



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 08:56 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 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

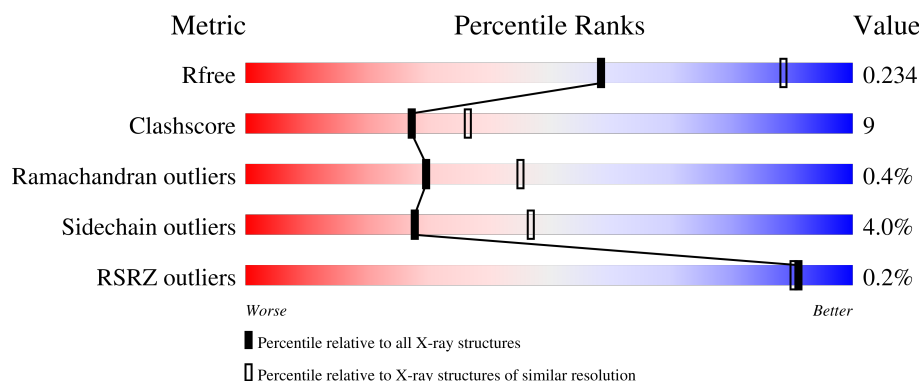
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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).

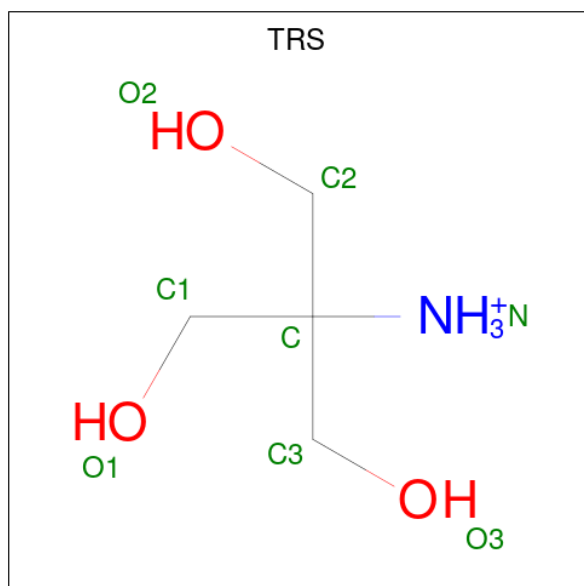
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0

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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		

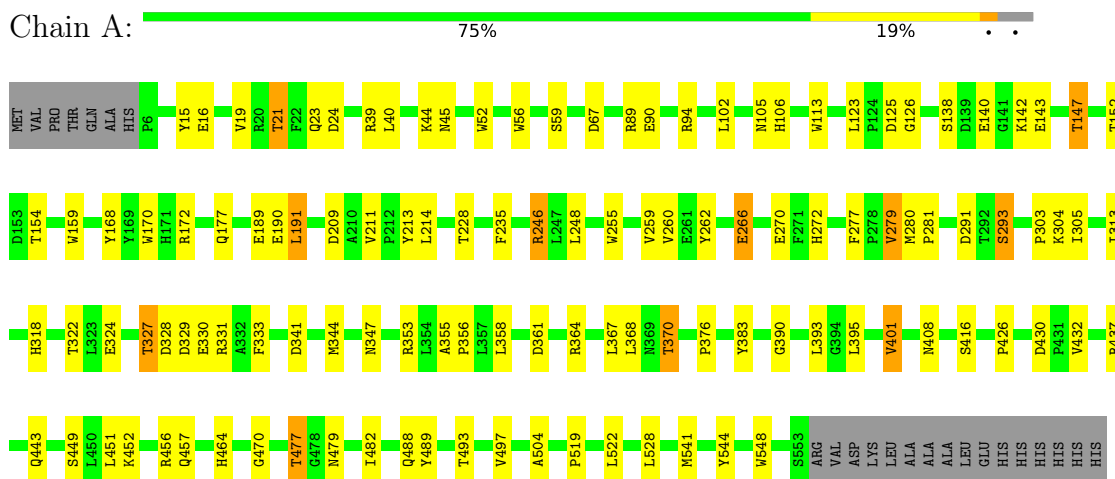
- Molecule 5 is water.

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		

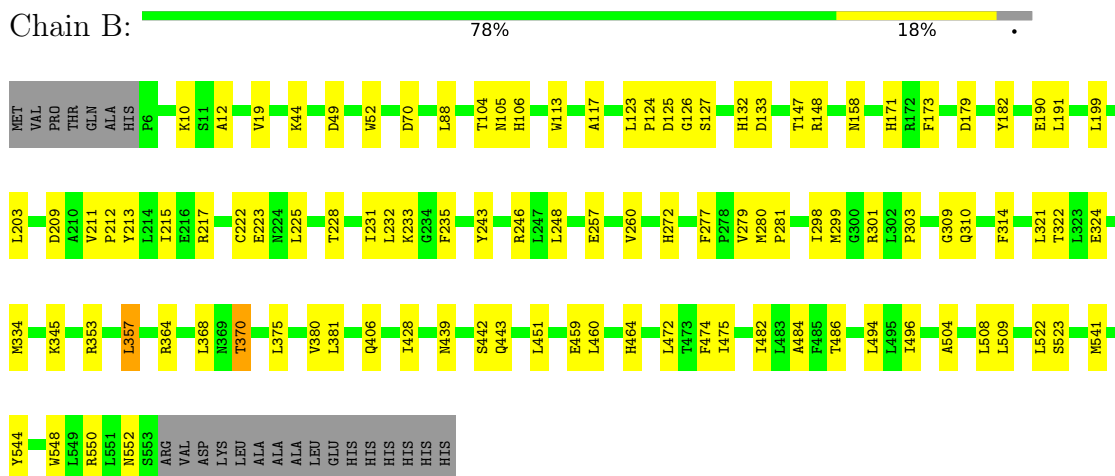
3 Residue-property plots

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.

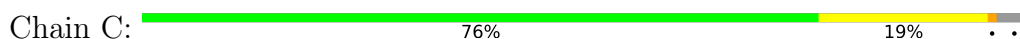
- Molecule 1: maltose alpha-D-glucosyltransferase

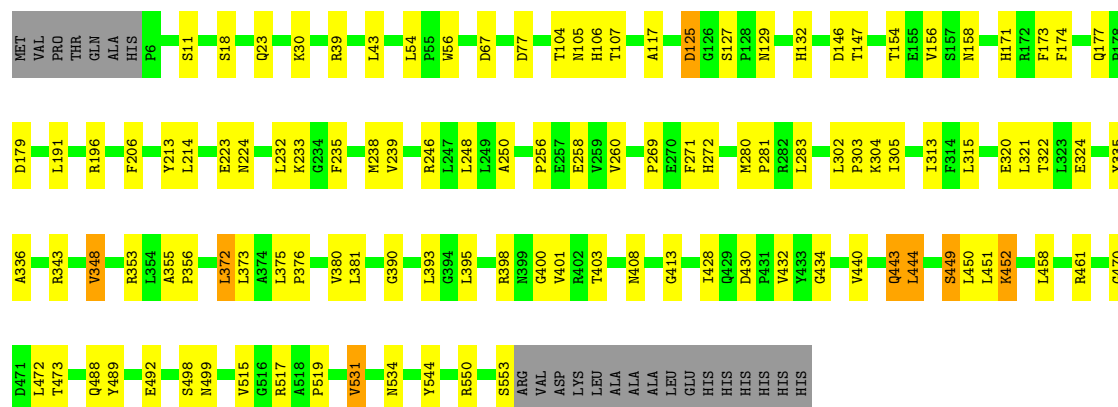


- Molecule 1: maltose alpha-D-glucosyltransferase



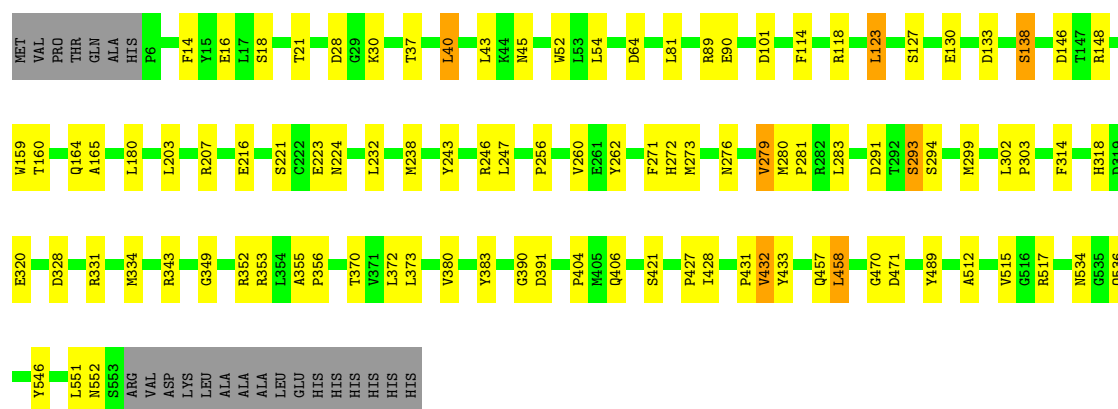
- Molecule 1: maltose alpha-D-glucosyltransferase





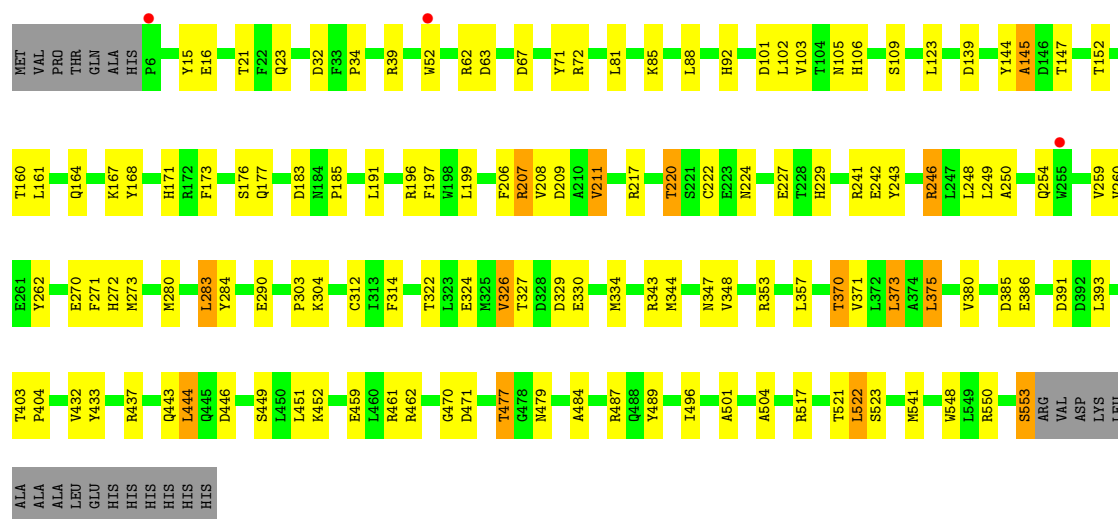
- Molecule 1: maltose alpha-D-glucosyltransferase

Chain D: 79% 16% . .



- Molecule 1: maltose alpha-D-glucosyltransferase

Chain E: 73% 21% . .



- Molecule 1: maltose alpha-D-glucosyltransferase

21% • •



22%



23%



ASP	L367
LYS	L368
LEU	L369
ALA	L370
ALA	L371
ALA	L372
LEU	L373
GLU	L374
HIS	L375
HIS	L376
HIS	L377
HIS	L378
HIS	L379
HIS	L380
HIS	L381
HIS	L382
HIS	L383
HIS	L384
HIS	L385
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HIS	L401
HIS	L402
HIS	L403
HIS	L404
HIS	L405
HIS	L406
HIS	L407
HIS	L408
HIS	L409
HIS	L410
HIS	L411
HIS	L412
HIS	L413
HIS	L414
HIS	L415
HIS	L416
HIS	L417
HIS	L418
HIS	L419
HIS	L420
HIS	L421
HIS	L422
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HIS	L424
HIS	L425
HIS	L426
HIS	L427
HIS	L428
HIS	L429
HIS	L430
HIS	L431
HIS	L432
HIS	L433
HIS	L434
HIS	L435
HIS	L436
HIS	L437
HIS	L438
HIS	L439
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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.

All (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
1	H	182	TYR	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	8	0	12	1	0
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.

