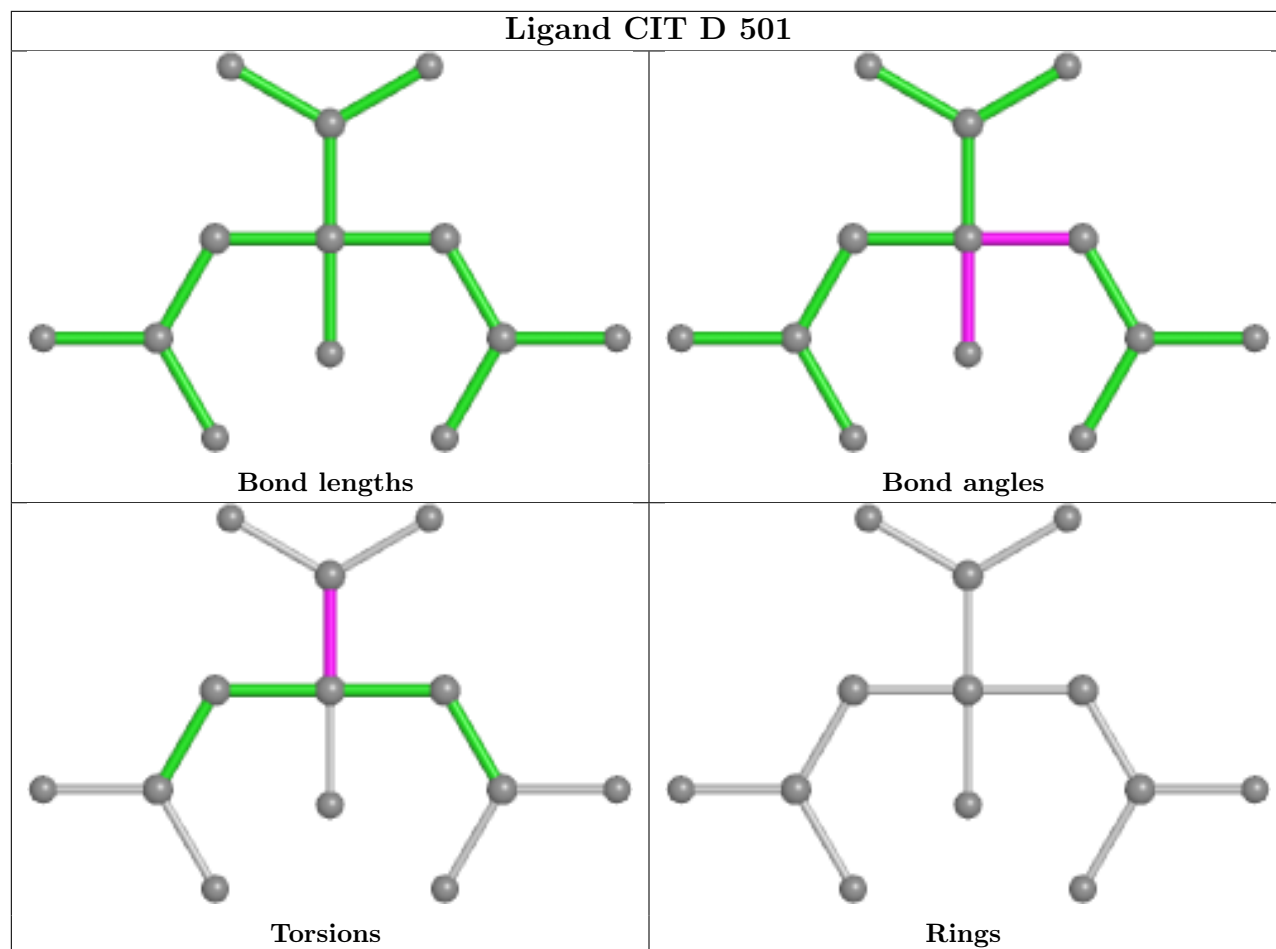
Mol	Chain	Res	Type	Atoms
2	A	501	CIT	O7-C3-C6-O5
2	A	501	CIT	O7-C3-C6-O6
2	A	501	CIT	C4-C3-C6-O6
2	G	501	CIT	O7-C3-C6-O6
2	G	501	CIT	C4-C3-C6-O6

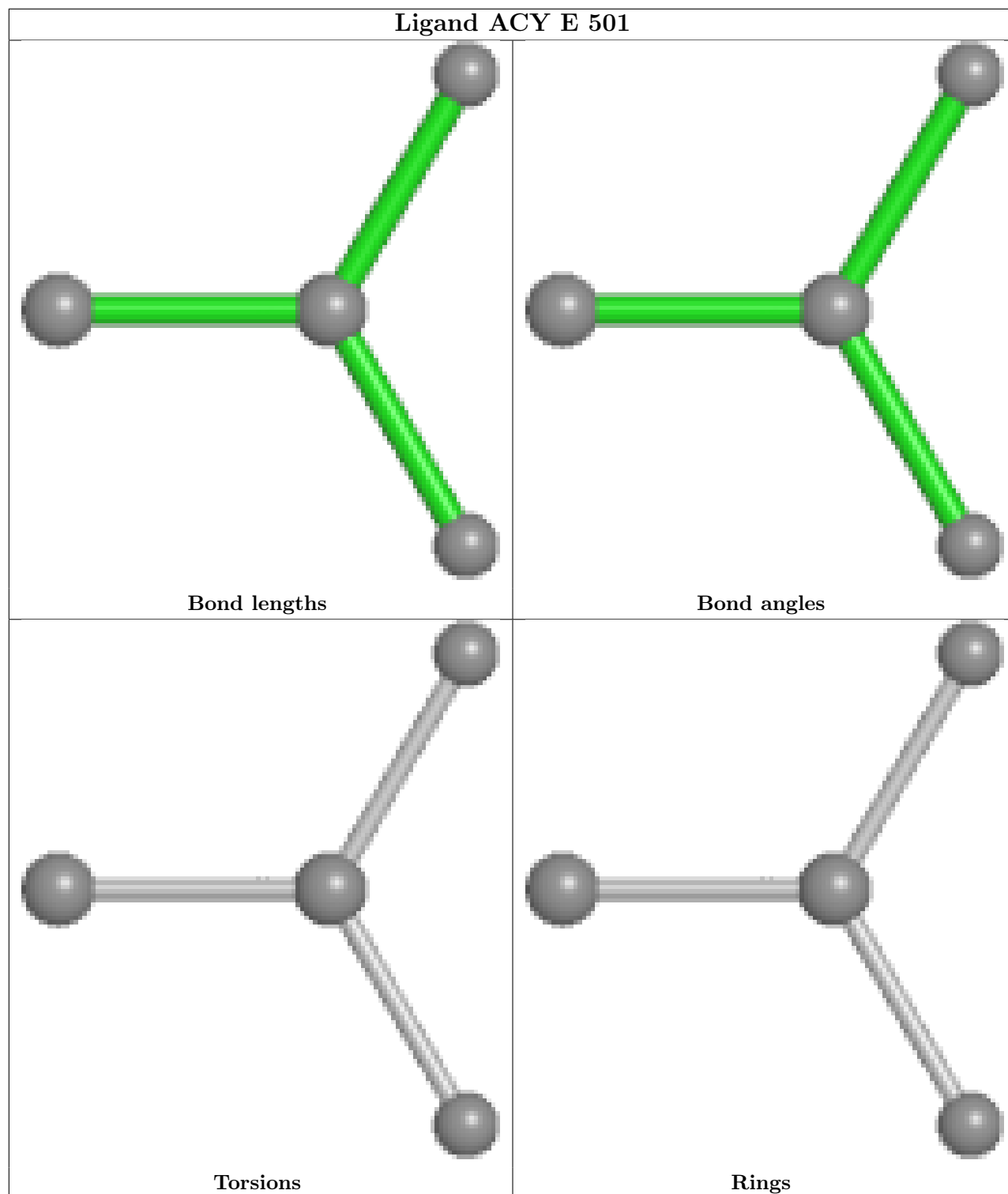
There are no ring outliers.

