



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 08:54 AM UTC

PDB ID : 8YWD / pdb_00008ywd
Title : Crystal structure of trehalose synthase mutant N253C from *Deinococcus radiodurans*
Authors : Ye, L.C.; Chen, S.C.
Deposited on : 2024-03-30
Resolution : 2.65 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 : 4-5-2 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

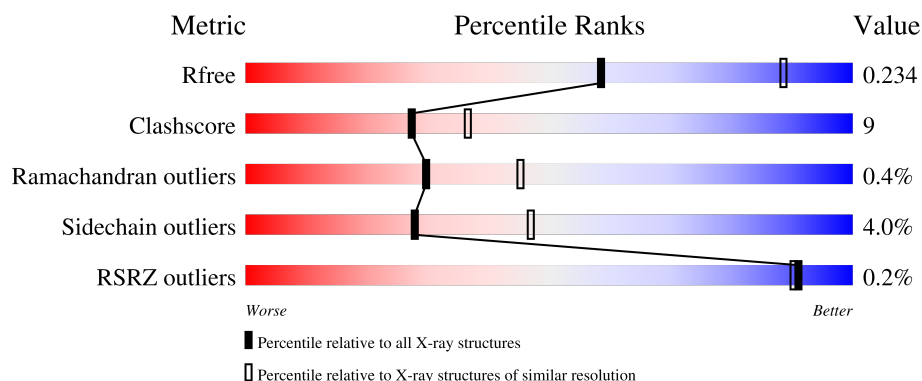
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	571	 75% 19% . .
1	B	571	 78% 18% .
1	C	571	 76% 19% . .
1	D	571	 79% 16% . .
1	E	571	 73% 21% . .

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Mol	Chain	Length	Quality of chain
1	F	571	73% 21%
1	G	571	74% 22%
1	H	571	% 71% 23%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 35405 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 maltose alpha-D-glucosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total	C	N	O	S	0	0	0
			4402	2817	750	818	17			
1	B	548	Total	C	N	O	S	0	0	0
			4402	2817	750	818	17			
1	C	548	Total	C	N	O	S	0	0	0
			4402	2817	750	818	17			
1	D	548	Total	C	N	O	S	0	0	0
			4402	2817	750	818	17			
1	E	548	Total	C	N	O	S	0	0	0
			4402	2817	750	818	17			
1	F	548	Total	C	N	O	S	0	0	0
			4402	2817	750	818	17			
1	G	548	Total	C	N	O	S	0	0	0
			4402	2817	750	818	17			
1	H	548	Total	C	N	O	S	0	0	0
			4402	2817	750	818	17			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP Q9RST7
A	0	VAL	-	expression tag	UNP Q9RST7
A	1	PRO	-	expression tag	UNP Q9RST7
A	97	TRP	ARG	engineered mutation	UNP Q9RST7
A	253	CYS	ASN	engineered mutation	UNP Q9RST7
A	313	ILE	THR	engineered mutation	UNP Q9RST7
A	380	VAL	ILE	engineered mutation	UNP Q9RST7
A	553	SER	-	expression tag	UNP Q9RST7
A	554	ARG	-	expression tag	UNP Q9RST7
A	555	VAL	-	expression tag	UNP Q9RST7
A	556	ASP	-	expression tag	UNP Q9RST7
A	557	LYS	-	expression tag	UNP Q9RST7
A	558	LEU	-	expression tag	UNP Q9RST7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	559	ALA	-	expression tag	UNP Q9RST7
A	560	ALA	-	expression tag	UNP Q9RST7
A	561	ALA	-	expression tag	UNP Q9RST7
A	562	LEU	-	expression tag	UNP Q9RST7
A	563	GLU	-	expression tag	UNP Q9RST7
A	564	HIS	-	expression tag	UNP Q9RST7
A	565	HIS	-	expression tag	UNP Q9RST7
A	566	HIS	-	expression tag	UNP Q9RST7
A	567	HIS	-	expression tag	UNP Q9RST7
A	568	HIS	-	expression tag	UNP Q9RST7
A	569	HIS	-	expression tag	UNP Q9RST7
B	-1	MET	-	initiating methionine	UNP Q9RST7
B	0	VAL	-	expression tag	UNP Q9RST7
B	1	PRO	-	expression tag	UNP Q9RST7
B	97	TRP	ARG	engineered mutation	UNP Q9RST7
B	253	CYS	ASN	engineered mutation	UNP Q9RST7
B	313	ILE	THR	engineered mutation	UNP Q9RST7
B	380	VAL	ILE	engineered mutation	UNP Q9RST7
B	553	SER	-	expression tag	UNP Q9RST7
B	554	ARG	-	expression tag	UNP Q9RST7
B	555	VAL	-	expression tag	UNP Q9RST7
B	556	ASP	-	expression tag	UNP Q9RST7
B	557	LYS	-	expression tag	UNP Q9RST7
B	558	LEU	-	expression tag	UNP Q9RST7
B	559	ALA	-	expression tag	UNP Q9RST7
B	560	ALA	-	expression tag	UNP Q9RST7
B	561	ALA	-	expression tag	UNP Q9RST7
B	562	LEU	-	expression tag	UNP Q9RST7
B	563	GLU	-	expression tag	UNP Q9RST7
B	564	HIS	-	expression tag	UNP Q9RST7
B	565	HIS	-	expression tag	UNP Q9RST7
B	566	HIS	-	expression tag	UNP Q9RST7
B	567	HIS	-	expression tag	UNP Q9RST7
B	568	HIS	-	expression tag	UNP Q9RST7
B	569	HIS	-	expression tag	UNP Q9RST7
C	-1	MET	-	initiating methionine	UNP Q9RST7
C	0	VAL	-	expression tag	UNP Q9RST7
C	1	PRO	-	expression tag	UNP Q9RST7
C	97	TRP	ARG	engineered mutation	UNP Q9RST7
C	253	CYS	ASN	engineered mutation	UNP Q9RST7
C	313	ILE	THR	engineered mutation	UNP Q9RST7
C	380	VAL	ILE	engineered mutation	UNP Q9RST7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	553	SER	-	expression tag	UNP Q9RST7
C	554	ARG	-	expression tag	UNP Q9RST7
C	555	VAL	-	expression tag	UNP Q9RST7
C	556	ASP	-	expression tag	UNP Q9RST7
C	557	LYS	-	expression tag	UNP Q9RST7
C	558	LEU	-	expression tag	UNP Q9RST7
C	559	ALA	-	expression tag	UNP Q9RST7
C	560	ALA	-	expression tag	UNP Q9RST7
C	561	ALA	-	expression tag	UNP Q9RST7
C	562	LEU	-	expression tag	UNP Q9RST7
C	563	GLU	-	expression tag	UNP Q9RST7
C	564	HIS	-	expression tag	UNP Q9RST7
C	565	HIS	-	expression tag	UNP Q9RST7
C	566	HIS	-	expression tag	UNP Q9RST7
C	567	HIS	-	expression tag	UNP Q9RST7
C	568	HIS	-	expression tag	UNP Q9RST7
C	569	HIS	-	expression tag	UNP Q9RST7
D	-1	MET	-	initiating methionine	UNP Q9RST7
D	0	VAL	-	expression tag	UNP Q9RST7
D	1	PRO	-	expression tag	UNP Q9RST7
D	97	TRP	ARG	engineered mutation	UNP Q9RST7
D	253	CYS	ASN	engineered mutation	UNP Q9RST7
D	313	ILE	THR	engineered mutation	UNP Q9RST7
D	380	VAL	ILE	engineered mutation	UNP Q9RST7
D	553	SER	-	expression tag	UNP Q9RST7
D	554	ARG	-	expression tag	UNP Q9RST7
D	555	VAL	-	expression tag	UNP Q9RST7
D	556	ASP	-	expression tag	UNP Q9RST7
D	557	LYS	-	expression tag	UNP Q9RST7
D	558	LEU	-	expression tag	UNP Q9RST7
D	559	ALA	-	expression tag	UNP Q9RST7
D	560	ALA	-	expression tag	UNP Q9RST7
D	561	ALA	-	expression tag	UNP Q9RST7
D	562	LEU	-	expression tag	UNP Q9RST7
D	563	GLU	-	expression tag	UNP Q9RST7
D	564	HIS	-	expression tag	UNP Q9RST7
D	565	HIS	-	expression tag	UNP Q9RST7
D	566	HIS	-	expression tag	UNP Q9RST7
D	567	HIS	-	expression tag	UNP Q9RST7
D	568	HIS	-	expression tag	UNP Q9RST7
D	569	HIS	-	expression tag	UNP Q9RST7
E	-1	MET	-	initiating methionine	UNP Q9RST7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	0	VAL	-	expression tag	UNP Q9RST7
E	1	PRO	-	expression tag	UNP Q9RST7
E	97	TRP	ARG	engineered mutation	UNP Q9RST7
E	253	CYS	ASN	engineered mutation	UNP Q9RST7
E	313	ILE	THR	engineered mutation	UNP Q9RST7
E	380	VAL	ILE	engineered mutation	UNP Q9RST7
E	553	SER	-	expression tag	UNP Q9RST7
E	554	ARG	-	expression tag	UNP Q9RST7
E	555	VAL	-	expression tag	UNP Q9RST7
E	556	ASP	-	expression tag	UNP Q9RST7
E	557	LYS	-	expression tag	UNP Q9RST7
E	558	LEU	-	expression tag	UNP Q9RST7
E	559	ALA	-	expression tag	UNP Q9RST7
E	560	ALA	-	expression tag	UNP Q9RST7
E	561	ALA	-	expression tag	UNP Q9RST7
E	562	LEU	-	expression tag	UNP Q9RST7
E	563	GLU	-	expression tag	UNP Q9RST7
E	564	HIS	-	expression tag	UNP Q9RST7
E	565	HIS	-	expression tag	UNP Q9RST7
E	566	HIS	-	expression tag	UNP Q9RST7
E	567	HIS	-	expression tag	UNP Q9RST7
E	568	HIS	-	expression tag	UNP Q9RST7
E	569	HIS	-	expression tag	UNP Q9RST7
F	-1	MET	-	initiating methionine	UNP Q9RST7
F	0	VAL	-	expression tag	UNP Q9RST7
F	1	PRO	-	expression tag	UNP Q9RST7
F	97	TRP	ARG	engineered mutation	UNP Q9RST7
F	253	CYS	ASN	engineered mutation	UNP Q9RST7
F	313	ILE	THR	engineered mutation	UNP Q9RST7
F	380	VAL	ILE	engineered mutation	UNP Q9RST7
F	553	SER	-	expression tag	UNP Q9RST7
F	554	ARG	-	expression tag	UNP Q9RST7
F	555	VAL	-	expression tag	UNP Q9RST7
F	556	ASP	-	expression tag	UNP Q9RST7
F	557	LYS	-	expression tag	UNP Q9RST7
F	558	LEU	-	expression tag	UNP Q9RST7
F	559	ALA	-	expression tag	UNP Q9RST7
F	560	ALA	-	expression tag	UNP Q9RST7
F	561	ALA	-	expression tag	UNP Q9RST7
F	562	LEU	-	expression tag	UNP Q9RST7
F	563	GLU	-	expression tag	UNP Q9RST7
F	564	HIS	-	expression tag	UNP Q9RST7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	565	HIS	-	expression tag	UNP Q9RST7
F	566	HIS	-	expression tag	UNP Q9RST7
F	567	HIS	-	expression tag	UNP Q9RST7
F	568	HIS	-	expression tag	UNP Q9RST7
F	569	HIS	-	expression tag	UNP Q9RST7
G	-1	MET	-	initiating methionine	UNP Q9RST7
G	0	VAL	-	expression tag	UNP Q9RST7
G	1	PRO	-	expression tag	UNP Q9RST7
G	97	TRP	ARG	engineered mutation	UNP Q9RST7
G	253	CYS	ASN	engineered mutation	UNP Q9RST7
G	313	ILE	THR	engineered mutation	UNP Q9RST7
G	380	VAL	ILE	engineered mutation	UNP Q9RST7
G	553	SER	-	expression tag	UNP Q9RST7
G	554	ARG	-	expression tag	UNP Q9RST7
G	555	VAL	-	expression tag	UNP Q9RST7
G	556	ASP	-	expression tag	UNP Q9RST7
G	557	LYS	-	expression tag	UNP Q9RST7
G	558	LEU	-	expression tag	UNP Q9RST7
G	559	ALA	-	expression tag	UNP Q9RST7
G	560	ALA	-	expression tag	UNP Q9RST7
G	561	ALA	-	expression tag	UNP Q9RST7
G	562	LEU	-	expression tag	UNP Q9RST7
G	563	GLU	-	expression tag	UNP Q9RST7
G	564	HIS	-	expression tag	UNP Q9RST7
G	565	HIS	-	expression tag	UNP Q9RST7
G	566	HIS	-	expression tag	UNP Q9RST7
G	567	HIS	-	expression tag	UNP Q9RST7
G	568	HIS	-	expression tag	UNP Q9RST7
G	569	HIS	-	expression tag	UNP Q9RST7
H	-1	MET	-	initiating methionine	UNP Q9RST7
H	0	VAL	-	expression tag	UNP Q9RST7
H	1	PRO	-	expression tag	UNP Q9RST7
H	97	TRP	ARG	engineered mutation	UNP Q9RST7
H	253	CYS	ASN	engineered mutation	UNP Q9RST7
H	313	ILE	THR	engineered mutation	UNP Q9RST7
H	380	VAL	ILE	engineered mutation	UNP Q9RST7
H	553	SER	-	expression tag	UNP Q9RST7
H	554	ARG	-	expression tag	UNP Q9RST7
H	555	VAL	-	expression tag	UNP Q9RST7
H	556	ASP	-	expression tag	UNP Q9RST7
H	557	LYS	-	expression tag	UNP Q9RST7
H	558	LEU	-	expression tag	UNP Q9RST7

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Chain	Residue	Modelled	Actual	Comment	Reference
H	559	ALA	-	expression tag	UNP Q9RST7
H	560	ALA	-	expression tag	UNP Q9RST7
H	561	ALA	-	expression tag	UNP Q9RST7
H	562	LEU	-	expression tag	UNP Q9RST7
H	563	GLU	-	expression tag	UNP Q9RST7
H	564	HIS	-	expression tag	UNP Q9RST7
H	565	HIS	-	expression tag	UNP Q9RST7
H	566	HIS	-	expression tag	UNP Q9RST7
H	567	HIS	-	expression tag	UNP Q9RST7
H	568	HIS	-	expression tag	UNP Q9RST7
H	569	HIS	-	expression tag	UNP Q9RST7

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0
2	G	1	Total Ca 1 1	0	0
2	H	1	Total Ca 1 1	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

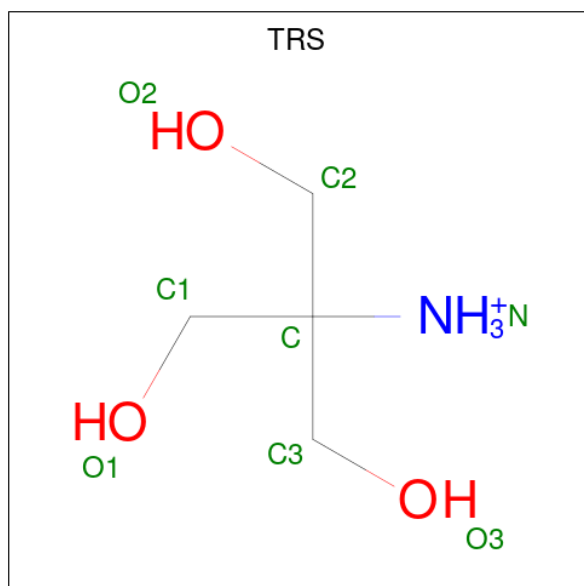
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		
3	G	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃) (labeled as "Ligand of Interest" by depositor).