All (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
1:E:220:THR:HG23	1:E:222:CYS:H	1.42	0.85
1:B:248:LEU:H	1:B:272:HIS:HD2	1.19	0.85
1:A:23:GLN:HE21	1:A:39:ARG:HE	1.27	0.82
1:H:105:ASN:HD22	1:H:106:HIS:HD2	1.22	0.82
1:A:327:THR:HG22	1:A:330:GLU:H	1.43	0.82
1:G:191:LEU:HG	1:G:235:PHE:HZ	1.45	0.81
1:G:304:LYS:HD2	1:G:305:ILE:H	1.45	0.81
1:F:104:THR:HG22	1:F:191:LEU:HD11	1.63	0.81
1:G:444:LEU:O	1:G:452:LYS:NZ	2.13	0.80
1:B:105:ASN:HD22	1:B:106:HIS:HD2	1.30	0.79
1:C:449:SER:HB2	1:C:452:LYS:HB2	1.65	0.79
1:E:52:TRP:HH2	1:E:207:ARG:HD2	1.43	0.79
1:D:243:TYR:HB3	1:D:246:ARG:HD2	1.65	0.79
1:G:280:MET:HG3	1:G:281:PRO:HD3	1.64	0.78
1:E:477:THR:HG22	1:E:479:ASN:H	1.48	0.77
1:E:304:LYS:H	1:E:304:LYS:HD2	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:63:ASP:OD2	4:E:603:TRS:O2	2.03	0.76
1:A:248:LEU:H	1:A:272:HIS:HD2	1.32	0.74
1:H:254:GLN:HB2	1:H:259:VAL:HG22	1.70	0.73
1:F:256:PRO:HB3	1:F:302:LEU:HD23	1.70	0.73
1:G:23:GLN:NE2	1:G:39:ARG:HE	1.87	0.73
1:C:125:ASP:OD1	1:C:125:ASP:N	2.22	0.73
1:D:123:LEU:HD22	1:D:127:SER:HB2	1.69	0.72
1:H:44:LYS:NZ	1:H:94:ARG:O	2.18	0.72
1:C:373:LEU:HG	1:C:461:ARG:HD2	1.70	0.72
1:F:288:LYS:HG2	1:F:337:ALA:HB1	1.70	0.72
1:G:23:GLN:HE21	1:G:39:ARG:HE	1.37	0.72
1:A:143:GLU:OE2	1:A:143:GLU:N	2.19	0.72
1:D:232:LEU:HD13	1:D:271:PHE:HE2	1.55	0.71
1:H:343:ARG:H	1:H:343:ARG:HD2	1.55	0.71
1:D:279:VAL:CG1	1:D:299:MET:HE3	2.20	0.71
1:G:207:ARG:HB2	1:G:249:LEU:HD23	1.72	0.71
1:H:248:LEU:H	1:H:272:HIS:HD2	1.36	0.70
1:H:389:MET:SD	1:H:406:GLN:HG3	2.31	0.70
1:B:280:MET:HG3	1:B:281:PRO:HD3	1.71	0.70
1:D:353:ARG:NH2	1:D:383:TYR:O	2.23	0.70
1:D:279:VAL:HG13	1:D:299:MET:HE3	1.74	0.70
1:D:224:ASN:ND2	1:D:262:TYR:OH	2.23	0.69
1:C:322:THR:OG1	1:C:324:GLU:HG3	1.92	0.69
1:D:320:GLU:HG3	1:D:349:GLY:HA3	1.75	0.69
1:E:217:ARG:O	1:E:220:THR:HG22	1.93	0.69
1:E:224:ASN:ND2	1:E:262:TYR:OH	2.25	0.69
1:E:88:LEU:HD22	1:E:92:HIS:CE1	2.28	0.69
1:F:260:VAL:HG21	1:F:303:PRO:HG2	1.75	0.69
1:A:113:TRP:CZ2	1:A:190:GLU:HG2	2.28	0.68
1:E:81:LEU:HD12	1:E:85:LYS:HE3	1.75	0.68
1:C:515:VAL:HA	1:C:531:VAL:HG22	1.75	0.68
1:D:148:ARG:NH1	1:D:223:GLU:OE1	2.26	0.68
1:B:248:LEU:H	1:B:272:HIS:CD2	2.06	0.67
1:F:329:ASP:HA	1:F:332:ALA:HB3	1.76	0.67
1:G:224:ASN:ND2	1:G:258:GLU:OE1	2.27	0.67
1:A:477:THR:HG22	1:A:479:ASN:H	1.60	0.67
1:A:125:ASP:OD2	1:A:126:GLY:N	2.27	0.67
1:C:191:LEU:HD23	1:C:235:PHE:CE2	2.30	0.67
1:H:343:ARG:HD2	1:H:343:ARG:N	2.10	0.67
1:E:443:GLN:NE2	1:E:451:LEU:H	1.93	0.66
1:D:14:PHE:CZ	1:D:273:MET:HE1	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:52:TRP:NE1	1:F:101:ASP:OD2	2.28	0.66
1:D:37:THR:HA	1:D:40:LEU:HD22	1.77	0.66
1:G:104:THR:HG22	1:G:191:LEU:HD11	1.76	0.66
1:C:105:ASN:HD22	1:C:106:HIS:HD2	1.43	0.66
1:C:470:GLY:HA2	1:C:489:TYR:HB2	1.78	0.65
1:C:23:GLN:NE2	1:C:39:ARG:HH21	1.95	0.65
1:E:23:GLN:HE21	1:E:39:ARG:HE	1.42	0.65
1:E:248:LEU:H	1:E:272:HIS:HD2	1.42	0.65
1:F:199:LEU:HD22	1:F:246:ARG:HG2	1.79	0.65
1:D:247:LEU:HD11	1:D:273:MET:HG3	1.79	0.65
1:H:256:PRO:HB3	1:H:302:LEU:HD12	1.79	0.65
1:H:495:LEU:HD23	1:H:549:LEU:HD12	1.78	0.64
1:G:160:THR:OG1	1:G:171:HIS:HE1	1.80	0.64
1:A:260:VAL:HG21	1:A:303:PRO:HG2	1.78	0.64
1:E:229:HIS:ND1	1:E:270:GLU:OE2	2.25	0.64
1:B:364:ARG:HD2	1:B:544:TYR:CZ	2.32	0.64
1:A:322:THR:OG1	1:A:324:GLU:HG3	1.98	0.64
1:B:191:LEU:HD23	1:B:235:PHE:HE2	1.64	0.63
1:C:256:PRO:HB3	1:C:302:LEU:HD23	1.80	0.63
1:C:280:MET:HE1	1:C:321:LEU:HG	1.80	0.63
1:F:265:THR:HG23	1:F:268:GLU:H	1.63	0.63
1:C:191:LEU:HD23	1:C:235:PHE:HE2	1.64	0.63
1:H:111:HIS:HD2	1:H:112:PRO:HD2	1.62	0.63
1:A:488:GLN:HG2	1:A:493:THR:HG23	1.80	0.63
1:B:334:MET:HA	1:B:334:MET:HE2	1.79	0.63
1:H:101:ASP:OD1	1:H:207:ARG:HD2	1.99	0.63
1:F:63:ASP:OD2	4:F:603:TRS:O2	2.18	0.62
1:G:232:LEU:HD13	1:G:271:PHE:HE2	1.63	0.62
1:B:171:HIS:HD2	1:B:173:PHE:O	1.82	0.62
1:C:23:GLN:HE21	1:C:39:ARG:HE	1.45	0.62
1:D:256:PRO:HB3	1:D:302:LEU:HD23	1.81	0.62
1:H:113:TRP:CH2	1:H:190:GLU:HG2	2.34	0.62
1:H:260:VAL:HG21	1:H:303:PRO:HG2	1.81	0.62
1:F:293:SER:O	1:F:297:GLU:HG3	1.99	0.62
1:G:143:GLU:OE1	1:G:143:GLU:N	2.32	0.62
1:G:456:ARG:HH22	1:G:457:GLN:HE21	1.44	0.62
1:B:117:ALA:O	1:B:132:HIS:HD2	1.83	0.62
1:F:229:HIS:O	1:F:233:LYS:HG3	2.00	0.62
1:H:373:LEU:HD22	1:H:461:ARG:HD2	1.81	0.62
1:D:130:GLU:OE2	1:D:130:GLU:N	2.21	0.62
1:B:299:MET:HE2	1:B:375:LEU:HD22	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:171:HIS:HD2	1:G:173:PHE:O	1.84	0.61
1:A:23:GLN:NE2	1:A:39:ARG:HE	1.94	0.61
1:B:257:GLU:H	1:B:257:GLU:CD	2.07	0.61
1:H:105:ASN:HD22	1:H:106:HIS:CD2	2.12	0.61
1:G:470:GLY:HA2	1:G:489:TYR:HB2	1.81	0.61
1:H:341:ASP:HB3	1:H:344:MET:HE3	1.83	0.61
1:C:304:LYS:HE3	1:C:305:ILE:H	1.66	0.60
1:C:313:ILE:HG22	1:C:372:LEU:HD12	1.83	0.60
1:F:248:LEU:H	1:F:272:HIS:HD2	1.49	0.60
1:H:113:TRP:CZ2	1:H:190:GLU:HG2	2.37	0.60
1:B:10:LYS:HA	1:B:310:GLN:HG3	1.82	0.59
1:A:364:ARG:HD2	1:A:544:TYR:CZ	2.36	0.59
1:C:23:GLN:HE22	1:C:39:ARG:HH21	1.50	0.59
1:C:280:MET:HE2	1:C:315:LEU:O	2.02	0.59
1:G:467:PHE:O	1:G:487:ARG:NH2	2.35	0.59
1:H:145:ALA:C	1:H:147:THR:H	2.10	0.59
1:F:322:THR:OG1	1:F:324:GLU:HG3	2.03	0.59
1:G:313:ILE:HG22	1:G:372:LEU:HD12	1.84	0.59
1:H:224:ASN:OD1	1:H:262:TYR:OH	2.21	0.59
1:H:227:GLU:N	1:H:227:GLU:OE1	2.36	0.59
1:D:52:TRP:NE1	1:D:101:ASP:OD2	2.24	0.58
1:H:59:SER:HB2	1:H:67:ASP:O	2.03	0.58
1:H:472:LEU:HD12	1:H:473:THR:N	2.18	0.58
1:H:358:LEU:HD11	1:H:368:LEU:HD12	1.85	0.58
1:C:171:HIS:HD2	1:C:173:PHE:O	1.86	0.58
1:F:116:ALA:O	1:F:119:ARG:HG2	2.02	0.58
1:F:464:HIS:HD2	1:F:492:GLU:OE2	1.86	0.58
1:A:113:TRP:CH2	1:A:190:GLU:HG2	2.39	0.58
1:E:23:GLN:NE2	1:E:39:ARG:HE	2.00	0.58
1:H:55:PRO:HD3	1:H:101:ASP:OD2	2.03	0.58
1:B:280:MET:HE1	1:B:321:LEU:HD12	1.85	0.58
1:E:105:ASN:HD22	1:E:106:HIS:HD2	1.51	0.58
1:C:196:ARG:HG3	1:C:238:MET:HE1	1.85	0.58
1:G:118:ARG:O	1:G:165:ALA:HB2	2.03	0.58
1:G:353:ARG:HD3	1:G:390:GLY:O	2.03	0.58
1:G:88:LEU:HG	1:G:92:HIS:CE1	2.39	0.57
1:E:254:GLN:HB2	1:E:259:VAL:HG23	1.85	0.57
1:B:148:ARG:NH1	1:B:324:GLU:OE1	2.32	0.57
1:B:443:GLN:NE2	1:B:451:LEU:H	2.02	0.57
1:E:290:GLU:CG	1:E:501:ALA:HA	2.30	0.57
1:H:495:LEU:HB3	1:H:549:LEU:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ASN:HD22	1:A:106:HIS:HD2	1.53	0.57
1:C:248:LEU:H	1:C:272:HIS:CD2	2.21	0.57
1:E:284:TYR:HB2	1:E:334:MET:HE1	1.87	0.57
1:H:89:ARG:NH2	1:H:90:GLU:OE2	2.34	0.57
1:H:211:VAL:HG13	1:H:232:LEU:HD21	1.87	0.56
1:C:248:LEU:H	1:C:272:HIS:HD2	1.52	0.56
1:D:118:ARG:O	1:D:165:ALA:HB2	2.06	0.56
1:E:273:MET:HE2	1:E:312:CYS:HB2	1.85	0.56
1:B:222:CYS:HA	1:B:225:LEU:HD11	1.86	0.56
1:D:471:ASP:OD1	1:D:471:ASP:N	2.27	0.56
1:F:299:MET:HE2	1:F:299:MET:HA	1.88	0.56
1:F:493:THR:HG22	1:F:551:LEU:HD12	1.88	0.56
1:G:153:ASP:OD2	1:G:347:ASN:N	2.39	0.56
1:A:358:LEU:HD11	1:A:368:LEU:HD12	1.88	0.56
1:G:90:GLU:HG3	1:G:94:ARG:NH1	2.21	0.55
1:H:183:ASP:O	1:H:184:ASN:HB3	2.06	0.55
1:E:52:TRP:CZ2	1:E:207:ARG:HD2	2.40	0.55
1:F:65:GLY:C	1:F:67:ASP:H	2.13	0.55
1:C:260:VAL:HG21	1:C:303:PRO:HD2	1.87	0.55
1:G:191:LEU:HG	1:G:235:PHE:CZ	2.35	0.55
1:F:442:SER:HB2	1:G:431:PRO:O	2.06	0.55
1:E:52:TRP:CH2	1:E:207:ARG:HB3	2.42	0.55
1:A:443:GLN:NE2	1:A:451:LEU:H	2.05	0.54
1:E:52:TRP:CZ3	1:E:207:ARG:HB3	2.41	0.54
1:C:517:ARG:HD3	1:C:553:SER:HB3	1.90	0.54
1:H:137:TRP:HB3	1:H:167:LYS:HD3	1.90	0.54
1:E:171:HIS:HD2	1:E:173:PHE:O	1.90	0.54
1:F:257:GLU:CD	1:F:257:GLU:H	2.16	0.54
1:B:215:ILE:HG23	1:B:217:ARG:HH21	1.72	0.54
1:D:279:VAL:HG11	1:D:299:MET:HE3	1.90	0.54
1:H:248:LEU:H	1:H:272:HIS:CD2	2.22	0.54
1:H:459:GLU:HG3	1:H:462:ARG:HH12	1.73	0.54
1:A:89:ARG:NH1	1:A:90:GLU:OE2	2.42	0.54
1:F:486:THR:HA	1:F:494:LEU:O	2.07	0.53
1:H:163:GLU:O	1:H:165:ALA:N	2.41	0.53
1:A:395:LEU:HD21	1:A:426:PRO:HD2	1.90	0.53
1:D:28:ASP:OD1	1:D:30:LYS:HD2	2.07	0.53
1:D:517:ARG:HG2	1:D:552:ASN:C	2.33	0.53
1:C:488:GLN:HA	1:C:492:GLU:O	2.08	0.53
1:E:62:ARG:NH1	1:E:176:SER:OG	2.42	0.53
1:F:224:ASN:HD21	1:F:254:GLN:HG3	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:113:TRP:CZ2	1:G:190:GLU:HG2	2.43	0.53
1:A:470:GLY:HA2	1:A:489:TYR:HB2	1.90	0.53
1:E:432:VAL:HG13	1:E:433:TYR:CD2	2.44	0.53
1:A:140:GLU:CD	1:A:142:LYS:HE2	2.34	0.53
1:C:443:GLN:HE21	1:C:451:LEU:H	1.57	0.53
1:E:326:VAL:HG13	1:E:330:GLU:HB2	1.91	0.52
1:G:182:TYR:OH	1:G:191:LEU:HD22	2.10	0.52
1:H:209:ASP:HA	1:H:251:GLU:HG2	1.91	0.52
1:A:67:ASP:HB3	1:A:177:GLN:HG2	1.92	0.52
1:B:209:ASP:OD2	4:B:603:TRS:O3	2.27	0.52
1:F:67:ASP:O	1:F:108:SER:HB2	2.10	0.52
1:G:443:GLN:HE21	1:G:451:LEU:H	1.56	0.52
1:H:361:ASP:HB3	1:H:364:ARG:HG2	1.91	0.52
1:G:171:HIS:CD2	1:G:173:PHE:O	2.63	0.52
1:G:341:ASP:HB2	1:G:344:MET:HE3	1.91	0.52
1:G:490:ASP:CG	1:G:490:ASP:O	2.52	0.52
1:C:395:LEU:HD12	1:C:400:GLY:HA2	1.92	0.52
1:H:262:TYR:O	1:H:271:PHE:HB2	2.09	0.52
1:H:255:TRP:HB2	1:H:258:GLU:OE1	2.10	0.52
1:A:191:LEU:HG	1:A:235:PHE:CE1	2.45	0.52
1:B:406:GLN:HE22	1:B:428:ILE:HB	1.73	0.52
1:D:16:GLU:OE2	1:D:318:HIS:ND1	2.42	0.52
1:D:299:MET:HA	1:D:299:MET:HE2	1.92	0.52
1:E:220:THR:HG23	1:E:222:CYS:N	2.17	0.52
1:F:146:ASP:O	1:F:146:ASP:OD2	2.26	0.52
1:H:199:LEU:HD22	1:H:246:ARG:HG2	1.92	0.52
1:A:23:GLN:NE2	1:A:39:ARG:HH21	2.08	0.52
1:F:107:THR:HG21	1:F:135:TYR:OH	2.10	0.52
1:H:343:ARG:H	1:H:343:ARG:CD	2.23	0.52
1:H:472:LEU:HD12	1:H:473:THR:H	1.75	0.52
1:F:125:ASP:HB2	1:F:127:SER:H	1.73	0.51
1:H:122:THR:OG1	1:H:125:ASP:O	2.29	0.51
1:C:224:ASN:ND2	1:C:258:GLU:HG2	2.26	0.51
1:G:114:PHE:O	1:G:118:ARG:HB2	2.11	0.51
1:H:341:ASP:OD2	1:H:342:ALA:N	2.43	0.51
1:C:117:ALA:O	1:C:132:HIS:HD2	1.93	0.51
1:C:428:ILE:HG22	1:C:434:GLY:HA2	1.92	0.51
1:E:373:LEU:O	1:E:461:ARG:NH1	2.38	0.51
1:H:362:ARG:HD2	1:H:450:LEU:HD13	1.92	0.51
1:C:443:GLN:HG2	1:C:449:SER:HB3	1.93	0.51
1:F:107:THR:HG23	1:F:111:HIS:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:ARG:NH1	1:D:343:ARG:HG3	2.25	0.51
1:E:139:ASP:OD1	1:E:167:LYS:HE2	2.10	0.51
1:C:18:SER:HB2	1:C:54:LEU:HD22	1.93	0.51
1:F:444:LEU:HD13	1:F:451:LEU:HD21	1.93	0.51
1:A:522:LEU:HD12	1:A:548:TRP:HB3	1.92	0.51
1:E:246:ARG:HD3	1:E:246:ARG:N	2.26	0.50
1:G:266:GLU:OE1	1:G:307:SER:OG	2.27	0.50
1:A:291:ASP:OD1	1:A:293:SER:OG	2.28	0.50
1:B:257:GLU:OE2	1:B:301:ARG:NH2	2.38	0.50
1:F:143:GLU:N	1:F:143:GLU:OE1	2.44	0.50
1:A:344:MET:HG2	1:A:393:LEU:HD21	1.94	0.50
1:B:248:LEU:N	1:B:272:HIS:HD2	1.98	0.50
1:B:211:VAL:HG23	1:B:212:PRO:HD3	1.94	0.50
1:F:280:MET:SD	1:F:321:LEU:HD13	2.52	0.50
1:H:171:HIS:CD2	1:H:175:ALA:HA	2.46	0.50
1:A:443:GLN:HE21	1:A:451:LEU:H	1.59	0.50
1:B:147:THR:HG23	1:B:158:ASN:ND2	2.27	0.50
1:D:314:PHE:HB3	1:D:380:VAL:CG1	2.41	0.50
1:F:145:ALA:O	1:F:146:ASP:HB3	2.12	0.50
1:H:257:GLU:CD	1:H:257:GLU:H	2.19	0.50
1:F:248:LEU:H	1:F:272:HIS:CD2	2.30	0.50
1:F:467:PHE:O	1:F:487:ARG:NH2	2.45	0.50
1:G:140:GLU:HG3	1:G:142:LYS:HG3	1.92	0.50
1:E:260:VAL:HG11	1:E:303:PRO:HG2	1.94	0.50
1:F:304:LYS:H	1:F:304:LYS:CE	2.19	0.50
1:F:321:LEU:HD12	1:F:322:THR:N	2.27	0.50
1:G:90:GLU:HG3	1:G:94:ARG:HH12	1.77	0.50
1:B:550:ARG:HD2	1:B:552:ASN:OD1	2.11	0.49
1:G:370:THR:HG23	1:G:548:TRP:HE1	1.75	0.49
1:C:430:ASP:OD1	1:C:432:VAL:N	2.44	0.49
1:F:264:GLY:HA3	1:F:270:GLU:HB2	1.94	0.49
1:A:21:THR:HG21	1:A:383:TYR:OH	2.11	0.49
1:A:255:TRP:O	1:A:259:VAL:HG23	2.11	0.49
1:A:449:SER:HB2	1:A:452:LYS:HB2	1.95	0.49
1:E:250:ALA:HB2	1:E:271:PHE:CD1	2.47	0.49
1:E:322:THR:OG1	1:E:324:GLU:HG2	2.12	0.49
1:A:23:GLN:HE22	1:A:39:ARG:HH21	1.61	0.49
1:C:154:THR:HG21	1:C:174:PHE:CE1	2.47	0.49
1:D:101:ASP:OD1	1:D:207:ARG:HD2	2.12	0.49
1:E:484:ALA:HA	1:E:496:ILE:O	2.13	0.49
1:H:108:SER:C	1:H:110:ASP:H	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:353:ARG:HD3	1:H:390:GLY:O	2.13	0.49
1:B:504:ALA:HA	1:B:541:MET:O	2.12	0.49
1:D:404:PRO:HD2	1:D:427:PRO:HA	1.95	0.49
1:E:353:ARG:HG3	1:E:391:ASP:HB3	1.95	0.49
1:G:269:PRO:HB3	1:G:308:PHE:CE2	2.48	0.49
1:A:367:LEU:O	1:A:370:THR:HB	2.13	0.49
1:G:182:TYR:HB3	1:G:231:ILE:CD1	2.43	0.49
1:G:428:ILE:HG22	1:G:434:GLY:HA2	1.95	0.49
1:F:213:TYR:HE1	1:F:223:GLU:HG2	1.78	0.49
1:A:260:VAL:HG11	1:A:303:PRO:CG	2.43	0.49
1:E:32:ASP:HB2	1:E:34:PRO:HD2	1.95	0.49
1:E:241:ARG:O	1:E:241:ARG:HG2	2.13	0.49
1:G:232:LEU:HD13	1:G:271:PHE:CE2	2.46	0.49
1:H:75:HIS:HB3	1:H:78:LEU:HD22	1.94	0.49
1:H:121:PRO:O	1:H:128:PRO:HA	2.13	0.49
1:B:260:VAL:HG11	1:B:303:PRO:HB2	1.95	0.48
1:D:343:ARG:HG3	1:D:343:ARG:HH11	1.78	0.48
1:F:220:THR:OG1	1:F:221:SER:N	2.46	0.48
1:F:376:PRO:HA	1:F:487:ARG:NH2	2.28	0.48
1:A:147:THR:HG21	1:A:170:TRP:HH2	1.78	0.48
1:A:353:ARG:NH2	1:A:383:TYR:O	2.31	0.48
1:E:432:VAL:HA	1:E:437:ARG:HH11	1.78	0.48
1:F:123:LEU:C	1:F:125:ASP:H	2.21	0.48
1:A:191:LEU:HG	1:A:235:PHE:HE1	1.77	0.48
1:A:353:ARG:HD3	1:A:390:GLY:O	2.14	0.48
1:F:499:ASN:O	1:F:544:TYR:HA	2.14	0.48
1:C:443:GLN:NE2	1:C:450:LEU:HB3	2.27	0.48
1:G:443:GLN:NE2	1:G:451:LEU:H	2.10	0.48
1:A:172:ARG:HG3	1:A:213:TYR:HB3	1.96	0.48
1:C:499:ASN:O	1:C:544:TYR:HA	2.14	0.48
1:D:406:GLN:HE22	1:D:428:ILE:HB	1.78	0.48
1:E:15:TYR:OH	1:E:386:GLU:OE2	2.32	0.48
1:E:284:TYR:CB	1:E:334:MET:HE1	2.43	0.48
1:G:9:TYR:CD2	1:G:247:LEU:HD13	2.48	0.48
1:G:50:CYS:HA	1:G:97:TRP:O	2.13	0.48
1:A:456:ARG:NH2	1:A:457:GLN:OE1	2.47	0.48
1:H:471:ASP:O	1:H:487:ARG:HA	2.14	0.48
1:B:133:ASP:OD1	1:B:133:ASP:N	2.41	0.48
1:B:243:TYR:HB3	1:B:246:ARG:HG2	1.96	0.48
1:C:376:PRO:HD3	1:C:472:LEU:HD22	1.94	0.48
1:D:432:VAL:HG22	1:D:433:TYR:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:260:VAL:HG11	1:H:303:PRO:HG2	1.96	0.48
1:C:23:GLN:NE2	1:C:39:ARG:HE	2.10	0.48
1:C:440:VAL:HG12	1:C:444:LEU:HD22	1.95	0.48
1:H:145:ALA:O	1:H:146:ASP:HB2	2.14	0.48
1:C:67:ASP:HB3	1:C:177:GLN:HG2	1.96	0.48
1:D:164:GLN:O	1:D:164:GLN:HG3	2.14	0.47
1:E:227:GLU:H	1:E:227:GLU:CD	2.21	0.47
1:D:247:LEU:HD11	1:D:273:MET:HE2	1.95	0.47
1:H:56:TRP:CD1	1:H:74:ILE:HD13	2.49	0.47
1:A:246:ARG:N	1:A:246:ARG:HD3	2.30	0.47
1:G:408:ASN:O	1:G:413:GLY:HA2	2.13	0.47
1:H:236:ARG:O	1:H:239:VAL:N	2.47	0.47
1:H:297:GLU:O	1:H:301:ARG:HG3	2.13	0.47
1:A:456:ARG:HB3	1:A:456:ARG:CZ	2.45	0.47
1:C:213:TYR:CE1	1:C:223:GLU:HG2	2.50	0.47
1:G:406:GLN:HE22	1:G:428:ILE:HB	1.79	0.47
1:B:105:ASN:HD22	1:B:106:HIS:CD2	2.19	0.47
1:E:446:ASP:O	1:E:452:LYS:HD2	2.15	0.47
1:B:104:THR:CG2	1:B:191:LEU:HD21	2.36	0.47
1:B:199:LEU:HD22	1:B:246:ARG:HG3	1.96	0.47
1:C:353:ARG:HD2	1:C:390:GLY:O	2.15	0.47
1:E:327:THR:HG22	1:E:329:ASP:H	1.79	0.47
1:G:88:LEU:HD21	1:G:202:GLY:O	2.14	0.47
1:H:255:TRP:O	1:H:259:VAL:HG23	2.15	0.47
1:H:328:ASP:OD1	1:H:331:ARG:NH1	2.47	0.47
1:A:430:ASP:OD1	1:A:432:VAL:N	2.44	0.47
1:E:208:VAL:HG12	1:E:211:VAL:HG23	1.97	0.47
1:E:443:GLN:HE21	1:E:451:LEU:H	1.61	0.47
1:H:121:PRO:HD3	1:H:132:HIS:CD2	2.50	0.47
1:G:497:VAL:HG12	1:G:541:MET:SD	2.55	0.47
1:C:408:ASN:O	1:C:413:GLY:HA2	2.15	0.47
1:A:504:ALA:HA	1:A:541:MET:O	2.14	0.46
1:G:118:ARG:HG2	1:G:164:GLN:OE1	2.15	0.46
1:A:152:THR:HG22	1:A:347:ASN:CA	2.35	0.46
1:D:260:VAL:HG21	1:D:303:PRO:HD2	1.96	0.46
1:E:471:ASP:O	1:E:487:ARG:HA	2.16	0.46
1:G:52:TRP:CZ2	1:G:207:ARG:HD3	2.50	0.46
1:H:276:ASN:HD21	1:H:299:MET:HE1	1.81	0.46
1:A:138:SER:HB2	1:A:159:TRP:CZ3	2.51	0.46
1:A:328:ASP:OD2	1:A:331:ARG:NH2	2.48	0.46
1:A:370:THR:HG23	1:A:548:TRP:HE1	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:160:THR:OG1	1:G:171:HIS:CE1	2.66	0.46
1:B:439:ASN:ND2	1:B:442:SER:H	2.13	0.46
1:D:291:ASP:OD1	1:D:293:SER:OG	2.34	0.46
1:H:145:ALA:C	1:H:147:THR:N	2.74	0.46
1:D:334:MET:HE3	1:D:334:MET:HB3	1.90	0.46
1:F:464:HIS:CD2	1:F:492:GLU:OE2	2.67	0.46
1:B:213:TYR:CE1	1:B:223:GLU:HG2	2.50	0.46
1:C:56:TRP:CD1	1:C:56:TRP:C	2.94	0.46
1:G:104:THR:HG22	1:G:191:LEU:CD1	2.44	0.46
1:A:44:LYS:HD2	1:A:44:LYS:HA	1.67	0.46
1:B:301:ARG:O	1:B:303:PRO:HD3	2.16	0.46
1:F:213:TYR:CE1	1:F:223:GLU:HG2	2.50	0.46
1:G:88:LEU:HD21	1:G:202:GLY:C	2.41	0.46
1:G:369:ASN:O	1:G:373:LEU:HG	2.15	0.46
1:H:279:VAL:HB	1:H:299:MET:HE2	1.96	0.46
1:A:341:ASP:OD2	1:A:341:ASP:N	2.49	0.46
1:F:80:THR:N	1:F:83:ASP:OD2	2.48	0.46
1:F:471:ASP:O	1:F:487:ARG:HD2	2.16	0.46
1:H:111:HIS:CD2	1:H:112:PRO:HD2	2.47	0.46
1:H:117:ALA:O	1:H:132:HIS:CD2	2.69	0.46
1:A:105:ASN:HB3	1:A:106:HIS:CD2	2.51	0.46
1:C:280:MET:HB3	1:C:281:PRO:HD3	1.98	0.46
1:C:355:ALA:HB3	1:C:356:PRO:HD3	1.98	0.46
1:E:16:GLU:HB2	1:E:52:TRP:CD1	2.50	0.46
1:E:71:TYR:OH	1:E:103:VAL:O	2.13	0.46
1:H:367:LEU:HD11	1:H:498:SER:HB3	1.97	0.46
1:A:24:ASP:HB3	1:A:416:SER:HB2	1.98	0.45
1:E:370:THR:HG23	1:E:548:TRP:HE1	1.81	0.45
1:E:327:THR:HG22	1:E:329:ASP:N	2.31	0.45
1:E:504:ALA:HA	1:E:541:MET:O	2.16	0.45
1:G:40:LEU:HD21	1:G:87:PHE:HE1	1.82	0.45
1:H:518:ALA:HB2	1:H:530:VAL:HG22	1.98	0.45
1:A:189:GLU:OE2	1:A:189:GLU:O	2.35	0.45
1:B:123:LEU:HB3	1:B:124:PRO:CD	2.47	0.45
1:G:16:GLU:HB2	1:G:52:TRP:CE3	2.51	0.45
1:G:519:PRO:HB2	1:G:528:LEU:HB2	1.97	0.45
1:A:456:ARG:HB3	1:A:456:ARG:NH1	2.32	0.45
1:D:89:ARG:NH2	1:D:90:GLU:OE2	2.33	0.45
1:E:446:ASP:HB3	1:E:449:SER:HB3	1.99	0.45
1:F:122:THR:HG22	1:F:123:LEU:O	2.16	0.45
1:A:16:GLU:HB2	1:A:52:TRP:CE3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:HIS:O	1:B:309:GLY:HA2	2.16	0.45
1:B:314:PHE:HB3	1:B:380:VAL:HG13	1.99	0.45
1:F:446:ASP:HB3	1:F:449:SER:HB3	1.98	0.45
1:A:16:GLU:OE2	1:A:318:HIS:HD2	1.99	0.45
1:A:90:GLU:HG3	1:A:94:ARG:NH1	2.32	0.45
1:F:321:LEU:HD12	1:F:321:LEU:C	2.41	0.45
1:E:290:GLU:HG2	1:E:501:ALA:CA	2.31	0.45
1:G:101:ASP:OD2	1:G:101:ASP:N	2.47	0.45
1:A:497:VAL:HG12	1:A:541:MET:SD	2.57	0.45
1:B:228:THR:O	1:B:232:LEU:HG	2.17	0.45
1:C:173:PHE:CE1	4:C:603:TRS:H12	2.52	0.45
1:D:247:LEU:HD12	1:D:272:HIS:HB2	1.99	0.45
1:E:81:LEU:HD13	1:E:81:LEU:O	2.17	0.45
1:F:182:TYR:OH	1:F:191:LEU:HD13	2.17	0.45
1:H:163:GLU:HB3	1:H:164:GLN:OE1	2.17	0.45
1:H:236:ARG:HH12	1:H:308:PHE:HE1	1.65	0.45
1:H:251:GLU:O	1:H:251:GLU:HG3	2.17	0.45
1:C:430:ASP:OD1	1:C:430:ASP:C	2.61	0.44
1:E:67:ASP:HB3	1:E:177:GLN:HG2	1.99	0.44
1:F:398:ARG:HH12	4:F:603:TRS:H21	1.81	0.44
1:H:107:THR:O	1:H:178:PRO:HD2	2.17	0.44
1:A:105:ASN:HB3	1:A:106:HIS:HD2	1.81	0.44
1:C:238:MET:HG3	1:C:239:VAL:N	2.33	0.44
1:F:472:LEU:HD12	1:F:473:THR:N	2.31	0.44
1:G:248:LEU:HD23	1:G:248:LEU:HA	1.74	0.44
1:H:148:ARG:HG3	1:H:149:ILE:N	2.32	0.44
1:D:238:MET:HE3	1:D:238:MET:HB3	1.86	0.44
1:D:260:VAL:HG11	1:D:303:PRO:HB2	1.99	0.44
1:F:233:LYS:NZ	1:F:268:GLU:O	2.51	0.44
1:A:262:TYR:O	1:A:270:GLU:HB3	2.18	0.44
1:B:52:TRP:CD1	1:B:52:TRP:C	2.96	0.44
1:F:344:MET:HG2	1:F:393:LEU:HD11	1.99	0.44
1:G:446:ASP:HB3	1:G:449:SER:HB3	1.99	0.44
1:D:353:ARG:HD3	1:D:390:GLY:O	2.18	0.44
1:E:72:ARG:HG2	1:E:197:PHE:CG	2.53	0.44
1:E:207:ARG:HA	1:E:249:LEU:O	2.17	0.44
1:E:262:TYR:O	1:E:270:GLU:HB3	2.18	0.44
1:E:470:GLY:HA2	1:E:489:TYR:HB2	1.98	0.44
1:G:277:PHE:O	1:G:278:PRO:C	2.60	0.44
1:B:472:LEU:HD21	1:B:474:PHE:CE2	2.52	0.44
1:D:114:PHE:O	1:D:118:ARG:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:SER:HB3	1:D:159:TRP:CZ3	2.53	0.44
1:D:280:MET:HB3	1:D:281:PRO:HD3	1.99	0.44
1:F:262:TYR:O	1:F:270:GLU:HB3	2.18	0.44
1:F:526:SER:HA	1:F:527:PRO:HD3	1.80	0.44
1:E:23:GLN:HE22	1:E:39:ARG:HH21	1.66	0.44
1:F:21:THR:HG21	1:F:383:TYR:OH	2.18	0.44
1:H:108:SER:C	1:H:110:ASP:N	2.76	0.44
1:E:161:LEU:HB2	1:E:168:TYR:CE2	2.53	0.44
1:G:280:MET:HG3	1:G:281:PRO:CD	2.44	0.44
1:H:278:PRO:HB3	1:H:298:ILE:HD11	2.00	0.44
1:A:266:GLU:H	1:A:266:GLU:HG2	1.66	0.43
1:G:192:HIS:CD2	1:G:238:MET:HE3	2.53	0.43
1:H:499:ASN:O	1:H:544:TYR:HA	2.18	0.43
1:A:327:THR:CG2	1:A:330:GLU:H	2.23	0.43
1:A:477:THR:HG22	1:A:479:ASN:N	2.30	0.43
1:C:30:LYS:HE2	1:C:77:ASP:CG	2.43	0.43
1:F:132:HIS:CE1	1:F:167:LYS:NZ	2.86	0.43
1:G:320:GLU:HG3	1:G:349:GLY:HA3	1.99	0.43
1:C:104:THR:CG2	1:C:191:LEU:HD21	2.48	0.43
1:C:343:ARG:NH2	1:C:393:LEU:O	2.43	0.43
1:C:534:ASN:OD1	1:C:534:ASN:N	2.51	0.43
1:D:232:LEU:HD13	1:D:271:PHE:CE2	2.45	0.43
1:E:270:GLU:HB3	1:E:271:PHE:H	1.68	0.43
1:E:371:VAL:HG12	1:E:375:LEU:HD22	1.98	0.43
1:C:343:ARG:HD2	1:C:343:ARG:HA	1.76	0.43
1:D:40:LEU:HD12	1:D:40:LEU:HA	1.76	0.43
1:E:144:TYR:C	1:E:145:ALA:O	2.62	0.43
1:H:441:GLN:HE21	1:H:445:GLN:NE2	2.17	0.43
1:E:250:ALA:HB2	1:E:271:PHE:CE1	2.53	0.43
1:G:215:ILE:HG21	1:G:227:GLU:HG3	1.99	0.43
1:G:266:GLU:CD	1:G:307:SER:HG	2.27	0.43
1:G:403:THR:HG21	1:G:428:ILE:HD11	2.00	0.43
1:F:490:ASP:CG	1:F:490:ASP:O	2.61	0.43
1:A:45:ASN:OD1	1:D:431:PRO:HD3	2.18	0.43
1:B:12:ALA:HA	1:B:49:ASP:OD2	2.18	0.43
1:B:443:GLN:HE21	1:B:451:LEU:H	1.66	0.43
1:C:335:TYR:OH	1:C:348:VAL:HA	2.18	0.43
1:E:444:LEU:HD12	1:E:444:LEU:HA	1.82	0.43
1:F:228:THR:O	1:F:232:LEU:HD22	2.19	0.43
1:F:367:LEU:HD11	1:F:498:SER:HB2	2.01	0.43
1:A:364:ARG:HD2	1:A:544:TYR:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:236:ARG:HG2	1:H:270:GLU:O	2.18	0.43
1:A:277:PHE:O	1:A:281:PRO:HD3	2.19	0.43
1:E:102:LEU:HA	1:E:102:LEU:HD12	1.73	0.43
1:F:134:TYR:OH	1:F:186:LYS:HG3	2.18	0.43
1:G:269:PRO:HB3	1:G:308:PHE:CZ	2.54	0.43
1:G:275:PHE:HA	1:G:312:CYS:HB3	2.01	0.43
1:G:334:MET:HE3	1:G:334:MET:HB3	1.92	0.43
1:G:470:GLY:CA	1:G:489:TYR:HB2	2.47	0.43
1:H:508:LEU:HD12	1:H:508:LEU:HA	1.86	0.43
1:C:147:THR:HG22	1:C:158:ASN:ND2	2.34	0.43
1:D:355:ALA:HB3	1:D:356:PRO:HD3	2.01	0.43
1:D:512:ALA:O	1:D:515:VAL:HG23	2.19	0.43
1:G:28:ASP:OD1	1:G:28:ASP:N	2.52	0.43
1:H:373:LEU:HA	1:H:373:LEU:HD23	1.75	0.43
1:A:23:GLN:HE21	1:A:39:ARG:NE	2.06	0.42
1:H:272:HIS:O	1:H:309:GLY:HA2	2.19	0.42
1:A:324:GLU:HG3	1:A:324:GLU:H	1.69	0.42
1:D:18:SER:HB2	1:D:54:LEU:HD22	2.01	0.42
1:D:203:LEU:HD12	1:D:203:LEU:HA	1.94	0.42
1:E:196:ARG:HG2	1:E:243:TYR:HE1	1.83	0.42
1:A:313:ILE:HD11	1:A:376:PRO:O	2.19	0.42
1:A:355:ALA:HB3	1:A:356:PRO:HD3	2.01	0.42
1:F:72:ARG:HG2	1:F:197:PHE:CG	2.54	0.42
1:H:446:ASP:HB3	1:H:449:SER:HB3	2.01	0.42
1:B:125:ASP:O	1:B:127:SER:N	2.52	0.42
1:E:81:LEU:CD1	1:E:85:LYS:HE3	2.47	0.42
1:F:17:LEU:HD12	1:F:17:LEU:C	2.45	0.42
1:F:52:TRP:CD1	1:F:52:TRP:C	2.96	0.42
1:F:343:ARG:C	1:F:345:LYS:H	2.28	0.42
1:G:541:MET:HE2	1:G:541:MET:HB3	1.93	0.42
1:H:239:VAL:C	1:H:241:ARG:H	2.27	0.42
1:A:353:ARG:HG3	1:A:401:VAL:HG22	2.01	0.42
1:C:233:LYS:HG2	1:C:269:PRO:O	2.19	0.42
1:A:280:MET:HB3	1:A:280:MET:HE3	1.87	0.42
1:B:280:MET:SD	1:B:321:LEU:HD12	2.59	0.42
1:D:247:LEU:HD21	1:D:273:MET:HE2	2.01	0.42
1:F:214:LEU:HB2	1:F:228:THR:HG23	2.02	0.42
1:A:361:ASP:OD1	1:A:364:ARG:HD3	2.19	0.42
1:B:474:PHE:O	1:B:475:ILE:HD13	2.20	0.42
1:C:472:LEU:HD12	1:C:473:THR:N	2.35	0.42
1:E:327:THR:HB	1:E:330:GLU:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:452:LYS:O	1:F:456:ARG:HD2	2.19	0.42
1:G:165:ALA:O	1:G:167:LYS:HG3	2.20	0.42
1:F:521:THR:O	1:F:525:ALA:HA	2.20	0.42
1:G:101:ASP:OD1	1:G:207:ARG:NH1	2.53	0.42
1:G:335:TYR:CE1	1:G:345:LYS:HG2	2.54	0.42
1:H:67:ASP:O	1:H:108:SER:HB2	2.20	0.42
1:H:161:LEU:HA	1:H:168:TYR:HD1	1.85	0.42
1:A:102:LEU:HD12	1:A:102:LEU:HA	1.74	0.42
1:A:327:THR:HG23	1:A:329:ASP:H	1.85	0.42
1:B:459:GLU:HB3	1:E:343:ARG:HH12	1.85	0.42
1:B:460:LEU:HD12	1:B:460:LEU:HA	1.87	0.42
1:D:81:LEU:HD12	1:D:81:LEU:HA	1.82	0.42
1:F:541:MET:HE3	1:F:547:TYR:CD2	2.55	0.42
1:C:320:GLU:CD	1:C:320:GLU:H	2.27	0.41
1:D:328:ASP:OD1	1:D:331:ARG:NH2	2.53	0.41
1:E:353:ARG:NH2	1:E:385:ASP:OD1	2.41	0.41
1:E:459:GLU:HA	1:E:462:ARG:CG	2.50	0.41
1:H:296:ARG:HG2	1:H:474:PHE:CG	2.54	0.41
1:G:161:LEU:HD23	1:G:168:TYR:CE1	2.55	0.41
1:H:145:ALA:HA	1:H:147:THR:HG22	2.03	0.41
1:A:260:VAL:HG23	1:A:305:ILE:HG22	2.02	0.41
1:D:52:TRP:CD1	1:D:52:TRP:C	2.97	0.41
1:H:192:HIS:HD2	1:H:238:MET:HG3	1.85	0.41
1:A:519:PRO:HB2	1:A:528:LEU:HB2	2.02	0.41
1:B:182:TYR:HB3	1:B:231:ILE:CD1	2.50	0.41
1:C:250:ALA:HB2	1:C:271:PHE:CD2	2.55	0.41
1:E:196:ARG:HG2	1:E:243:TYR:CE1	2.55	0.41
1:E:344:MET:HG2	1:E:393:LEU:HD21	2.02	0.41
1:F:231:ILE:H	1:F:231:ILE:HD12	1.85	0.41
1:C:320:GLU:OE2	1:C:398:ARG:HD3	2.20	0.41
1:D:470:GLY:HA2	1:D:489:TYR:HB2	2.03	0.41
1:F:196:ARG:HD3	1:F:242:GLU:OE2	2.21	0.41
1:G:508:LEU:HD12	1:G:508:LEU:HA	1.86	0.41
1:H:91:ALA:O	1:H:96:LEU:HB2	2.20	0.41
1:A:333:PHE:CE1	1:C:336:ALA:HB2	2.56	0.41
1:B:123:LEU:HB3	1:B:124:PRO:HD2	2.02	0.41
1:B:203:LEU:O	1:B:246:ARG:NH1	2.53	0.41
1:D:130:GLU:H	1:D:130:GLU:CD	2.20	0.41
1:D:352:ARG:HA	1:D:391:ASP:OD1	2.20	0.41
1:B:147:THR:CG2	1:B:158:ASN:HD22	2.33	0.41
1:B:464:HIS:NE2	1:B:522:LEU:HD22	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:458:LEU:HD12	1:D:458:LEU:HA	1.91	0.41
1:G:214:LEU:HD23	1:G:214:LEU:HA	1.84	0.41
1:G:273:MET:HE1	1:G:378:SER:HB2	2.02	0.41
1:G:502:GLY:C	1:G:543:LYS:HB2	2.46	0.41
1:A:138:SER:OG	1:A:143:GLU:OE1	2.36	0.41
1:A:279:VAL:O	1:A:280:MET:C	2.61	0.41
1:B:44:LYS:HD2	1:B:44:LYS:HA	1.82	0.41
1:B:277:PHE:O	1:B:281:PRO:HD3	2.20	0.41
1:E:52:TRP:CH2	1:E:101:ASP:OD1	2.73	0.41
1:E:314:PHE:HB3	1:E:380:VAL:CG1	2.51	0.41
1:F:302:LEU:HD23	1:F:302:LEU:HA	1.78	0.41
1:H:259:VAL:O	1:H:262:TYR:HD1	2.04	0.41
1:A:56:TRP:CD1	1:A:56:TRP:C	2.99	0.41
1:A:214:LEU:HB2	1:A:228:THR:HG23	2.03	0.41
1:B:353:ARG:O	1:B:357:LEU:HD22	2.20	0.41
1:B:508:LEU:HD12	1:B:508:LEU:HA	1.93	0.41
1:D:276:ASN:CG	1:D:279:VAL:HG22	2.46	0.41
1:E:21:THR:O	1:E:404:PRO:HA	2.21	0.41
1:E:152:THR:HG22	1:E:347:ASN:HA	2.03	0.41
1:E:196:ARG:HD3	1:E:242:GLU:OE2	2.20	0.41
1:E:211:VAL:HG21	1:E:271:PHE:CZ	2.55	0.41
1:E:248:LEU:H	1:E:272:HIS:CD2	2.30	0.41
1:E:280:MET:HA	1:E:283:LEU:HD22	2.03	0.41
1:E:459:GLU:HA	1:E:462:ARG:HG2	2.03	0.41
1:E:522:LEU:CD1	1:E:550:ARG:HB2	2.51	0.41
1:F:273:MET:HE1	1:F:378:SER:HB2	2.03	0.41
1:F:495:LEU:HB3	1:F:549:LEU:HB2	2.02	0.41
1:G:453:TRP:CZ2	1:G:457:GLN:HG3	2.56	0.41
1:B:541:MET:HE2	1:B:541:MET:HB3	1.91	0.41
1:C:107:THR:O	1:C:177:GLN:HA	2.20	0.41
1:G:531:VAL:HG22	1:G:537:TYR:CD1	2.56	0.41
1:H:138:SER:O	1:H:167:LYS:HB2	2.20	0.41
1:H:467:PHE:O	1:H:487:ARG:NH2	2.52	0.41
1:D:221:SER:O	1:D:223:GLU:HG3	2.22	0.40
1:D:534:ASN:ND2	1:D:536:GLN:HG2	2.37	0.40
1:F:226:PRO:O	1:F:230:GLU:HG2	2.21	0.40
1:F:272:HIS:O	1:F:309:GLY:HA2	2.21	0.40
1:H:66:TYR:CG	4:H:603:TRS:H32	2.56	0.40
1:H:426:PRO:HA	1:H:427:PRO:HD3	1.94	0.40
1:A:15:TYR:CZ	1:A:383:TYR:HA	2.56	0.40
1:A:52:TRP:CD1	1:A:52:TRP:C	2.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:SER:HB3	1:A:168:TYR:HB2	2.02	0.40
1:A:477:THR:HG21	1:A:482:ILE:HB	2.03	0.40
1:B:113:TRP:CZ2	1:B:190:GLU:CG	3.05	0.40
1:F:42:TYR:HD2	1:F:43:LEU:HD13	1.85	0.40
1:F:471:ASP:O	1:F:487:ARG:NH1	2.40	0.40
1:H:67:ASP:C	1:H:108:SER:HB2	2.46	0.40
1:H:341:ASP:OD2	1:H:343:ARG:HD3	2.20	0.40
1:B:88:LEU:HA	1:B:88:LEU:HD12	1.84	0.40
1:B:314:PHE:HB3	1:B:380:VAL:CG1	2.51	0.40
1:C:519:PRO:HA	1:C:550:ARG:O	2.21	0.40
1:D:370:THR:HG21	1:D:546:TYR:CD2	2.55	0.40
1:E:517:ARG:HG2	1:E:553:SER:HA	2.02	0.40
1:F:46:LEU:HD22	1:F:46:LEU:HA	1.84	0.40
1:F:299:MET:O	1:F:302:LEU:HB2	2.22	0.40
1:F:404:PRO:HB3	1:F:415:PHE:CG	2.57	0.40
1:G:443:GLN:HG2	1:G:449:SER:HB2	2.04	0.40
1:H:29:GLY:HA3	1:H:423:CYS:HA	2.02	0.40
1:H:44:LYS:HD2	1:H:44:LYS:HA	1.83	0.40
1:H:57:PHE:HB2	1:H:68:VAL:HG13	2.02	0.40
1:A:280:MET:C	1:A:280:MET:SD	3.04	0.40
1:A:464:HIS:NE2	1:A:522:LEU:HD22	2.37	0.40
1:B:484:ALA:HA	1:B:496:ILE:O	2.21	0.40
1:B:486:THR:HA	1:B:494:LEU:O	2.22	0.40
1:D:373:LEU:HD12	1:D:457:GLN:HG3	2.03	0.40
1:E:183:ASP:O	1:E:185:PRO:HD3	2.20	0.40
1:G:10:LYS:O	1:G:468:ALA:HB1	2.22	0.40
1:G:44:LYS:HA	1:G:44:LYS:HD2	1.90	0.40
1:H:282:ARG:CZ	1:H:326:VAL:HG12	2.52	0.40
1:H:495:LEU:O	1:H:496:ILE:HD13	2.21	0.40
1:A:432:VAL:HA	1:A:437:ARG:HH11	1.86	0.40
1:B:370:THR:HG23	1:B:548:TRP:HE1	1.87	0.40

