



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 13, 2026 – 05:10 pm BST

PDB ID : 9HXT / pdb_00009hxt
Title : Crystal structure of bifunctional catalase-phenol oxidase from a marine-derived Cladosporium species
Authors : Kosinas, C.; Ferousi, C.; Pantelakis, O.I.; Topakas, E.; Dimarogona, M.
Deposited on : 2025-01-08
Resolution : 1.60 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 : 1.8.4, CSD as541be (2020)
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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

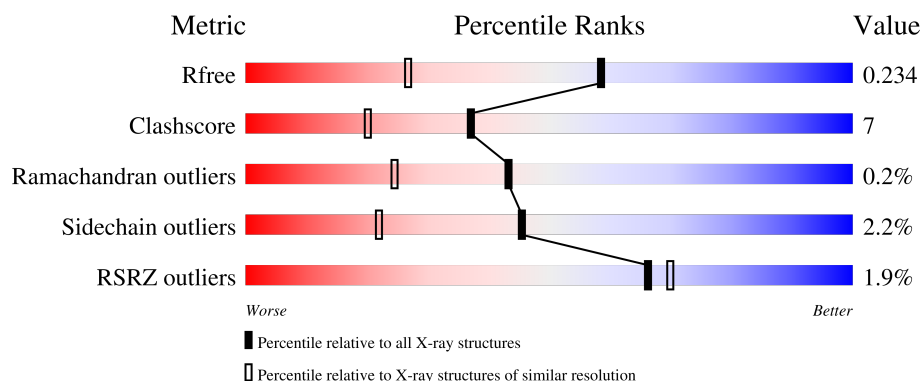
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	545	0% 78% 13% 8%
1	B	545	0% 80% 11% 8%
1	C	545	0% 80% 11% 7%
1	D	545	2% 80% 12% 7%
1	E	545	3% 81% 10% 7%

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Mol	Chain	Length	Quality of chain
1	F	545	
1	G	545	
1	H	545	
2	I	2	
2	K	2	
3	J	7	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	B	604	-	-	X	-
9	ALA	A	603	-	-	X	-

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 71000 atoms, of which 32119 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 Catalase-phenol oxidase from Cladosporium sp.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	H	507	Total	C	H	N	O	S	117	15	0
			8105	2610	3954	735	797	9			
1	A	503	Total	C	H	N	O	S	117	17	0
			8090	2603	3951	736	791	9			
1	B	501	Total	C	H	N	O	S	116	9	0
			7979	2573	3889	725	783	9			
1	C	506	Total	C	H	N	O	S	116	12	0
			8047	2595	3919	729	794	10			
1	D	506	Total	C	H	N	O	S	119	14	0
			8071	2601	3939	728	794	9			
1	E	505	Total	C	H	N	O	S	119	15	0
			8079	2602	3944	730	793	10			
1	F	507	Total	C	H	N	O	S	116	13	0
			8097	2607	3947	737	797	9			
1	G	505	Total	C	H	N	O	S	116	8	0
			8020	2585	3911	728	787	9			

There are 200 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-14	SER	-	expression tag	UNP A0AB34KRF0
H	-13	MET	-	expression tag	UNP A0AB34KRF0
H	508	ALA	-	expression tag	UNP A0AB34KRF0
H	509	LEU	-	expression tag	UNP A0AB34KRF0
H	510	GLU	-	expression tag	UNP A0AB34KRF0
H	511	GLN	-	expression tag	UNP A0AB34KRF0
H	512	LYS	-	expression tag	UNP A0AB34KRF0
H	513	LEU	-	expression tag	UNP A0AB34KRF0
H	514	ILE	-	expression tag	UNP A0AB34KRF0
H	515	SER	-	expression tag	UNP A0AB34KRF0
H	516	GLU	-	expression tag	UNP A0AB34KRF0
H	517	GLU	-	expression tag	UNP A0AB34KRF0
H	518	ASP	-	expression tag	UNP A0AB34KRF0

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Chain	Residue	Modelled	Actual	Comment	Reference
H	519	LEU	-	expression tag	UNP A0AB34KRF0
H	520	ASN	-	expression tag	UNP A0AB34KRF0
H	521	SER	-	expression tag	UNP A0AB34KRF0
H	522	ALA	-	expression tag	UNP A0AB34KRF0
H	523	VAL	-	expression tag	UNP A0AB34KRF0
H	524	ASP	-	expression tag	UNP A0AB34KRF0
H	525	HIS	-	expression tag	UNP A0AB34KRF0
H	526	HIS	-	expression tag	UNP A0AB34KRF0
H	527	HIS	-	expression tag	UNP A0AB34KRF0
H	528	HIS	-	expression tag	UNP A0AB34KRF0
H	529	HIS	-	expression tag	UNP A0AB34KRF0
H	530	HIS	-	expression tag	UNP A0AB34KRF0
A	-14	SER	-	expression tag	UNP A0AB34KRF0
A	-13	MET	-	expression tag	UNP A0AB34KRF0
A	508	ALA	-	expression tag	UNP A0AB34KRF0
A	509	LEU	-	expression tag	UNP A0AB34KRF0
A	510	GLU	-	expression tag	UNP A0AB34KRF0
A	511	GLN	-	expression tag	UNP A0AB34KRF0
A	512	LYS	-	expression tag	UNP A0AB34KRF0
A	513	LEU	-	expression tag	UNP A0AB34KRF0
A	514	ILE	-	expression tag	UNP A0AB34KRF0
A	515	SER	-	expression tag	UNP A0AB34KRF0
A	516	GLU	-	expression tag	UNP A0AB34KRF0
A	517	GLU	-	expression tag	UNP A0AB34KRF0
A	518	ASP	-	expression tag	UNP A0AB34KRF0
A	519	LEU	-	expression tag	UNP A0AB34KRF0
A	520	ASN	-	expression tag	UNP A0AB34KRF0
A	521	SER	-	expression tag	UNP A0AB34KRF0
A	522	ALA	-	expression tag	UNP A0AB34KRF0
A	523	VAL	-	expression tag	UNP A0AB34KRF0
A	524	ASP	-	expression tag	UNP A0AB34KRF0
A	525	HIS	-	expression tag	UNP A0AB34KRF0
A	526	HIS	-	expression tag	UNP A0AB34KRF0
A	527	HIS	-	expression tag	UNP A0AB34KRF0
A	528	HIS	-	expression tag	UNP A0AB34KRF0
A	529	HIS	-	expression tag	UNP A0AB34KRF0
A	530	HIS	-	expression tag	UNP A0AB34KRF0
B	-14	SER	-	expression tag	UNP A0AB34KRF0
B	-13	MET	-	expression tag	UNP A0AB34KRF0
B	508	ALA	-	expression tag	UNP A0AB34KRF0
B	509	LEU	-	expression tag	UNP A0AB34KRF0
B	510	GLU	-	expression tag	UNP A0AB34KRF0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	511	GLN	-	expression tag	UNP A0AB34KRF0
B	512	LYS	-	expression tag	UNP A0AB34KRF0
B	513	LEU	-	expression tag	UNP A0AB34KRF0
B	514	ILE	-	expression tag	UNP A0AB34KRF0
B	515	SER	-	expression tag	UNP A0AB34KRF0
B	516	GLU	-	expression tag	UNP A0AB34KRF0
B	517	GLU	-	expression tag	UNP A0AB34KRF0
B	518	ASP	-	expression tag	UNP A0AB34KRF0
B	519	LEU	-	expression tag	UNP A0AB34KRF0
B	520	ASN	-	expression tag	UNP A0AB34KRF0
B	521	SER	-	expression tag	UNP A0AB34KRF0
B	522	ALA	-	expression tag	UNP A0AB34KRF0
B	523	VAL	-	expression tag	UNP A0AB34KRF0
B	524	ASP	-	expression tag	UNP A0AB34KRF0
B	525	HIS	-	expression tag	UNP A0AB34KRF0
B	526	HIS	-	expression tag	UNP A0AB34KRF0
B	527	HIS	-	expression tag	UNP A0AB34KRF0
B	528	HIS	-	expression tag	UNP A0AB34KRF0
B	529	HIS	-	expression tag	UNP A0AB34KRF0
B	530	HIS	-	expression tag	UNP A0AB34KRF0
C	-14	SER	-	expression tag	UNP A0AB34KRF0
C	-13	MET	-	expression tag	UNP A0AB34KRF0
C	508	ALA	-	expression tag	UNP A0AB34KRF0
C	509	LEU	-	expression tag	UNP A0AB34KRF0
C	510	GLU	-	expression tag	UNP A0AB34KRF0
C	511	GLN	-	expression tag	UNP A0AB34KRF0
C	512	LYS	-	expression tag	UNP A0AB34KRF0
C	513	LEU	-	expression tag	UNP A0AB34KRF0
C	514	ILE	-	expression tag	UNP A0AB34KRF0
C	515	SER	-	expression tag	UNP A0AB34KRF0
C	516	GLU	-	expression tag	UNP A0AB34KRF0
C	517	GLU	-	expression tag	UNP A0AB34KRF0
C	518	ASP	-	expression tag	UNP A0AB34KRF0
C	519	LEU	-	expression tag	UNP A0AB34KRF0
C	520	ASN	-	expression tag	UNP A0AB34KRF0
C	521	SER	-	expression tag	UNP A0AB34KRF0
C	522	ALA	-	expression tag	UNP A0AB34KRF0
C	523	VAL	-	expression tag	UNP A0AB34KRF0
C	524	ASP	-	expression tag	UNP A0AB34KRF0
C	525	HIS	-	expression tag	UNP A0AB34KRF0
C	526	HIS	-	expression tag	UNP A0AB34KRF0
C	527	HIS	-	expression tag	UNP A0AB34KRF0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	528	HIS	-	expression tag	UNP A0AB34KRF0
C	529	HIS	-	expression tag	UNP A0AB34KRF0
C	530	HIS	-	expression tag	UNP A0AB34KRF0
D	-14	SER	-	expression tag	UNP A0AB34KRF0
D	-13	MET	-	expression tag	UNP A0AB34KRF0
D	508	ALA	-	expression tag	UNP A0AB34KRF0
D	509	LEU	-	expression tag	UNP A0AB34KRF0
D	510	GLU	-	expression tag	UNP A0AB34KRF0
D	511	GLN	-	expression tag	UNP A0AB34KRF0
D	512	LYS	-	expression tag	UNP A0AB34KRF0
D	513	LEU	-	expression tag	UNP A0AB34KRF0
D	514	ILE	-	expression tag	UNP A0AB34KRF0
D	515	SER	-	expression tag	UNP A0AB34KRF0
D	516	GLU	-	expression tag	UNP A0AB34KRF0
D	517	GLU	-	expression tag	UNP A0AB34KRF0
D	518	ASP	-	expression tag	UNP A0AB34KRF0
D	519	LEU	-	expression tag	UNP A0AB34KRF0
D	520	ASN	-	expression tag	UNP A0AB34KRF0
D	521	SER	-	expression tag	UNP A0AB34KRF0
D	522	ALA	-	expression tag	UNP A0AB34KRF0
D	523	VAL	-	expression tag	UNP A0AB34KRF0
D	524	ASP	-	expression tag	UNP A0AB34KRF0
D	525	HIS	-	expression tag	UNP A0AB34KRF0
D	526	HIS	-	expression tag	UNP A0AB34KRF0
D	527	HIS	-	expression tag	UNP A0AB34KRF0
D	528	HIS	-	expression tag	UNP A0AB34KRF0
D	529	HIS	-	expression tag	UNP A0AB34KRF0
D	530	HIS	-	expression tag	UNP A0AB34KRF0
E	-14	SER	-	expression tag	UNP A0AB34KRF0
E	-13	MET	-	expression tag	UNP A0AB34KRF0
E	508	ALA	-	expression tag	UNP A0AB34KRF0
E	509	LEU	-	expression tag	UNP A0AB34KRF0
E	510	GLU	-	expression tag	UNP A0AB34KRF0
E	511	GLN	-	expression tag	UNP A0AB34KRF0
E	512	LYS	-	expression tag	UNP A0AB34KRF0
E	513	LEU	-	expression tag	UNP A0AB34KRF0
E	514	ILE	-	expression tag	UNP A0AB34KRF0
E	515	SER	-	expression tag	UNP A0AB34KRF0
E	516	GLU	-	expression tag	UNP A0AB34KRF0
E	517	GLU	-	expression tag	UNP A0AB34KRF0
E	518	ASP	-	expression tag	UNP A0AB34KRF0
E	519	LEU	-	expression tag	UNP A0AB34KRF0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	520	ASN	-	expression tag	UNP A0AB34KRF0
E	521	SER	-	expression tag	UNP A0AB34KRF0
E	522	ALA	-	expression tag	UNP A0AB34KRF0
E	523	VAL	-	expression tag	UNP A0AB34KRF0
E	524	ASP	-	expression tag	UNP A0AB34KRF0
E	525	HIS	-	expression tag	UNP A0AB34KRF0
E	526	HIS	-	expression tag	UNP A0AB34KRF0
E	527	HIS	-	expression tag	UNP A0AB34KRF0
E	528	HIS	-	expression tag	UNP A0AB34KRF0
E	529	HIS	-	expression tag	UNP A0AB34KRF0
E	530	HIS	-	expression tag	UNP A0AB34KRF0
F	-14	SER	-	expression tag	UNP A0AB34KRF0
F	-13	MET	-	expression tag	UNP A0AB34KRF0
F	508	ALA	-	expression tag	UNP A0AB34KRF0
F	509	LEU	-	expression tag	UNP A0AB34KRF0
F	510	GLU	-	expression tag	UNP A0AB34KRF0
F	511	GLN	-	expression tag	UNP A0AB34KRF0
F	512	LYS	-	expression tag	UNP A0AB34KRF0
F	513	LEU	-	expression tag	UNP A0AB34KRF0
F	514	ILE	-	expression tag	UNP A0AB34KRF0
F	515	SER	-	expression tag	UNP A0AB34KRF0
F	516	GLU	-	expression tag	UNP A0AB34KRF0
F	517	GLU	-	expression tag	UNP A0AB34KRF0
F	518	ASP	-	expression tag	UNP A0AB34KRF0
F	519	LEU	-	expression tag	UNP A0AB34KRF0
F	520	ASN	-	expression tag	UNP A0AB34KRF0
F	521	SER	-	expression tag	UNP A0AB34KRF0
F	522	ALA	-	expression tag	UNP A0AB34KRF0
F	523	VAL	-	expression tag	UNP A0AB34KRF0
F	524	ASP	-	expression tag	UNP A0AB34KRF0
F	525	HIS	-	expression tag	UNP A0AB34KRF0
F	526	HIS	-	expression tag	UNP A0AB34KRF0
F	527	HIS	-	expression tag	UNP A0AB34KRF0
F	528	HIS	-	expression tag	UNP A0AB34KRF0
F	529	HIS	-	expression tag	UNP A0AB34KRF0
F	530	HIS	-	expression tag	UNP A0AB34KRF0
G	-14	SER	-	expression tag	UNP A0AB34KRF0
G	-13	MET	-	expression tag	UNP A0AB34KRF0
G	508	ALA	-	expression tag	UNP A0AB34KRF0
G	509	LEU	-	expression tag	UNP A0AB34KRF0
G	510	GLU	-	expression tag	UNP A0AB34KRF0
G	511	GLN	-	expression tag	UNP A0AB34KRF0

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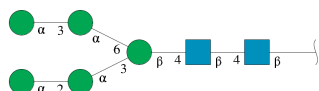
Chain	Residue	Modelled	Actual	Comment	Reference
G	512	LYS	-	expression tag	UNP A0AB34KRF0
G	513	LEU	-	expression tag	UNP A0AB34KRF0
G	514	ILE	-	expression tag	UNP A0AB34KRF0
G	515	SER	-	expression tag	UNP A0AB34KRF0
G	516	GLU	-	expression tag	UNP A0AB34KRF0
G	517	GLU	-	expression tag	UNP A0AB34KRF0
G	518	ASP	-	expression tag	UNP A0AB34KRF0
G	519	LEU	-	expression tag	UNP A0AB34KRF0
G	520	ASN	-	expression tag	UNP A0AB34KRF0
G	521	SER	-	expression tag	UNP A0AB34KRF0
G	522	ALA	-	expression tag	UNP A0AB34KRF0
G	523	VAL	-	expression tag	UNP A0AB34KRF0
G	524	ASP	-	expression tag	UNP A0AB34KRF0
G	525	HIS	-	expression tag	UNP A0AB34KRF0
G	526	HIS	-	expression tag	UNP A0AB34KRF0
G	527	HIS	-	expression tag	UNP A0AB34KRF0
G	528	HIS	-	expression tag	UNP A0AB34KRF0
G	529	HIS	-	expression tag	UNP A0AB34KRF0
G	530	HIS	-	expression tag	UNP A0AB34KRF0