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

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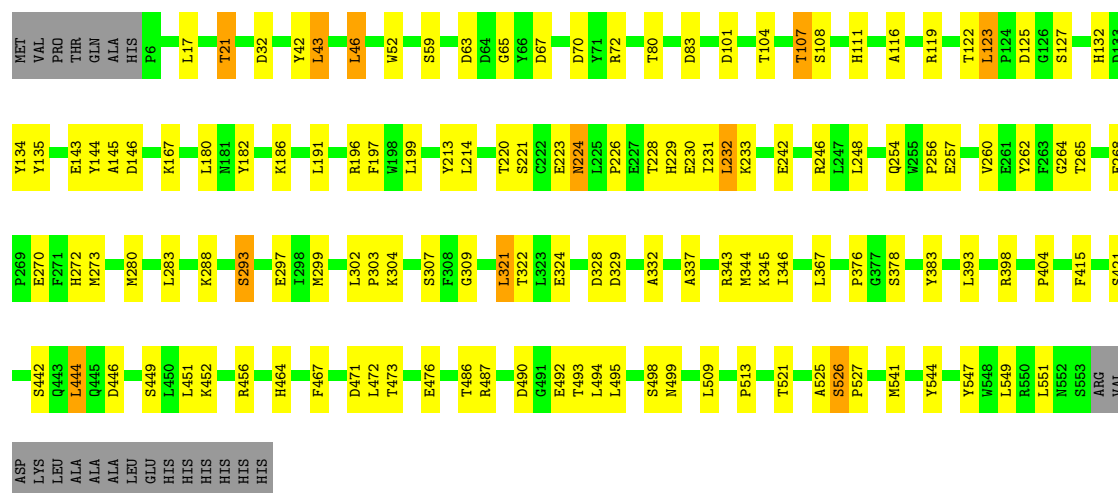
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	F	1	Total	C	N	O	0	0
			8	4	1	3		
4	G	1	Total	C	N	O	0	0
			8	4	1	3		
4	H	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	24	Total	O	0	0
			24	24		
5	B	19	Total	O	0	0
			19	19		
5	C	7	Total	O	0	0
			7	7		
5	D	21	Total	O	0	0
			21	21		
5	E	10	Total	O	0	0
			10	10		
5	F	13	Total	O	0	0
			13	13		
5	G	5	Total	O	0	0
			5	5		
5	H	10	Total	O	0	0
			10	10		

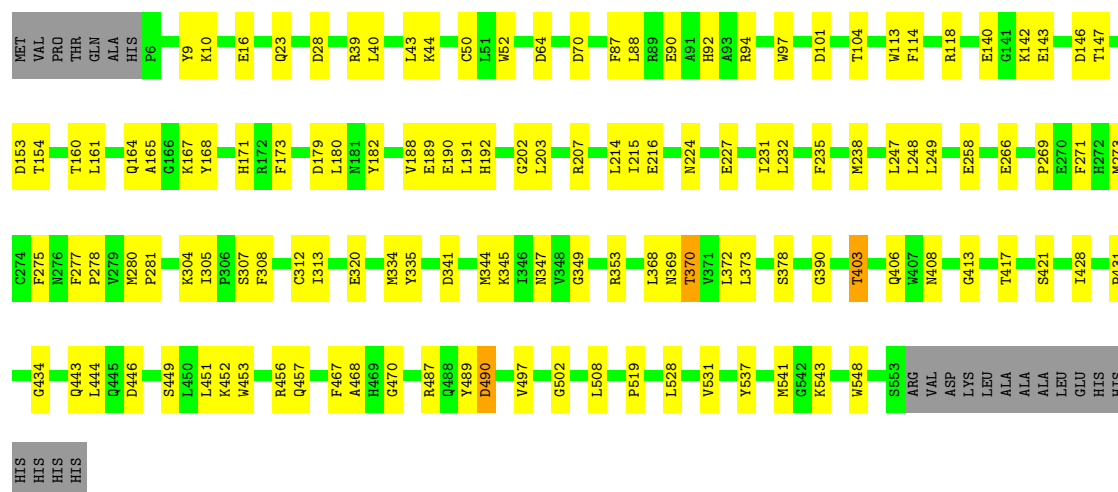


Chain F: 



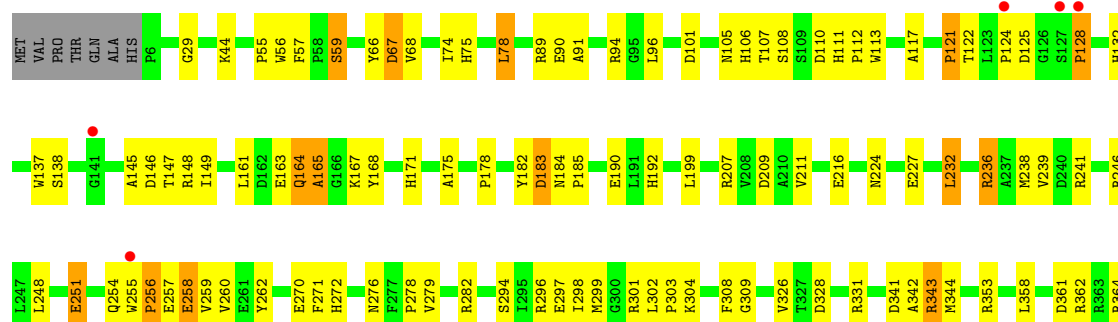
- Molecule 1: maltose alpha-D-glucosyltransferase

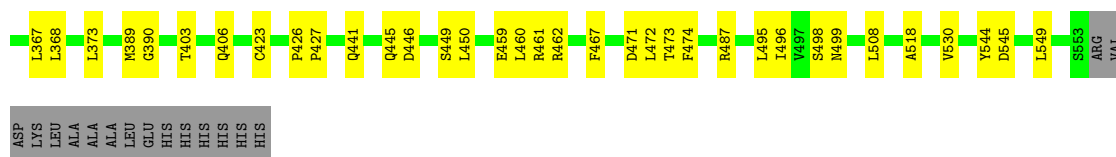
Chain G: 



- Molecule 1: maltose alpha-D-glucosyltransferase

Chain H: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.32Å 196.85Å 131.19Å 90.00° 93.07° 90.00°	Depositor
Resolution (Å)	22.33 – 2.65 22.33 – 2.65	Depositor EDS
% Data completeness (in resolution range)	96.2 (22.33-2.65) 96.0 (22.33-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 2.67Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.172 , 0.234 0.172 , 0.234	Depositor DCC
R_{free} test set	6707 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	35405	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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: TRS, CA, MG

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	0.43	0/4535	0.61	0/6179
1	B	0.41	0/4535	0.60	0/6179
1	C	0.40	0/4535	0.57	0/6179
1	D	0.43	0/4535	0.61	0/6179
1	E	0.40	0/4535	0.61	0/6179
1	F	0.40	0/4535	0.61	0/6179
1	G	0.38	0/4535	0.58	0/6179
1	H	0.37	0/4535	0.60	1/6179 (0.0%)
All	All	0.40	0/36280	0.60	1/49432 (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	C	0	1
1	E	0	2
1	F	0	1
1	H	0	2
All	All	0	6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	343	ARG	CG-CD-NE	5.41	123.90	112.00

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	206	PHE	Peptide
1	E	206	PHE	Peptide
1	E	207	ARG	Sidechain
1	F	144	TYR	Peptide
1	H	165	ALA	Peptide

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	4402	0	4200	89	1
1	B	4402	0	4200	64	1
1	C	4402	0	4200	63	0
1	D	4402	0	4200	62	0
1	E	4402	0	4200	89	0
1	F	4402	0	4200	82	0
1	G	4402	0	4200	84	0
1	H	4402	0	4200	97	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	8	0	12	0	0
4	B	8	0	12	1	0
4	C	8	0	12	1	0
4	D	8	0	12	0	0
4	E	8	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	8	0	12	2	0
4	G	8	0	12	0	0
4	H	8	0	12	1	0
5	A	24	0	0	0	0
5	B	19	0	0	0	0
5	C	7	0	0	0	0
5	D	21	0	0	0	0
5	E	10	0	0	0	0
5	F	13	0	0	0	0
5	G	5	0	0	0	0
5	H	10	0	0	0	0
All	All	35405	0	33696	626	1

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 9.

The worst 5 of 626 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:E:52:TRP:CH2	1:E:207:ARG:HD2	1.88	1.09
1:E:290:GLU:HG2	1:E:501:ALA:HA	1.47	0.95
1:A:152:THR:HG22	1:A:347:ASN:HA	1.52	0.91
1:F:304:LYS:HE2	1:F:304:LYS:H	1.37	0.89
1:B:104:THR:HG22	1:B:191:LEU:HD21	1.55	0.87

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:LYS:NZ	1:B:125:ASP:OD1[2_556]	2.18	0.02

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	546/571 (96%)	521 (95%)	25 (5%)	0	100	100
1	B	546/571 (96%)	528 (97%)	16 (3%)	2 (0%)	30	45
1	C	546/571 (96%)	522 (96%)	22 (4%)	2 (0%)	30	45
1	D	546/571 (96%)	527 (96%)	17 (3%)	2 (0%)	30	45
1	E	546/571 (96%)	524 (96%)	20 (4%)	2 (0%)	30	45
1	F	546/571 (96%)	510 (93%)	33 (6%)	3 (0%)	24	39
1	G	546/571 (96%)	516 (94%)	29 (5%)	1 (0%)	43	60
1	H	546/571 (96%)	492 (90%)	47 (9%)	7 (1%)	9	16
All	All	4368/4568 (96%)	4140 (95%)	209 (5%)	19 (0%)	30	45

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	146	ASP
1	H	164	GLN
1	B	70	ASP
1	B	126	GLY
1	C	129	ASN

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	465/484 (96%)	446 (96%)	19 (4%)	27	46
1	B	465/484 (96%)	451 (97%)	14 (3%)	36	57
1	C	465/484 (96%)	441 (95%)	24 (5%)	21	36
1	D	465/484 (96%)	446 (96%)	19 (4%)	27	46
1	E	465/484 (96%)	441 (95%)	24 (5%)	21	36
1	F	465/484 (96%)	445 (96%)	20 (4%)	26	44
1	G	465/484 (96%)	448 (96%)	17 (4%)	30	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	465/484 (96%)	452 (97%)	13 (3%)	38 60
All	All	3720/3872 (96%)	3570 (96%)	150 (4%)	28 47

5 of 150 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	421	SER
1	H	236	ARG
1	F	526	SER
1	G	216	GLU
1	C	381	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	158	ASN
1	G	132	HIS
1	F	181	ASN
1	F	443	GLN
1	G	443	GLN

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 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 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	$\# Z > 2$
4	TRS	H	603	-	7,7,7	0.34	0	9,9,9	0.99	0
4	TRS	G	603	-	7,7,7	0.33	0	9,9,9	0.63	0
4	TRS	B	603	-	7,7,7	0.24	0	9,9,9	0.81	0
4	TRS	D	603	-	7,7,7	0.27	0	9,9,9	0.66	0
4	TRS	F	603	-	7,7,7	0.36	0	9,9,9	0.60	0
4	TRS	A	602	-	7,7,7	0.52	0	9,9,9	1.40	1 (11%)
4	TRS	C	603	-	7,7,7	0.29	0	9,9,9	0.82	0
4	TRS	E	603	-	7,7,7	0.31	0	9,9,9	0.67	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
4	TRS	H	603	-	-	4/9/9/9	-
4	TRS	G	603	-	-	7/9/9/9	-
4	TRS	B	603	-	-	0/9/9/9	-
4	TRS	D	603	-	-	1/9/9/9	-
4	TRS	F	603	-	-	7/9/9/9	-
4	TRS	A	602	-	-	2/9/9/9	-
4	TRS	C	603	-	-	2/9/9/9	-
4	TRS	E	603	-	-	5/9/9/9	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	TRS	O2-C2-C	-2.44	104.08	110.88

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

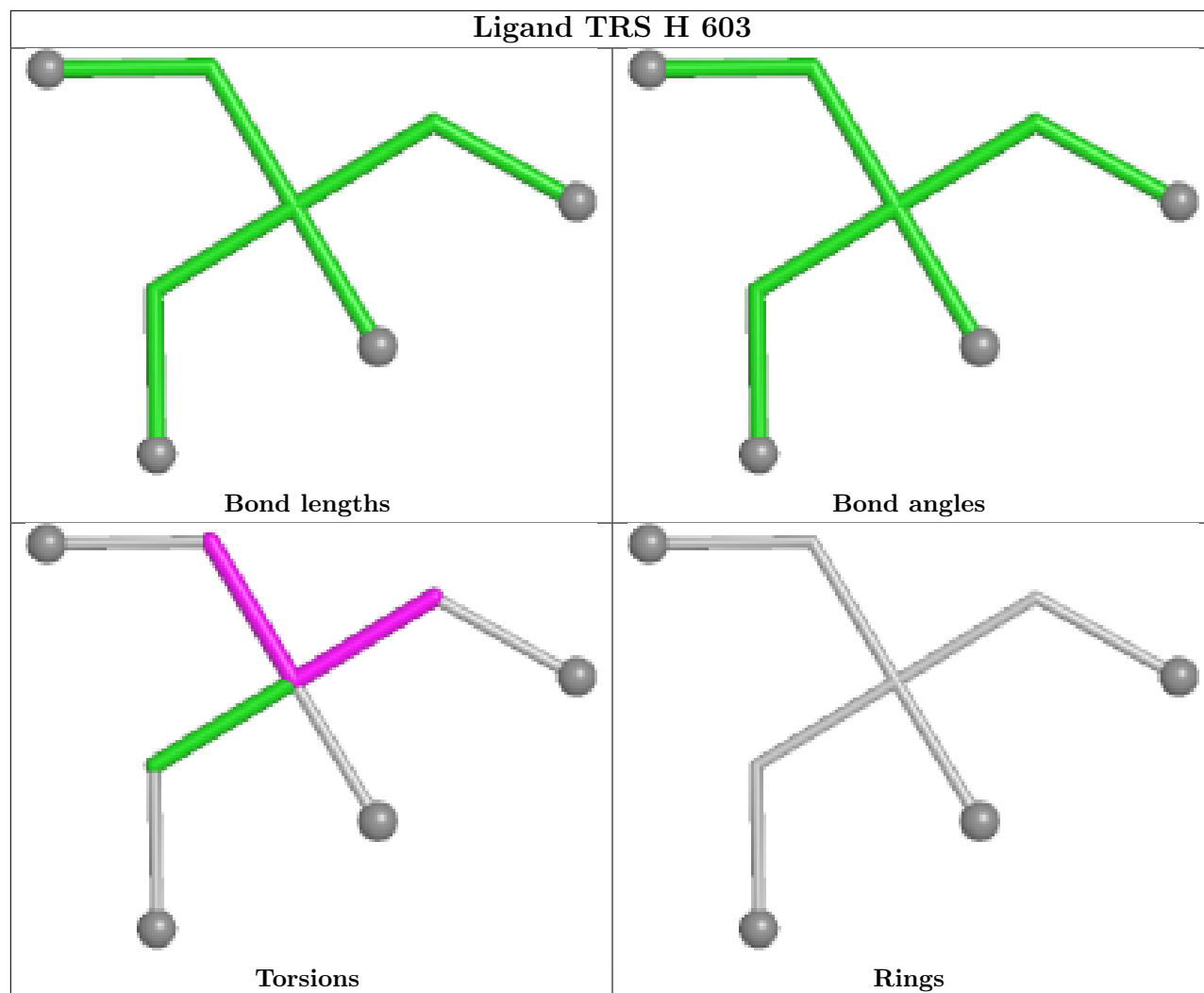
Mol	Chain	Res	Type	Atoms
4	F	603	TRS	C1-C-C3-O3
4	F	603	TRS	C2-C-C3-O3
4	G	603	TRS	C3-C-C1-O1
4	G	603	TRS	N-C-C1-O1
4	E	603	TRS	C2-C-C3-O3

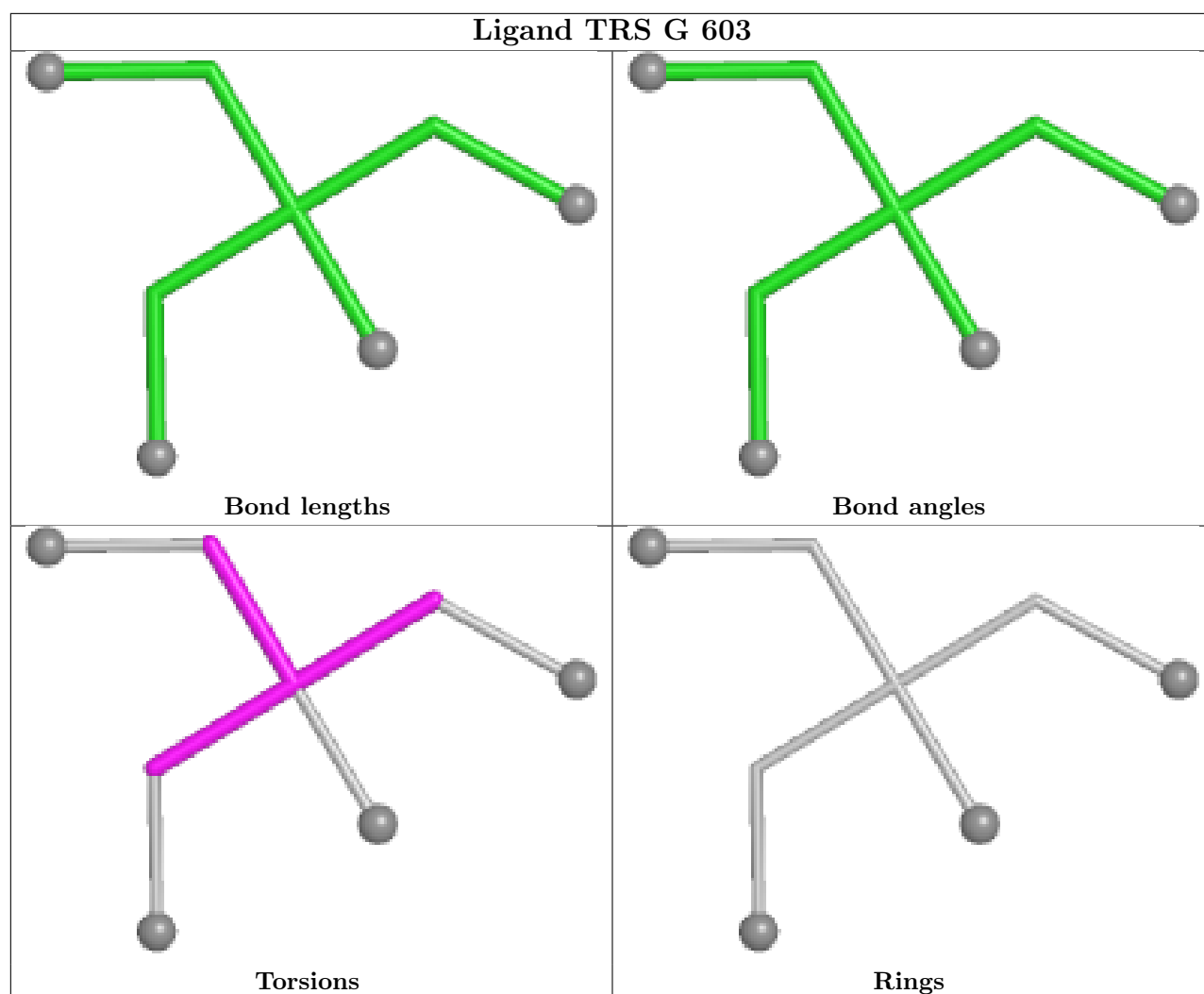
There are no ring outliers.