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

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	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

All (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
1	C	449	SER
1	G	70	ASP
1	E	109	SER
1	E	145	ALA
1	H	128	PRO
1	H	304	LYS
1	F	70	ASP
1	D	123	LEU
1	F	328	ASP
1	H	185	PRO
1	H	124	PRO
1	F	513	PRO

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Mol	Chain	Res	Type
1	H	121	PRO
1	H	256	PRO

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
1	H	465/484 (96%)	452 (97%)	13 (3%)	38	60
All	All	3720/3872 (96%)	3570 (96%)	150 (4%)	28	47

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	VAL
1	A	21	THR
1	A	40	LEU
1	A	59	SER
1	A	123	LEU
1	A	147	THR
1	A	154	THR
1	A	191	LEU
1	A	209	ASP
1	A	211	VAL
1	A	246	ARG
1	A	266	GLU
1	A	279	VAL

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Mol	Chain	Res	Type
1	A	293	SER
1	A	327	THR
1	A	370	THR
1	A	401	VAL
1	A	408	ASN
1	A	477	THR
1	B	19	VAL
1	B	179	ASP
1	B	233	LYS
1	B	279	VAL
1	B	298	ILE
1	B	322	THR
1	B	345	LYS
1	B	357	LEU
1	B	368	LEU
1	B	370	THR
1	B	381	LEU
1	B	482	ILE
1	B	509	LEU
1	B	523	SER
1	C	11	SER
1	C	43	LEU
1	C	125	ASP
1	C	127	SER
1	C	146	ASP
1	C	156	VAL
1	C	179	ASP
1	C	214	LEU
1	C	232	LEU
1	C	246	ARG
1	C	283	LEU
1	C	348	VAL
1	C	372	LEU
1	C	375	LEU
1	C	380	VAL
1	C	381	LEU
1	C	401	VAL
1	C	403	THR
1	C	443	GLN
1	C	444	LEU
1	C	452	LYS
1	C	458	LEU

