



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 13, 2026 – 05:23 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 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:

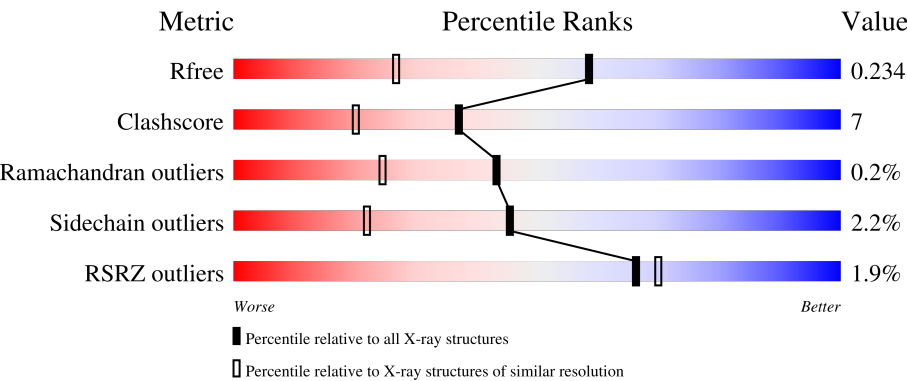
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

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	% 78%13%•8%
1	B	545	% 80%11%•8%
1	C	545	% 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

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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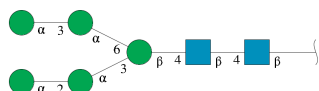
Chain	Residue	Modelled	Actual	Comment	Reference
G	512	LYS	-	expression tag	UNP A0AB34KRF0
G	513	LEU	-	expression tag	UNP A0AB34KRF0
G	514	ILE	-	expression tag	UNP A0AB34KRF0
G	515	SER	-	expression tag	UNP A0AB34KRF0
G	516	GLU	-	expression tag	UNP A0AB34KRF0
G	517	GLU	-	expression tag	UNP A0AB34KRF0
G	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.



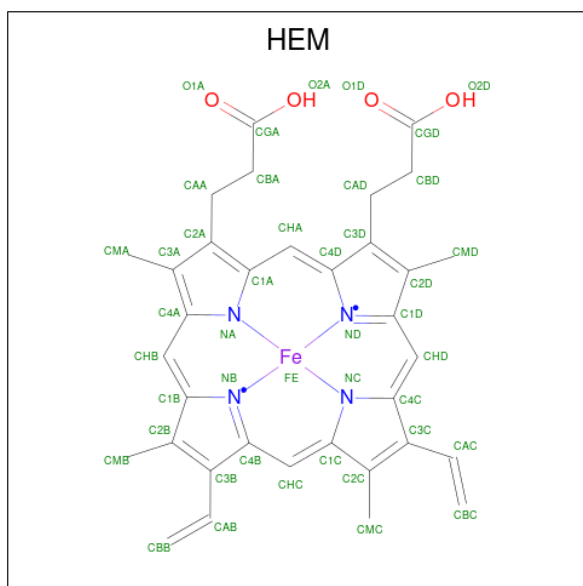
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	2	Total	C	H	N	O	12	0	0
			55	16	27	2	10			
2	K	2	Total	C	H	N	O	12	0	0
			55	16	27	2	10			

- 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.



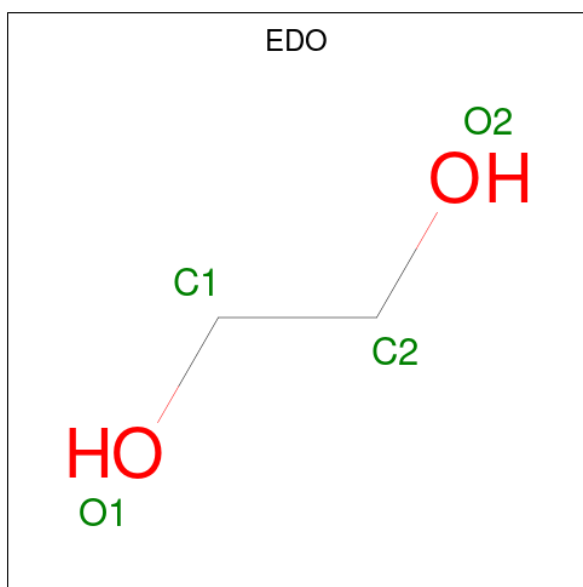
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	7	Total	C	H	N	O	26	0	0
			160	46	77	2	35			

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



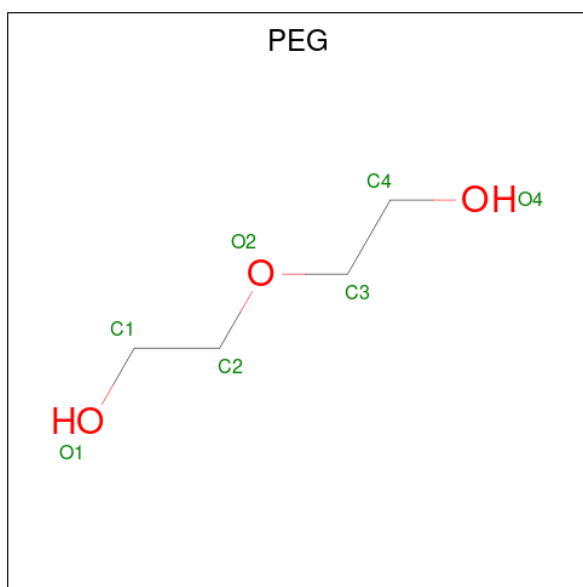
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	H	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
4	A	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
4	B	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
4	C	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
4	D	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
4	E	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
4	F	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
4	G	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



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).

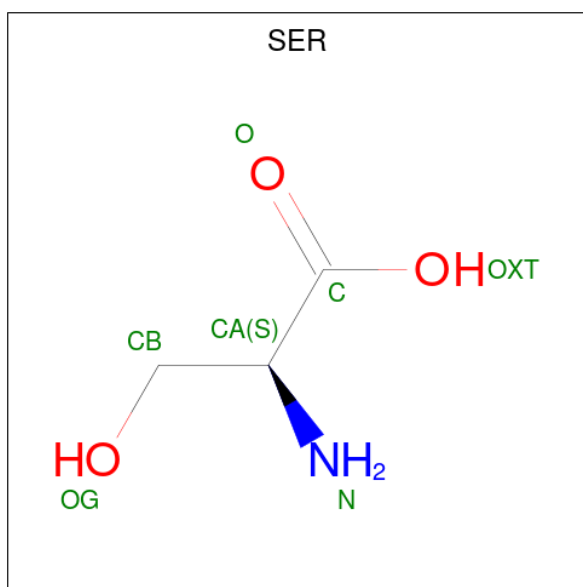


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	H	1	Total	C	H	O	2	0
			17	4	10	3		
6	H	1	Total	C	H	O	2	0
			17	4	10	3		
6	A	1	Total	C	H	O	2	0
			17	4	10	3		
6	D	1	Total	C	H	O	2	0
			17	4	10	3		
6	D	1	Total	C	H	O	2	0
			17	4	10	3		
6	E	1	Total	C	H	O	2	0
			17	4	10	3		

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

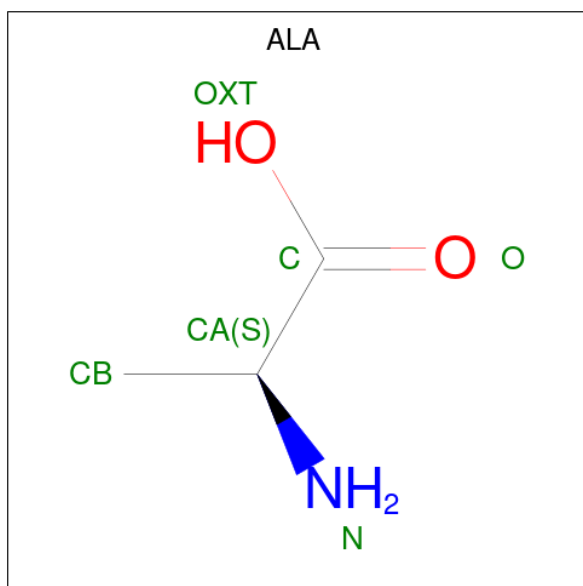
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	1	Total	Na	0	0
			1	1		

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



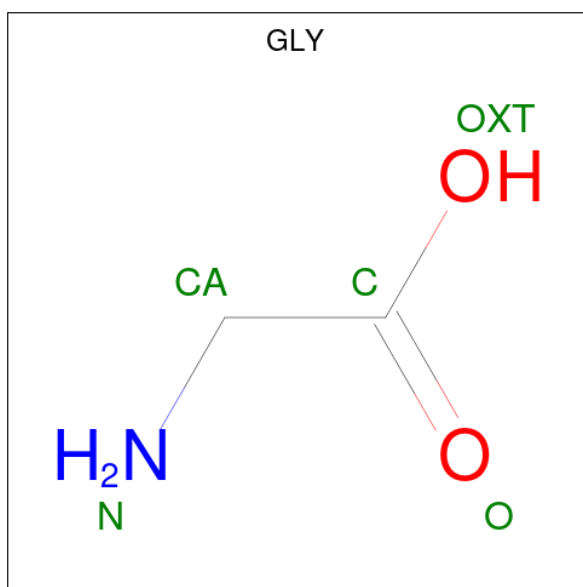
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	H	N	O	1	0
			14	3	7	1	3		

- Molecule 9 is ALANINE (CCD ID: ALA) (formula: $\text{C}_3\text{H}_7\text{NO}_2$).



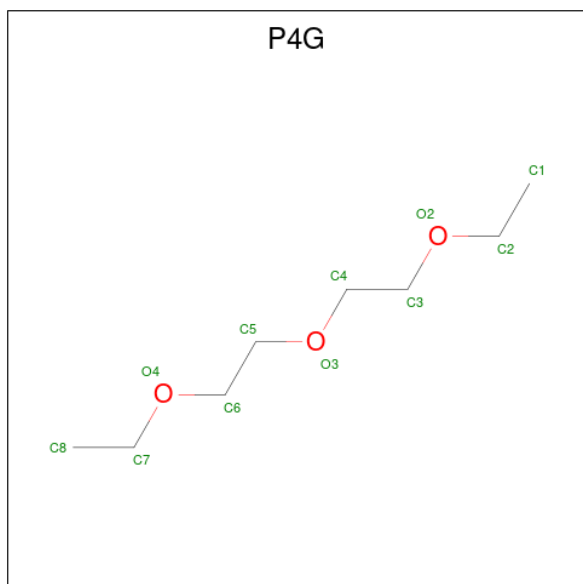
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	H	N	O	0	0
			13	3	7	1	2		

- Molecule 10 is GLYCINE (CCD ID: GLY) (formula: $\text{C}_2\text{H}_5\text{NO}_2$).



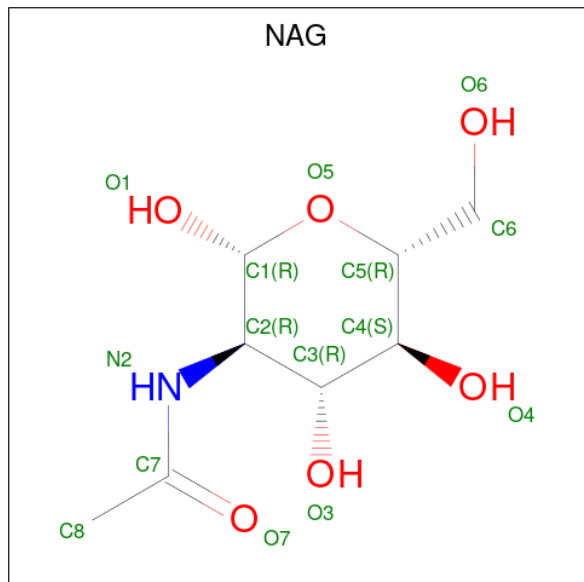
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	A	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
10	F	1	Total	C	H	N	O	0	0
			10	2	5	1	2		

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



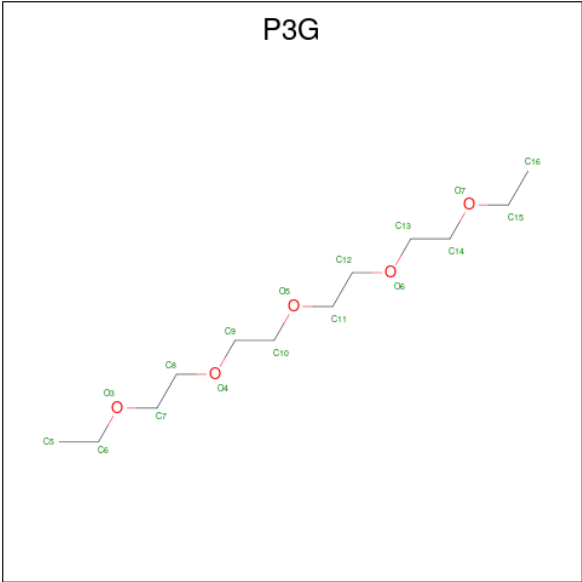
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	H	O	0	0
			29	8	18	3		

- 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		

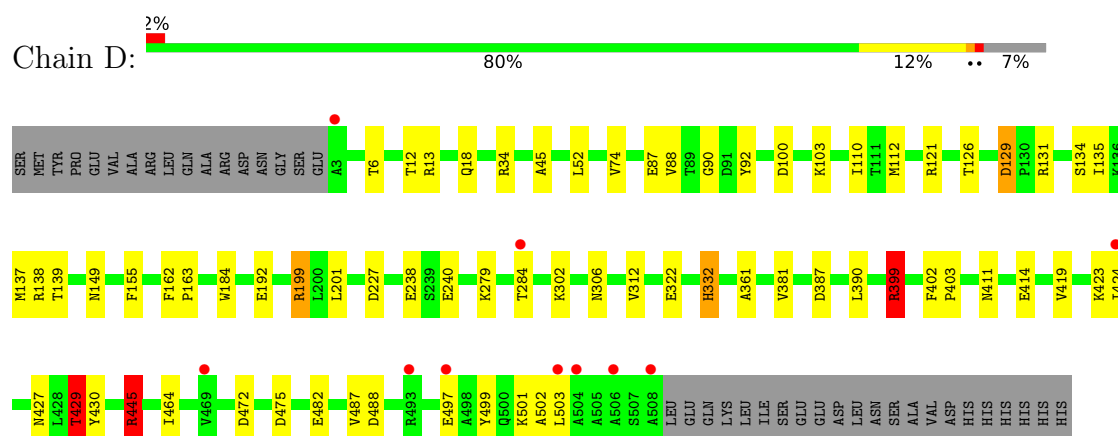
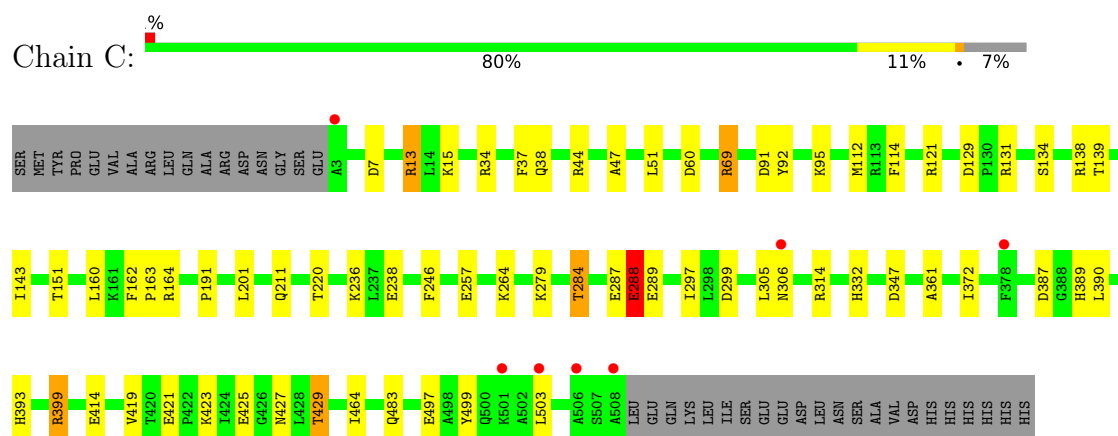
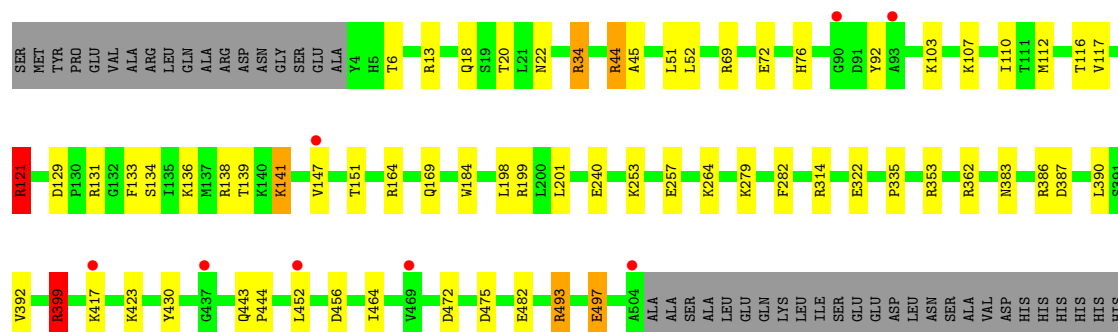
- Molecule 13 is 3,6,9,12,15-PENTAOXAHEPTADECANE (CCD ID: P3G) (formula: $C_{12}H_{26}O_5$).