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



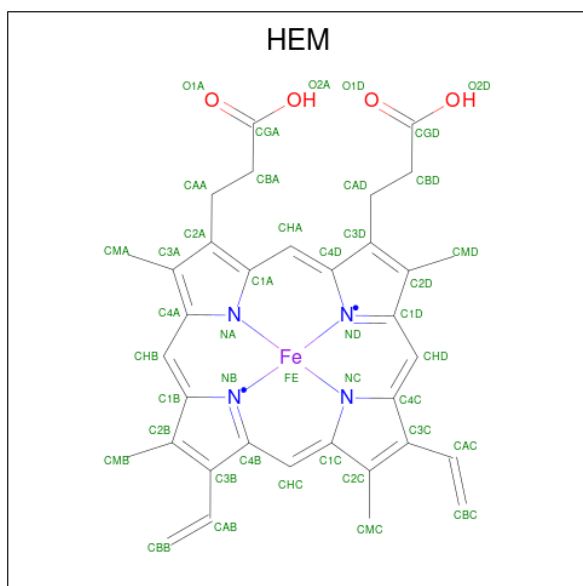
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	2	Total	C	H	N	O	12	0	0
			55	16	27	2	10			
2	K	2	Total	C	H	N	O	12	0	0
			55	16	27	2	10			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



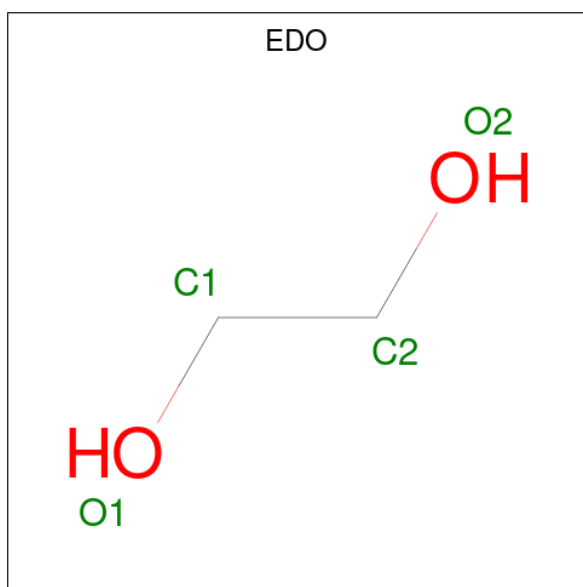
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	7	Total	C	H	N	O	26	0	0
			160	46	77	2	35			

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



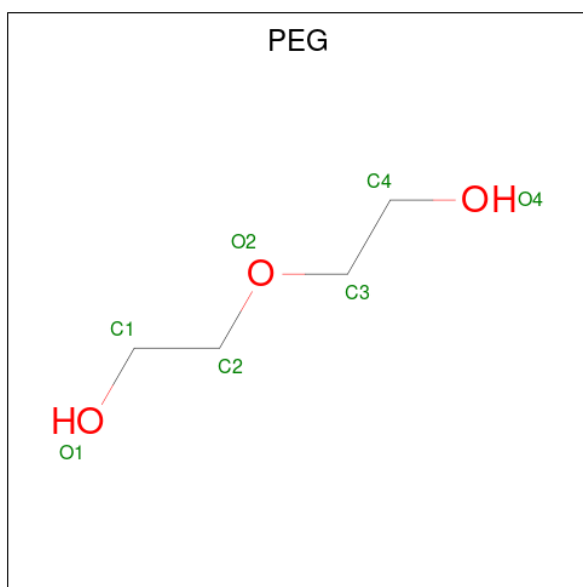
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	H	1	Total	C	Fe	H	N	O	
			73	34	1	30	4	4	
4	A	1	Total	C	Fe	H	N	O	
			73	34	1	30	4	4	
4	B	1	Total	C	Fe	H	N	O	
			73	34	1	30	4	4	
4	C	1	Total	C	Fe	H	N	O	
			73	34	1	30	4	4	
4	D	1	Total	C	Fe	H	N	O	
			73	34	1	30	4	4	
4	E	1	Total	C	Fe	H	N	O	
			73	34	1	30	4	4	
4	F	1	Total	C	Fe	H	N	O	
			73	34	1	30	4	4	
4	G	1	Total	C	Fe	H	N	O	
			73	34	1	30	4	4	

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).

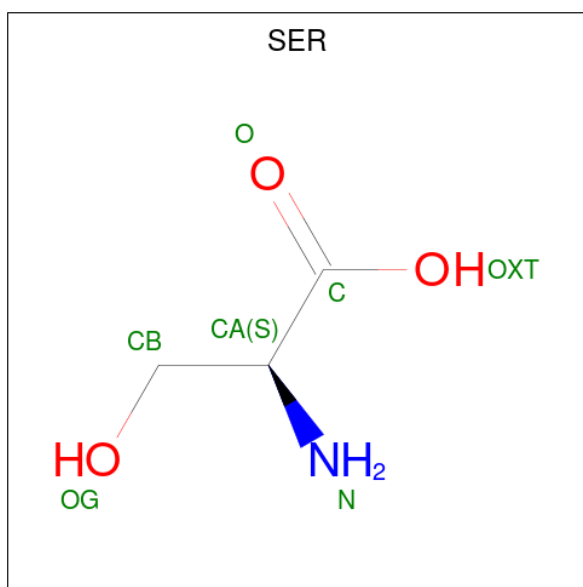


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	H	1	Total	C	H	O	2	0
			17	4	10	3		
6	H	1	Total	C	H	O	2	0
			17	4	10	3		
6	A	1	Total	C	H	O	2	0
			17	4	10	3		
6	D	1	Total	C	H	O	2	0
			17	4	10	3		
6	D	1	Total	C	H	O	2	0
			17	4	10	3		
6	E	1	Total	C	H	O	2	0
			17	4	10	3		

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

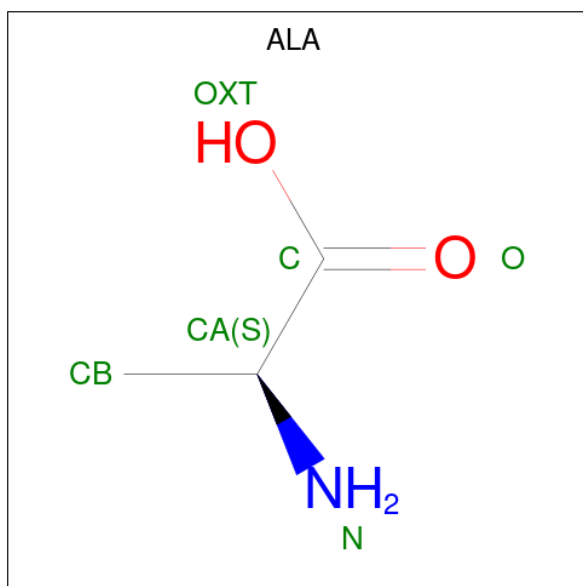
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	1	Total	Na	0	0
			1	1		

- Molecule 8 is SERINE (CCD ID: SER) (formula: C₃H₇NO₃).



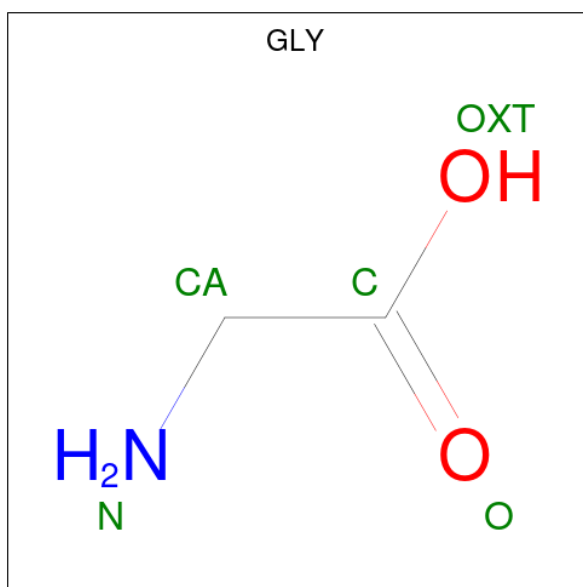
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
8	A	1	14	3	7	1	3	1	0

- Molecule 9 is ALANINE (CCD ID: ALA) (formula: $C_3H_7NO_2$).



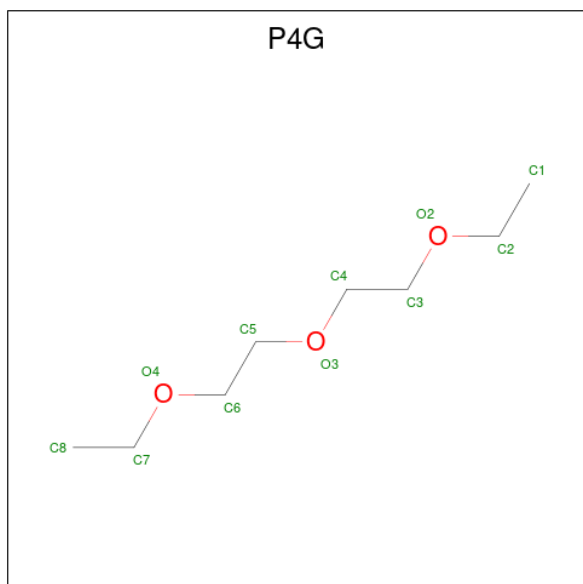
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
9	A	1	13	3	7	1	2	0	0

- Molecule 10 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$).



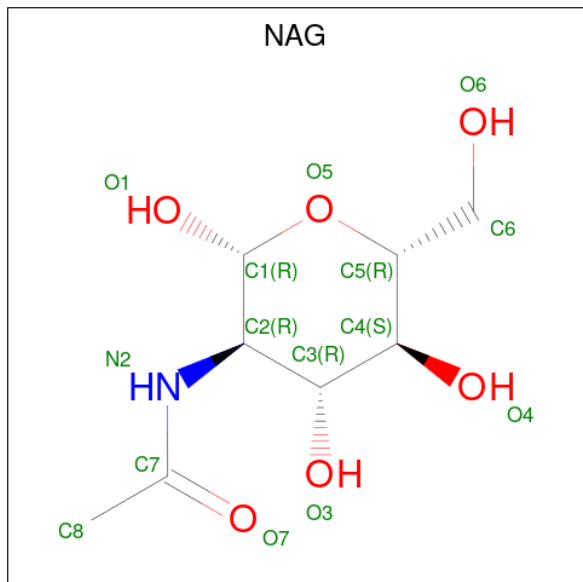
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	A	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
10	F	1	Total	C	H	N	O	0	0
			10	2	5	1	2		

- Molecule 11 is 1-ETHOXY-2-(2-ETHOXYETHOXY)ETHANE (CCD ID: P4G) (formula: $C_8H_{18}O_3$).



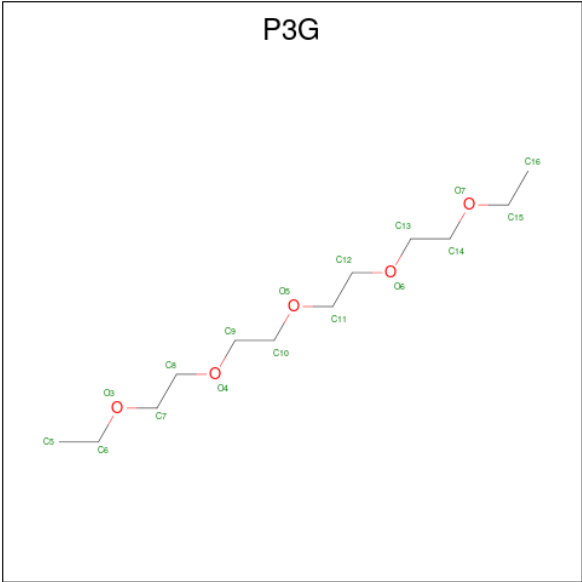
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	H	O	0	0
			29	8	18	3		

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	B	1	Total	C	H	N	O	6	0
			28	8	14	1	5		
12	B	1	Total	C	H	N	O	7	0
			28	8	14	1	5		
12	C	1	Total	C	H	N	O	6	0
			28	8	14	1	5		
12	C	1	Total	C	H	N	O	7	0
			28	8	14	1	5		
12	D	1	Total	C	H	N	O	7	0
			28	8	14	1	5		
12	D	1	Total	C	H	N	O	7	0
			28	8	14	1	5		
12	E	1	Total	C	H	N	O	7	0
			28	8	14	1	5		
12	G	1	Total	C	H	N	O	7	0
			28	8	14	1	5		

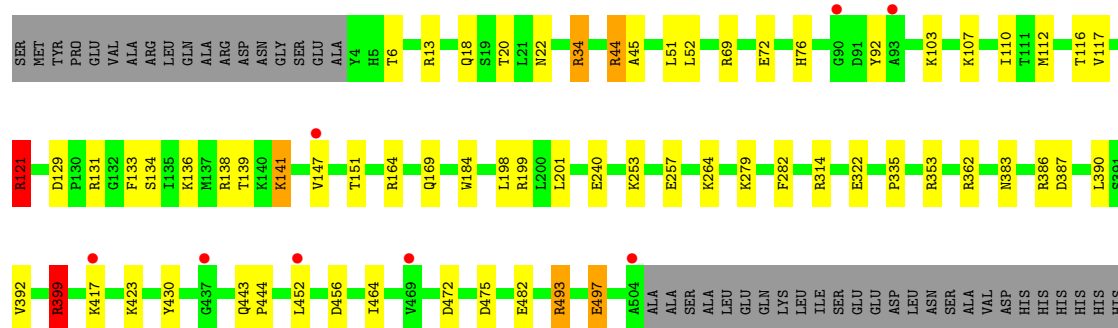
- Molecule 13 is 3,6,9,12,15-PENTAOXAHEPTADECANE (CCD ID: P3G) (formula: $C_{12}H_{26}O_5$).



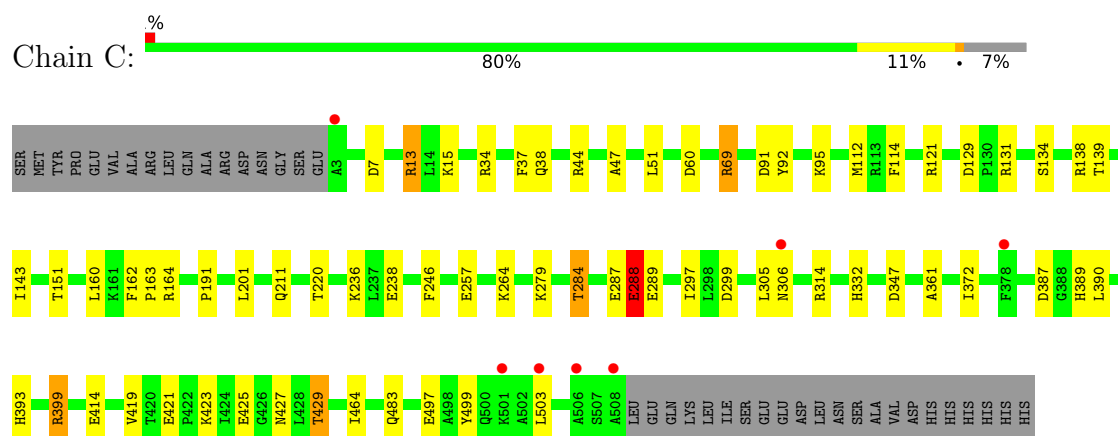
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	C	1	Total	C	H	O	0	0
			43	12	26	5		

- Molecule 14 is water.