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Mol	Chain	Res	Type
1	C	498	SER
1	C	531	VAL
1	D	21	THR
1	D	40	LEU
1	D	43	LEU
1	D	45	ASN
1	D	64	ASP
1	D	133	ASP
1	D	138	SER
1	D	160	THR
1	D	180	LEU
1	D	216	GLU
1	D	279	VAL
1	D	283	LEU
1	D	293	SER
1	D	294	SER
1	D	372	LEU
1	D	421	SER
1	D	432	VAL
1	D	458	LEU
1	D	551	LEU
1	E	123	LEU
1	E	147	THR
1	E	160	THR
1	E	164	GLN
1	E	191	LEU
1	E	199	LEU
1	E	209	ASP
1	E	211	VAL
1	E	220	THR
1	E	246	ARG
1	E	283	LEU
1	E	326	VAL
1	E	348	VAL
1	E	357	LEU
1	E	370	THR
1	E	373	LEU
1	E	375	LEU
1	E	403	THR
1	E	444	LEU
1	E	477	THR
1	E	521	THR

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Mol	Chain	Res	Type
1	E	522	LEU
1	E	523	SER
1	E	553	SER
1	F	21	THR
1	F	32	ASP
1	F	43	LEU
1	F	46	LEU
1	F	59	SER
1	F	107	THR
1	F	123	LEU
1	F	180	LEU
1	F	224	ASN
1	F	232	LEU
1	F	283	LEU
1	F	293	SER
1	F	307	SER
1	F	321	LEU
1	F	346	ILE
1	F	421	SER
1	F	444	LEU
1	F	476	GLU
1	F	509	LEU
1	F	526	SER
1	G	43	LEU
1	G	64	ASP
1	G	146	ASP
1	G	147	THR
1	G	154	THR
1	G	179	ASP
1	G	180	LEU
1	G	188	VAL
1	G	189	GLU
1	G	203	LEU
1	G	216	GLU
1	G	368	LEU
1	G	370	THR
1	G	403	THR
1	G	417	THR
1	G	421	SER
1	G	490	ASP
1	H	59	SER
1	H	67	ASP

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Mol	Chain	Res	Type
1	H	78	LEU
1	H	183	ASP
1	H	216	GLU
1	H	232	LEU
1	H	236	ARG
1	H	251	GLU
1	H	258	GLU
1	H	294	SER
1	H	403	THR
1	H	460	LEU
1	H	545	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	45	ASN
1	A	106	HIS
1	A	115	GLN
1	A	272	HIS
1	A	318	HIS
1	A	347	ASN
1	A	406	GLN
1	A	443	GLN
1	A	445	GLN
1	A	488	GLN
1	A	503	ASN
1	B	106	HIS
1	B	115	GLN
1	B	132	HIS
1	B	158	ASN
1	B	171	HIS
1	B	192	HIS
1	B	272	HIS
1	B	406	GLN
1	B	439	ASN
1	B	443	GLN
1	C	23	GLN
1	C	45	ASN
1	C	106	HIS
1	C	115	GLN
1	C	132	HIS

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Mol	Chain	Res	Type
1	C	171	HIS
1	C	272	HIS
1	C	318	HIS
1	C	360	ASN
1	C	406	GLN
1	C	443	GLN
1	D	115	GLN
1	D	224	ASN
1	D	406	GLN
1	D	429	GLN
1	D	441	GLN
1	D	443	GLN
1	D	445	GLN
1	D	464	HIS
1	E	23	GLN
1	E	106	HIS
1	E	132	HIS
1	E	158	ASN
1	E	164	GLN
1	E	171	HIS
1	E	192	HIS
1	E	224	ASN
1	E	272	HIS
1	E	318	HIS
1	E	347	ASN
1	E	406	GLN
1	E	443	GLN
1	E	464	HIS
1	F	115	GLN
1	F	132	HIS
1	F	158	ASN
1	F	164	GLN
1	F	181	ASN
1	F	229	HIS
1	F	272	HIS
1	F	347	ASN
1	F	399	ASN
1	F	406	GLN
1	F	443	GLN
1	F	445	GLN
1	F	464	HIS
1	F	488	GLN

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Mol	Chain	Res	Type
1	F	536	GLN
1	G	23	GLN
1	G	132	HIS
1	G	171	HIS
1	G	229	HIS
1	G	406	GLN
1	G	443	GLN
1	G	445	GLN
1	G	457	GLN
1	G	503	ASN
1	G	536	GLN
1	H	105	ASN
1	H	106	HIS
1	H	111	HIS
1	H	272	HIS
1	H	399	ASN
1	H	406	GLN
1	H	419	GLN
1	H	441	GLN
1	H	443	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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.

All (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

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Mol	Chain	Res	Type	Atoms
4	G	603	TRS	C3-C-C1-O1
4	G	603	TRS	N-C-C1-O1
4	E	603	TRS	C2-C-C3-O3
4	H	603	TRS	C2-C-C1-O1
4	E	603	TRS	C1-C-C3-O3
4	F	603	TRS	N-C-C3-O3
4	G	603	TRS	C2-C-C1-O1
4	G	603	TRS	C1-C-C3-O3
4	H	603	TRS	C3-C-C1-O1
4	G	603	TRS	C2-C-C3-O3
4	E	603	TRS	C3-C-C2-O2
4	E	603	TRS	N-C-C2-O2
4	E	603	TRS	N-C-C3-O3
4	G	603	TRS	N-C-C3-O3
4	H	603	TRS	N-C-C1-O1
4	H	603	TRS	C3-C-C2-O2
4	A	602	TRS	C3-C-C2-O2
4	C	603	TRS	C3-C-C2-O2
4	D	603	TRS	C2-C-C1-O1
4	F	603	TRS	C3-C-C1-O1
4	F	603	TRS	C3-C-C2-O2
4	G	603	TRS	C1-C-C2-O2
4	A	602	TRS	N-C-C2-O2
4	C	603	TRS	N-C-C2-O2
4	F	603	TRS	N-C-C1-O1
4	F	603	TRS	N-C-C2-O2

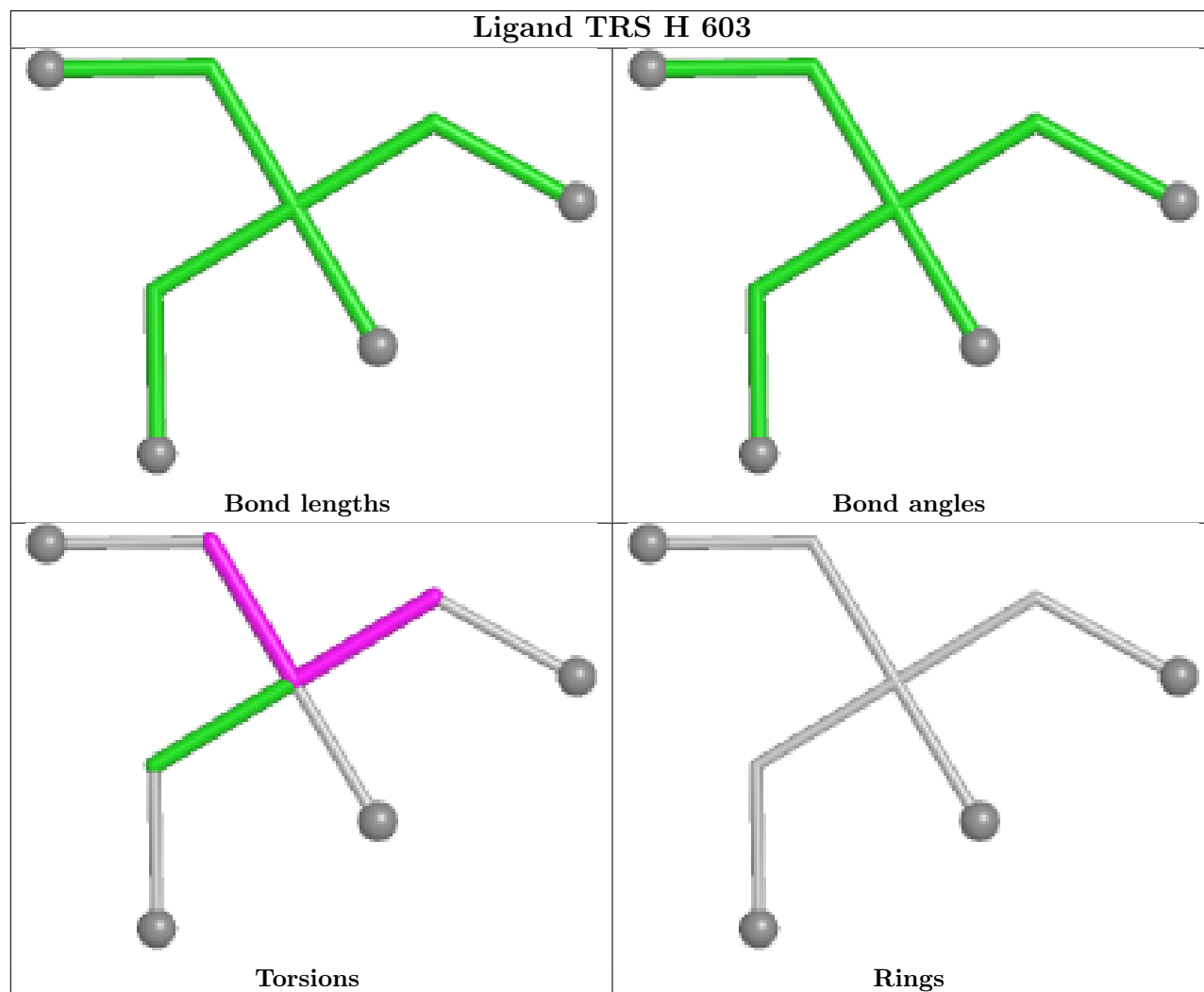
There are no ring outliers.

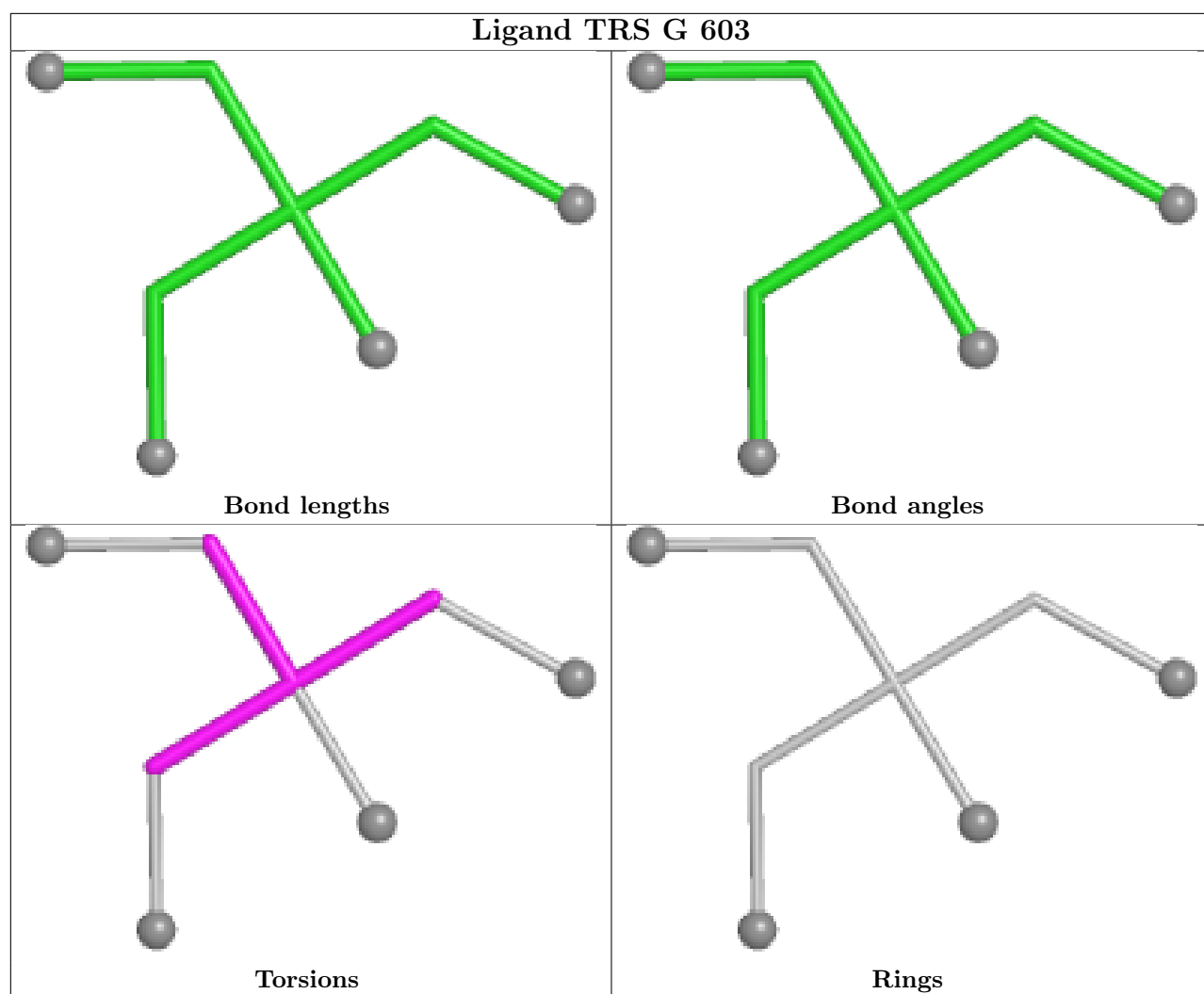
5 monomers are involved in 6 short contacts:

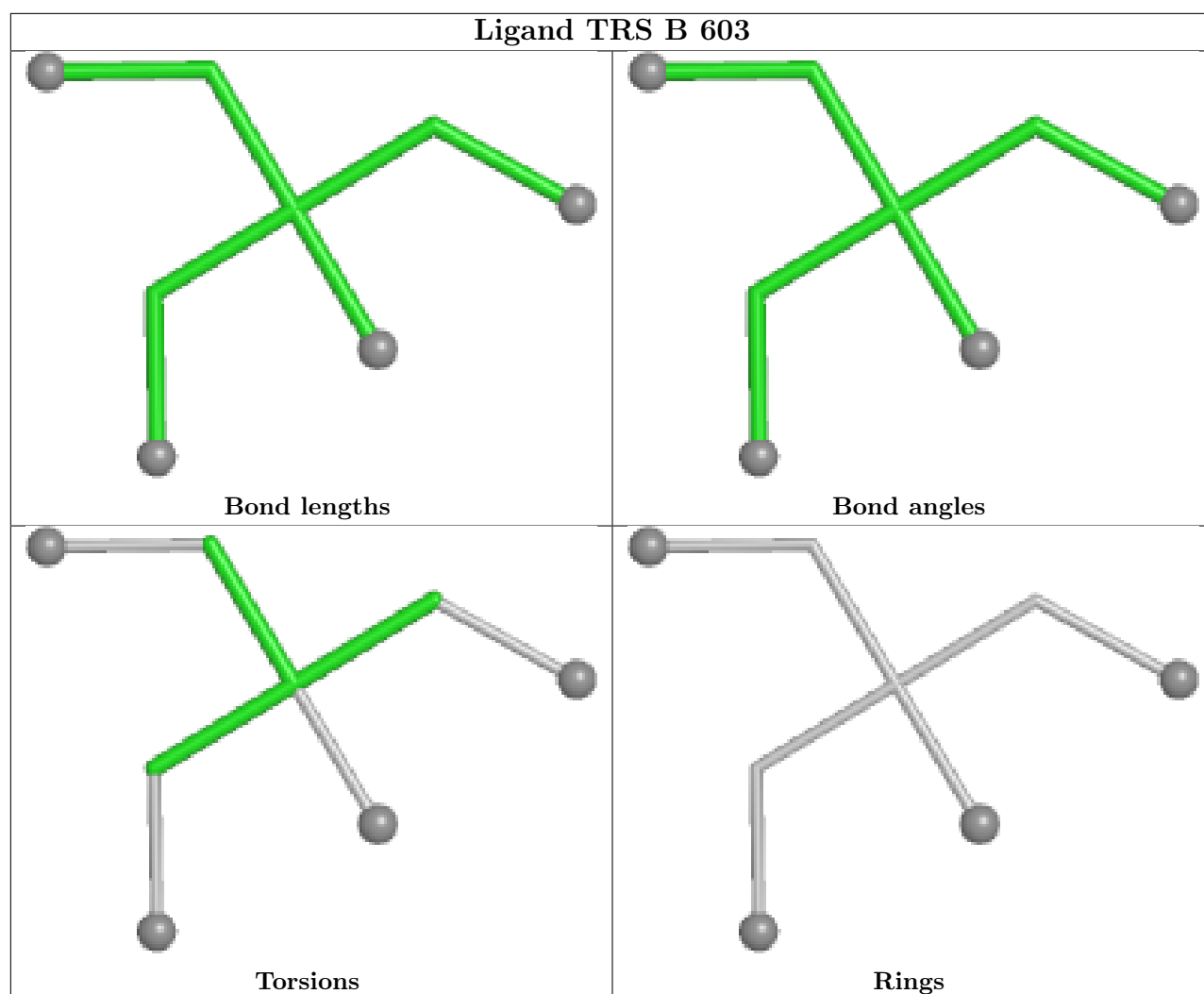
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	603	TRS	1	0
4	B	603	TRS	1	0
4	F	603	TRS	2	0
4	C	603	TRS	1	0
4	E	603	TRS	1	0

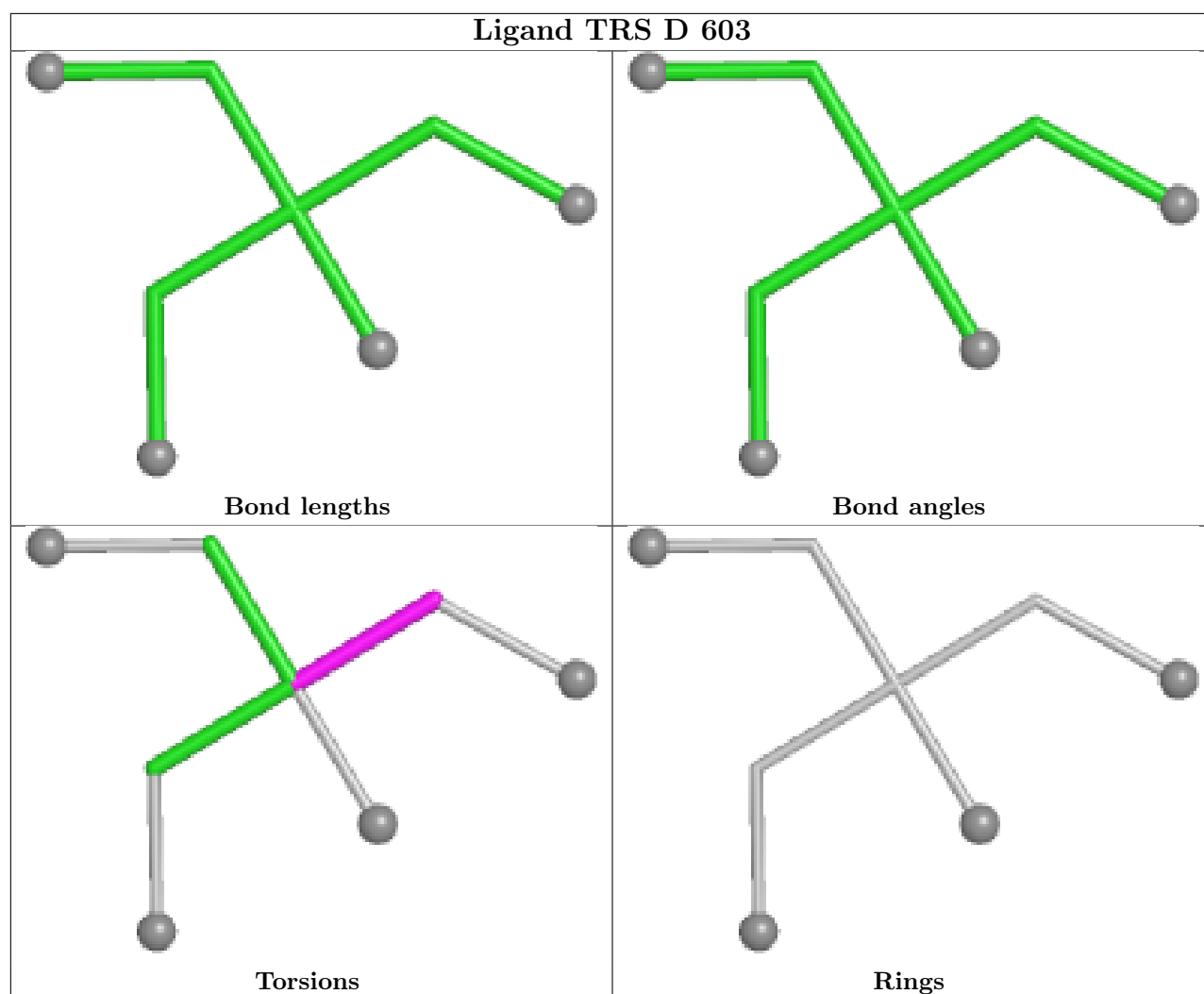
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