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 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

All (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
1	H	399	ARG	NE-CZ-NH2	-9.78	110.40	119.20
1	D	445	ARG	CD-NE-CZ	9.64	137.90	124.40
1	E	100	ASP	CA-CB-CG	9.29	121.89	112.60
1	A	211	GLN	CB-CA-C	-9.17	93.66	110.63
1	D	6	THR	CA-CB-OG1	9.13	123.30	109.60
1	D	199	ARG	CD-NE-CZ	9.03	137.04	124.40
1	E	100	ASP	CB-CA-C	8.81	125.82	110.85
1	D	429	THR	CA-CB-OG1	8.74	122.71	109.60
1	E	226	ASP	CA-CB-CG	8.72	121.32	112.60
1	F	303	ASP	CA-CB-CG	8.54	121.14	112.60
1	D	6	THR	OG1-CB-CG2	-8.32	92.65	109.30
1	E	284	THR	N-CA-CB	-7.73	97.30	111.13
1	C	288	GLU	N-CA-CB	7.64	121.47	110.16
1	B	199	ARG	CD-NE-CZ	7.57	134.99	124.40
1	F	108	THR	CA-CB-OG1	7.50	120.84	109.60
1	C	34	ARG	N-CA-CB	7.33	120.74	109.97
1	C	289	GLU	CB-CA-C	-7.06	99.79	110.88
1	A	472	ASP	CA-CB-CG	7.00	119.60	112.60
1	H	445	ARG	NE-CZ-NH1	6.87	128.37	121.50
1	F	121	ARG	N-CA-CB	-6.82	98.66	109.78
1	G	121	ARG	N-CA-CB	-6.82	98.97	110.49
1	D	129	ASP	CA-CB-CG	6.80	119.40	112.60
1	D	445	ARG	NE-CZ-NH2	-6.71	113.16	119.20
1	E	429	THR	CA-CB-OG1	6.70	119.65	109.60
1	B	482	GLU	CB-CA-C	-6.68	99.70	110.79
1	A	299	ASP	CA-CB-CG	6.63	119.23	112.60
1	B	282[A]	PHE	CA-CB-CG	6.63	120.43	113.80
1	B	282[B]	PHE	CA-CB-CG	6.63	120.43	113.80
1	H	303	ASP	CA-CB-CG	6.56	119.16	112.60
1	D	227	ASP	CA-CB-CG	6.54	119.14	112.60
1	G	211	GLN	N-CA-CB	6.45	121.09	110.39
1	F	442	GLU	CB-CG-CD	-6.38	101.76	112.60
1	C	246	PHE	CA-CB-CG	6.33	120.13	113.80
1	C	121	ARG	N-CA-CB	-6.31	99.49	109.78
1	C	305	LEU	CA-C-N	-6.20	113.19	122.24
1	C	305	LEU	C-N-CA	-6.20	113.19	122.24
1	E	268	ASP	CA-CB-CG	6.19	118.79	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	386	ARG	CD-NE-CZ	6.17	133.04	124.40
1	G	347	ASP	CA-CB-CG	6.10	118.70	112.60
1	B	456	ASP	CA-CB-CG	6.09	118.69	112.60
1	B	92	TYR	N-CA-CB	6.07	118.76	109.91
1	H	445	ARG	NE-CZ-NH2	-5.95	113.84	119.20
1	C	288	GLU	CB-CA-C	-5.95	100.73	110.85
1	H	340	GLU	CB-CG-CD	-5.94	102.50	112.60
1	H	399	ARG	NE-CZ-NH1	5.85	127.35	121.50
1	A	458	ASP	CA-CB-CG	5.84	118.44	112.60
1	E	148	PHE	CA-CB-CG	5.84	119.64	113.80
1	E	456	ASP	CA-CB-CG	5.82	118.42	112.60
1	D	497	GLU	CB-CG-CD	5.82	122.49	112.60
1	C	7	ASP	CA-CB-CG	5.79	118.39	112.60
1	G	60	ASP	CA-CB-CG	5.78	118.38	112.60
1	D	121	ARG	NE-CZ-NH2	5.76	124.39	119.20
1	G	129	ASP	CA-CB-CG	5.76	118.36	112.60
1	C	60	ASP	CA-CB-CG	5.76	118.36	112.60
1	G	211	GLN	CB-CA-C	-5.72	98.36	110.31
1	G	141	LYS	CB-CA-C	-5.71	102.26	111.28
1	A	474	ASP	CA-CB-CG	5.70	118.30	112.60
1	A	60	ASP	CA-CB-CG	5.67	118.27	112.60
1	D	121	ARG	N-CA-CB	-5.67	100.92	110.49
1	B	121	ARG	CA-C-O	5.65	126.19	120.88
1	G	286	THR	CA-CB-OG1	-5.62	101.17	109.60
1	A	385	ASP	CA-CB-CG	5.59	118.19	112.60
1	C	389	HIS	CA-CB-CG	5.56	119.36	113.80
1	B	475	ASP	CA-CB-CG	5.55	118.15	112.60
1	F	347	ASP	CA-CB-CG	5.53	118.13	112.60
1	B	399	ARG	CB-CA-C	-5.53	99.73	109.62
1	D	399	ARG	NE-CZ-NH1	-5.47	116.03	121.50
1	F	347	ASP	CB-CA-C	5.47	117.86	109.60
1	D	149	ASN	CA-CB-CG	5.44	118.04	112.60
1	A	7	ASP	CA-CB-CG	5.43	118.03	112.60
1	C	211	GLN	CB-CA-C	-5.40	99.02	110.31
1	G	329	GLU	N-CA-CB	5.40	118.05	110.12
1	A	246	PHE	CA-CB-CG	5.39	119.19	113.80
1	D	475	ASP	CA-CB-CG	5.38	117.98	112.60
1	C	299	ASP	CA-CB-CG	5.34	117.94	112.60
1	D	488	ASP	CA-CB-CG	5.32	117.92	112.60
1	B	497	GLU	CB-CG-CD	5.28	121.57	112.60
1	D	192	GLU	CB-CG-CD	5.27	121.56	112.60
1	C	121	ARG	CG-CD-NE	-5.26	100.42	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	179	ASP	CA-CB-CG	5.25	117.85	112.60
1	B	133	PHE	CB-CA-C	5.25	118.58	111.70
1	E	274	ASP	CA-CB-CG	5.24	117.84	112.60
1	E	284	THR	CB-CA-C	5.23	120.00	109.38
1	H	347	ASP	CA-CB-CG	5.22	117.82	112.60
1	F	171	THR	CA-CB-OG1	-5.21	101.78	109.60
1	A	34	ARG	CG-CD-NE	-5.19	100.59	112.00
1	F	287	GLU	CG-CD-OE2	-5.18	106.48	118.40
1	A	484	PHE	CA-CB-CG	5.17	118.97	113.80
1	F	423	LYS	N-CA-CB	5.15	117.58	110.17
1	H	484	PHE	CA-CB-CG	5.14	118.94	113.80
1	C	306	ASN	CB-CA-C	5.13	118.77	111.74
1	A	65	PHE	CA-CB-CG	5.13	118.93	113.80
1	E	130	PRO	N-CA-CB	5.12	108.20	103.39
1	C	284	THR	OG1-CB-CG2	5.12	119.54	109.30
1	F	461	HIS	CA-CB-CG	5.09	118.89	113.80
1	F	129	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	157	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	D	155	PHE	CA-CB-CG	5.08	118.88	113.80
1	C	347	ASP	CA-CB-CG	5.08	117.68	112.60
1	E	44	ARG	CB-CA-C	-5.07	98.31	109.56
1	H	312	VAL	N-CA-CB	-5.07	102.87	111.23
1	B	164	ARG	CA-C-N	5.06	127.02	120.44
1	B	164	ARG	C-N-CA	5.06	127.02	120.44
1	C	429	THR	CA-CB-OG1	5.02	117.13	109.60
1	F	152	PRO	N-CA-CB	-5.02	98.69	103.41
1	H	325	HIS	CA-C-N	5.02	126.96	120.44
1	H	325	HIS	C-N-CA	5.02	126.96	120.44
1	D	472	ASP	CA-CB-CG	5.01	117.61	112.60
1	E	165	PHE	CA-CB-CG	-5.01	108.79	113.80
1	H	129	ASP	CA-CB-CG	5.01	117.61	112.60
1	A	343	GLU	O-C-N	-5.01	117.64	121.55

There are no chirality outliers.