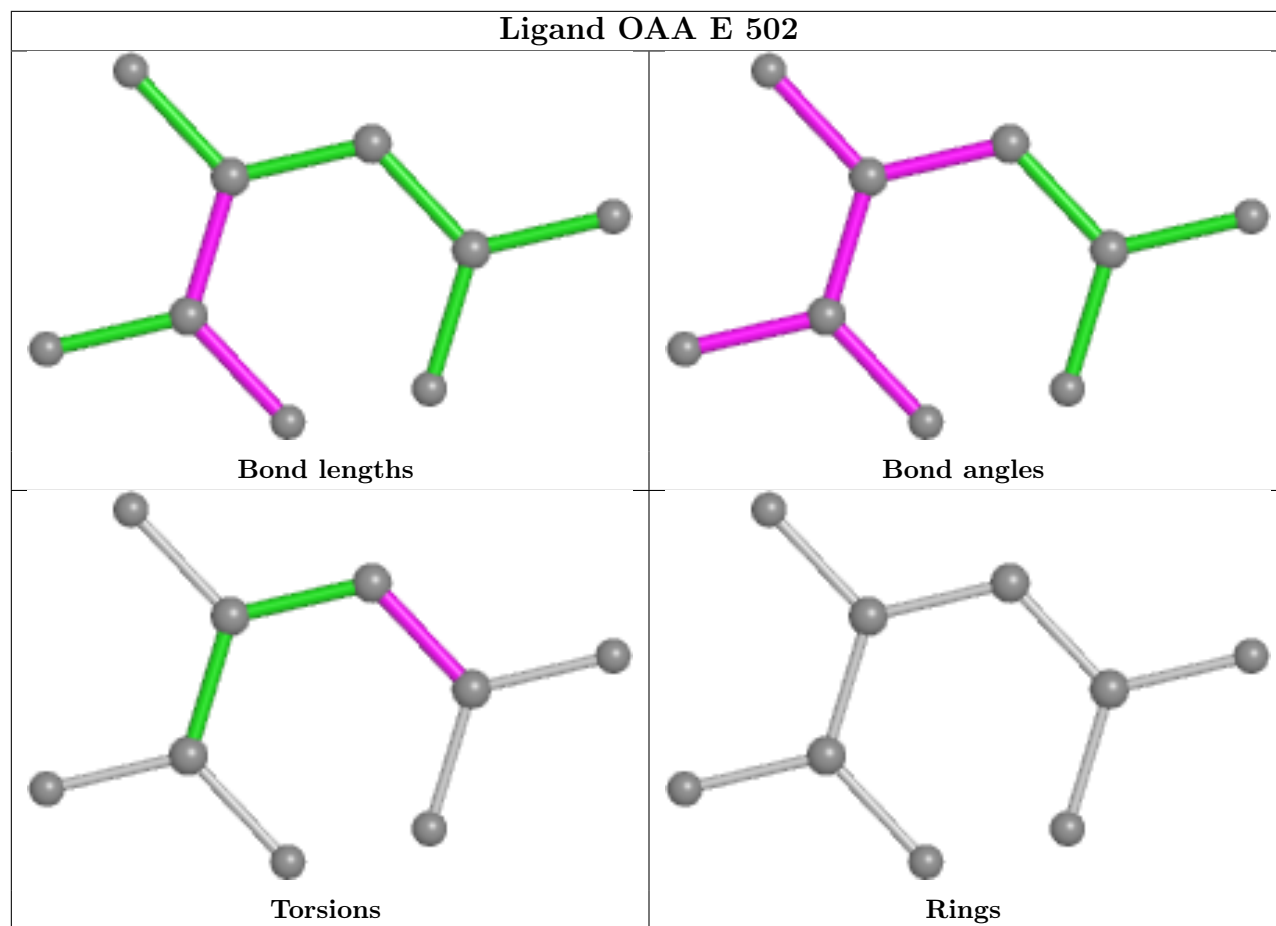
5 monomers are involved in 10 short contacts:

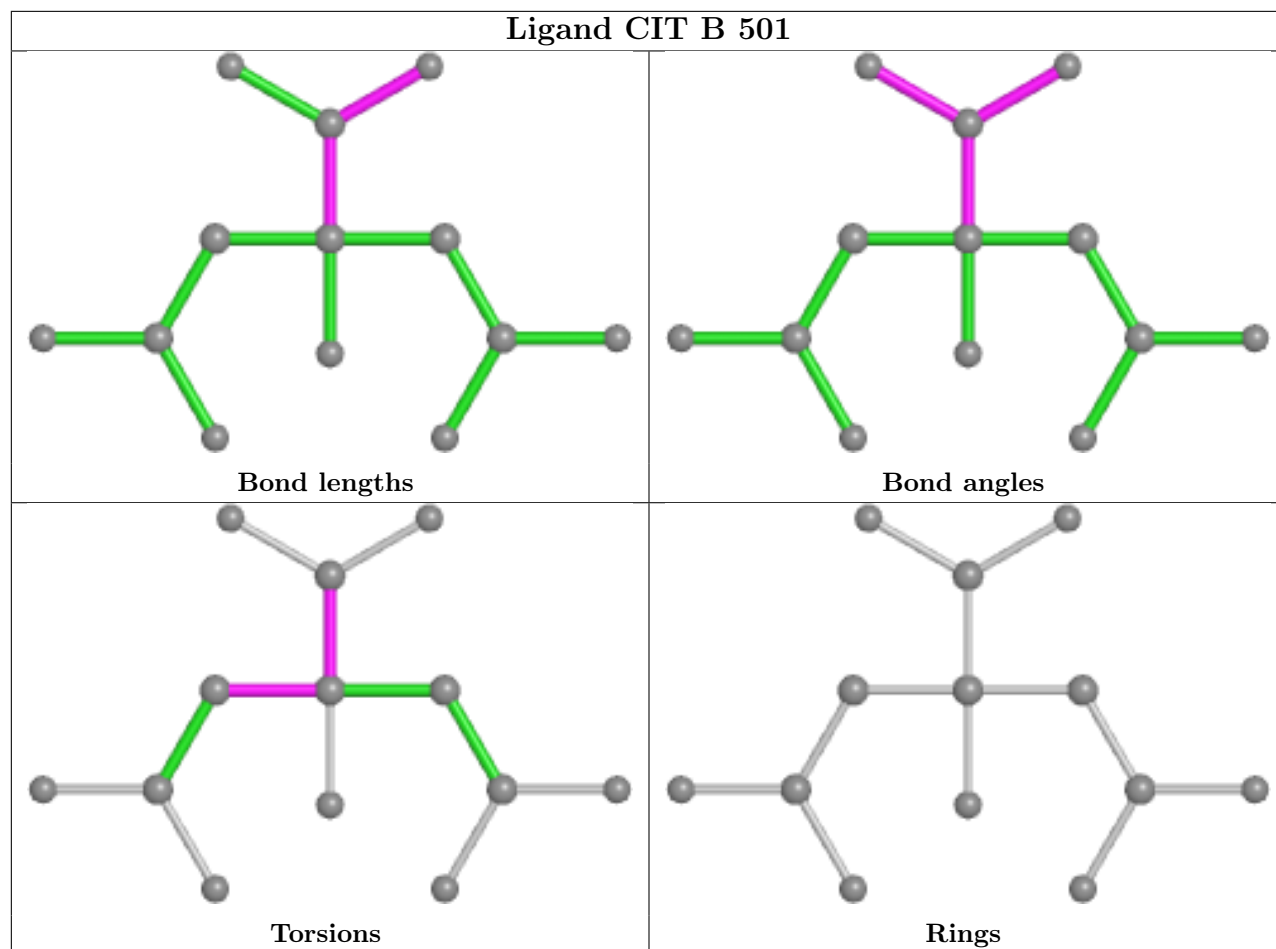
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	CIT	6	0
2	C	501	CIT	1	0
2	G	501	CIT	1	0
2	A	501	CIT	1	0
2	H	501	CIT	1	0