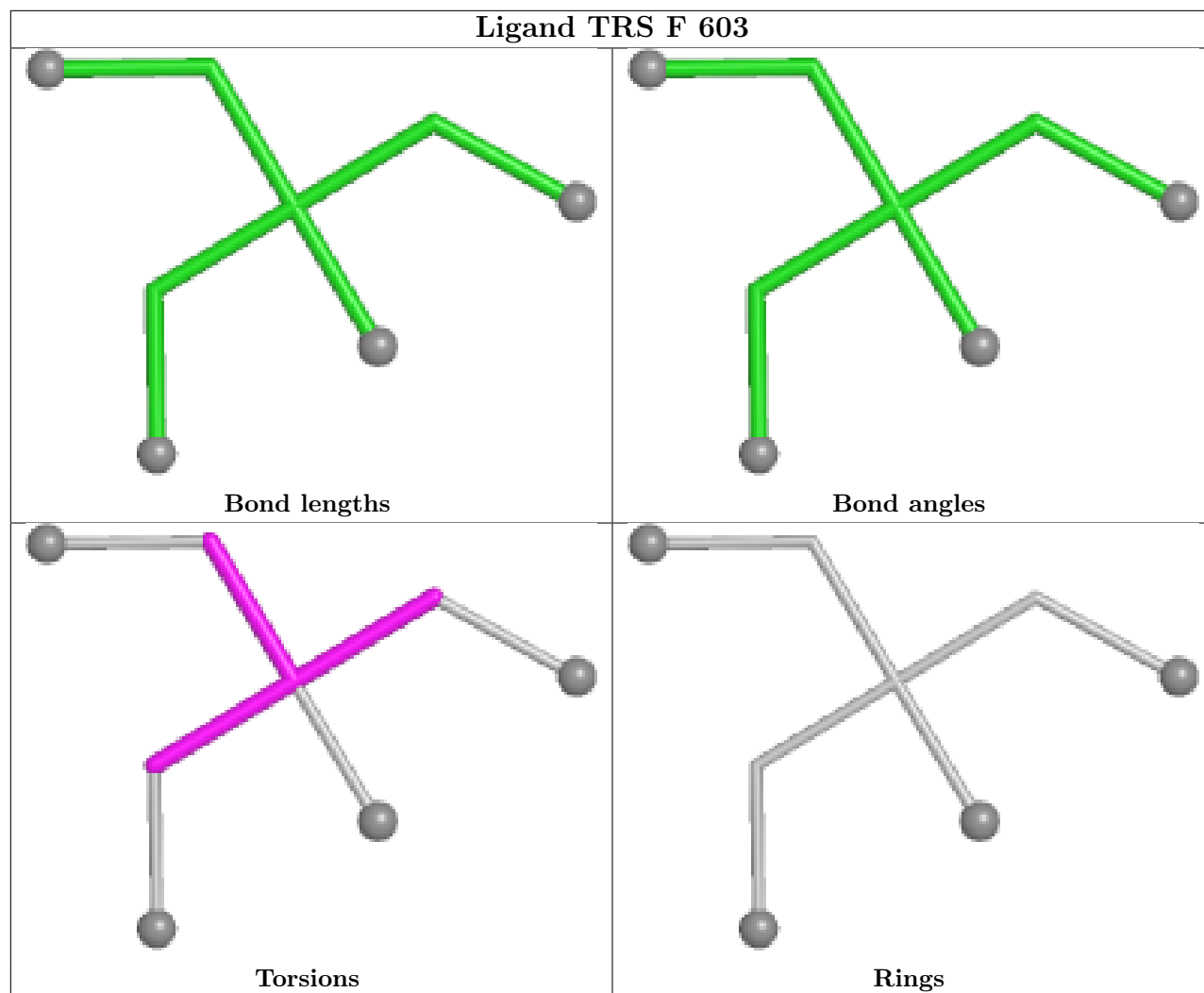
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

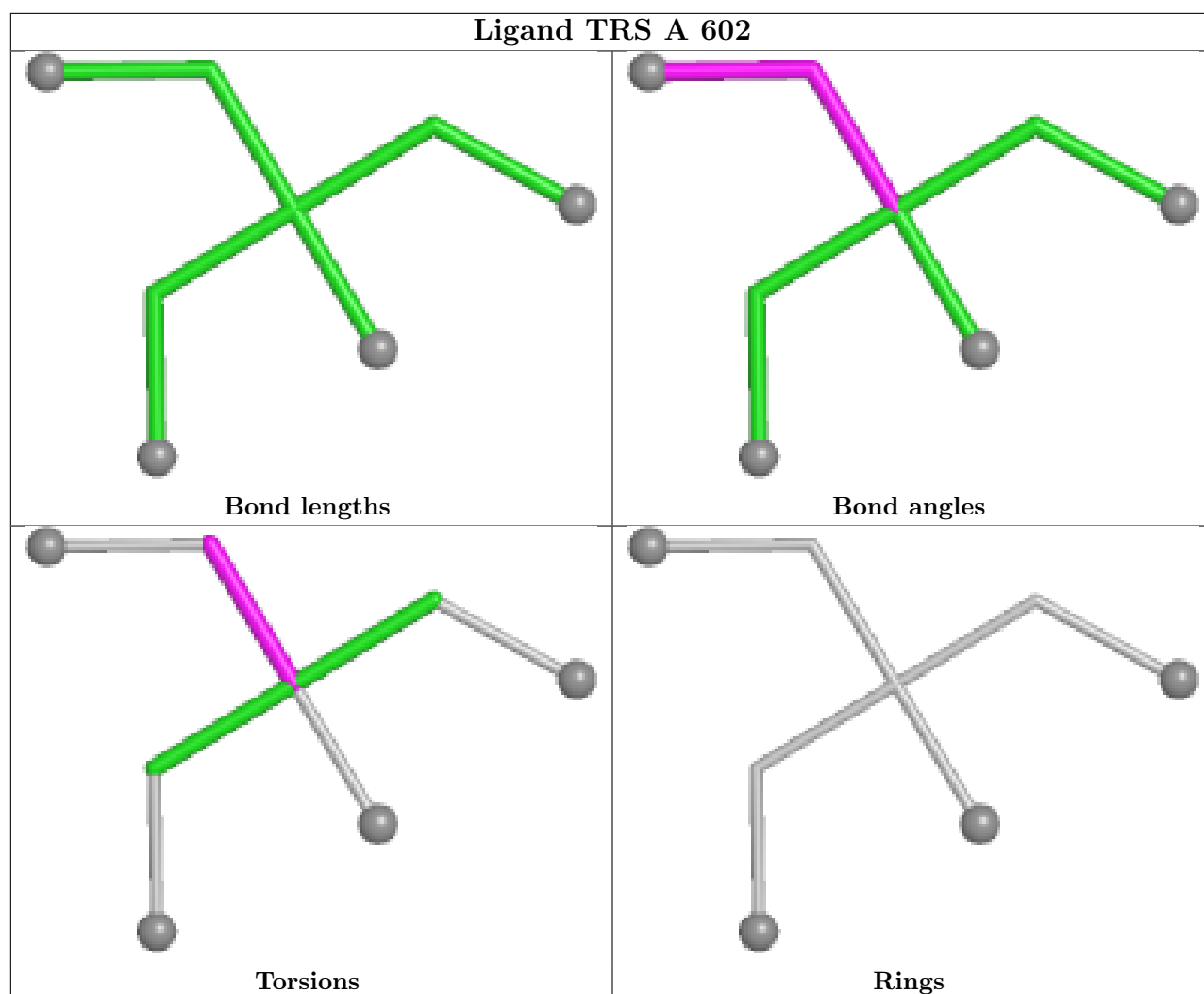


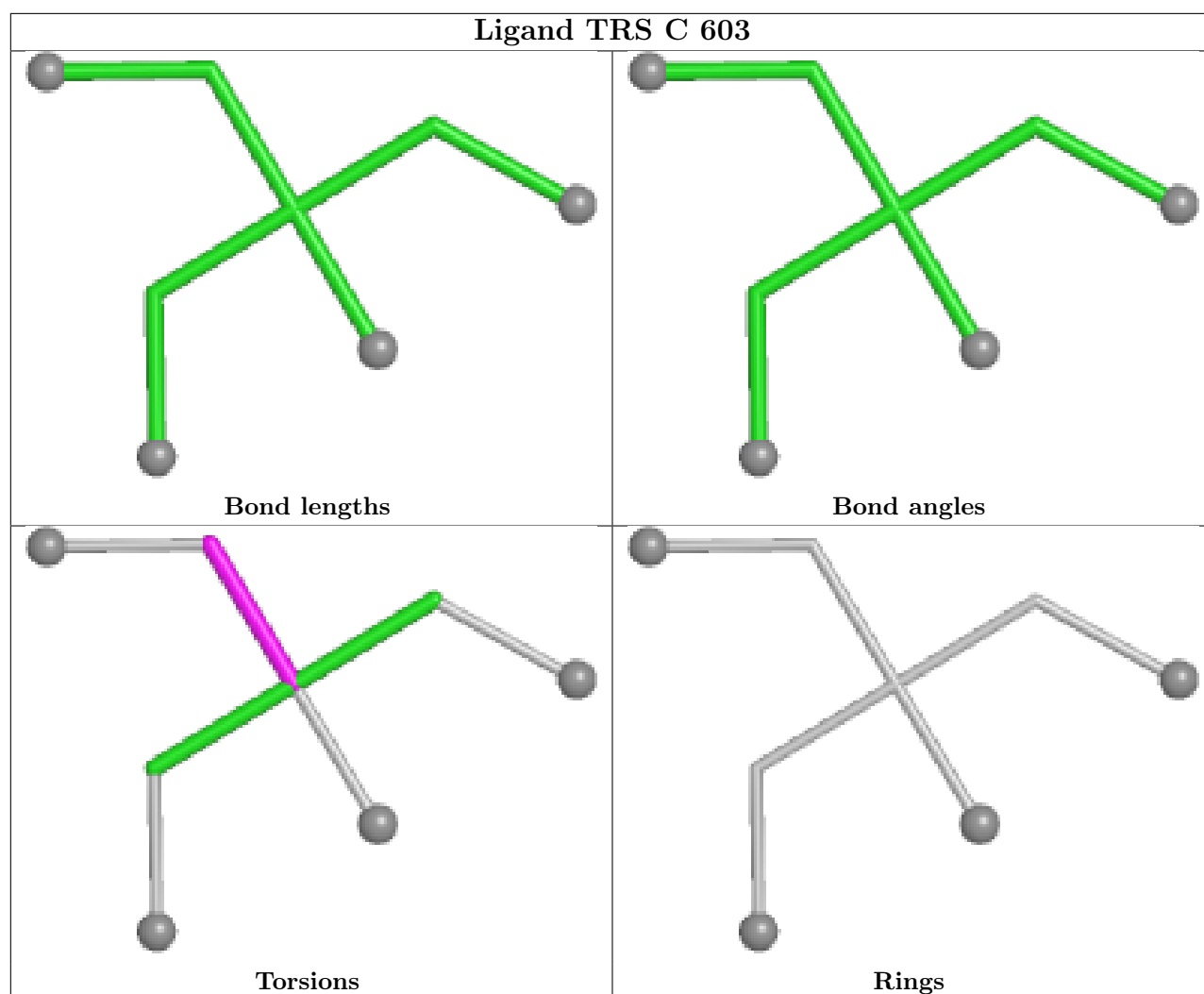


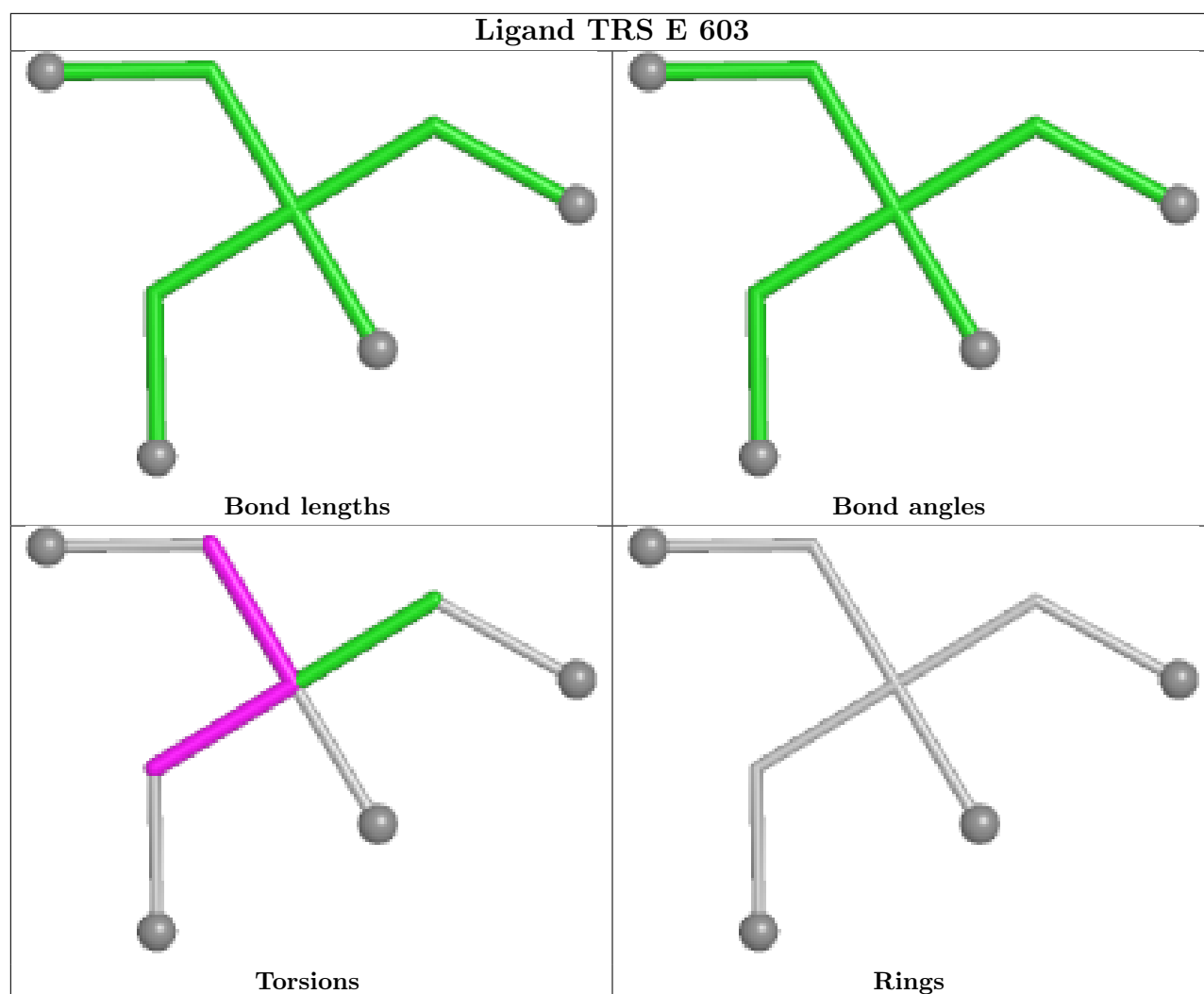












5.7 Other polymers [i](#)

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%)

All (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
1	E	255	TRP	2.2
1	H	141	GLY	2.1
1	H	255	TRP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

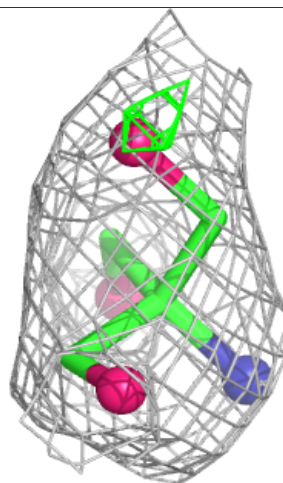
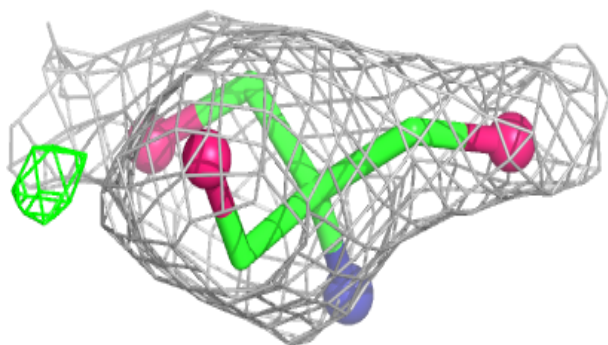
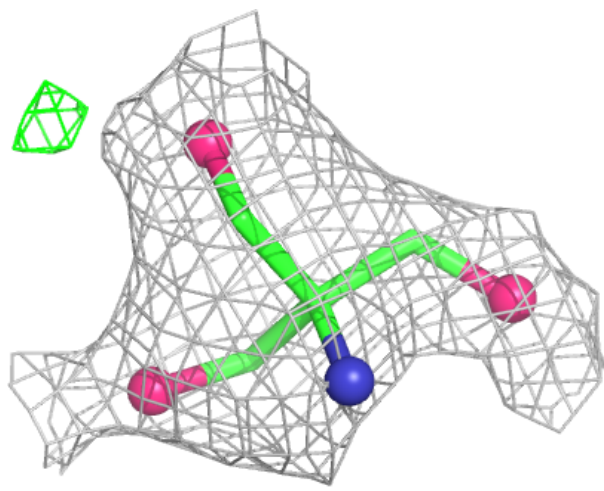
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(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.

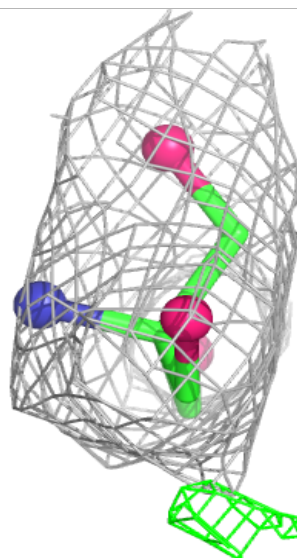
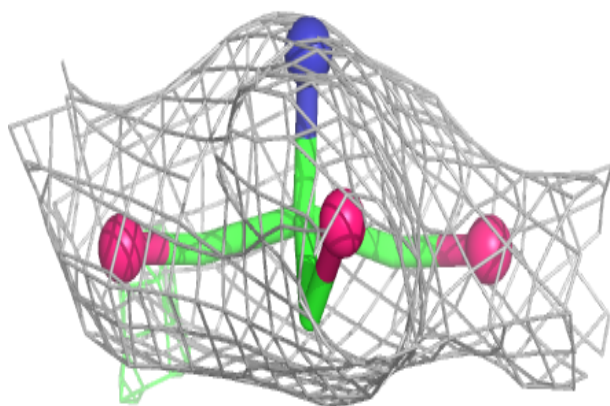
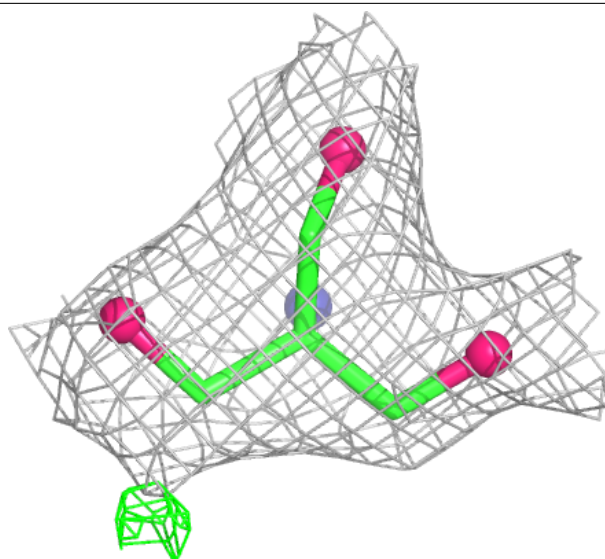
Electron density around TRS H 603:

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



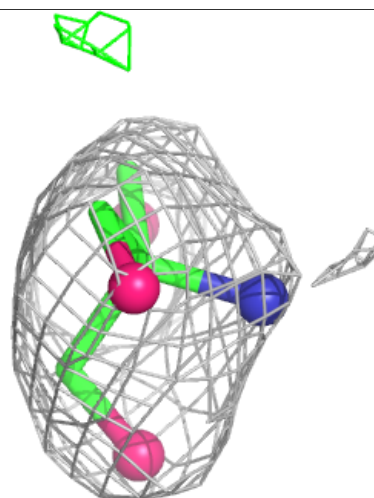
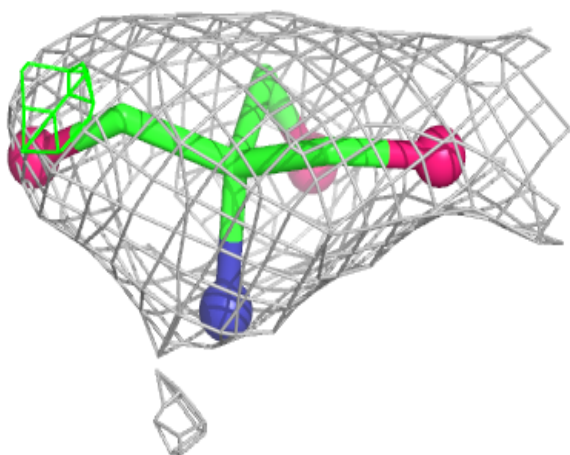
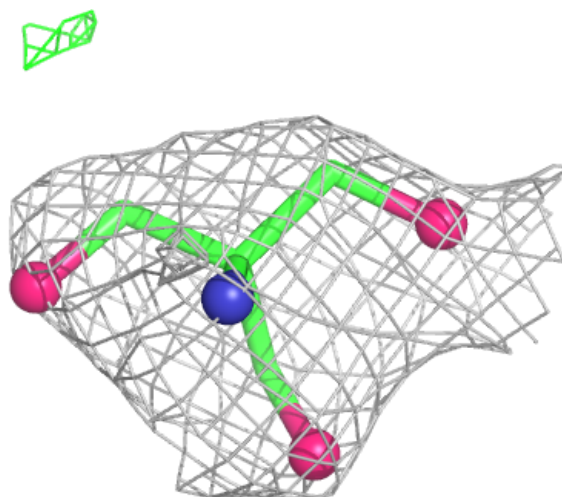
Electron density around TRS F 603:

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



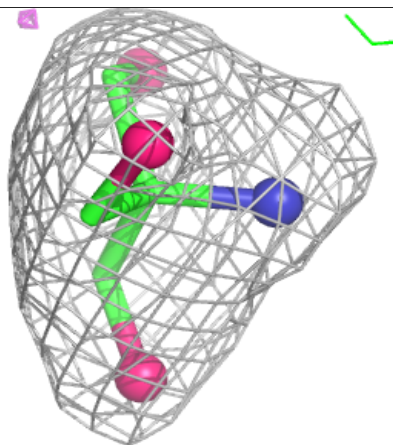
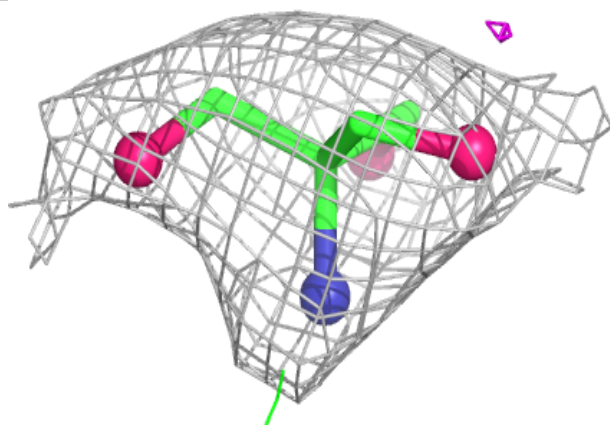
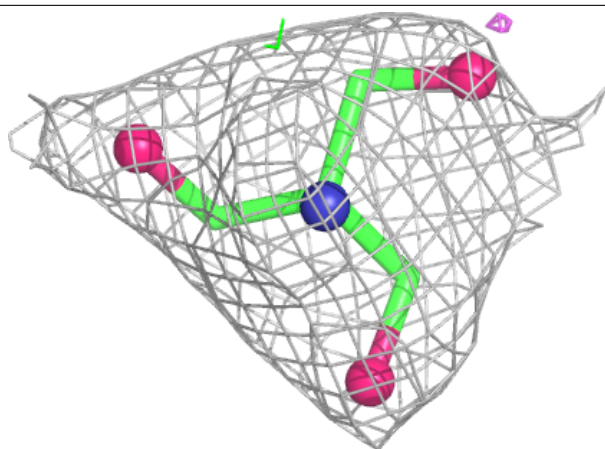
Electron density around TRS E 603:

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



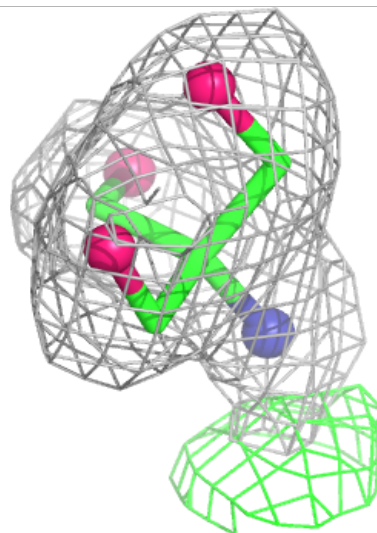
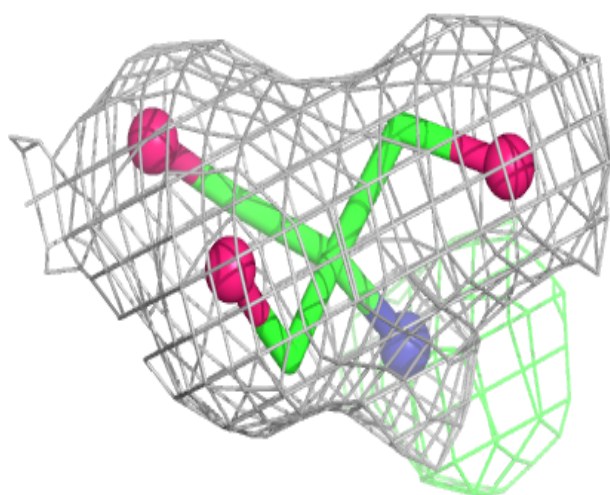
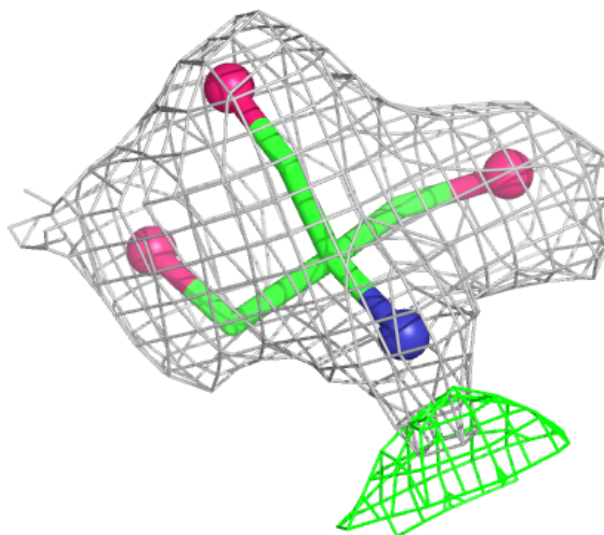
Electron density around TRS A 602:

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



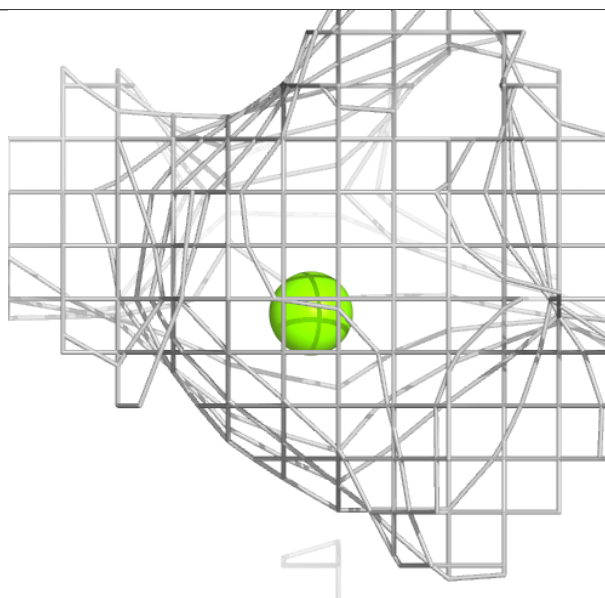
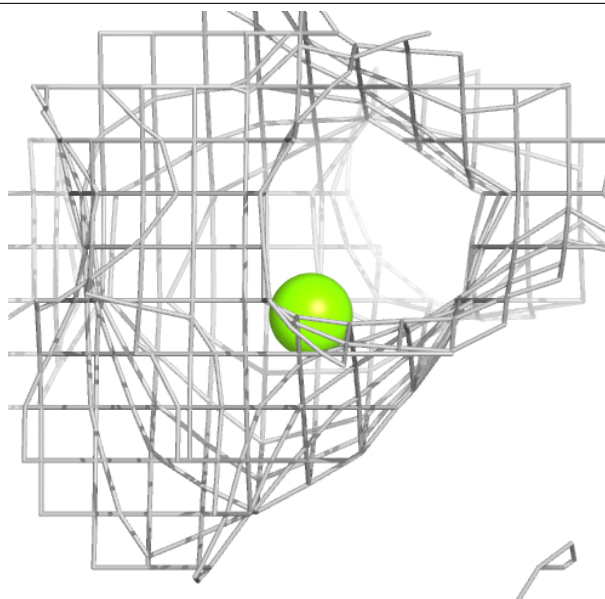
Electron density around TRS D 603:

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and green (positive)



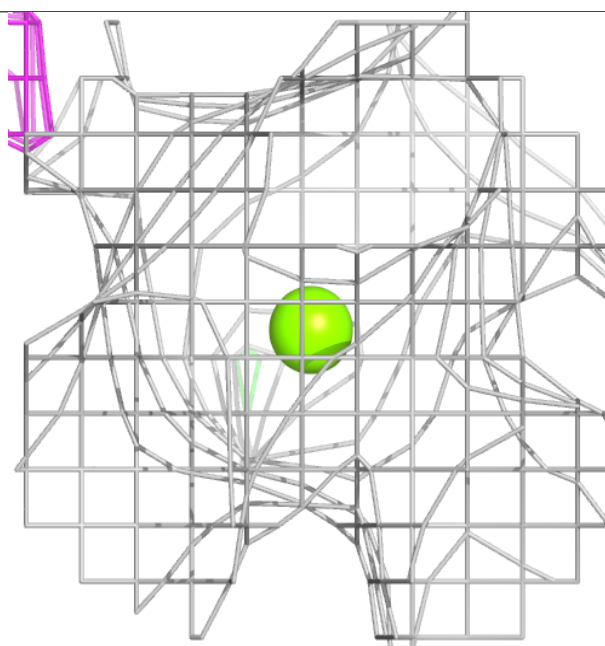
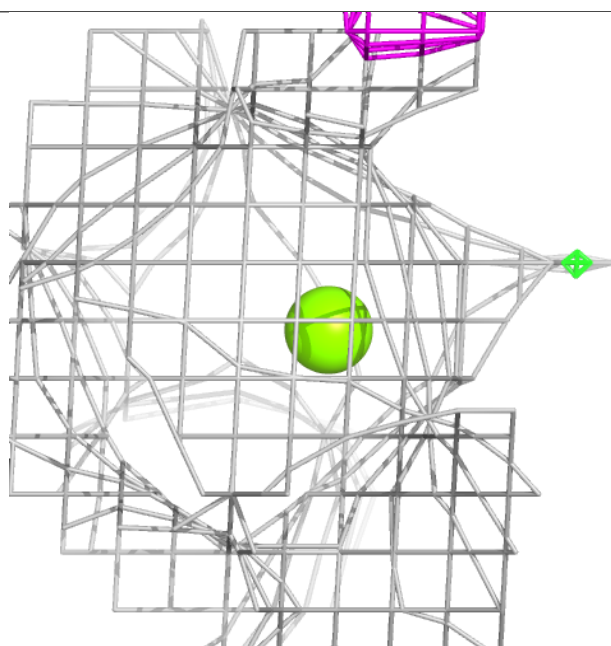
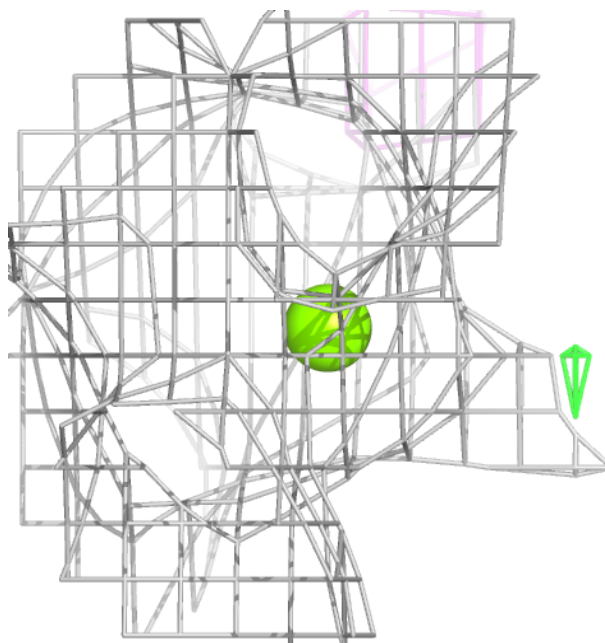
Electron density around MG H 602:

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and green (positive)



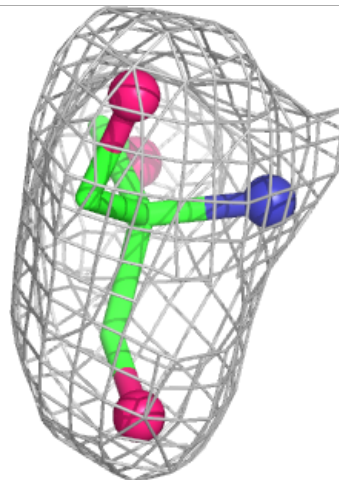
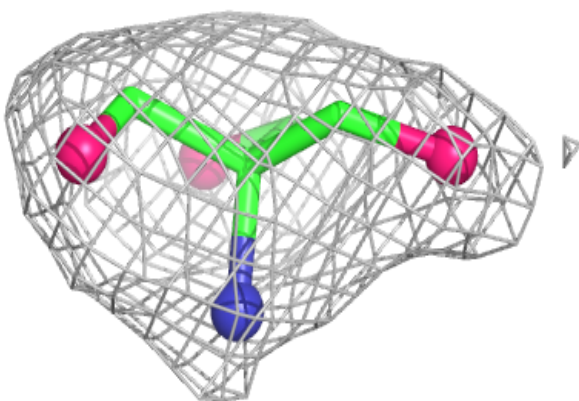
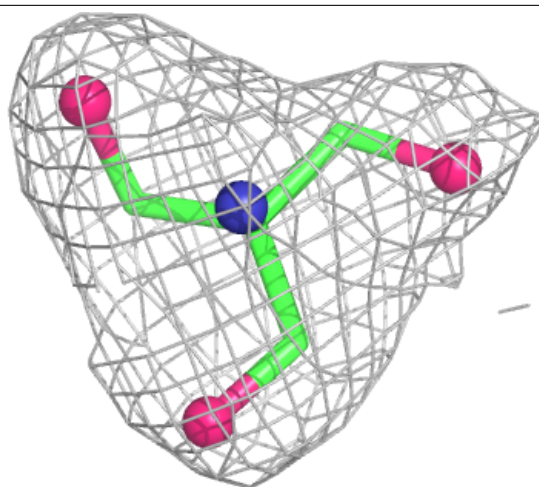
Electron density around MG E 602:

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



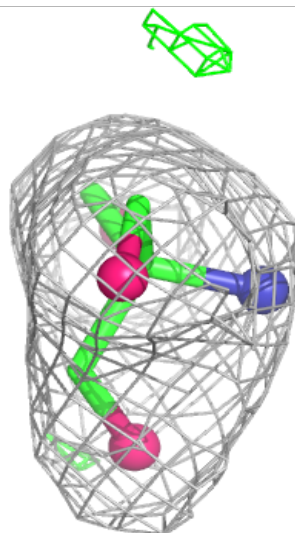
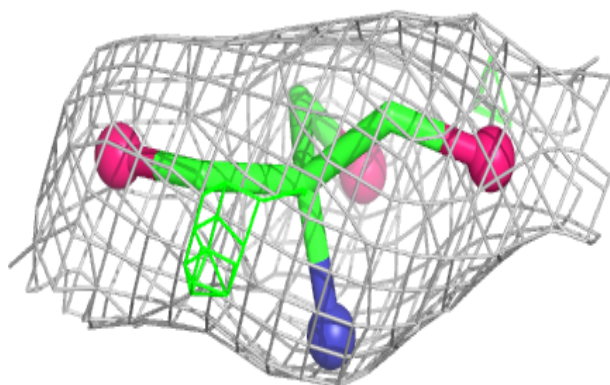
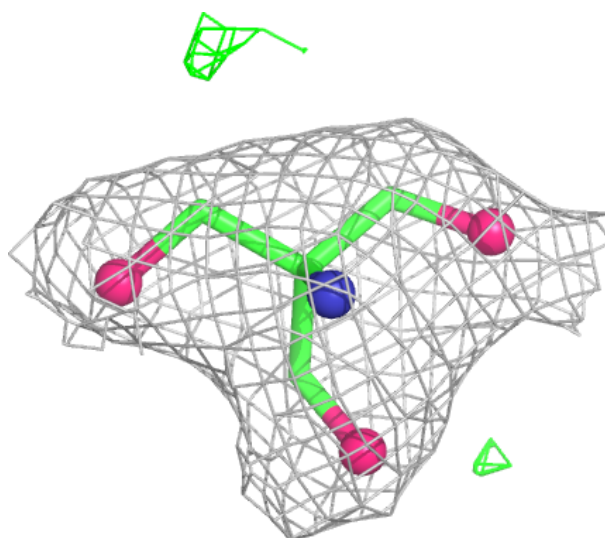
Electron density around TRS C 603:

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



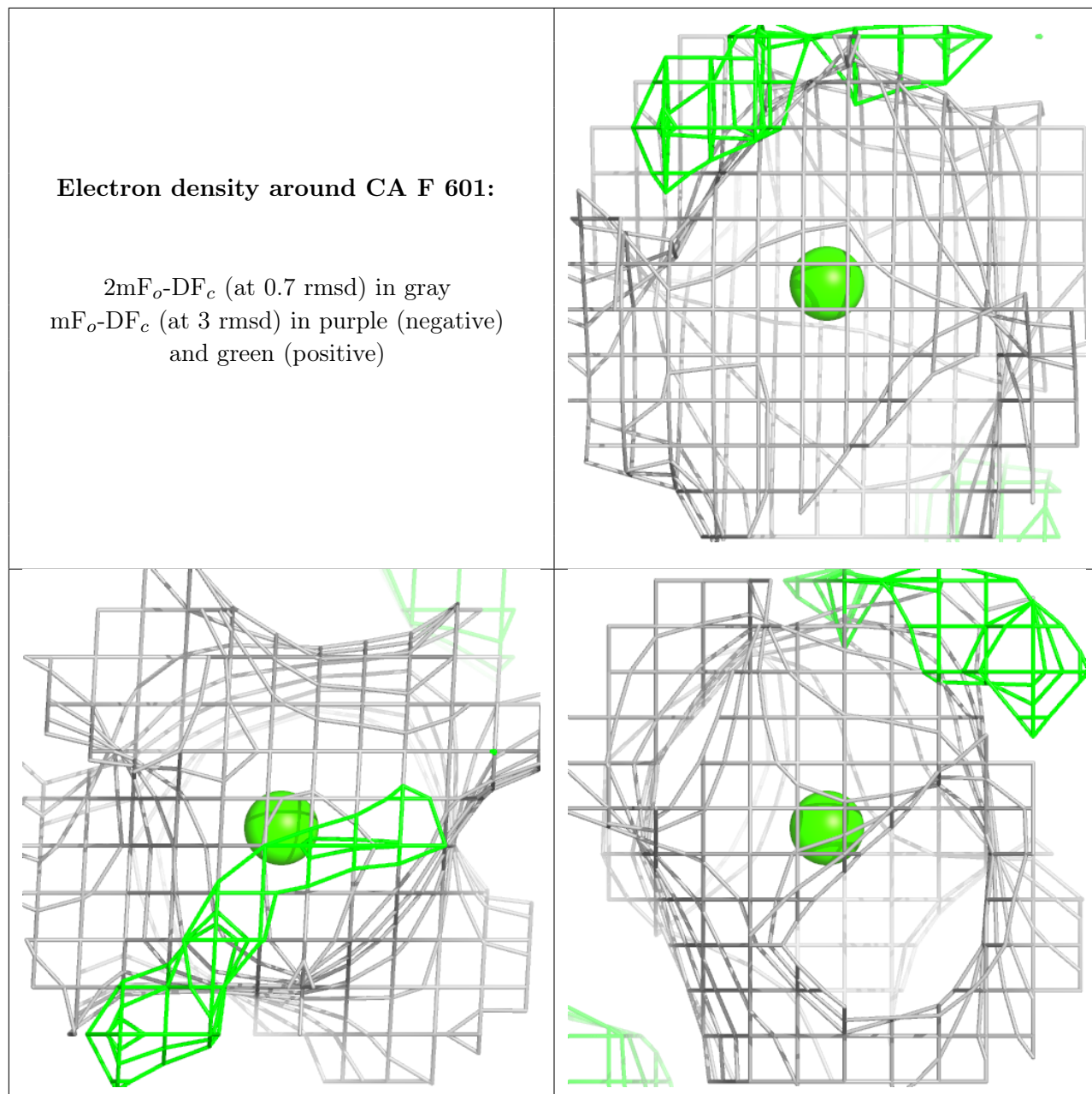
Electron density around TRS G 603:

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and green (positive)



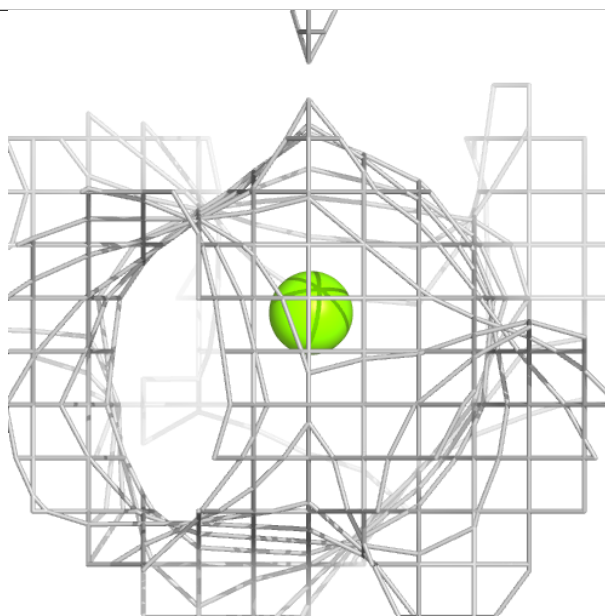
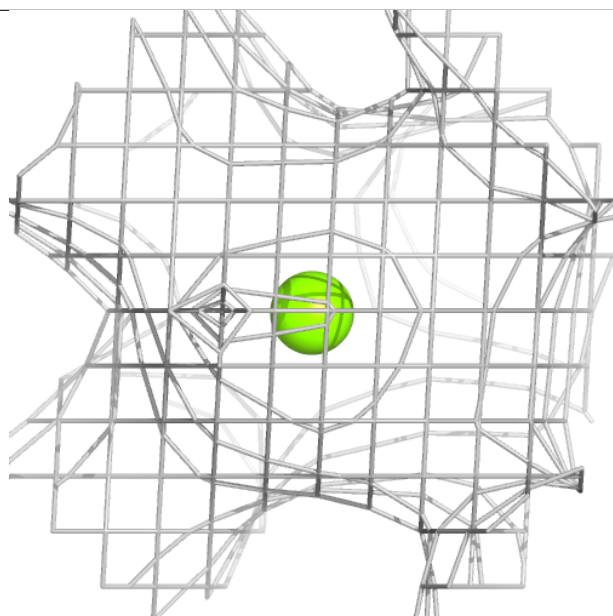
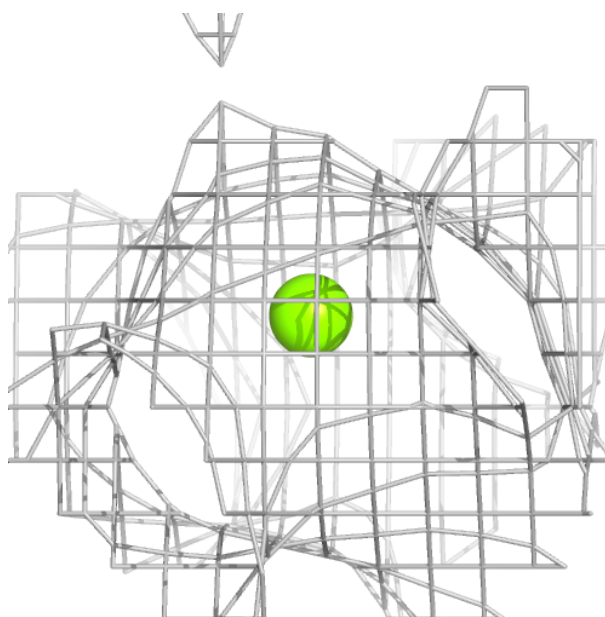
Electron density around CA F 601:

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



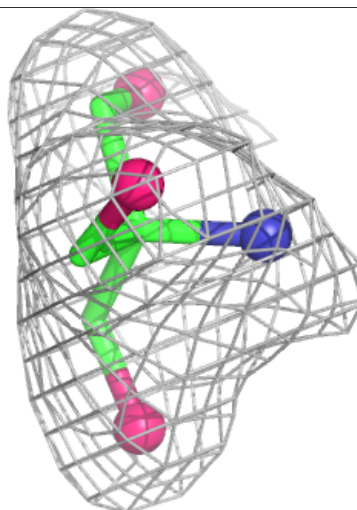
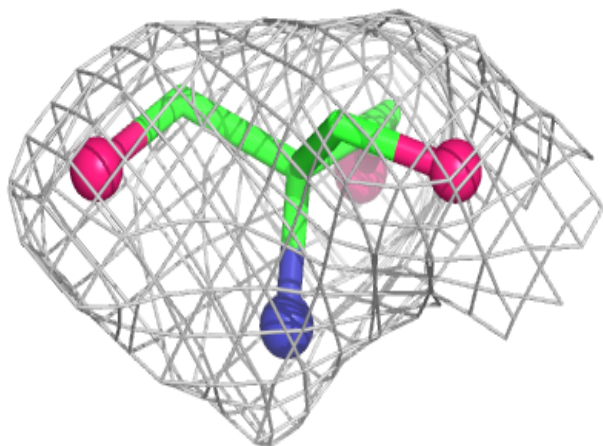
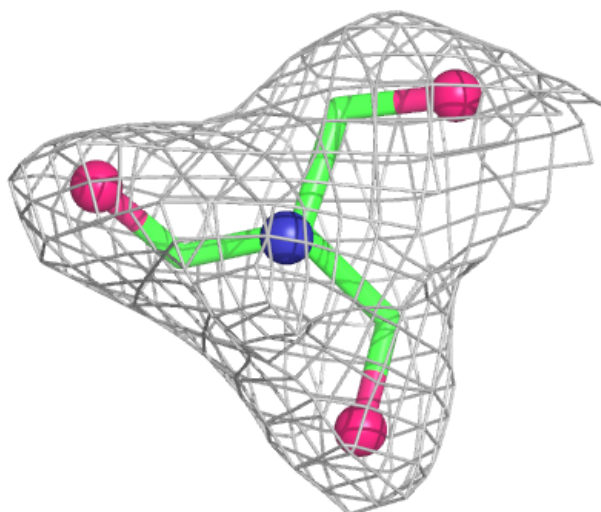
Electron density around MG C 602:

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



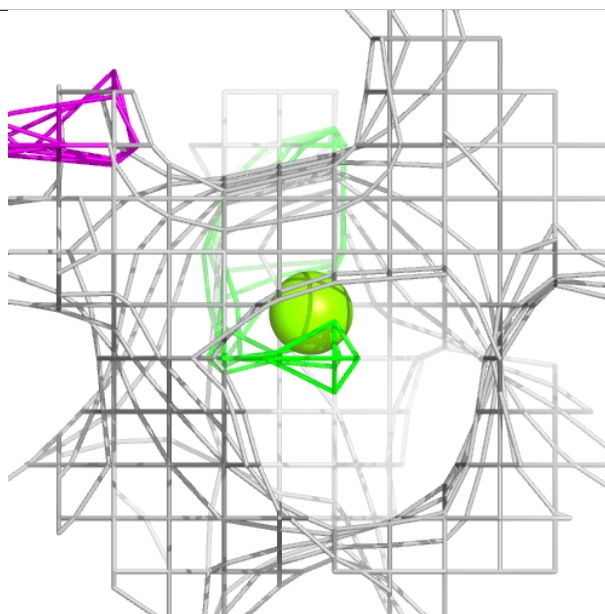
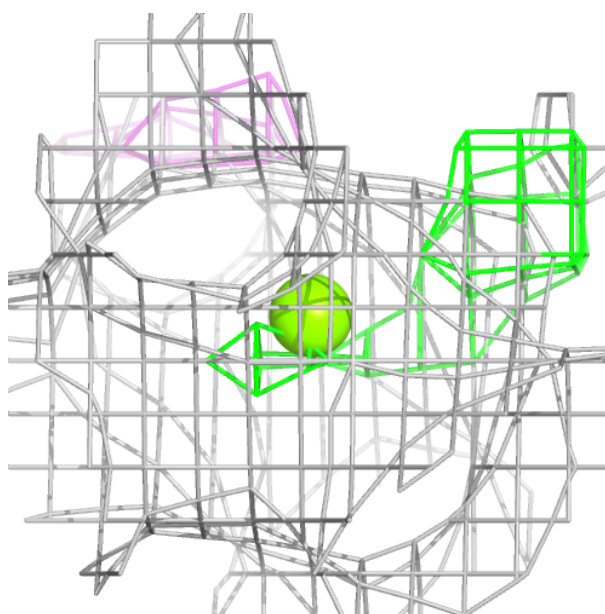
Electron density around TRS B 603:

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and green (positive)



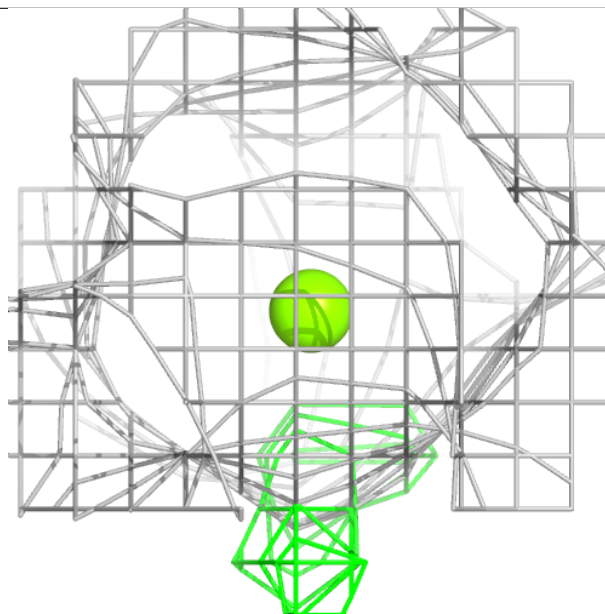
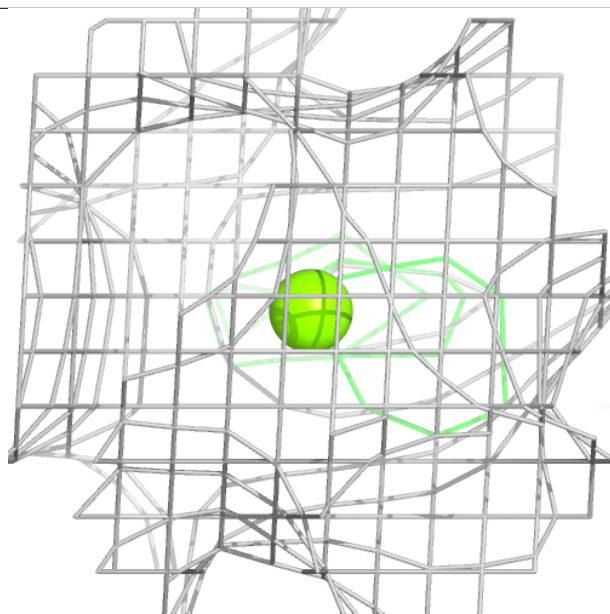
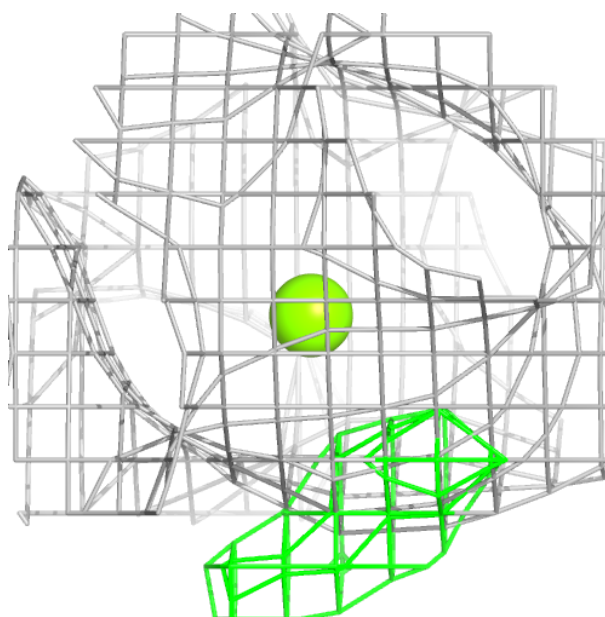
Electron density around MG A 601:

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and green (positive)



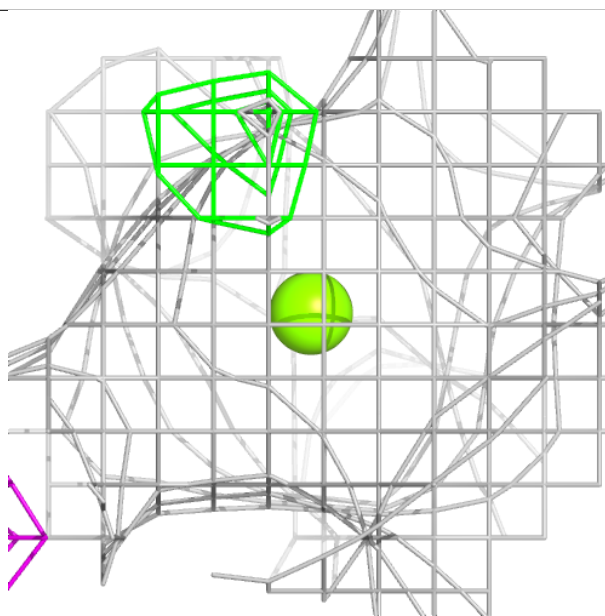
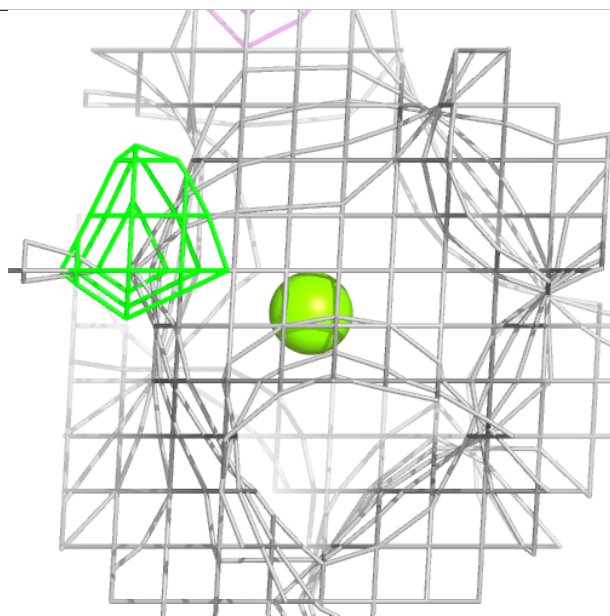
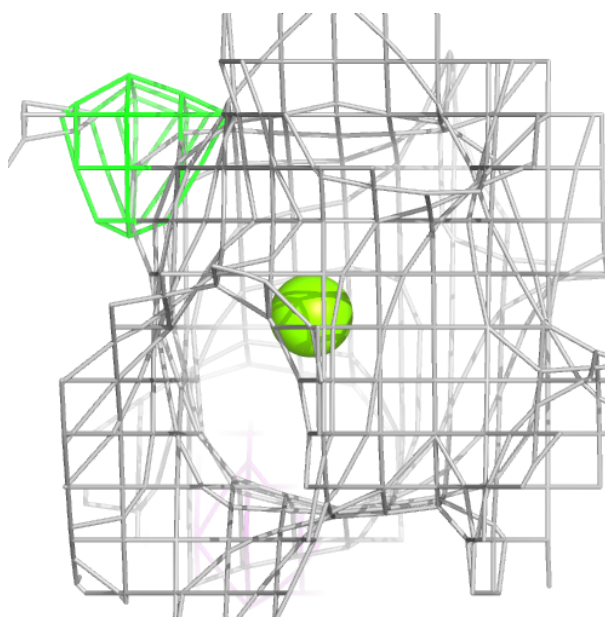
Electron density around MG B 602:

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and green (positive)



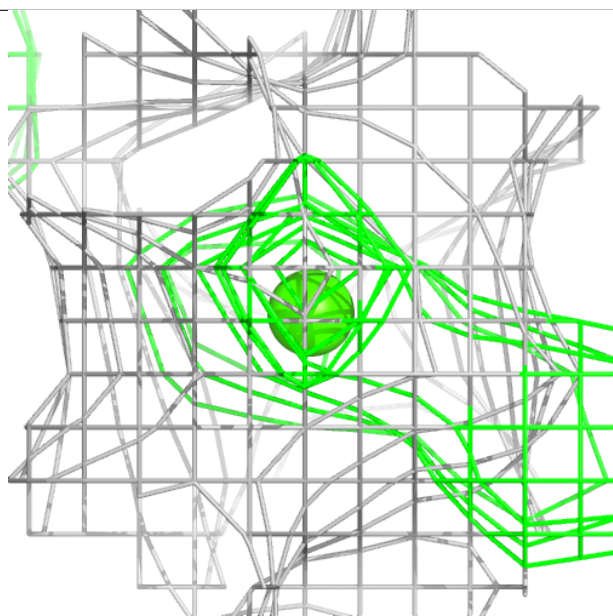
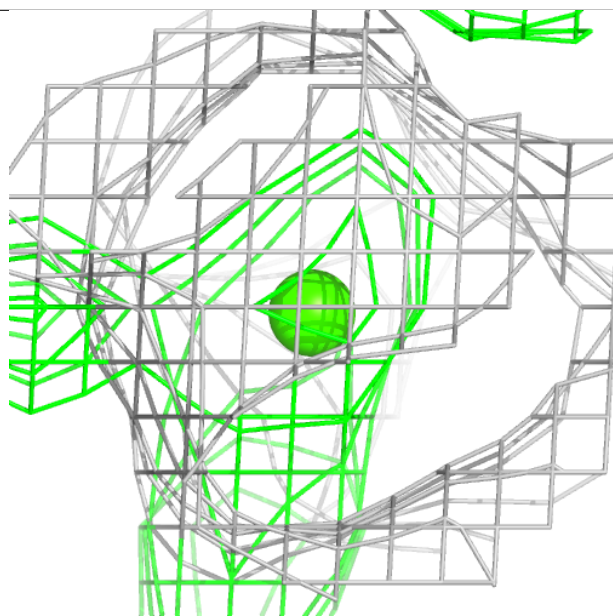
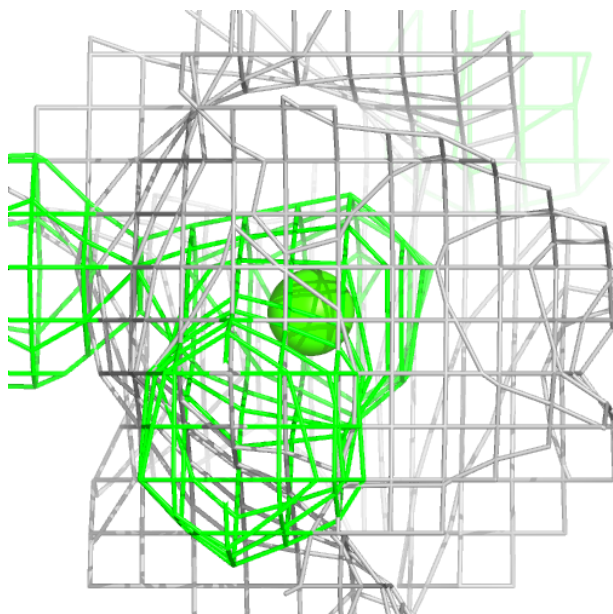
Electron density around MG F 602:

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and green (positive)



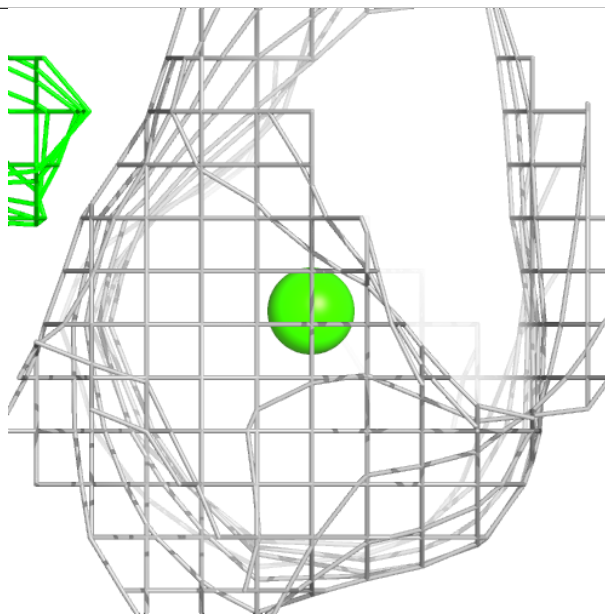
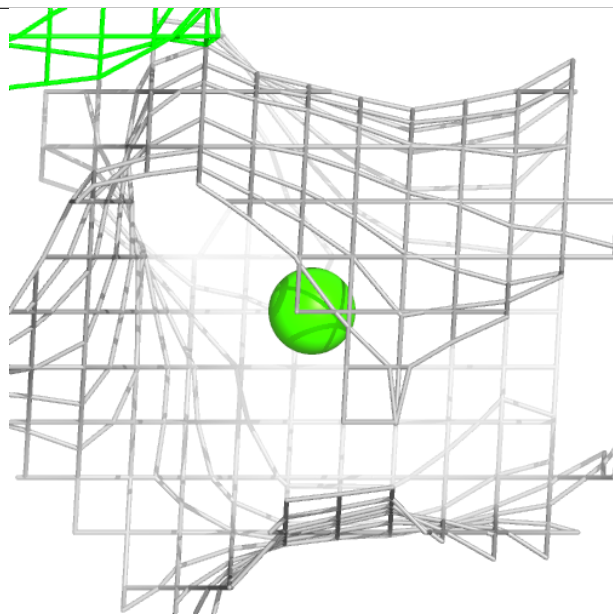
Electron density around CA A 600:

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and green (positive)



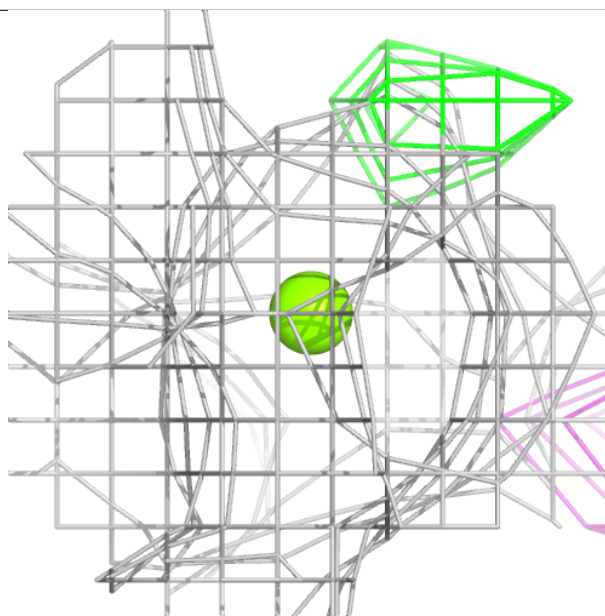
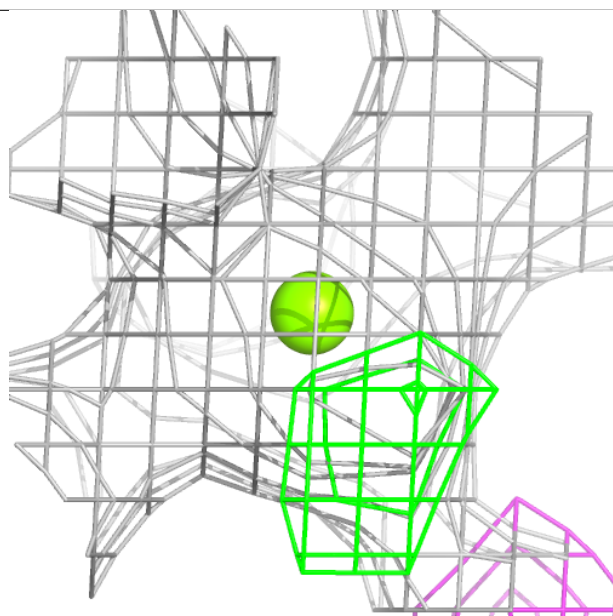
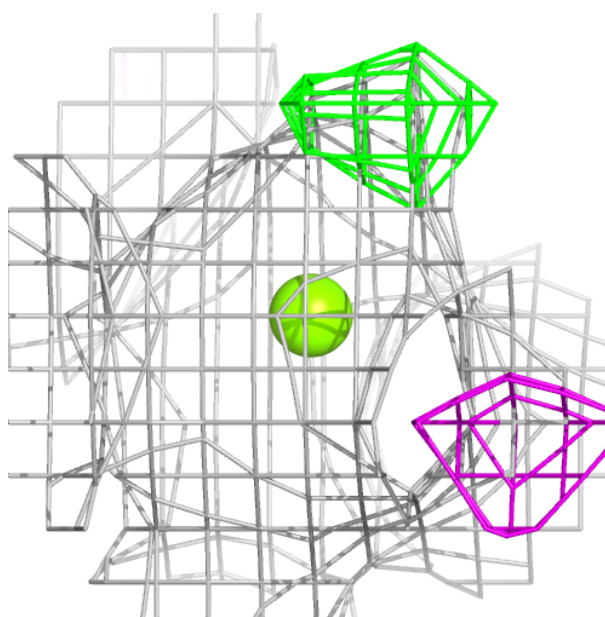
Electron density around CA H 601:

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and green (positive)



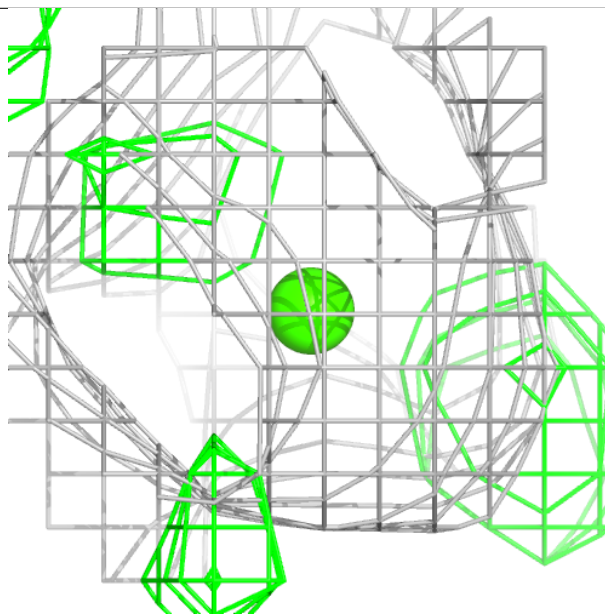
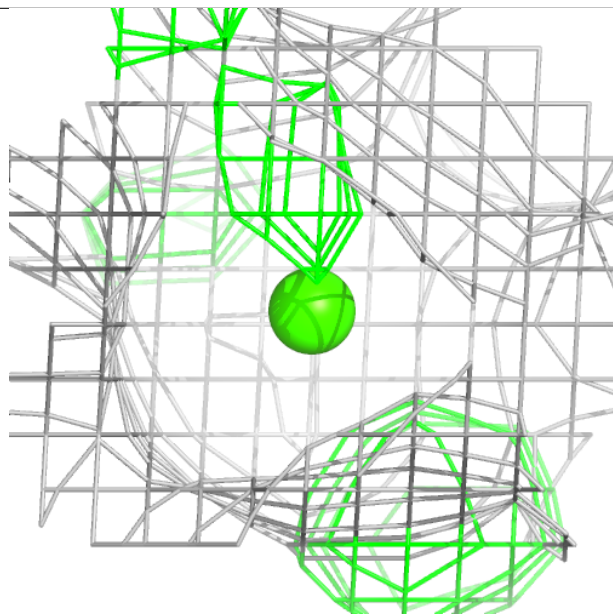
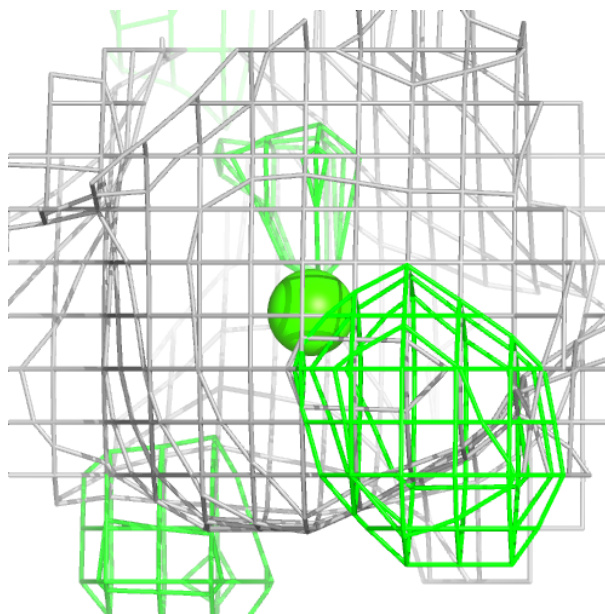
Electron density around MG D 602:

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



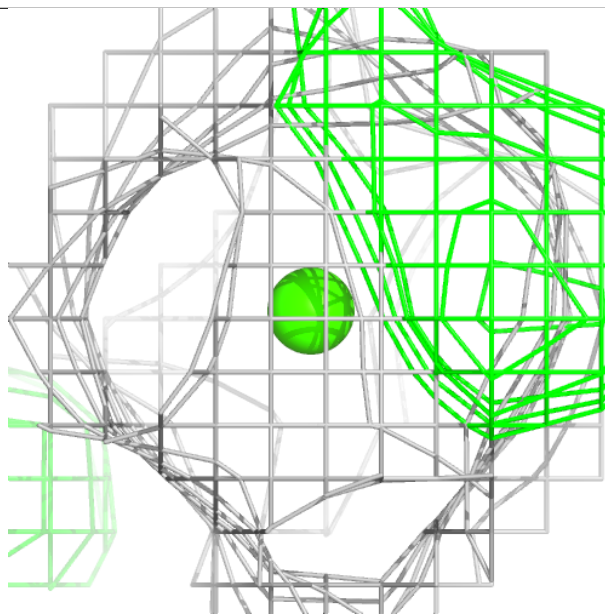
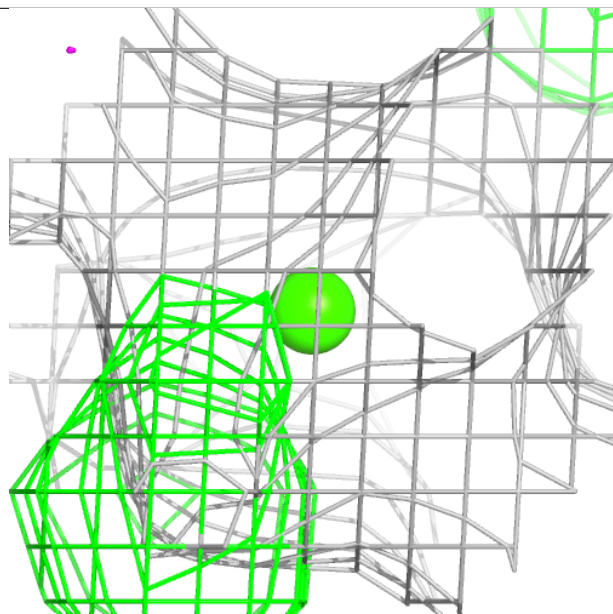
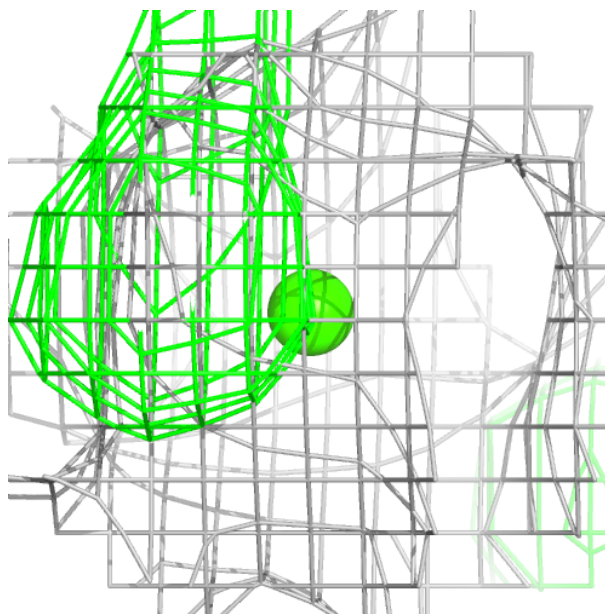
Electron density around CA E 601:

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



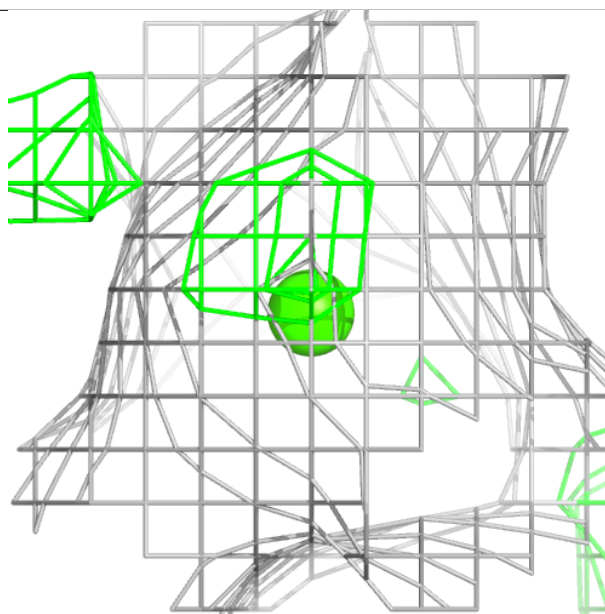
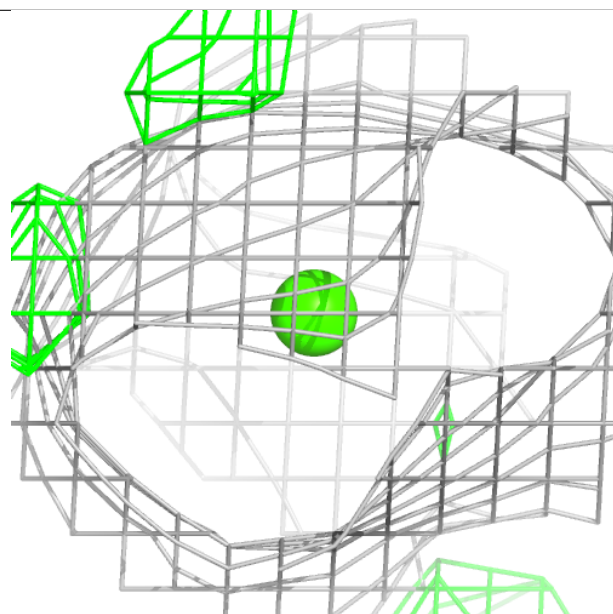
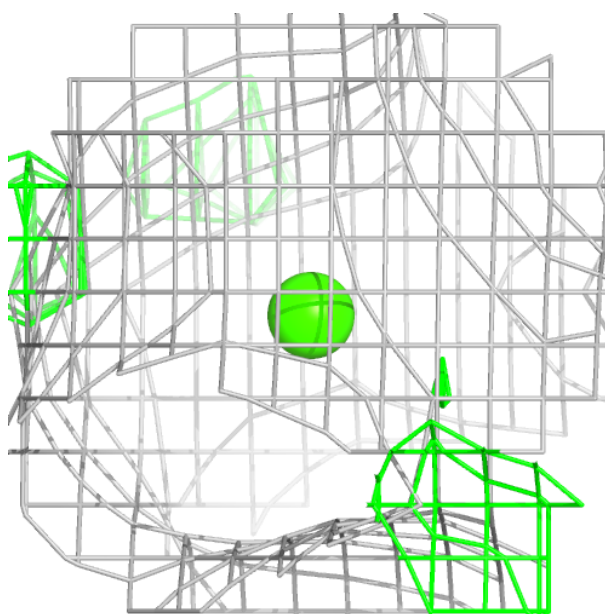
Electron density around CA D 601:

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



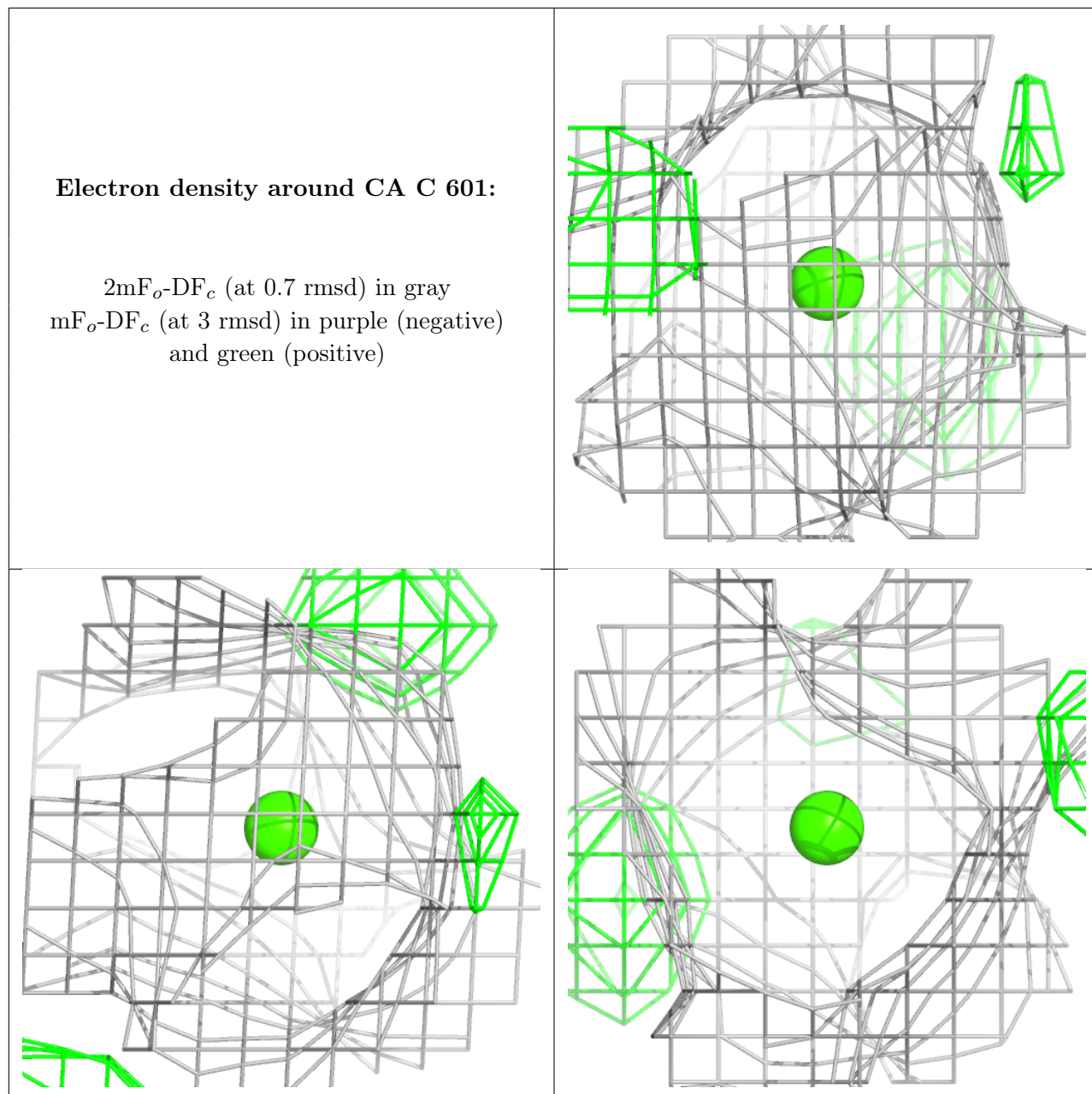
Electron density around CA G 601:

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



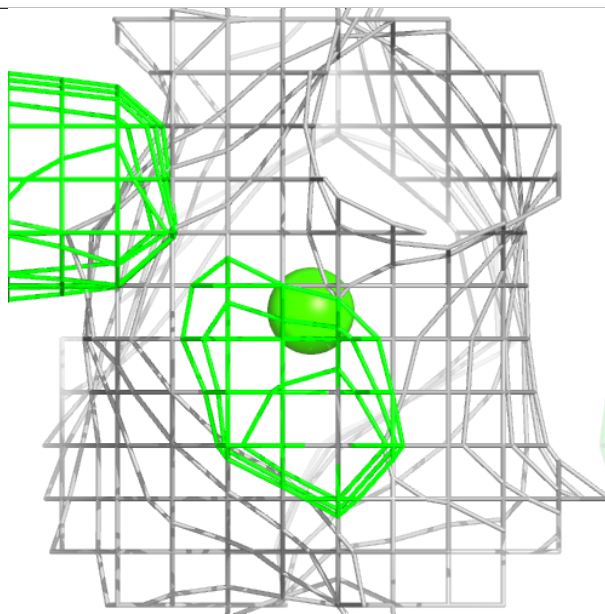
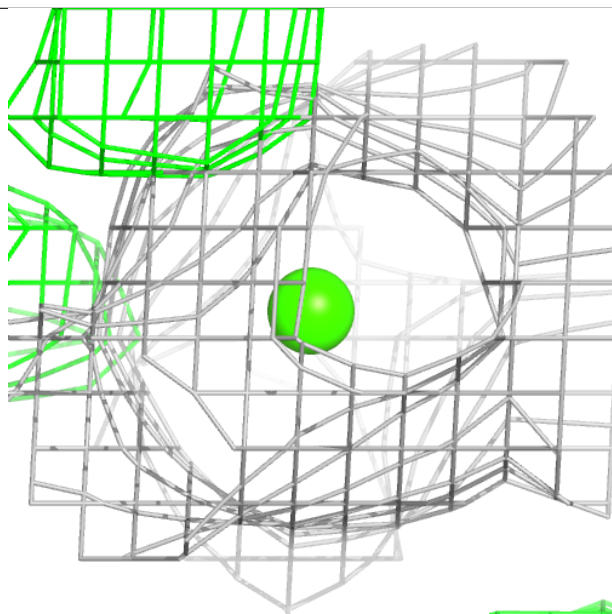
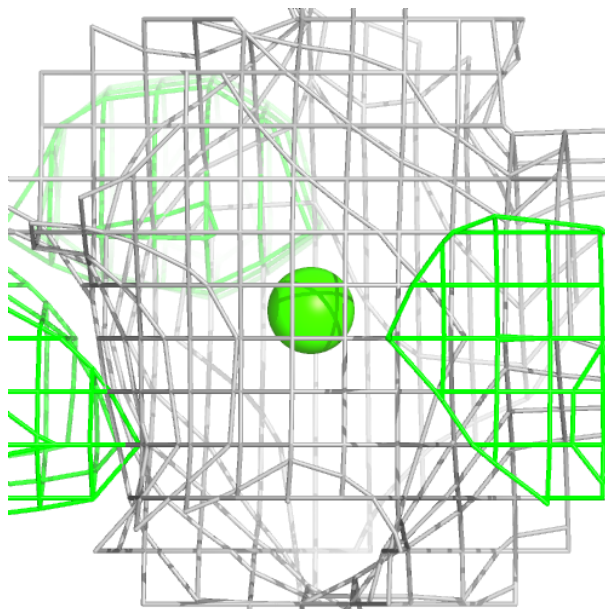
Electron density around CA C 601:

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



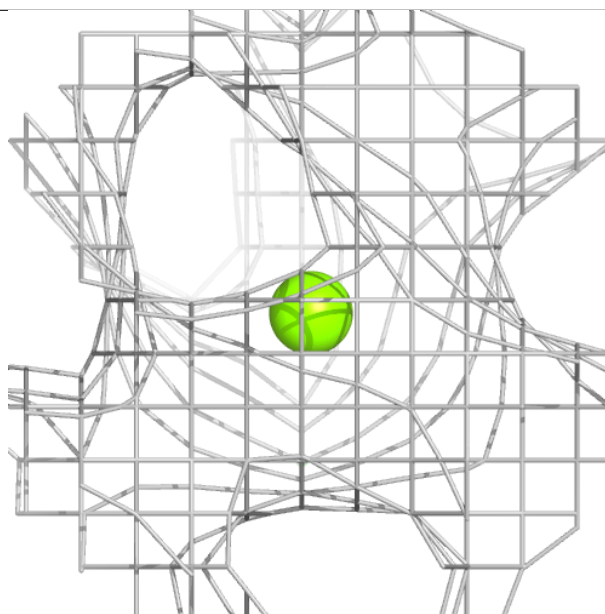
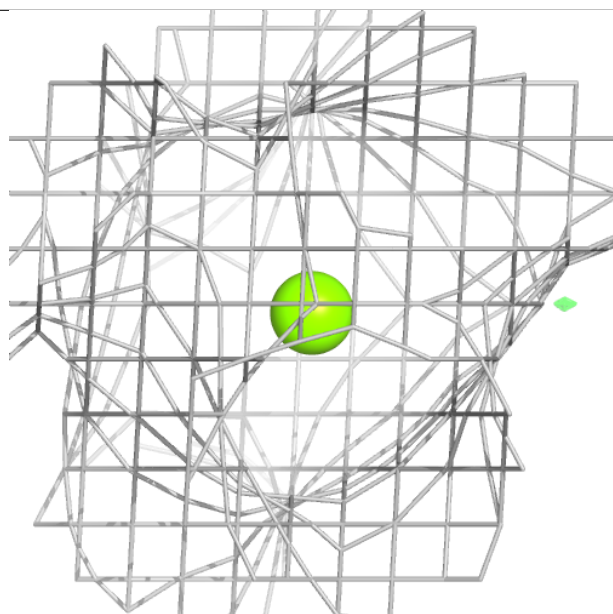
Electron density around CA B 601:

$2mF_o-DF_c$ (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.