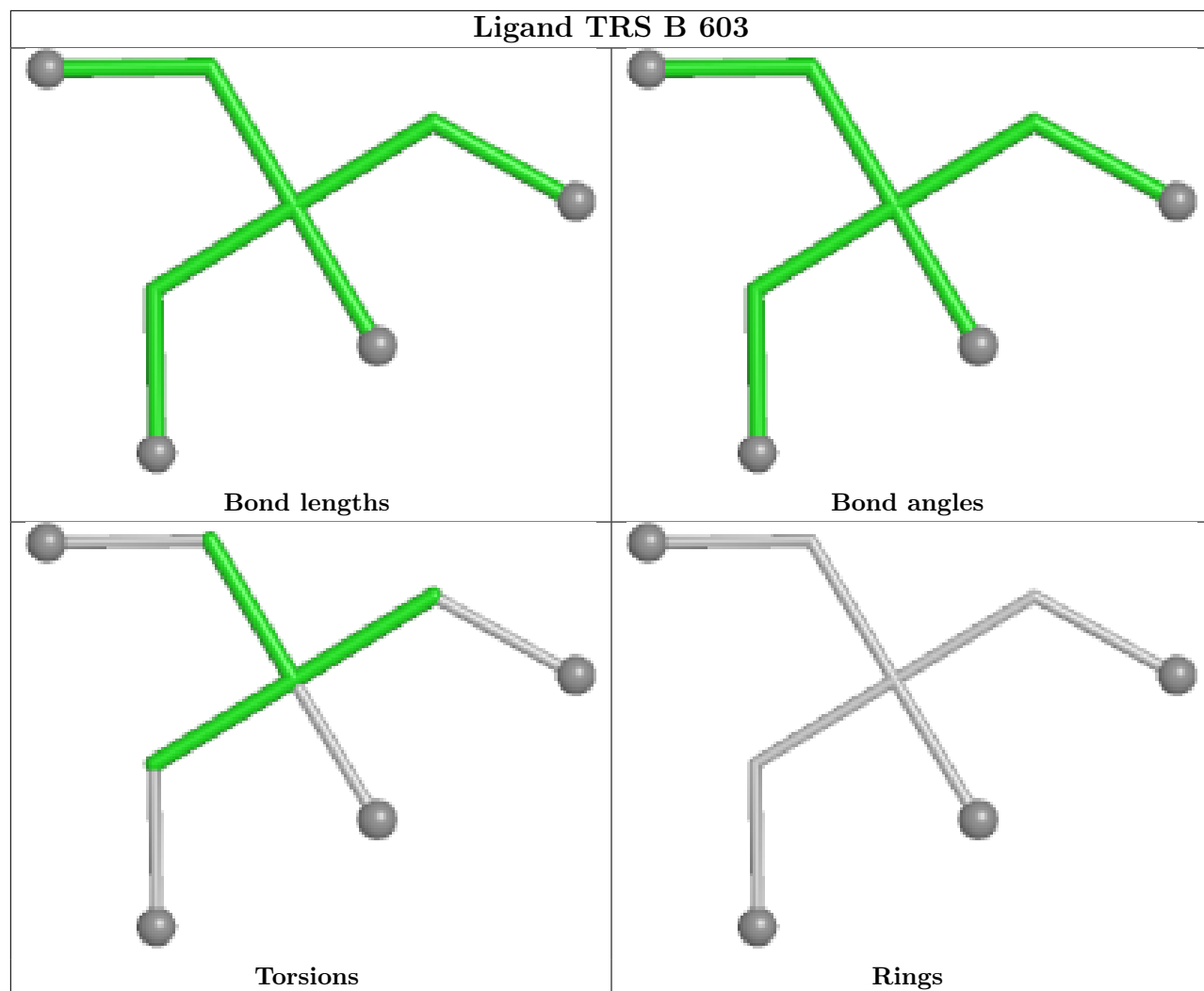
5 monomers are involved in 6 short contacts:

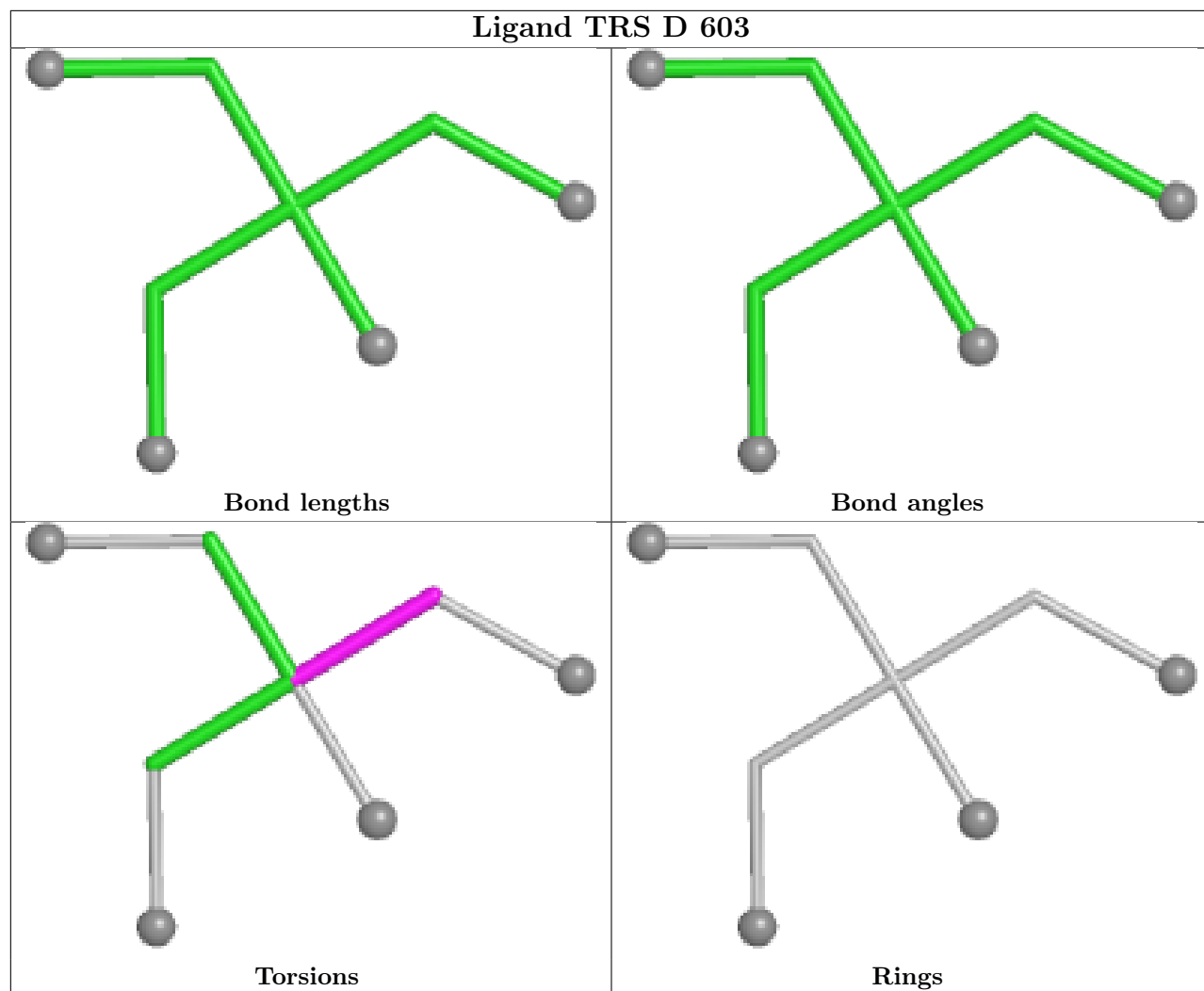
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	603	TRS	1	0
4	B	603	TRS	1	0
4	F	603	TRS	2	0
4	C	603	TRS	1	0
4	E	603	TRS	1	0

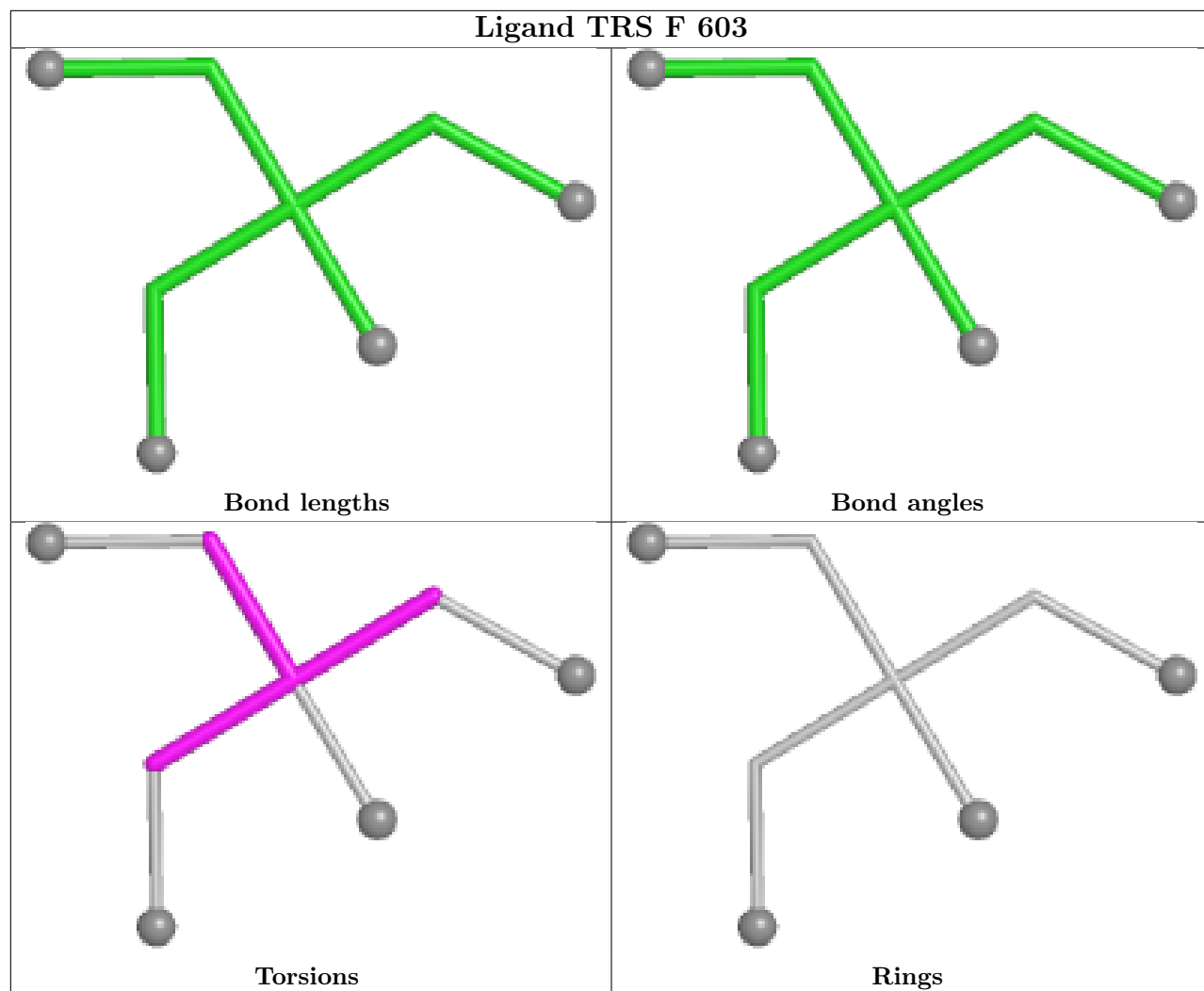
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