All (52) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	ARG	Sidechain
1	A	131	ARG	Sidechain
1	A	138	ARG	Sidechain
1	A	34	ARG	Sidechain
1	A	364	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	493[A]	ARG	Sidechain
1	A	493[B]	ARG	Sidechain
1	A	69	ARG	Sidechain
1	B	121	ARG	Sidechain
1	B	131	ARG	Sidechain
1	B	138	ARG	Sidechain
1	B	314	ARG	Sidechain
1	B	362	ARG	Sidechain
1	B	399	ARG	Sidechain
1	B	44	ARG	Sidechain
1	B	493[A]	ARG	Sidechain
1	B	69	ARG	Sidechain
1	C	13[A]	ARG	Sidechain
1	C	131	ARG	Sidechain
1	C	399	ARG	Sidechain
1	C	69	ARG	Sidechain
1	D	131	ARG	Sidechain
1	D	138	ARG	Sidechain
1	D	34	ARG	Sidechain
1	D	399	ARG	Sidechain
1	D	445	ARG	Sidechain
1	E	13	ARG	Sidechain
1	E	131	ARG	Sidechain
1	E	138	ARG	Sidechain
1	E	199[A]	ARG	Sidechain
1	E	493	ARG	Sidechain
1	E	67	ARG	Sidechain
1	E	69	ARG	Sidechain
1	F	121	ARG	Sidechain
1	F	131	ARG	Sidechain
1	F	199[A]	ARG	Sidechain
1	F	44	ARG	Sidechain
1	F	69	ARG	Sidechain
1	G	121	ARG	Sidechain
1	G	131	ARG	Sidechain
1	G	34[A]	ARG	Sidechain
1	G	493	ARG	Sidechain
1	G	69	ARG	Sidechain
1	H	121	ARG	Sidechain
1	H	131	ARG	Sidechain
1	H	138	ARG	Sidechain
1	H	34[A]	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	H	34[B]	ARG	Sidechain
1	H	399	ARG	Sidechain
1	H	445	ARG	Sidechain
1	H	493	ARG	Sidechain
1	H	69	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
1:G:445:ARG:HD3	1:G:487:VAL:O	1.52	1.09
1:C:427:ASN:ND2	12:C:603:NAG:C1	2.17	1.08
1:H:445:ARG:HD3	1:H:487:VAL:O	1.65	0.96
1:C:427:ASN:HD21	12:C:603:NAG:C1	1.77	0.95
1:B:6:THR:HG23	14:B:1204:HOH:O	1.68	0.94
1:E:264:LYS:HG3	14:E:1117:HOH:O	1.65	0.94
1:H:399:ARG:HD2	14:H:1034:HOH:O	1.68	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6:THR:HG23	14:F:1200:HOH:O	1.67	0.93
1:D:445:ARG:CD	1:D:487:VAL:O	2.17	0.92
1:C:112[A]:MET:HE1	1:C:114:PHE:CZ	2.04	0.90
1:E:13:ARG:HD2	1:F:13:ARG:CZ	2.02	0.89
1:A:390:LEU:HD12	1:B:390:LEU:HD12	1.52	0.88
1:E:201[A]:LEU:HD22	1:E:464:ILE:HG12	1.56	0.87
1:H:264:LYS:HG3	14:H:1128:HOH:O	1.73	0.87
1:A:399[A]:ARG:NH2	1:B:18:GLN:O	2.08	0.85
14:C:995:HOH:O	5:D:606:EDO:H11	1.76	0.85
14:C:1105:HOH:O	1:D:390:LEU:CD1	2.24	0.85
1:A:493[A]:ARG:HB3	1:A:493[A]:ARG:CZ	2.06	0.84
1:C:427:ASN:HD21	12:C:603:NAG:C2	1.91	0.84
1:D:88:VAL:HG13	1:D:312:VAL:HG12	1.59	0.84
1:B:399:ARG:HD3	14:B:1062:HOH:O	1.77	0.83
11:A:607:P4G:H42	14:A:1118:HOH:O	1.79	0.83
1:B:147[B]:VAL:HG23	1:B:353:ARG:NH2	1.94	0.83
1:B:423:LYS:HD2	1:C:427:ASN:OD1	1.79	0.82
1:B:147[B]:VAL:CG2	1:B:335:PRO:HG3	2.10	0.82
1:G:284[A]:THR:HG22	14:G:1007:HOH:O	1.79	0.81
1:D:87:GLU:HG3	14:D:862:HOH:O	1.78	0.81
1:A:287:GLU:HG3	14:A:712:HOH:O	1.79	0.81
1:B:22:ASN:ND2	14:B:702:HOH:O	2.11	0.81
1:C:112[A]:MET:CE	1:C:114:PHE:CZ	2.63	0.81
1:E:74[A]:VAL:HG12	14:G:969:HOH:O	1.79	0.80
1:C:112[A]:MET:HE1	1:C:114:PHE:CE1	2.15	0.80
1:H:288:GLU:HG3	14:H:1075:HOH:O	1.81	0.80
11:A:607:P4G:H61	14:A:830:HOH:O	1.83	0.79
1:A:287:GLU:CG	14:A:712:HOH:O	2.31	0.78
1:H:34[B]:ARG:NH2	14:H:703:HOH:O	2.16	0.78
1:A:13:ARG:CZ	1:B:13:ARG:HD2	2.13	0.78
14:B:876:HOH:O	1:D:424:ILE:HG23	1.83	0.77
1:C:287:GLU:OE2	14:C:701:HOH:O	2.02	0.77
1:C:421:GLU:OE1	14:C:702:HOH:O	2.04	0.76
1:H:274[B]:ASP:OD1	14:H:701:HOH:O	2.03	0.76
1:A:486:LYS:HA	11:A:607:P4G:H31	1.66	0.76
1:H:6:THR:HG23	14:H:1149:HOH:O	1.84	0.76
1:D:92:TYR:OH	1:D:284[A]:THR:HG22	1.86	0.76
1:C:257[B]:GLU:CD	14:C:703:HOH:O	2.29	0.75
1:D:284[A]:THR:HG23	14:D:997:HOH:O	1.85	0.75
1:E:272:LYS:HG3	14:E:720:HOH:O	1.85	0.75
1:G:105:GLY:HA3	14:G:1113:HOH:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:500:GLN:HG2	14:F:976:HOH:O	1.88	0.74
1:E:108[A]:THR:HG22	14:E:868:HOH:O	1.87	0.74
1:A:100:ASP:HB3	14:A:891:HOH:O	1.89	0.73
1:F:284:THR:HG23	14:F:1112:HOH:O	1.88	0.73
1:H:244:ARG:HD2	14:H:741:HOH:O	1.88	0.73
1:E:13:ARG:CD	1:F:13:ARG:CZ	2.67	0.73
1:B:147[B]:VAL:HG21	1:B:335:PRO:HG3	1.71	0.72
1:H:100:ASP:CG	14:H:711:HOH:O	2.31	0.72
1:H:13:ARG:CZ	1:G:13:ARG:HD2	2.20	0.71
1:B:147[B]:VAL:HG23	1:B:353:ARG:HH22	1.55	0.71
1:C:427:ASN:ND2	12:C:603:NAG:N2	2.39	0.71
14:C:1105:HOH:O	1:D:390:LEU:HD12	1.84	0.71
1:B:257:GLU:OE1	14:B:701:HOH:O	2.08	0.71
14:H:714:HOH:O	1:G:10:GLU:HG2	1.90	0.71
1:E:74[A]:VAL:CG1	14:G:969:HOH:O	2.37	0.71
1:A:257:GLU:HG2	14:A:946:HOH:O	1.90	0.70
1:C:499:TYR:O	1:C:503:LEU:HD13	1.90	0.70
1:C:499:TYR:CE1	1:C:503:LEU:HD11	2.27	0.70
1:B:103:LYS:HE2	14:B:894:HOH:O	1.91	0.69
1:F:101:VAL:HG23	1:F:108:THR:HG21	1.74	0.69
1:F:108:THR:HG23	14:F:916:HOH:O	1.93	0.69
1:A:390:LEU:HD22	14:B:1194:HOH:O	1.91	0.69
1:A:482:GLU:HG3	14:A:787:HOH:O	1.92	0.69
1:A:253[B]:LYS:NZ	14:A:703:HOH:O	2.24	0.69
1:B:184:TRP:HZ2	1:B:201:LEU:HD21	1.58	0.68
1:A:108[A]:THR:HG23	14:A:939:HOH:O	1.92	0.68
1:B:103:LYS:HE3	14:B:1130:HOH:O	1.93	0.68
1:A:430:TYR:CE1	1:D:419:VAL:CG1	2.77	0.68
1:C:390:LEU:HD12	1:D:390:LEU:HD12	1.76	0.67
1:F:112:MET:HG2	1:F:135:ILE:HD13	1.76	0.67
1:B:201:LEU:HD22	1:B:464:ILE:HG12	1.76	0.67
1:G:112:MET:HG2	1:G:135:ILE:HD12	1.77	0.67
1:D:502:ALA:O	14:D:701:HOH:O	2.12	0.66
1:C:497:GLU:HG3	14:C:1115:HOH:O	1.95	0.66
1:E:6:THR:HG21	1:F:109:SER:OG	1.95	0.66
1:D:90:GLY:O	1:D:312:VAL:HG13	1.96	0.66
1:C:390:LEU:CD1	1:D:390:LEU:HB2	2.25	0.66
1:H:13:ARG:HD2	1:G:13:ARG:CZ	2.26	0.66
1:C:390:LEU:HD13	1:D:390:LEU:HB2	1.77	0.66
1:H:427:ASN:O	1:H:429[A]:THR:HG23	1.96	0.65
1:H:14:LEU:HD21	6:H:604:PEG:H21	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:500:GLN:NE2	14:F:704:HOH:O	2.30	0.65
1:B:257:GLU:HG2	14:B:869:HOH:O	1.97	0.64
1:B:493[B]:ARG:O	1:B:497:GLU:HG3	1.96	0.64
1:E:13:ARG:CZ	1:F:13:ARG:HD2	2.27	0.64
1:A:493[A]:ARG:CZ	1:A:493[A]:ARG:CB	2.73	0.64
1:D:74[B]:VAL:HG23	14:D:825:HOH:O	1.97	0.63
1:C:287:GLU:HG3	14:C:736:HOH:O	1.99	0.63
1:D:427:ASN:OD1	12:D:605:NAG:O5	2.15	0.63
1:D:427:ASN:CG	12:D:605:NAG:C1	2.71	0.63
1:H:425:GLU:OE1	14:H:702:HOH:O	2.15	0.63
1:B:20:THR:HG23	14:B:890:HOH:O	1.97	0.63
1:E:13:ARG:NE	1:F:13:ARG:CD	2.61	0.63
1:E:108[A]:THR:HG23	14:E:905:HOH:O	1.98	0.62
1:G:287:GLU:HG3	14:G:750:HOH:O	1.99	0.62
1:H:34[B]:ARG:HH11	1:H:34[B]:ARG:HB2	1.63	0.62
1:E:112[A]:MET:HE1	1:E:133:PHE:CE1	2.34	0.62
1:F:92:TYR:OH	1:F:284:THR:HG22	1.98	0.62
1:H:452:LEU:HG	1:H:456:ASP:HB3	1.81	0.62
1:A:13:ARG:CZ	1:B:13:ARG:CD	2.78	0.62
1:A:15:LYS:O	1:A:18[B]:GLN:HG3	1.99	0.62
1:C:427:ASN:ND2	12:C:603:NAG:C2	2.56	0.61
1:F:100:ASP:HA	1:F:103[C]:LYS:HD3	1.82	0.61
1:A:390:LEU:HD12	1:B:390:LEU:CD1	2.27	0.61
1:A:493[B]:ARG:NH1	14:A:707:HOH:O	2.33	0.61
1:D:302:LYS:NZ	14:D:706:HOH:O	2.29	0.61
1:B:253:LYS:O	1:B:257:GLU:HG3	1.99	0.61
1:H:107:LYS:HD3	14:H:1272:HOH:O	2.01	0.61
12:E:602:NAG:H81	14:E:1175:HOH:O	2.01	0.60
1:H:399:ARG:CD	14:H:1034:HOH:O	2.40	0.60
1:H:252[A]:LYS:NZ	14:H:710:HOH:O	2.34	0.60
1:A:279:LYS:NZ	14:A:708:HOH:O	2.35	0.60
1:A:101:VAL:HG23	1:A:108[A]:THR:HG21	1.83	0.60
1:A:385:ASP:O	9:A:603:ALA:HB3	2.02	0.60
1:A:424:ILE:HD12	1:B:45:ALA:HB1	1.83	0.60
1:B:201:LEU:CD2	1:B:464:ILE:HG12	2.31	0.60
1:C:399:ARG:NH2	1:D:18:GLN:O	2.35	0.60
1:D:238:GLU:OE1	14:D:702:HOH:O	2.17	0.60
1:A:13:ARG:NH1	1:B:13:ARG:HD2	2.18	0.59
1:A:237[A]:LEU:N	1:A:237[A]:LEU:HD12	2.18	0.59
1:A:86:PHE:HB3	1:A:108[B]:THR:CG2	2.32	0.59
1:C:279:LYS:HD3	1:C:314:ARG:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:LYS:NZ	14:B:703:HOH:O	2.23	0.58
1:F:245:ASN:ND2	2:K:1:NAG:C2	2.60	0.58
1:B:201:LEU:HD23	1:B:464:ILE:HA	1.83	0.58
1:B:240:GLU:OE1	1:B:279:LYS:HD3	2.03	0.58
1:D:88:VAL:HG13	1:D:312:VAL:CG1	2.31	0.58
1:D:322:GLU:HG2	14:D:1199:HOH:O	2.03	0.58
1:A:109:SER:OG	1:B:6:THR:HG21	2.03	0.58
1:E:227:ASP:HB3	6:E:604:PEG:H42	1.84	0.58
1:H:13:ARG:CD	1:G:13:ARG:NE	2.67	0.58
1:A:390:LEU:HB3	14:B:1194:HOH:O	2.03	0.58
1:F:419:VAL:CG1	1:G:430:TYR:CE1	2.86	0.58
1:C:47:ALA:HB1	5:C:604:EDO:H12	1.84	0.58
1:G:112:MET:HG2	1:G:135:ILE:CD1	2.33	0.58
1:A:396:GLN:HG3	9:A:603:ALA:HB2	1.85	0.57
1:E:284:THR:CG2	14:E:1150:HOH:O	2.51	0.57
1:F:110:ILE:HG22	1:F:137:MET:HG2	1.85	0.57
1:A:493[A]:ARG:HG3	14:A:1315:HOH:O	2.03	0.57
5:B:604:EDO:C2	14:B:774:HOH:O	2.51	0.57
1:G:427:ASN:O	1:G:429:THR:HG22	2.05	0.57
14:C:1105:HOH:O	1:D:390:LEU:HD11	1.94	0.57
1:D:399:ARG:HD3	14:D:955:HOH:O	2.03	0.57
14:E:992:HOH:O	1:F:34[B]:ARG:HG3	2.04	0.57
1:H:13:ARG:NE	1:G:13:ARG:CD	2.68	0.57
1:E:101:VAL:HG23	1:E:108[A]:THR:HG21	1.85	0.57
1:F:436[A]:GLU:O	1:F:436[A]:GLU:HG2	2.04	0.57
1:E:184:TRP:HZ2	1:E:201[A]:LEU:HD21	1.70	0.57
14:E:889:HOH:O	1:F:390:LEU:CD1	2.51	0.57
1:G:110:ILE:HG22	1:G:137:MET:HG2	1.85	0.56
1:C:162:PHE:HB3	1:C:163:PRO:HD3	1.86	0.56
1:A:419:VAL:CG1	1:D:430:TYR:CE1	2.89	0.56
1:D:184:TRP:HZ2	1:D:201[A]:LEU:HD21	1.70	0.56
1:H:237:LEU:N	1:H:237:LEU:HD12	2.21	0.56
1:A:390:LEU:HD13	1:B:390:LEU:HB2	1.87	0.56
1:D:92:TYR:OH	1:D:284[A]:THR:CG2	2.53	0.56
1:G:445:ARG:CD	1:G:487:VAL:O	2.42	0.56
1:A:288:GLU:HG3	14:A:1070:HOH:O	2.05	0.56
1:A:395:ASN:OD1	9:A:603:ALA:HB1	2.06	0.56
14:B:893:HOH:O	1:D:74[B]:VAL:HG22	2.05	0.56
1:F:112:MET:HE2	1:F:135:ILE:HD12	1.88	0.56
1:D:201[A]:LEU:HD22	1:D:464:ILE:HG12	1.88	0.55
1:F:245:ASN:CG	2:K:1:NAG:C1	2.67	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:240:GLU:OE1	1:G:279:LYS:HD3	2.06	0.55
1:H:308:THR:HG21	14:H:1186:HOH:O	2.05	0.55
1:C:112[A]:MET:HE2	1:C:114:PHE:CZ	2.42	0.55
1:A:279:LYS:HD3	1:A:314:ARG:HG2	1.88	0.55
1:D:399:ARG:CD	14:D:955:HOH:O	2.55	0.55
1:H:424:ILE:HG22	1:E:424:ILE:HG21	1.90	0.54
1:F:430:TYR:CE1	1:G:419:VAL:HG13	2.42	0.54
1:B:147[B]:VAL:CG2	1:B:353:ARG:NH2	2.70	0.54
1:D:381:VAL:HG12	5:D:606:EDO:H21	1.89	0.54
5:H:603:EDO:H12	1:G:141:LYS:HD2	1.90	0.54
1:F:423:LYS:CD	1:G:427:ASN:OD1	2.56	0.54
1:B:147[B]:VAL:HG23	1:B:147[B]:VAL:O	2.08	0.54
1:F:257:GLU:HG3	10:F:602:GLY:HA3	1.89	0.54
1:A:257:GLU:CG	14:A:946:HOH:O	2.52	0.54
1:C:112[A]:MET:CE	1:C:114:PHE:CE1	2.86	0.54
1:F:34[A]:ARG:O	1:F:34[A]:ARG:HG3	2.07	0.53
1:H:199[B]:ARG:HD2	14:H:756:HOH:O	2.09	0.53
1:A:178:ARG:NH2	8:A:602:SER:HA	2.23	0.53
1:E:107:LYS:HB3	14:E:1124:HOH:O	2.08	0.53
1:F:231:VAL:HG21	1:F:284:THR:OG1	2.08	0.53
1:H:34[B]:ARG:HB2	1:H:34[B]:ARG:NH1	2.24	0.53
1:G:121:ARG:NH1	14:G:705:HOH:O	2.36	0.53
1:H:72:GLU:OE1	1:H:121:ARG:HB2	2.08	0.53
1:E:13:ARG:CD	1:F:13:ARG:NE	2.71	0.53
14:C:1015:HOH:O	1:D:390:LEU:HD11	2.08	0.53
14:E:913:HOH:O	1:F:390:LEU:HD11	2.09	0.53
1:D:414:GLU:OE1	6:D:604:PEG:O1	2.15	0.52
14:E:865:HOH:O	1:G:74:VAL:CG1	2.57	0.52
1:F:295:TYR:OH	1:F:442:GLU:OE2	2.19	0.52
1:F:92:TYR:OH	1:F:284:THR:CG2	2.57	0.52
1:A:214:HIS:HE2	5:A:605:EDO:H22	1.74	0.52
4:B:601:HEM:CMB	4:B:601:HEM:HBB2	2.40	0.51
1:A:430:TYR:CE1	1:D:419:VAL:HG13	2.44	0.51
1:F:430:TYR:CE1	1:G:419:VAL:CG1	2.93	0.51
1:G:306:ASN:HA	14:G:812:HOH:O	2.09	0.51
1:H:107:LYS:CD	14:H:1272:HOH:O	2.58	0.51
1:B:169:GLN:NE2	14:B:707:HOH:O	2.37	0.51
1:B:184:TRP:CZ2	1:B:201:LEU:HD21	2.42	0.51
1:G:34[A]:ARG:HG3	1:G:34[A]:ARG:O	2.09	0.51
1:H:44:ARG:HG2	1:H:51:LEU:HD23	1.93	0.51
1:G:112:MET:SD	1:G:135:ILE:HD12	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:PHE:HB3	1:D:163:PRO:HD3	1.93	0.51
1:D:332:HIS:CE1	1:D:361:ALA:HB2	2.46	0.51
1:E:13:ARG:CZ	1:F:13:ARG:CD	2.89	0.51
1:F:428:LEU:C	1:F:428:LEU:HD23	2.36	0.51
1:B:423:LYS:HG2	14:B:1098:HOH:O	2.10	0.50
1:C:287:GLU:CG	14:C:736:HOH:O	2.57	0.50
4:D:601:HEM:HBB2	4:D:601:HEM:HMB2	1.93	0.50
1:A:314:ARG:NH1	14:A:718:HOH:O	2.44	0.50
1:G:244:ARG:HG2	14:G:1145:HOH:O	2.10	0.50
1:A:390:LEU:HB2	1:B:390:LEU:HD13	1.93	0.50
1:H:212:HIS:CD2	1:H:244:ARG:HD3	2.46	0.50
1:B:430:TYR:CE1	1:C:419:VAL:CG1	2.95	0.50
1:C:390:LEU:HD11	14:D:951:HOH:O	2.12	0.50
1:E:284:THR:HG23	14:E:1150:HOH:O	2.11	0.50
1:C:332:HIS:CE1	1:C:361:ALA:HB2	2.47	0.50
1:E:201[A]:LEU:CD2	1:E:464:ILE:HG12	2.36	0.50
1:D:184:TRP:CZ2	1:D:201[A]:LEU:HD21	2.47	0.50
1:D:482:GLU:HG3	14:D:709:HOH:O	2.11	0.50
1:B:423:LYS:CD	1:C:427:ASN:OD1	2.58	0.49
1:G:112:MET:CG	1:G:135:ILE:HD12	2.42	0.49
1:F:436[A]:GLU:O	1:F:436[A]:GLU:CG	2.58	0.49
1:B:103:LYS:CE	14:B:894:HOH:O	2.57	0.49
1:G:493:ARG:O	1:G:497:GLU:HG3	2.12	0.49
1:E:281[B]:SER:OG	1:E:309:TYR:HB3	2.12	0.49
1:A:390:LEU:HD11	14:B:902:HOH:O	2.11	0.49
1:F:245:ASN:ND2	2:K:1:NAG:O5	2.40	0.49
1:F:114:PHE:HB3	1:F:210:PHE:CD1	2.47	0.49
1:E:13:ARG:HD2	1:F:13:ARG:NH1	2.28	0.49
1:E:238:GLU:HG3	14:E:815:HOH:O	2.11	0.49
1:H:419:VAL:CG1	1:E:430:TYR:CE1	2.96	0.48
14:H:826:HOH:O	1:F:424:ILE:HG23	2.13	0.48
1:E:140:LYS:NZ	14:E:708:HOH:O	2.36	0.48
1:E:429:THR:CG2	14:E:1191:HOH:O	2.61	0.48
1:F:231:VAL:CG2	1:F:284:THR:OG1	2.62	0.48
1:A:13:ARG:NE	1:B:13:ARG:CD	2.76	0.48
1:A:95:LYS:HE2	14:A:1212:HOH:O	2.13	0.48
1:C:47:ALA:HB1	5:C:604:EDO:C1	2.44	0.48
1:C:91:ASP:OD2	1:C:95:LYS:NZ	2.47	0.48
1:F:44:ARG:HG2	1:F:51:LEU:HD23	1.96	0.48
1:F:245:ASN:HB2	2:K:1:NAG:C1	2.43	0.48
1:F:423:LYS:HD3	1:G:427:ASN:OD1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:112:MET:SD	1:G:135:ILE:CD1	3.01	0.48
1:A:430:TYR:CZ	1:D:419:VAL:HG13	2.48	0.48
14:E:889:HOH:O	1:F:390:LEU:HD12	2.14	0.48
1:A:279:LYS:HD3	14:A:706:HOH:O	2.13	0.48
1:E:427:ASN:O	1:E:429:THR:HG22	2.13	0.48
1:H:13:ARG:CD	1:G:13:ARG:CZ	2.91	0.48
1:A:110:ILE:HG22	1:A:137:MET:HG2	1.96	0.48
1:A:493[A]:ARG:CG	14:A:1315:HOH:O	2.62	0.47
1:C:236:LYS:HE2	1:C:238[A]:GLU:CG	2.44	0.47
1:H:477:ARG:HD2	14:H:704:HOH:O	2.13	0.47
1:A:162:PHE:HB3	1:A:163:PRO:HD3	1.96	0.47
1:C:257[B]:GLU:HG2	14:C:830:HOH:O	2.13	0.47
1:F:112:MET:CG	1:F:135:ILE:HD13	2.43	0.47
1:B:72:GLU:OE1	1:B:121:ARG:HB2	2.14	0.47
1:E:68:GLU:HG2	1:F:386:ARG:O	2.14	0.47
1:B:147[B]:VAL:HG22	1:B:335:PRO:HG3	1.96	0.47
14:H:1328:HOH:O	2:I:2:NAG:H5	2.15	0.47
1:C:13[A]:ARG:CZ	1:D:13:ARG:CD	2.93	0.47
1:C:13[A]:ARG:CZ	1:D:13:ARG:HD3	2.45	0.47
1:C:92:TYR:OH	1:C:284:THR:CG2	2.63	0.47
1:G:288:GLU:CD	14:G:724:HOH:O	2.57	0.47
1:G:258:ASN:ND2	1:G:260:ALA:H	2.13	0.47
1:H:85:TYR:CE2	1:H:107:LYS:HE3	2.50	0.47
1:C:37:PHE:CE2	1:C:38:GLN:HB2	2.50	0.47
1:G:369:TYR:CE1	1:G:370:GLN:HG3	2.50	0.47
1:A:493[A]:ARG:HB3	1:A:493[A]:ARG:NH1	2.28	0.47
1:B:44:ARG:HG2	1:B:51:LEU:HD23	1.97	0.47
1:B:45:ALA:HB2	1:B:52:LEU:HD21	1.97	0.47
1:H:95:LYS:NZ	14:H:719:HOH:O	2.44	0.46
1:B:184:TRP:HZ2	1:B:201:LEU:CD2	2.28	0.46
1:F:91:ASP:HB3	14:F:1160:HOH:O	2.15	0.46
1:G:22:ASN:ND2	14:G:707:HOH:O	2.47	0.46
4:G:601:HEM:CMB	4:G:601:HEM:HBB2	2.45	0.46
1:A:34:ARG:O	1:A:34:ARG:HG3	2.15	0.46
1:F:199[A]:ARG:NH2	1:F:204:LEU:HD13	2.30	0.46
1:E:13:ARG:NE	1:F:13:ARG:HD3	2.30	0.46
1:F:162:PHE:HB3	1:F:163:PRO:HD3	1.97	0.46
1:H:452:LEU:HG	1:H:456:ASP:CB	2.44	0.46
1:C:13[A]:ARG:HD2	1:D:13:ARG:CZ	2.45	0.46
1:D:100:ASP:HA	1:D:103:LYS:HD3	1.96	0.46
1:E:100:ASP:OD1	14:E:701:HOH:O	2.20	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:424:ILE:CD1	1:F:45:ALA:HA	2.46	0.46
1:E:12:THR:HB	1:F:393:HIS:CE1	2.51	0.46
4:B:601:HEM:HBB2	4:B:601:HEM:HMB2	1.96	0.46
1:E:112[A]:MET:CE	1:E:133:PHE:CE1	2.98	0.46
1:H:34[B]:ARG:HH11	1:H:34[B]:ARG:CB	2.29	0.46
1:E:390:LEU:HD13	1:F:390:LEU:HB2	1.97	0.46
14:E:865:HOH:O	1:G:74:VAL:HG12	2.15	0.46
1:C:164:ARG:N	1:C:164:ARG:HD2	2.31	0.45
1:F:423:LYS:HD2	1:G:427:ASN:OD1	2.16	0.45
1:H:13:ARG:NE	1:G:13:ARG:HD2	2.31	0.45
1:E:110:ILE:HG22	1:E:137:MET:HG2	1.97	0.45
1:E:201[A]:LEU:HD22	1:E:464:ILE:CG1	2.37	0.45
1:F:100:ASP:HA	1:F:103[C]:LYS:CE	2.46	0.45
1:H:219:HIS:CE1	1:H:300:LEU:HD22	2.51	0.45
1:C:15:LYS:HE2	5:D:606:EDO:H22	1.99	0.45
1:E:148:PHE:CD1	1:E:217:SER:HA	2.52	0.45
1:E:227:ASP:HB3	6:E:604:PEG:C4	2.47	0.45
1:H:216:TRP:CZ2	1:H:236:LYS:HE3	2.51	0.45
1:H:332:HIS:CE1	1:H:361:ALA:HB2	2.51	0.45
1:A:390:LEU:CD1	1:B:390:LEU:HB2	2.47	0.45
1:E:74[B]:VAL:HG21	1:G:66:ASN:HA	1.97	0.45
1:G:58:LEU:HD23	1:G:58:LEU:C	2.41	0.45
1:G:436:GLU:O	1:G:436:GLU:HG3	2.16	0.45
1:B:110:ILE:HA	1:B:136:LYS:O	2.17	0.45
1:H:13:ARG:CZ	1:G:13:ARG:CD	2.93	0.45
1:E:390:LEU:HB2	1:F:390:LEU:CD1	2.47	0.45
1:E:13:ARG:NH1	1:F:13:ARG:HD2	2.32	0.45
1:H:393:HIS:CE1	1:G:12:THR:HB	2.52	0.45
1:C:44:ARG:HG2	1:C:51:LEU:HD23	1.99	0.45
1:E:162:PHE:HB3	1:E:163:PRO:HD3	1.99	0.45
1:F:281:SER:OG	1:F:311:ASP:OD1	2.31	0.44
1:H:30:GLN:OE1	1:H:34[B]:ARG:HD3	2.17	0.44
1:H:34[B]:ARG:NH1	14:H:703:HOH:O	2.49	0.44
1:A:322:GLU:HG2	14:A:1113:HOH:O	2.17	0.44
1:A:396:GLN:HE21	9:A:603:ALA:N	2.15	0.44
1:H:65:PHE:CG	1:F:163:PRO:HB3	2.52	0.44
1:F:110:ILE:HA	1:F:136:LYS:O	2.17	0.44
1:H:110:ILE:HG22	1:H:137:MET:HG2	1.99	0.44
1:C:257[A]:GLU:HG2	14:C:703:HOH:O	2.16	0.44
1:E:74[B]:VAL:HG23	14:E:780:HOH:O	2.17	0.44
1:B:141:LYS:HE2	14:B:1207:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:61:THR:HB	1:G:160:LEU:HD11	2.00	0.44
4:E:601:HEM:HBB2	4:E:601:HEM:HMB2	1.98	0.44
1:F:199[B]:ARG:HD3	1:F:447:PHE:CE1	2.53	0.44
1:A:13:ARG:CD	1:B:13:ARG:NE	2.81	0.44
1:G:44:ARG:HG2	1:G:51:LEU:HD23	1.99	0.44
1:H:176:ASN:HB2	1:F:324:TYR:CD2	2.53	0.44
1:C:112[A]:MET:HE2	1:C:112[A]:MET:HB3	1.43	0.44
1:H:423:LYS:HD2	1:E:427:ASN:OD1	2.18	0.43
1:A:279:LYS:CD	14:A:706:HOH:O	2.66	0.43
1:E:112[A]:MET:HE2	1:E:112[A]:MET:HB3	1.47	0.43
1:F:271:GLU:OE2	14:F:701:HOH:O	2.20	0.43
1:A:138:ARG:HA	1:A:143:ILE:HD13	1.99	0.43
1:C:138:ARG:HA	1:C:143:ILE:HD13	1.99	0.43
1:C:220:THR:HG21	1:C:297:ILE:HD12	1.98	0.43
1:F:100:ASP:HA	1:F:103[C]:LYS:CD	2.47	0.43
1:F:160:LEU:HD12	1:F:160:LEU:HA	1.81	0.43
1:A:244:ARG:CG	14:A:1220:HOH:O	2.66	0.43
1:D:45:ALA:HB2	1:D:52:LEU:HD21	2.00	0.43
1:D:110:ILE:HG22	1:D:137:MET:HG2	1.99	0.43
4:G:601:HEM:HBB2	4:G:601:HEM:HMB2	1.99	0.43
1:B:417:LYS:HA	1:B:417:LYS:HD2	1.62	0.43
1:E:390:LEU:HB2	1:F:390:LEU:HD13	1.99	0.43
1:B:184:TRP:CZ2	1:B:201:LEU:CD2	3.01	0.43
4:C:601:HEM:HBB2	4:C:601:HEM:HMB2	2.00	0.43
1:E:478:GLU:O	1:E:482:GLU:HG3	2.19	0.43
1:A:148:PHE:CD1	1:A:217:SER:HA	2.53	0.43
1:C:191:PRO:HB3	1:C:483:GLN:HE21	1.83	0.43
4:D:601:HEM:HBB2	4:D:601:HEM:CMB	2.47	0.43
1:H:107:LYS:HB3	14:H:1272:HOH:O	2.19	0.43
1:H:254:GLN:CD	1:H:261:TRP:CD1	2.97	0.43
1:B:443:GLN:N	1:B:444:PRO:HD2	2.33	0.43
1:E:184:TRP:CZ2	1:E:201[A]:LEU:HD21	2.50	0.43
1:E:386:ARG:O	1:F:68:GLU:HG2	2.19	0.43
1:H:414:GLU:HG2	14:H:1097:HOH:O	2.18	0.43
1:A:44:ARG:HG2	1:A:51:LEU:HD23	2.01	0.43
5:B:604:EDO:H22	14:B:774:HOH:O	2.15	0.43
1:E:164:ARG:HD2	1:E:164:ARG:N	2.34	0.42
1:E:497:GLU:HG2	14:E:930:HOH:O	2.18	0.42
4:A:601:HEM:HMB2	4:A:601:HEM:HBB2	2.01	0.42
1:C:393:HIS:CE1	1:D:12:THR:HB	2.54	0.42
1:D:427:ASN:O	1:D:429:THR:HG22	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:417:LYS:NZ	14:F:715:HOH:O	2.50	0.42
1:F:452:LEU:HG	1:F:456:ASP:HB3	2.01	0.42
1:G:422:PRO:HG2	14:G:1133:HOH:O	2.19	0.42
1:H:35:THR:OG1	5:H:603:EDO:H21	2.18	0.42
1:H:386:ARG:O	1:G:68:GLU:HG2	2.20	0.42
1:A:138:ARG:HD3	1:A:378:PHE:CZ	2.54	0.42
1:B:76:HIS:HA	1:B:116:THR:O	2.18	0.42
1:C:414:GLU:HG2	14:C:1218:HOH:O	2.18	0.42
1:F:236[A]:LYS:NZ	14:F:707:HOH:O	2.39	0.42
1:A:110:ILE:HA	1:A:136:LYS:O	2.19	0.42
1:E:389:HIS:CE1	14:E:1097:HOH:O	2.73	0.42
1:H:13:ARG:NH1	1:G:13:ARG:HD2	2.35	0.42
1:H:424:ILE:HG23	14:F:773:HOH:O	2.20	0.42
1:B:76:HIS:CE1	1:B:117:VAL:HG22	2.55	0.42
1:F:430:TYR:CZ	1:G:419:VAL:HG13	2.55	0.42
1:B:257:GLU:HG3	14:B:765:HOH:O	2.20	0.42
1:G:369:TYR:CD1	1:G:370:GLN:HG3	2.54	0.42
1:H:222:LYS:HE2	1:H:230:TRP:CZ3	2.55	0.41
1:C:288:GLU:HG3	14:C:1127:HOH:O	2.21	0.41
1:D:499:TYR:CZ	1:D:503:LEU:HD11	2.55	0.41
1:C:92:TYR:OH	1:C:284:THR:HG21	2.21	0.41
1:F:332:HIS:CE1	1:F:361:ALA:HB2	2.55	0.41
1:G:112:MET:CG	1:G:135:ILE:CD1	2.98	0.41
1:H:138:ARG:HD3	1:H:378:PHE:CE1	2.55	0.41
1:A:141:LYS:HG2	14:A:891:HOH:O	2.20	0.41
1:B:430:TYR:CZ	1:C:419:VAL:HG13	2.55	0.41
1:C:201:LEU:HD22	1:C:464:ILE:HA	2.01	0.41
1:C:264:LYS:NZ	14:C:716:HOH:O	2.51	0.41
1:D:402:PHE:HB2	1:D:403:PRO:HD2	2.02	0.41
1:G:45:ALA:O	1:G:49:GLY:HA3	2.21	0.41
1:G:264[B]:LYS:NZ	14:G:703:HOH:O	2.31	0.41
1:A:363:HIS:HE1	1:C:69:ARG:O	2.03	0.41
1:C:372:ILE:HD11	1:D:390:LEU:HD23	2.01	0.41
1:G:88:VAL:HG12	1:G:104:PRO:HA	2.01	0.41
1:H:204:LEU:HD21	2:I:1:NAG:C8	2.51	0.41
1:A:214:HIS:NE2	5:A:605:EDO:H22	2.36	0.41
1:D:411:ASN:ND2	14:D:712:HOH:O	2.42	0.41
1:H:34[B]:ARG:CZ	14:H:703:HOH:O	2.63	0.41
1:A:392:VAL:HG21	1:B:392:VAL:HG21	2.03	0.41
1:C:164:ARG:N	1:C:164:ARG:CD	2.84	0.41
1:D:240:GLU:OE1	1:D:279[A]:LYS:HE3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:436:GLU:O	1:G:436:GLU:CG	2.68	0.41
1:F:76:HIS:HA	1:F:116:THR:O	2.20	0.41
1:F:112:MET:HA	1:F:134:SER:O	2.21	0.41
1:F:245:ASN:CB	2:K:1:NAG:C1	2.99	0.41
1:G:501:LYS:NZ	14:G:715:HOH:O	2.54	0.41
5:H:603:EDO:C1	1:G:141:LYS:HB3	2.51	0.41
1:A:279:LYS:CE	14:A:1007:HOH:O	2.69	0.41
1:F:264:LYS:HG3	14:F:1080:HOH:O	2.21	0.41
10:A:606:GLY:HA3	1:B:322:GLU:HG2	2.03	0.40
1:H:140:LYS:HD3	14:H:778:HOH:O	2.21	0.40
1:A:369:TYR:CE2	1:A:370:GLN:HG3	2.56	0.40
1:B:112:MET:HA	1:B:134:SER:O	2.22	0.40
1:C:160:LEU:HD12	1:C:160:LEU:HA	1.92	0.40
1:E:22:ASN:OD1	14:E:702:HOH:O	2.22	0.40
1:A:76:HIS:CE1	1:A:117:VAL:HG22	2.57	0.40
1:A:424:ILE:HD12	1:B:45:ALA:CB	2.49	0.40
1:B:264:LYS:HE2	14:D:896:HOH:O	2.22	0.40
1:B:134:SER:OG	4:B:601:HEM:HBD2	2.21	0.40
5:B:604:EDO:H21	14:B:774:HOH:O	2.17	0.40
1:C:112[A]:MET:HA	1:C:134:SER:O	2.21	0.40
4:F:601:HEM:CMC	4:F:601:HEM:HBC2	2.52	0.40
1:G:112:MET:HG3	1:G:317:LEU:HD21	2.03	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: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