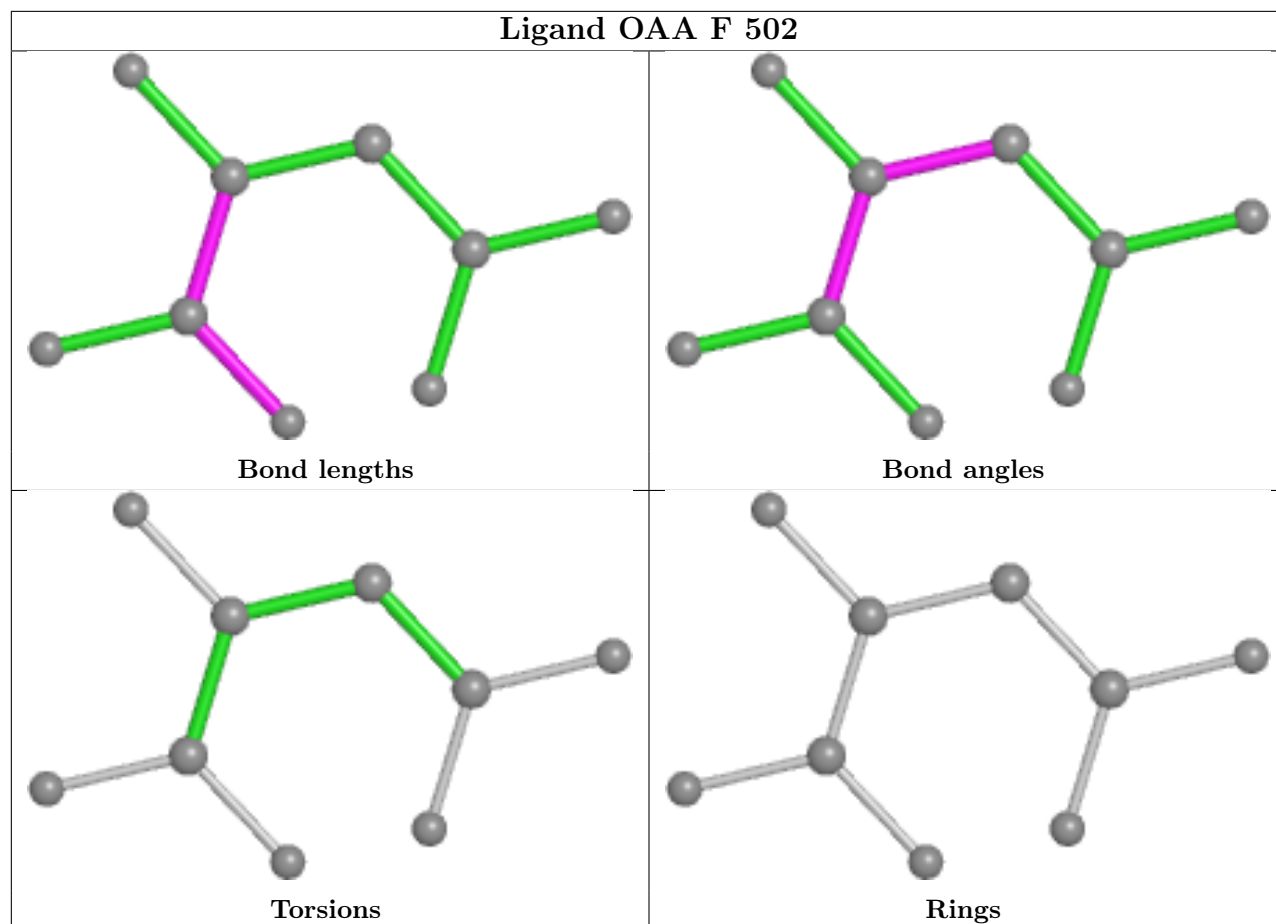
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