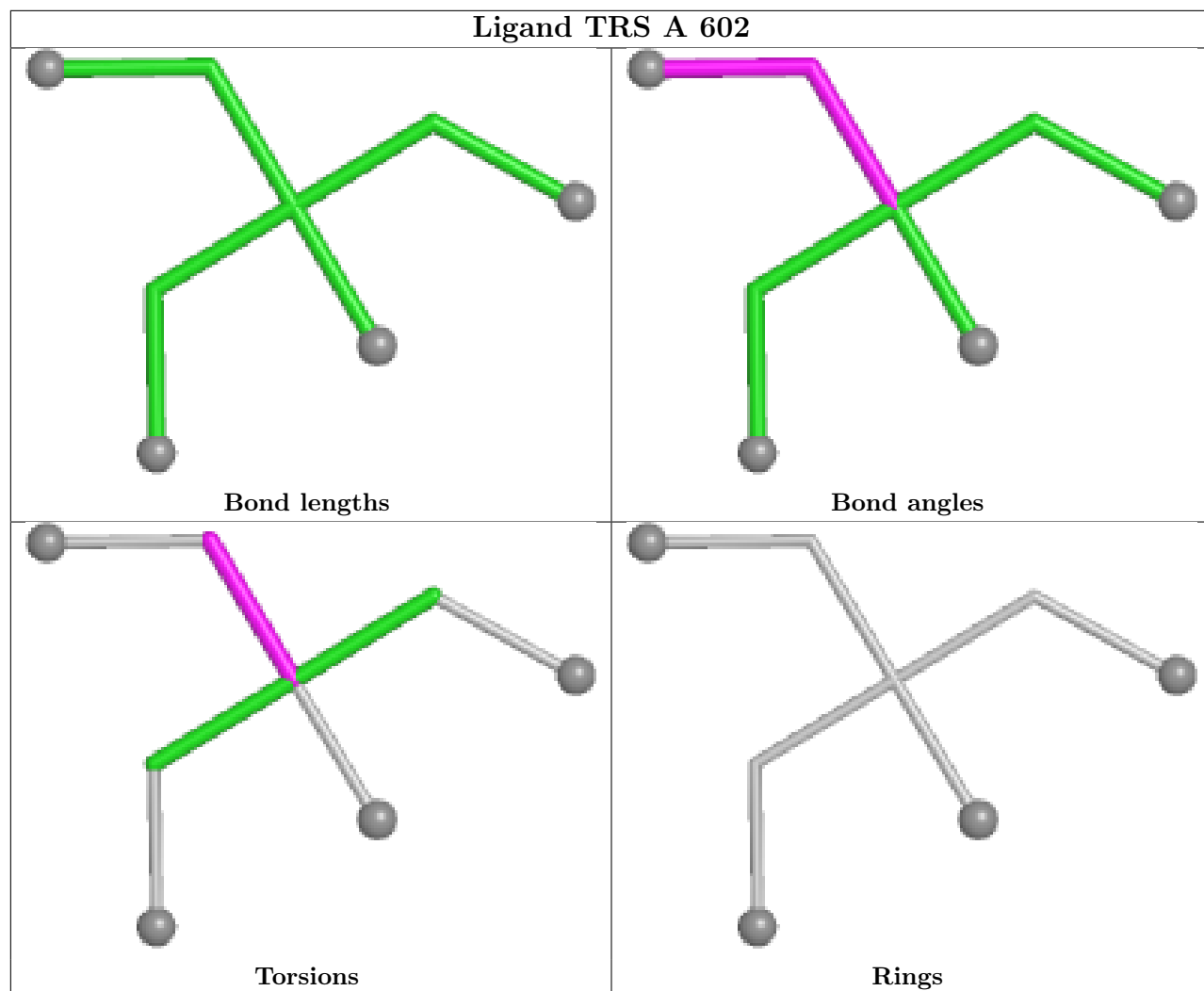


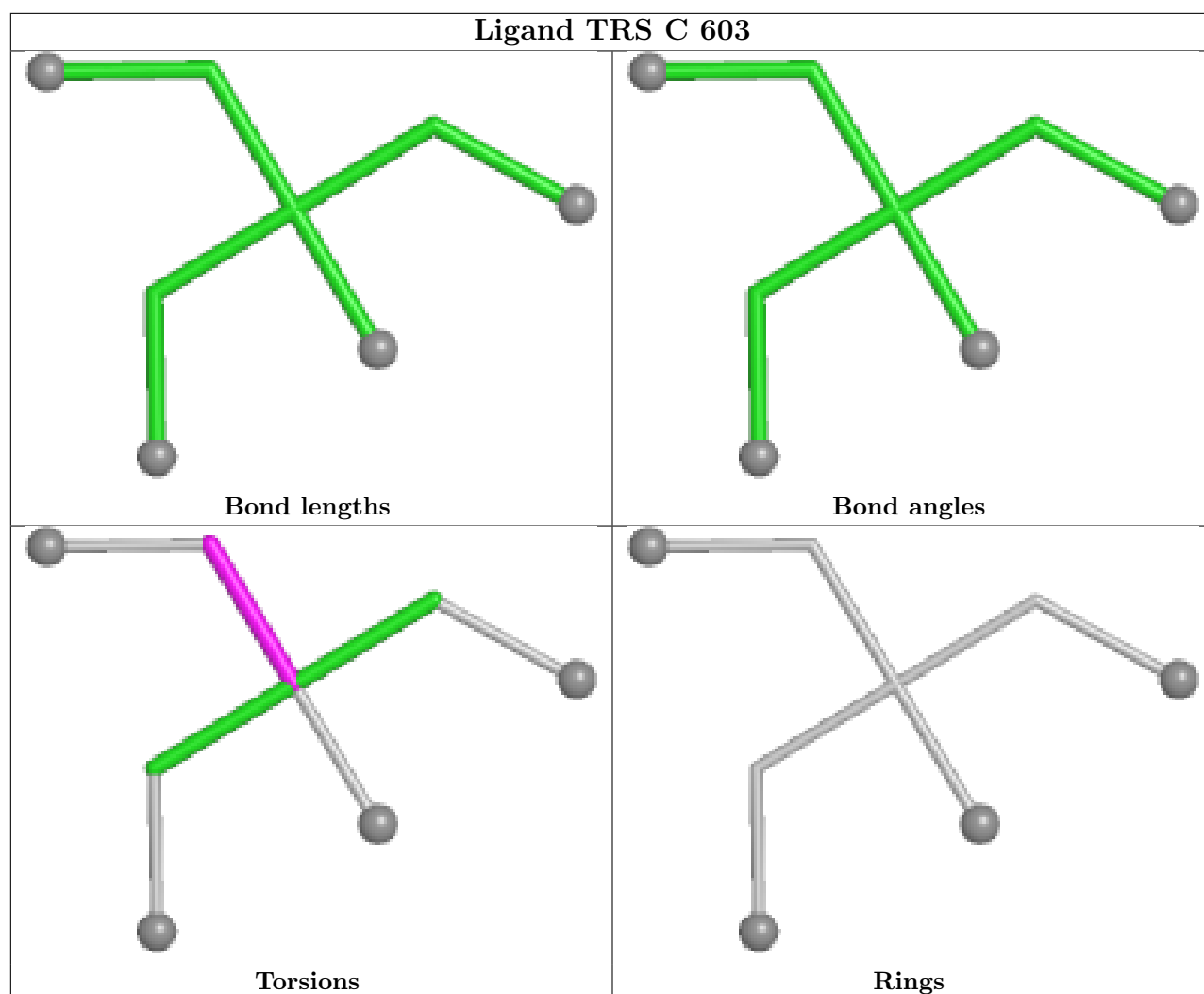


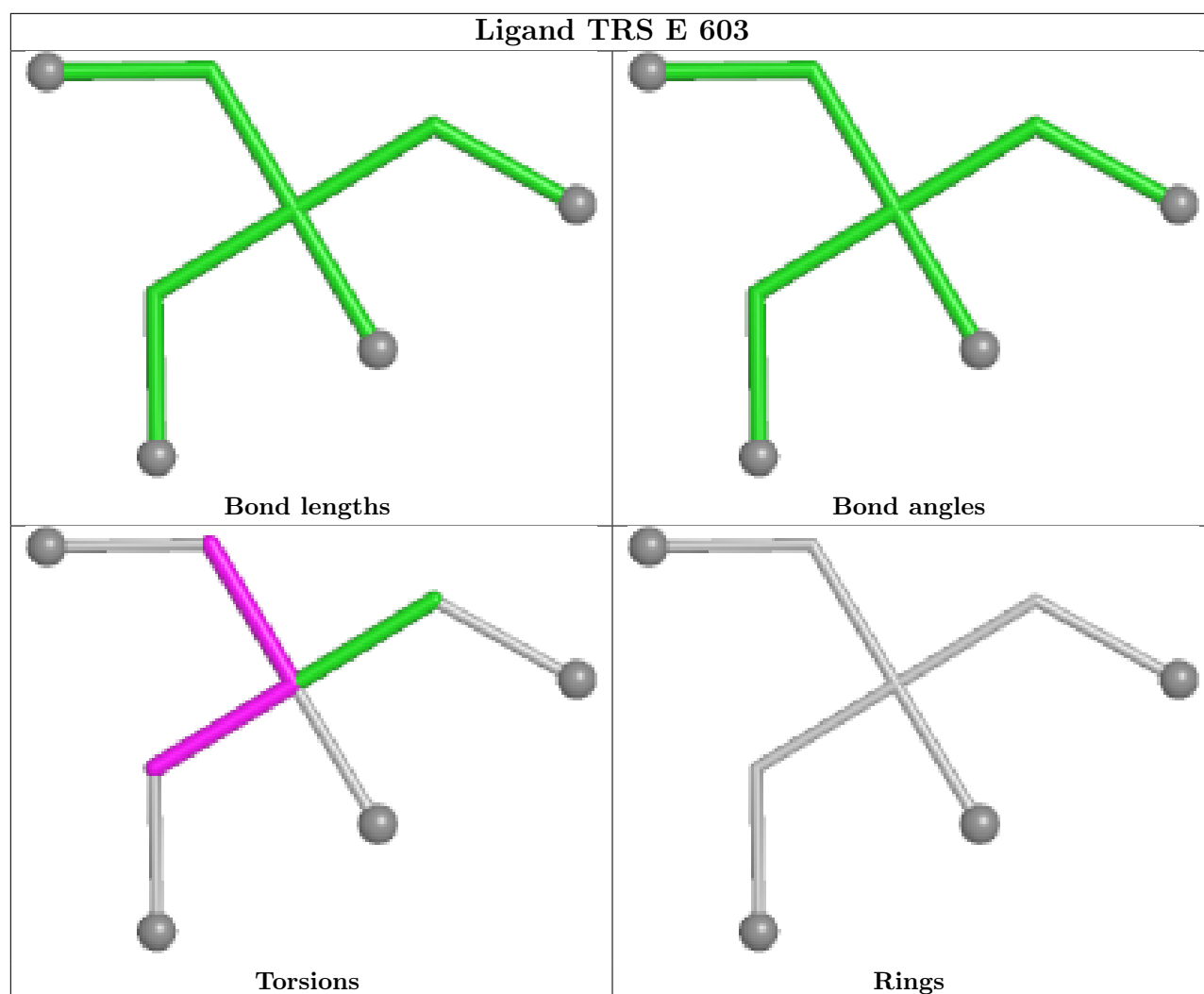












5.7 Other polymers [i](#)

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	548/571 (95%)	-0.68	0	100 100	23, 35, 50, 77	1 (0%)
1	B	548/571 (95%)	-0.64	0	100 100	24, 36, 52, 66	0
1	C	548/571 (95%)	-0.61	0	100 100	26, 39, 56, 95	0
1	D	548/571 (95%)	-0.59	0	100 100	23, 38, 58, 107	1 (0%)
1	E	548/571 (95%)	-0.49	3 (0%)	87 85	26, 42, 62, 88	1 (0%)
1	F	548/571 (95%)	-0.33	0	100 100	23, 46, 69, 101	1 (0%)
1	G	548/571 (95%)	-0.32	0	100 100	28, 47, 67, 85	0
1	H	548/571 (95%)	-0.17	5 (0%)	81 78	29, 50, 78, 112	0
All	All	4384/4568 (95%)	-0.48	8 (0%)	91 90	23, 41, 66, 112	4 (0%)

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	128	PRO	5.2
1	H	124	PRO	2.7
1	E	52	TRP	2.3
1	E	6	PRO	2.2
1	H	127	SER	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

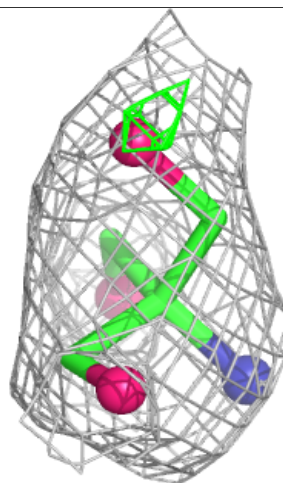
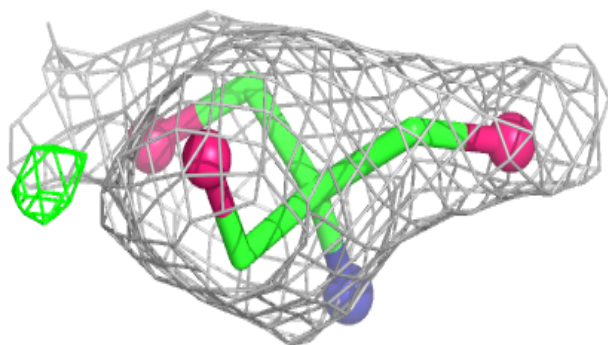
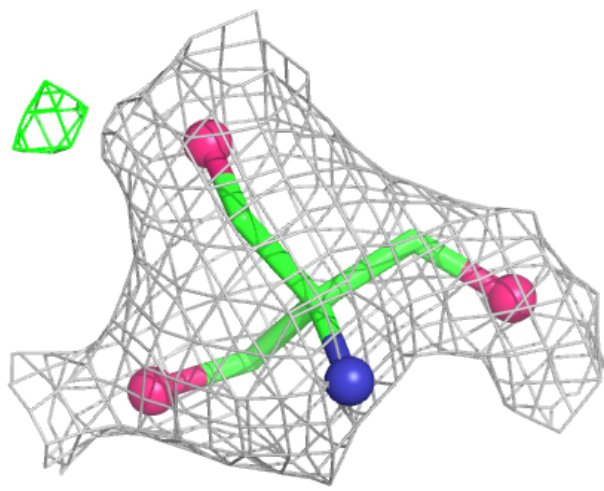
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	TRS	H	603	8/8	0.85	0.10	59,65,69,71	0
4	TRS	F	603	8/8	0.90	0.09	48,51,54,54	0
4	TRS	E	603	8/8	0.91	0.10	50,54,57,58	0
4	TRS	A	602	8/8	0.91	0.09	34,37,41,47	0
4	TRS	D	603	8/8	0.91	0.09	40,48,54,56	0
3	MG	H	602	1/1	0.92	0.08	55,55,55,55	0
3	MG	E	602	1/1	0.93	0.07	45,45,45,45	0
4	TRS	C	603	8/8	0.93	0.07	43,45,47,47	0
4	TRS	G	603	8/8	0.93	0.08	41,48,49,53	0
2	CA	F	601	1/1	0.93	0.05	55,55,55,55	0
3	MG	C	602	1/1	0.96	0.06	35,35,35,35	0
4	TRS	B	603	8/8	0.96	0.06	32,41,43,46	0
3	MG	A	601	1/1	0.96	0.12	44,44,44,44	0
3	MG	B	602	1/1	0.96	0.08	34,34,34,34	0
3	MG	F	602	1/1	0.97	0.05	36,36,36,36	0
2	CA	A	600	1/1	0.97	0.14	58,58,58,58	0
2	CA	H	601	1/1	0.97	0.04	64,64,64,64	0
3	MG	D	602	1/1	0.97	0.04	35,35,35,35	0
2	CA	E	601	1/1	0.97	0.09	43,43,43,43	0
2	CA	D	601	1/1	0.98	0.07	35,35,35,35	0
2	CA	G	601	1/1	0.98	0.06	51,51,51,51	0
2	CA	C	601	1/1	0.99	0.03	38,38,38,38	0
2	CA	B	601	1/1	0.99	0.04	35,35,35,35	0
3	MG	G	602	1/1	0.99	0.04	36,36,36,36	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.

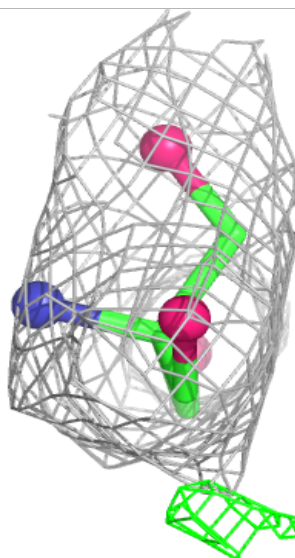
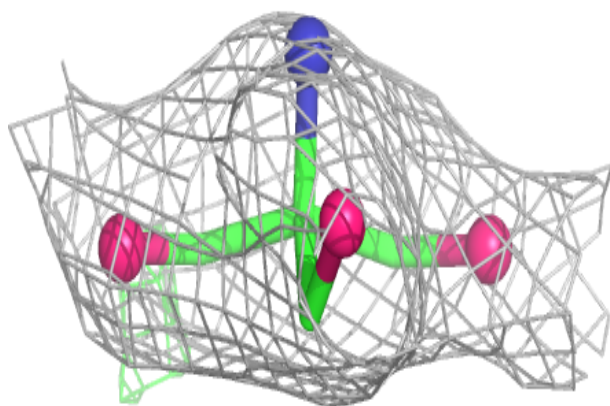
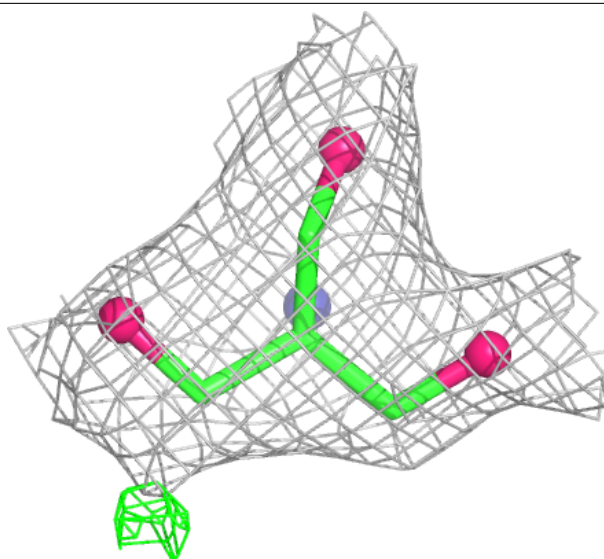
Electron density around TRS H 603:

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



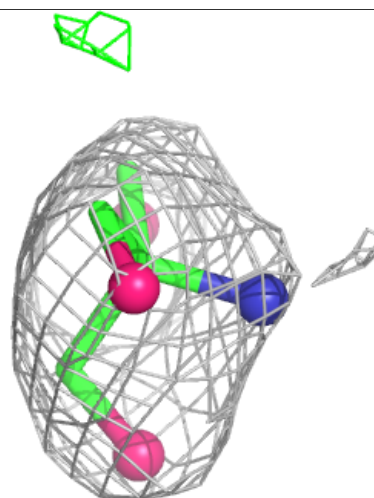
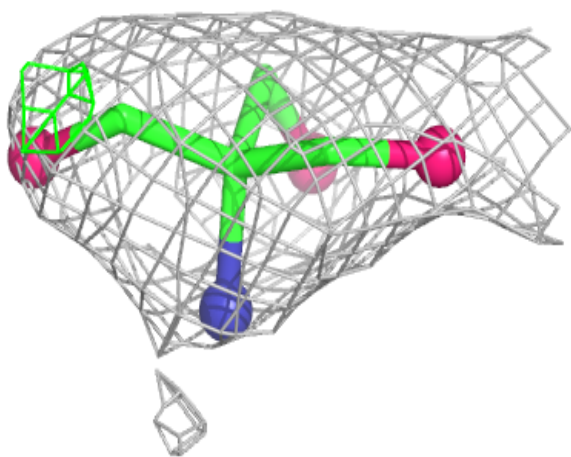
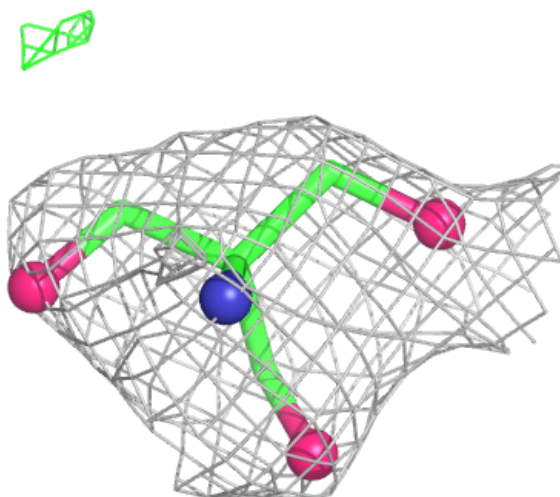
Electron density around TRS F 603:

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



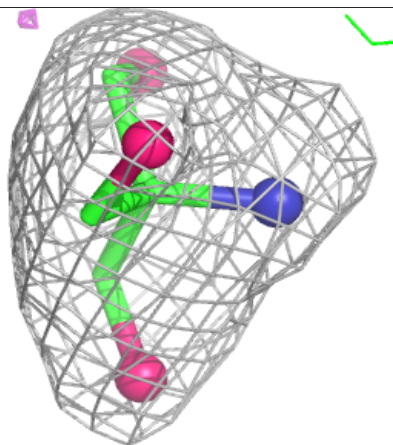
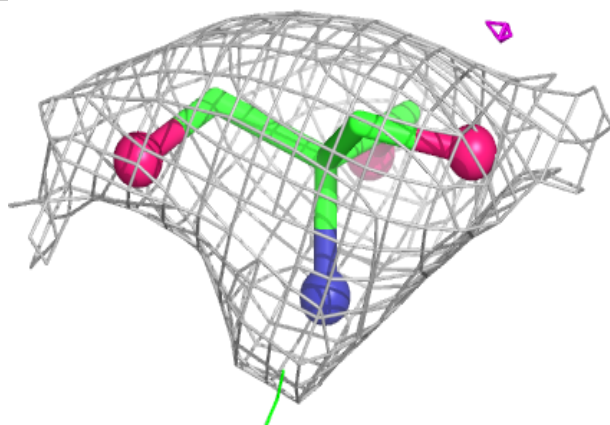
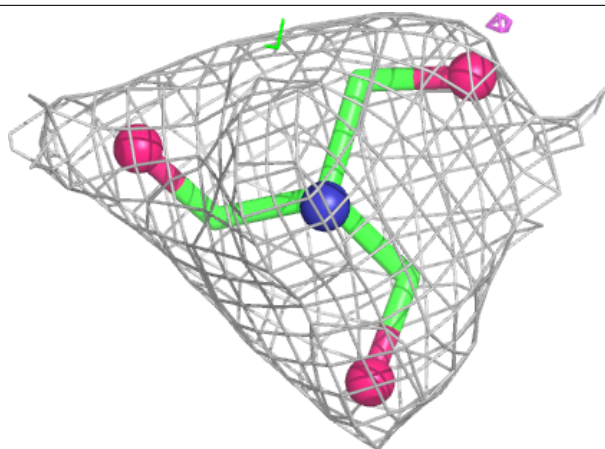
Electron density around TRS E 603:

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and green (positive)



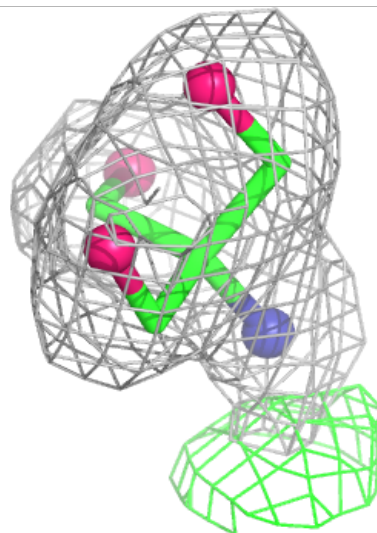
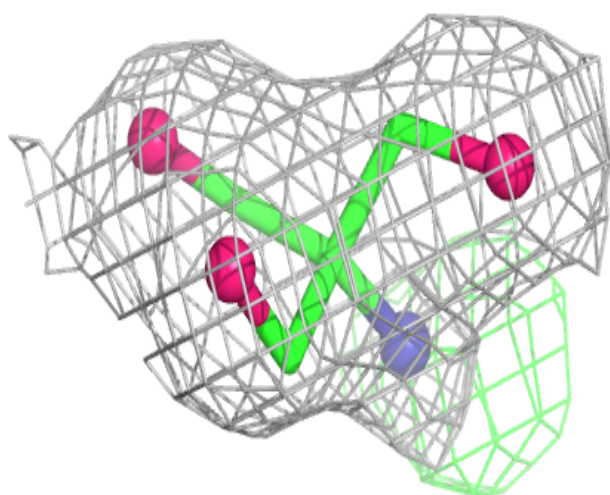
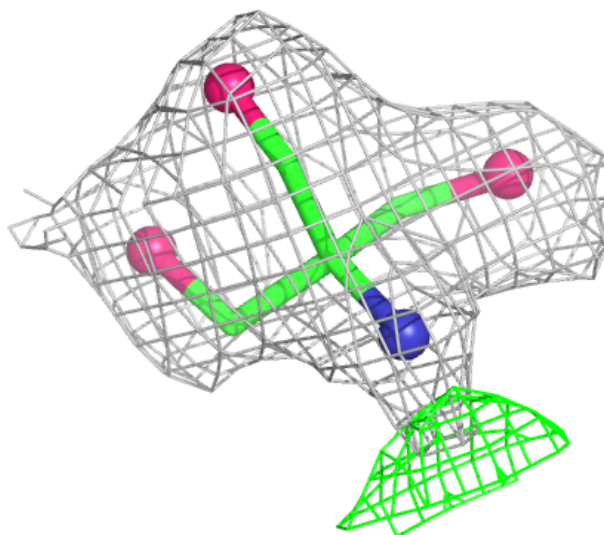
Electron density around TRS A 602:

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



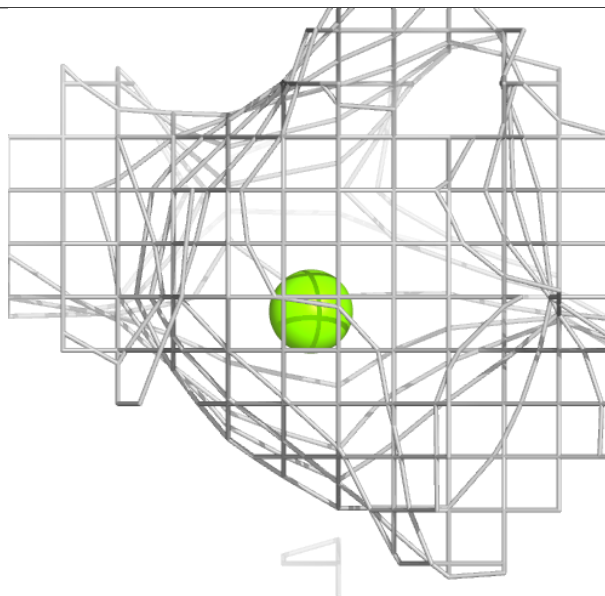
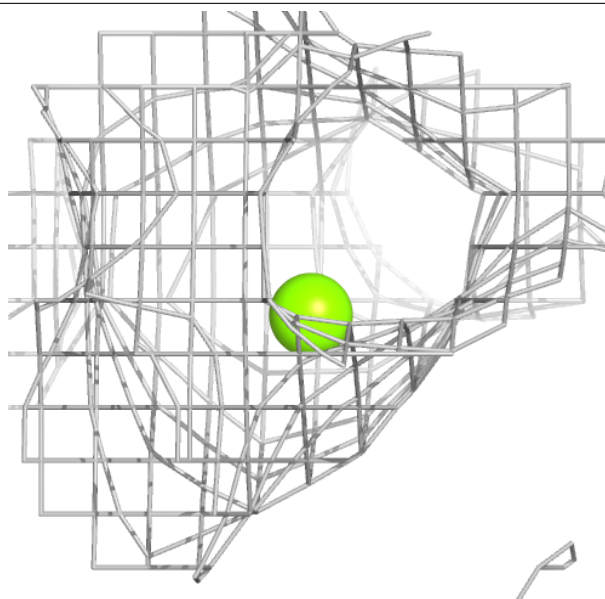
Electron density around TRS D 603:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



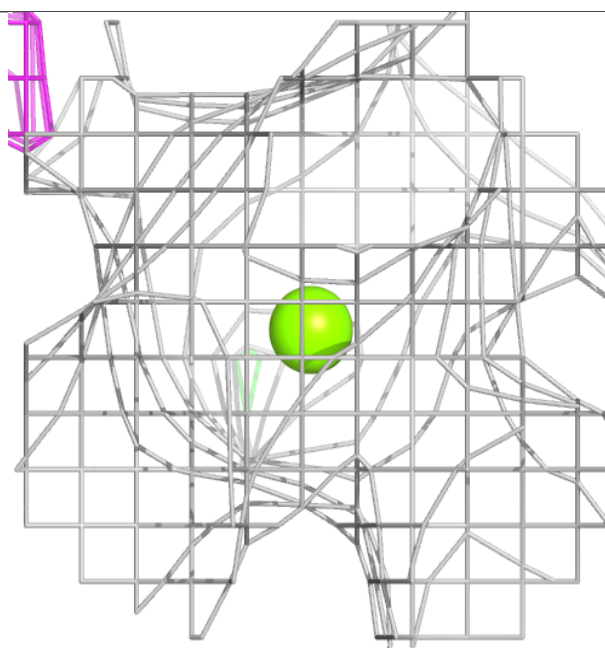
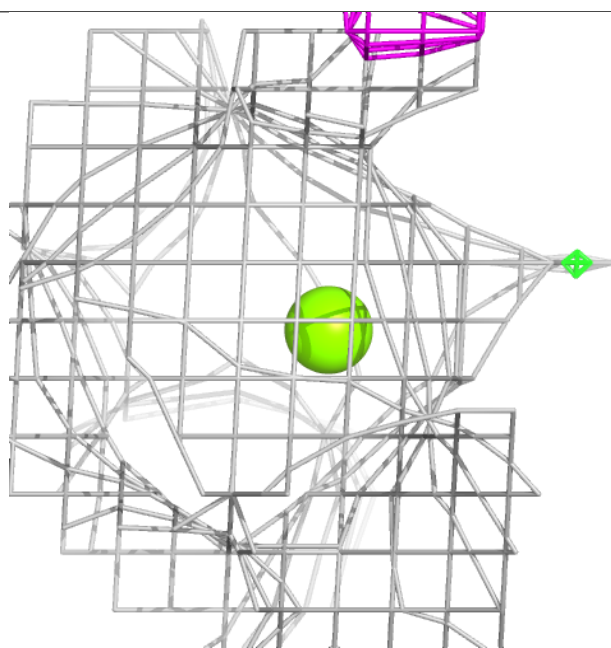
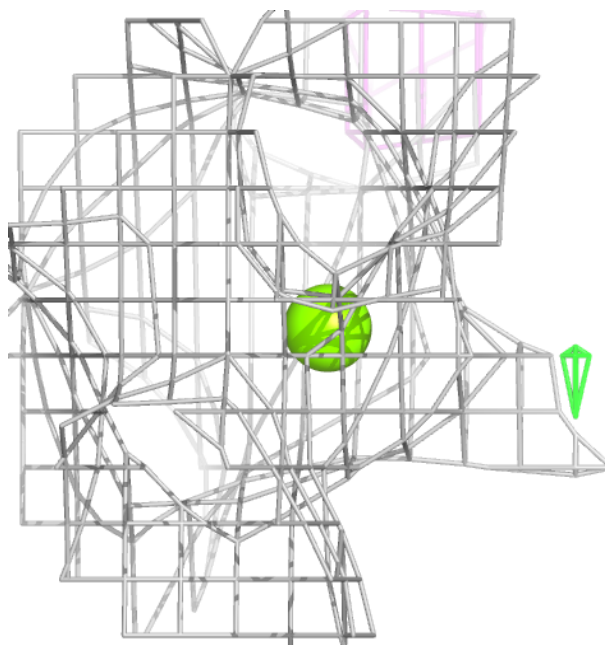
Electron density around MG H 602:

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



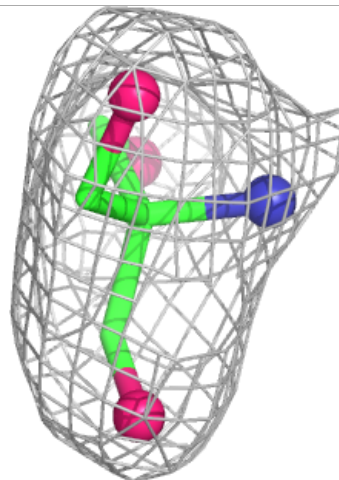
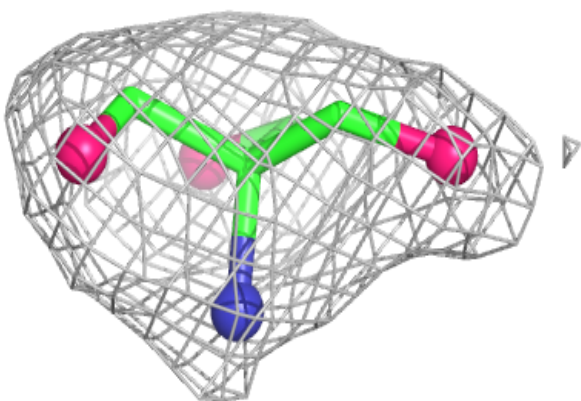
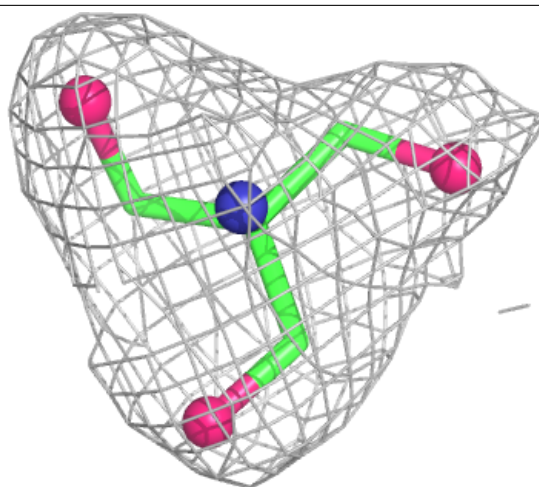
Electron density around MG E 602:

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



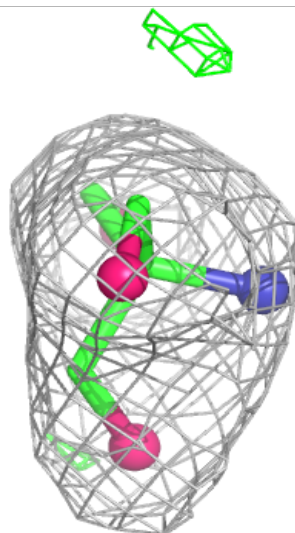
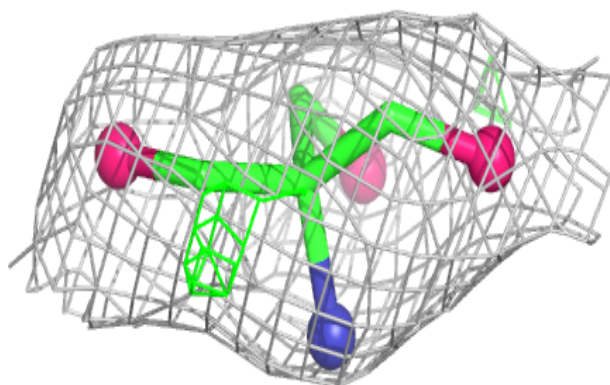
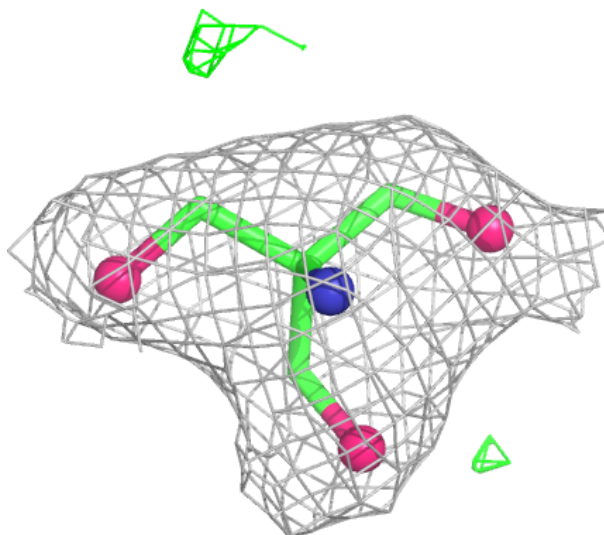
Electron density around TRS C 603:

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



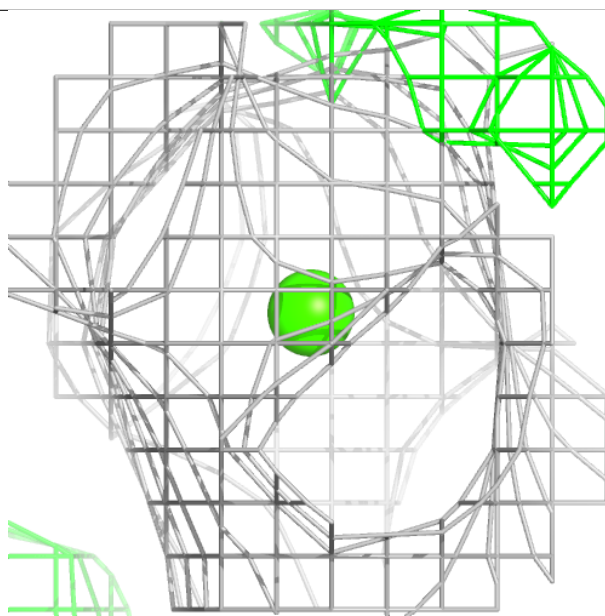
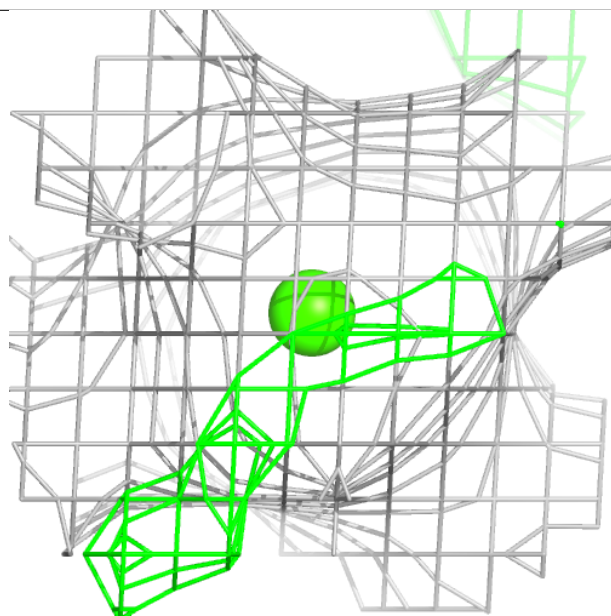
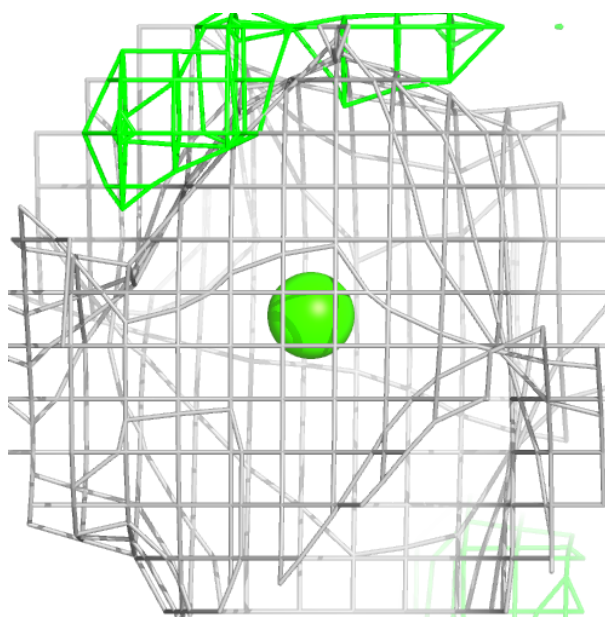
Electron density around TRS G 603:

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



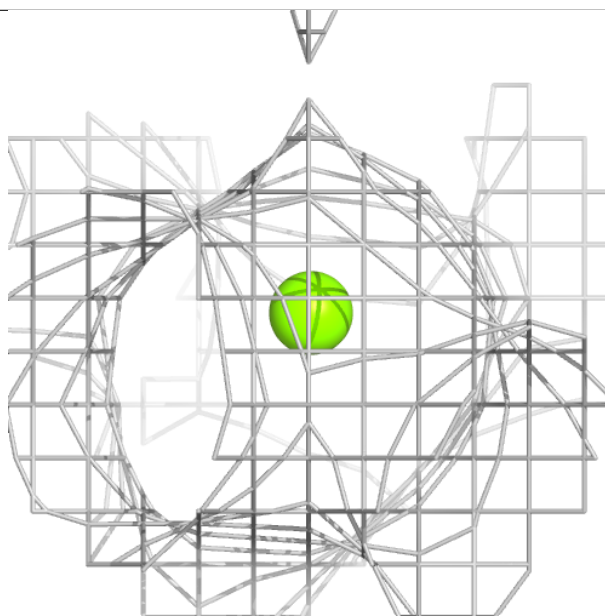
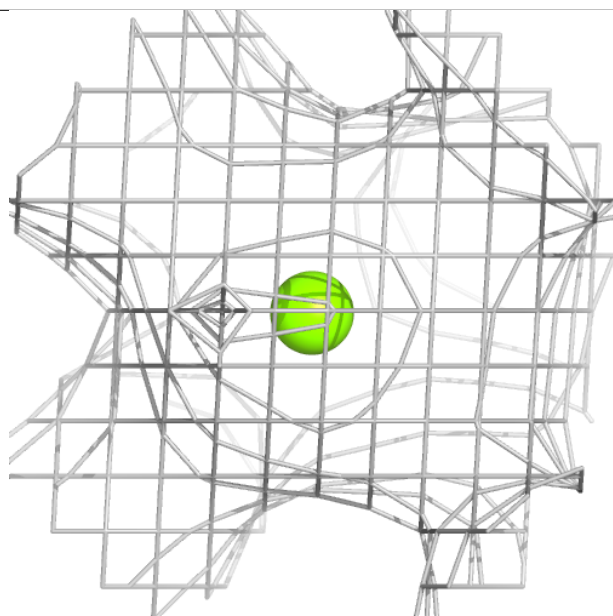
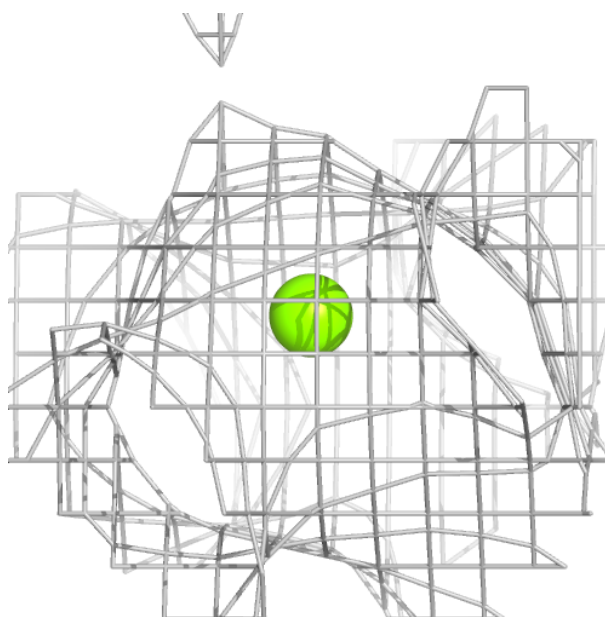
Electron density around CA F 601:

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



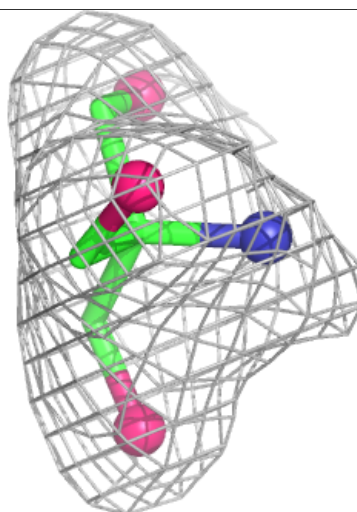
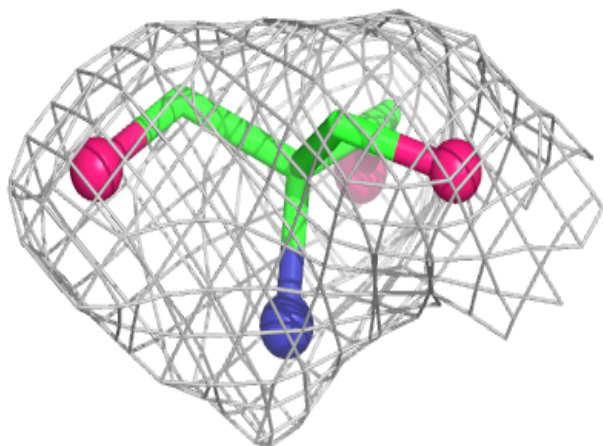
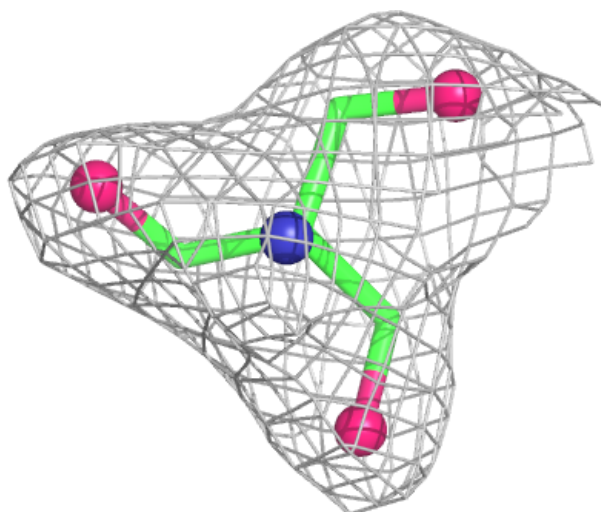
Electron density around MG C 602:

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



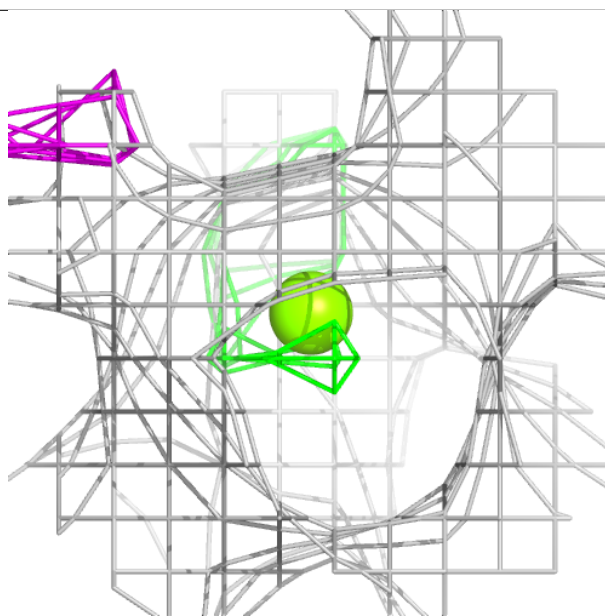
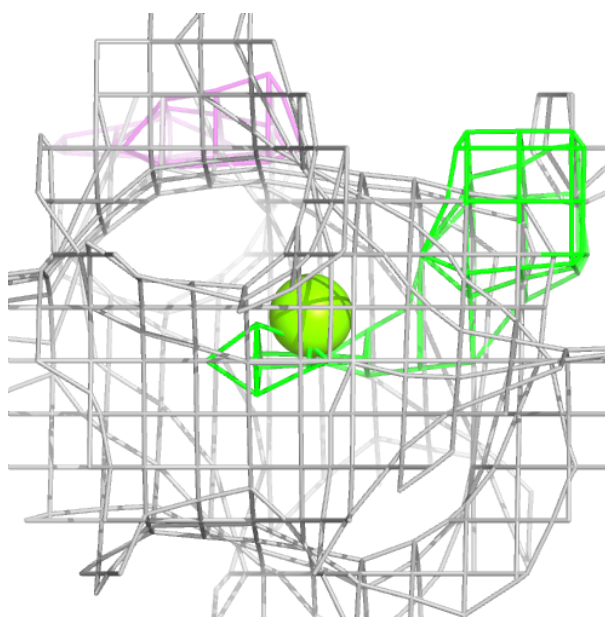
Electron density around TRS B 603:

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



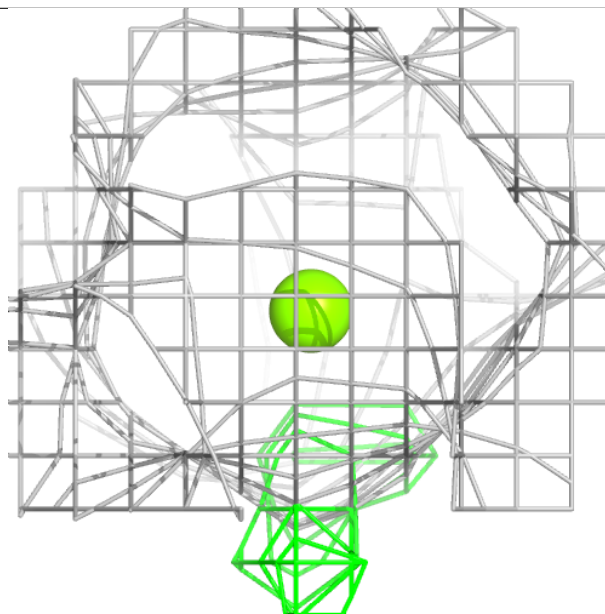
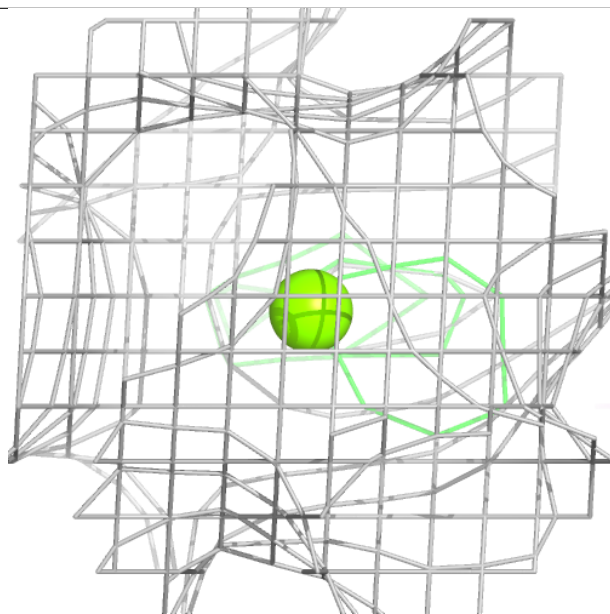
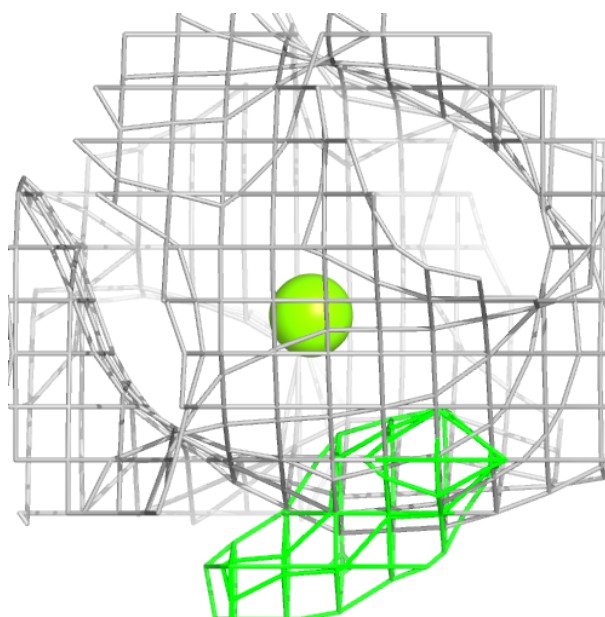
Electron density around MG A 601:

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



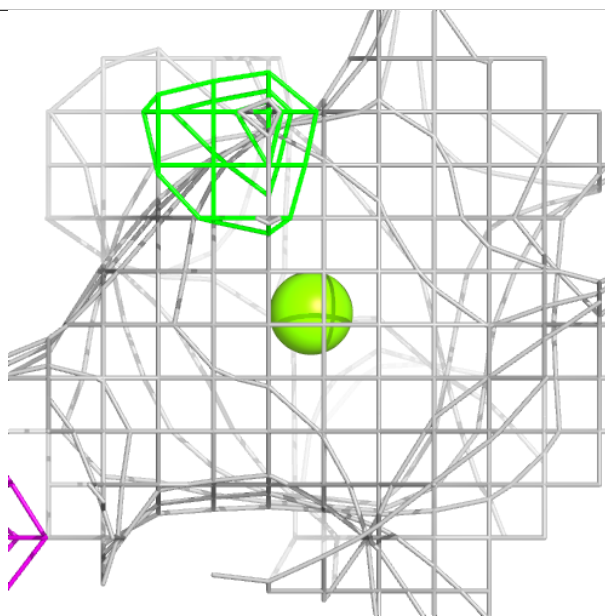
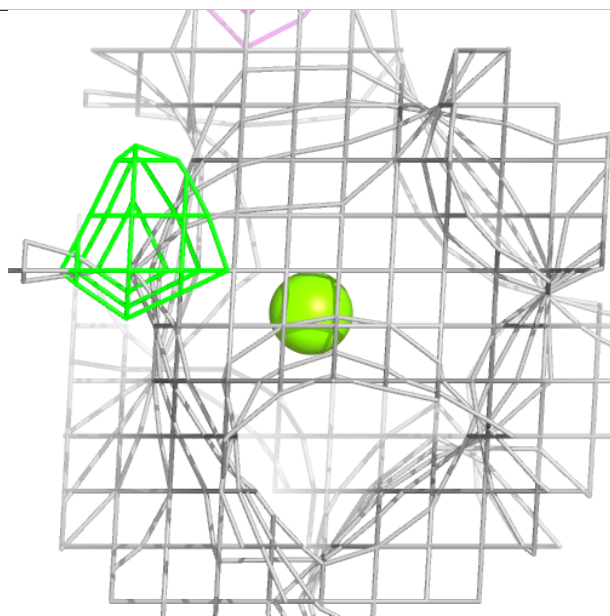
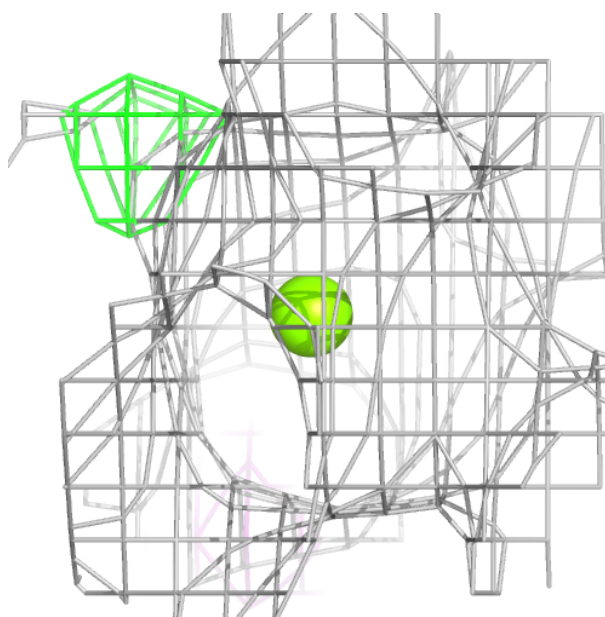
Electron density around MG B 602:

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



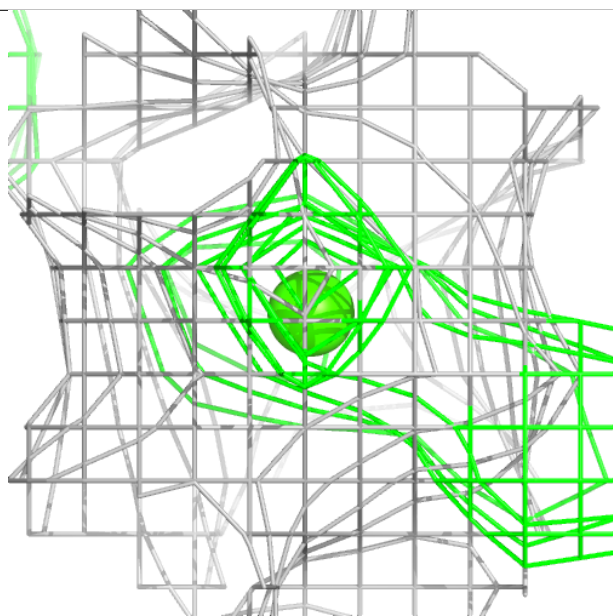
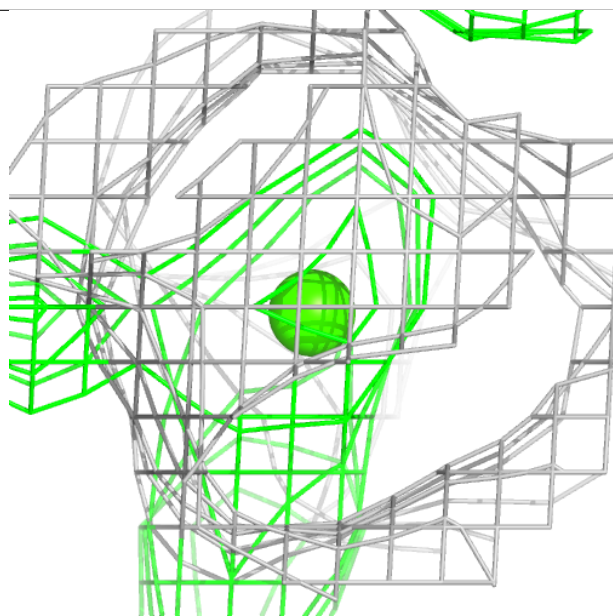
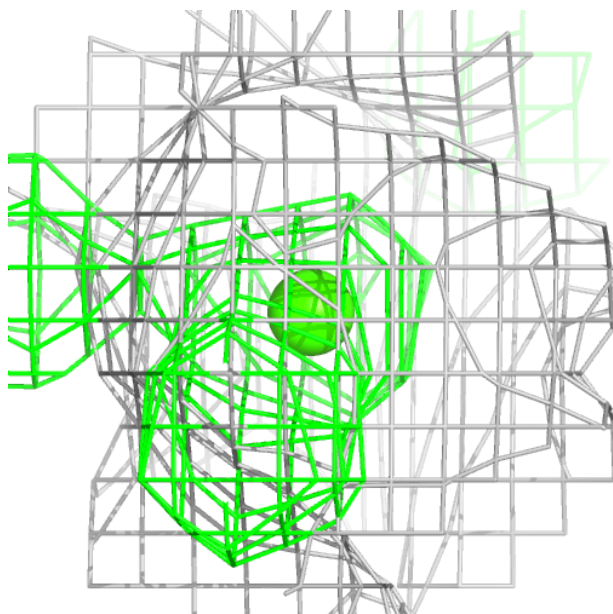
Electron density around MG F 602:

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



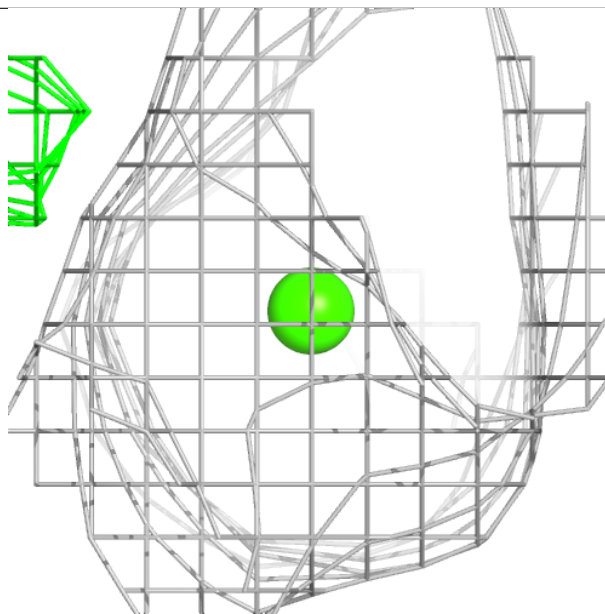
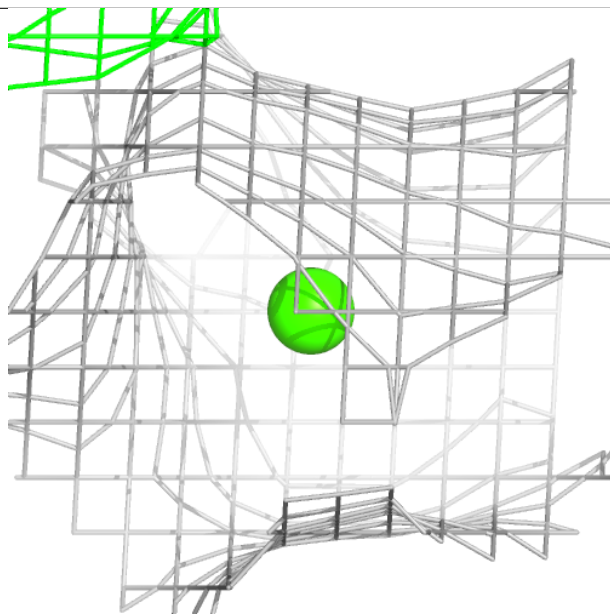
Electron density around CA A 600:

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



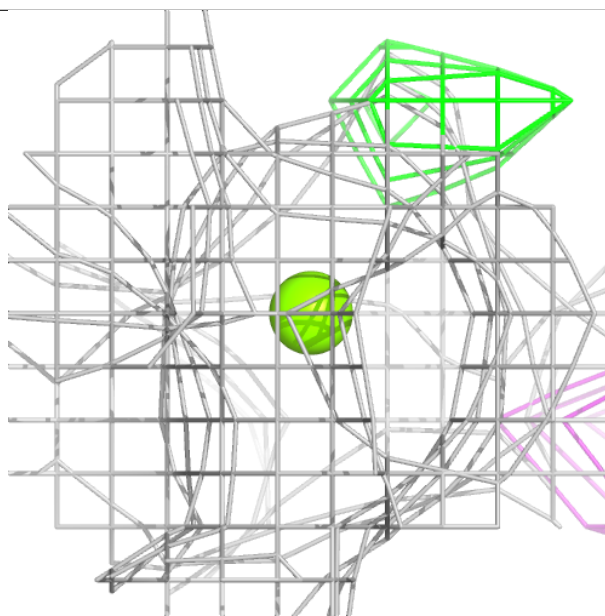
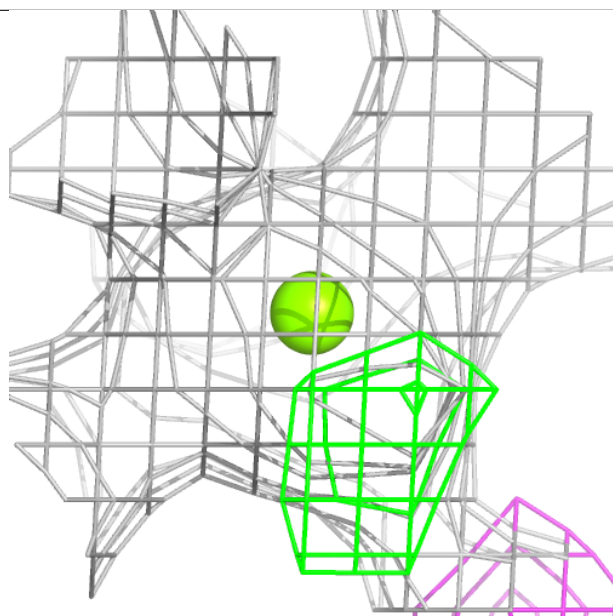
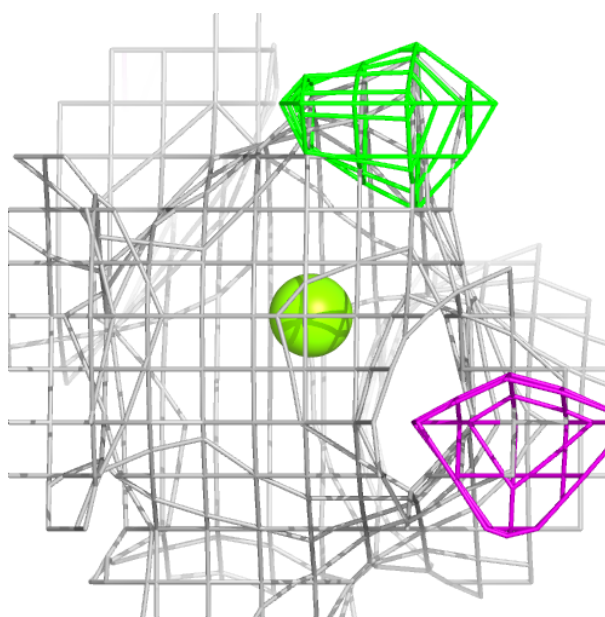
Electron density around CA H 601:

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



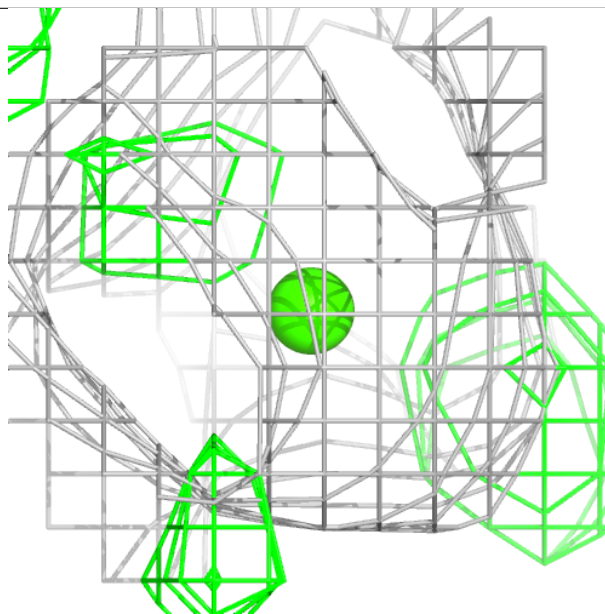
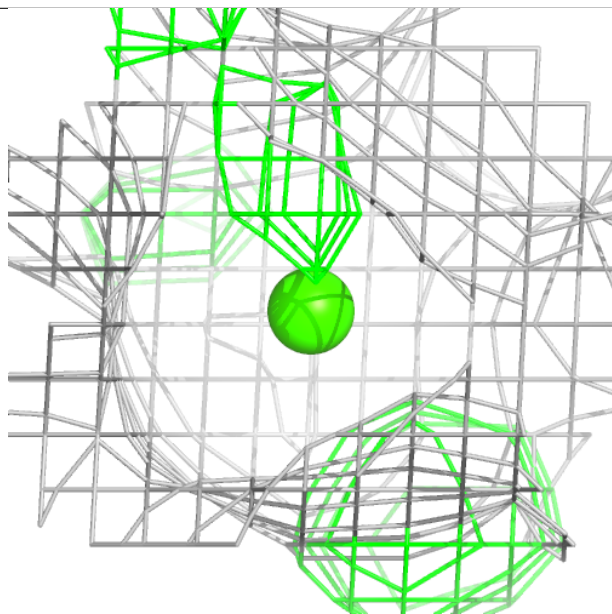
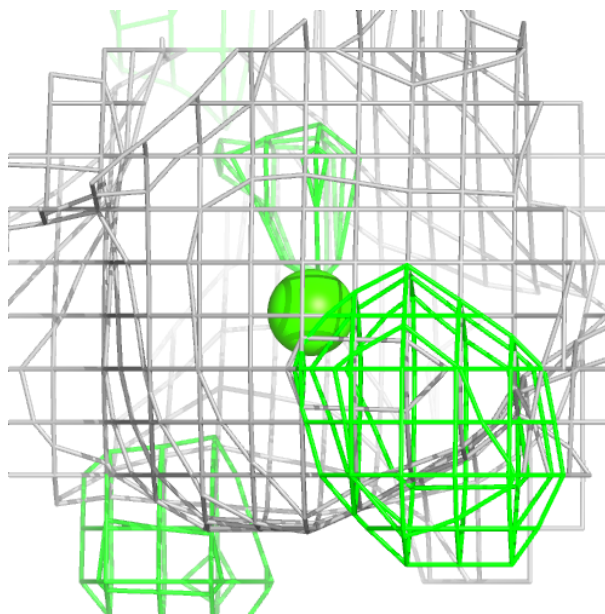
Electron density around MG D 602:

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



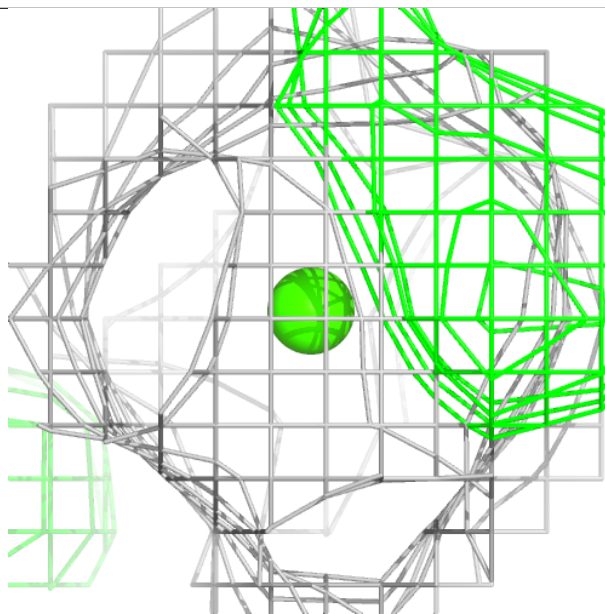
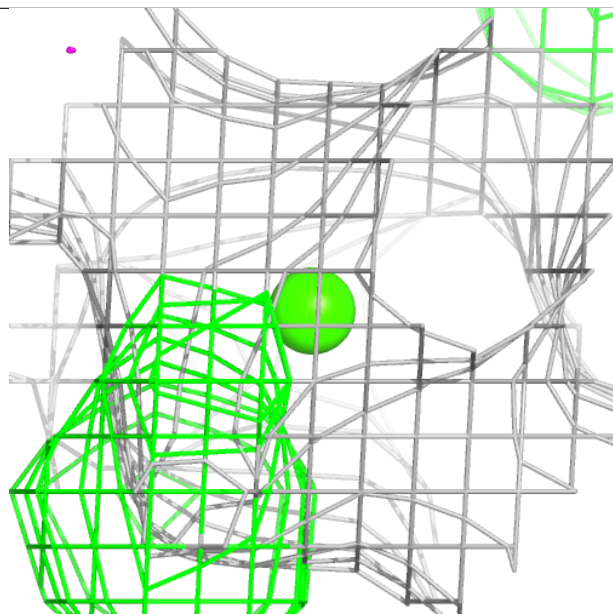
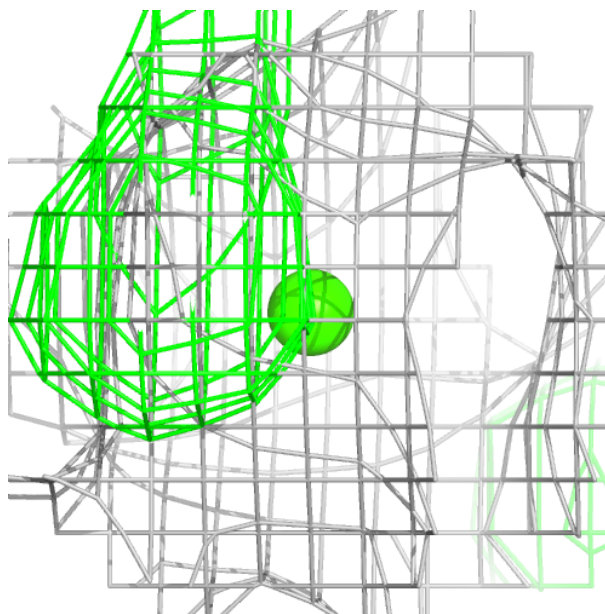
Electron density around CA E 601:

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



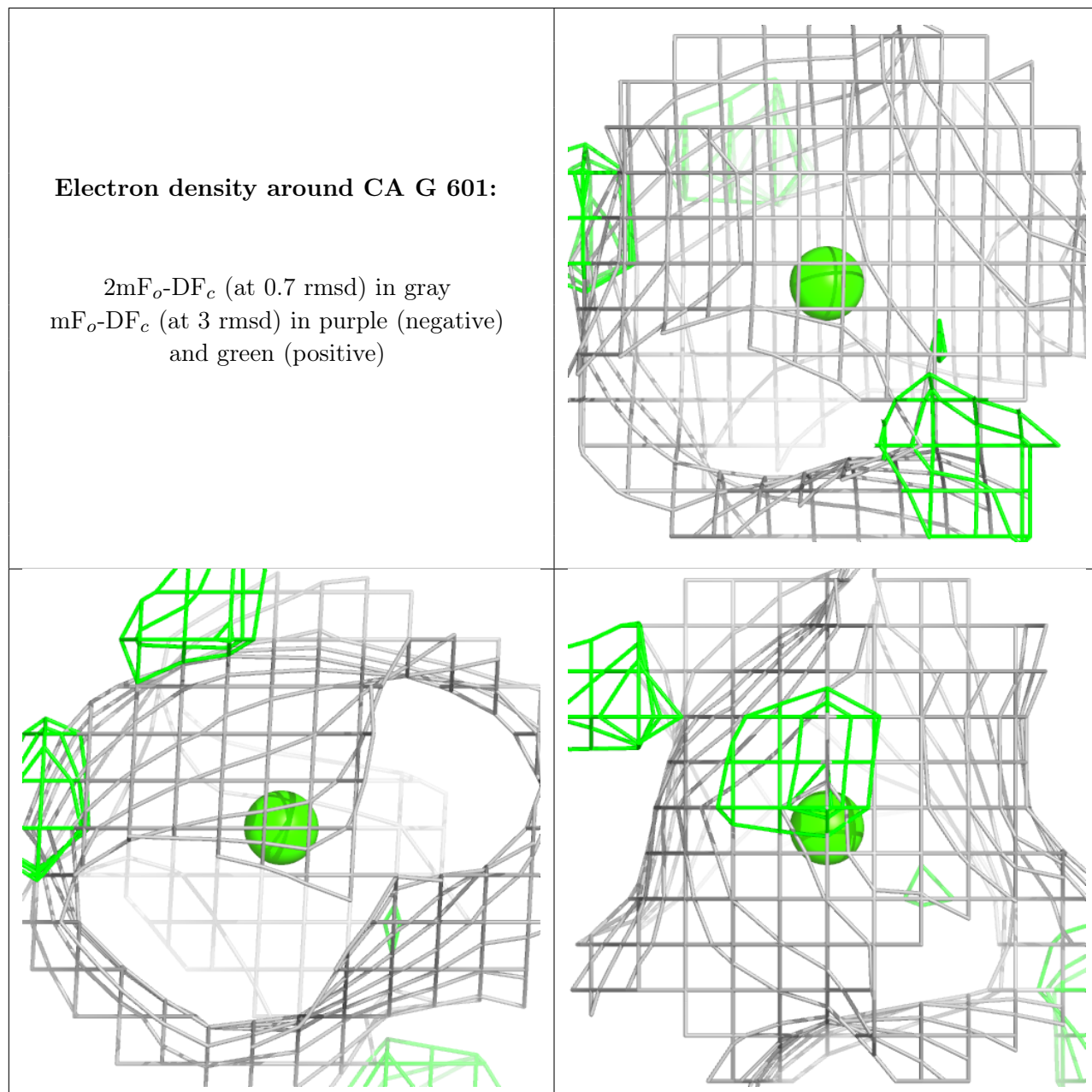
Electron density around CA D 601:

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



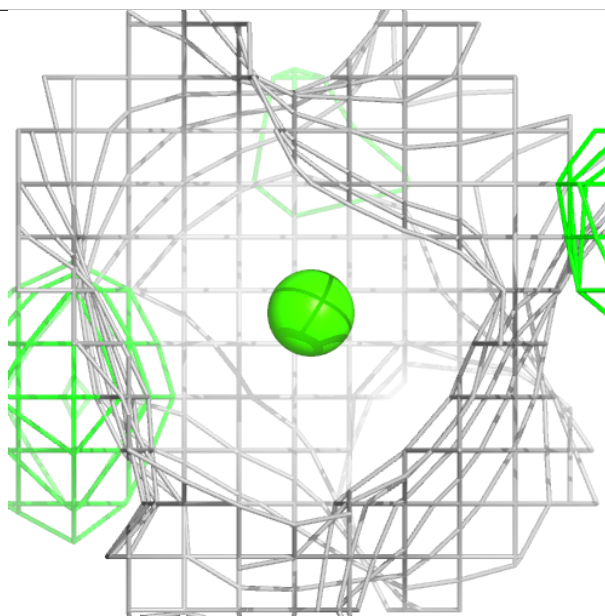
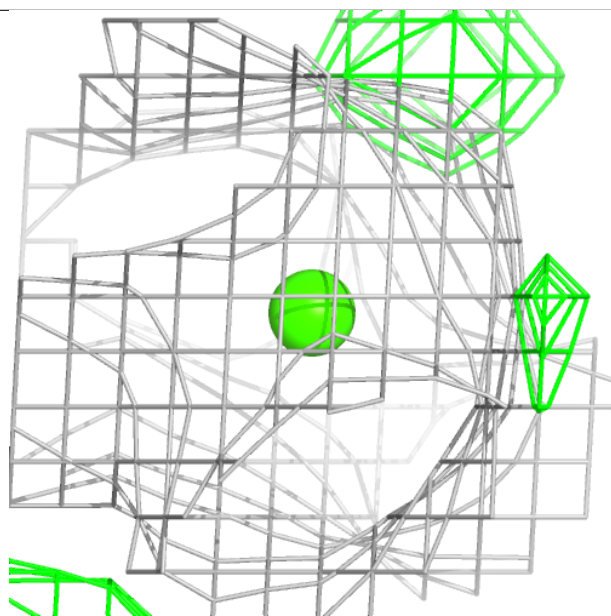
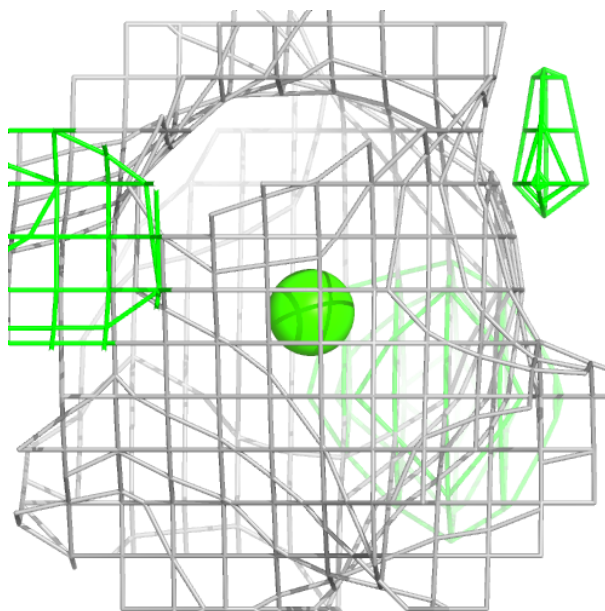
Electron density around CA G 601:

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



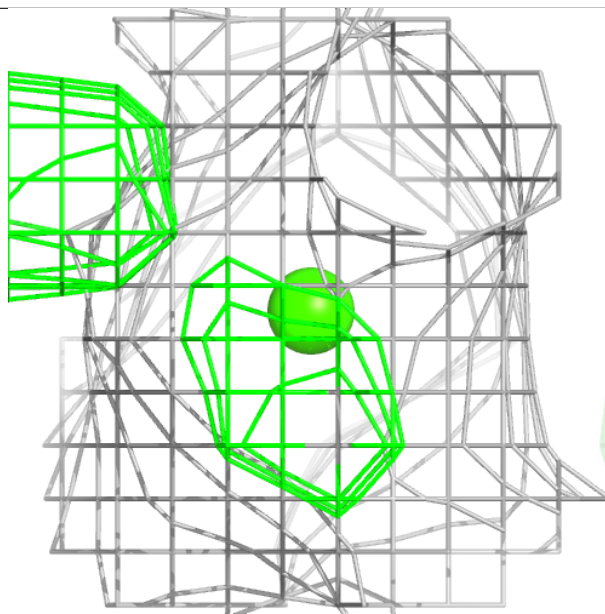
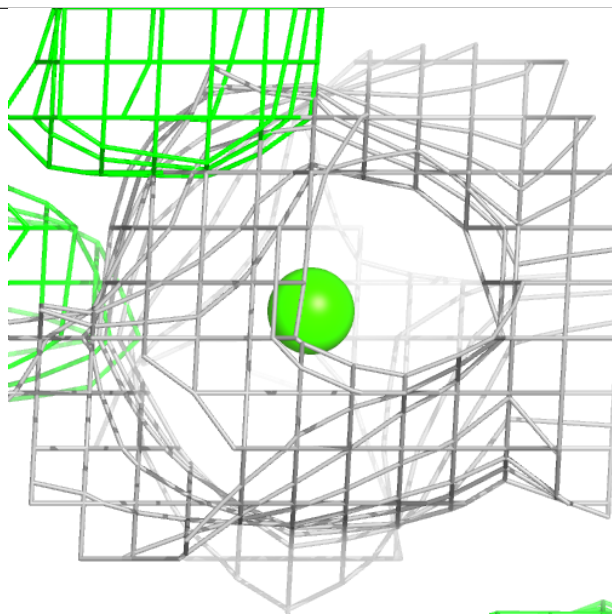
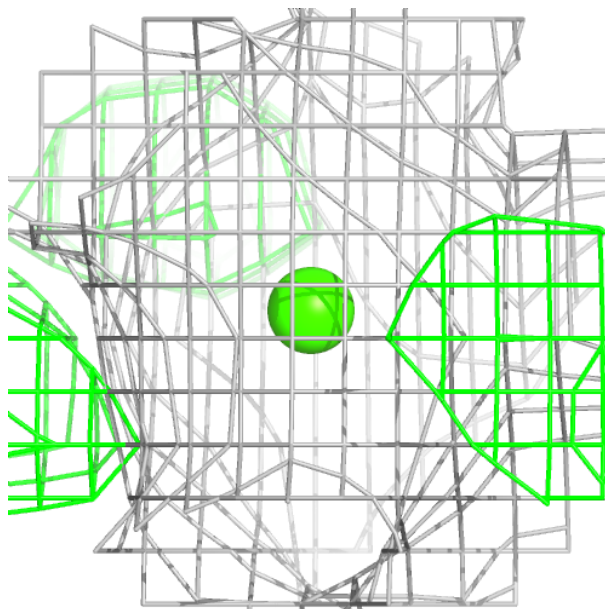
Electron density around CA C 601:

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



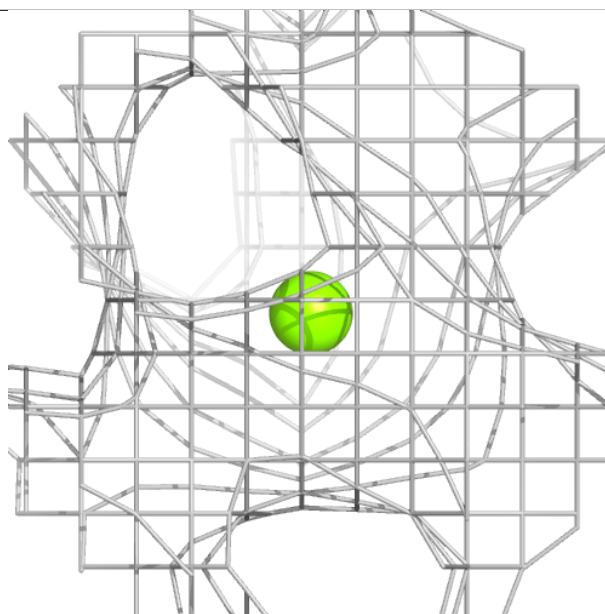
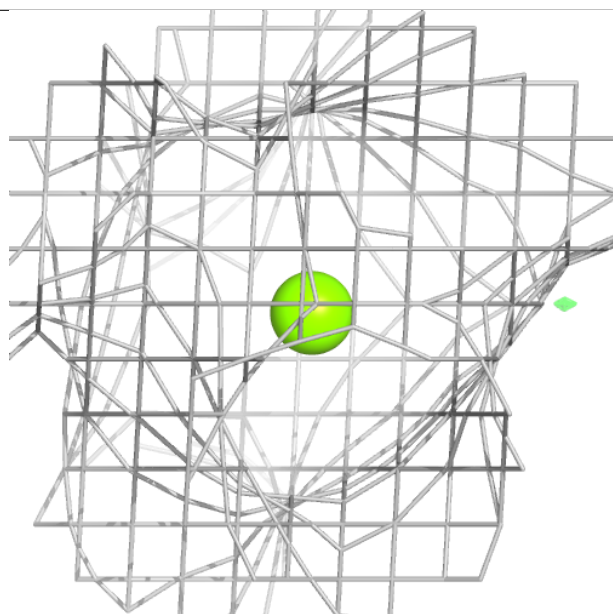
Electron density around CA B 601:

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



Electron density around MG G 602:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.