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	387	ASP
1	B	387	ASP
1	E	387	ASP
1	A	387	ASP
1	C	387	ASP
1	D	387	ASP
1	F	387	ASP
1	G	387	ASP
1	B	383	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	104	PRO
1	H	129	ASP
1	H	139	THR
1	H	151	THR
1	H	226[A]	ASP
1	H	226[B]	ASP
1	H	306	ASN
1	H	312	VAL
1	H	390	LEU
1	H	436	GLU
1	H	452	LEU
1	H	503[A]	LEU
1	H	503[B]	LEU
1	A	34	ARG
1	A	104	PRO
1	A	108[A]	THR
1	A	108[B]	THR
1	A	129	ASP
1	A	139	THR
1	A	151	THR
1	A	306	ASN
1	A	308	THR
1	A	424	ILE
1	A	493[A]	ARG
1	A	493[B]	ARG
1	A	503	LEU
1	B	34[A]	ARG
1	B	34[B]	ARG
1	B	129	ASP
1	B	139	THR
1	B	141	LYS
1	B	151	THR
1	B	198	LEU

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Mol	Chain	Res	Type
1	B	452	LEU
1	B	472	ASP
1	C	129	ASP
1	C	139	THR
1	C	151	THR
1	C	288	GLU
1	C	423	LYS
1	C	425	GLU
1	C	429	THR
1	D	129	ASP
1	D	135[A]	ILE
1	D	135[B]	ILE
1	D	139	THR
1	D	199	ARG
1	D	306	ASN
1	D	423	LYS
1	D	429	THR
1	D	501[A]	LYS
1	D	501[B]	LYS
1	E	100	ASP
1	E	129	ASP
1	E	139	THR
1	E	151	THR
1	E	198	LEU
1	E	201[A]	LEU
1	E	201[B]	LEU
1	E	284	THR
1	E	429	THR
1	E	501	LYS
1	F	103[A]	LYS
1	F	103[C]	LYS
1	F	108	THR
1	F	129	ASP
1	F	135	ILE
1	F	139	THR
1	F	199[A]	ARG
1	F	199[B]	ARG
1	F	287	GLU
1	F	416	PRO
1	F	452	LEU
1	F	503	LEU
1	G	34[A]	ARG

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Mol	Chain	Res	Type
1	G	34[B]	ARG
1	G	100	ASP
1	G	129	ASP
1	G	139	THR
1	G	201	LEU
1	G	284[A]	THR
1	G	284[B]	THR
1	G	429	THR
1	G	439	ILE
1	G	452	LEU
1	G	503	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	400	GLN
1	A	189	GLN
1	A	363	HIS
1	A	370	GLN
1	B	31	GLN
1	C	31	GLN
1	C	189	GLN
1	C	483	GLN
1	D	306	ASN
1	D	370	GLN
1	D	434	GLN
1	D	483	GLN
1	E	18	GLN
1	E	22	ASN
1	E	306	ASN
1	E	411	ASN
1	F	18	GLN
1	F	212	HIS
1	F	483	GLN
1	F	500	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (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
3	J	3	BMA	O5-C5-C6	-3.05	102.42	107.20
2	K	2	NAG	C3-C4-C5	-2.99	104.90	110.24
3	J	4	MAN	O4-C4-C5	2.93	116.57	109.30
3	J	2	NAG	O4-C4-C5	-2.83	102.28	109.30
2	K	1	NAG	O5-C1-C2	-2.59	107.20	111.29
3	J	4	MAN	O4-C4-C3	-2.58	104.38	110.35
2	K	2	NAG	O3-C3-C2	2.54	114.72	109.47
2	K	2	NAG	C4-C3-C2	-2.52	107.33	111.02
3	J	3	BMA	O3-C3-C2	-2.47	105.26	109.99
3	J	7	MAN	O3-C3-C2	2.37	114.54	109.99
3	J	7	MAN	C3-C4-C5	-2.35	106.04	110.24
3	J	2	NAG	C1-O5-C5	2.31	115.32	112.19
3	J	4	MAN	O2-C2-C1	2.24	113.73	109.15
3	J	4	MAN	O3-C3-C4	2.16	115.35	110.35
2	K	2	NAG	C2-N2-C7	2.00	125.75	122.90

There are no chirality outliers.

All (8) torsion outliers are listed below:

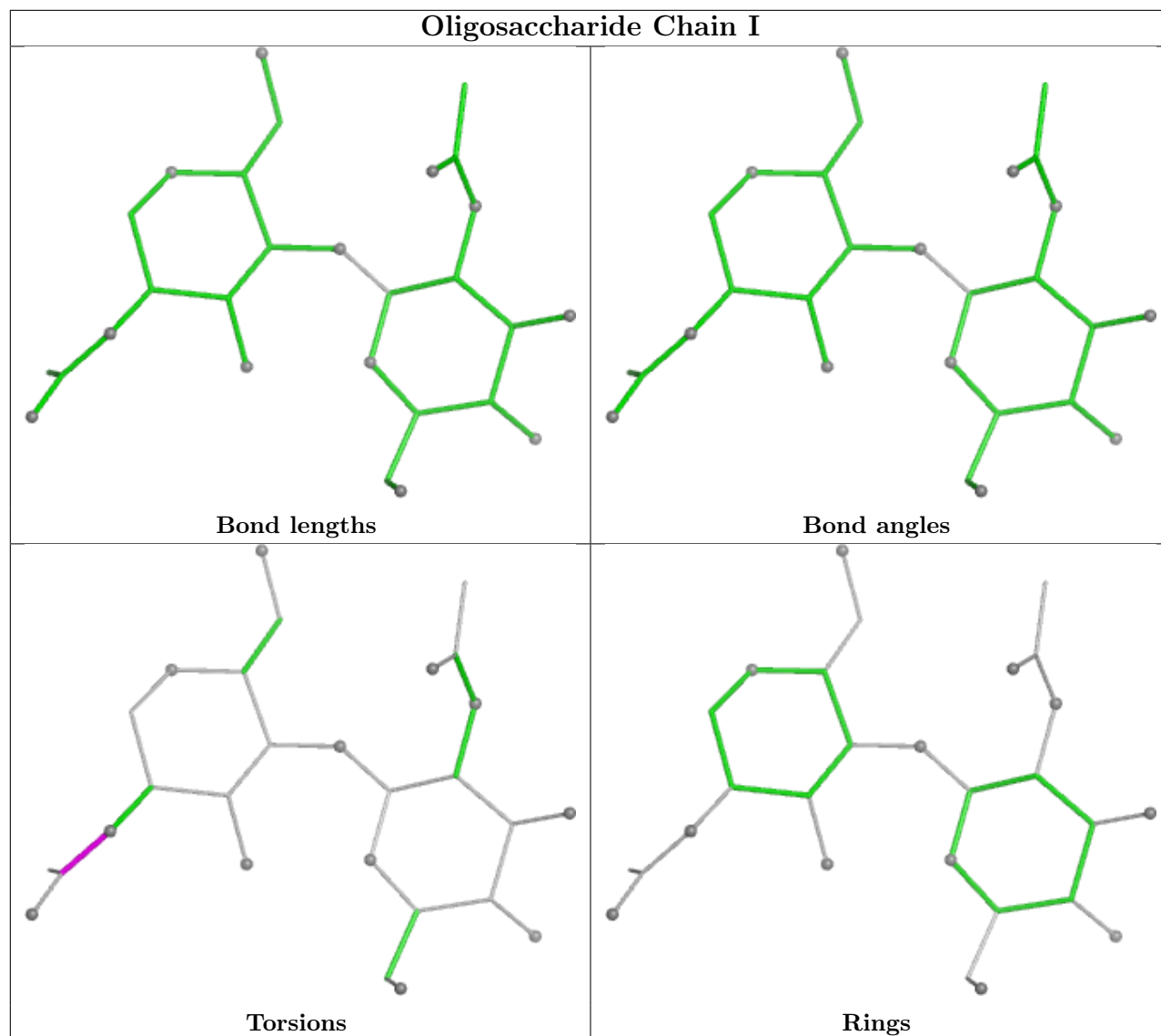
Mol	Chain	Res	Type	Atoms
3	J	7	MAN	O5-C5-C6-O6
3	J	5	MAN	O5-C5-C6-O6
3	J	4	MAN	O5-C5-C6-O6
3	J	7	MAN	C4-C5-C6-O6
2	I	1	NAG	C8-C7-N2-C2
2	I	1	NAG	O7-C7-N2-C2
3	J	4	MAN	C4-C5-C6-O6
3	J	5	MAN	C4-C5-C6-O6

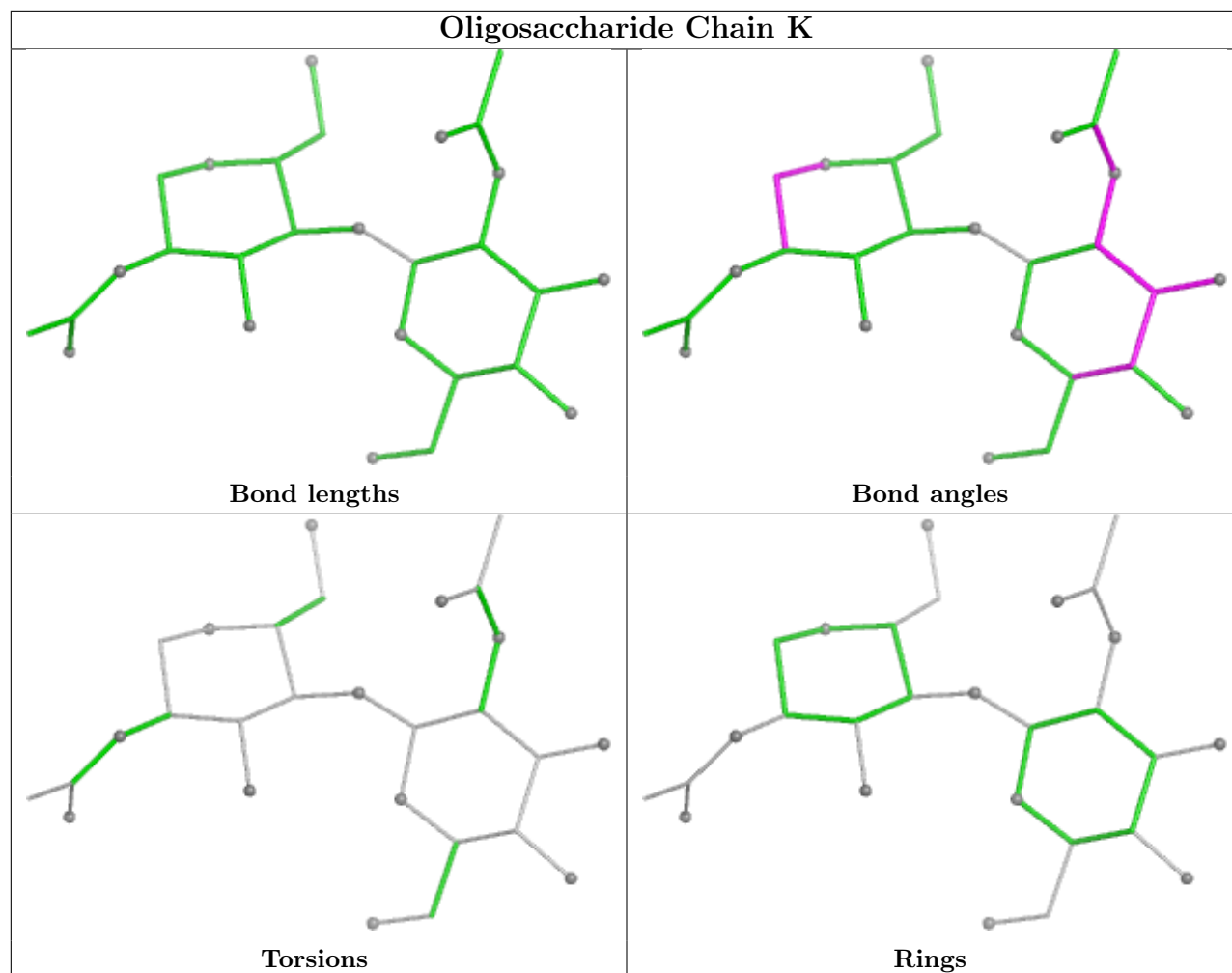
There are no ring outliers.

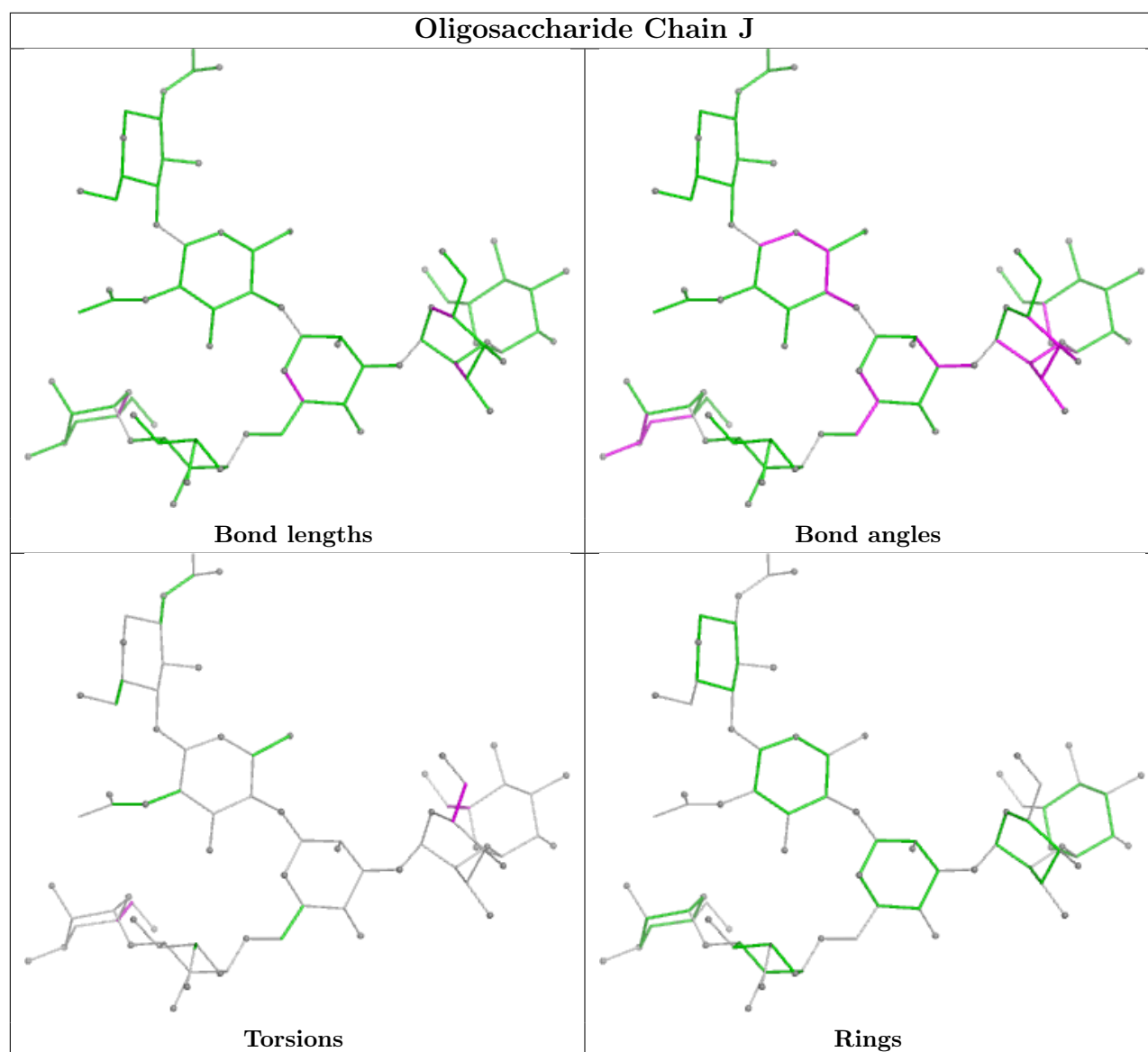
4 monomers are involved in 9 short contacts:

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

All (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
4	A	601	HEM	C4D-C3D	4.73	1.53	1.45
4	G	601	HEM	C1B-NB	-4.64	1.32	1.40
4	F	601	HEM	FE-NB	4.62	2.09	1.94
4	G	601	HEM	FE-NC	4.59	2.10	1.95
4	A	601	HEM	FE-NB	4.35	2.08	1.94
4	D	601	HEM	FE-NB	4.25	2.08	1.94
4	A	601	HEM	FE-NC	4.16	2.09	1.95
4	H	601	HEM	FE-NC	4.16	2.09	1.95
4	E	601	HEM	C4D-ND	-4.15	1.33	1.40
4	B	601	HEM	FE-NC	4.07	2.08	1.95
4	F	601	HEM	FE-NC	3.98	2.08	1.95
4	D	601	HEM	FE-NA	3.92	2.08	1.95
4	C	601	HEM	FE-NC	3.90	2.08	1.95
4	G	601	HEM	C1C-C2C	-3.85	1.37	1.45
4	G	601	HEM	FE-NB	3.84	2.06	1.94
4	H	601	HEM	C1C-C2C	-3.80	1.37	1.45
4	A	601	HEM	C1C-C2C	-3.56	1.38	1.45
4	B	601	HEM	C1D-ND	-3.53	1.31	1.38
4	D	601	HEM	CHA-C4D	3.51	1.45	1.38
4	H	601	HEM	C1B-NB	-3.49	1.34	1.40
4	A	601	HEM	C4B-NB	-3.35	1.31	1.38
4	B	601	HEM	C1B-NB	-3.25	1.34	1.40
4	E	601	HEM	FE-NC	3.24	2.06	1.95
4	H	601	HEM	CHB-C4A	-3.20	1.32	1.39
4	C	601	HEM	C4D-C3D	3.18	1.50	1.45
4	A	601	HEM	C4C-NC	-3.17	1.33	1.39
4	H	601	HEM	FE-NA	3.13	2.05	1.95
4	H	601	HEM	CHB-C1B	3.06	1.44	1.38
4	D	601	HEM	C4D-C3D	3.01	1.50	1.45
4	G	601	HEM	CAA-C2A	3.01	1.59	1.51
4	F	601	HEM	FE-NA	2.99	2.05	1.95
4	F	601	HEM	C3B-C2B	2.81	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	606	GLY	OXT-C	-2.77	1.21	1.30
4	D	601	HEM	C3B-C4B	2.72	1.50	1.44
4	A	601	HEM	C4D-ND	-2.72	1.35	1.40
4	A	601	HEM	C1B-NB	-2.68	1.35	1.40
4	G	601	HEM	FE-NA	2.63	2.04	1.95
4	H	601	HEM	CMC-C2C	2.59	1.56	1.50
4	H	601	HEM	C3B-C4B	2.57	1.50	1.44
4	E	601	HEM	C4A-NA	-2.57	1.34	1.39
4	D	601	HEM	C1D-C2D	2.56	1.49	1.44
4	C	601	HEM	CHB-C1B	2.55	1.43	1.38
4	F	601	HEM	O2D-CGD	-2.55	1.22	1.30
4	D	601	HEM	C4B-NB	-2.52	1.33	1.38
4	A	601	HEM	FE-NA	2.50	2.03	1.95
4	C	601	HEM	CBA-CGA	2.46	1.56	1.50
4	D	601	HEM	O1D-CGD	2.45	1.30	1.22
4	C	601	HEM	C1B-NB	-2.44	1.36	1.40
4	F	601	HEM	CHB-C1B	2.38	1.43	1.38
4	E	601	HEM	CAC-C3C	2.37	1.53	1.47
4	E	601	HEM	CMD-C2D	-2.36	1.45	1.50
4	C	601	HEM	C1C-C2C	-2.36	1.40	1.45
4	H	601	HEM	C4D-C3D	2.31	1.49	1.45
4	E	601	HEM	C4B-NB	-2.31	1.34	1.38
4	D	601	HEM	C4A-NA	-2.30	1.35	1.39
4	A	601	HEM	O2D-CGD	-2.30	1.23	1.30
4	B	601	HEM	C4B-NB	-2.30	1.34	1.38
4	H	601	HEM	C3B-C2B	2.30	1.41	1.37
4	F	601	HEM	CHA-C4D	2.29	1.43	1.38
4	A	601	HEM	C4A-NA	-2.28	1.35	1.39
4	H	601	HEM	CHC-C4B	2.26	1.44	1.39
4	H	601	HEM	C4A-NA	-2.26	1.35	1.39
9	A	603	ALA	OXT-C	-2.22	1.23	1.30
4	B	601	HEM	O1D-CGD	2.20	1.29	1.22
4	A	601	HEM	C1D-C2D	2.20	1.48	1.44
4	F	601	HEM	C4D-ND	-2.18	1.36	1.40
4	E	601	HEM	C1C-NC	-2.16	1.35	1.39
4	B	601	HEM	C4C-NC	-2.16	1.35	1.39
4	C	601	HEM	CHA-C4D	2.13	1.42	1.38
4	H	601	HEM	CHA-C4D	2.10	1.42	1.38
4	D	601	HEM	O2A-CGA	-2.10	1.23	1.30
4	C	601	HEM	FE-NA	2.09	2.02	1.95
4	B	601	HEM	FE-NA	2.08	2.02	1.95
4	F	601	HEM	C4A-NA	-2.06	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	602	SER	CB-CA	2.04	1.58	1.53
4	F	601	HEM	C1B-NB	-2.03	1.36	1.40
4	F	601	HEM	C2A-C3A	-2.03	1.33	1.38
4	A	601	HEM	C3B-C4B	2.02	1.48	1.44
4	F	601	HEM	C3C-C4C	-2.01	1.42	1.46
4	G	601	HEM	O2D-CGD	-2.00	1.24	1.30
4	B	601	HEM	C1D-C2D	2.00	1.48	1.44

All (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
4	H	601	HEM	CHC-C4B-NB	5.20	130.07	124.42
12	C	603	NAG	C1-C2-N2	5.18	119.33	110.49
4	D	601	HEM	CHC-C4B-NB	5.16	130.02	124.42
4	B	601	HEM	CHC-C4B-NB	5.07	129.93	124.42
4	F	601	HEM	C4A-NA-C1A	5.00	110.25	105.35
4	G	601	HEM	C4C-NC-C1C	4.98	110.22	105.35
4	E	601	HEM	C4A-NA-C1A	4.86	110.11	105.35
4	E	601	HEM	CHD-C1D-ND	4.74	129.57	124.42
4	G	601	HEM	CHD-C4C-NC	4.70	129.53	124.44
4	F	601	HEM	C4C-NC-C1C	4.55	109.80	105.35
4	B	601	HEM	C1B-NB-C4B	4.46	109.68	105.07
4	H	601	HEM	CHD-C4C-NC	4.27	129.06	124.44
4	D	601	HEM	CAD-CBD-CGD	-4.12	104.74	113.60
4	H	601	HEM	C4C-NC-C1C	4.04	109.31	105.35
4	A	601	HEM	CHB-C1B-NB	3.87	129.15	124.37
8	A	602	SER	OG-CB-CA	3.82	120.97	110.85
4	C	601	HEM	C1B-NB-C4B	3.80	109.00	105.07
4	E	601	HEM	CHA-C1A-NA	3.77	130.79	123.85
4	F	601	HEM	CHC-C4B-NB	3.74	128.48	124.42
4	D	601	HEM	CHD-C4C-NC	3.72	128.46	124.44
4	B	601	HEM	CMB-C2B-C1B	3.63	130.57	125.04
4	D	601	HEM	O2D-CGD-O1D	-3.56	114.42	123.30
4	F	601	HEM	C3D-C4D-ND	3.55	114.12	110.17
12	B	602	NAG	C1-O5-C5	3.48	116.90	112.19
4	H	601	HEM	CHA-C4D-ND	3.42	128.59	124.37
4	F	601	HEM	C2D-C1D-ND	3.42	113.97	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	601	HEM	CHD-C4C-NC	3.34	128.06	124.44
4	E	601	HEM	C1B-NB-C4B	3.30	108.48	105.07
4	H	601	HEM	CAD-C3D-C4D	3.28	130.38	124.66
4	C	601	HEM	C2D-C1D-ND	3.28	113.81	109.88
4	F	601	HEM	CHD-C1D-C2D	-3.24	119.91	124.98
4	D	601	HEM	C4A-NA-C1A	3.21	108.50	105.35
4	C	601	HEM	C4C-NC-C1C	3.17	108.46	105.35
4	F	601	HEM	C4D-ND-C1D	-3.16	101.81	105.07
4	E	601	HEM	C4C-NC-C1C	3.09	108.38	105.35
4	F	601	HEM	C2A-C1A-NA	-3.07	106.72	110.15
4	F	601	HEM	CHD-C4C-NC	3.06	127.75	124.44
4	A	601	HEM	CAD-CBD-CGD	-2.92	107.32	113.60
4	C	601	HEM	CHD-C1D-C2D	-2.92	120.42	124.98
4	F	601	HEM	O2A-CGA-CBA	2.88	123.30	114.03
4	B	601	HEM	C3B-C2B-C1B	-2.87	104.36	106.49
4	C	601	HEM	C1A-CHA-C4D	-2.85	119.58	126.34
4	E	601	HEM	CHD-C1D-C2D	-2.83	120.56	124.98
4	C	601	HEM	O1D-CGD-CBD	-2.83	113.99	123.08
4	E	601	HEM	CHC-C1C-NC	2.81	127.48	124.44
4	H	601	HEM	CHA-C4D-C3D	-2.80	120.07	125.33
12	D	605	NAG	O5-C1-C2	-2.79	106.89	111.29
4	B	601	HEM	CAD-CBD-CGD	-2.77	107.65	113.60
4	B	601	HEM	CAA-C2A-C1A	2.74	130.28	124.89
4	D	601	HEM	CMB-C2B-C1B	2.73	129.20	125.04
4	B	601	HEM	CHD-C1D-C2D	-2.71	120.74	124.98
4	F	601	HEM	CHA-C1A-NA	2.71	128.83	123.85
4	C	601	HEM	C1D-C2D-C3D	-2.71	104.11	106.96
4	D	601	HEM	CHA-C4D-ND	2.69	127.69	124.37
4	G	601	HEM	CAD-C3D-C4D	2.69	129.36	124.66
12	B	603	NAG	O3-C3-C2	-2.65	103.98	109.47
4	F	601	HEM	C3A-C4A-NA	-2.65	106.05	110.08
4	F	601	HEM	C1B-NB-C4B	2.62	107.78	105.07
4	C	601	HEM	CHB-C1B-NB	2.55	127.52	124.37
4	G	601	HEM	CAD-C3D-C2D	-2.52	123.18	127.88
4	C	601	HEM	CHA-C4D-ND	2.52	127.48	124.37
4	A	601	HEM	CHA-C4D-ND	2.51	127.47	124.37
12	G	602	NAG	C2-N2-C7	2.49	126.44	122.90
4	G	601	HEM	CMB-C2B-C1B	2.47	128.80	125.04
4	E	601	HEM	CAD-CBD-CGD	-2.46	108.32	113.60
4	H	601	HEM	CAA-C2A-C1A	2.46	129.72	124.89
4	C	601	HEM	CMB-C2B-C1B	2.45	128.78	125.04
12	C	603	NAG	O3-C3-C2	-2.45	104.39	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	601	HEM	C1B-NB-C4B	2.45	107.60	105.07
4	G	601	HEM	CAD-CBD-CGD	-2.44	108.35	113.60
4	G	601	HEM	CHC-C4B-NB	2.44	127.07	124.42
12	C	602	NAG	O5-C5-C6	-2.43	103.39	107.20
4	B	601	HEM	CAA-CBA-CGA	2.43	118.82	113.60
4	A	601	HEM	C4C-NC-C1C	2.42	107.72	105.35
12	B	602	NAG	C2-N2-C7	2.40	126.32	122.90
4	B	601	HEM	C4D-C3D-C2D	-2.39	103.42	106.90
4	B	601	HEM	CHD-C1D-ND	2.37	126.99	124.42
12	B	602	NAG	C1-C2-N2	-2.36	106.46	110.49
4	A	601	HEM	CHD-C1D-C2D	-2.35	121.31	124.98
4	E	601	HEM	C4C-CHD-C1D	-2.34	121.00	126.06
4	F	601	HEM	CHA-C4D-C3D	-2.33	120.95	125.33
4	E	601	HEM	CHD-C4C-NC	2.33	126.96	124.44
4	H	601	HEM	CMB-C2B-C1B	2.31	128.56	125.04
4	E	601	HEM	C2A-C1A-NA	-2.30	107.58	110.15
4	E	601	HEM	C1A-CHA-C4D	-2.29	120.92	126.34
4	C	601	HEM	O2D-CGD-CBD	2.28	121.34	114.03
4	H	601	HEM	C4C-CHD-C1D	-2.25	121.20	126.06
4	A	601	HEM	O2A-CGA-CBA	2.25	121.25	114.03
8	A	602	SER	OXT-C-CA	2.22	120.96	113.38
12	B	603	NAG	C2-N2-C7	-2.22	119.74	122.90
12	E	602	NAG	C2-N2-C7	2.22	126.06	122.90
4	B	601	HEM	C4A-NA-C1A	2.20	107.50	105.35
4	A	601	HEM	CHD-C4C-C3C	2.19	129.00	125.26
4	C	601	HEM	CMA-C3A-C4A	2.16	128.67	125.37
4	A	601	HEM	C2D-C1D-ND	2.16	112.47	109.88
4	G	601	HEM	C4C-C3C-C2C	-2.16	104.98	106.75
8	A	602	SER	O-C-CA	-2.16	114.53	122.14
4	D	601	HEM	C4C-NC-C1C	2.15	107.45	105.35
4	G	601	HEM	CBA-CAA-C2A	-2.14	106.67	112.63
4	A	601	HEM	CMB-C2B-C1B	2.13	128.29	125.04
4	C	601	HEM	CHA-C1A-NA	2.09	127.70	123.85
4	B	601	HEM	C4A-C3A-C2A	2.07	109.25	106.83
4	F	601	HEM	CHB-C4A-NA	2.04	127.61	123.85
4	A	601	HEM	O2D-CGD-O1D	-2.04	118.21	123.30
4	D	601	HEM	CAA-C2A-C1A	2.04	128.90	124.89
4	A	601	HEM	CMA-C3A-C4A	-2.03	122.28	125.37

There are no chirality outliers.

All (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
11	A	607	P4G	O3-C5-C6-O4
6	D	604	PEG	O1-C1-C2-O2
6	E	604	PEG	O2-C3-C4-O4
12	E	602	NAG	C8-C7-N2-C2
12	E	602	NAG	O7-C7-N2-C2
10	F	602	GLY	OXT-C-CA-N
6	A	608	PEG	O1-C1-C2-O2
10	F	602	GLY	O-C-CA-N
5	B	604	EDO	O1-C1-C2-O2
5	D	606	EDO	O1-C1-C2-O2
9	A	603	ALA	OXT-C-CA-N
6	H	604	PEG	O1-C1-C2-O2
6	H	605	PEG	O2-C3-C4-O4
9	A	603	ALA	O-C-CA-CB
5	H	602	EDO	O1-C1-C2-O2
13	C	605	P3G	C16-C15-O7-C14
12	D	605	NAG	O5-C5-C6-O6
6	H	605	PEG	C1-C2-O2-C3
13	C	605	P3G	C11-C12-O6-C13
13	C	605	P3G	C10-C9-O4-C8
6	E	604	PEG	O1-C1-C2-O2
6	A	608	PEG	O2-C3-C4-O4
13	C	605	P3G	C8-C7-O3-C6
13	C	605	P3G	C12-C11-O5-C10
6	H	605	PEG	O1-C1-C2-O2
11	A	607	P4G	C1-C2-O2-C3
4	B	601	HEM	CAD-CBD-CGD-O1D
4	F	601	HEM	CAD-CBD-CGD-O1D
4	B	601	HEM	CAD-CBD-CGD-O2D
4	H	601	HEM	CAD-CBD-CGD-O1D
4	D	601	HEM	CAD-CBD-CGD-O1D
4	D	601	HEM	CAD-CBD-CGD-O2D
4	H	601	HEM	CAD-CBD-CGD-O2D
4	C	601	HEM	CAD-CBD-CGD-O2D
4	E	601	HEM	CAD-CBD-CGD-O1D
4	F	601	HEM	CAD-CBD-CGD-O2D
11	A	607	P4G	C4-C3-O2-C2
4	E	601	HEM	CAD-CBD-CGD-O2D

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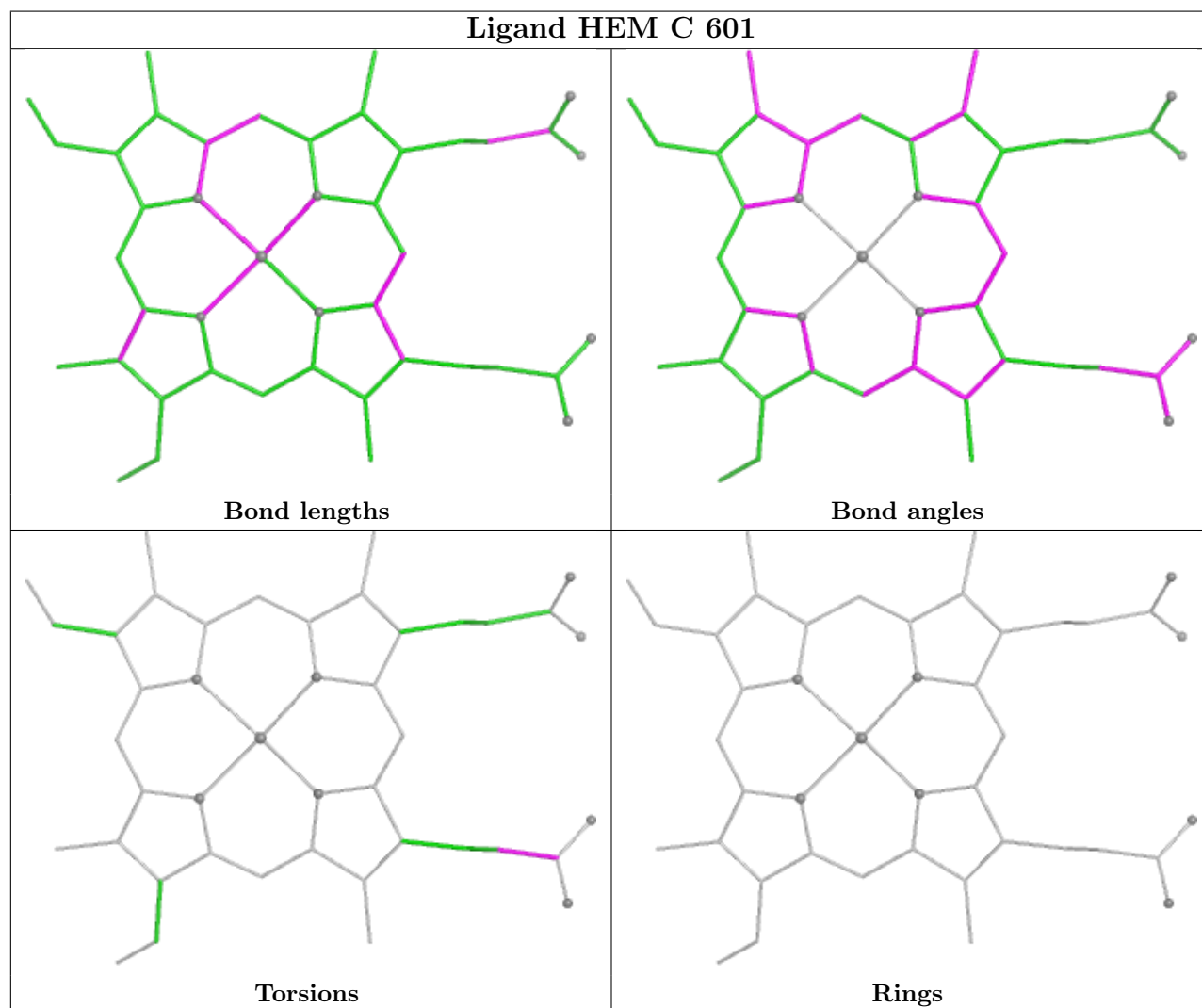
Mol	Chain	Res	Type	Atoms
4	C	601	HEM	CAD-CBD-CGD-O1D
4	G	601	HEM	CAD-CBD-CGD-O2D
4	G	601	HEM	CAD-CBD-CGD-O1D
4	A	601	HEM	CAD-CBD-CGD-O2D
13	C	605	P3G	O5-C11-C12-O6
5	A	604	EDO	O1-C1-C2-O2
6	D	603	PEG	O1-C1-C2-O2
4	A	601	HEM	CAD-CBD-CGD-O1D
6	H	604	PEG	C1-C2-O2-C3
11	A	607	P4G	C3-C4-O3-C5
11	A	607	P4G	O2-C3-C4-O3
4	D	601	HEM	CAA-CBA-CGA-O1A
4	A	601	HEM	CAA-CBA-CGA-O2A
4	E	601	HEM	CAA-CBA-CGA-O1A