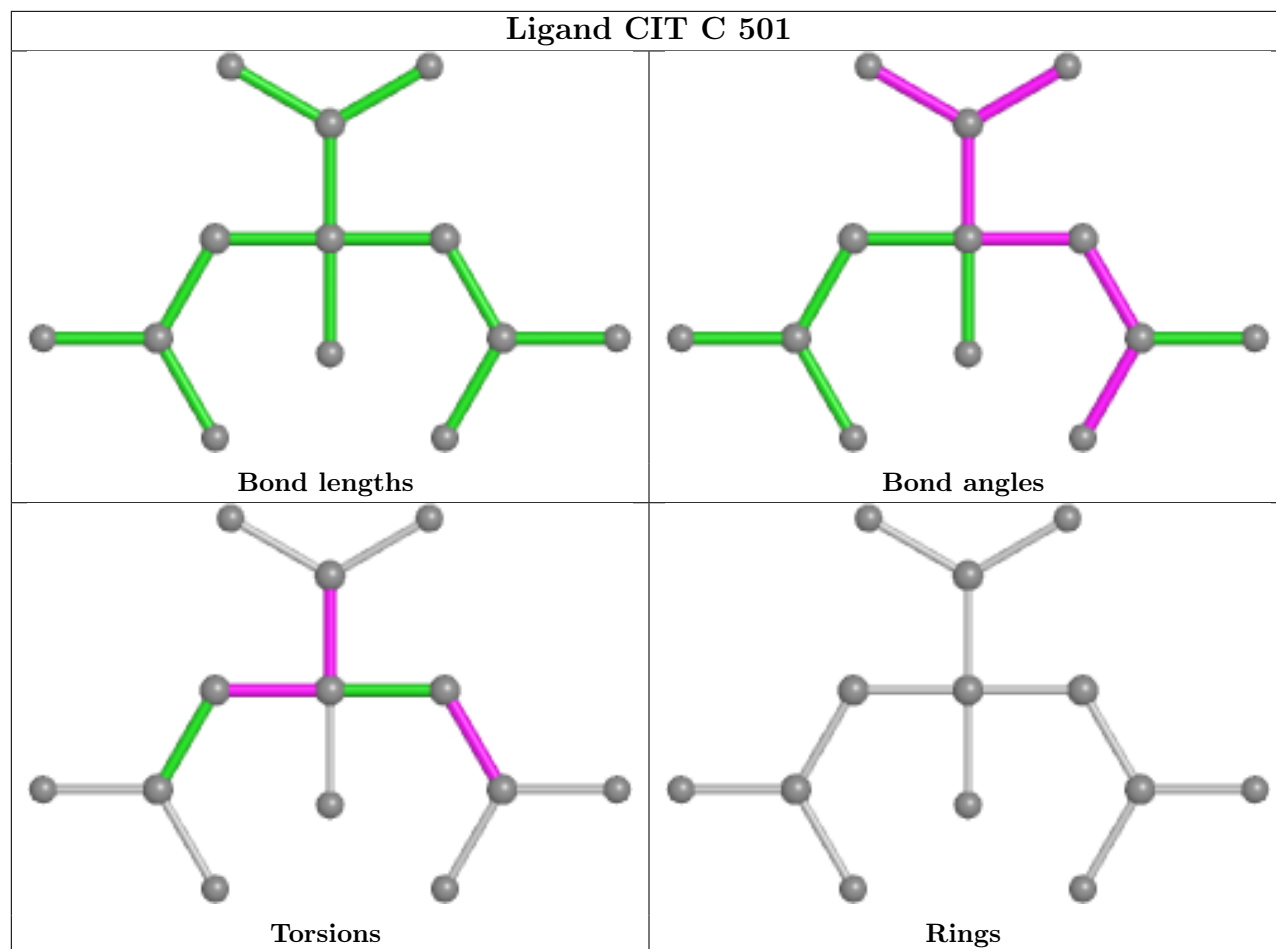


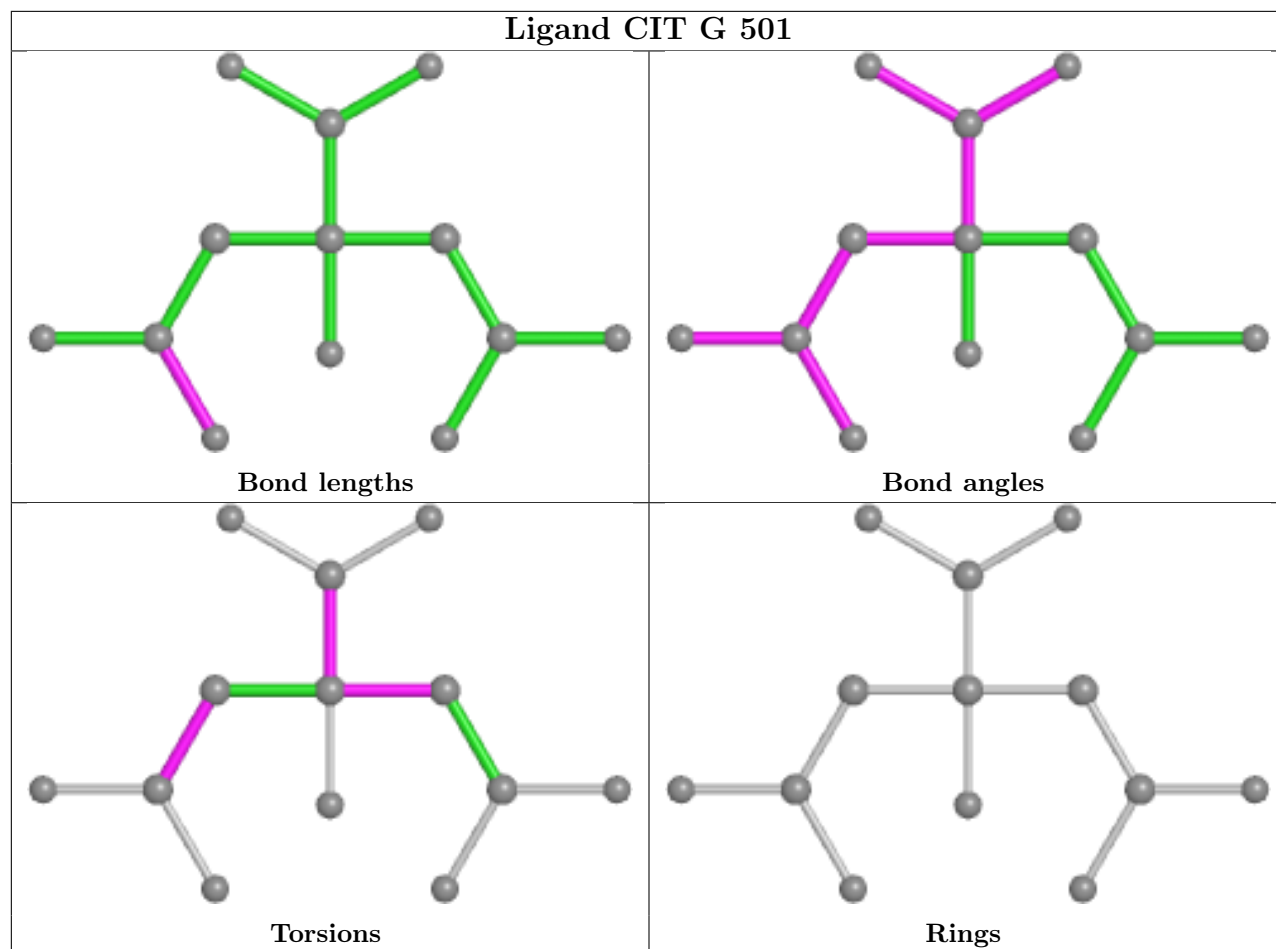


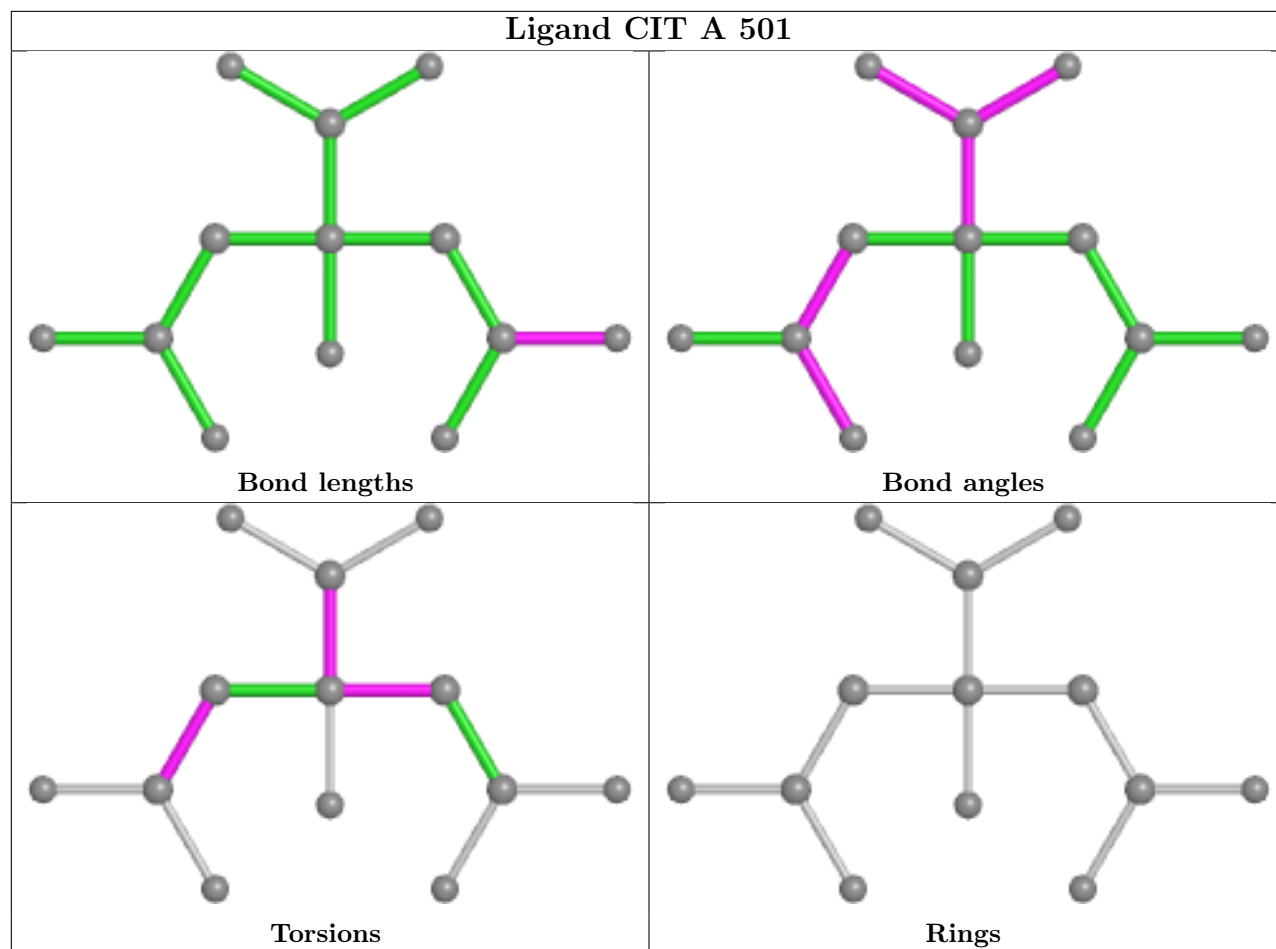


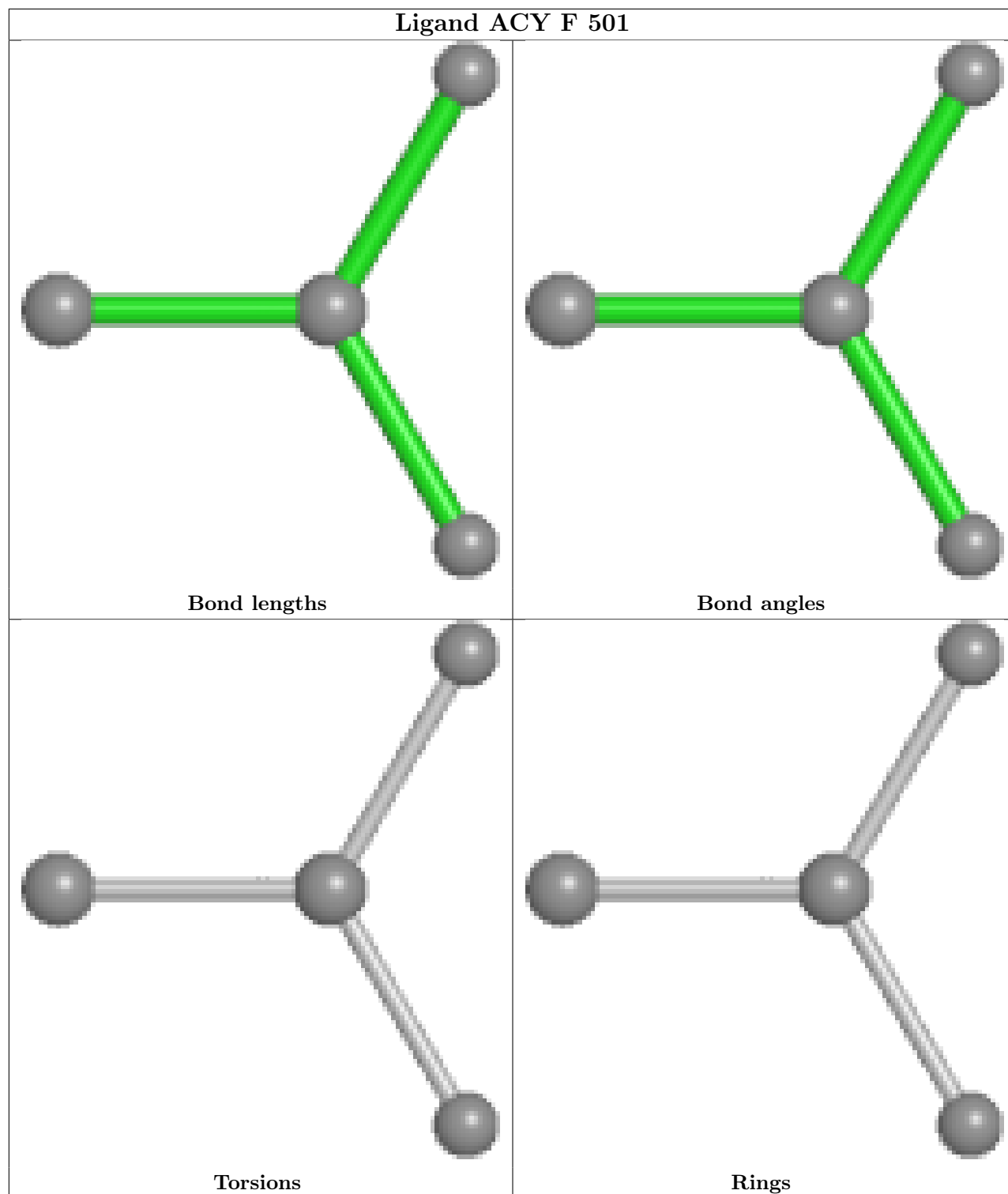


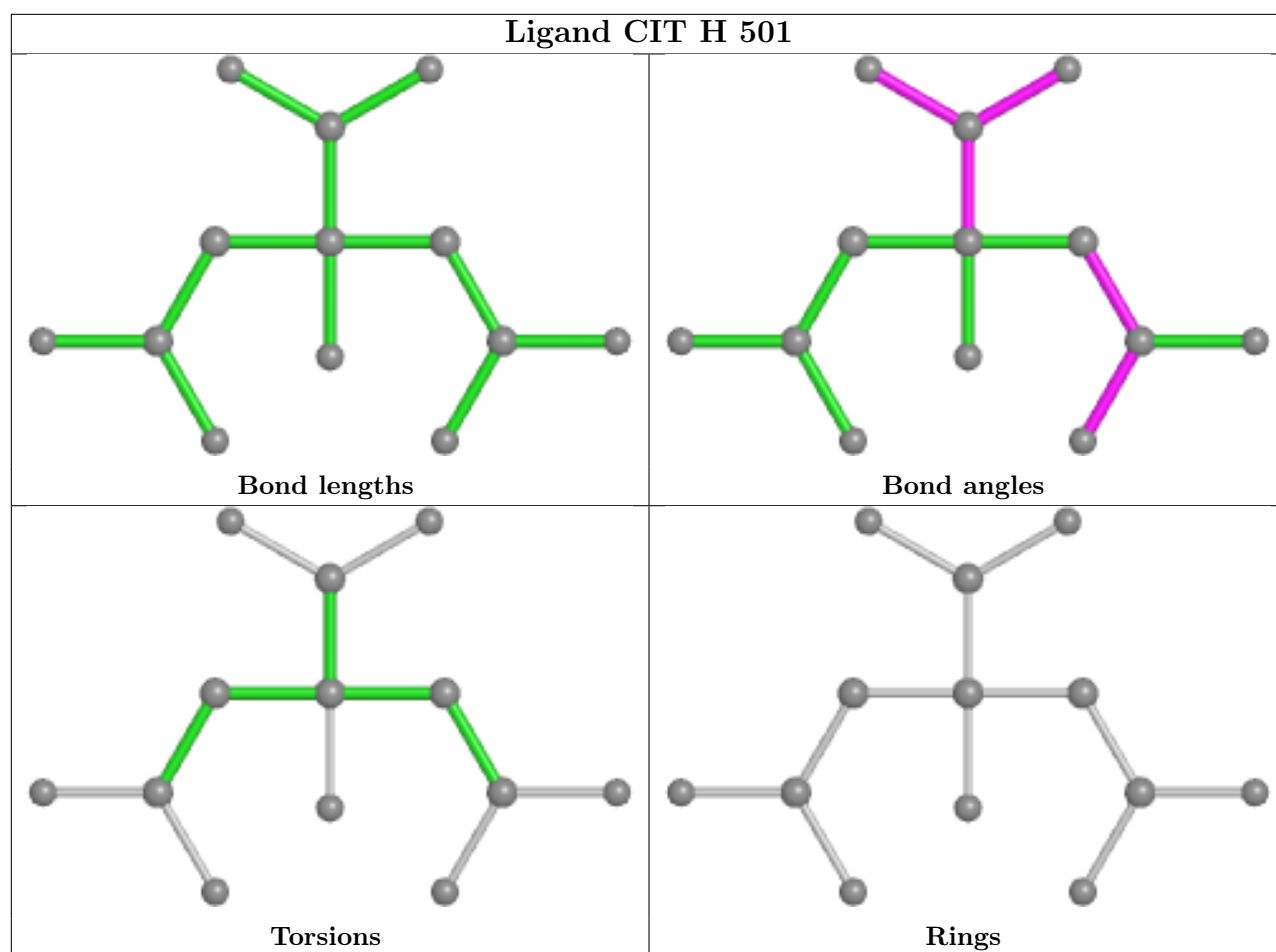












5.7 Other polymers [i](#)

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 [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	435/435 (100%)	-0.35	4 (0%) 81 81	11, 24, 59, 80	0
1	B	434/435 (99%)	-0.20	10 (2%) 61 60	12, 24, 66, 99	0
1	C	435/435 (100%)	-0.14	5 (1%) 77 77	14, 29, 62, 83	0
1	D	435/435 (100%)	0.27	44 (10%) 14 13	13, 34, 93, 132	0
1	E	434/435 (99%)	0.39	19 (4%) 39 39	21, 42, 74, 96	0
1	F	434/435 (99%)	0.49	21 (4%) 36 36	20, 45, 79, 116	0
1	G	434/435 (99%)	-0.24	3 (0%) 84 84	14, 26, 57, 92	0
1	H	434/435 (99%)	-0.17	10 (2%) 61 60	13, 27, 67, 110	0
All	All	3475/3480 (99%)	0.01	116 (3%) 49 48	11, 31, 71, 132	0