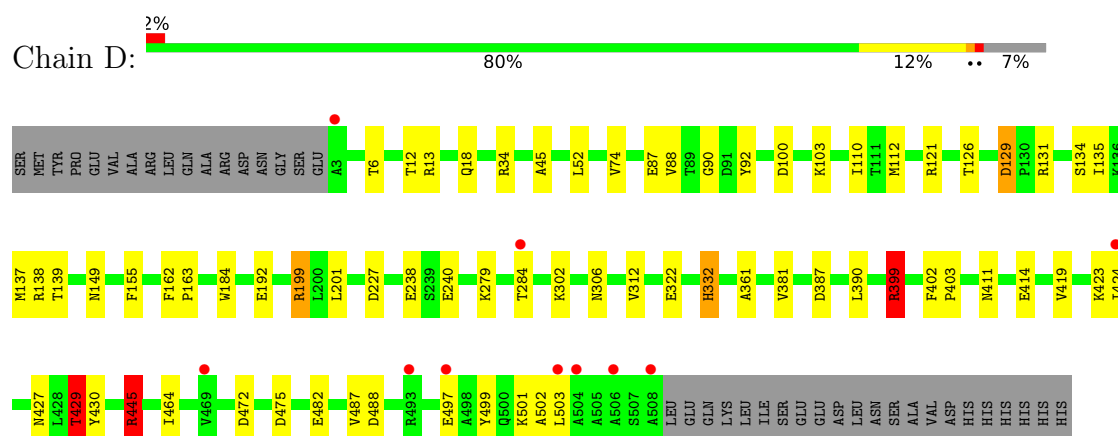
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	H	628	Total	O	0	0
			628	628		
14	A	672	Total	O	0	0
			672	672		
14	B	639	Total	O	0	0
			639	639		
14	C	667	Total	O	0	0
			667	667		
14	D	684	Total	O	0	0
			684	684		
14	E	608	Total	O	0	0
			608	608		
14	F	640	Total	O	0	0
			640	640		
14	G	584	Total	O	0	0
			584	584		



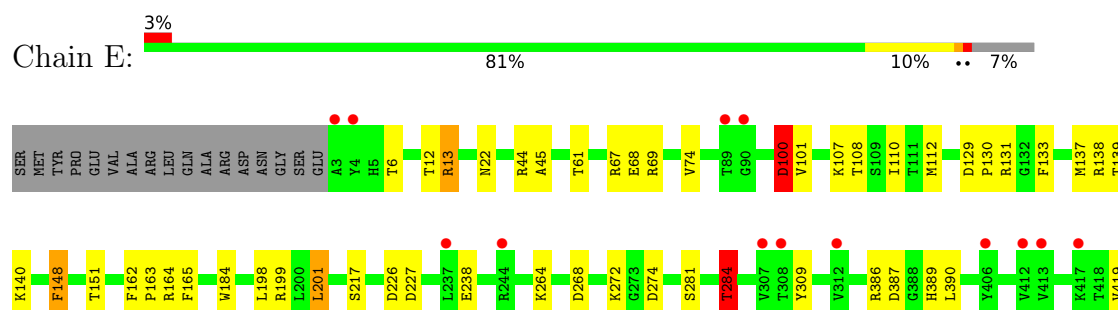
- Molecule 1: Catalase-phenol oxidase from *Cladosporium* sp

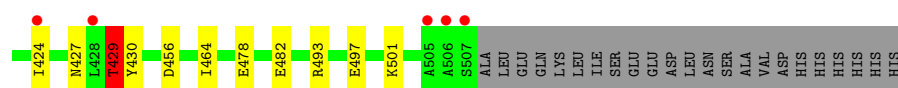


- Molecule 1: Catalase-phenol oxidase from *Cladosporium* sp

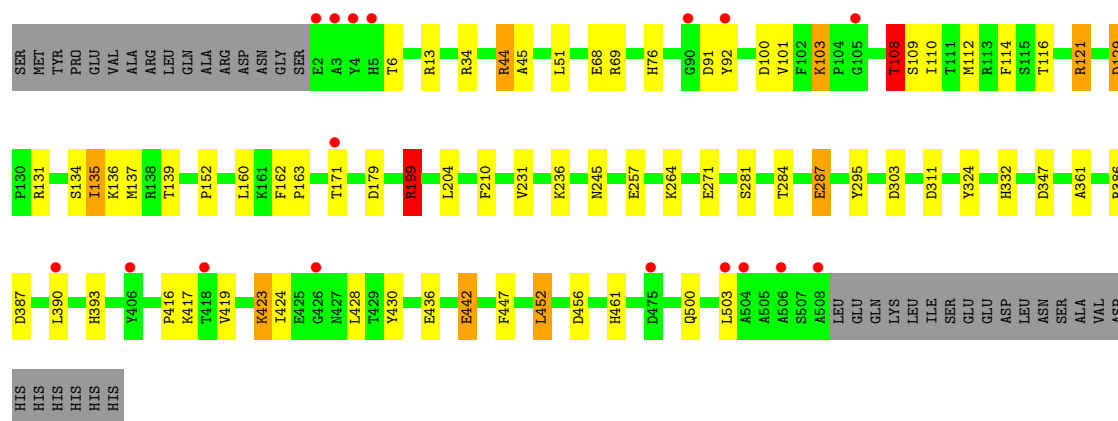
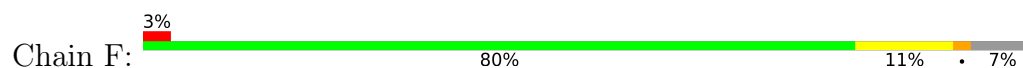


- Molecule 1: Catalase-phenol oxidase from *Cladosporium* sp

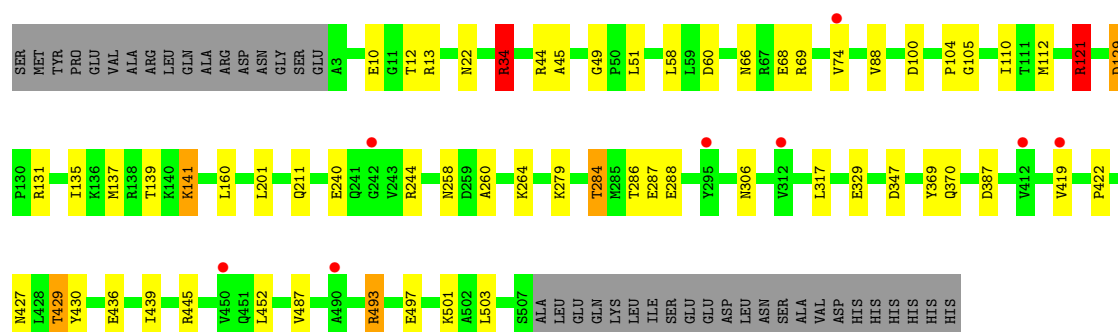
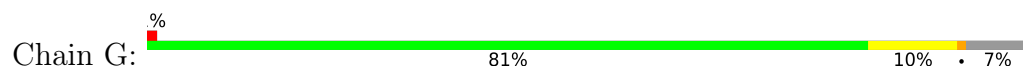




- Molecule 1: Catalase-phenol oxidase from *Cladosporium* sp



- Molecule 1: Catalase-phenol oxidase from *Cladosporium* sp



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-3)- α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain J:  14% 86%

MAG1
MAG2
EMA3
MAN4
MAN5
MAN6
MAN7

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	92.55Å 92.66Å 169.23Å 83.31° 78.18° 60.33°	Depositor
Resolution (Å)	82.94 – 1.60 82.94 – 1.60	Depositor EDS
% Data completeness (in resolution range)	91.5 (82.94-1.60) 89.7 (82.94-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0425, REFMAC 5.8.0425	Depositor
R, R_{free}	0.199 , 0.236 0.197 , 0.234	Depositor DCC
R_{free} test set	29071 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	18.2	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 63.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.025 for -h,-h+k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	71000	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.25% 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: MAN, BMA, HEM, NAG, P3G, NA, P4G, EDO, PEG

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	0.76	0/4317	1.20	15/5859 (0.3%)
1	B	0.74	0/4234	1.20	15/5748 (0.3%)
1	C	0.74	0/4286	1.18	18/5819 (0.3%)
1	D	0.73	1/4298 (0.0%)	1.23	19/5837 (0.3%)
1	E	0.68	0/4292	1.19	13/5828 (0.2%)
1	F	0.68	0/4301	1.17	13/5839 (0.2%)
1	G	0.69	0/4255	1.19	9/5776 (0.2%)
1	H	0.70	0/4331	1.19	14/5881 (0.2%)
All	All	0.71	1/34314 (0.0%)	1.19	116/46587 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	9
1	C	0	4
1	D	0	5
1	E	0	7
1	F	0	5
1	G	0	5
1	H	0	9
All	All	0	52

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	332	HIS	CG-CD2	-5.10	1.30	1.35

The worst 5 of 116 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	MET	CG-SD-CE	-13.20	71.86	100.90
1	B	399	ARG	CB-CG-CD	-11.77	84.23	111.30
1	H	399	ARG	CD-NE-CZ	11.75	140.84	124.40
1	H	445	ARG	CD-NE-CZ	10.78	139.49	124.40
1	D	399	ARG	CB-CG-CD	-10.49	87.17	111.30

There are no chirality outliers.

5 of 52 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	121	ARG	Sidechain
1	H	131	ARG	Sidechain
1	H	34[A]	ARG	Sidechain
1	H	34[B]	ARG	Sidechain
1	H	69	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4139	3951	3870	70	0
1	B	4090	3889	3844	63	0
1	C	4128	3919	3847	59	0
1	D	4132	3939	3860	62	0
1	E	4135	3944	3875	62	0
1	F	4150	3947	3877	80	0
1	G	4109	3911	3857	58	0
1	H	4151	3954	3870	62	1
2	I	28	27	25	2	0
2	K	28	27	25	6	0
3	J	83	77	70	0	1
4	A	43	30	30	1	0
4	B	43	30	30	3	0
4	C	43	30	30	1	0
4	D	43	30	30	2	0
4	E	43	30	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	43	30	30	1	0
4	G	43	30	30	2	0
4	H	43	30	30	0	0
5	A	8	12	12	2	0
5	B	4	6	6	4	0
5	C	4	6	6	2	0
5	D	4	6	6	3	0
5	E	8	12	11	0	0
5	H	8	12	12	3	0
6	A	7	10	10	0	0
6	D	14	20	20	1	0
6	E	7	10	10	2	0
6	H	14	20	20	1	0
7	H	1	0	0	0	0
8	A	7	7	4	1	0
9	A	6	7	4	4	0
10	A	5	5	2	1	0
10	F	5	5	2	1	0
11	A	11	18	18	3	0
12	B	28	28	26	0	0
12	C	28	28	26	5	0
12	D	28	28	26	3	0
12	E	14	14	13	1	0
12	G	14	14	13	0	0
13	C	17	26	26	0	0
14	A	672	0	0	23	0
14	B	639	0	0	23	0
14	C	667	0	0	17	0
14	D	684	0	0	13	0
14	E	608	0	0	22	0
14	F	640	0	0	11	0
14	G	584	0	0	13	0
14	H	628	0	0	25	0
All	All	38881	32119	31533	462	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 7.

The worst 5 of 462 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:F:245:ASN:ND2	2:K:1:NAG:C1	1.70	1.52
1:D:445:ARG:HD3	1:D:487:VAL:O	1.35	1.21
1:D:427:ASN:OD1	12:D:605:NAG:C1	1.93	1.16
1:H:474:ASP:OD1	1:H:477:ARG:NH2	1.82	1.13
5:B:604:EDO:H21	14:B:1014:HOH:O	1.51	1.10

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:H:409:LYS:HZ3	3:J:6:MAN:HO2[1_465]	1.08	0.52

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	518/545 (95%)	502 (97%)	15 (3%)	1 (0%)	43	24
1	B	508/545 (93%)	490 (96%)	16 (3%)	2 (0%)	30	14
1	C	516/545 (95%)	500 (97%)	15 (3%)	1 (0%)	43	24
1	D	518/545 (95%)	499 (96%)	18 (4%)	1 (0%)	43	24
1	E	518/545 (95%)	500 (96%)	17 (3%)	1 (0%)	43	24
1	F	518/545 (95%)	503 (97%)	14 (3%)	1 (0%)	43	24
1	G	511/545 (94%)	495 (97%)	15 (3%)	1 (0%)	43	24
1	H	520/545 (95%)	505 (97%)	14 (3%)	1 (0%)	43	24
All	All	4127/4360 (95%)	3994 (97%)	124 (3%)	9 (0%)	43	24

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	387	ASP

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Mol	Chain	Res	Type
1	B	387	ASP
1	E	387	ASP
1	A	387	ASP
1	C	387	ASP

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	442/462 (96%)	429 (97%)	13 (3%)	37	14
1	B	433/462 (94%)	424 (98%)	9 (2%)	47	23
1	C	439/462 (95%)	432 (98%)	7 (2%)	55	33
1	D	441/462 (96%)	431 (98%)	10 (2%)	44	20
1	E	441/462 (96%)	431 (98%)	10 (2%)	44	20
1	F	440/462 (95%)	428 (97%)	12 (3%)	39	16
1	G	435/462 (94%)	423 (97%)	12 (3%)	38	15
1	H	442/462 (96%)	429 (97%)	13 (3%)	37	14
All	All	3513/3696 (95%)	3427 (98%)	86 (2%)	45	19

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	201[A]	LEU
1	F	416	PRO
1	E	284	THR
1	F	129	ASP
1	G	34[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	306	ASN

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Mol	Chain	Res	Type
1	F	212	HIS
1	F	500	GLN
1	F	483	GLN
1	C	189	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 ⓘ

11 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	I	1	2	14,14,15	0.47	0	17,19,21	0.59	0
2	NAG	I	2	2	14,14,15	0.35	0	17,19,21	1.12	0
3	NAG	J	1	3,1	14,14,15	0.47	0	17,19,21	0.90	0
3	NAG	J	2	3	14,14,15	0.42	0	17,19,21	1.14	2 (11%)
3	BMA	J	3	3	11,11,12	0.90	1 (9%)	15,15,17	1.37	2 (13%)
3	MAN	J	4	3	11,11,12	1.77	2 (18%)	15,15,17	2.26	7 (46%)
3	MAN	J	5	3	11,11,12	0.65	0	15,15,17	1.19	1 (6%)
3	MAN	J	6	3	11,11,12	0.73	0	15,15,17	0.71	0
3	MAN	J	7	3	11,11,12	1.25	1 (9%)	15,15,17	1.56	3 (20%)
2	NAG	K	1	2	14,14,15	0.57	0	17,19,21	1.23	1 (5%)
2	NAG	K	2	2	14,14,15	0.36	0	17,19,21	1.51	4 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	I	1	2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
3	NAG	J	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
3	BMA	J	3	3	-	0/2/19/22	0/1/1/1
3	MAN	J	4	3	-	2/2/19/22	0/1/1/1
3	MAN	J	5	3	-	2/2/19/22	0/1/1/1
3	MAN	J	6	3	-	0/2/19/22	0/1/1/1
3	MAN	J	7	3	-	2/2/19/22	0/1/1/1
2	NAG	K	1	2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	4	MAN	C2-C3	-4.75	1.45	1.52
3	J	7	MAN	O5-C5	3.70	1.50	1.43
3	J	4	MAN	O5-C5	2.59	1.48	1.43
3	J	3	BMA	O5-C5	2.35	1.48	1.43

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	4	MAN	C2-C3-C4	-4.47	103.16	110.89
3	J	7	MAN	C2-C3-C4	-3.78	104.36	110.89
3	J	5	MAN	C1-O5-C5	3.65	117.14	112.19
3	J	4	MAN	C1-C2-C3	-3.55	105.30	109.67
3	J	4	MAN	O2-C2-C3	-3.09	103.95	110.14