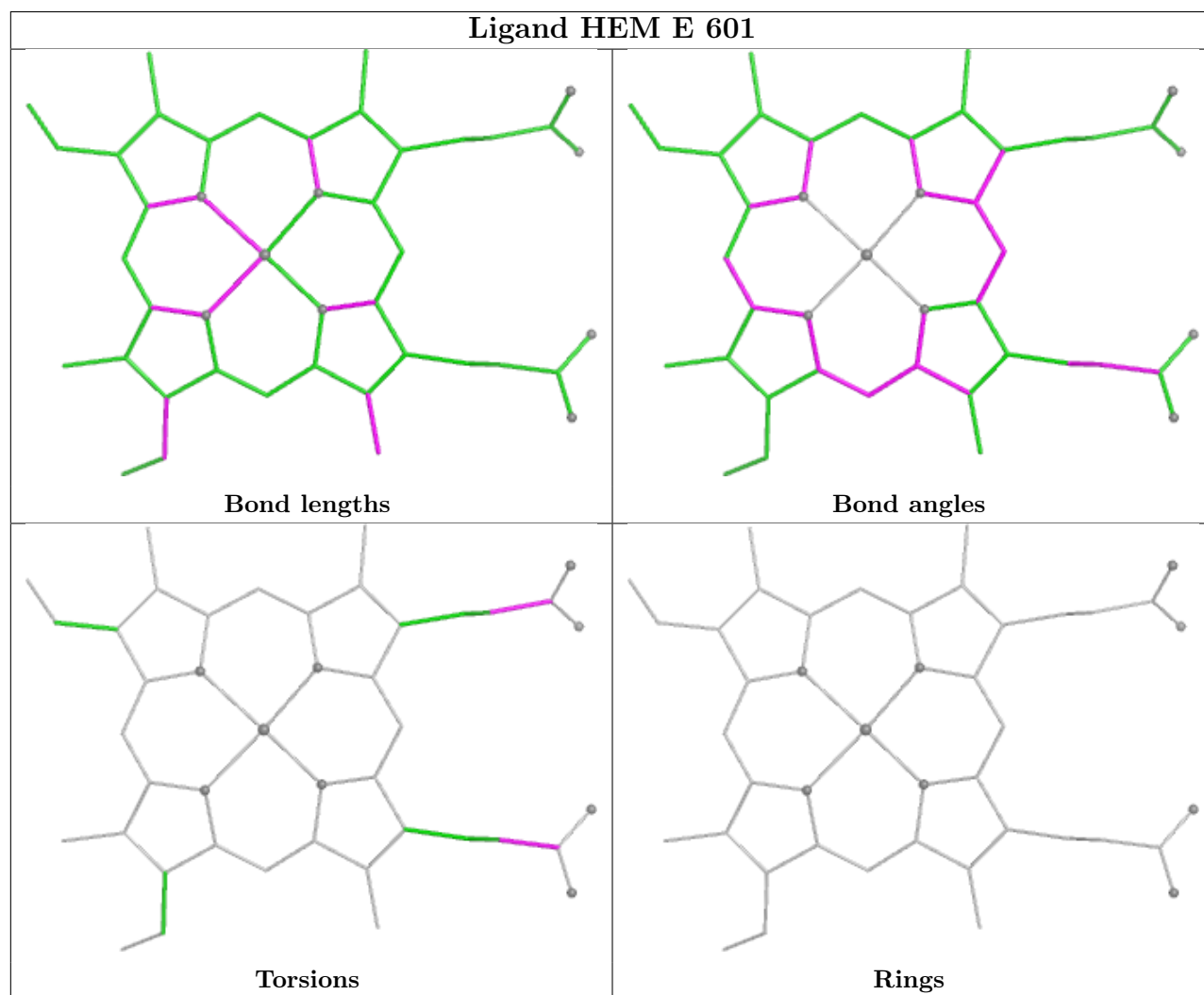
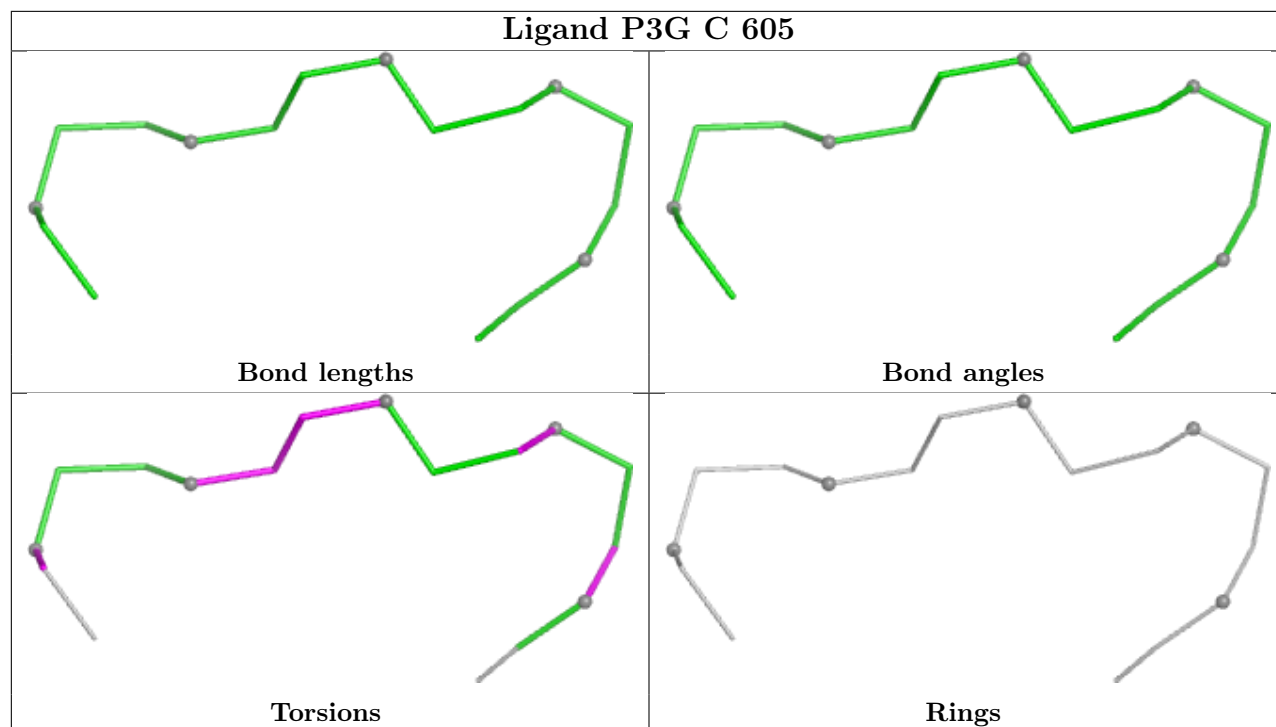
There are no ring outliers.

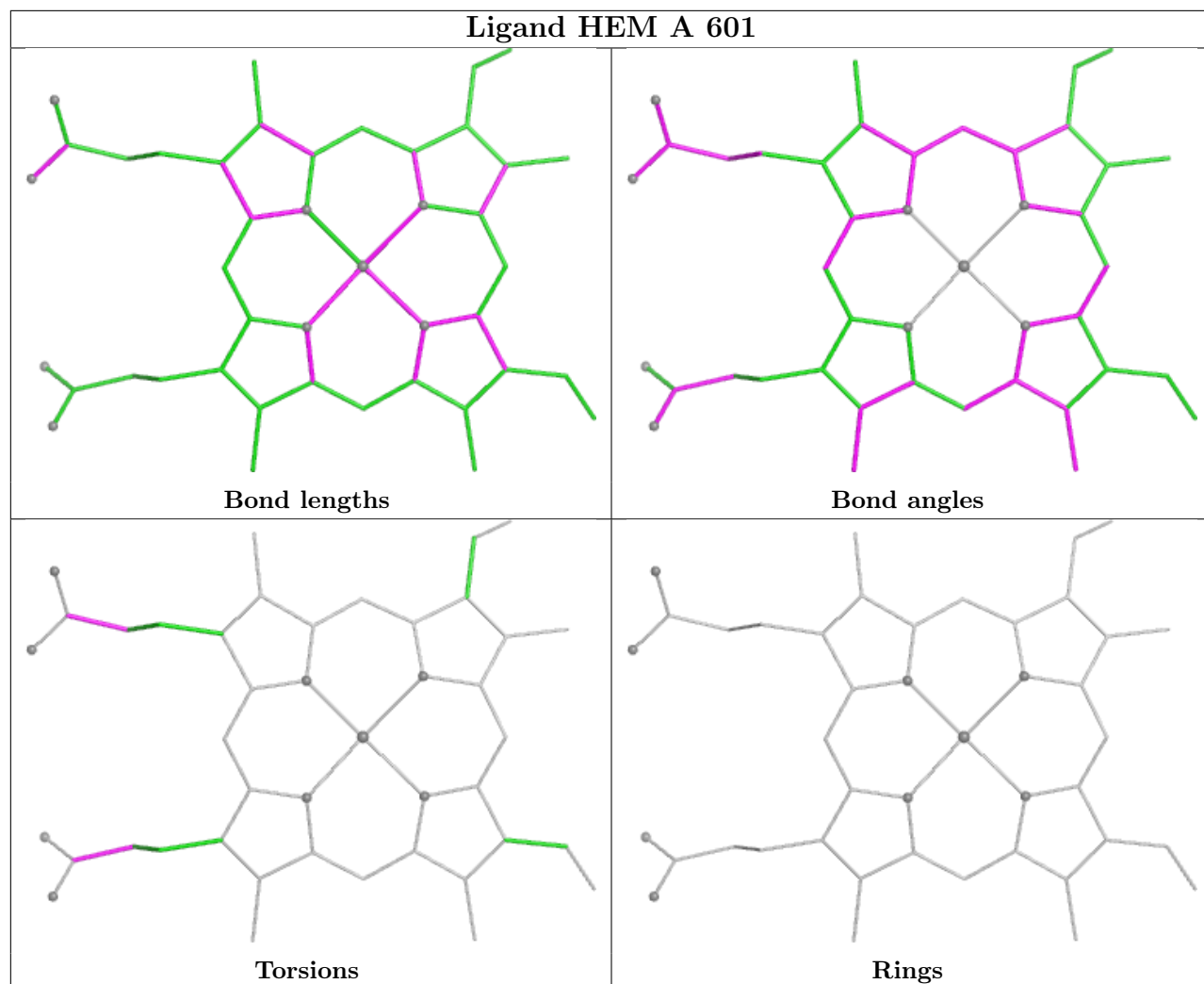
23 monomers are involved in 48 short contacts:

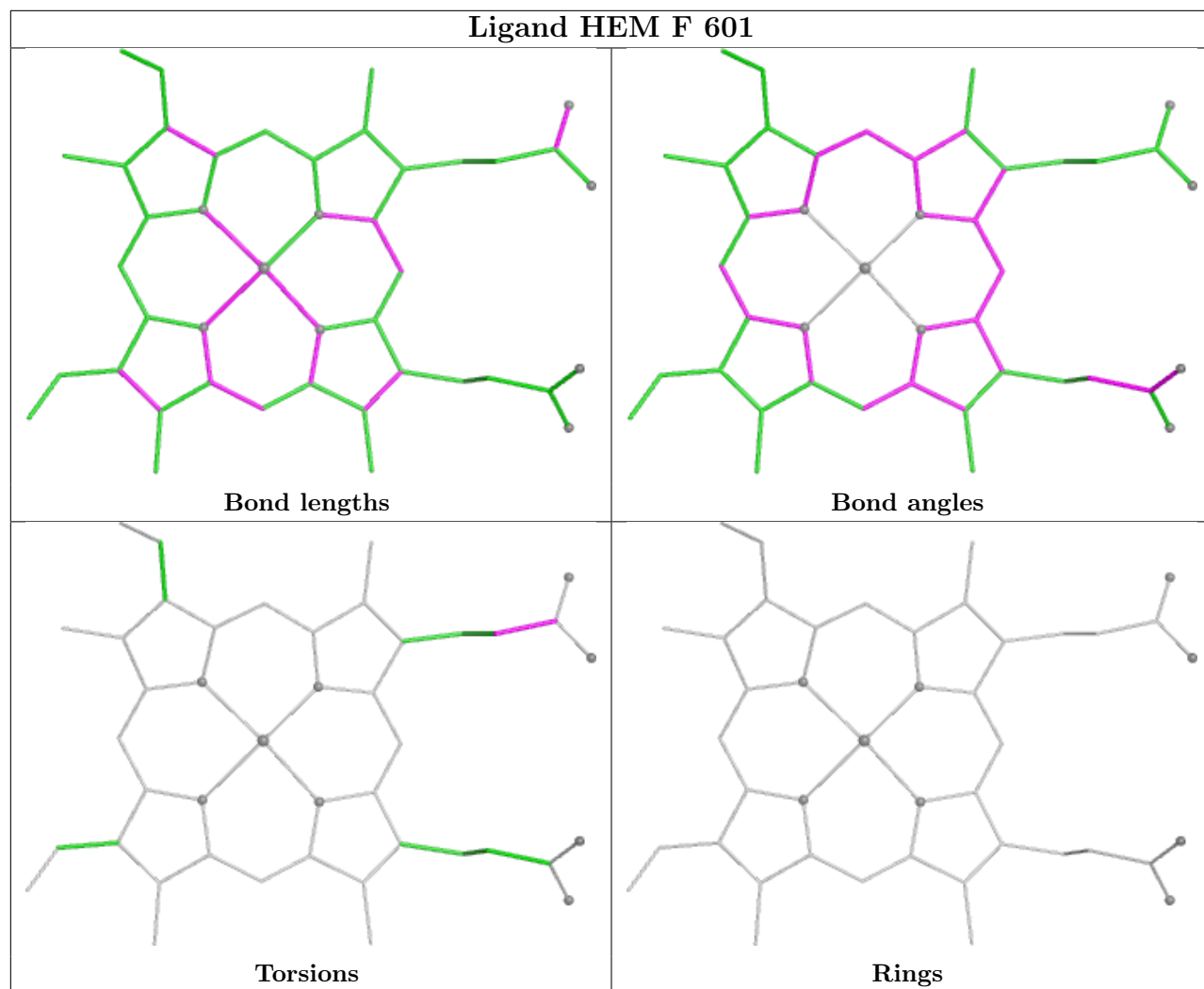
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	601	HEM	1	0
5	B	604	EDO	4	0
6	E	604	PEG	2	0
10	F	602	GLY	1	0
10	A	606	GLY	1	0
8	A	602	SER	1	0
4	E	601	HEM	1	0
4	A	601	HEM	1	0
4	F	601	HEM	1	0
4	G	601	HEM	2	0
5	H	603	EDO	3	0
11	A	607	P4G	3	0
5	A	605	EDO	2	0
5	D	606	EDO	3	0
6	H	604	PEG	1	0
6	D	604	PEG	1	0
4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

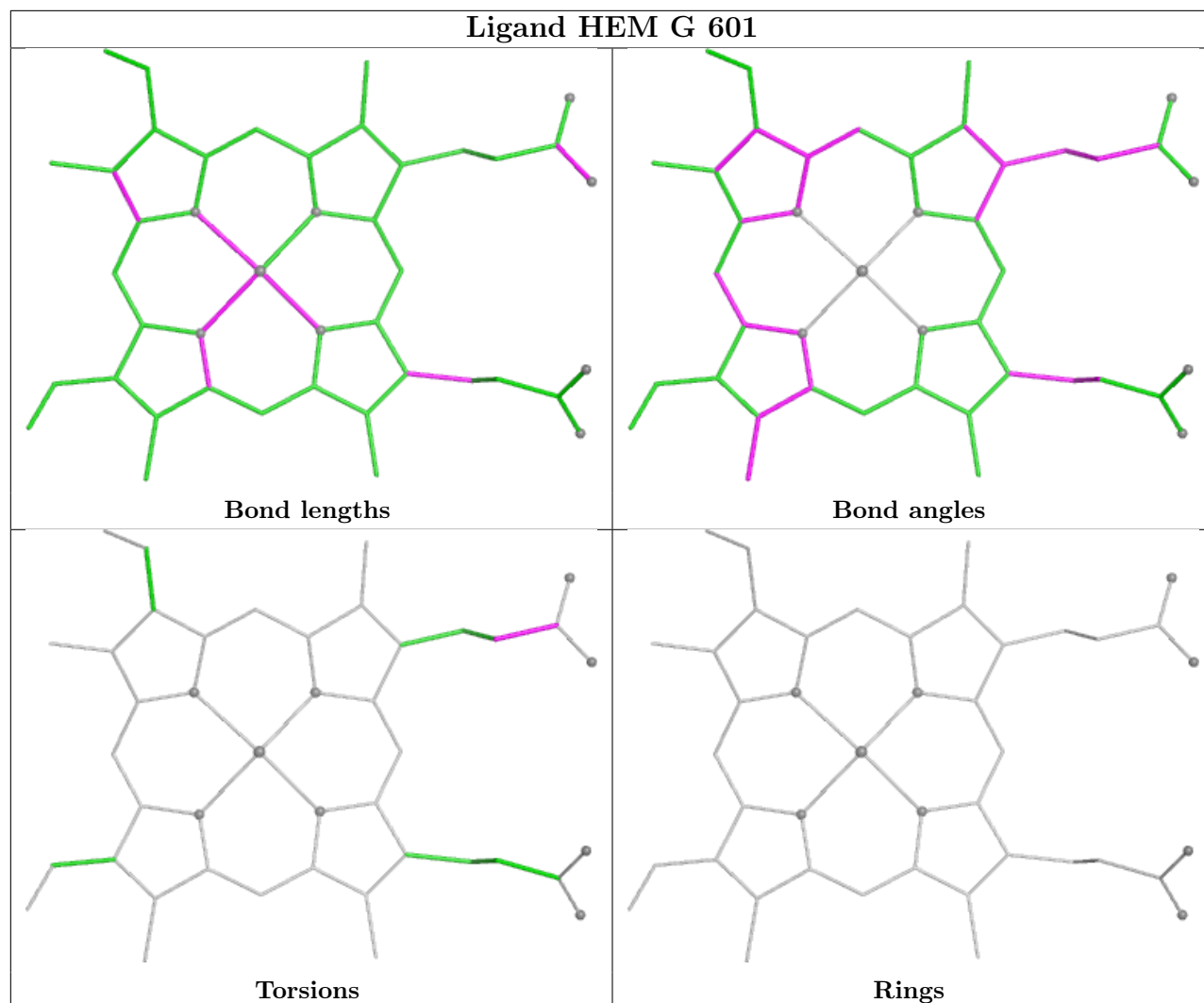
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