The worst 5 of 116 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	2	SER	8.4
1	D	2	SER	4.7
1	F	2	SER	4.6
1	D	303	PHE	4.6
1	D	296	THR	4.5

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands

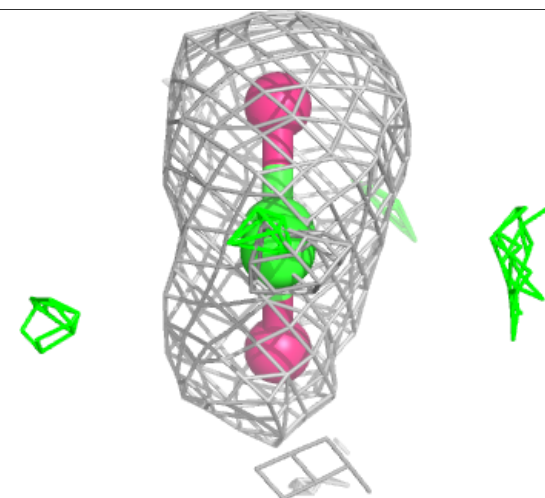
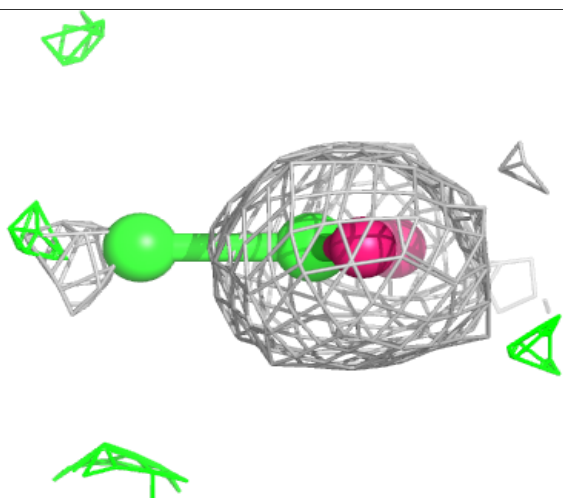
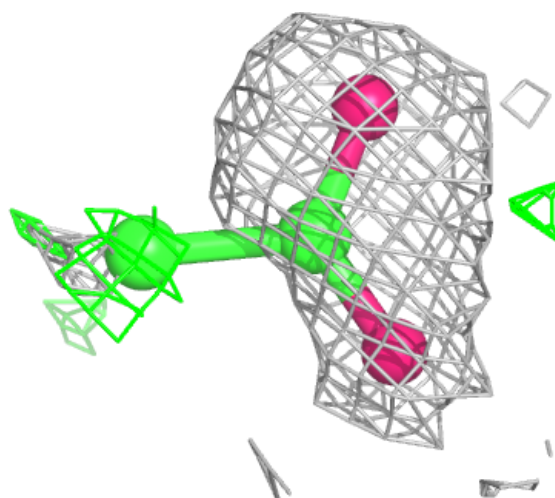
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ACY	F	501	4/4	0.80	0.17	44,52,52,54	0
3	ACY	E	501	4/4	0.82	0.20	36,51,52,54	0
4	OAA	E	502	9/9	0.87	0.11	29,32,34,35	0
2	CIT	D	501	13/13	0.88	0.12	30,44,51,55	0
4	OAA	F	502	9/9	0.93	0.07	31,35,38,40	0
2	CIT	B	501	13/13	0.94	0.07	19,26,34,35	0
2	CIT	C	501	13/13	0.95	0.07	21,24,29,29	0
2	CIT	G	501	13/13	0.95	0.07	19,22,30,31	0
2	CIT	H	501	13/13	0.96	0.06	21,25,29,31	0
2	CIT	A	501	13/13	0.97	0.05	16,19,26,26	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.