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

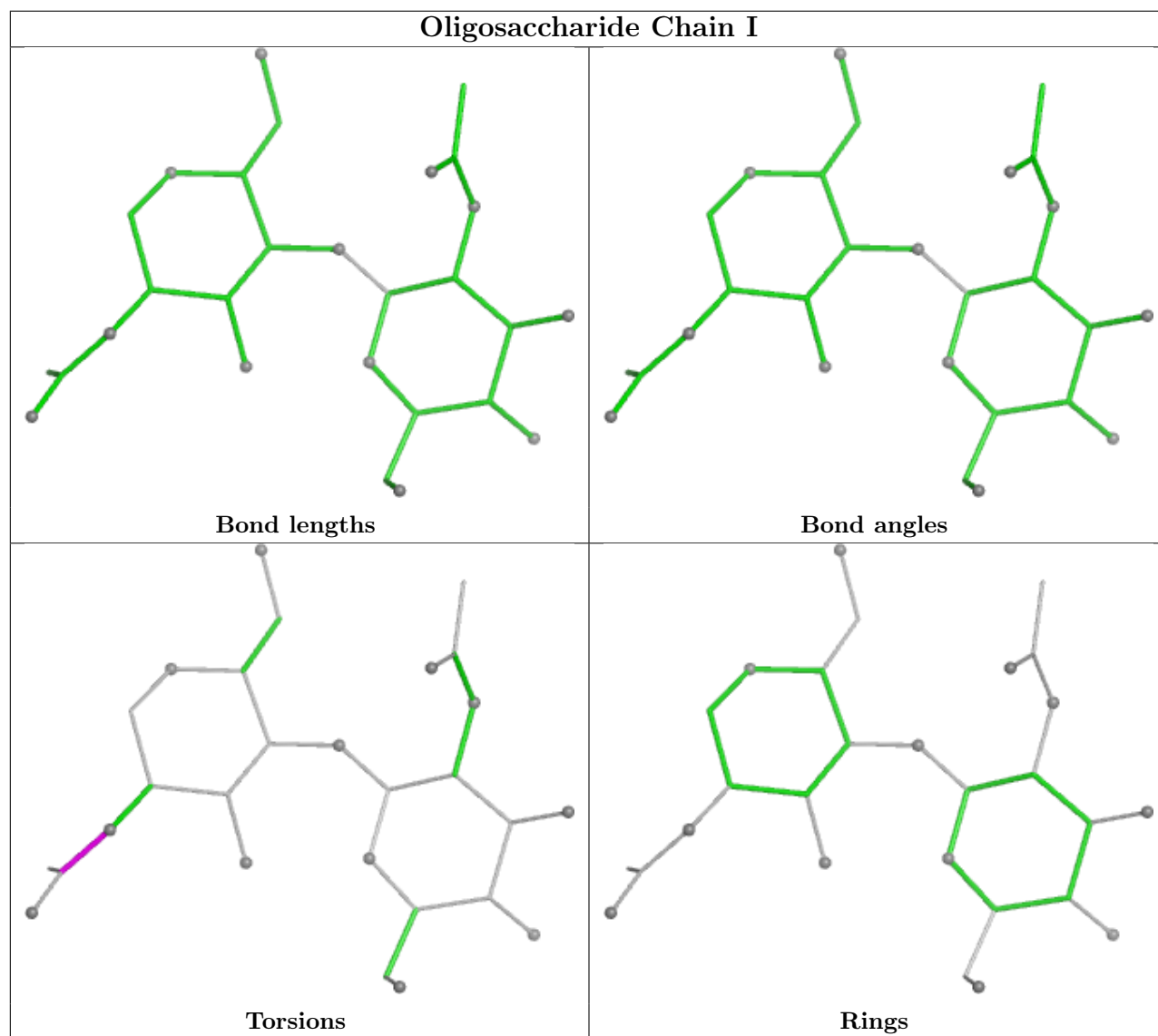
Mol	Chain	Res	Type	Atoms
3	J	7	MAN	O5-C5-C6-O6
3	J	5	MAN	O5-C5-C6-O6
3	J	4	MAN	O5-C5-C6-O6
3	J	7	MAN	C4-C5-C6-O6
2	I	1	NAG	C8-C7-N2-C2

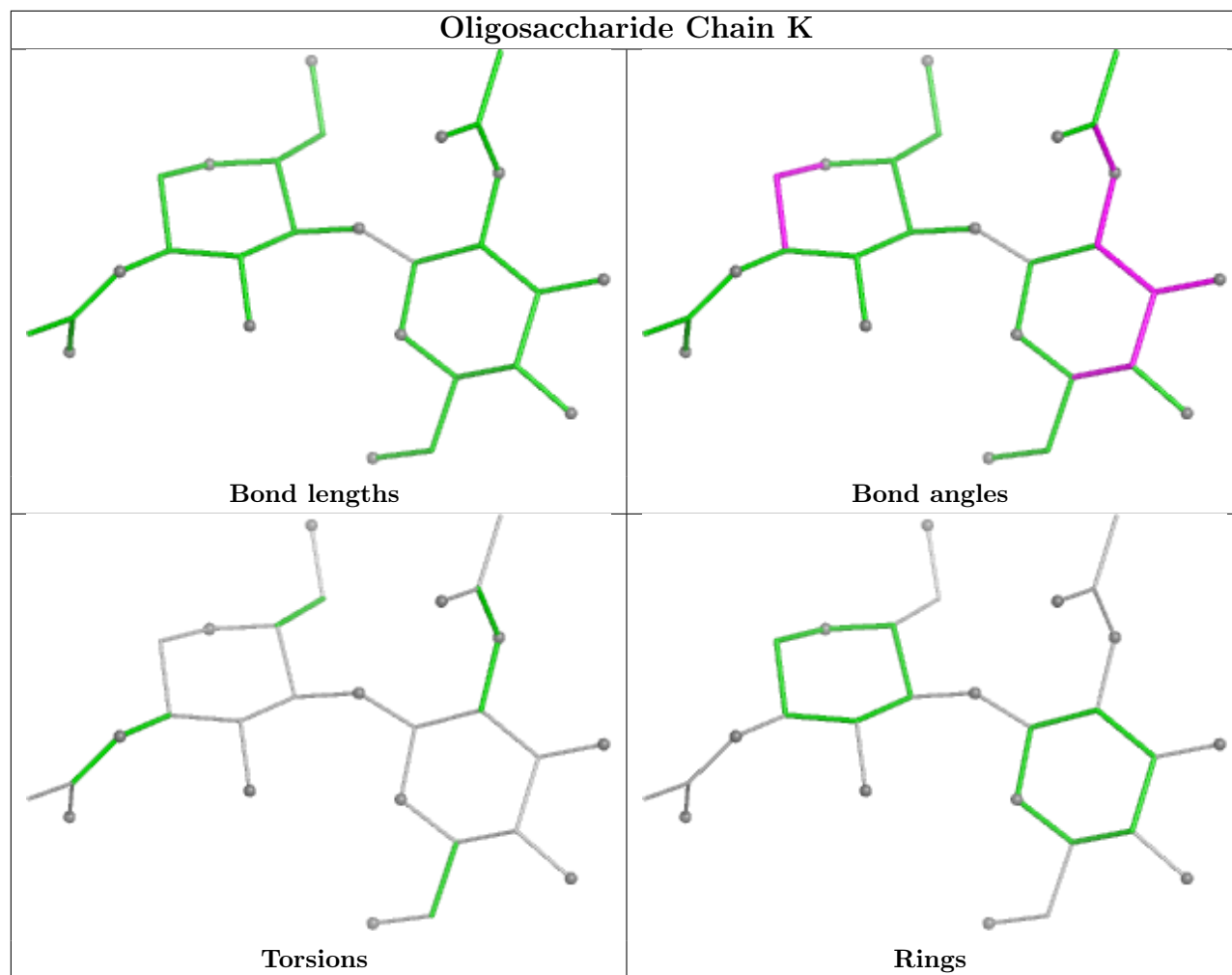
There are no ring outliers.

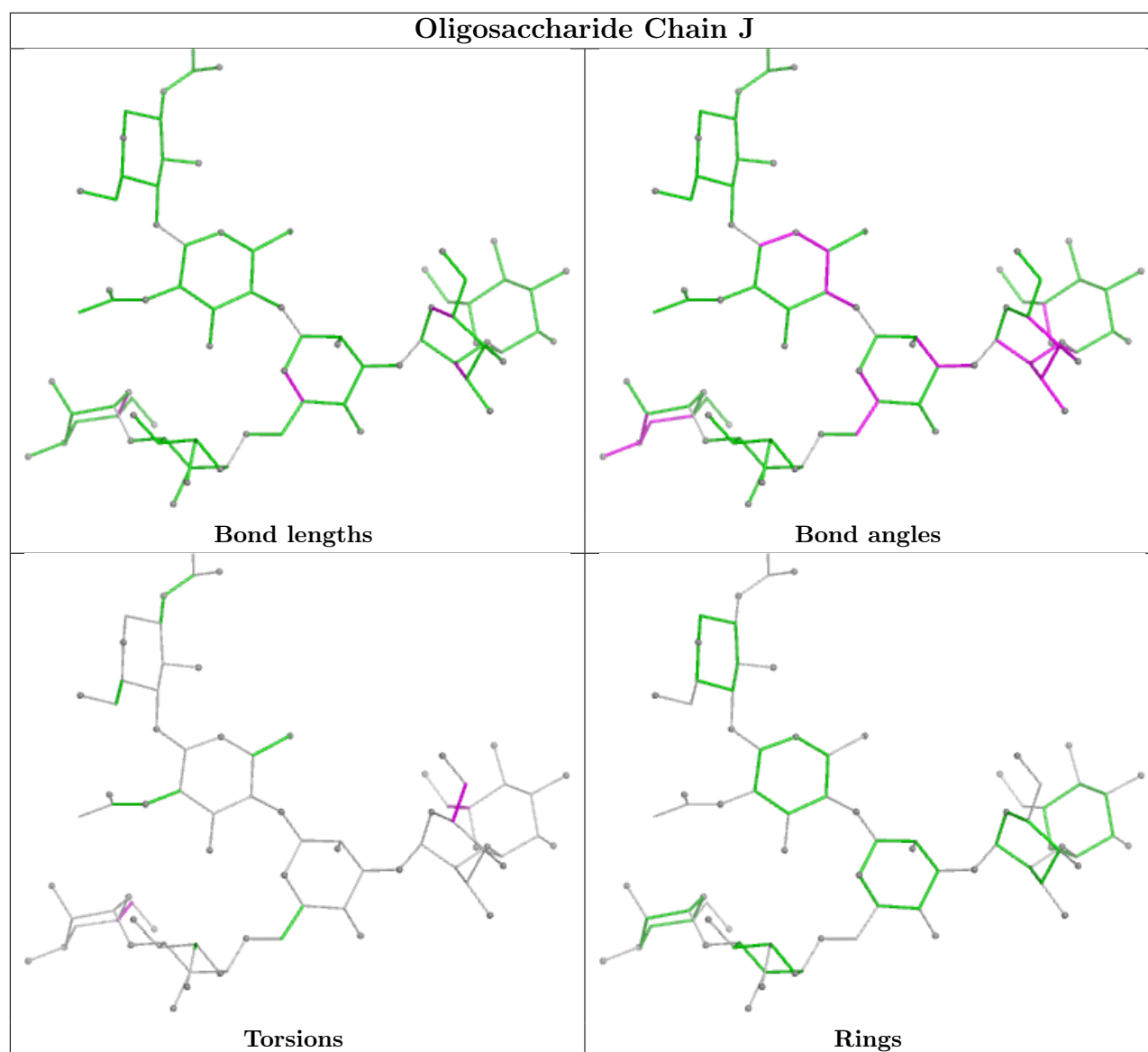
4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	2	NAG	1	0
2	K	1	NAG	6	0
3	J	6	MAN	0	1
2	I	1	NAG	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 oligosaccharide.







5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 1 is monoatomic - leaving 37 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	HEM	C	601	14,1	50,50,50	1.63	9 (18%)	66,82,82	1.47	13 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	B	604	-	3,3,3	0.40	0	2,2,2	0.54	0
6	PEG	E	604	-	6,6,6	0.28	0	5,5,5	0.20	0
5	EDO	H	602	-	3,3,3	0.42	0	2,2,2	0.40	0
6	PEG	A	608	-	6,6,6	0.26	0	5,5,5	0.34	0
10	GLY	F	602	-	4,4,4	0.80	0	3,4,4	1.40	0
10	GLY	A	606	-	4,4,4	1.56	1 (25%)	3,4,4	0.69	0
13	P3G	C	605	-	16,16,16	0.20	0	15,15,15	0.24	0
8	SER	A	602	-	5,6,6	1.30	1 (20%)	5,7,7	2.29	3 (60%)
4	HEM	E	601	1	50,50,50	1.50	8 (16%)	66,82,82	1.66	12 (18%)
4	HEM	A	601	1	50,50,50	1.81	13 (26%)	66,82,82	1.64	13 (19%)
4	HEM	F	601	1	50,50,50	1.67	12 (24%)	66,82,82	1.85	15 (22%)
4	HEM	G	601	1	50,50,50	1.66	7 (14%)	66,82,82	1.46	10 (15%)
5	EDO	H	603	-	3,3,3	0.20	0	2,2,2	0.48	0
12	NAG	B	603	-	14,14,15	0.37	0	17,19,21	1.14	2 (11%)
11	P4G	A	607	-	10,10,10	0.18	0	9,9,9	0.34	0
5	EDO	A	605	-	3,3,3	0.06	0	2,2,2	0.36	0
12	NAG	G	602	-	14,14,15	0.36	0	17,19,21	0.85	1 (5%)
5	EDO	D	606	-	3,3,3	0.10	0	2,2,2	0.59	0
6	PEG	H	604	-	6,6,6	0.21	0	5,5,5	0.19	0
4	HEM	H	601	7,14,1	50,50,50	1.87	14 (28%)	66,82,82	1.76	10 (15%)
5	EDO	A	604	-	3,3,3	0.17	0	2,2,2	0.22	0
6	PEG	D	604	-	6,6,6	0.31	0	5,5,5	0.19	0
4	HEM	D	601	1	50,50,50	1.79	11 (22%)	66,82,82	1.70	10 (15%)
9	ALA	A	603	-	5,5,5	1.32	1 (20%)	6,6,6	0.76	0
12	NAG	C	602	1	14,14,15	0.31	0	17,19,21	0.78	1 (5%)
5	EDO	E	603	-	3,3,3	0.29	0	2,2,2	0.48	0
6	PEG	D	603	-	6,6,6	0.19	0	5,5,5	0.10	0
12	NAG	D	602	-	14,14,15	0.40	0	17,19,21	0.78	0
6	PEG	H	605	-	6,6,6	0.18	0	5,5,5	0.27	0
4	HEM	B	601	1	50,50,50	1.60	9 (18%)	66,82,82	1.80	14 (21%)
12	NAG	C	603	-	14,14,15	0.39	0	17,19,21	1.54	2 (11%)
12	NAG	B	602	1	14,14,15	0.57	0	17,19,21	1.38	3 (17%)
12	NAG	D	605	-	14,14,15	0.39	0	17,19,21	1.03	1 (5%)
5	EDO	C	604	-	3,3,3	0.18	0	2,2,2	0.31	0
5	EDO	E	605	-	3,3,3	1.26	0	2,2,2	0.47	0
12	NAG	E	602	-	14,14,15	0.39	0	17,19,21	0.90	1 (5%)

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	HEM	C	601	14,1	-	2/14/54/54	-
5	EDO	B	604	-	-	1/1/1/1	-
6	PEG	E	604	-	-	2/4/4/4	-
5	EDO	H	602	-	-	1/1/1/1	-
6	PEG	A	608	-	-	2/4/4/4	-
10	GLY	F	602	-	-	2/2/2/2	-
10	GLY	A	606	-	-	2/2/2/2	-
13	P3G	C	605	-	-	6/14/14/14	-
8	SER	A	602	-	-	0/6/6/6	-
4	HEM	E	601	1	-	3/14/54/54	-
4	HEM	A	601	1	-	3/14/54/54	-
4	HEM	F	601	1	-	2/14/54/54	-
4	HEM	G	601	1	-	2/14/54/54	-
5	EDO	H	603	-	-	0/1/1/1	-
12	NAG	B	603	-	-	2/6/23/26	0/1/1/1
11	P4G	A	607	-	-	5/8/8/8	-
5	EDO	A	605	-	-	0/1/1/1	-
12	NAG	G	602	-	-	0/6/23/26	0/1/1/1
5	EDO	D	606	-	-	1/1/1/1	-
6	PEG	H	604	-	-	2/4/4/4	-
4	HEM	H	601	7,14,1	-	2/14/54/54	-
5	EDO	A	604	-	-	1/1/1/1	-
6	PEG	D	604	-	-	1/4/4/4	-
4	HEM	D	601	1	-	3/14/54/54	-
9	ALA	A	603	-	-	3/4/4/4	-
12	NAG	C	602	1	-	0/6/23/26	0/1/1/1
5	EDO	E	603	-	-	0/1/1/1	-
6	PEG	D	603	-	-	1/4/4/4	-
12	NAG	D	602	-	-	0/6/23/26	0/1/1/1
6	PEG	H	605	-	-	3/4/4/4	-
4	HEM	B	601	1	-	2/14/54/54	-
12	NAG	C	603	-	-	0/6/23/26	0/1/1/1
12	NAG	B	602	1	-	0/6/23/26	0/1/1/1
12	NAG	D	605	-	-	1/6/23/26	0/1/1/1
5	EDO	C	604	-	-	0/1/1/1	-
5	EDO	E	605	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	E	602	-	-	2/6/23/26	0/1/1/1

The worst 5 of 86 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	HEM	FE-NB	5.12	2.10	1.94
4	D	601	HEM	FE-NC	5.04	2.12	1.95
4	C	601	HEM	FE-NB	5.03	2.10	1.94
4	H	601	HEM	FE-NB	4.96	2.10	1.94
4	E	601	HEM	FE-NB	4.90	2.10	1.94

The worst 5 of 111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	601	HEM	C1B-NB-C4B	6.85	112.14	105.07
4	D	601	HEM	C1B-NB-C4B	5.60	110.85	105.07
4	A	601	HEM	CHC-C4B-NB	5.49	130.38	124.42
4	B	601	HEM	C4C-NC-C1C	5.41	110.64	105.35
4	A	601	HEM	C1B-NB-C4B	5.33	110.58	105.07

There are no chirality outliers.