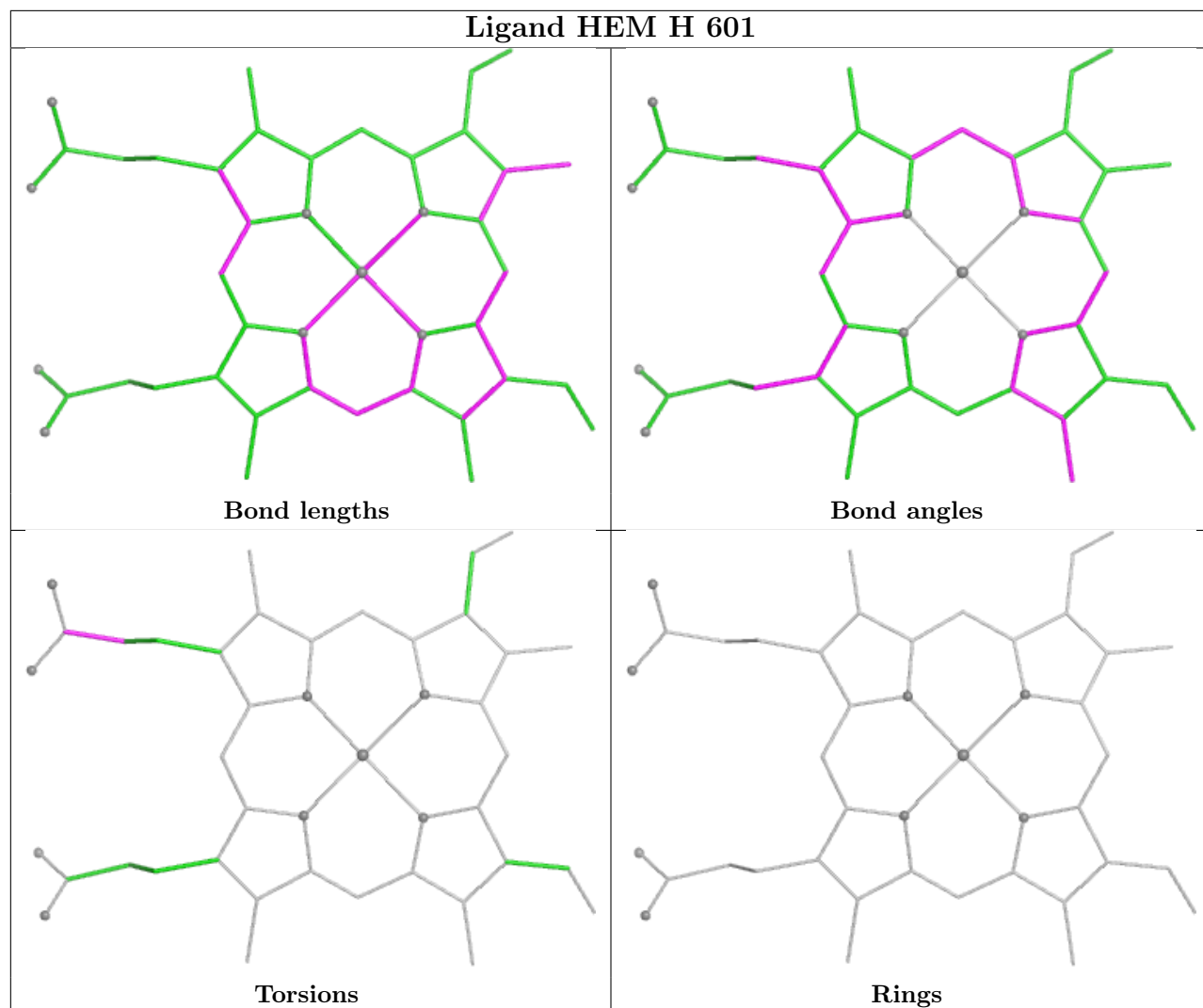


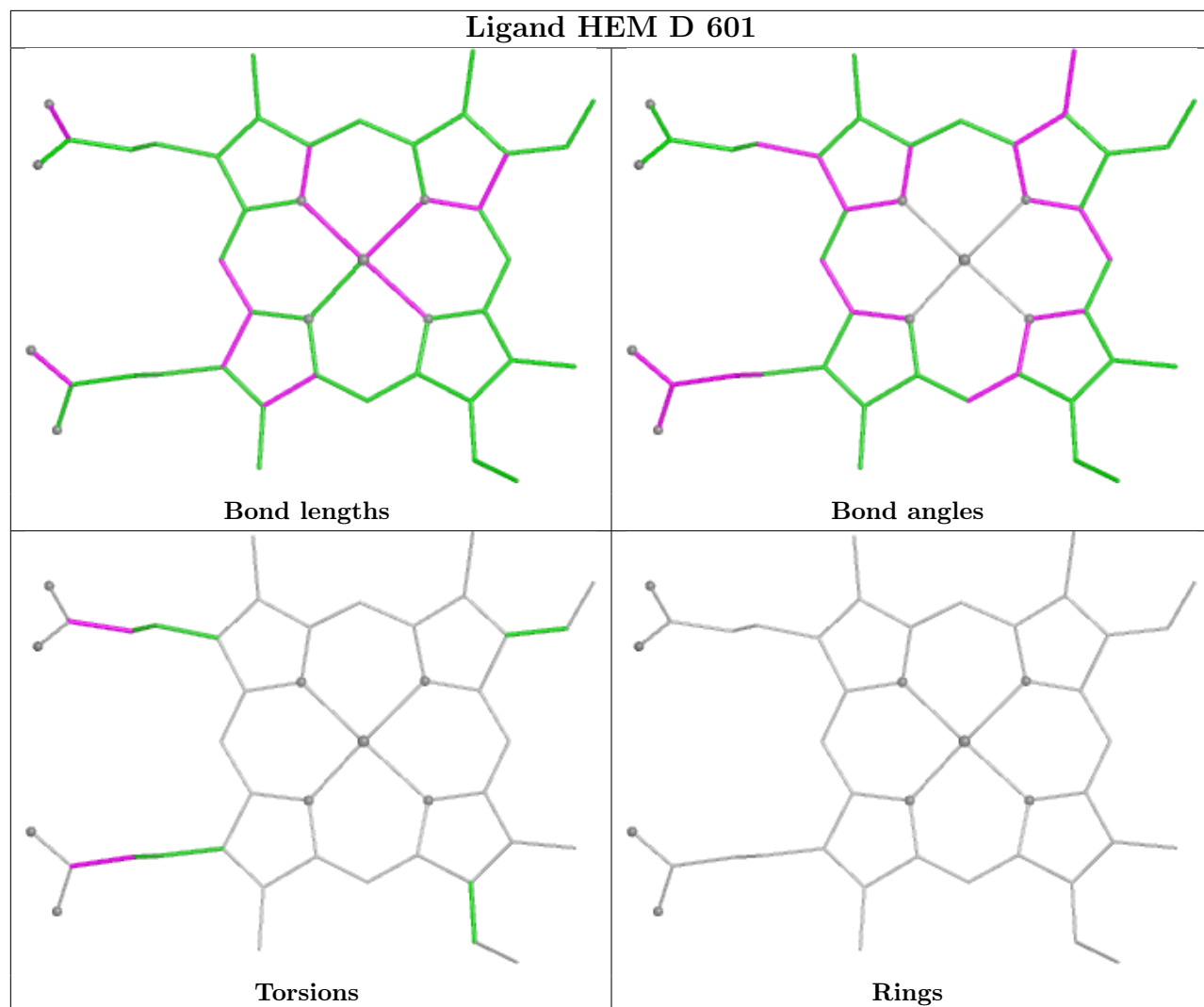


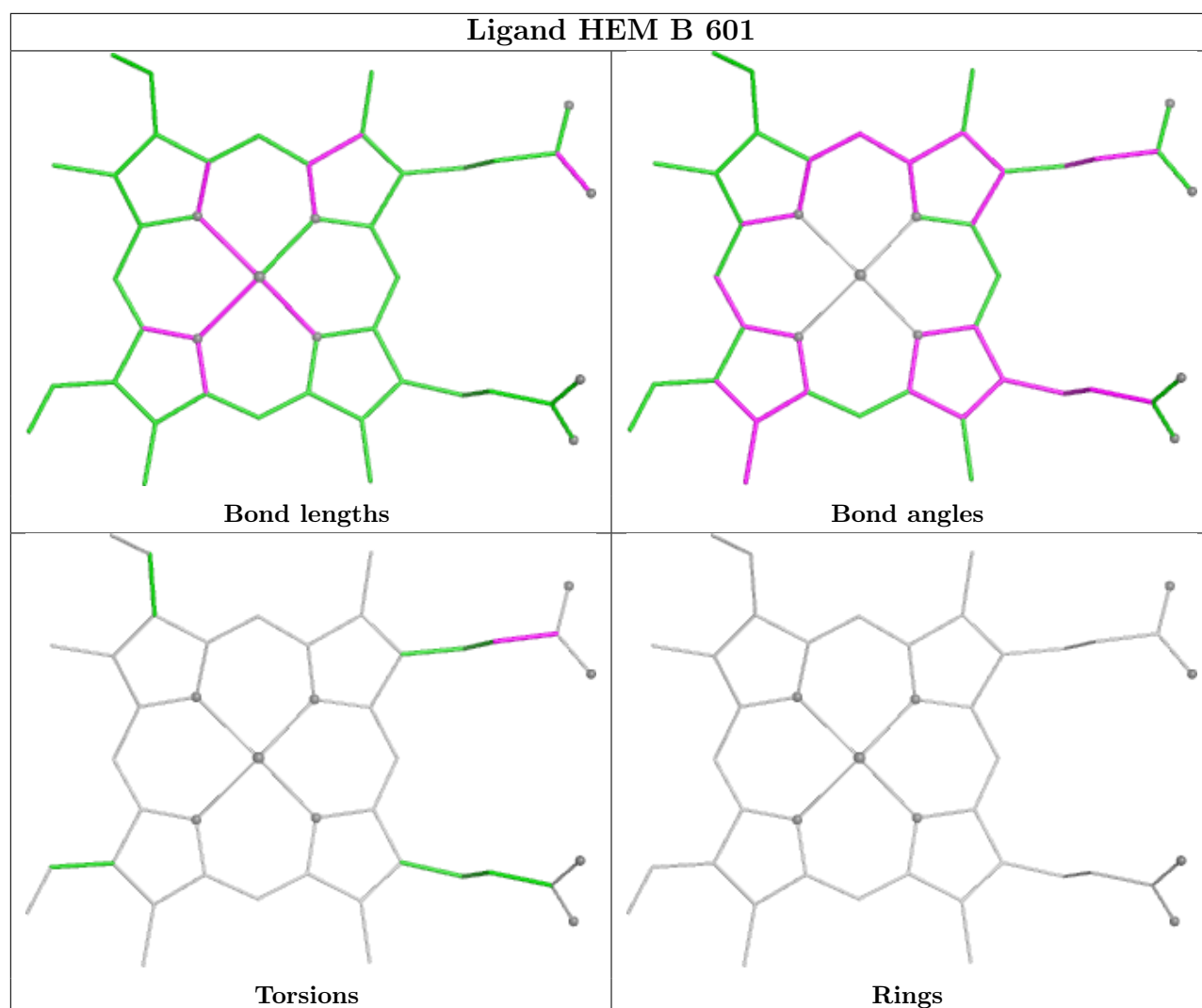












5.7 Other polymers [i](#)

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%)

All (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
1	F	390	LEU	3.5
1	C	508	ALA	3.5
1	D	424	ILE	3.4
1	A	506	ALA	3.3
1	E	4	TYR	3.3
1	F	4	TYR	3.3
1	F	426	GLY	3.3
1	C	306	ASN	3.2
1	A	505	ALA	3.2
1	H	3	ALA	3.1
1	F	406	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	390	LEU	3.0
1	D	504	ALA	3.0
1	D	3	ALA	2.9
1	A	90	GLY	2.8
1	D	503	LEU	2.8
1	C	501	LYS	2.8
1	B	504	ALA	2.8
1	E	424	ILE	2.8
1	G	295	TYR	2.8
1	C	503	LEU	2.8
1	D	508	ALA	2.7
1	E	505	ALA	2.7
1	F	90	GLY	2.7
1	E	506	ALA	2.7
1	E	90	GLY	2.6
1	D	497	GLU	2.6
1	F	2	GLU	2.5
1	A	504	ALA	2.5
1	F	506	ALA	2.5
1	B	417	LYS	2.5
1	D	469	VAL	2.5
1	D	493	ARG	2.5
1	B	437	GLY	2.5
1	E	244	ARG	2.4
1	A	419	VAL	2.4
1	E	507	SER	2.4
1	F	3	ALA	2.4
1	G	490	ALA	2.4
1	E	308	THR	2.3
1	E	307	VAL	2.3
1	F	504	ALA	2.3
1	E	413	VAL	2.3
1	F	475	ASP	2.3
1	D	284[A]	THR	2.3
1	C	3	ALA	2.3
1	B	147[A]	VAL	2.3
1	G	74	VAL	2.3
1	G	312	VAL	2.3
1	F	171	THR	2.2
1	H	497	GLU	2.2
1	G	450	VAL	2.2
1	D	506	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	452	LEU	2.2
1	F	5	HIS	2.2
1	E	417	LYS	2.2
1	F	92	TYR	2.2
1	E	89	THR	2.2
1	C	506	ALA	2.1
1	F	105	GLY	2.1
1	F	503	LEU	2.1
1	C	378	PHE	2.1
1	E	406	TYR	2.1
1	B	93	ALA	2.1
1	E	428	LEU	2.1
1	B	469	VAL	2.1
1	E	237	LEU	2.1
1	G	242	GLY	2.0
1	E	312	VAL	2.0
1	G	412	VAL	2.0
1	F	418	THR	2.0
1	E	412	VAL	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 [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.

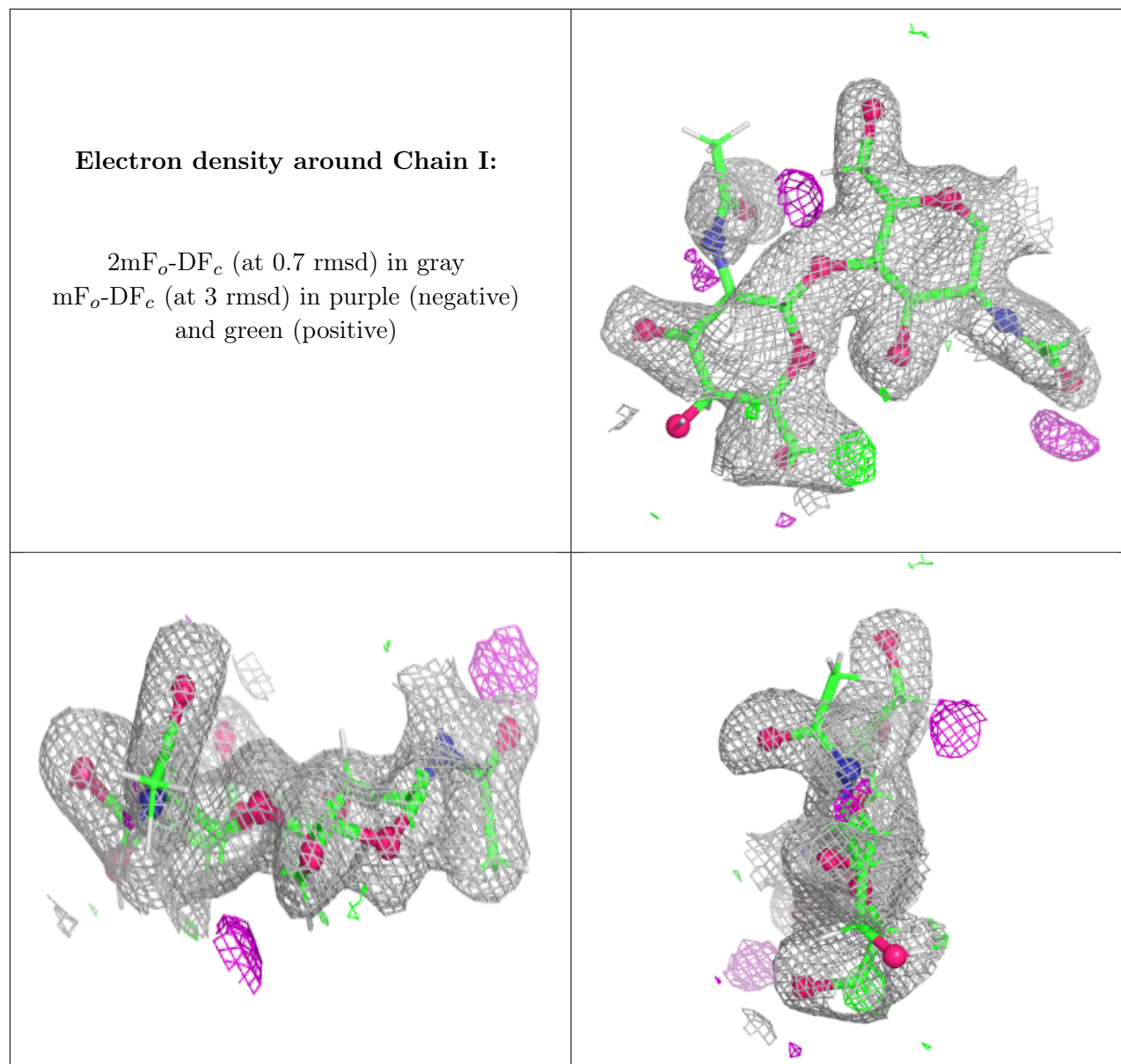
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MAN	J	5	11/12	0.74	0.14	35,42,45,51	4
2	NAG	K	2	14/15	0.75	0.15	34,39,46,53	6
3	MAN	J	7	11/12	0.77	0.17	32,38,43,47	4
2	NAG	I	2	14/15	0.79	0.15	32,42,48,57	6
3	MAN	J	4	11/12	0.80	0.14	30,36,41,45	3
3	BMA	J	3	11/12	0.90	0.09	22,25,35,35	2
3	MAN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

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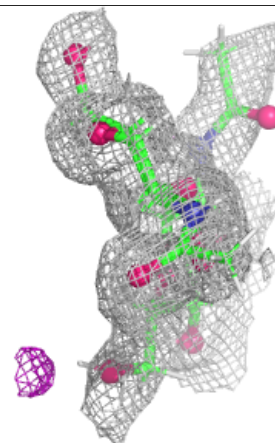
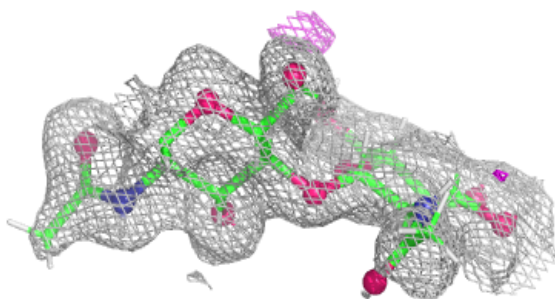
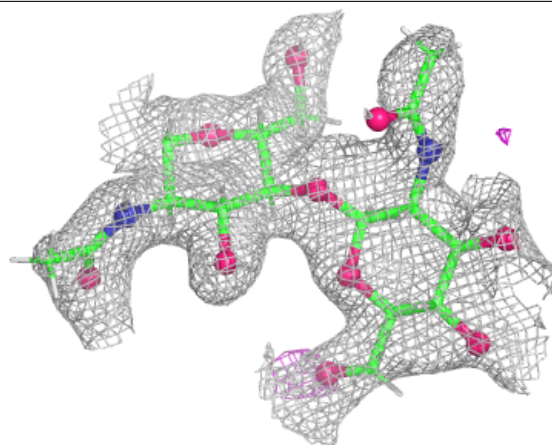
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	J	1	14/15	0.94	0.06	12,15,35,35	5
2	NAG	I	1	14/15	0.95	0.07	17,21,35,35	6