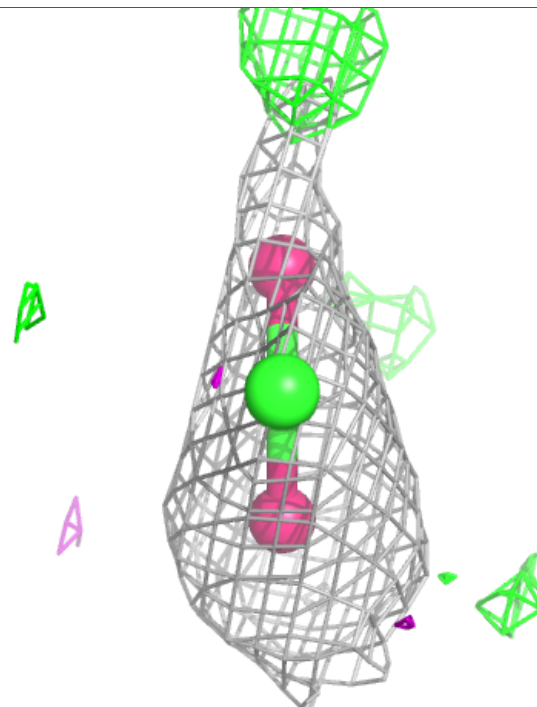
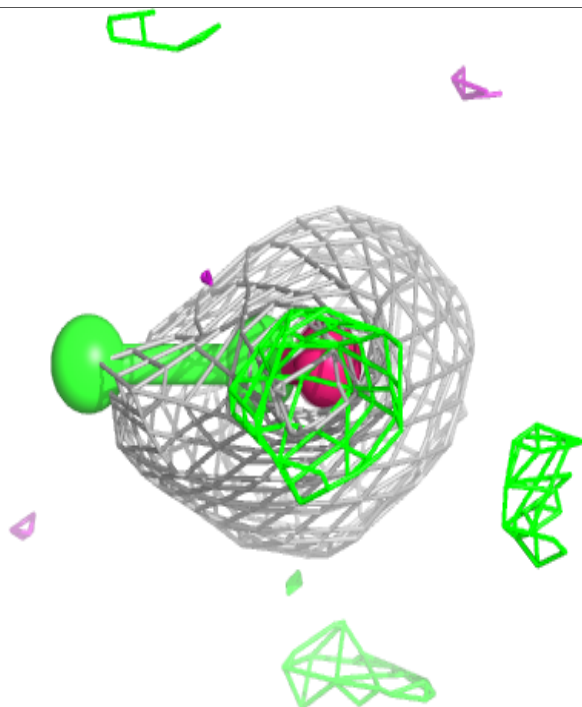
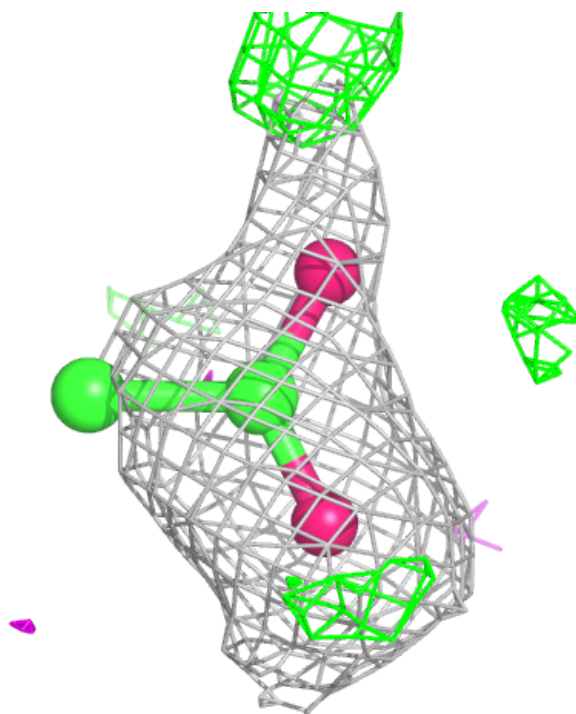
Electron density around ACY F 501:

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



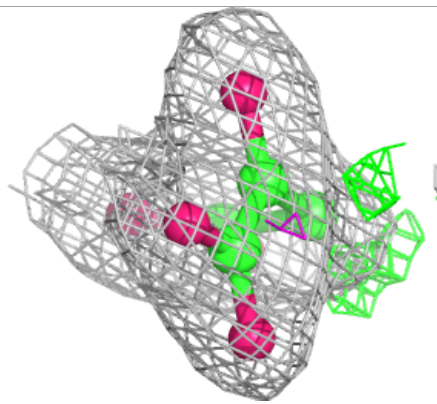
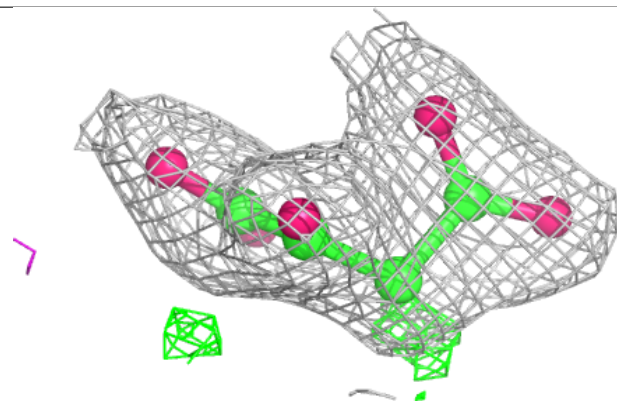
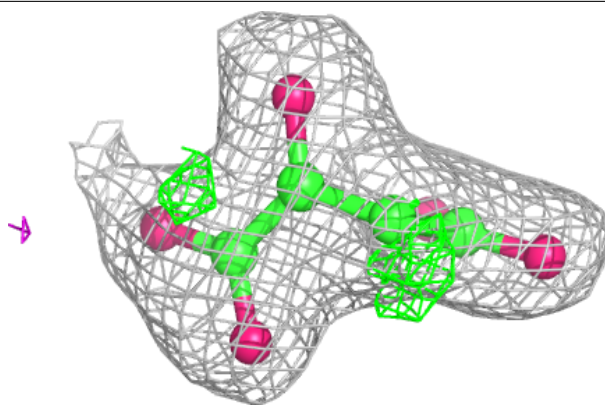
Electron density around ACY E 501:

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



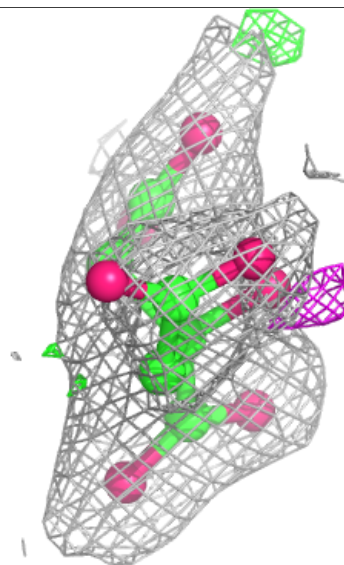
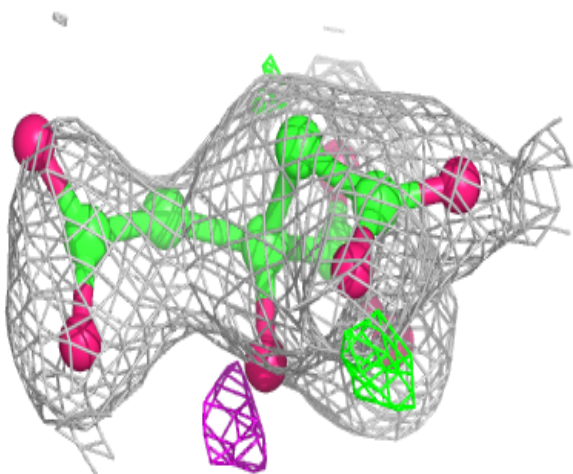
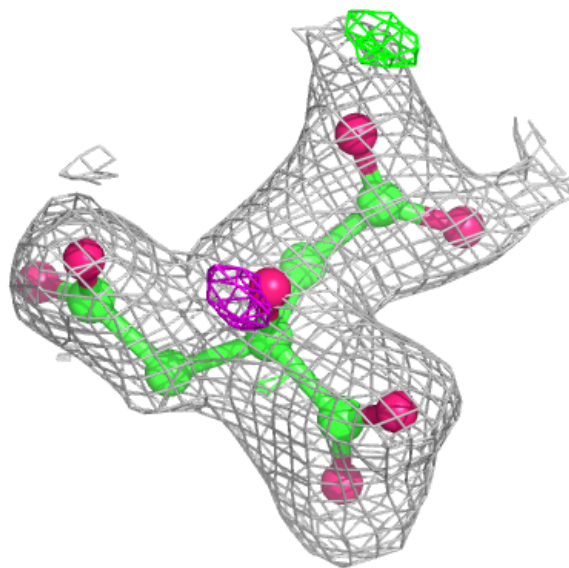
Electron density around OAA E 502:

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



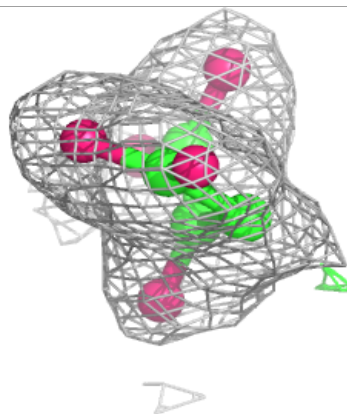
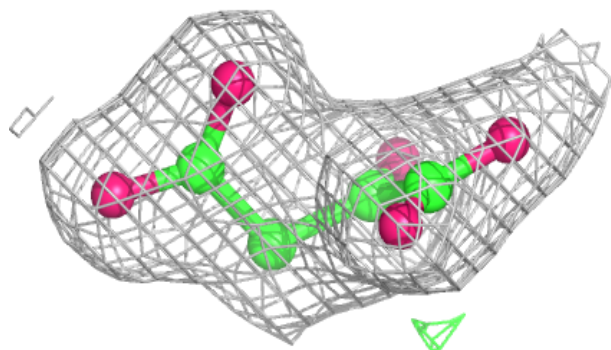
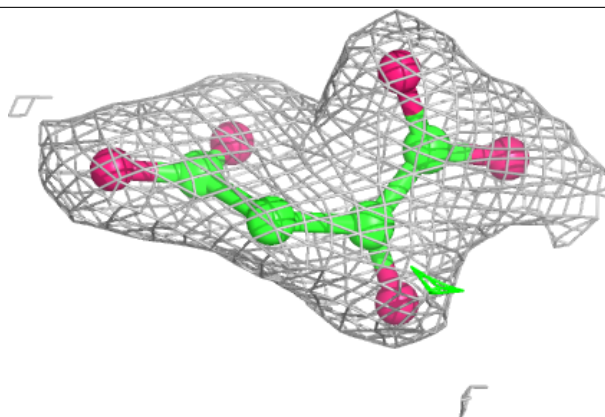
Electron density around CIT D 501:

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



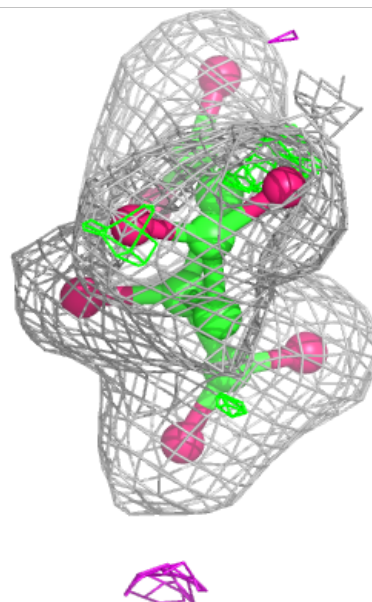
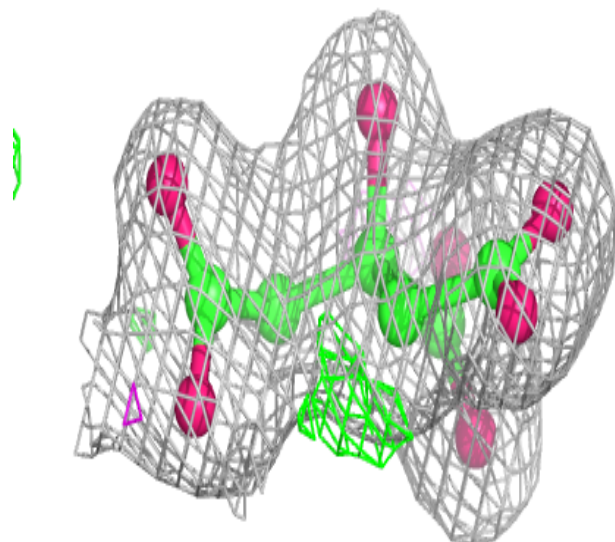
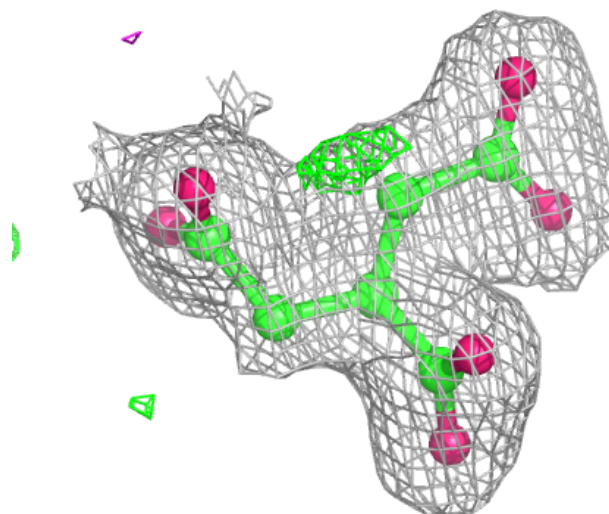
Electron density around OAA F 502:

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



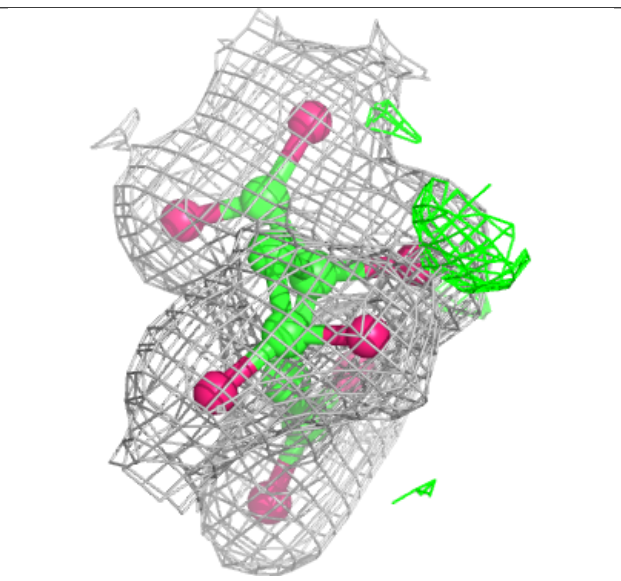
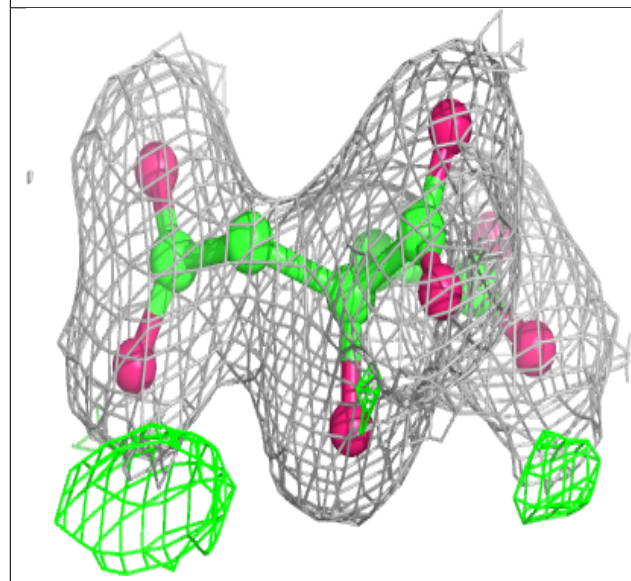
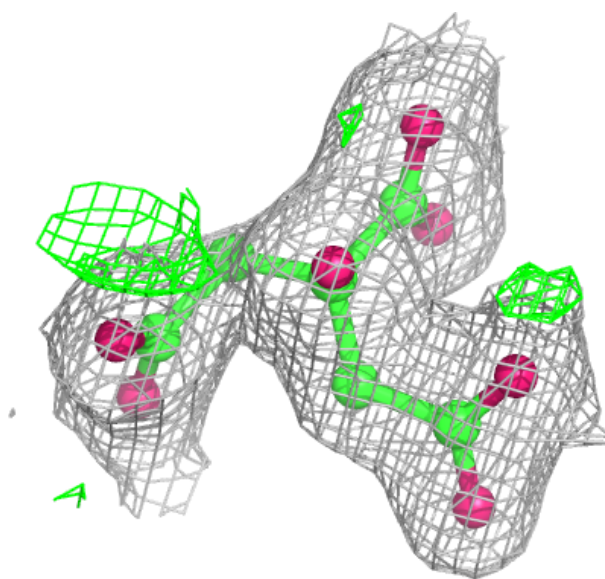
Electron density around CIT B 501:

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



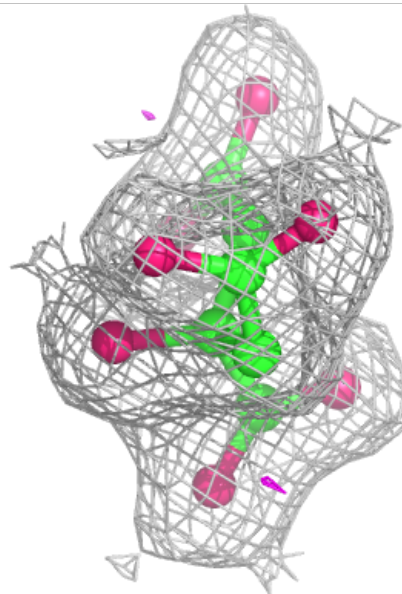
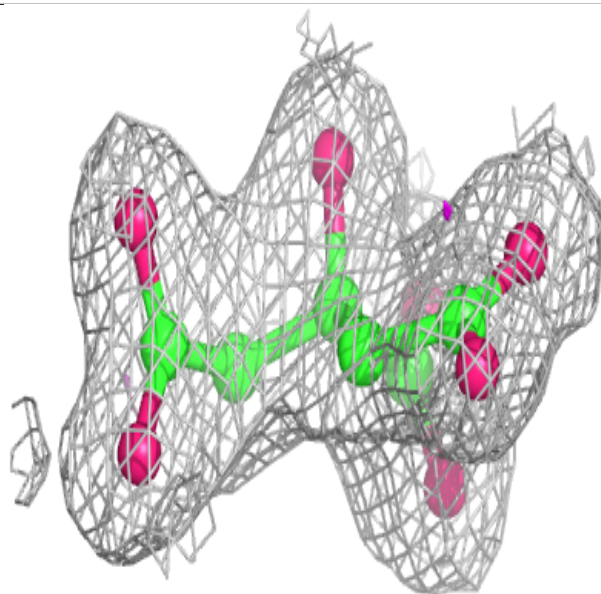
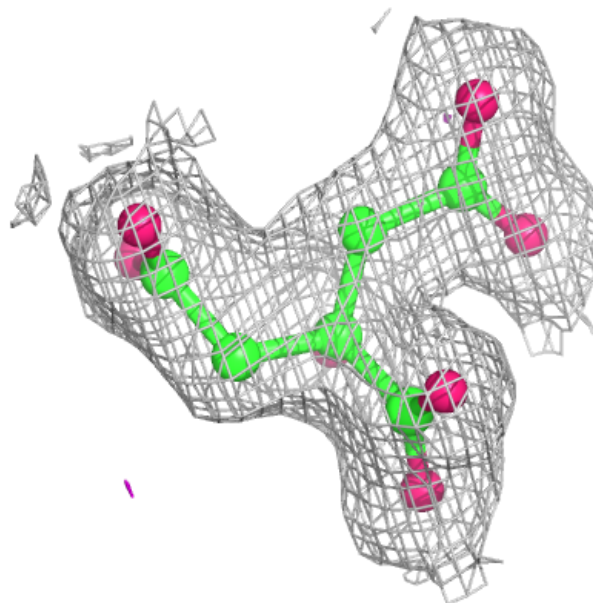
Electron density around CIT C 501:

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



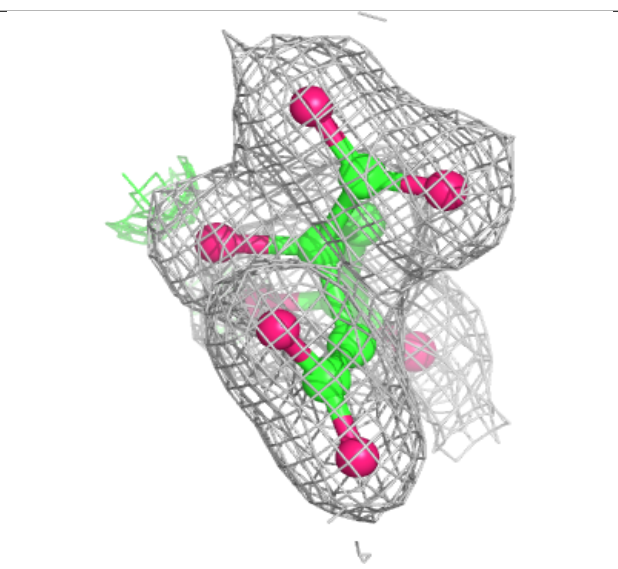
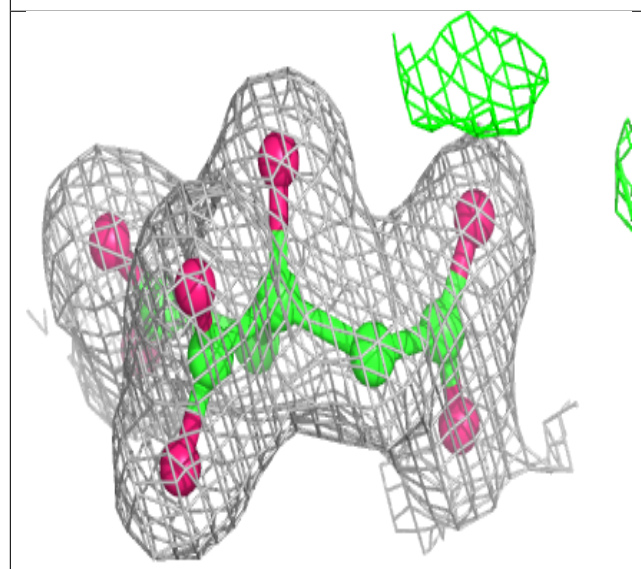
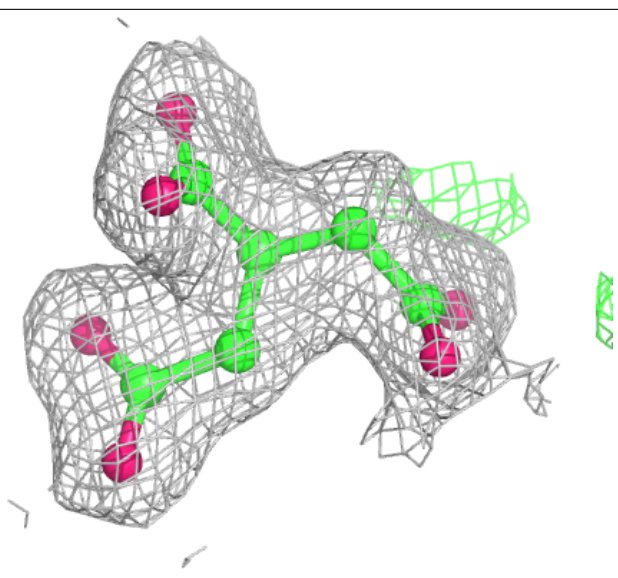
Electron density around CIT G 501:

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



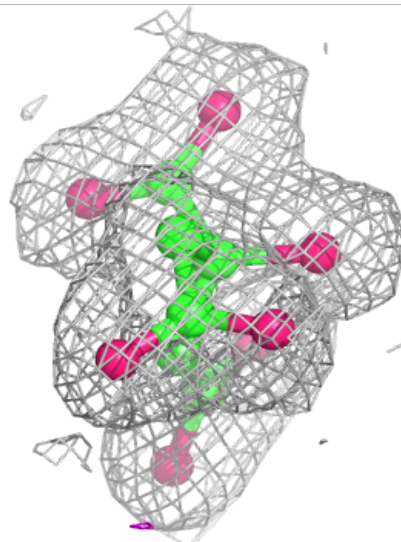
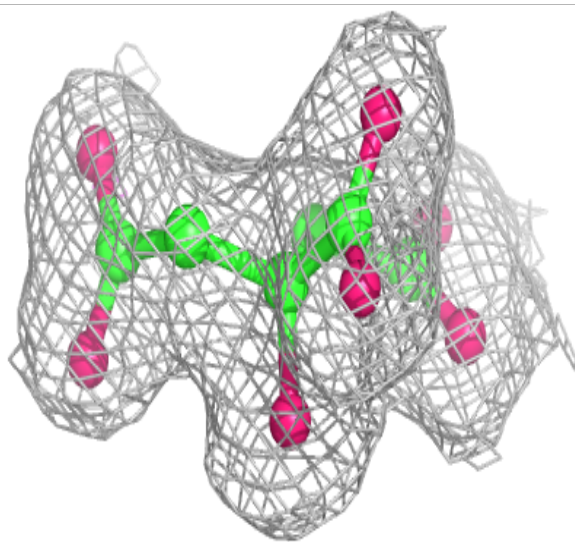
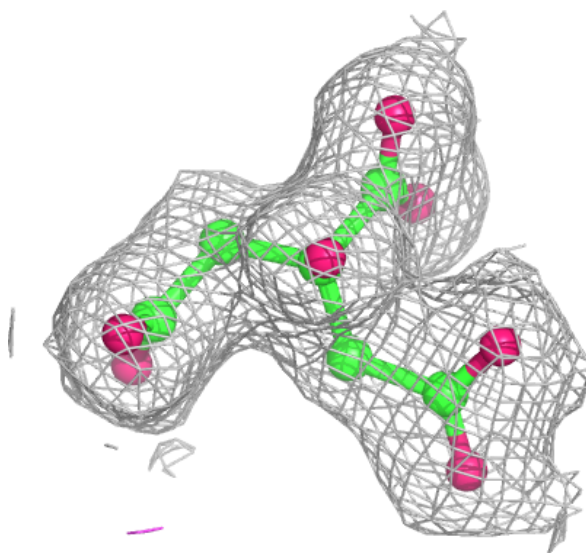
Electron density around CIT H 501:

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



Electron density around CIT A 501:

$2mF_o-DF_c$ (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.