5 of 57 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	603	ALA	OXT-C-CA-CB
10	A	606	GLY	O-C-CA-N
10	A	606	GLY	OXT-C-CA-N
12	B	603	NAG	C8-C7-N2-C2
12	B	603	NAG	O7-C7-N2-C2

There are no ring outliers.

23 monomers are involved in 48 short contacts:

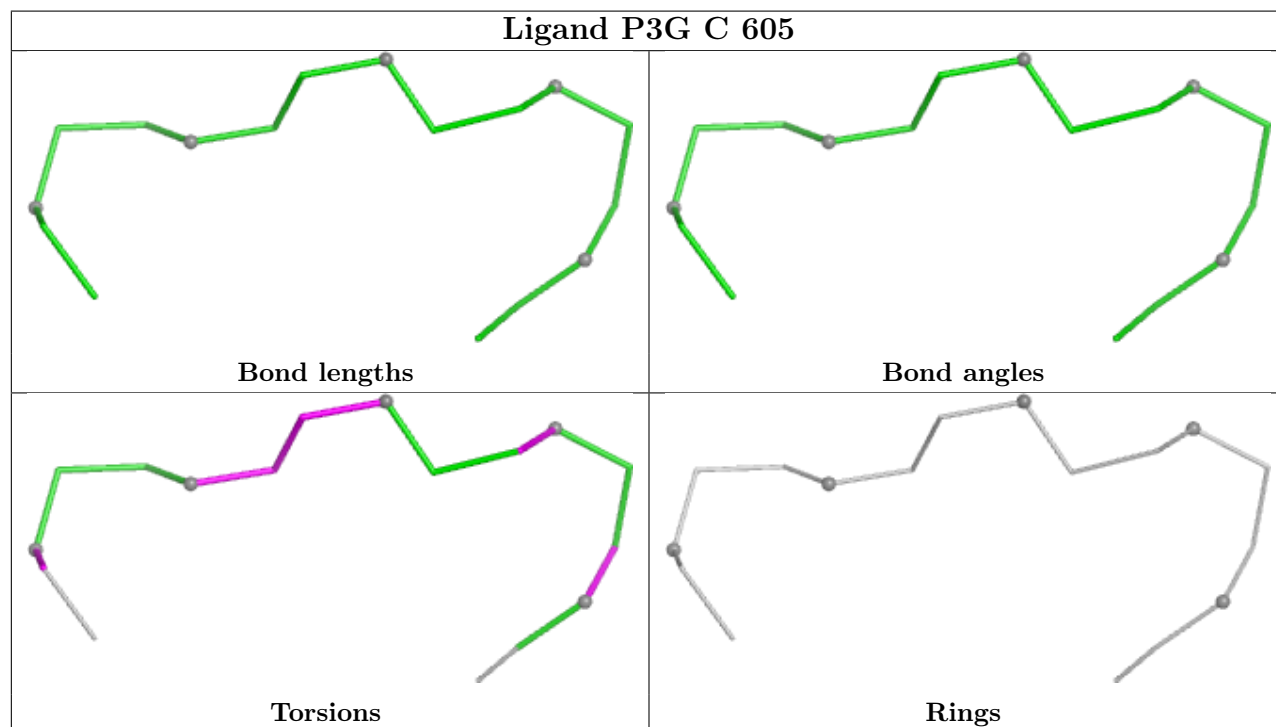
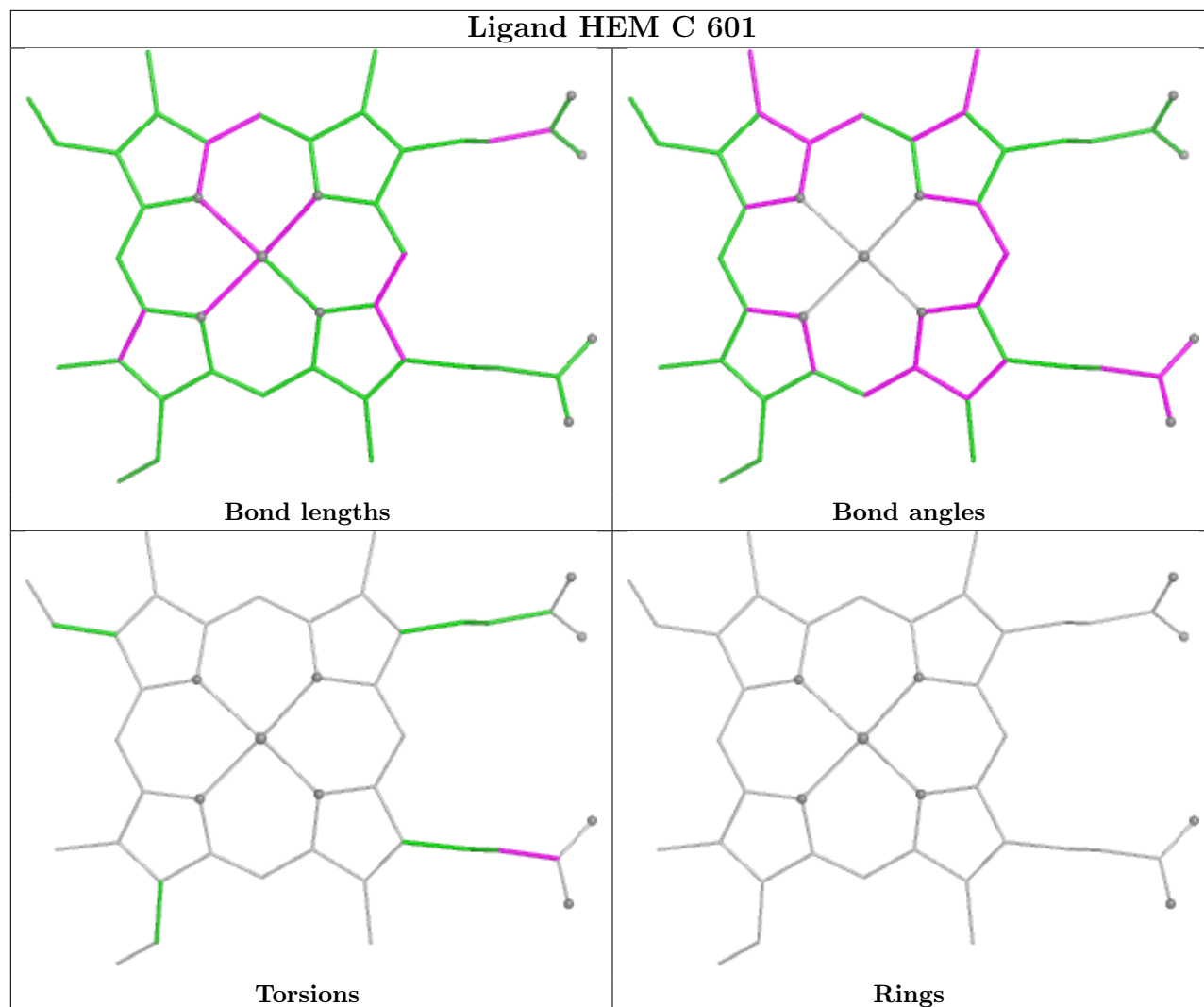
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	601	HEM	1	0
5	B	604	EDO	4	0
6	E	604	PEG	2	0
10	F	602	GLY	1	0
10	A	606	GLY	1	0
8	A	602	SER	1	0
4	E	601	HEM	1	0

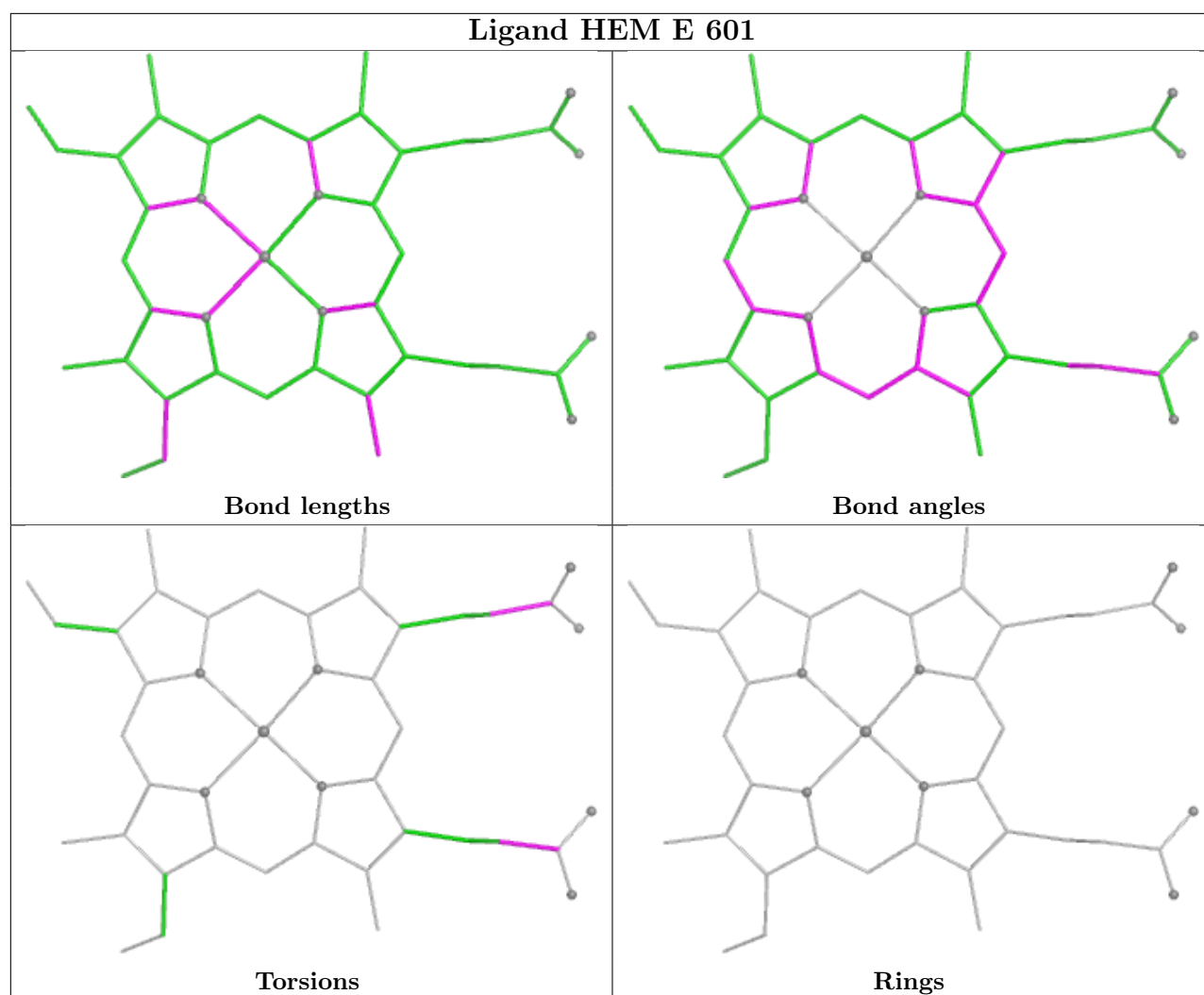
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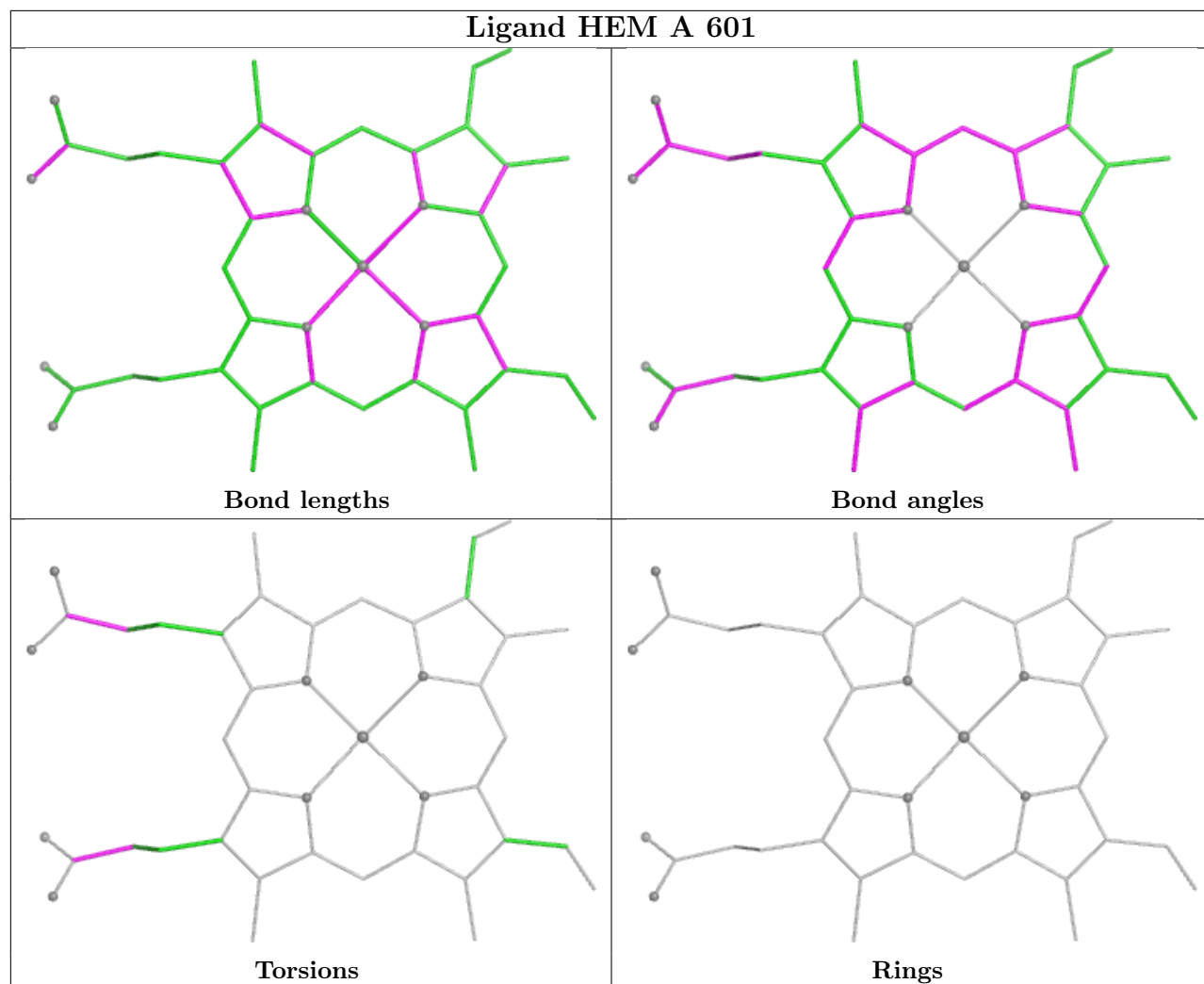
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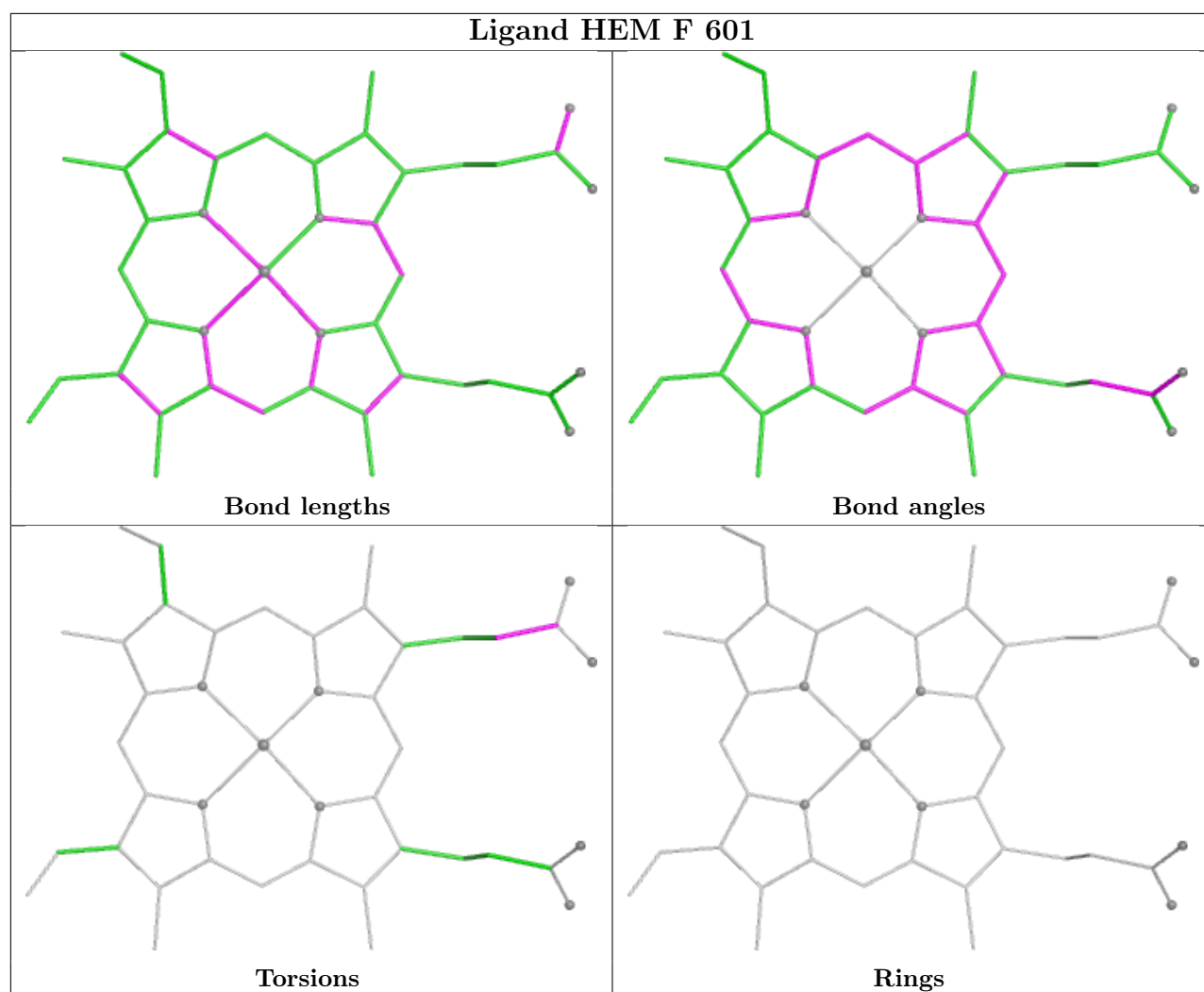
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	HEM	1	0
4	F	601	HEM	1	0
4	G	601	HEM	2	0
5	H	603	EDO	3	0
11	A	607	P4G	3	0
5	A	605	EDO	2	0
5	D	606	EDO	3	0
6	H	604	PEG	1	0
6	D	604	PEG	1	0
4	D	601	HEM	2	0
9	A	603	ALA	4	0
4	B	601	HEM	3	0
12	C	603	NAG	5	0
12	D	605	NAG	3	0
5	C	604	EDO	2	0
12	E	602	NAG	1	0