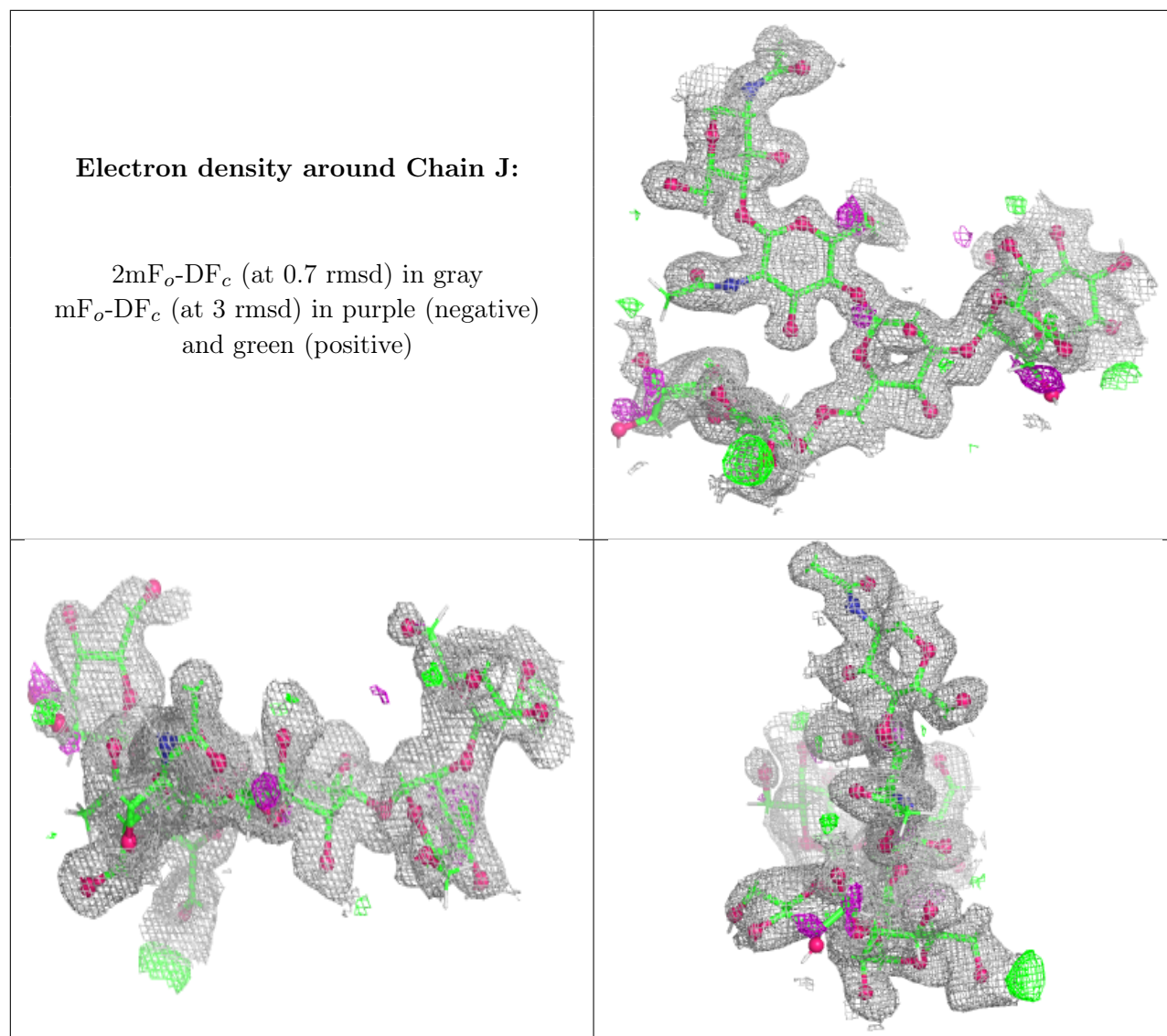
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain 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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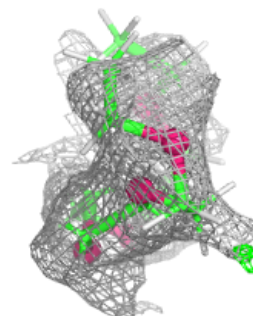
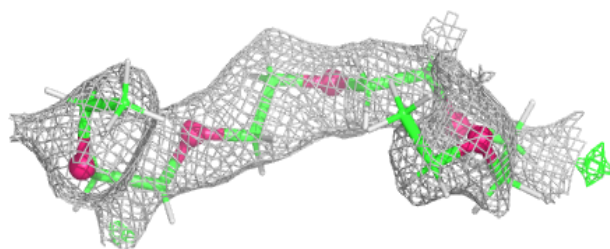
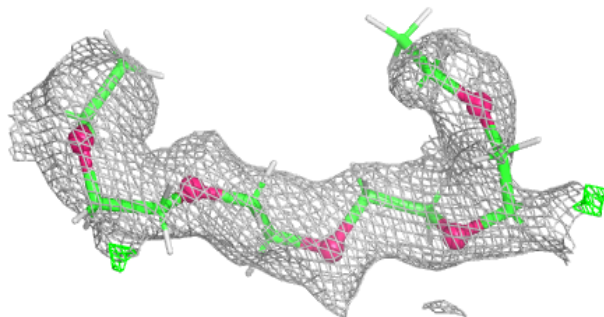
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	D	606	4/4	0.82	0.15	26,30,32,32	2
6	PEG	H	605	7/7	0.83	0.11	30,45,47,47	2
12	NAG	D	605	14/15	0.84	0.12	30,40,44,47	7
9	ALA	A	603	6/6	0.85	0.14	25,29,35,37	0
5	EDO	E	605	4/4	0.86	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.

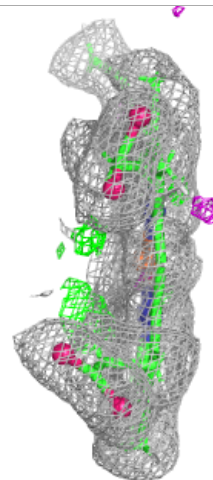
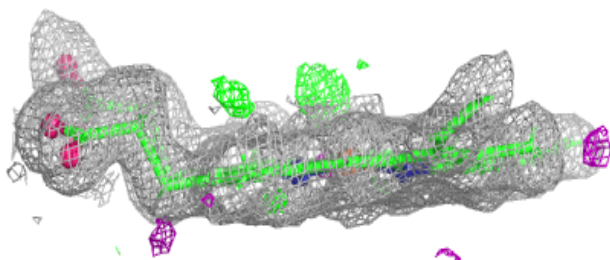
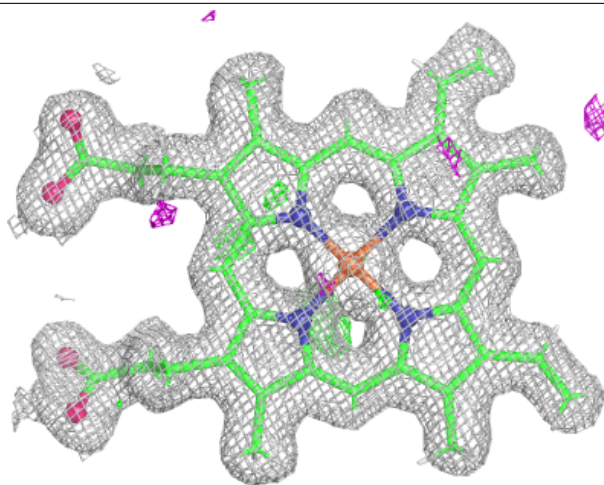
Electron density around P3G C 605:

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



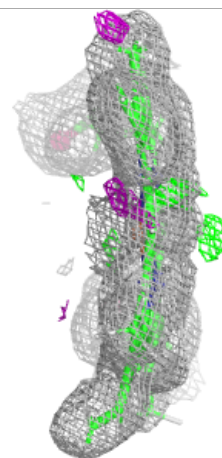
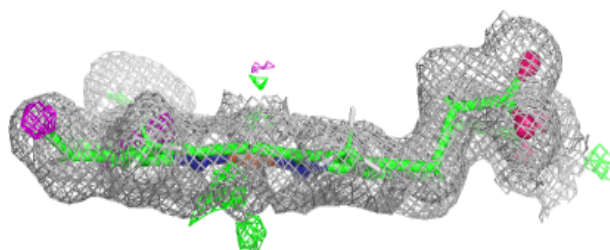
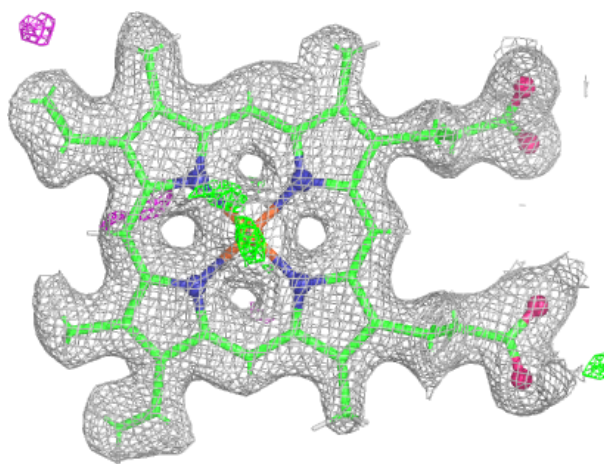
Electron density around HEM F 601:

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



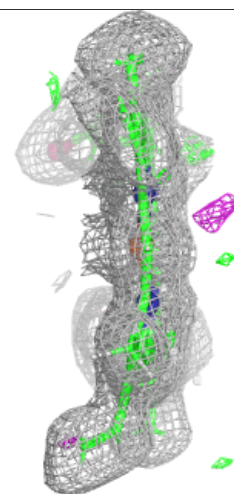
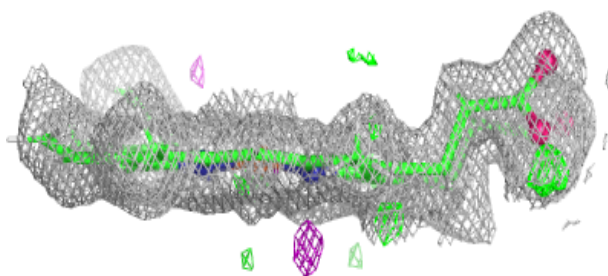
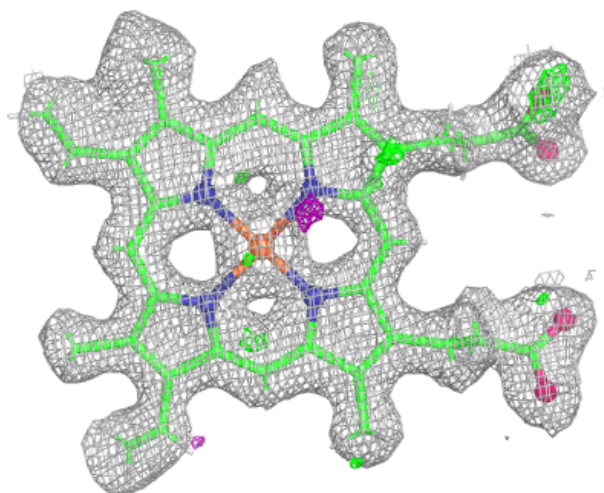
Electron density around HEM G 601:

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



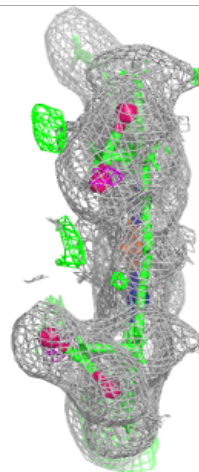
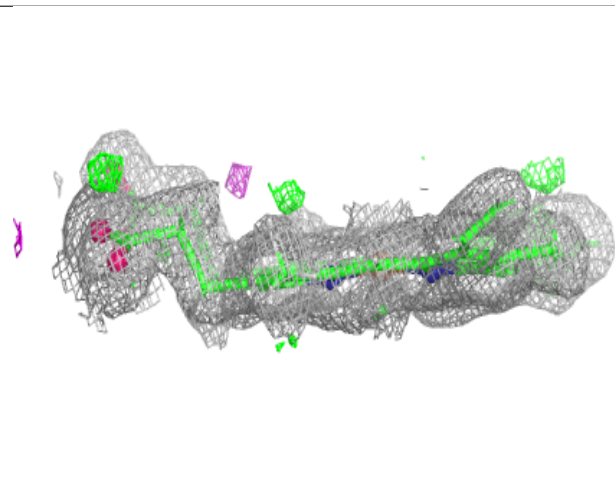
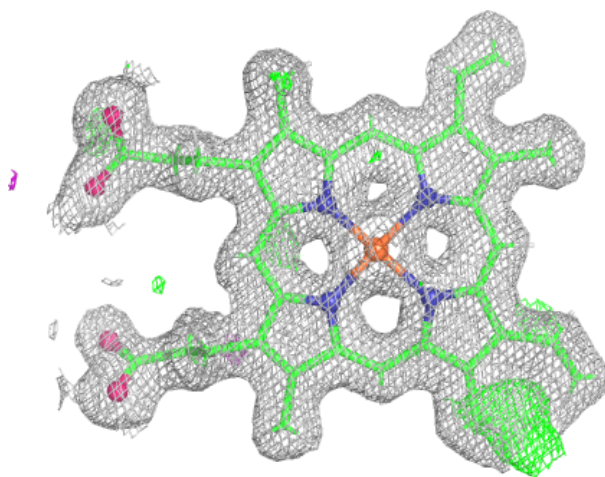
Electron density around HEM A 601:

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



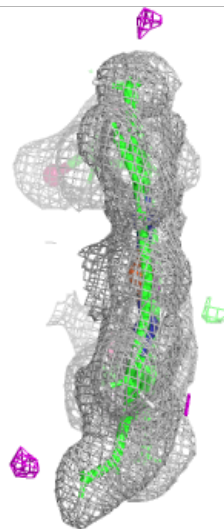
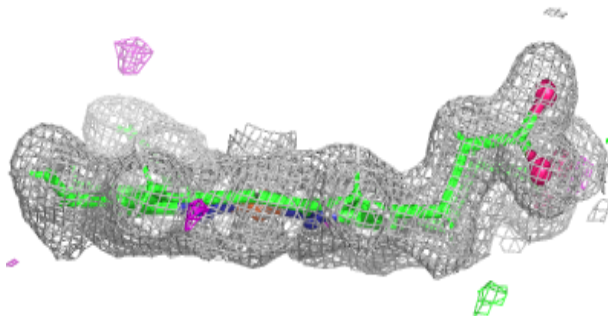
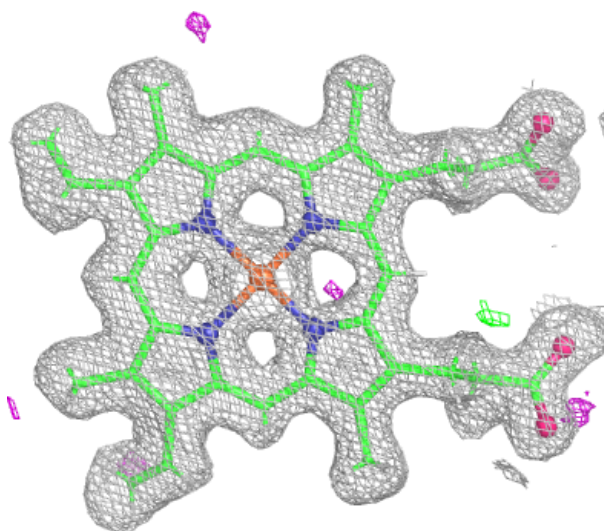
Electron density around HEM C 601:

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



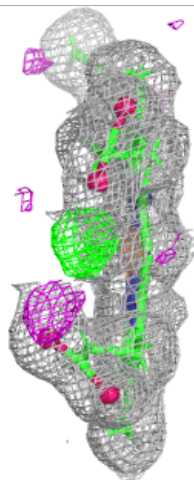
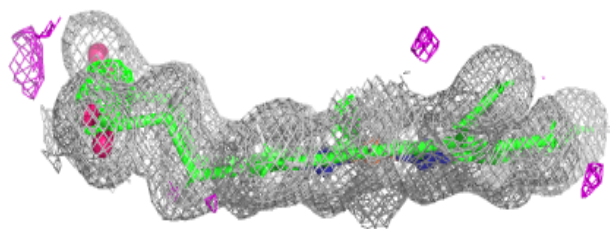
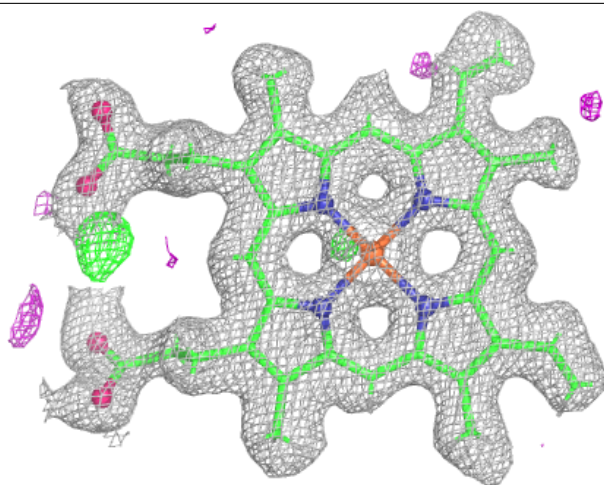
Electron density around HEM B 601:

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



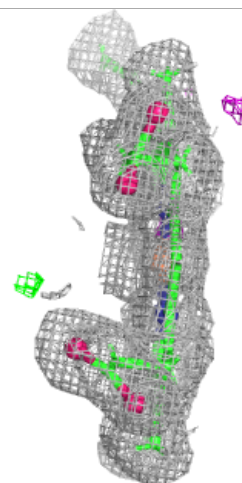
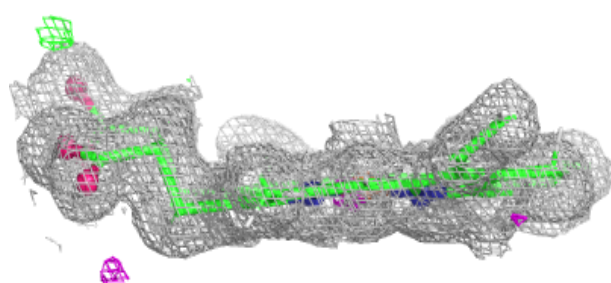
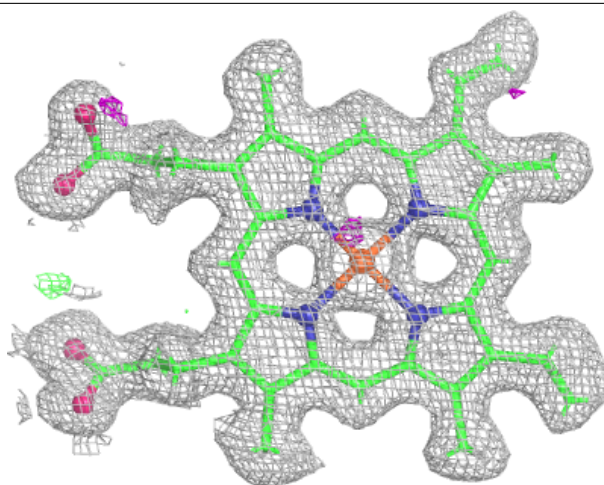
Electron density around HEM H 601:

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



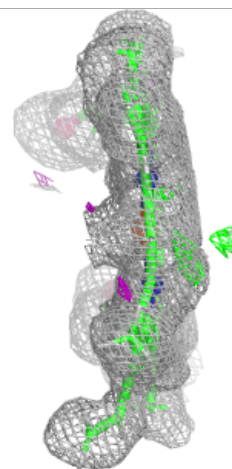
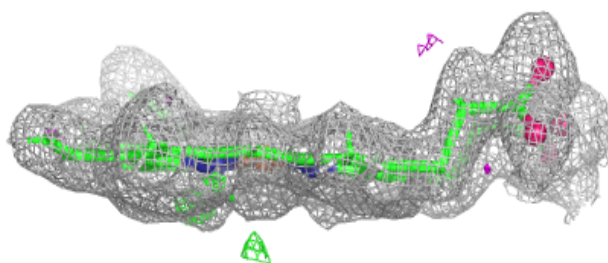
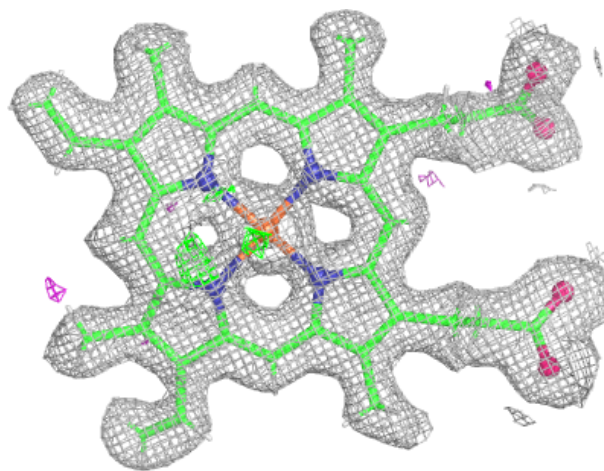
Electron density around HEM D 601:

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



Electron density around HEM 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.