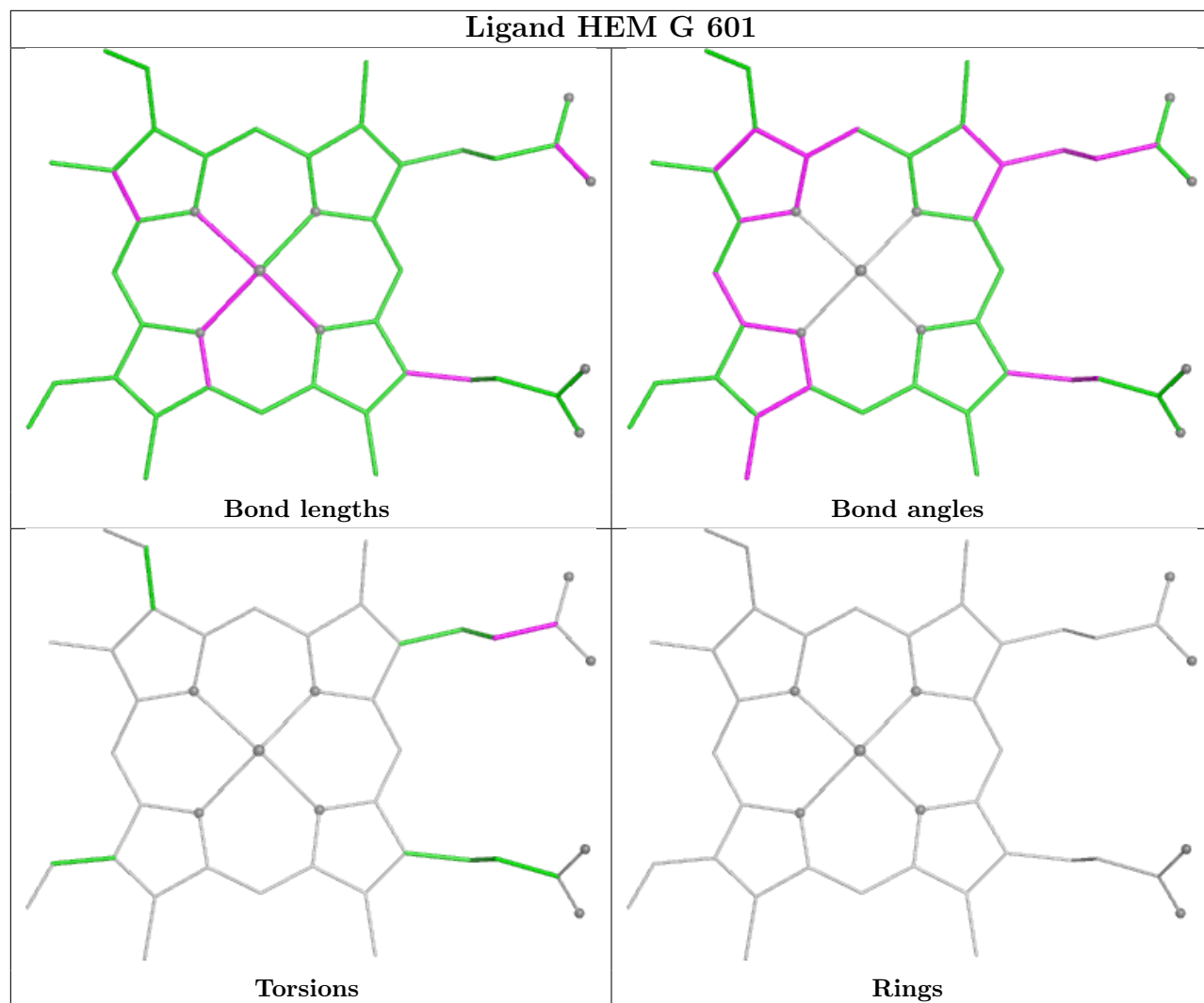
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

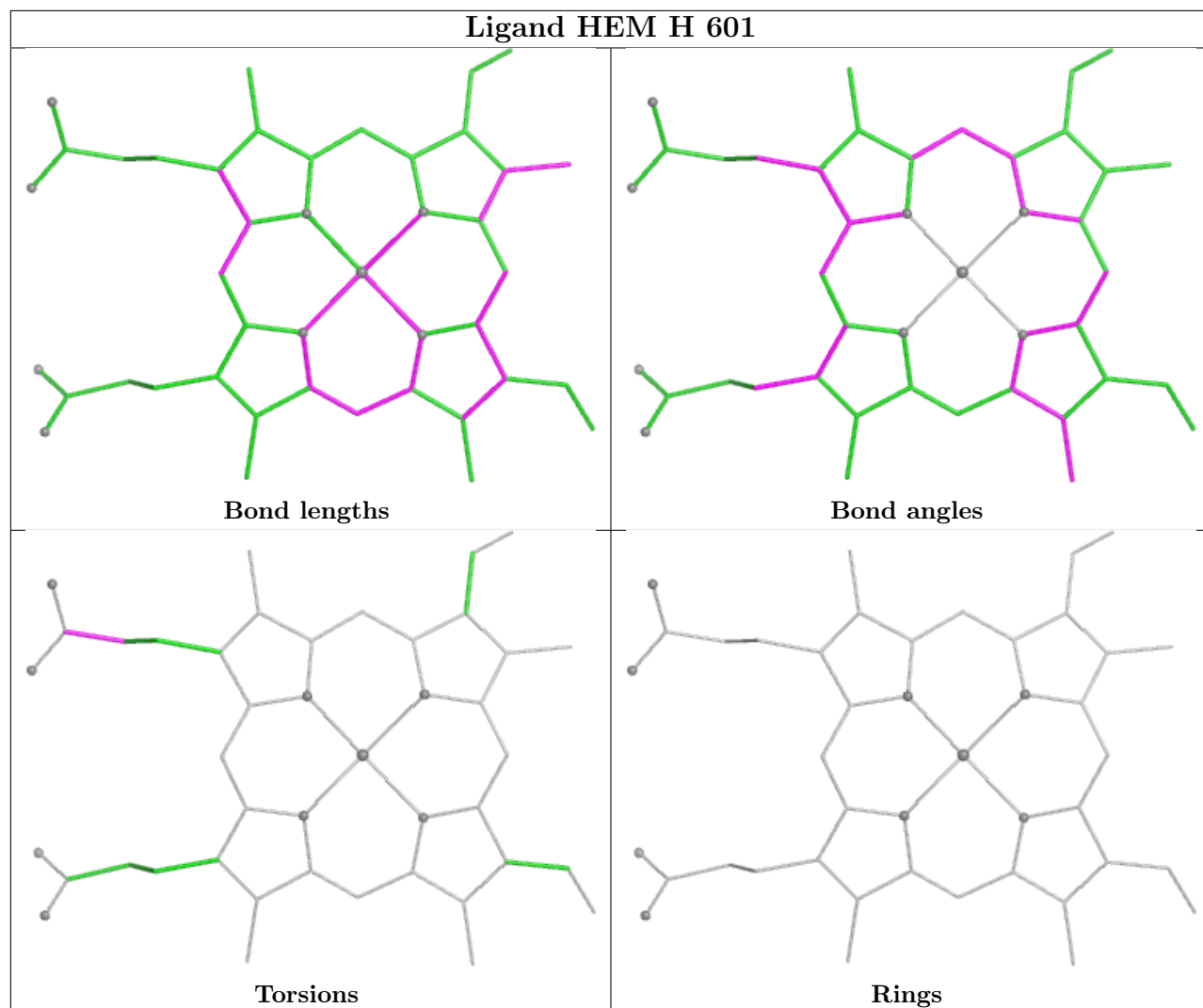


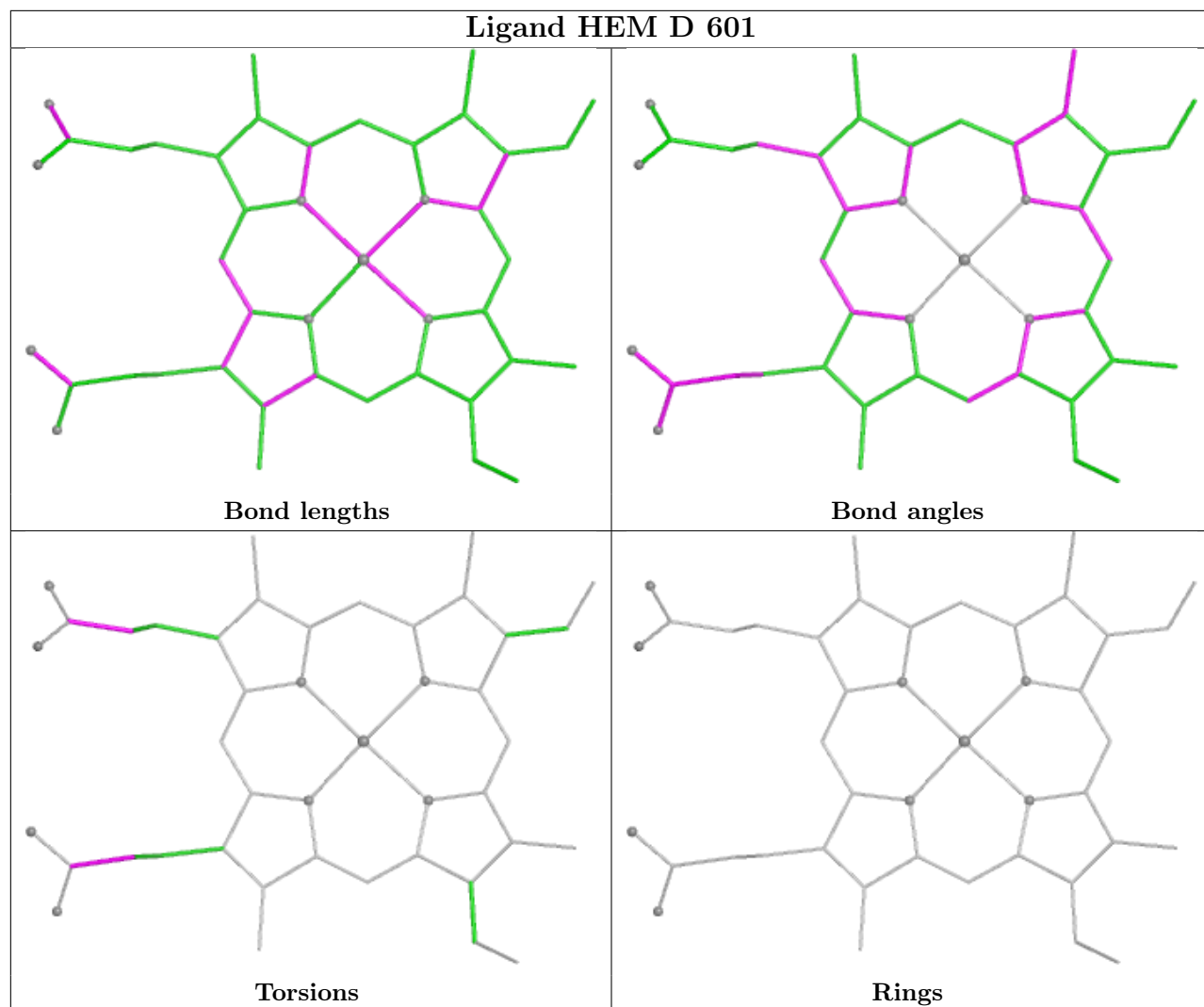


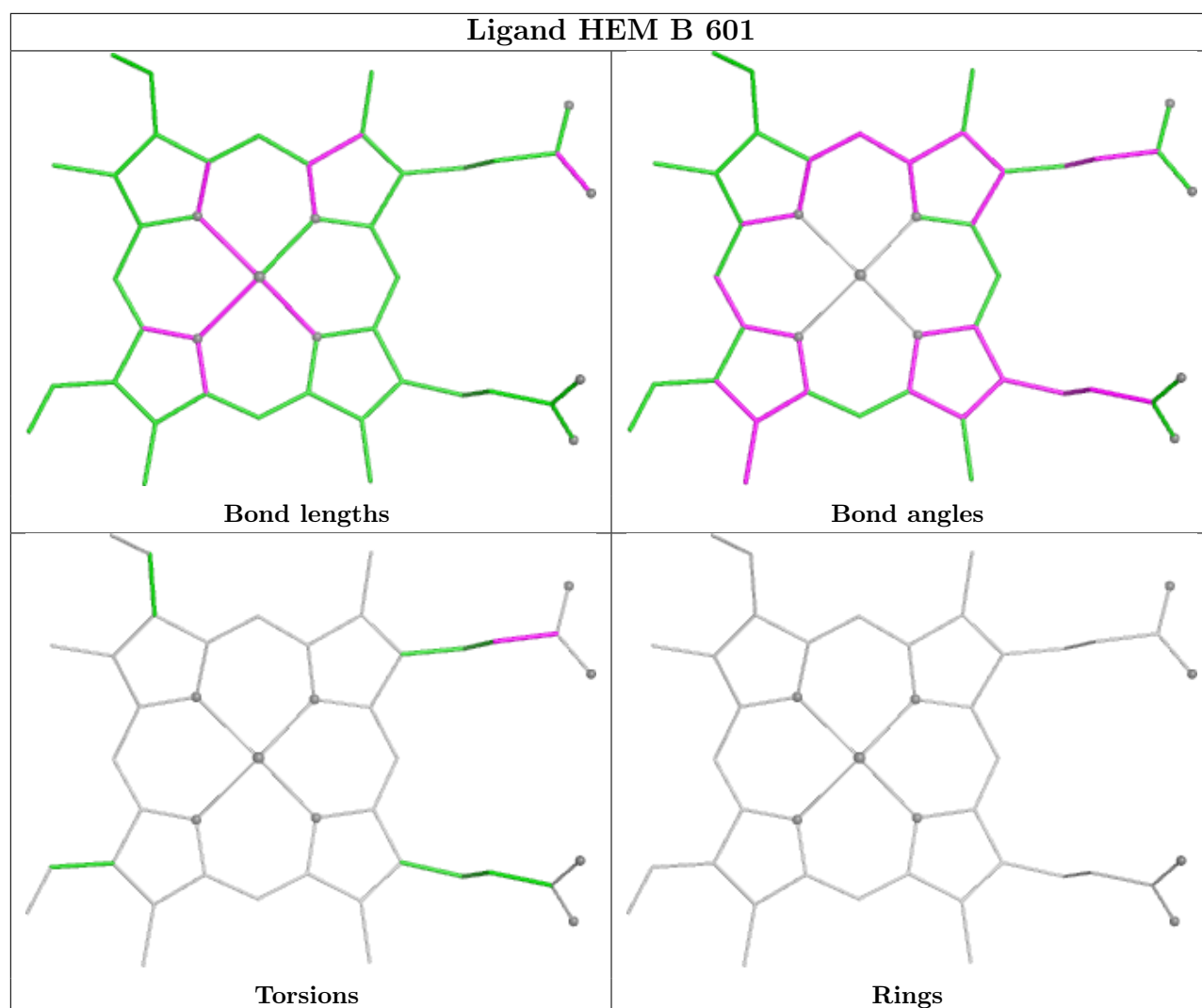












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	503/545 (92%)	0.06	7 (1%) 73 78	5, 15, 26, 39	10 (1%)
1	B	501/545 (91%)	0.24	8 (1%) 70 74	6, 18, 28, 43	5 (0%)
1	C	506/545 (92%)	0.12	7 (1%) 73 78	7, 17, 28, 50	6 (1%)
1	D	506/545 (92%)	0.16	10 (1%) 65 69	6, 17, 28, 53	8 (1%)
1	E	505/545 (92%)	0.32	18 (3%) 46 48	6, 19, 31, 50	9 (1%)
1	F	507/545 (93%)	0.27	17 (3%) 48 50	8, 19, 32, 51	7 (1%)
1	G	505/545 (92%)	0.34	8 (1%) 70 74	9, 19, 31, 47	4 (0%)
1	H	507/545 (93%)	0.21	2 (0%) 88 91	8, 19, 30, 45	8 (1%)
All	All	4040/4360 (92%)	0.21	77 (1%) 66 70	5, 18, 30, 53	57 (1%)

The worst 5 of 77 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	3	ALA	4.8
1	B	90	GLY	4.5
1	A	502	ALA	4.3
1	F	508	ALA	3.9
1	G	419	VAL	3.7

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

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

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

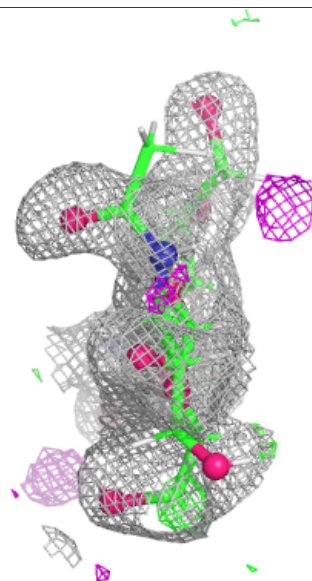
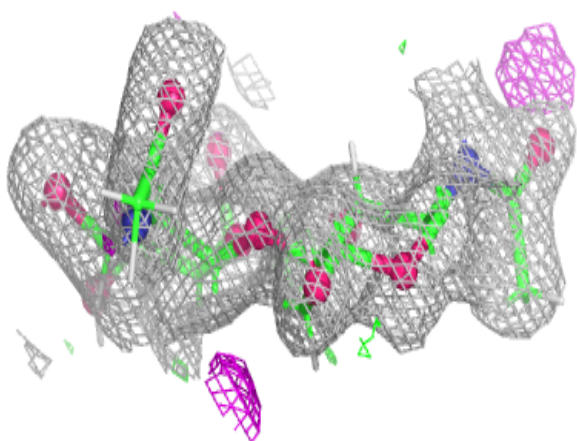
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MAN	J	5	11/12	0.74	0.14	35,42,45,51	4
2	NAG	K	2	14/15	0.75	0.15	34,39,46,53	6
3	MAN	J	7	11/12	0.77	0.17	32,38,43,47	4
2	NAG	I	2	14/15	0.79	0.15	32,42,48,57	6
3	MAN	J	4	11/12	0.80	0.14	30,36,41,45	3
3	BMA	J	3	11/12	0.90	0.09	22,25,35,35	2
3	MAN	J	6	11/12	0.90	0.09	24,28,35,35	3
3	NAG	J	2	14/15	0.90	0.10	17,22,35,35	5
2	NAG	K	1	14/15	0.92	0.09	17,20,35,35	6
3	NAG	J	1	14/15	0.94	0.06	12,15,35,35	5
2	NAG	I	1	14/15	0.95	0.07	17,21,35,35	6

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

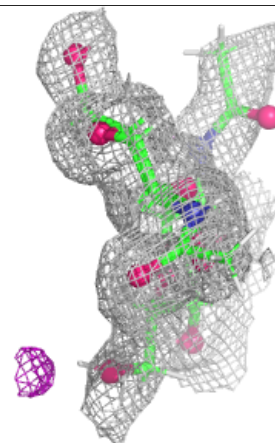
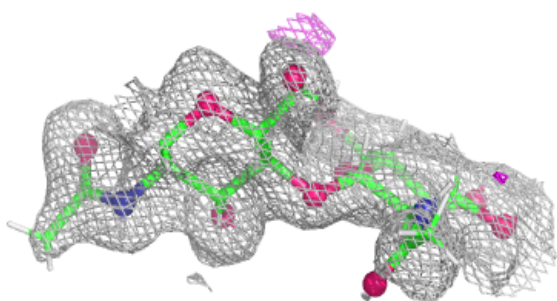
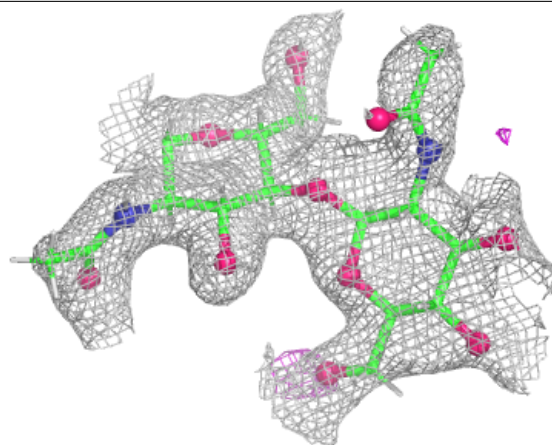
Electron density around Chain I:

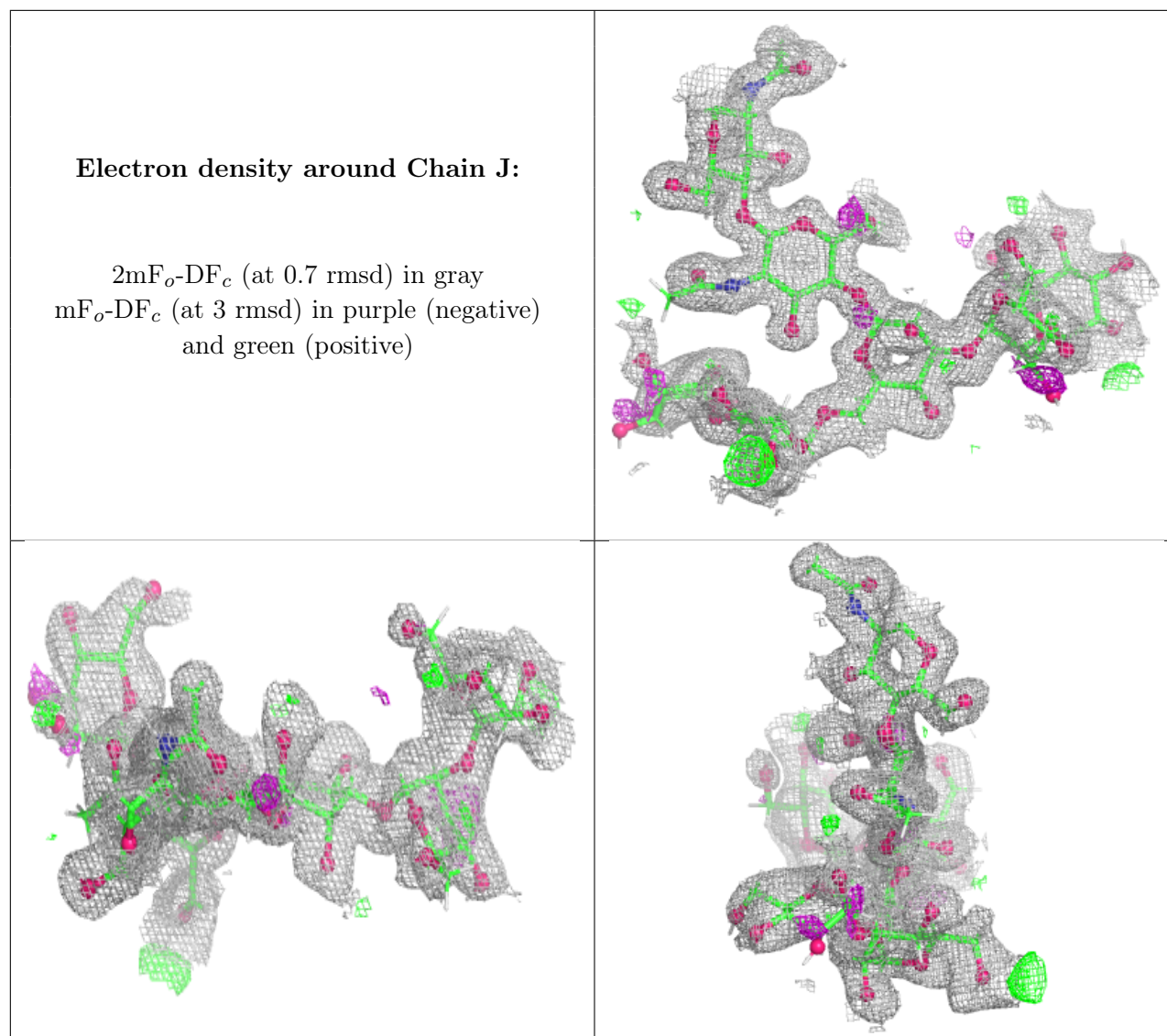
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain K:

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





6.4 Ligands [i](#)

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
12	NAG	C	603	14/15	0.75	0.14	30,40,44,47	7
6	PEG	E	604	7/7	0.76	0.14	30,44,48,49	2
5	EDO	E	603	4/4	0.80	0.15	30,38,39,39	2
8	SER	A	602	7/7	0.80	0.14	26,28,31,33	1
6	PEG	D	603	7/7	0.80	0.15	30,45,55,59	2
13	P3G	C	605	17/17	0.81	0.14	47,50,55,56	0
6	PEG	A	608	7/7	0.82	0.12	30,42,43,43	2

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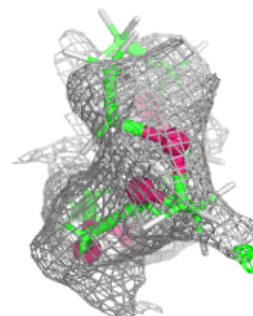
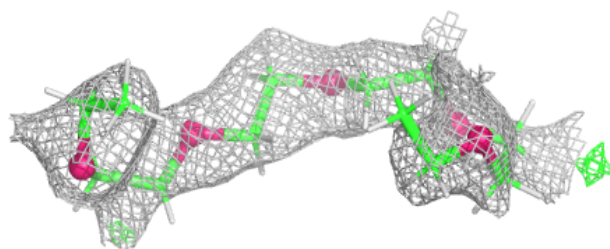
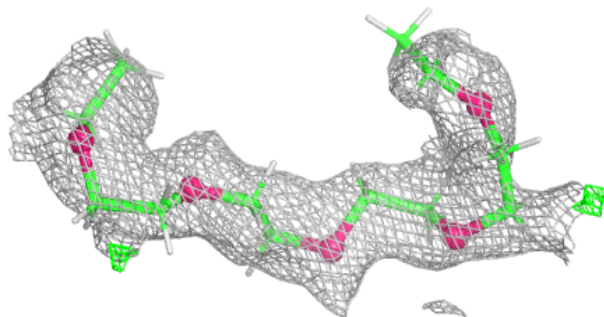
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	D	606	4/4	0.82	0.15	26,30,32,32	2
6	PEG	H	605	7/7	0.83	0.11	30,45,47,47	2
12	NAG	D	605	14/15	0.84	0.12	30,40,44,47	7
9	ALA	A	603	6/6	0.85	0.14	25,29,35,37	0
5	EDO	E	605	4/4	0.86	0.14	25,29,30,31	2
10	GLY	F	602	5/5	0.86	0.13	36,40,43,45	0
12	NAG	B	603	14/15	0.86	0.11	27,30,40,40	7
6	PEG	D	604	7/7	0.87	0.12	30,35,39,39	2
6	PEG	H	604	7/7	0.87	0.11	30,36,39,39	2
5	EDO	A	604	4/4	0.87	0.13	30,38,39,39	2
5	EDO	B	604	4/4	0.88	0.11	23,30,32,32	2
11	P4G	A	607	11/11	0.88	0.10	30,34,41,43	0
5	EDO	H	602	4/4	0.89	0.11	30,34,35,37	2
5	EDO	A	605	4/4	0.90	0.10	30,38,41,43	2
10	GLY	A	606	5/5	0.90	0.14	26,31,33,33	0
5	EDO	C	604	4/4	0.91	0.11	30,37,38,39	2
12	NAG	B	602	14/15	0.91	0.08	20,23,30,30	6
5	EDO	H	603	4/4	0.91	0.11	29,33,35,36	2
12	NAG	G	602	14/15	0.93	0.07	21,25,30,30	7
12	NAG	D	602	14/15	0.93	0.08	19,22,30,30	7
7	NA	H	606	1/1	0.94	0.10	20,20,20,20	0
12	NAG	E	602	14/15	0.94	0.07	19,24,30,30	7
12	NAG	C	602	14/15	0.95	0.07	18,20,30,30	6
4	HEM	F	601	43/43	0.97	0.06	12,14,16,17	0
4	HEM	G	601	43/43	0.97	0.07	12,14,16,17	0
4	HEM	A	601	43/43	0.97	0.07	10,12,14,16	0
4	HEM	C	601	43/43	0.97	0.06	11,12,14,15	0
4	HEM	B	601	43/43	0.98	0.06	11,13,16,17	0
4	HEM	H	601	43/43	0.98	0.06	12,13,15,16	0
4	HEM	D	601	43/43	0.98	0.06	11,12,13,14	0
4	HEM	E	601	43/43	0.98	0.07	12,13,15,15	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.

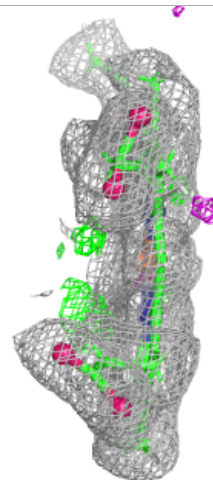
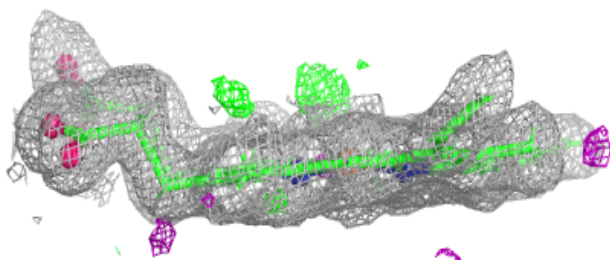
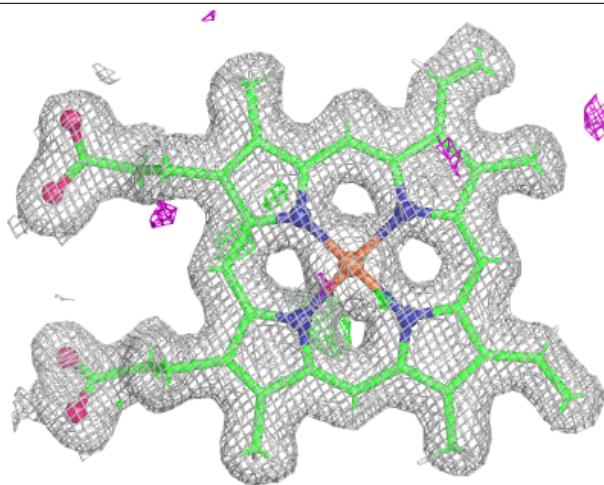
Electron density around P3G C 605:

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



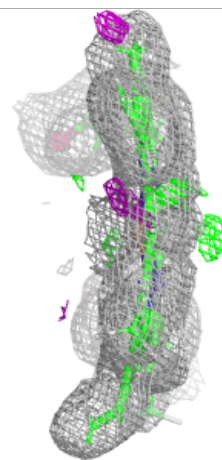
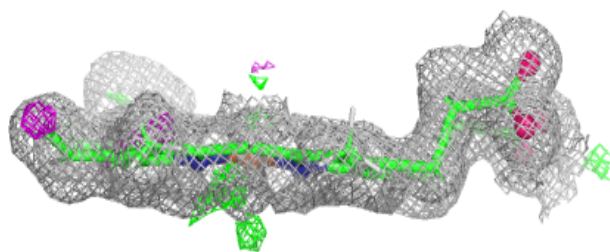
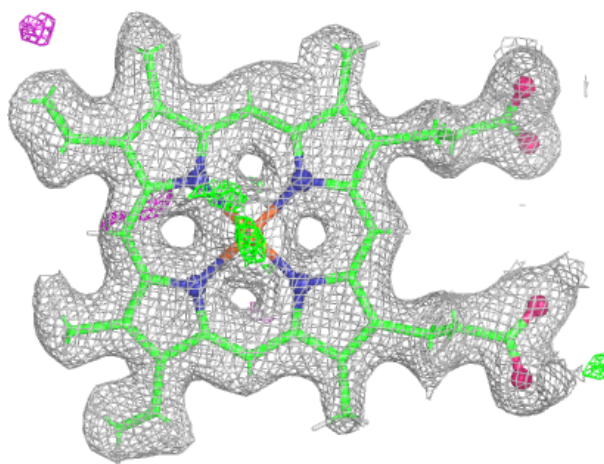
Electron density around HEM F 601:

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



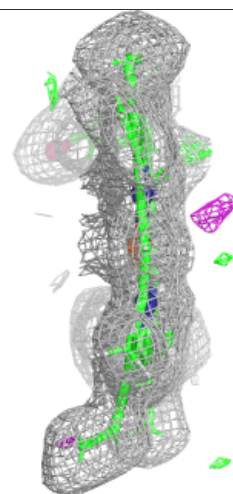
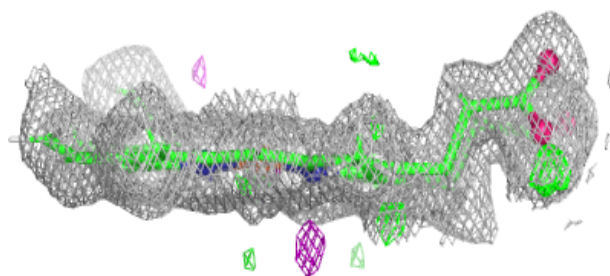
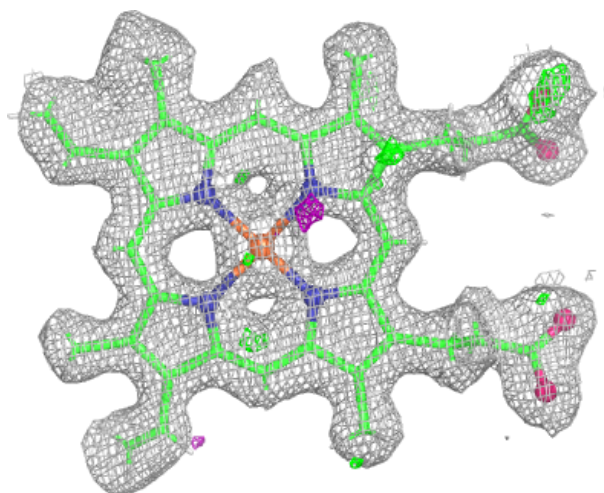
Electron density around HEM G 601:

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



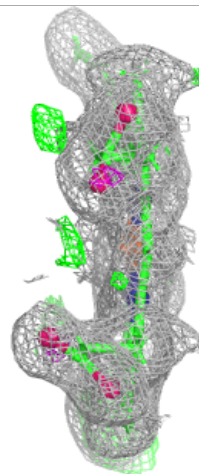
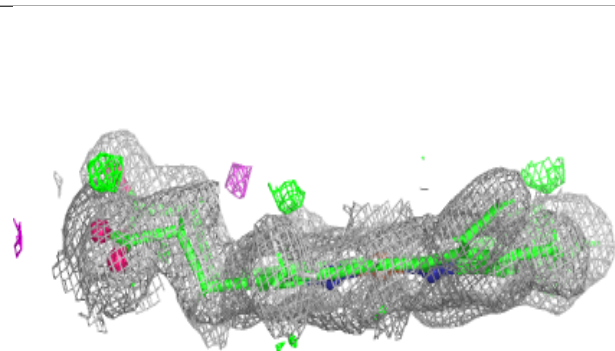
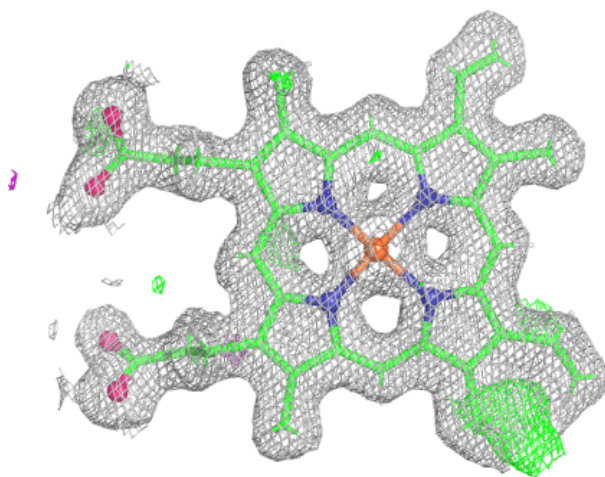
Electron density around HEM A 601:

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



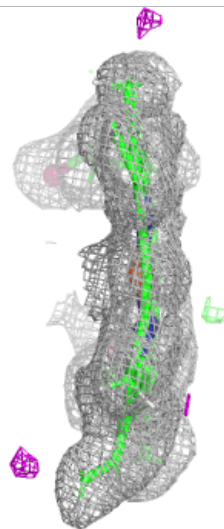
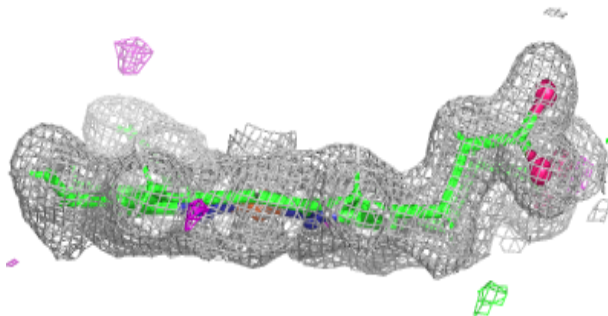
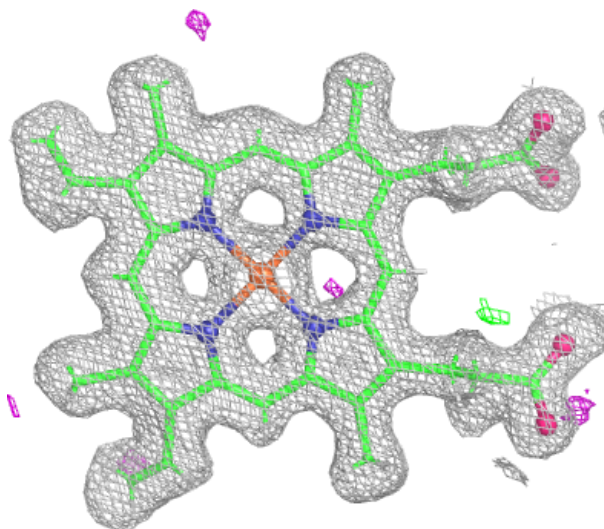
Electron density around HEM C 601:

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



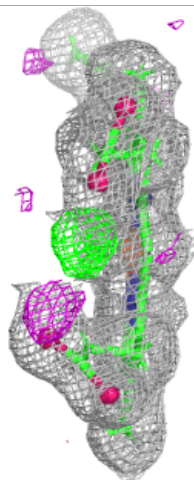
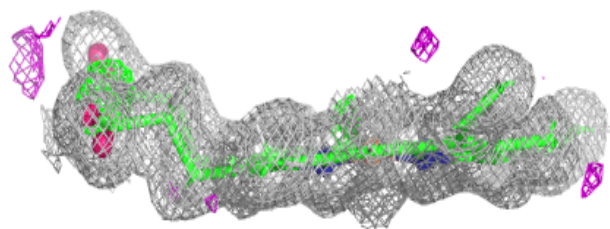
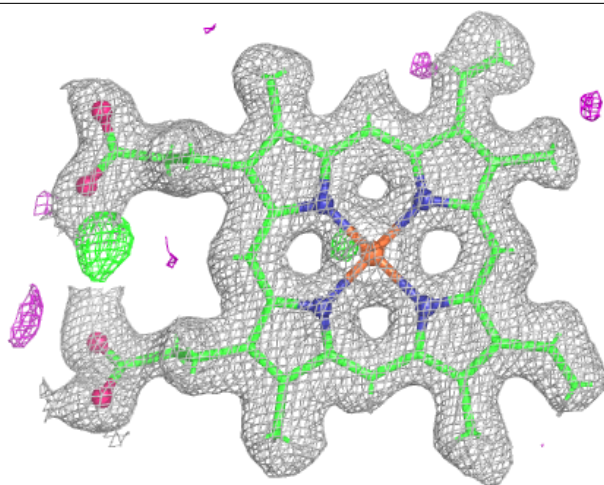
Electron density around HEM B 601:

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



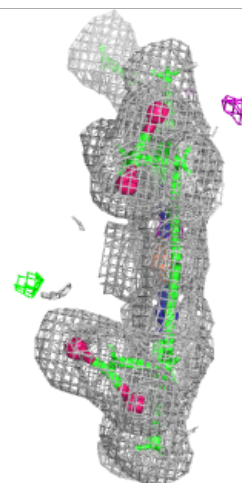
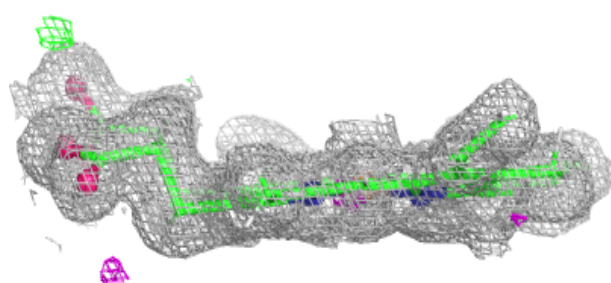
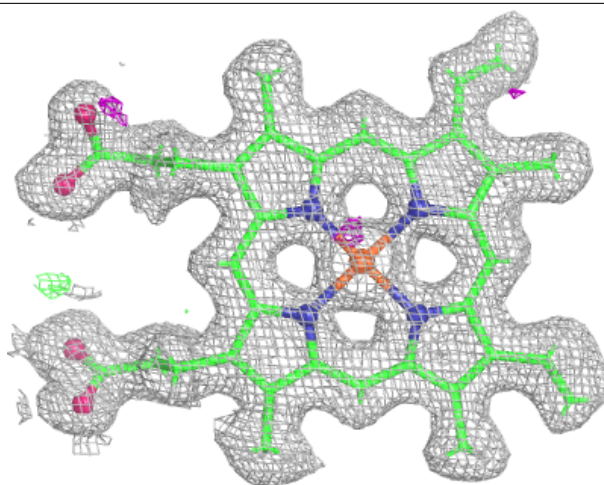
Electron density around HEM H 601:

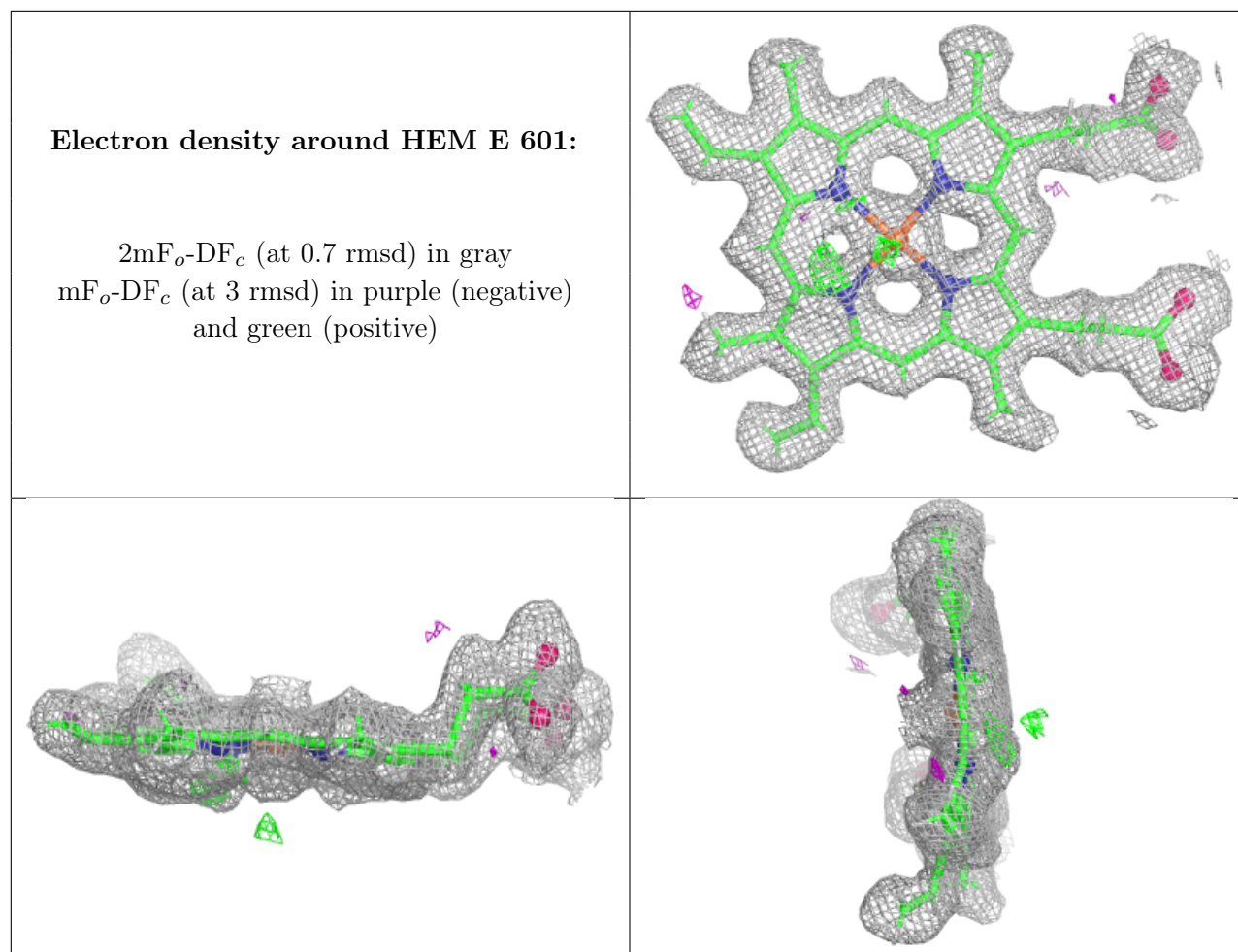
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.